MULTI-POINT PADÉ APPROXIMATION AND ITS APPLICATIONS IN PROBABILITY THEORY AND FINANCE

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Abstract

This thesis proposes a computational framework for constructing and applying multi-point Padé approximations to study Stieltjes functions, distribution functions including generalized gamma convolutions (GGCs), and other special functions through their Laplace transforms. We establish algorithmic foundations for multi-point Padé approximation via both matrix-based and continued-fraction approaches, with particular emphasis on an efficient reduced-parameter continued-fraction scheme.

Numerical implementations are performed using high-precision arithmetic to ensure the accuracy of results. The practical applicability of the method is demonstrated through a range of examples, including the approximation of Gaussian, lognormal, and gamma densities, as well as completely monotone functions, hockey-stick functions, and unit step functions by sums of exponentials. As a consequence, we introduce a new approach for approximating cumulative distribution functions (cdfs) through the Laplace transform of the underlying distribution.

We further propose approximation methods for several well-known risk measures widely used in insurance and finance, based on the approximations of hockey-stick and unit step functions. The examples include expected shortfall, individual economic capital allocation, tail standard deviation and expectiles.

The thesis also investigates dependence structures of GGCs through their lower and upper tail dependence coefficients, and finally, we present a new Laplace inversion relation for GGCs.

I dedicate this work to my family and friends

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Chapter 1

Introduction

Approximation of functions by rational functions and by finite sum of exponentials are classical topics with a long history, motivated by applications across signal processing [13], probability theory [24], numerical analysis and mathematical physics [54]. Many functions encountered in practice, such as Laplace transforms, special functions and cumulative distribution functions, do not admit closed-form representations suitable for computation. Rational and exponential approximations therefore serve as powerful surrogates that enable fast evaluation, analytic manipulation, and efficient simulation.

Among the most influential tools in this area are Padé approximations, introduced by Henri Padé in the late nineteenth century. A Padé approximant represents a function by a ratio of two polynomials determined so that the function's series expansion is matched to the highest possible degree. Since their introduction, Padé approximants have become central in diverse areas including quantum chemistry, statistical physics, special function theory, and numerical solution of differential equations. Their popularity stems from their ability to capture the behaviour, including singularities, far more effectively than polynomial approximations. Comprehensive treatments of their analytic theory and numerical properties can be found in classic works such as the monographs of Baker and Graves-Morris [7].

Beyond the classical single-point setting, researchers soon realized that imposing approximation conditions at multiple interpolation points could yield more flexible and accurate

approximations, particularly for functions with complicated analytic structure. This led to the development of multi-point Padé approximations, with early milestones contributed by Montessus de Ballore [8] and later by Gonchar and Stahl [36, 70]. Multi-point Padé approximants allow the user to prescribe interpolation at several complex points simultaneously, enabling precise control over the approximation on large domains. This feature is essential when approximating Laplace or Stieltjes transforms or functions possessing branch cuts or singularities distributed over a region. Classical methods based on solving moment-matching systems or constructing multi-point continued fractions often suffer from numerical instability or are restricted to specialized cases.

One of the central goals of this thesis is proposing a computational framework for multi-point Padé approximation, including matrix-based approaches, robust continued-fraction formulations, and an investigation of their numerical performance.

Parallel to rational approximation is the problem of representing functions by finite sums of exponentials. This topic traces back to the work of Prony [31] in the late eighteenth century. Exponential sums have played important roles in harmonic analysis, numerical PDEs, and various applied disciplines. Their practical importance arises from the fact that exponentials are especially convenient for computation, since they interact well with differentiation, convolution, and transform methods. Classical algorithms such as Prony's method and the matrix pencil method [65] are widely used in signal processing and system identification. However, these methods often impose restrictive data requirements, such as evenly spaced samples.

A key conceptual observation linking rational approximation and exponential approximation is that rational approximations of a Laplace transform automatically generate approximations of its inverse in the form of exponential mixtures. In this sense, Padé approximation provides a clean and systematic method for exponential fitting. One of the main contributions of this thesis is to develop this connection in a general setting, showing that multi-point Padé approximations can produce remarkably accurate exponential-sum approximations for a broad class of functions, including many that arise in probability and

statistical applications.

Chapters 2 and 3 provide background on several important function classes that are used throughout this work. These include completely monotone functions, Bernstein and complete Bernstein functions, Stieltjes functions, and Thorin–Bernstein functions. These classes are unified by their integral representation properties. Although these chapters primarily provide background material, they also illustrate why the functions studied later are especially amenable to approximation by rational functions and exponential sums.

A major focus of this thesis is the class of generalized gamma convolutions (GGCs). This family of probability distributions was introduced by Thorin [76] in the 1970s in connection with infinite divisibility and self-decomposability. GGCs include gamma distributions, log-normal distributions, and many heavy-tailed families of interest in finance, queueing theory, and Bayesian statistics. Bondesson's monograph [16] on GGCs provides a comprehensive treatment of their properties and applications. Despite their importance, explicit formulas for their cumulative distribution functions or Laplace transforms are rarely available. Most numerical work with GGCs relies on Laplace transform inversion or simulation-based methods, each of which has limitations in terms of accuracy, robustness, or computational efficiency.

This thesis demonstrates that multi-point Padé approximation offers a highly effective computational tool for GGCs. By approximating the associated Laplace transforms with rational functions, one obtains arbitrarily close approximations of distribution functions. Furthermore, the thesis presents new analytic results concerning tail coefficient of dependent GGCs.

Another significant set of applications considered in this thesis concerns risk measures in actuarial science and quantitative finance. Measures such as expected shortfall, tail variance and expectiles play a central role in modern risk management. The theoretical foundations for these measures have been developed extensively over the past two decades, with key contributions from Artzner and collaborators [2] and Föllmer and Schied [34]. Computing these measures for heavy-tailed or structurally complex distributions, however, remains challenging. Many of these quantities can be expressed in terms of integrals of tail functions

or transforms that are difficult to evaluate directly.

Recent work in actuarial science has explored transform-based techniques and saddlepoint approximations for evaluating such risk measures. Nevertheless, these approaches may suffer from instability or limited applicability, especially for distributions with slowly decaying tails. A major contribution of this thesis is to show that our approximations of hockey stick and unit step functions provide a flexible and accurate framework for approximating a wide range of risk measures without resorting to simulation or fragile numerical inversion techniques. This includes new approximation methods for expected shortfall, economic capital allocation, tail standard deviation and expectiles.

The main contributions of this thesis can be summarized as follows. First, a comprehensive algorithmic framework for multi-point Padé approximation is developed in Chapter 4, including both matrix-based methods and continued-fraction approaches, together with detailed numerical comparisons. Second, a systematic connection between Padé approximation and exponential-sum approximation is established in Chapter 5, yielding high-quality approximations for a wide variety of completely monotone functions, special functions, and distributional models. Third, new computational methods are introduced for generalized gamma convolutions and mixtures of exponentials in Chapter 5, allowing efficient approximation of densities and distribution functions. Fourth, new methods are developed for approximating important risk measures in insurance and finance in Chapter 6. Finally, new analytic results concerning tail coefficient of dependent GGCs and a new inversion formula for Laplace transform of generalized gamma convolutions are proved in Chapter 7.

Chapter 2

Bernstein functions and Stieltjes transform

2.1 Completely monotone functions

The class of functions defined on $(0, \infty)$ whose derivatives alternate in sign at every point was first developed by S. Bernstein [11], F. Hausdorff [39], and V. Widder [80] in relation to the moment problem. The connection between these functions and infinitely divisible measures makes them particularly interesting, as such measures are fundamental to the definition of Lévy processes, which have wide applications in financial modeling and physics [9], and biology [51]. Beyond probability and measure theory, these functions are also used in approximation theory, particularly in scattered data interpolation problems [28].

Definition 1. A function $f : (0, \infty) \to \mathbb{R}$ is called a completely monotone function if f is of class C^∞ and

$$(-1)^n f^{(n)}(\lambda) \geq 0, \tag{2.1}$$

for all $n \in \mathbb{N} \cup \{0\}$ and $\lambda > 0$.

The class of completely monotone functions is denoted by $\mathcal{CM}$. Condition (2.1) is known as the Bernstein–Hausdorff–Widder condition. The definition immediately implies that each

$\mathcal{CM}$ function is positive and decreasing.

The following theorem, which establishes a bijection between $\mathcal{CM}$ functions and finite Laplace transforms, is known as Bernstein's theorem.

Theorem 1 (Theorem 1.4 in [67]). *Let $f : (0, \infty) \to \mathbb{R}$ be a completely monotone function. Then it is the Laplace transform of a unique measure μ on $[0, \infty)$. That is, for all $\lambda > 0$,*

$$f(\lambda) = \mathcal{L}(\mu, \lambda) = \int_0^\infty e^{-\lambda t} \mu(dt). \tag{2.2}$$

Conversely, whenever $\mathcal{L}(\mu, \lambda) < \infty$ for every $\lambda > 0$, the function $\lambda \mapsto \mathcal{L}(\mu, \lambda)$ is completely monotone.

Examples of $\mathcal{CM}$ functions include $\exp(-ax)$, $\exp(a/x)$, $\ln(1 + a/x)$, $\ln(1 + x)/x$, and $1/(b + ax)^c$, where $a > 0$ and $b, c \geq 0$.

2.2 Bernstein functions and complete Bernstein functions

A class of functions closely related to completely monotone functions is that of Bernstein functions. These functions originated from the potential theory school of A. Beurling and J. Deny [67].

Definition 2. A function $f : (0, \infty) \to \mathbb{R}$ is a Bernstein function if f is of class C^∞, $f(\lambda) \geq 0$ for all $\lambda > 0$, and

$$(-1)^{n-1} f^{(n)}(\lambda) \geq 0,$$

for all $n \in \mathbb{N}$ and $\lambda > 0$.

The set of Bernstein functions is denoted by $\mathcal{BF}$. From this definition, it follows that a non-negative C^∞ function f defined on the positive reals belongs to $\mathcal{BF}$ if and only if f' belongs to $\mathcal{CM}$. However, the primitive of a completely monotone function is a Bernstein function only if it is positive. For example, the primitive of the completely monotone function λ^{-2}, which is $-\lambda^{-1}$, is not a Bernstein function.

Next, we present the Lévy–Khintchine representation for Bernstein functions.

Theorem 2 (Theorem 3.2 in [67]). *A function $f : (0,\infty) \to \mathbb{R}$ is a Bernstein function if and only if it admits the representation*

$$f(\lambda) = a + b\lambda + \int_0^\infty (1 - e^{-\lambda t})\mu(dt), \tag{2.3}$$

where $a, b \geq 0$ and μ is a measure (called the Lévy measure) on $(0,\infty)$ satisfying $\int_0^\infty \min(1,t)\mu(dt) < \infty$.

Remark 1. (i) Applying Fubini's theorem to (2.3) yields another representation of Bernstein functions:

$$f(\lambda) = a + b\lambda + \lambda \int_0^\infty e^{-\lambda t} M(t)dt,$$

where $M(t) = \mu(t,\infty)$.

(ii) The coefficients a and b can be computed as $a = f(0^+)$ and $b = \lim_{\lambda\to\infty} f(\lambda)/\lambda$.

Examples of Bernstein functions include λ, λ^α for $0 < \alpha < 1$, $\lambda/(1+\lambda)$, $\lambda/(\lambda+a)^\alpha$ for $a > 0$, $\ln(1+\lambda)$, $\lambda \ln(1 + a/\lambda)$ for $a > 0$, $\sqrt{\lambda}\arctan(\sqrt{\lambda/a})$ for $a > 0$ and $\sinh^{-1}(\lambda)$.

The following theorem was first established by Bochner [14].

Theorem 3 (Theorem 3.6 in [67]). *Let f be a positive function on $(0,\infty)$. Then f is a Bernstein function if and only if $e^{-uf} \in \mathcal{C}M$ for every $u > 0$.*

An important subclass of Bernstein functions is that of complete Bernstein functions, a notion first introduced by Prüss [59] in connection with Volterra-type integral equations.

Definition 3. A Bernstein function f is said to be a complete Bernstein function if its Lévy measure μ in (2.3) has a completely monotone density $m(t)$ with respect to Lebesgue measure,

$$f(\lambda) = a + b\lambda + \int_0^\infty (1 - e^{-\lambda t})m(t)dt. \tag{2.4}$$

This class of functions is denoted by $\mathcal{CBF}$. Many functions in $\mathcal{BF}$ also belong to $\mathcal{CBF}$. Examples include λ^α for $0 < \alpha < 1$, $\lambda/(a+\lambda)$ for $a > 0$, $\lambda/\sqrt{a+\lambda}$ for $a > 0$, and $\ln(1+\lambda/a)$ for $a > 0$.

2.3 Stieltjes functions

Stieltjes functions, a subclass of completely monotone functions, are closely related to the $\mathcal{CBF}$ class and serve as the main analytical tools in Chapters 4 and 5. Stieltjes transforms first appeared in the works of T. J. Stieltjes, who investigated continued fractions to solve the Stieltjes moment problem [72].

Definition 4. A (non-negative) Stieltjes function is a function $f : (0, \infty) \to [0, \infty)$ that can be written in the form

$$f(\lambda) = \frac{a}{\lambda} + b + \int_0^\infty \frac{1}{\lambda + t}\sigma(dt), \tag{2.5}$$

where $a, b \geq 0$ are constants and σ is a measure on $(0, \infty)$ such that $\int_0^\infty (1 + t)^{-1}\sigma(dt) < \infty$.

The class of Stieltjes functions is denoted by $\mathcal{S}$. The integral in (2.5) is called the Stieltjes transform of the measure σ, a term introduced independently by G. Doetsch [21] and by Widder [79].

Some examples of Stieltjes functions are $\lambda^{\alpha-1}$ for $0 \leq \alpha \leq 1$, $1/(\lambda + a)$ for $a > 0$, and $(\ln(1 + \lambda))/\lambda$. For instance, by letting

$$\sigma(dt) = \frac{\mathbf{1}_{(1,\infty)}(t)}{t}dt,$$

as the representing measure in (2.5), we see that the condition $\int_0^\infty (1 + t)^{-1}\sigma(dt) < \infty$ is clearly satisfied, and the corresponding Stieltjes function is

$$\int_0^\infty \frac{1}{\lambda + t}\frac{\mathbf{1}_{(1,\infty)}(t)}{t}dt = \frac{\ln(1 + \lambda)}{\lambda}.$$

Remark 2. The Stieltjes transform in (2.5) can be expressed as a double Laplace transform by applying Fubini's theorem. In fact, $\mathcal{S}$ consists precisely of all completely monotone functions whose representing measures have completely monotone densities on $(0, \infty)$.

The following theorem characterizes the relationship between Stieltjes and complete Bernstein functions. In what follows, $\mathbb{H}^\uparrow$ denotes the open upper complex half-plane, where $\mathrm{Im}(z) > 0$.

Theorem 4 (Theorem 6.2. in [67]). *For a non-negative function f on $(0,\infty)$, the following conditions are equivalent:*

1. *f is a complete Bernstein function.*
2. *The function $\lambda \to f(\lambda)/\lambda$ belongs to $\mathcal{S}$.*
3. *f has an analytic continuation to $\mathbb{H}^{\uparrow}$ such that $Imf(z) \geq 0$ for all $z \in \mathbb{H}^{\uparrow}$. Moreover, $f(0^+) = \lim_{z \downarrow 0} f(z)$ exists and is real.*
4. *f has an analytic continuation to $\mathbb{H}^{\uparrow}$ given by*

$$f(z) = a + bz + \int_0^{\infty} \frac{z}{z+t}\sigma(dt), \tag{2.6}$$

where $a, b \geq 0$ are constants and σ is a measure on $(0,\infty)$ satisfying

$$\int_0^{\infty} (1+t)^{-1}\sigma(dt) < \infty.$$

Proposition 1 (Proposition 7.1. in [67]). *A non-zero function f is a complete Bernstein function if and only if the function $\lambda \to \lambda/f(\lambda)$ is also a complete Bernstein function.*

Due to the duality stated in Proposition 1, $f(\lambda)$ and $\lambda/f(\lambda)$ are called a conjugate pair in the $\mathcal{CBF}$ class. The following theorem, which is a characterization of Stieltjes functions, follows directly from Theorem 4 and Proposition 1.

Theorem 5 (Theorem 7.3. in [67]). *A non-zero function f is a complete Bernstein function if and only if $1/f$ is a non-zero Stieltjes function.*

2.4 Thorin–Bernstein functions

A subclass of $\mathcal{CBF}$ that is particularly important from a probabilistic perspective is the class of Thorin–Bernstein functions. This class first appeared in Thorin's paper [76] as the Laplace exponents of a class of probability distributions, which will be discussed in the next chapter.

Definition 5. A Bernstein function f is called a Thorin–Bernstein function if the Lévy measure μ from (2.3) has a density $m(t)$ such that $t \mapsto t \times m(t)$ is completely monotone, i.e.,

$$f(\lambda) = a + b\lambda + \int_0^\infty (1 - e^{-\lambda t}) m(t) dt,$$

where $a, b \geq 0$, $\int_0^\infty \min(1, t) m(t) dt < \infty$, and $t \mapsto t \times m(t)$ is completely monotone.

We denote the family of Thorin–Bernstein functions by $\mathcal{TBF}$. Note that when $t \times m(t)$ is completely monotone, so is $m(t)$; hence, every Thorin–Bernstein function is also a complete Bernstein function. The following theorem shows the connection between the $\mathcal{S}$ and $\mathcal{TBF}$ classes and provides alternative representations for $\mathcal{TBF}$ functions.

Theorem 6 (Theorem 8.2. in [67])**.** *For a non-negative function f on $(0, \infty)$, the following conditions are equivalent:*

1. *$f \in \mathcal{TBF}$.*
2. *$f' \in \mathcal{S}$ and $f(0^+) = \lim_{\lambda \to 0^+} f(\lambda)$ exists.*
3. *f admits the representation*

$$f(z) = a + bz + \int_0^\infty \ln\left(1 + \frac{z}{t}\right) U(dt), \tag{2.7}$$

   where $a, b \geq 0$ and U is a unique measure on $(0, \infty)$ satisfying

$$\int_0^1 |\ln(t)| U(dt) + \int_1^\infty \frac{1}{t} U(dt) < \infty. \tag{2.8}$$

4. *$f \in \mathcal{CBF}$ and $f' \in \mathcal{S}$.*
5. *f is of the form*

$$f(z) = a + bz + \int_0^\infty \frac{z}{z + t} \frac{w(t)}{t} (dt), \tag{2.9}$$

   where $a, b \geq 0$ and $w : (0, \infty) \to [0, \infty)$ is a non-decreasing function such that $\int_0^\infty \frac{w(t)}{t(1+t)} dt < \infty$, and if w is left-continuous, then it is unique.

We call the measure U appearing in (2.7) the *Thorin measure* of f. Note that the m, U, and w above satisfy the following relations:

$$m(t) = \mathcal{L}(w, t),\ t \times m(t) = \mathcal{L}(U, t),\ w(t) = U(0, t).$$

Some examples of Thorin–Bernstein functions are λ^α for $0 < \alpha < 1$, $\ln(1 + \lambda/a)$ for $a > 0$, $\ln(1 + \lambda^\alpha)$ for $0 < \alpha < 1$ and $\sqrt{\lambda}\arctan(\sqrt{\lambda/a})$ for $a > 0$. Another important observation is that $\mathcal{TBF}$ is a proper subset of $\mathcal{CBF}$. For instance, the complete Bernstein function $f(x) = \sqrt{x}\arctan(\frac{1}{\sqrt{x}}) = \frac{1}{2}\int_0^1 \frac{x}{x+t}\frac{\sqrt{t}}{t}dt$ has a derivative that is not a Stieltjes function; hence, by the above theorem, f does not belong to $\mathcal{TBF}$.

The theorem above connects the $\mathcal{TBF}$ class with the $\mathcal{S}$ class, which will be used in the next chapter.

Chapter 3

Generalized Gamma Convolutions and Mixtures of Exponentials

As mentioned earlier, the class of generalized gamma convolutions (GGC) was introduced by Olof Thorin in 1977 [76] as a tool to show that lognormal and Pareto distributions are infinitely divisible. For example, lognormal distributions have been used to model total insurance claims [27], where infinite divisibility is required.

Following [67], we define this class of distributions through their Laplace transform to clarify their connection with Stieltjes and Thorin–Bernstein functions. The Laplace transform (LT) of a random variable X is defined by

$$\mathcal{L}_X(s) = \phi_X(s) = \mathbb{E}[\exp(-sX)].$$

Definition 6. A *Generalized Gamma Convolution* (GGC) is a probability distribution F on $\mathbb{R}^+$ with Laplace transform of the form

$$\phi_X(z) = \exp\Big(- az - \int_0^\infty \ln\Big(1 + \frac{z}{t}\Big) U(\mathrm{d}t)\Big), \quad z \in \mathbb{C} \setminus (-\infty, 0), \tag{3.1}$$

where $a \geq 0$ and the Thorin measure $U(\mathrm{d}t)$ on $(0, \infty)$ satisfies

$$\int_0^\infty \min(|\ln(t)|, 1/t)\, U(dt) < \infty.$$

Equation (3.1) implies $\phi(0) = 1$ and

$$\frac{\phi'(z)}{\phi(z)} = -a - \int_0^\infty \frac{1}{t+z} U(dt),$$

so that

$$-\frac{\phi'(s)}{\phi(s)} \in \mathcal{S}.$$

The expectation and variance of a GGC can also be expressed via the Thorin measure. Specifically, for a r.v. X with Laplace transform as in (3.1), a is the left-extremity of the distribution, and

$$\mathbb{E}[X] = a + \int_0^\infty \frac{1}{t} U(dt), \quad \mathrm{Var}[X] = \int_0^\infty \frac{1}{t^2} U(dt).$$

The GGC class is closed under right-translation, scaling, convolution, and convolution roots, as explained in the following theorem.

Theorem 7 (Proposition 9.10. in [67])**.**

- *A random variable X is a GGC if and only if $\mathcal{L}_X(s) = e^{-f(s)}$ for some f in the Thorin–Bernstein class.*
- *The GGC class contains all gamma distributions $Gamma(\alpha, \beta)$, with $\alpha, \beta > 0$.*
- *The GGC class is closed under convolution: the sum of two independent GGCs is a GGC.*

The Laplace transform of a finite convolution of gamma distributions $Gamma(\alpha_i, \beta_i), 1 \leq i \leq n$, is

$$\phi(z) = \prod_{i=1}^n \left(1 + \frac{z}{\beta_i}\right)^{-\alpha_i} = \exp\Big(- \sum_{i=1}^n \alpha_i \ln(1 + \frac{z}{\beta_i})\Big).$$

For a degenerate distribution at $a > 0$, the Laplace transform is $\exp(-az)$. Weak limits of such convolutions then yield the LT in (3.1). The following theorem formalizes that GGC is the minimal class with this property.

Theorem 8 (Theorem 9.12. in [67]). *The GGC class is the closure of all finite convolutions of gamma distributions. In particular, it is the smallest class containing all gamma distributions and closed under convolutions and weak limits.*

A probability distribution F is *infinitely divisible* (ID) if, for each $n \geq 1$, it can be decomposed into n identical convolution factors F_n. Its Laplace transform satisfies $\phi(z) = (\phi_n(z))^n$, where $\phi_n(z)$ is the Laplace transform of a probability distribution. Examples of ID distributions include gamma, negative binomial, and stable distributions. The LT of an ID distribution on $\mathbb{R}^+$ can be represented as

$$\phi(z) = \exp\Big(- az - \int_0^\infty (1 - e^{-yz}) L(dy) \Big),$$

where $a \geq 0$ and L (the Lévy measure) is non-negative with $\int_0^\infty \min(1, y) L(dy) < \infty$. The class of ID distributions is closed under convolution and weak limits.

Theorem 9 (Theorem 3.1.1. in [16]). *A probability distribution on $\mathbb{R}^+$ is a GGC if and only if it is ID and its Lévy measure has a density l such that $y \times l(y)$ is completely monotone for $y > 0$. In fact,*

$$y \times l(y) = \int_0^\infty e^{-yt} U(dt).$$

Remark 3. For the LT $\phi(z) = \exp(-z^\alpha)$, $0 < \alpha < 1$, of a strictly stable distribution on $(0, \infty)$, we have

$$y \times l(y) = \frac{\alpha}{\Gamma(1-\alpha)} y^{-\alpha},$$

which is completely monotone. Hence, this distribution is a GGC.

The following two theorems characterize a GGC only by behavior of its moment generating gunction (mgf) defined by $\varphi_X(s) = \mathbb{E}[\exp(sX)]$.

Theorem 10 (Theorem 3.1.3. in [16]). *(Main characterization theorem). The mgf φ of a probability distribution on $\mathbb{R}^+$ corresponds to a GGC if and only if φ is analytic in $\mathbb{C} \setminus [0, \infty)$ and*

$$\mathrm{Im}\left[\varphi'(s)\overline{\varphi(s)}\right] \geq 0, \quad \mathrm{Im}(s) > 0.$$

Theorem 11 (Theorem 3.1.4. in [16]). *(Inversion theorem). Let φ be the mgf of a probability distribution F on $\mathbb{R}^+$. Assume:*

a) φ is analytic and zero-free in $\mathbb{C} \setminus [0, \infty)$ and continuously differentiable up to the cut with non-zero boundary values.

b) $\varphi'(s)/\varphi(s) \to a$ uniformly as $|s| \to \infty$, $s \in \mathbb{C} \setminus [0, \infty)$.

c) $\arg[\varphi(s)]$ is increasing for $s > 0$, equivalently, $\mathrm{Im}[\varphi'(s)/\varphi(s)] \geq 0$ for $s > 0$.

Then F is a GGC with left-extremity a, and

$$\int_0^s U(dt) = \frac{1}{\pi} \arg[\varphi(s)], \quad s > 0.$$

Moreover, U has a density

$$u(t) = \frac{1}{\pi} \mathrm{Im} \left[\frac{\varphi'(t)}{\varphi(t)} \right].$$

These theorems are key tools for identifying a GGC distribution.

To address weak convergence of GGCs, we define a nonnegative measure $v(dt)$ on $[0, \infty]$ by

$$v(\{0\}) = 0, \quad v(\{\infty\}) = a, \quad v(dt) = \ln(1 + t^{-1}) U(dt), \ \ 0 < t < \infty.$$

Then we have

$$\varphi(s) = \exp\left(\int_0^\infty \frac{1}{\ln(1 + t^{-1})} \ln\left(\frac{t}{t - s} \right) v(dt) \right).$$

The following theorem about weak convergence of GGCs will be used in chapter 7 for proving a conjecture about GGCs.

Theorem 12 (Theorem 3.1.5. in [16]). *(Closure theorem). Let F_n in GGCs, $n = 1, 2, \ldots$, be defined by the measures $v_n, n = 1, 2, \ldots$. If $F_n \to F$ weakly (with F non-defective), then F is a GGC and the corresponding measure v is a vague limit of v_n on $[0, \infty]$. Conversely, if $v_n \to v$ vaguely on $[0, \infty]$ and $v(\{0\}) = 0$, then $F_n \to F$ weakly, where F in GGC corresponds to v.*

For the non-degenerate GGCs starting from zero with finite total Thorin measure ($U(\mathbb{R}^+) < \infty$), we have the next theorem helpful in both characterizing the distribution as well as generating such a distribution.

Theorem 13 (Theorem 4.1.1. in [16]). *(Gamma mixture representation). The pdf f of a GGC with $a = 0$ and $\int_0^\infty U(dt) = \beta$, $0 < \beta < \infty$, admits the representation*

$$f(x) = x^{\beta-1}h(x),$$

where h is completely monotone. Equivalently, if X is a GGC (with α, β as above), then

$$X \stackrel{d}{=} Y\,Z,$$

where $Y \sim Gamma(\beta, 1)$ and $Z > 0$ are independent r.v.s.

Concerning smoothness of density of GGC's, the following theorem states that GGC's starting from zero and with Thorin measure greater than 1 are infinitely differentiable on $(0, \infty)$.

Theorem 14 (Theorem 4.1.3. in [16]). *Let f be the pdf of a GGC with $a = 0$ and $U((0, \infty)) = \beta$, $1 < \beta \leq \infty$. Let $k \geq 0$ be an integer such that $k < \beta - 1$. Then f is continuously differentiable any number of times on $(0, \infty)$ and at 0 at least k times with $f^{(j)}(0) = 0$ for $j \leq k$.*

One immediate result of Theorem 14 is that if $f(0^+) > 0$, then $U(0, \infty) \leq 1$ and from Theorem 13 it follows that f is decreasing.

The next theorem gives the relation between total Thorin measure of a GGC and behaviour of its density function at zero.

Theorem 15 (Theorem 4.1.4. in [16]). *For a non-degenerate GGC with pdf f and $a = 0$, we have*

$$\int_0^\infty U(dt) = \sup\left\{\alpha;\ \lim_{x \downarrow 0} \frac{f(x)}{x^{\alpha-1}} = 0\right\}.$$

Let f_n, $n = 1, 2, \ldots$, be a sequence of densities of GGCs. If f_n converges pointwise to a probability density function f, then, by Scheffé's theorem [66], the convergence is weak as well. There is also a converse.

Theorem 16 (Theorem 4.1.5. in [16]). *Let densities f_n in GGC, $n = 1, 2, \ldots$, converge to f in GGC weakly. Let a and U be the left-extremity and the Thorin measure, respectively, corresponding to f.*

1. *if $\int_0^\infty U(dt) > 1$, then $f_n(x) \to f(x)$ for all $x \in \mathbb{R}$.*
2. *if $\int_0^\infty U(dt) \leq 1$, then $f_n(x) \to f(x)$ for all $x \neq a$.*

Not only is the GGC class closed under weak limits and addition of independent elements, it is also closed under multiplication of independent elements as the following theorem by Bondesson states.

Theorem 17 (Theorem 1 in [15]). *Let X in GGC and Y in GGC be independent r.v.'s. Then XY is a GGC and in particular XY is infinitely divisible and self-decomposable. In other words, the GGC class is closed w.r.t. convolution as well as multiplicative convolution.*

An important consequence of Theorem 17 appears in Theorem 3 in [15] stating that if random variable X is in GGC, so is e^X.

A probability distribution on $[0, \infty)$ with cumulative distribution function (cdf) F is said to be a mixture of Exponential distributions (MED) if

$$F(x) = \int_0^\infty (1 - e^{-xt}) M(dt), \ x > 0,$$

where $M(dt)$ is a probability measure. If $M(\{\infty\}) > 0$, then the distribution has an atom at 0. From the definition it immediately follows that for $x > 0$, it has a pdf

$$f(x) = \int_0^\infty t e^{-xt} M(dt).$$

Also, Bernstein's theorem 2.3 gives that any completely monotone pdf is an MED. The mgf of an MED equals

$$\varphi(s) = M(\{\infty\}) + \int_0^\infty \frac{t}{t - s} M(dt).$$

Remark 4. Every GGC with left-extremity zero ($a = 0$) and $U((0,\infty)) \leq 1$ is a MED.

The following result about MED characterization can be found in [16]. Before going over the theorem we need definition of Pick functions.

A function is called a Pick function if it is analytic in the upper half-plane and has positive imaginary part. Also, for $a \leq b$, $P(a,b)$ denotes the class of functions $f(z)$ which are analytic in $\mathbb{C} \setminus ((-\infty, a] \cup [b,\infty))$ and satisfy $f(\mathbb{H}^{\uparrow}) \subset \mathbb{H}^{\uparrow}$, and $f(\bar{z}) = \overline{f(z)}$ for $z \in \mathbb{H}^{\uparrow}$. Moreover, as canonical representation of Pick functions (Theorem 1 in [63]), a function f is a Pick function, $f \in P(a,b)$, if and only if it can be written as

$$f(z) = \alpha z + \beta + \int_{-\infty}^{\infty} \Big[\frac{1}{t-z} - \frac{t}{t^2+1}\Big] d\mu(t), \tag{3.2}$$

where $\alpha \geq 0$, β is real and μ is a positive measure on the real axis which puts no mass on (a,b) such that $\int (1+t^2)^{-1} d\mu(t) < \infty$. Now we are ready to state the theorem about characterizing an MED via Pick functions.

Theorem 18 (Theorem 2.4.2. in [16])**.** *(MED-characterization theorem). A function $\varphi(s)$ is the mgf of an MED iff $\varphi(s) \in P(-\infty, 0)$ and $\lim_{s\uparrow 0} \varphi(s) = 1$ and $\lim_{s\downarrow -\infty} \varphi(s) \geq 0$. In particular, an mgf φ (of a distribution on $\mathbb{R}^+$) belongs to $P(-\infty,0)$ iff it corresponds to an MED.*

Remark 5. If X is an MED and $Y \geq 0$ are independent r.v.'s, then XY is an MED.

Remark 6. If X is an MED, then for $q \geq 1$, X^q is also an MED.

From Theorem 18 the next theorem easily follows.

Theorem 19 (Theorem 2.4.3. in [16])**.** *An MED is infinitely divisible (ID) and its convolution roots are MED's.*

A result of the above theorem is that the Pareto distribution with the pdf $f(x) = C(1+x)^{-\lambda}$, for $\lambda > 1$ and the Weibull distribution with the pdf $f(x) = Cx^{\alpha-1}e^{-x^{\alpha}}$, for $0 < \alpha \leq 1$, are ID distributions.

Lastly, by Theorem 9.5. in [67] one can conclude that a cdf measure F on $[0,\infty)$ is a mixture of exponential distribution if and only if, $\mathcal{L}(F,t) \in \mathcal{S}$ and $\mathcal{L}(F,0^+) \leq 1$.

Chapter 4

Padé Approximations

In this chapter, we first review the concept of Padé approximation and its relation to Stieltjes functions. In Section 4.1, we discuss the connection between single-point Padé approximation and Gaussian quadrature. We then introduce two new approaches for approximating a Stieltjes function using multi-point Padé approximations. In Section 4.2, we present a matrix-based method for constructing the Padé approximant, which involves matrix multiplications and solving a system of linear equations. In Section 4.3, we develop a continued-fraction approach for obtaining the Padé approximant. This method relies solely on vector operations, making it more efficient than the matrix-based approach. Finally, Section 4.3.1 addresses a special case of the method in Section 4.3, which is treated separately due to its computational simplicity and minimal parameter requirements.

In general, a rational function that interpolates given function values at several (not necessarily distinct) points is called a *multi-point Padé approximant*. The associated interpolation problem for rational functions is known as the *Cauchy–Jacobi problem*.

Padé approximation was first introduced by Georg Frobenius to study the properties of rational approximations of power series and was later developed by Henri Padé around 1890. A Padé approximant provides the best local approximation of a function near a specific point by a rational function of prescribed order. It often yields a more accurate representation of the function than a truncated Taylor series and can remain valid over a wider domain, even

where the Taylor series fails to converge.

For a given function f and two non-negative integers m and n, the classical $[m/n]$ Padé approximant is a rational function R of the form

$$R(x) = \frac{\sum_{j=0}^{m} a_j x^j}{1 + \sum_{j=1}^{n} b_j x^j}, \tag{4.1}$$

which agrees with f to the highest possible order, meaning that

$$f(0) = R(0), \quad f'(0) = R'(0), \quad \ldots, \quad f^{(m+n)}(0) = R^{(m+n)}(0).$$

Note that it is possible that the $[m/n]$ Padé approximant does not exist if the constant term on the denominator is 0. For instance, as shown in Section 1.4 of [7], consider constructing a rational $[1/1]$ approximant $R(z) = P(z)/Q(z)$ to the function $f(z) = 1 + z^2$. If R exists, it takes the form $P(z) = a_0 + a_1 z$ and $Q(z) = b_0 + b_1 z$, and satisfy

$$\frac{a_0 + a_1 z}{b_0 + b_1 z} = 1 + z^2 + O(z^3),$$

or equivalently,

$$a_0 + a_1 z = b_0 + b_1 z + b_0 z^2 + O(z^3).$$

Equating coefficients yields $a_0 = b_0$, $a_1 = b_1$, and $b_0 = 0$. Consequently, the rational approximant reduces to $R(z) = 1$, which clearly fails to satisfy the condition $R^{(2)}(0) = 2$. Therefore, no such rational approximant to f exists.

The $[m/n]$ *multi-point Padé approximation* to a function f at points $z_1, z_2, \ldots, z_N$ and corresponding positive integers $n_1, n_2, \ldots, n_N$, where $m + n + 1 = \sum_{i=1}^{N} n_i$, is a rational function of the form $R(z) = P(z)/Q(z)$, where $P(z)$ and $Q(z)$ are polynomials of degree at most m and n, respectively, with the constant term of $Q(z)$ equal to 1, and

$$f^{(j)}(z_i) = R^{(j)}(z_i), \quad 1 \le i \le N,\ 0 \le j \le n_i - 1. \tag{4.2}$$

We call $[m/n]$ the degree of the Padé approximant. In this thesis we only seek the Padé approximations of degree $[M-1/M]$ for some natural number M.

From the perspective of multi-point summation, the Padé approximation generally provides a superior alternative to the truncated Taylor series, as it improves accuracy across multiple

points and accommodates functions with specific asymptotic behaviors. Notably, the Padé method can approximate divergent series, unlike Taylor expansions, which are valid only for convergent series.

The above definition of multi-point Padé approximant can be extended to complex numbers, where the interpolation points z_i and the function values may be complex. To establish the uniqueness and other properties of the rational approximant, we first state the necessary conditions guaranteeing these features and throughout all algorithms and applications that we provide, these conditions are assumed.

Assume we have N complex numbers $\{z_i\}_{1\le i\le N}$. For each $i \in \{1, 2, \dots, N\}$, there are n_i complex numbers $\{a_{i,j}\}_{0\le j<n_i}$, where $a_{i,j} = f^{(j)}(z_i)/j!$. The complex numbers z_i and $a_{i,j}$ appear in conjugate pairs: if for some $1 \le i_1 \le N$ we have $\mathrm{Im}(z_{i_1}) \neq 0$, then there exists $i_2 \in \{1, 2, \dots, N\}$ such that $z_{i_2} = \bar{z}_{i_1}$, $n_{i_2} = n_{i_1}$, and $a_{i_2,j} = \bar{a}_{i_1,j}$ for all $j \in \{0, 1, 2, \dots, n_{i_1} - 1\}$. Moreover, if $z_i \in \mathbb{R}$ for some i, then $a_{i,j} \in \mathbb{R}$ for all $0 \le j \le n_i - 1$. We also have n_∞ real numbers $\{\xi_i\}_{0\le i\le n_\infty-1}$ (assuming $\xi_0 \neq 0$).

We seek a Padé approximant $R(z) = P(z)/Q(z)$ satisfying

$$\deg(P) = M - 1 \quad \text{and} \quad \deg(Q) = M, \tag{4.3}$$

such that for every $i \in \{1, 2, \dots, N\}$,

$$R(z_i + w) = \sum_{j=0}^{n_i-1} a_{i,j} w^j + O(w^{n_i}), \quad w \to 0, \tag{4.4}$$

and

$$R(z) = \sum_{j=0}^{n_\infty-1} \xi_j z^{-j-1} + O(z^{-n_\infty-1}), \quad z \to \infty. \tag{4.5}$$

Note that here we are looking for a rational function of the form

$$R(z) = \frac{c_0 + c_1 z + \cdots + c_{M-1} z^{M-1}}{1 + d_1 z + \cdots + d_{M-1} z^{M-1} + d_M z^M},$$

and is thus defined by $2M$ complex coefficients $\{c_i\}_{0\le i<M}$, $\{d_i\}_{1\le i\le M}$. Also, there are

$$S = n_1 + n_2 + \cdots + n_N + n_\infty$$

conditions imposed on this rational function by (4.4) and (4.5). We now state the following proposition:

Proposition 2. *Assume that $S = 2M$ and that there exists a rational interpolating function $R(z) = P(z)/Q(z)$ satisfying (4.3), (4.4), and (4.5). Then such a function R is unique and $R \in \mathbb{R}(x)$ (meaning that P and Q have real coefficients).*

Proof. Suppose there exist two such rational interpolating functions $R_1(z) = P_1(z)/Q_1(z)$ and $R_2(z) = P_2(z)/Q_2(z)$ satisfying (4.3), (4.4), and (4.5). Then from equation

$$\frac{d^j}{dz^j}(R_1 - R_2)\Big|_{z=z_i} = \frac{d^j}{dz^j}\Big(\frac{P_1Q_2 - P_2Q_1}{Q_1Q_2}\Big)\Big|_{z=z_i} = 0,\ 0 \le j < n_i, \tag{4.6}$$

it implies that their difference

$$G(z) := R_1(z) - R_2(z) = \frac{P_1(z)Q_2(z) - P_2(z)Q_1(z)}{Q_1(z)Q_2(z)}$$

has $n_1+n_2+\cdots+n_N$ roots $z_1, \ldots, z_N$ (counting multiplicities), and satisfies $G(z) = O(z^{-n_\infty-1})$ as $z \to \infty$. Consequently, the numerator $P_1Q_2 - P_2Q_1$ is a polynomial with $n_1+n_2+\cdots+n_N$ distinct zeros, yet

$$\deg(P_1Q_2 - P_2Q_1) \le \deg(Q_1Q_2) - n_\infty - 1 = 2M - n_\infty - 1 = n_1 + n_2 + \cdots + n_N - 1.$$

Thus by Fundamental Theorem of Algebra the polynomial must vanish identically, and we conclude that $R_1(z) \equiv R_2(z)$.

To show that the coefficients of P and Q are real, consider $\overline{R(\bar{z})}$, the complex conjugate of $R(z)$ evaluated at $\bar{z}$. It clearly satisfies (4.3). For an arbitrary $i \in \{1, 2, \ldots, N\}$, there exists k such that $\bar{z}_i = z_k$, hence $a_{i,j} = \bar{a}_{k,j}$. Using (4.4), when $w \to 0$ and w is real, we have

$$\overline{R(\overline{z_i + w})} = \overline{R(\overline{z_i} + w)} = \overline{R(z_k + w)} = \overline{\sum_{j=0}^{n_i-1} a_{k,j}w^j + O(w^{n_i})} = \sum_{j=0}^{n_i-1} a_{i,j}w^j + O(w^{n_i}),$$

so it satisfies (4.4). Finally, as $z \to \infty$,

$$\overline{R(\bar{z})} = \overline{\sum_{j=0}^{n_\infty-1} \xi_j \bar{z}^{-j-1} + O(\bar{z}^{-n_\infty-1})} = \sum_{j=0}^{n_\infty-1} \xi_j z^{-j-1} + O(z^{-n_\infty-1}),$$

where the last equality follows from ξ_j being real. Therefore, $\overline{R(\bar{z})}$ satisfies all three conditions in the proposition, and by uniqueness, $\overline{R(\bar{z})} \equiv R(z)$. This identity implies that replacing every coefficient in $R(z)$ by its conjugate yields the same function, hence $R \in \mathbb{R}(x)$. □

The following theorem by W. Donoghue [22] is instrumental to our work, as we repeatedly use it whenever questions of existence and uniqueness arise in our approximations.

Theorem 20. *Suppose $n_1 + \cdots + n_N = 2k+1$ is odd and the interpolation points are all in the open interval (a, b). Then the multi-point Padé approximation for the interpolation problem of a Pick function on the interval (a, b), where degrees of both numerator and denominator are less than or equal to k, exists, is unique and it also belongs to $P(a, b)$.*

Proof. The uniqueness proof is straightforward. If another solution R_2 existed, the difference $R - R_2$ would be a rational function of degree of both numerator and denominator less than $2k + 1$, having at least $2k + 1$ zeros, and hence must vanish identically. The existence comes from Theorem 2 and 3 in [22]. The Pick function property comes from Theorem 4 in [22]. □

More can be said about the Padé approximant under the conditions of Theorem 20. If a rational function $g \in P(a, b)$, then all its poles are simple, located on the real axis outside (a, b), and have negative residues [22].

It can further be shown that for a Pick function f with representation (3.2), f belongs to $P(0, \infty)$ if and only if the corresponding measure μ has no mass in $(0, \infty)$. Moreover, when the number of interpolation conditions (here $2k + 1$) is odd, the unique Padé approximant also lies in $P(0, \infty)$. For detailed proofs, we refer the reader to [22, 23].

The following theorem concerning rational approximants of Stieltjes functions is a consequence of the preceding result.

Theorem 21. *Suppose $n_1 + \cdots + n_N = 2k$ is even and the interpolation points are all real positive numbers. Then the $[k - 1/k]$ multi-point Padé approximation of a Stieltjes function*

exists, is unique and it is also a Stieltjes function. Its poles are simple, lie on the negative real axis, and have positive residues.

Proof. For the given Stieltjes function f, consider the Pick function $g(z) = zf(z)$, $g \in P(0,\infty)$. It is easy to see that, in general for arbitrary functions f and h, the conditions $f^{(i)}(a) = h^{(i)}(a)$ for $i = 0, 1, \ldots, k$ hold if and only if the conditions $F^{(i)}(a) = G^{(i)}(a)$ hold for $F(z) = zf(z)$ and $G(z) = zh(z)$. Due to $g(0) = 0$, via adding zero to other $2k$ interpolation points, by Theorem 20 and the discussion following it, there exists rational approximation $R(z) = zP(z)/Q(z)$ in such a way that $R(z)$ is the $[k/k]$ multi-point Padé approximation to $g(z)$, $R(z) \in P(0,\infty)$, and $Q(z)$ has simple poles outside $(0,\infty)$ and negative residues. That is, if α is a pole, then $\alpha P(\alpha)/Q'(\alpha) < 0$, so $P(\alpha)/Q'(\alpha) > 0$. Therefore $R(z)/z = P(z)/Q(z)$ is the desired $[k-1/k]$ multi-point Padé approximation of f. □

Similar statements can be formulated for general $[m/n]$ Padé approximants of Stieltjes functions.

Theorem 22 (Corollary 1 in §5.1 and Theorem 5.2.1 in [7])**.** *If $f(z)$ is a Stieltjes function, then the $[M + J/M]$ Padé approximants (with $J \geq -1$) to $f(z)$ exist, have simple poles lying on the negative real axis, and possess positive residues.*

To have a better understanding of the above results, we now show why multi-point Padé approximation of a Stieltjes function is also Stieltjes for the simplest case $k = 1$, and demonstrate that the statement of Theorem 21 fails when the number of conditions is odd. In particular, we present an example where the number of conditions is odd and the resulting continued-fraction approximant is not Stieltjes.

When $k = 1$, the continued fraction has the form $\frac{a_1}{1+a_2(z-z_1)}$. This represents a Stieltjes function if and only if its pole, $z_1 - 1/a_2$, is negative. There are two cases to consider: $n_1 = n_2 = 1$ or $n_1 = 2$.

If $n_1 = n_2 = 1$, define the function g by

$$g(z) = \left(\frac{f(z_1)}{f(z)} - 1\right) \frac{1}{(z - z_1)}.$$

By construction, $a_2 = g(z_2) = -\frac{f(z_2)-f(z_1)}{z_2-z_1}\frac{1}{f(z_2)}$. The condition $z_1 - 1/a_2 < 0$ is equivalent to

$$z_1 < \frac{f(z_2)(z_2 - z_1)}{f(z_1) - f(z_2)} \quad \iff \quad f(z_2)z_2 > f(z_1)z_1.$$

However, by Theorem 4, we know that $zf(z) \in \text{CBF}$, meaning it is a Bernstein function. By Definition 2, it is therefore increasing, as required.

If $n_1 = 2$, then $a_2 = g(z_1)$, and the condition $z_1 - 1/a_2 < 0$ becomes $z_1 < 1/g(z_1)$. Since $g(z_1) = -f'(z_1)/f(z_1)$ and f is a Stieltjes function (implying $f'(z_1) < 0$), this inequality is equivalent to

$$z_1 f'(z_1) > -f(z_1) \quad \iff \quad (zf(z))' > 0 \text{ at } z = z_1,$$

which again holds by the previous argument. This completes the proof for $k = 1$.

Now for providing an example where the number of conditions is odd and the Padé approximant to the Stieltjes function is not Stieltjes, consider the Stieltjes function

$$f(z) = \int_0^\infty \frac{e^{-zx}}{1+x} dx$$

Take interpolation points $z_1 = 0.0013, z_2 = 0.003$, and $z_3 = 0.3$ and require that the rational approximant

$$R(z) = \frac{a_0 + a_1 z + a_2 z^2 + a_3 z^3 + a_4 z^4}{1 + b_1 z + b_2 z^2 + b_3 z^3 + b_4 z^4}$$

satisfies the nine conditions $R(z_1) = f(z_1)$, $R^{(j)}(z_2) = f^{(j)}(z_2)$ $0 \le j \le 2$, and $R^{(k)}(z_3) = f^{(k)}(z_3)$ $0 \le k \le 4$. Solving the resulting linear system yields

$$R(z) \approx \frac{7.0289 + 1283.4z - 7232.8z^2 - 124842.7z^3 - 11235.44z^4}{1 + 347.4354z + 2465.9z^2 - 75497.9z^3 - 164458.16z^4}$$

The poles of R are

$$z_1^{\text{pole}} \approx -0.481163,\ z_2^{\text{pole}} \approx -0.0541696,\ z_3^{\text{pole}} \approx -0.00294532,\ z_4^{\text{pole}} \approx 0.0792071.$$

One pole of R is not a negative real number. If R was a Stieltjes function, by representation (2.5), the measure σ would be a finite sum of atoms

$$\sigma = \sum_{k=1}^{n} c_k \delta_{t_k},$$

for some $c_k, t_k > 0$. Thus, R would have the form

$$R(z) = b + \sum_{k=1}^{n} \frac{c_k}{z + t_k},$$

for some $b > 0$, where poles, $z = -t_k$, are non-positive. Therefore R is not a Stieltjes function, even though it interpolates the Stieltjes function f at the prescribed points.

As for the computational method, consider the single-point $[m/n]$ Padé approximant $P(x)/Q(x)$ of f. Let $T(x) = c_0 + c_1 x + \cdots + c_{m+n} x^{m+n}$ denote the Taylor series of f up to degree $m + n$. Then we set $P(x) = Q(x)T(x) \bmod x^{m+n}$, meaning that the coefficients of $1, x, \ldots, x^{m+n}$ are identical on both sides of the equation.

The multi-point Padé approximant is treated in a similar fashion. For arbitrary points $z_1, z_2, \ldots, z_N$, we can first write the Taylor expansion of f around any of these points up to a prescribed degree, then equate the coefficients of the power series of the rational Padé approximant and the Taylor expansion around that point up to that order. Note that the last point can even take the value ∞, in which case the power series is expressed in negative powers. Through this method, we can achieve any desired order of accuracy at any finite number of points, including ∞.

4.1 Single-point Padé approximation via orthogonal polynomials

The material and formulas in this section regarding Gaussian quadrature can be found in Section 4.6 of [58]. To elaborate on the connection between Padé approximants and orthogonal polynomials, we begin by defining Gaussian quadrature. A quadrature is an approximate evaluation of a definite integral $\int_a^b f(z)\, dz$ with a specified degree of accuracy. Since our focus is on the interval $(0, \infty)$, we restrict attention to integrals of the form $\int_0^\infty f(z)\, dz$.

For a given finite positive measure $\sigma(dz)$ on $(0, \infty)$, an n-point Gaussian quadrature rule is constructed such that the approximation $Q(f) = \sum_{i=1}^{n} w_i f(z_i)$ of $\int_0^\infty f(z)\, \sigma(dz)$ is exact for all polynomials of degree less than or equal to $2n - 1$, through an appropriate choice of the

nodes z_i and weights w_i for $i = 1, \ldots, n$. In other words, for a finite positive measure $\sigma(dz)$, the Gaussian quadrature of order n is the measure $\tilde{\sigma}(dz)$ supported on n points in $(0, \infty)$, matching the first $2n-1$ moments of $\sigma(dz)$. For a proof of the existence and uniqueness of the Gaussian quadrature see Theorem 3.4.1 in [74].

To construct the Gaussian quadrature, for each positive integer n we define the orthogonal polynomial $P_n(z)$ of degree n by

$$\int_0^\infty P_n(z)\, z^k\, \sigma(dz) = 0, \qquad k = 0, 1, \ldots, n-1. \tag{4.7}$$

See Theorem 2.1.1 in [74] for a proof that at least one family of orthogonal polynomials exists. Let z_i denote the roots of P_n. Then there exist corresponding weights w_i, given by the formula below, such that the resulting Gaussian quadrature is exact for all polynomials of degree up to $2n-1$. Moreover, the roots z_i are positive and distinct (see Section 3.6. in [73]), and the orthogonal polynomials can be obtained recursively.

Define the inner product of two functions $f(z)$ and $g(z)$ with respect to the measure $\sigma(dz)$ as $\langle f(z), g(z)\rangle = \int_0^\infty f(z)g(z)\,\sigma(dz)$. Then the weights w_i are given by

$$w_i = \frac{p_n}{p_{n-1}} \frac{\langle P_{n-1}, P_{n-1}\rangle}{P_n'(z_i)\, P_{n-1}(z_i)},$$

where p_i denotes the coefficient of x^i in $P_i(z)$. The orthogonal polynomials with leading coefficient one satisfy the recurrence relation

$$P_{n+1}(z) = (z - a_{n,n})P_n(z) - a_{n,n-1}P_{n-1}(z),$$

where $a_{i,j} = \langle zP_i, P_j\rangle / \langle P_j, P_j\rangle$.

We now describe how the single-point Padé approximants of a Stieltjes function can be derived from orthogonal polynomials, and the connection between the partial fraction decomposition of the Padé approximant and the coefficients and nodes of the Gaussian quadrature. We also use Watson's Lemma [81]. In the simplified form applicable here, the lemma states: suppose that $g(x)$ has infinitely many derivatives near zero and that $g(0) \neq 0$. Furthermore, assume that either $\int_0^\infty |g(x)|\, dx < \infty$ or $|g(x)| < ke^{bx}$ for all $x > 0$, where k, b

are constants. Then, for all complex z such that $|\arg(z)| < \pi/2$, and $|z|$ is large enough, we have

$$\left| \int_0^\infty e^{-zx} g(x)\, dx \right| < \infty,$$

and the following asymptotic expansion holds:

$$\int_0^\infty e^{-zx} g(x)\, dx \approx \sum_{n=0}^{\infty} \frac{g^{(n)}(0)}{z^{n+1}}, \qquad |z| \to \infty. \tag{4.8}$$

Now consider a Stieltjes function

$$f(z) = \int_0^\infty \frac{1}{z+t}\, \sigma(dt).$$

Then the $[n-1/n]$ Padé approximant of $f(z)$ is given by

$$Q\Big(\frac{1}{z+t}\Big) = \sum_{i=1}^{n} \frac{w_i}{z+z_i},$$

where w_i are the Gaussian quadrature weights and z_i are the roots of the orthogonal polynomial P_n with respect to σ.

Also, we can write f as

$$\int_0^\infty \int_0^\infty e^{-zu} e^{-tu} du\, \sigma(dt) = \int_0^\infty e^{-zu} \int_0^\infty e^{-tu} \sigma(dt)\, du, \tag{4.9}$$

where we have used Fubini's Theorem. By Stieltjes assumption we can conclude $\int_0^\infty \int_0^\infty e^{-tu}\sigma(dt)du < \infty$, therefore we can use Watson's lemma (4.8), which gives the expansion of f at ∞:

$$f(z) = \sum_{n=0}^{\infty} \frac{g^{(n)}(0)}{z^{n+1}} \qquad z \to \infty,$$

where $g(u) = \int_0^\infty e^{-tu}\sigma(dt)$, therefore $g^{(n)}(0) = \int_0^\infty (-t)^n \sigma(dt)$.

Assuming the expansion of $f(z)$ at ∞ is $\sum_{i=1}^{\infty} a_i z^{-i}$, by the above discussion we obtain

$$a_i = \int_0^\infty (-t)^{i-1}\, \sigma(dt), \qquad i = 1, 2, \ldots.$$

Moreover, since the quadrature formula is exact for all polynomials of degree up to $2n-1$, we obtain

$$Q((-t)^j) = \int_0^\infty (-t)^j\, \sigma(dt) = a_{j+1}, \qquad j = 0, 1, \ldots, 2n-1.$$

By linearity of the quadrature and the relation above, we have

$$Q\Big(\frac{1}{z+t}\Big) = Q\Big(\sum_{j=1}^{2n-1}(-t)^{j-1}z^{-j} + \frac{(-t)^{2n-1}z^{-2n}}{1+t/z}\Big) = \sum_{j=1}^{2n-1} a_j z^{-j} + z^{-2n}Q\Big(\frac{(-t)^{2n-1}}{1+t/z}\Big).$$

Letting $z \to \infty$ gives

$$Q\Big(\frac{1}{z+t}\Big) = \sum_{j=1}^{2n-1} a_j z^{-j} + O(z^{-2n}),$$

which shows that the quadrature—being a rational function with a numerator of degree $n-1$ and denominator of degree n—matches the expansion of f at ∞ up to $2n-1$ terms. This satisfies the definition of the Padé approximant of f, confirming that it is indeed the $[n-1/n]$ Padé approximant of f.

4.2 Computing Multi-Point Padé Approximations via a Matrix Approach

In this section, we describe how to compute the multi-point Padé approximant to a function by forming certain matrices and then solving a corresponding matrix equation.

For a given set of points $z_1, z_2, \ldots, z_N$, we assume that the function f is at least n_j times differentiable at each z_j. Hence, it can be expanded into a Taylor series around z_j as follows:

$$f(z) = \sum_{l=0}^{n_j-1} s_{j,l}(z-z_j)^l + O\Big((z-z_j)^{n_j}\Big). \tag{4.10}$$

Now, setting $w = z - z_j$ in (4.10) and substituting this into (4.2) gives

$$\frac{a_0 + a_1(w+z_j) + a_2(w+z_j)^2 + \cdots + a_{m-1}(w+z_j)^{m-1}}{b_0 + b_1(w+z_j) + b_2(w+z_j)^2 + \cdots + b_m(w+z_j)^m} = \sum_{l=0}^{n_j-1} s_{j,l}w^l + O(w^{n_j}), \tag{4.11}$$

where we set $b_0 = 1$. Also at ∞ by (4.5) we can write

$$\frac{a_0 + a_1\, z + a_2\, z^2 + \cdots + a_{m-1}\, z^{m-1}}{1 + b_1\, z + b_2\, z^2 + \cdots + b_m\, z^m} = \sum_{j=0}^{n_\infty-1} \xi_j z^{-j-1} + O(z^{-n_\infty-1}), \quad z \to \infty. \tag{4.12}$$

We set $u = 1/z$ where $u \to 0$ in (4.12). Multiplying both numerator and denominator of left side of (4.12) to u^m yields

$$\frac{a_{m-1} + a_{m-2}\, u + \cdots + a_0\, u^{m-1}}{b_m + b_{m-1}\, u + \cdots + 1\, u^m} = \sum_{j=0}^{n_\infty-1} \xi_j u^j + O(u^{n_\infty}), \quad u \to 0. \tag{4.13}$$

Comparing the coefficients of powers of u in both sides of the last equation gives

$$a_{m-l} = \sum_{j=0}^{l-1} b_{m-j}\xi_{l-1-j}, \quad 1 \le l \le n_\infty.$$

We put these equations into the matrix form. Define matrix $C^{(\infty,m)}$ as follows

$$C(i,j) = \begin{cases} 1, & \text{if } j = m+1-i, \\ -\xi_{i-1-l}, & \text{if for some } 0 \le l \le i-1,\ j+l = 2m+1, \\ 0, & \text{otherwise,} \end{cases} \tag{4.14}$$

for $1 \le i \le n_\infty$ and $1 \le j \le 2m+1$. Then, the system of equations at ∞ can be written as

$$C^{(\infty,m)} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_{m-1} \\ 1 \\ \vdots \\ b_m \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{4.15}$$

Now, note that in general, for a polynomial of the form $T(z) = A_0 + A_1 z + A_2 z^2 + \cdots + A_m z^m$ and for a constant c, we can write

$$T(z+c) = \tilde{A}_0 + \tilde{A}_1 z + \tilde{A}_2 z^2 + \cdots + \tilde{A}_m z^m,$$

where

$$\begin{bmatrix} \tilde{A}_0 \\ \tilde{A}_1 \\ \vdots \\ \tilde{A}_m \end{bmatrix} = B^{(c,m)} \begin{bmatrix} A_0 \\ A_1 \\ \vdots \\ A_m \end{bmatrix}. \tag{4.16}$$

Here, $B^{(c,m)}$ is an $(m+1) \times (m+1)$ matrix with entries

$$B^{(c,m)}_{i,j} = \mathbf{1}_{(i \le j)} \binom{j-1}{i-1} c^{j-i}, \qquad 1 \le i, j \le m+1.$$

We can now rewrite equation (4.11) as

$$\frac{\tilde{a}_{0,j} + \tilde{a}_{1,j}w + \cdots + \tilde{a}_{m-1,j}w^{m-1}}{\tilde{b}_{0,j} + \tilde{b}_{1,j}w + \tilde{b}_{2,j}w^2 + \cdots + \tilde{b}_{m,j}w^m} = \sum_{l=0}^{n_j-1} s_{j,l}w^l + O(w^{n_j}), \qquad j = 1, 2, \ldots, N, \tag{4.17}$$

where

$$\begin{bmatrix} \tilde{a}_{0,j} \\ \tilde{a}_{1,j} \\ \vdots \\ \tilde{a}_{m-1,j} \\ \tilde{b}_{0,j} \\ \vdots \\ \tilde{b}_{m,j} \end{bmatrix} = \Lambda^{(z_j,m)} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_{m-1} \\ 1 \\ \vdots \\ b_m \end{bmatrix}, \qquad \Lambda^{(z_j,m)} = \begin{bmatrix} B^{(z_j,m-1)} & O \\ O & B^{(z_j,m)} \end{bmatrix}, \tag{4.18}$$

where $\Lambda^{(z_j,m)}$ is a $(2m+1) \times (2m+1)$ matrix. By equating coefficients of powers of w on both sides of (4.17), we obtain: for w^0,

$$\tilde{a}_{0,j} = \tilde{b}_{0,j}s_{j,0},$$

and for w^l with $1 \le l \le n_j - 1$,

$$\tilde{a}_{l,j} = \sum_{y=0}^{l} \tilde{b}_{y,j}\, s_{j,l-y}.$$

Hence, defining the matrix $A^{(z_r,m)}$ by

$$A(i,j) = \begin{cases} 1, & \text{if } i = j, \\ -s_{r,i-k}, & \text{if for some } 1 \le k \le i,\ j = k + m, \\ 0, & \text{otherwise,} \end{cases} \tag{4.19}$$

for $1 \le i \le n_r$ and $1 \le j \le 2m+1$, where $A^{(z_r,m)}$ is a $n_r \times (2m+1)$ matrix, the above system

of equations can be written compactly as

$$A^{(z_j,m)} \begin{bmatrix} \tilde{a}_{0,j} \\ \tilde{a}_{1,j} \\ \vdots \\ \tilde{a}_{m-1,j} \\ \tilde{b}_{0,j} \\ \vdots \\ \tilde{b}_{m,j} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{4.20}$$

Combining all such matrix identities for each point z_j as well as ∞ into one system gives the final matrix representation:

$$\begin{bmatrix} A^{(z_1,m)}\Lambda^{(z_1,m)} \\ \vdots \\ A^{(z_N,m)}\Lambda^{(z_N,m)} \\ C^{(\infty,m)} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_{m-1} \\ 1 \\ \vdots \\ b_m \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{4.21}$$

The matrix on the left-hand side is of size $2m \times (2m+1)$. By removing the $(m+1)$-th column of this matrix and moving it to the right-hand side, we see that the coefficients a_i and b_i are determined by Gaussian elimination method on the resulting square matrix. Consequently, we obtain the Padé polynomials $P(z)$ and $Q(z)$.

Here we summarize the steps of the algorithm for obtaining the rational approximant:

Step 1: Compute the coefficients $s_{j,k}$ for $j = 1, \ldots, N$ and $k = 1, \ldots, n_j - 1$ from the Taylor expansion of f around each point z_j and coeffients ξ_i for $i = 0, \ldots, n_\infty - 1$. from the expansion of f at infinity.

Step 2: Construct the matrices $C^{(\infty,m)}$ using (4.14).

Step 3: Construct the matrices $A^{(z_j,m)}$ for $j = 1, \ldots, N$ using (4.19).

Step 4: Define $B^{(c,m)}$ by $B^{(c,m)}_{i,j} = \mathbf{1}_{(i\le j)}\binom{j-1}{i-1}c^{j-i}$ for $1 \le i, j \le m+1$, and construct $\Lambda^{(z_j,m)}$ as in (4.18). Let

$$\Lambda \coloneqq \begin{bmatrix} A^{(z_1,m)}\Lambda^{(z_1,m)} \\ \vdots \\ A^{(z_N,m)}\Lambda^{(z_N,m)} \\ C^{(\infty,m)} \end{bmatrix},$$

and denote by C the $(m+1)$-th column of Λ. Let Λ_C be the matrix obtained by removing this column from Λ.

Step 5: Solve the matrix equation

$$\Lambda_C \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_{m-1} \\ b_1 \\ \vdots \\ b_m \end{bmatrix} = -C,$$

to obtain the coefficients $a_0, \dots, a_{m-1}$ and $b_1, \dots, b_m$.

Remark 7. The algorithm described in Section 4.2 requires high-precision computation. This is because, in Step 4, solving the system of linear equations may involve an ill-conditioned matrix, necessitating high-precision arithmetic. Moreover, when the Stieltjes function ψ is not explicitly known, computing the initial coefficients $s_{j,k}$ may also require high-precision evaluation.

4.3 Computing Multi-Point Padé Approximations via the Continued Fraction Approach

The continued fraction approach proposed here provides an efficient and transparent procedure for constructing multi-point Padé approximants. The method is fully recursive and avoids solving large linear systems, reducing the interpolation problem step by step via linear fractional transformations.

We consider an interpolation problem specified by an ordered collection of interpolation points $z_1, z_2, \ldots, z_N, \infty$. At each point z_j the value of the function and its derivatives up to order $n_j - 1$ are prescribed. In addition, asymptotic conditions at infinity are imposed through a prescribed expansion of the function as $z \to \infty$ up to order n_∞. The goal is to construct a rational approximation satisfying all the conditions (4.3), (4.4), and (4.5).

The construction is based on a recursive linear fractional transformation that removes one interpolation condition at a time. Fix a complex number c and define

$$\tilde{f}(z) = \frac{1}{z - c}\left(\frac{f(c)}{f(z)} - 1\right). \tag{4.22}$$

This transformation plays a central role in the algorithm. Applied at a finite interpolation point, it removes one condition at that point while transferring all remaining conditions to the transformed function $\tilde{f}$.

We begin by processing the first interpolation point z_1. If only the value of the function is prescribed at z_1, that is, if $n_1 = 1$, then the transformation (4.22) with $c = z_1$ eliminates the interpolation condition at z_1 entirely. The transformed function $\tilde{f}$ must then satisfy interpolation conditions at the remaining finite points $z_2, \ldots, z_N$, together with modified asymptotic conditions at infinity.

Let z_i be one of the remaining finite points with $i \geq 2$, and write local expansions

$$f(z_i + w) \approx \sum_{j=0}^{n_i - 1} a_j w^j, \qquad \tilde{f}(z_i + w) \approx \sum_{j=0}^{n_i - 1} b_j w^j \quad w \to 0.$$

Substituting these expansions into (4.22) with $c = z_1$ yields

$$f(z_i + w) + (w + z_i - z_1) f(z_i + w)\tilde{f}(z_i + w) = z_1.$$

Comparing coefficients gives

$$b_0 = \frac{z_1 - a_0}{a_0(z_i - z_1)},$$

and for $n \geq 1$,

$$b_n = -\frac{1}{a_0(z_i - z_1)} \left[a_n + \sum_{j=0}^{n-1} a_j b_{n-1-j} + (z_i - z_1) \sum_{j=1}^{n} a_j b_{n-j} \right]. \tag{4.23}$$

If, on the other hand, derivatives of order higher than zero are prescribed at z_1, so that $n_1 > 1$, then the point z_1 remains among the interpolation points but with its multiplicity reduced by one. In this case the transformed function $\tilde{f}$ is expanded locally at z_1. Writing

$$f(z_1 + w) \approx \sum_{j=0}^{n_1-1} a_j w^j, \qquad \tilde{f}(z_1 + w) \approx \sum_{j=0}^{n_1-2} A_j w^j \quad w \to 0,$$

and substituting into (4.22) with $c = z_1$, one finds

$$A_0 = -\frac{a_1}{a_0}, \tag{4.24}$$

and, for $n = 1, \ldots, n_1 - 2$,

$$A_n = -\frac{1}{a_0} \left[a_{n+1} + \sum_{i=1}^{n} a_i A_{n-i} \right]. \tag{4.25}$$

Thus, one derivative condition at z_1 is removed, while all other interpolation data are transferred to $\tilde{f}$.

The transformation (4.22) also induces a recursive update of the asymptotic expansion at infinity. Suppose that, as $z \to \infty$,

$$f(z) = \sum_{i \geq 0} a_i z^{-i}.$$

Then $\tilde{f}$ admits an expansion of the form

$$\tilde{f}(z) = \sum_{i \geq 0} \tilde{a}_i z^{-i}.$$

An recursion relation is obtained by comparing coefficients in the identity

$$f(z) - z_1 f(z)\tilde{f}(z) + z f(z)\tilde{f}(z) = c.$$

Comparing coefficient of z yields $a_0\tilde{a}_0 = 0$. From the coefficients of z^0 we obtain

$$a_0 - z_1 a_0\tilde{a}_0 + a_0\tilde{a}_1 + a_1\tilde{a}_0 = c, \tag{4.26}$$

and from the coefficients of z^{-n} we get

$$a_n - z_1 \sum_{i=0}^{n} a_i\tilde{a}_{n-i} + \sum_{i=0}^{n+1} a_i\tilde{a}_{n+1-i} = 0, \quad n \geq 1. \tag{4.27}$$

Putting together the above equations, we can obtain $\tilde{f}(z)$ coefficients recursively:

If $a_0 = 0$, then

$$\tilde{a}_0 = c/a_1 \quad \tilde{a}_n = -\frac{1}{a_1}\left[a_n - z_1 \sum_{i=1}^{n} a_i\tilde{a}_{n-i} + \sum_{i=2}^{n+1} a_i\tilde{a}_{n+1-i}\right], \quad n \geq 1. \tag{4.28}$$

If $a_0 \neq 0$, then $\tilde{a}_0 = 0$, and

$$\tilde{a}_1 = c/a_0 - 1 \quad \tilde{a}_{n+1} = -\frac{1}{a_0}\left[a_n - z_1 \sum_{i=0}^{n} a_i\tilde{a}_{n-i} + \sum_{i=1}^{n} a_i\tilde{a}_{n+1-i}\right], \quad n \geq 0. \tag{4.29}$$

Note that in the first case, where $a_0 = 0$, starting with M coefficients $\{a_i\}_{1\leq i\leq M}$ of the expansion of f at infinity (with $a_0 = 0$), we can compute M coefficients $\{\tilde{a}_i\}_{0\leq i\leq M-1}$ of $\tilde{f}$ (where the first coefficient is non-zero). In the second case, where $a_0 \neq 0$, starting with M coefficients $\{a_i\}_{0\leq i\leq M-1}$ of f at infinity (with $a_0 \neq 0$), we can compute M coefficients $\{\tilde{a}_i\}_{1\leq i\leq M}$ of $\tilde{f}$ (where $\tilde{a}_0 = 0$).

The above procedure is repeated recursively. At each step, one interpolation condition at a finite point is removed, either by eliminating the point entirely or by reducing its multiplicity by one. After all finite interpolation conditions have been exhausted, the remaining function is characterized solely by its expansion at infinity. The algorithm for given conditions (4.4) and (4.5) runs as follows.

Set $\gamma_0 = 0$ and $\gamma_j = \xi_{j-1}$ for $1 \geq j \geq \infty$. Then f has the following asymptotic expansion as $z \to \infty$:

$$f(z) = \sum_{j=0}^{n_\infty} \gamma_j z^{-j} + O(z^{-n_\infty - 1}). \tag{4.30}$$

Define f_1 by

$$f_1(z) = \frac{1}{z - z_1}\left(\frac{f(z_1)}{f(z)} - 1\right). \tag{4.31}$$

The expansion of f_1 at each finite point is obtained via equations (4.23) or (4.25), depending on $n_1 = 1$ or $n_1 > 1$. Given $\gamma_0 = 0$, the function f_1 has the following expansion at ∞:

$$f_1(z) = \sum_{j=0}^{n_\infty - 1} \gamma_j^{(1)} z^{-j} + O(z^{-n_\infty}), \tag{4.32}$$

where coefficients $\gamma_j^{(1)}$ are derived from equation (4.28), and the coefficient $\gamma_0^{(1)}$ is non-zero. Note that equation (4.31) can be rewritten by

$$f(z) = \frac{f(z_1)}{1 + (z - z_1) f_1(z)}. \tag{4.33}$$

Hence, the function on the right side, we call it R_1, satisfies $R_1(z_1) = f(z_1)$, on condition that f_1 does not have a pole at z_1.

Now if $n_1 = 1$, then all expansion coefficients of f_1 at $z_2, \ldots, z_N$ are calculated by (4.23). Next, we define

$$f_1(z) = \frac{f_1(z_2)}{1 + (z - z_2) f_2(z)},$$

and compute the coefficients for expansion of f_2 at each finite point by (4.23) or (4.25) again, depending on $n_2 = 1$ or $n_2 > 1$. Due to $\gamma_0^{(1)} \neq 0$, the expansion of f_2 at ∞ takes the form

$$f_2(z) = \sum_{j=0}^{n_\infty} \gamma_j^{(2)} z^{-j} + O(z^{-n_\infty - 1}), \qquad z \to \infty, \tag{4.34}$$

with $\gamma_0^{(2)} = 0$ and $\gamma_j^{(2)}$ coefficients come from equation (4.29).

If $n_1 > 1$, then the expansion coefficients of f_1 at z_1 are calculated by (4.25) and at all other points are calculated by (4.23). Then, f_2 is defined by

$$f_1(z) = \frac{f_1(z_1)}{1 + (z - z_1) f_2(z)},$$

and similarly the coefficients of expansion of f_2 at each interpolation point are calculated.

By doing this procedure $n_1 + \cdots + n_N - 2 = 2M - n_\infty - 2$ times, we define successively the functions $f_3, f_4, \ldots, f_{2M - n_\infty}$. Then we do backward substitution which renders the continued

fraction representation of f:

$$f(z) = \cfrac{c_1}{1 + \cfrac{(z-z_1)c_2}{1 + \cfrac{(z-z_1)c_3}{\ddots \cfrac{\cdots}{1 + \cfrac{(z-z_N)c_{2M-n_\infty}}{1 + (z-z_N)f_{2M-n_\infty}(z)}}}}}, \tag{4.35}$$

where the continued fraction contains $(z - z_N)$ repeated n_N times at the end and $(z - z_1)$ repeated n_1 times at the beginning and $c_1 = f(z_1)$, $c_2 = f_1(z_2)$ or $c_2 = f_1(z_1)$ (depending on value of n_1) and so forth.

Also f has the asymptotic expansion (4.30) iff f_{2M-n_∞} satisfies

$$f_{2M-n_\infty}(z) = \sum_{j=0}^{K} \gamma_j^{(2M-n_\infty)} z^{-j} + O(z^{-K-1}), \qquad z \to \infty, \tag{4.36}$$

where the coefficients $\gamma_j^{(2M-n_\infty)}$ are computed iteratively similar to the procedure above, and

$$K = \begin{cases} n_\infty, & \text{if } \sum_{i=1}^{N} n_i \text{ is even}, \\ n_\infty - 1, & \text{if } \sum_{i=1}^{N} n_i \text{ is odd}, \end{cases}$$

which implies that K is always an even integer, since $\sum_{i=1}^{N} n_i + n_\infty = 2M$ is even.

Finally, we express $f_{2M-n_\infty}(z)$, satisfying (4.36), as a continued fraction:

$$f_{2M-n_\infty}(z) = \gamma_0^{(2M-n_\infty)} + \cfrac{d_1 z^{-1}}{1 + \cfrac{d_2 z^{-1}}{\ddots \cfrac{\cdots}{1 + \cfrac{d_{K-1} z^{-1}}{1 + d_K z^{-1}}}}}, \tag{4.37}$$

where $d_1 := \gamma_1^{(2M-n_\infty)}$, and the remaining coefficients $\{d_j\}_{2 \le j \le K}$ are computed iteratively similar to (4.33). That is, define $f_{2M-n_\infty+1}(z)$ by

$$f_{2M-n_\infty}(z) = \gamma_0^{2M-n_\infty} + \frac{d_1}{z f_{2M-n_\infty+1}(z)},$$

From (4.36) and this relation, we compute the expansion of $f_{2M-n_\infty+1}(z)$ as $z \to \infty$:

$$f_{2M-n_\infty+1}(z)(z) = 1 + \sum_{j=1}^{K-1} \gamma_j^{2M-n_\infty+1} z^{-j} + O(z^{-K}). \tag{4.38}$$

Then set $d_2 := \gamma_1^{2M-n_\infty+1}$ and repeat the step. Next, we define

$$f_{2M-n_\infty+1}(z) = 1 + \frac{d_2}{z f_{2M-n_\infty+2}(z)},$$

compute the expansion of $f_{2M-n_\infty+2}(z)$ at ∞, and set $d_3 := \gamma_1^{2M-n_\infty+2}$. Continuing this procedure for K steps yields the coefficients $\{d_j\}_{1\le j\le K}$ of the continued fraction (4.37) and substituting f_{2M-n_∞} from (4.37) into (4.35) gives the desired rational function.

Here we illustrate, through an example, how to obtain the continued fraction and consequently the multi-point Padé approximant given the initial points, corresponding integers, and coefficient matrix. Assume $z_1 = 1$, $z_2 = 2$, $z_3 = \infty$, $n_1 = 1$, $n_2 = 2$, $n_3 = 1$, with expansion coefficients as defined by equations (4.4) and (4.5), $a_{1,0} = -2$, $a_{2,0} = -3$, $a_{2,1} = -4$, $\xi_0 = 1$.

Since $n_1 = 1$, by transformation (4.33), the coefficients of f_1 at z_2 which we denote by b_0, b_1, are obtained by equation (4.23):

$$b_0 = \frac{-2-(-3)}{-3(2-1)} = -\frac{1}{3},$$

and

$$b_1 = \frac{-1}{-3(2-1)}\Big(-4 + (-3)\times\frac{-1}{3} + (2-1)\times(-4)\times\frac{-1}{3}\Big) = -\frac{5}{9}.$$

For the coefficient $\gamma_0^{(1)}$ of expansion of f_1 at ∞, note that due to $\gamma_0 = 0$, we conclude $\gamma_0^{(1)} \neq 0$ and by equation (4.28) $\gamma_0^{(1)} = -2/1 = -2$.

Next, we compute coefficient of expansion of f_2 at z_2 denoted by A_0. It is calculated through (4.24)

$$A_0 = -\frac{-5/9}{-1/3} = -\frac{5}{3}.$$

To compute the coefficient of expansion of f_2 as $z \to \infty$, since $\gamma_0^{(1)} \neq 0$, we use (4.29) and get

$$\gamma_1^{(2)} = \frac{-1/3}{-2} - 1 = -\frac{5}{6},$$

Finally, when there is no condition at finite points for f_3 and $\gamma_0^{(2)} = 0$, to derive coefficient of expansion of f_3 at ∞, we use (4.28) to find

$$\gamma_0^{(3)} = \frac{-5/3}{-5/6} = 2.$$

As a result, the continued fraction coefficients are $c_1 = -2$, $c_2 = -1/3$, $c_3 = -5/3$, and $f_3 = 2$ (corresponding to the ∞ constant). The overall continued fraction representation is therefore

$$R(z) = \cfrac{-2}{1 + \cfrac{\frac{-1}{3}(z-1)}{1 + \cfrac{\frac{-5}{3}(z-2)}{1 + 2(z-2)}}}. \tag{4.39}$$

If we simplify this representation to a rational function, we obtain

$$R(z) = \frac{z+1}{z^2 - 3z + 1},$$

as the multi-point Padé approximant for the given data.

Remark 8. We assert that the method introduced above yields the desired continued fraction approximation of f. Indeed, we show that for any point z_i, the part of the continued fraction from z_1 up to and including z_i matches the derivatives of f at points $\{z_1, \ldots, z_i\}$ up to orders $\{n_1, \ldots, n_i\}$ respectively.

First, note that $d_1 = f(z_1)$, so they match in value at z_1. Now, by induction, assume that they match at points $\{z_1, \ldots, z_i\}$ up to derivatives $\{n_1, \ldots, n_i - l\}$ respectively, where $1 \leq l \leq n_i$. Let $g(z)$ denote the continued fraction constructed by the method above, such that up to the $(n_i - l + 1)$ occurrences of $(z - z_i)$ appear in the continued fraction tail. Then, by equation (4.22) with $c = z_i$, we obtain $(z - z_i)\tilde{g}(z) = g(z_i)/g(z) - 1$.

By assumption, we can write

$$g(z)/g(z_i) = \sum_{j=0}^{n_i - l} \frac{g^{(j)}(z_i)}{g(z_i)} (z - z_i)^j,$$

where $g^{(j)}(z_i)$ are the same coefficients as in the expansion of f at z_i. If we set $\tilde{g}(z) \coloneqq \sum_{j=0}^{n_i - l} A_j (z - z_i)^j$, then it is straightforward that equations for finding coefficients A_i would

be the same as (4.24) and (4.25). Notice that we can continue expanding $g(z)$ at z_i because we know derivatives of $f(z)$ up to order n_i. This enables us to match the $(n_i - l + 1)$-th derivative of $g(z)$ at z_i, and consequently the $(n_i - l + 1)$-th derivative of $\tilde{g}(z)$ at z_i, to that of f.

For the expansion of $\tilde{g}(z)$ at other points, we proceed as in (4.23) and the method following it, ensuring that it matches the derivatives of f at the previous points.

4.3.1 Special case: multi-point Padé approximation with only values of the function

In this section, we describe the continued fraction approach for obtaining a multi-point Padé approximation when only the function values at interpolation points, together with a few terms from the expansion at infinity, are available. Owing to the small number of required parameters, this method will be employed for several applications in the next chapter.

Suppose the values of a function F at interpolation points are given, as well as the coefficients of its expansion at infinity:

$$F(z) = \sum_{j=0}^{n_\infty - 1} \xi_j z^{-j-1} + O(z^{-n_\infty - 1}), \qquad z \to \infty. \tag{4.40}$$

We impose the following constraints, requiring that R interpolates F at selected points z_j lying in the right half-plane $\mathrm{Re}(z) \geq 0$. Our goal is therefore to construct a rational function R satisfying the conditions below.

Interpolation conditions at finite points:

$$R(z_j) = F(z_j), \qquad j = 1, 2, \ldots, N, \tag{4.41}$$

where the interpolation points $\{z_j\}_{1 \leq j \leq N}$ lie in the half-plane $\mathrm{Re}(z) \geq 0$ and satisfy the symmetry condition $z_{N+1-j} = \overline{z}_j$ for all $j = 1, 2, \ldots, N$.

Expansion at infinity: as $z \to \infty$,

$$R(z) = \sum_{j=0}^{n_\infty - 1} \xi_j \, z^{-j-1} + O(z^{-n_\infty - 1}). \tag{4.42}$$

The above setup defines a multi-point Padé approximation problem with $N+1$ points, namely $\{z_1, z_2, \ldots, z_N, \infty\}$. At each finite interpolation point, we match only the value of the rational function R, while at infinity we match the first n_∞ coefficients of the power series expansion of R in z^{-1}.

Assume that the numerator and denominator of R are of degrees $M-1$ and M, respectively. The conditions (4.41) and (4.42) impose $N+n_\infty$ equations on R: N equations from interpolation at $\{z_j\}_{1\le j\le N}$ and n_∞ equations ensuring that the coefficients in the expansion of R in powers of z^{-1} coincide with the prescribed ξ_j. Thus, we obtain $N+n_\infty$ constraints for $2M$ unknowns. It is therefore natural to expect that when $N+n_\infty = 2M$, there exists at most one rational function R satisfying these conditions. By Proposition 2, provided such an R exists, its uniqueness and real-valuedness are guaranteed.

Although we have elaborated on continued fraction approach in section 4.3, we review the process once more here due to the simplicity of computations in this case.

We seek a rational function $R(z)$ of degree $[M-1/M]$ that satisfies N interpolation conditions

$$R(z_j) = a_j, \qquad j = 1, 2, \ldots, N, \tag{4.43}$$

together with an asymptotic expansion at infinity of the form

$$R(z) = \sum_{j=0}^{n_\infty - 1} \xi_j z^{-j-1} + O(z^{-n_\infty - 1}), \qquad z \to \infty. \tag{4.44}$$

The parameters $N, n_\infty \in \mathbb{N}$ (with $N + n_\infty = 2M$), the interpolation data $\{z_j, a_j\}_{1\le j\le N}$, and the coefficients $\{\xi_j\}_{0\le j\le n_\infty - 1}$ are assumed to be given, and they satisfy the symmetry conditions $z_{N+1-j} = \bar{z}_j$, $a_{N+1-j} = \bar{a}_j$.

As a first step, we define a rational function R_1 by

$$R(z) = \frac{a_1}{1 + (z - z_1)R_1(z)}, \tag{4.45}$$

which is equivalent to

$$R_1(z) = \frac{1}{z - z_1}\left[\frac{a_1}{R(z)} - 1\right]. \tag{4.46}$$

By construction, the function $R(z)$ defined through (4.45) satisfies $R(z_1) = a_1$, as long as R_1 does not have a pole at z_1. The remaining $N-1$ interpolation conditions for R (at the points $\{z_j\}_{2\le j\le N}$) are satisfied if and only if

$$R_1(z_j) = a_j^{(1)} := \frac{1}{z_j - z_1}\left[\frac{a_1}{a_j} - 1\right], \qquad j = 2, 3, \ldots, N. \tag{4.47}$$

Thus, the linear fractional transformation (4.45) reduces the problem from interpolation at N finite points to interpolation at $N-1$ points.

Next, we investigate the effect of the transformation (4.45) on the expansion of R as $z \to \infty$. For this purpose it is convenient to assume that R has a series expansion in powers of z^{-1} (valid for sufficiently large z):

$$R(z) = \sum_{j\ge 0} b_j z^{-j}. \tag{4.48}$$

We seek the coefficients $b_j^{(1)}$ of the corresponding expansion of $R_1(z)$:

$$R_1(z) = \sum_{j\ge 0} b_j^{(1)} z^{-j}. \tag{4.49}$$

Rewriting (4.45) gives

$$R(z) - z_1 R(z)R_1(z) + zR(z)R_1(z) = a_1. \tag{4.50}$$

We now obtain equations for $b_j^{(1)}$ by comparing coefficients of powers of z on both sides. Comparing coefficients of z in (4.50) yields

$$b_0 b_0^{(1)} = 0. \tag{4.51}$$

Comparing constant terms (coefficients of z^0) gives

$$b_0 - z_1 b_0 b_0^{(1)} + b_0 b_1^{(1)} + b_1 b_0^{(1)} = a_1, \tag{4.52}$$

and for coefficients of z^{-n} with $n \ge 1$ we obtain

$$b_n - z_1 \sum_{i=0}^{n} b_{n-i} b_i^{(1)} + \sum_{i=0}^{n+1} b_{n+1-i} b_i^{(1)} = 0, \qquad n \ge 1. \tag{4.53}$$

At this stage we must consider two separate cases.

Case 1: $b_0 = 0$. In this case, equation (4.51) is automatically satisfied, and from (4.52) we find $b_0^{(1)} = a_1/b_1$. The remaining coefficients are obtained iteratively from

$$b_n^{(1)} = -\frac{1}{b_1}\left[b_n + \sum_{i=0}^{n-1} b_i^{(1)}\Big(b_{n+1-i} - z_1 b_{n-i}\Big)\right], \qquad n \geq 1,$$

which follows from (4.53).

Case 2: $b_0 \neq 0$. Then (4.51) implies $b_0^{(1)} = 0$. From (4.52) and (4.53) we obtain

$$b_1^{(1)} = \frac{a_1}{b_0} - 1,$$

$$b_{n+1}^{(1)} = -\frac{1}{b_0}\left[b_n + \sum_{i=1}^{n} b_i^{(1)}\Big(b_{n+1-i} - z_1 b_{n-i}\Big)\right], \qquad n \geq 1.$$

We observe that in Case 1 (when $b_0 = 0$), if we know the next k coefficients $\{b_j\}_{1\leq j\leq k}$ of the expansion of $R(z)$ at $z = \infty$, then we can determine k coefficients $\{b_j^{(1)}\}_{0\leq j\leq k-1}$ of the corresponding expansion of $R_1(z)$. In this case, the first coefficient $b_0^{(1)}$ is non-zero. In Case 2 (when $b_0 \neq 0$), if we know k coefficients $\{b_j\}_{0\leq j\leq k-1}$ of the expansion of $R(z)$ at $z = \infty$, then necessarily $b_0^{(1)} = 0$, and we can compute the next k coefficients $\{b_j^{(1)}\}_{1\leq j\leq k}$ of the expansion of $R_1(z)$.

Now we can describe the general algorithm for finding the rational function $R(z)$ satisfying (4.43) and (4.44). Define $\gamma_0 = 0$ and $\gamma_j = \xi_{j-1}$ for $j = 1, 2, \ldots, n_\infty$, so that R has the following asymptotic expansion as $z \to \infty$:

$$R(z) = \sum_{j=0}^{n_\infty} \gamma_j z^{-j} + O(z^{-n_\infty - 1}). \tag{4.54}$$

We now define R_1 by

$$R(z) = \frac{a_1}{1 + (z - z_1)R_1(z)}, \tag{4.55}$$

with interpolation values $a_j^{(1)} = R_1(z_j)$ for $2 \leq j \leq N$, computed using (4.47). Since $\gamma_0 = 0$, the function R_1 has the following expansion for large z:

$$R_1(z) = \sum_{j=0}^{n_\infty - 1} \gamma_j^{(1)} z^{-j} + O(z^{-n_\infty}). \tag{4.56}$$

Here γ_j and $\gamma_j^{(1)}$ play the same role as b_j and $b_j^{(1)}$ in the preceding discussion, and the coefficient $\gamma_0^{(1)}$ is non-zero. Note that if a rational function R_1 does not have a pole at z_1, the function R constructed via (4.55) will satisfy the interpolation condition $R(z_1) = a_1$.

We then repeat the procedure, reducing the number of interpolation points at each step. Specifically, we define

$$R_1(z) = \frac{a_2^{(1)}}{1 + (z - z_2)R_2(z)}, \tag{4.57}$$

and compute $a_j^{(2)} = R_2(z_j)$ for $j = 3, 4, \ldots, N$ along with the coefficients of the expansion of $R_2(z)$ at $z = \infty$. Since $\gamma_0^{(1)} \neq 0$, the expansion of R_2 at infinity takes the form

$$R_2(z) = \sum_{j=0}^{n_\infty} \gamma_j^{(2)} z^{-j} + O(z^{-n_\infty - 1}), \qquad z \to \infty, \tag{4.58}$$

with $\gamma_0^{(2)} = 0$. The condition that R_1 does not have a pole at z_1 is equivalent to $R_2(z_1) \neq 1/(z_2 - z_1)$. As long as this condition is satisfied, the function R given by (4.55) will satisfy the interpolation condition $R(z_1) = a_1$. In order for R_1 to satisfy the interpolation condition $R_1(z_2) = a_2^{(1)}$, the function R_2 should not have a pole at $z = z_2$.

Repeating this procedure $N - 2$ times, we define successively the functions $R_3, R_4, \ldots, R_N$. Performing backward substitution (as in the illustrative example at the beginning of this section) yields the continued fraction representation of R:

$$R(z) = \cfrac{a_1}{1 + \cfrac{(z - z_1)a_2^{(1)}}{1 + \cfrac{(z - z_2)a_3^{(2)}}{\ddots \cfrac{\cdots}{1 + \cfrac{(z - z_{N-1})a_N^{(N-1)}}{1 + (z - z_N)R_N(z)}}}}}. \tag{4.59}$$

As long as R_N does not have a pole at z_N and $R_j(z_{j-1}) \neq 1/(z_j - z_{j-1})$ for $j = 2, 3, \ldots, N$, the rational function R will satisfy the interpolation conditions $R(z_j) = a_j$ for $j = 1, 2, \ldots, N$. Moreover, R has the prescribed asymptotics (4.54) if and only if R_N satisfies

$$R_N(z) = \sum_{j=0}^{K} \gamma_j^{(N)} z^{-j} + O(z^{-K-1}), \qquad z \to \infty, \tag{4.60}$$

where the coefficients $\gamma_j^{(N)}$ are computed by the iterative procedure above, and

$$K = \begin{cases} n_\infty, & \text{if } N \text{ is even,} \\ n_\infty - 1, & \text{if } N \text{ is odd.} \end{cases}$$

Note that K is always an even integer, since $N + n_\infty = 2M$ is even.

The last step of the algorithm is to express $R_N(z)$ (which must satisfy (4.60)) as a continued fraction:

$$R_N(z) = \gamma_0^{(N)} + \cfrac{d_1 z^{-1}}{1 + \cfrac{d_2 z^{-1}}{\ddots \cfrac{\cdots}{1 + \cfrac{d_{K-1} z^{-1}}{1 + d_K z^{-1}}}}}, \tag{4.61}$$

where $d_1 := \gamma_1^{(N)}$, and the remaining coefficients $\{d_j\}_{2 \le j \le K}$ are computed by an iterative scheme similar to (4.45). Specifically, we define $R_{N+1}(z)$ by

$$R_N(z) = \gamma_0^{(N)} + \frac{d_1}{z R_{N+1}(z)},$$

which is equivalent to

$$R_{N+1}(z) = \frac{d_1}{z\Big(R_N(z) - \gamma_0^{(N)}\Big)}.$$

From (4.60) and this relation, we compute the expansion of $R_{N+1}(z)$ as $z \to \infty$:

$$R_{N+1}(z) = 1 + \sum_{j=1}^{K-1} \gamma_j^{(N+1)} z^{-j} + O(z^{-K}). \tag{4.62}$$

We then set $d_2 := \gamma_1^{(N+1)}$ and repeat the step. Next, we define

$$R_{N+1}(z) = 1 + \frac{d_2}{z R_{N+2}(z)},$$

compute the expansion of $R_{N+2}(z)$ at $z = \infty$, and set $d_3 := \gamma_1^{(N+2)}$. Continuing this procedure for K steps yields the coefficients $\{d_j\}_{1 \le j \le K}$ of the continued fraction (4.61). Substituting R_N from (4.61) into (4.59) then gives the desired rational function $R(z)$.

There are some exceptional cases in which the algorithm may fail to produce a result, specifically when division by zero occurs. This can happen if, for some $1 \leq j \leq N-1$, the function R_j vanishes at one of the points z_i with $j+1 \leq i \leq N$. Failure can also occur if $\gamma_0^{(l)} = \gamma_1^{(l)} = 0$ for some l, since in that case the iteration cannot proceed to compute $\gamma_j^{(l+1)}$. There are also rare cases where the algorithm produces a rational function R, but the result fails to satisfy the interpolation conditions (4.43). As discussed above, this may occur when $R_j(z_{j-1}) = 1/(z_j - z_{j-1})$ for some $2 \leq j \leq N$ or if R_N has a pole at z_N. In all of our numerical experiments, however, such situations did not arise, and we do not regard them as a major practical concern.

We now claim that whenever the algorithm succeeds, the resulting rational function R has degree $[M-1/M]$. When $n_\infty = 2L$ is even, then $N = 2M - n_\infty$ is also even and $\gamma_0^{(N)} = 0$. By induction on L, one can show that in this case R_N has degree $[L-1/L]$, and hence R (constructed via (4.59)) has degree $[M-1/M]$. When $n_\infty = 2L+1$ is odd, N is also odd and $\gamma_0^{(N)} \neq 0$. A similar argument shows that R_N has degree $[L/L]$, and therefore R again has degree $[M-1/M]$. Thus, once we obtain the rational function R and verify that it satisfies the interpolation conditions (4.43), Proposition 2 ensures that R is the unique solution to the multi-point Padé approximation problem.

Remark 9. As noted earlier, the integer K appearing in (4.60) is always even. Writing $K = 2L$, we may identify the rational function $R_N^*(z) := R_N(1/z)$ as the $[L/L]$ Padé approximant at $z = 0$ to the power series $\sum_{j\geq 0} \gamma_j^{(N)} z^j$. There are several methods (besides the one described above) for computing the numerator and denominator coefficients of this Padé approximant. For instance, one can determine them by solving a linear system, as explained in [7]. An efficient alternative that also uses continued fractions is the Q.D. algorithm (see [7]) – this method may be preferable when n_∞ is large. In our examples n_∞ is relatively small, so we used the continued fraction approach described above, which is straightforward to implement.

Chapter 5

Applications of Multi-Point Padé Approximations

In this chapter, we demonstrate through several examples the implementation and applications of multi-point Padé approximations using the tools introduced in Chapter 4. Unless otherwise specified, a working precision of 100 decimal digits was used in all computations. High precision is essential due to the iterative nature of the continued fraction algorithm, where precision loss may accumulate, and because the computation of roots of relatively high-degree polynomials (up to degree 60 in some examples) requires numerical stability. The code was written in Fortran, employing D. H. Bailey's highly efficient MPFUN2020 [6] arbitrary-precision package. Polynomial roots were computed using the Ehrlich–Aberth method [1, 26].

5.1 Approximating Functions by Sums of Exponentials

Let f be a real-valued function defined on an interval $I \subseteq [0, \infty)$. The problem of approximating f by exponential sums of the form

$$\phi(x) = \sum_{j=1}^{M} c_j e^{-\lambda_j x}, \qquad c_j, \lambda_j \in \mathbb{C}, \tag{5.1}$$

has a long history. The earliest systematic method is due to Gaspard de Prony, dating back to the late eighteenth century. Prony's method [31] samples the function f on a regular grid of points inside the interval I and transforms the problem into one involving a linear difference equation with constant coefficients. Although Prony's method is general – it applies to a wide variety of functions – it suffers from solving a highly ill-conditioned system of linear equations. Numerous improvements and variants have since been developed; see [57] and the references therein.

Extensive work has also been done on studying optimal exponential-sum approximations in L_p spaces and on developing such approximations for specific functions. In this context, a more general class of approximants is often considered, in which the coefficients c_j in (5.1) may be polynomials in x. Rice [61] studied Chebyshev (i.e., $L_\infty(I, \mathrm{d}x)$) approximations on a finite interval. Kammler [42, 43] characterized optimal $L_p([0,1], \mathrm{d}x)$ approximations and investigated best $L_2((0,\infty), \mathrm{d}x)$ approximations of completely monotonic functions. Approximations to power functions $x^{-\beta}$ were studied in [19, 50, 37].

Another widely applicable approach was introduced in 2005 by Beylkin and Monzón [13, 12]. Their method also samples f on a regular grid, but then constructs a Hankel matrix from these values and applies singular value decomposition. This method has become very popular and has been applied in a broad range of contexts [29, 40, 50].

We use the algorithm in section 4.3.1 for approximating functions $f : [0,\infty) \to \mathbb{R}$ by exponential sums of the form (5.1) based on a multi-point Padé approximation of the Laplace transform of f, and it can be viewed as a generalization of the technique introduced in [45].

Let $F(z)$ and $R(z)$ denote the Laplace transforms of f and ϕ, respectively:

$$F(z) := \int_0^\infty f(x) e^{-zx} \mathrm{d}x, \qquad R(z) := \int_0^\infty \phi(x) e^{-zx} \mathrm{d}x. \tag{5.2}$$

We assume that $f \in L_1((0,\infty), \mathrm{d}x)$, so that F is well defined in the right half-plane $\mathrm{Re}(z) \geq 0$. If ϕ has the form (5.1), then $R(z)$ is a rational function with simple poles at $-\lambda_j$, and the coefficients c_j come from its partial fraction decomposition:

$$R(z) = \sum_{j=1}^{M} \frac{c_j}{z + \lambda_j}. \tag{5.3}$$

The key observation underlying our approach is that if the exponential sum ϕ is close (in some norm) to f, then the rational function R is close (in an appropriate sense) to the Laplace transform F, and vice versa. For example, if $\|f-\phi\|_p$ is small for some $p>1$, then by Hölder's inequality we have

$$\begin{aligned}|F(z)-R(z)| &= \left|\int_0^\infty (f(x)-\phi(x))e^{-zx}\mathrm{d}x\right| \\ &\le \|f-\phi\|_p \times \left(\int_0^\infty e^{-q\,\mathrm{Re}(z)x}\mathrm{d}x\right)^{1/q} = \frac{\|f-\phi\|_p}{(q\,\mathrm{Re}(z))^{1/q}},\end{aligned}$$

for all z in the right half-plane $\mathrm{Re}(z)>0$, where q is defined by $1/p+1/q=1$. When $p=1$, the same bound holds with the denominator replaced by 1. Thus, a good exponential-sum approximation to f in L_p norm produces a good rational approximation to F in L_∞ norm. Conversely, writing f and ϕ via the inverse Laplace transform yields, for any $c>0$,

$$|f(x)-\phi(x)| \le \frac{e^{cx}}{2\pi}\int_{\mathbb{R}} |F(c+\mathrm{i}y)-R(c+\mathrm{i}y)|\,\mathrm{d}y,$$

so if F is close to R in L_1 norm on some vertical line $c+\mathrm{i}\mathbb{R}$, then $e^{-cx}(f(x)-\phi(x))$ is small in L_∞ norm. This shows the close connection between rational approximation of Laplace transforms and exponential-sum approximation of the original function.

Having established this connection, let us examine what information about the original function f can be conveniently transferred to its Laplace transform. Suppose that f satisfies

$$f(x) = \sum_{j=0}^{n_\infty-1} \xi_j \frac{x^j}{j!} + O(x^{n_\infty}), \qquad x\to 0^+. \tag{5.4}$$

A sufficient condition for this expansion is the boundedness of the derivative $f^{(n_\infty)}(x)$ on some interval $(0,c)$; in that case we necessarily have $\xi_j = f^{(j)}(0+)$. Applying Watson's Lemma (4.8), we obtain

$$F(z) = \sum_{j=0}^{n_\infty-1} \xi_j z^{-j-1} + O(z^{-n_\infty-1}), \qquad z\to\infty, \tag{5.5}$$

uniformly in any sector

$$S_\theta := \{z\in\mathbb{C} : |\arg(z)|\le\theta\}, \qquad \theta\in(0,\pi/2).$$

We now require that the approximating rational function R satisfies the same asymptotic condition at $z = \infty$. By Watson's Lemma (4.8), this is equivalent to $f(x) - \phi(x) = O(x^{n_\infty})$ as $x \to 0^+$. Imposing this condition ensures that $R(z)$ is close to $F(z)$ for large values of z. Moreover, R interpolation of F at selected points z_j lying in the right half-plane $\mathrm{Re}(z) \geq 0$ guarantees closeness for moderate and small values of z as discussed in section 4.3.1.

A rational function $R(z)$ of the form (5.3) is determined by $2M$ complex parameters $\{c_j, \lambda_j\}_{1 \leq j \leq M}$. The multi-point Padé approximation problem described by (4.41) and (4.42) requires as input two positive integers, N and n_∞, together with N complex numbers $\{z_j\}_{1 \leq j \leq N}$. Even with the symmetry condition $z_{N+1-j} = \bar{z}_j$, this still leaves many degrees of freedom. To simplify the algorithm, we propose the following special choice of interpolation points z_j. We assume $N \geq 2$, take two numbers $A \geq 0$ and $B > 0$, and consider the piecewise linear curve $\gamma_{A,B}$ consisting of two intervals:

$$\gamma_{A,B} := [A - B\mathrm{i}, 0] \cup [0, A + B\mathrm{i}].$$

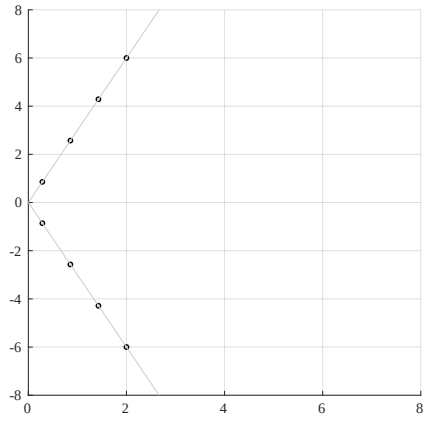
We then define $z_1 = A - B\mathrm{i}$, $z_N = A + B\mathrm{i}$, and place the remaining points $\{z_j\}_{2 \leq j \leq N-1}$ equidistantly along the curve $\gamma_{A,B}$; see Figure 5.1 for an illustration.

The motivation for this choice comes from the fact that when F admits the asymptotic expansion (5.5) for large z in any sector

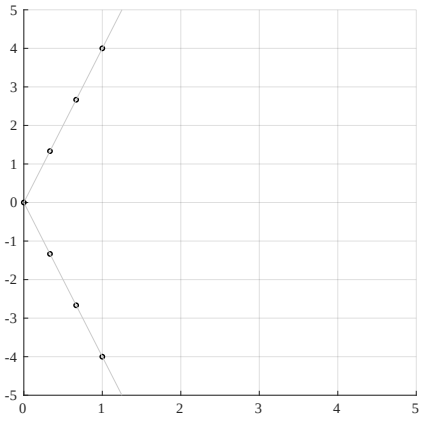
$$S_\theta := \{z \in \mathbb{C} \,:\, |\arg(z)| \leq \theta\}, \qquad \theta \in (0, \pi/2),$$

the farther z lies from the origin within such a sector, the more accurately $R(z)$ approximates $F(z)$ (since $F(z) - R(z) = O(z^{-n_\infty - 1})$ as $z \to \infty$); see Figure 5.1c. We therefore enforce N interpolation conditions along the boundary $\gamma_{A,B}$ of this sector (where $B/A = \tan(\theta)$). This allows us to control the error $F(z) - R(z)$ not only for large z, but also for moderate and small values of $z \in S_\theta$. By the maximum modulus principle, if F and R are close for large z and along the boundary of S_θ, they will also be close throughout the interior of this sector. Consequently, it is unnecessary to place interpolation points z_j inside S_θ.

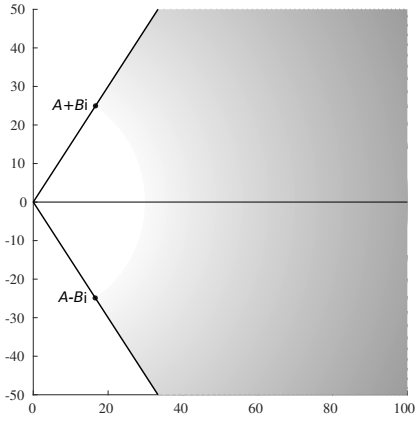
We can now summarize our algorithm:



(a) $N = 8$, $A = 2$, $B = 6$



(b) $N = 7$, $A = 1$, $B = 4$



(c) A sector $S_\theta \subset \mathbb{C}$

Figure 5.1: Configuration of points $\{z_j\}_{1 \le j \le N}$ for even and odd values of N. The points are indexed such that $\mathrm{Im}(z_j) < \mathrm{Im}(z_{j+1})$, and they satisfy the symmetry relation $z_{N+1-j} = \bar{z}_j$.

(i) Choose integers $N \geq 2$ and $n_\infty \geq 1$ such that $N + n_\infty = 2M$ is even;

(ii) Compute the coefficients $\{\xi_j\}_{0 \leq j < n_\infty}$ in the expansion (5.5);

(iii) Choose $A \geq 0$ and $B > 0$ and determine N interpolation points z_j, with $z_1 = A - B\mathrm{i}$, $z_N = A + B\mathrm{i}$, and the remaining $N - 2$ points chosen as shown in Figure 5.1;

(iv) Solve the multi-point Padé approximation problem: find a rational function R satisfying conditions (4.41) and (4.42) via continued fraction approach;

(v) If step (iv) is successful, compute the poles $\{-\lambda_j\}$ of R. If all poles are simple, write R in partial fraction form (5.3) and recover the coefficients c_j;

(vi) Verify whether R provides a sufficiently accurate approximation to F, using appropriate criteria. If R fails this test, repeat the above steps with different parameter values $\{N, n_\infty, A, B\}$.

The only drawback is that this approach requires the additional assumption $\xi_0 \neq 0$. This restriction is not severe, however, and in 5.1 we describe a simple workaround as an example.

The algorithm described above requires the values $F(z_j)$ of the Laplace transform of f. If $F(z)$ is not known in closed form, we evaluate $F(z_j)$ numerically by applying the double-exponential quadrature of Takahasi–Mori [75] to the integral in (5.2):

$$F(z) = \int_0^\infty f(x) e^{-zx} \, \mathrm{d}x \approx h \sum_{n \in \mathbb{Z}} x_n f(x_n) e^{-z x_n} \left(1 + e^{-nh}\right), \tag{5.6}$$

where $h > 0$ is a small step size and $x_n := \exp(nh - \exp(-nh))$. Formula (5.6) is obtained by applying the trapezoidal rule to the integral after the change of variables $x = \exp(u - \exp(-u))$. The infinite sum converges very rapidly and is truncated once its terms fall below the working precision.

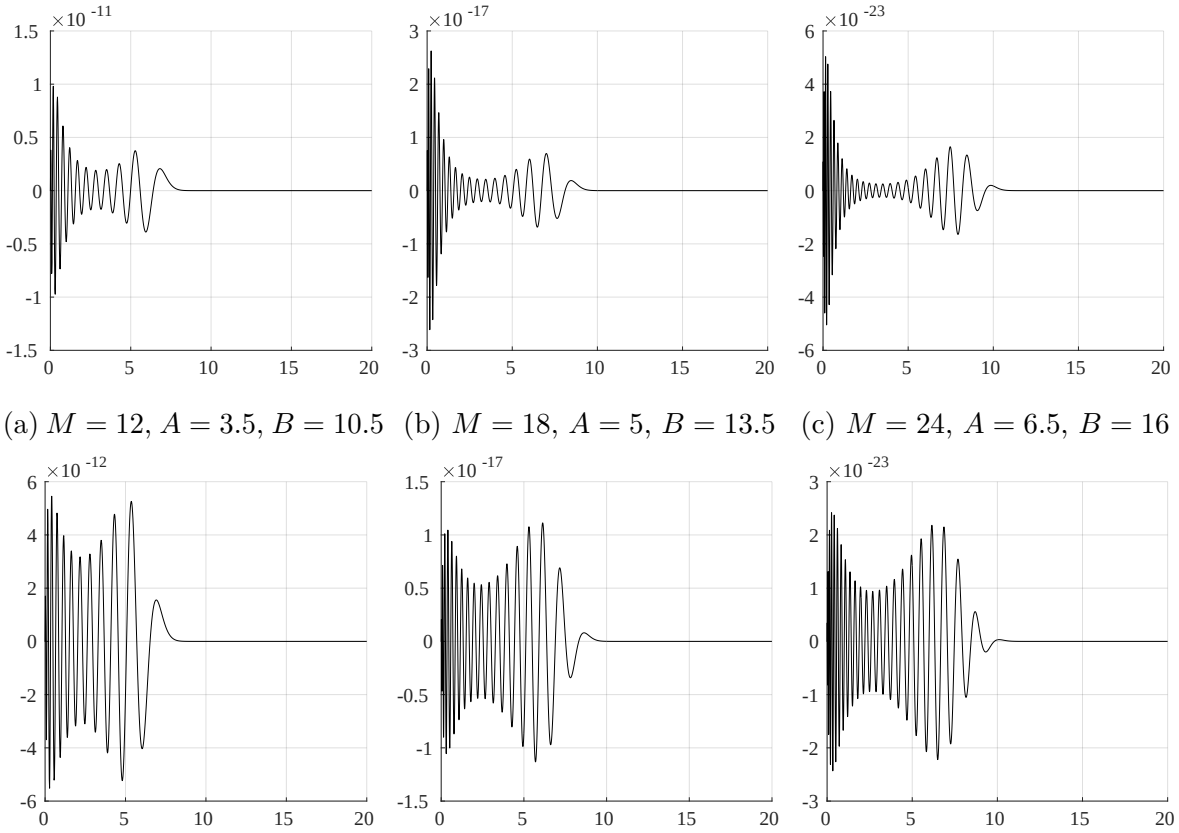
As mentioned earlier, we use the algorithm discussed in 4.3.1 for finding the rational approximant to F for which on top of high precision accuracy, the other important advantage is the speed of its implementation. Our implementation of the exponential sum approximation algorithm is reasonably fast. For example, finding the coefficients c_j and λ_j for the exponential

sum approximation to the hockey stick function (see subsection 5.1) with $M = 30$ ($M = 60$) terms took about 0.1 seconds (respectively, 1 second) on a standard laptop (Intel Core i5-1250P processor with 16GB of RAM). This example is relatively simple since the Laplace transform is known explicitly. When $F(z_j)$ must be computed numerically, the runtime increases substantially. In the lognormal example of subsection 5.1, computing the coefficients c_j and λ_j for $M = 30$ took 1.5 seconds. Fortunately, the computation of $F(z_j)$ for different values of j can be fully parallelized. With OpenMP parallelization (compiled using the `-fopenmp` flag), the same example with $M = 30$ took only 0.4 seconds instead of 1.5 seconds in serial execution.

Implementation of algorithm in section 4.3.1 depends on four parameters: two integers N and n_∞ (with the constraint that $N + n_\infty = 2M$ is even), and two real numbers $A \geq 0$ and $B > 0$. Based on extensive experiments, we can offer the following empirical guidelines for choosing these parameters:

- Larger values of M generally yield better approximations, corresponding to more terms in the exponential sum (5.1).
- Increasing n_∞ improves the accuracy of $f(x) - \phi(x)$ for small values of x, since $f(x) - \phi(x) = O(x^{n_\infty})$ as $x \to 0^+$.
- Increasing A has a similar effect, as it improves the approximation $F(z) - R(z)$ for large z, and Watson's Lemma relates the large-z behavior of the Laplace transform to the small-x behavior of the original function.
- In some cases (such as the hockey stick example of subsection 5.1), the algorithm produced exponential sums with very large coefficients c_j. Increasing B alleviated this issue and reduced the values of c_j to acceptable levels.

In the sequel we show the results of various numerical experiments.



(a) $M = 12$, $A = 3.5$, $B = 10.5$ (b) $M = 18$, $A = 5$, $B = 13.5$ (c) $M = 24$, $A = 6.5$, $B = 16$

(d) $M = 12$, $A = 4.5$, $B = 10$ (e) $M = 18$, $A = 6.5$, $B = 11$ (f) $M = 24$, $A = 8$, $B = 14.5$

Figure 5.2: The graphs of $\exp(-x^2) - \phi(x)$ for different values of M, A, and B. In each case we set $n_\infty = 2$.

Approximating the Gaussian function

As our first example, we consider the Gaussian function $f(x) = \exp(-x^2)$. Approximations of this function by exponential sums of the form (5.1) are widely used, for instance in the fast Gauss transform [44].

Since the Laplace transform of f is not known in closed form, we computed the values of $F(z_j)$ numerically using the double-exponential quadrature (5.6). We constructed exponential sum approximations with $M \in \{12, 18, 24\}$ terms, setting $n_\infty = 2$ in each case (corresponding to values of $N \in \{22, 34, 46\}$). For each M, we tested a range of parameters A and B and

selected those yielding the smallest L_1 or L_∞ error between f and ϕ.

The results are shown in Figure 5.2. The top row of graphs (5.2a–5.2c) shows approximations optimized for the smallest L_1 error $\|f-\phi\|_1$, while the bottom row (5.2d–5.2f) shows those optimized for the smallest L_∞ error.

For the approximation in Figure 5.2c, we obtained

$$\|f-\phi\|_1 \approx 6.4\times 10^{-23}, \qquad \|f-\phi\|_\infty \approx 5.0\times 10^{-23}.$$

For the approximation in Figure 5.2f, the errors were

$$\|f-\phi\|_1 \approx 8.5\times 10^{-23}, \qquad \|f-\phi\|_\infty \approx 2.4\times 10^{-23}.$$

We observe a slight improvement (by about a factor of two in the L_∞ error) when optimizing the parameters A and B. These results also suggest that both L_1 and L_∞ errors decay exponentially with M.

Approximations to the gamma function and the Barnes G-function

Gamma function is defined by

$$\Gamma(z) = \int_0^\infty e^{-x}x^{z-1}dx$$

for $\mathrm{Re}(z)>0$. There have been papers covering the approximation of the gamma function, including Lanczos approximation [46]. Kuznetsov ([45]) approximates it through approximating an auxiliary function by sum of exponentials by means of two-point Padé approximation. Here we take the multi-point Padé approach described in section 4.3.1 to obtain closer estimates. We provide a brief description of the method in the following.

We first try to approximate the function

$$f(x) = \frac{e^{-x}}{x^3}[\frac{1}{2}\coth(\frac{x}{2}) - \frac{1}{x} - \frac{x}{12}], \quad x>0, \tag{5.7}$$

by sum of exponential functions as in (5.1). The function f is smooth, decays exponentially as $x\to+\infty$, and has a removable singularity at $x=0$ (in fact, it is analytic in the disk $|x|<4\pi$). Exponential sum approximations to this function were used in [45] to construct

highly accurate approximations to the gamma function and the Barnes G-function. To see the connection between the aforementioned function and gamma function, a new function is defined $F(z) = \int_0^\infty e^{-zx} x f(x) dx$, then we have this equation for $\mathrm{Re}(z) > 0$ (proposition 1. in [45])

$$\ln(\Gamma(z)) = (z - \frac{1}{2}) \ln(z) - z + \frac{1}{2} \ln(2\pi) + \frac{1}{12z} - F'(z-1) \tag{5.8}$$

where $\ln(z)$ indicates the principal branch of the natural logarithm. Next, for a fixed M, assume the numbers c_j and λ_j have been found in a way that $\phi(x) = \sum_{j=1}^{M} c_j e^{-\lambda_j x}$ is an approximation to $f(x)$ on $x \in (0, \infty)$, then with defining the following new function for $\mathrm{Re}(z) > 0$

$$\Phi(z) = \sum_{j=1}^{n} \frac{c_j}{(z+\lambda_j)^2} = \int_0^\infty e^{-zx} x \phi(x) dx,$$

we will have this approximation of $\ln(\Gamma(z))$ and $\ln(G(z))$ by

$$\ln(\widehat{\Gamma}(z)) = \left(z - \frac{1}{2}\right) \ln(z) - z + \frac{1}{2} \ln(2\pi) + \frac{1}{12z} - \Phi'(z-1), \tag{5.9}$$

$$\begin{aligned} \ln(\widehat{G}(z)) = &\left(\frac{z^2}{2} - z + \frac{5}{12}\right) \ln(z) - \frac{3}{4} z^2 + \tfrac{1}{2} \ln(2\pi)(z-1) + z \\ &+ \tfrac{1}{12} - \ln(\mathcal{A}) - \tfrac{1}{12z} + \Phi(z-1) - (z-1)\Phi'(z-1), \end{aligned} \tag{5.10}$$

where $\mathcal{A} = 1.282427\ldots$ is the Glaisher–Kinkelin constant. Now define

$$\eta_1(x) := 2x^2\Big(f(x) - \phi(x)\Big), \quad \eta_2(x) := 6x\Big(f(x) - \phi(x)\Big) + 2x^2\Big(f'(x) - \phi'(x)\Big),$$

and set errors as

$$\epsilon_i = \|\eta_i\|_\infty = \sup\{|\eta_i(x)| : x \geq 0\},$$

then it can be proved in the half-plane $\mathrm{Re}(z) \geq 3/2$, we have (proposition 2. in [45]):

$$\Big|\ln(\Gamma(z)) - \ln(\widehat{\Gamma}(z))\Big| \leq \epsilon_1, \quad \Big|\ln(G(z)) - \ln(\widehat{G}(z))\Big| \leq \epsilon_2. \tag{5.11}$$

After approximating the gamma function on $\mathrm{Re}(z) \geq 3/2$, we can extend the domain to the strip $1/2 \leq \mathrm{Re}(z) < 3/2$ by equation

$$\ln(\Gamma(z)) = \ln(\Gamma(z+1)) - \ln(z).$$

Finally for the domain $\mathrm{Re}(z) < 1/2$, we apply the reflection identity

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin(\pi z)}.$$

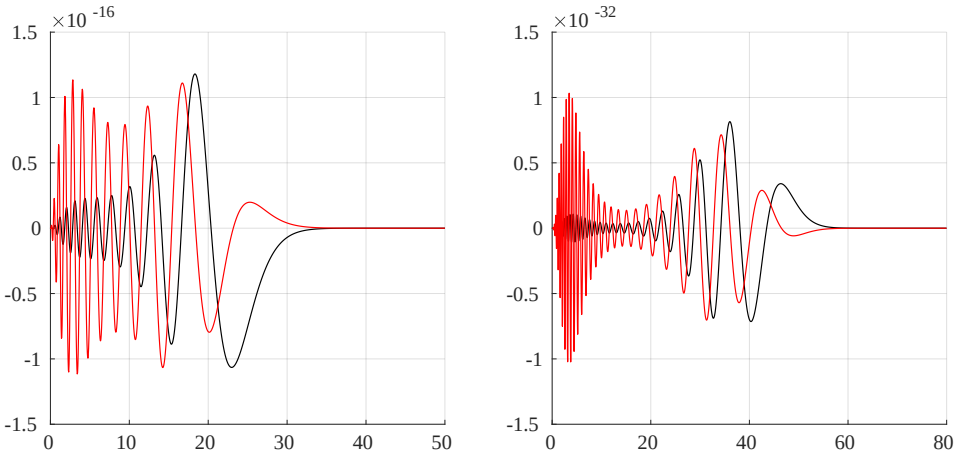
For the $\ln(\Gamma(z))$ to be analytic in $\mathbb{C} \setminus (-\infty, 0]$, we need to rewrite the right hand side of last equation in exponential form and choose the right branch, this way these approximations can then be extended to compute logarithms of $\Gamma(z)$ and $G(z)$ throughout the cut plane $\mathbb{C} \setminus (-\infty, 0]$ (details can be found in [45]). Next, to be able to approximate $f(x)$ by sum of exponentials, we first need to compute its derivatives at zero. By lemma 1 in [45] we get

$$f^{(n)}(0) = (-1)^n n! \sum_{k=0}^{[n/2]} \frac{B_{2k+4}}{(n-2k)!(2k+4)!},$$

where B_n are Bernoulli numbers.

To see the numerical results of the above method, first note that because the function f is not completely monotone, and consequently its Laplace transform is not Stieltjes function, then one cannot be sure of the Laplace transform of ϕ being Stieltjes due to the fact that there is no guarantee that all roots of the Padé approximant are simple and negative. Our comparison criteria are the results provided in [45].

The paper [45] employed a two-point Padé approximation (interpolating at 0 and ∞) to produce two exponential sum approximations to f. The first approximation had $M = 15$ terms with $\epsilon_1 \approx 9 \times 10^{-17}$ and $\epsilon_2 \approx 2.8 \times 10^{-16}$. According to (5.11), this guarantees double-precision accuracy for $\ln(\Gamma(z))$ and $\ln(G(z))$ in the half-plane $\mathrm{Re}(z) \geq 3/2$. Using the algorithm presented in section 4.3.1, we found an exponential sum ϕ with only $M = 12$ terms, yielding $\epsilon_1, \epsilon_2 \approx 1.2 \times 10^{-16}$ (see Figure 5.3a). Thus, we achieve the same double-precision accuracy as in [45] with 20% fewer terms, which is significant since it leads to faster evaluation of these functions. The second exponential sum approximation in [45] had $M = 45$ terms, with $\epsilon_1 \approx 5 \times 10^{-32}$ and $\epsilon_2 \approx 2.9 \times 10^{-31}$, providing nearly quadruple-precision accuracy for $\ln(\Gamma(z))$ and $\ln(G(z))$ via (5.9) and (5.10). Using our new method, we obtained an exponential sum ϕ with $M = 30$ terms and $\epsilon_1, \epsilon_2 \approx 10^{-32}$ (see Figure 5.3b), thus achieving the same accuracy with 33% fewer terms.



(a) $M = 12$, $n_\infty = 2$, $A = 2$, $B = 3.5$ (b) $M = 30$, $n_\infty = 4$, $A = 4.25$, $B = 5$

Figure 5.3: The graphs of $\eta_1(x)$ (black) and $\eta_2(x)$ (red) for different values of M, n_∞, A, and B.

Approximating the probability density function of the Gompertz–Makeham distribution

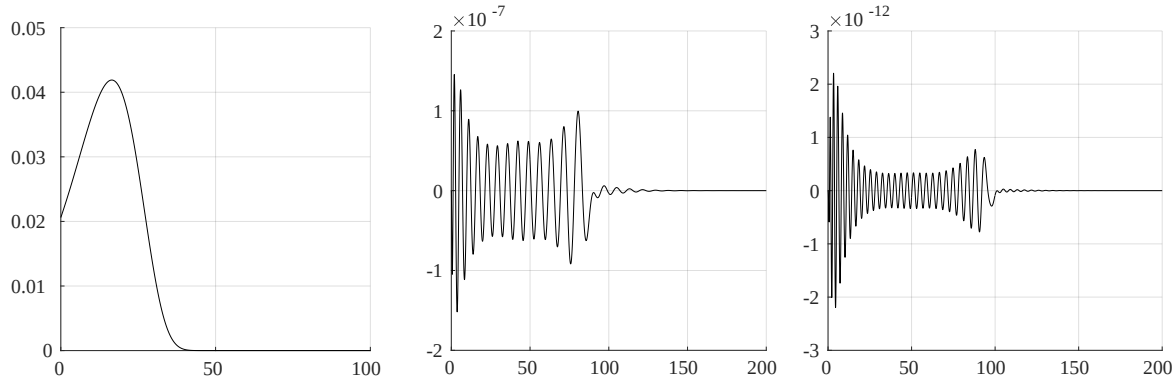
Consider the probability density function f of the Gompertz-Makeham law of mortality:

$$f(x) = (a + bc^{x_0+x}) \exp\left(-ax - \frac{b}{\ln(c)} c^{x_0}(c^x - 1)\right), \qquad x \geq 0.$$

A particular instance of this distribution with parameters $x_0 = 65$, $a = 0.0007$, $b = 0.00005$, and $c = 10^{0.04}$ was studied in [29, 30], where the authors used the Beylkin-Monzón method [13] to approximate f by exponential sums. Their approximation employed $M = 15$ terms and achieved an L_∞ error of approximately $\|f - \phi\|_\infty \approx 10^{-6}$.

Using our algorithm with $M = 14$ terms, we obtained an approximation with a smaller error, $\|f - \phi\|_\infty \approx 1.5 \times 10^{-7}$. Furthermore, with $M = 28$ terms we achieved $\|f - \phi\|_\infty \approx 2.2 \times 10^{-12}$. The density function f and the corresponding errors $f - \phi$ are shown in Figure 5.4.

Thus, in this example, our method improves upon the Beylkin-Monzón approximation, achieving smaller errors with fewer terms. The improvement comes from the fact that our



(a) Gompertz–Makeham pdf $f(x)$ (b) $M = 14$, $n_\infty = 2$, $A = 0.1$, $B = 0.9$ (c) $M = 28$, $n_\infty = 4$, $A = 0.12$, $B = 1.65$

Figure 5.4: Approximating the Gompertz–Makeham probability density function. Subplots (b) and (c) show the error $f(x) - \phi(x)$ for exponential sum approximations with 14 and 28 terms, respectively.

algorithm allows for better control of the approximation error $f(x) - \phi(x)$ for small values of x, through the parameter n_∞.

Approximating the density of the lognormal distribution

The probability density function of a lognormal distribution with parameter $\mu = 0$ is given by

$$g_\sigma(x) := \frac{1}{x\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2} \ln(x)^2\right), \qquad x > 0,$$

where $\sigma > 0$ is a parameter. Graphs of $g_\sigma(x)$ for $\sigma \in \{0.5, 1, 1.5\}$ are shown in Figure 5.5.

A key property of this density is that all derivatives $g_\sigma^{(j)}(x)$ vanish as $x \to 0^+$. In particular, our continued fraction algorithm cannot be applied directly since $g_\sigma(0+) = 0$. We address this difficulty by a simple modification: instead of approximating $g_\sigma(x)$, we approximate the function

$$f(x) = \int_x^\infty g_\sigma(y)\, \mathrm{d}y,$$

by an exponential sum $\phi(x)$ of the form (5.1), and then define

$$\widetilde{\phi}(x) = -\phi'(x) = \sum_{j=1}^{M} c_j \lambda_j e^{-\lambda_j x} \tag{5.12}$$

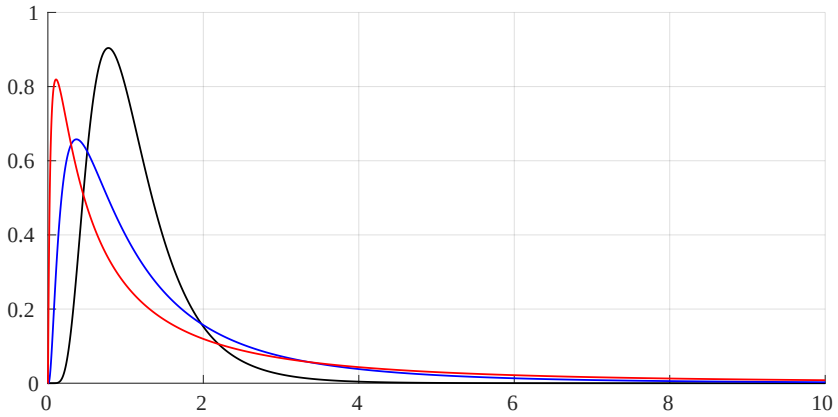


Figure 5.5: The lognormal pdf $g_\sigma(x)$ with $\sigma = 0.5$ (black), $\sigma = 1$ (blue), and $\sigma = 1.5$ (red).

as an exponential sum approximation to $g_\sigma(x) = -f'(x)$.

Since $f(0) = 1$ and $f'(x) = -g_\sigma(x)$, the coefficients ξ_j in (5.4) are given by

$$\xi_0 = 1, \qquad \xi_j = 0 \ \text{ for all } j \geq 1. \tag{5.13}$$

The Laplace transform of f can be expressed in terms of the Laplace transform of g_σ:

$$F(z) = \int_0^\infty e^{-zx} f(x)\,\mathrm{d}x = \frac{1}{z}\Big(1 - G(z)\Big), \tag{5.14}$$

where

$$G(z) := \int_0^\infty e^{-zx} g_\sigma(x)\,\mathrm{d}x$$

is the Laplace transform of g_σ. Formula (5.14) follows directly by integration by parts.

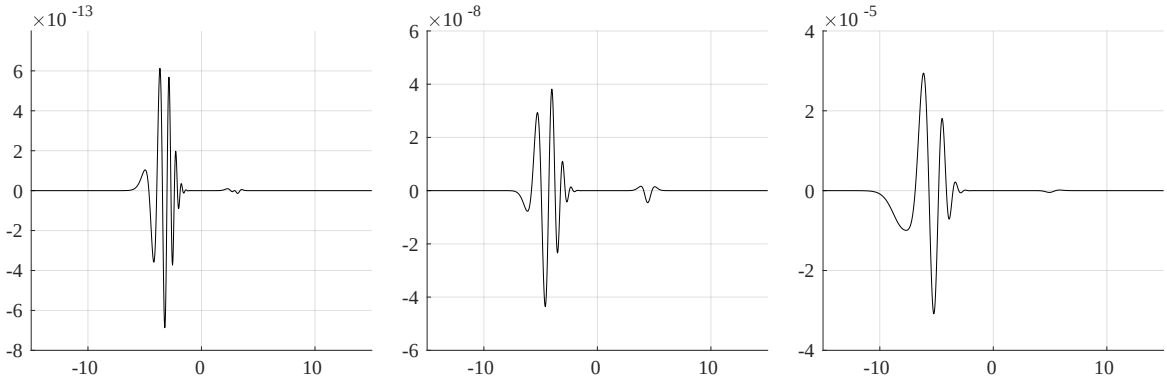
Now we can summarize the algorithm for approximating the lognormal pdf $g_\sigma(x)$ by exponential sums.

1. Compute the values of $G(z_j)$ numerically using the double exponential quadrature (5.6).

2. Use (5.14) to obtain the corresponding values of $F(z_j)$.

3. Define the coefficients ξ_j as in (5.13).

4. Run our continued fraction algorithm to compute the coefficients c_j and λ_j of $\phi(x)$.



(a) $\sigma = 0.5$, $A = 1.4$, $B = 21$ (b) $\sigma = 1$, $A = 1.7$, $B = 12$ (c) $\sigma = 1.5$, $A = 1.1$, $B = 8.5$

Figure 5.6: The graphs of $g_\sigma(x) - \widetilde{\phi}(x)$ with respect to $\ln(x)$. We set $M = 30$ in all cases, with $n_\infty = 6$ in (a), (b), and $n_\infty = 4$ in (c).

5. Finally, form $\widetilde{\phi}(x)$ according to (5.12), which gives the exponential sum approximation to $g_\sigma(x)$.

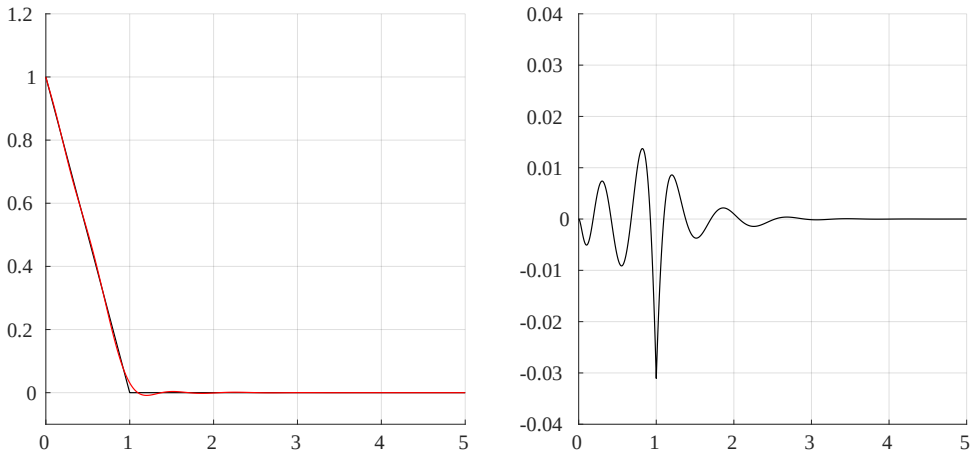
We constructed exponential sum approximations to g_σ for $\sigma \in \{0.5, 1, 1.5\}$. The results are shown in Figure 5.6. Note that the horizontal axis corresponds to $\ln(x)$. This logarithmic scale makes it easier to visualize the oscillations in the error $g_\sigma(x) - \widetilde{\phi}(x)$ that occur for very small values of x.

Approximating the hockey stick and the unit step functions

The hockey stick function is defined as

$$h(x) = \begin{cases} 1 - x & \text{if } \ 0 \leq x \leq 1 \\ 0 & \text{if } \ x > 1 \end{cases} \tag{5.15}$$

Exponential sum approximations to this function were obtained in [40] using the Beylkin-Monzón algorithm, with applications to pricing financial derivatives such as collateralized debt obligations (see [41]). This function is particularly well suited for the algorithm of section 4.3.1. Indeed, the coefficients ξ_j are easily computed since $h(x) = 1 - x$ for $0 \leq x \leq 1$,



(a) $h(x)$ (black) and $\phi(x)$ (red)

(b) $h(x) - \phi(x)$

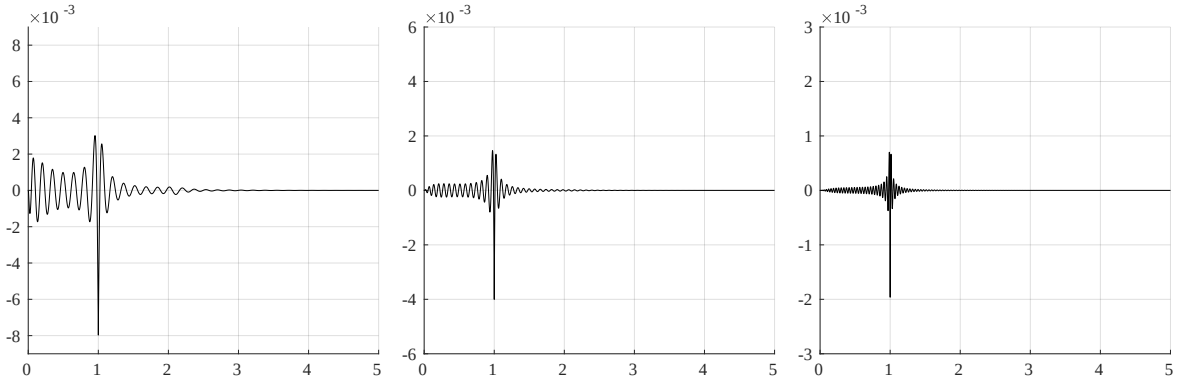
Figure 5.7: The graphs of $h(x)$, $\phi(x)$, and $h(x) - \phi(x)$ for $M = 5$, $n_\infty = 2$, $A = 0.5$, and $B = 8.5$.

giving $\xi_0 = 1$, $\xi_1 = -1$, and $\xi_j = 0$ for all $j \geq 2$. The Laplace transform of h is also available in closed form:

$$F(z) = \int_0^\infty e^{-zx} h(x)\,\mathrm{d}x = \int_0^1 e^{-zx}(1-x)\,\mathrm{d}x = z^{-2}\Big(e^{-z} + z - 1\Big).$$

Figure 5.7 shows the hockey stick function $h(x)$ and a 5-term exponential sum approximation $\phi(x)$ produced by our algorithm. We also computed approximations with $M \in \{15, 30, 60\}$ terms. In each case we optimized the parameters $\{A, B, n_\infty\}$ to minimize the L_1 error $\|h - \phi\|_1$. The errors and parameter choices are displayed in Figures 5.8a–5.8c. The L_1 errors for $M \in \{15, 30, 60\}$ were approximately 1.4×10^{-3}, 3.4×10^{-4}, and 9.7×10^{-5}, respectively.

A difficulty we encountered is that our algorithm sometimes produced exponential sums with very large coefficients c_j. For instance, with the parameters in Figure 5.8b, the largest coefficient $|c_j|$ is about 900, while the approximation shown on Figure 5.8c had the largest value of $|c_j|$ close to 1.5×10^6. Such large values are undesirable since they may cause loss of precision in applications of these approximations. By experimenting with the parameters, we found that increasing B significantly reduces $|c_j|$ without substantially increasing the L_1 error.



(a) $M = 15$, $n_\infty = 2$, $B = 39$ (b) $M = 30$, $n_\infty = 4$, $B = 78$ (c) $M = 60$, $n_\infty = 6$, $B = 160$

Figure 5.8: The graphs of $h(x) - \phi(x)$ for different values of M, n_∞, and B ($A = 0$ in all cases).

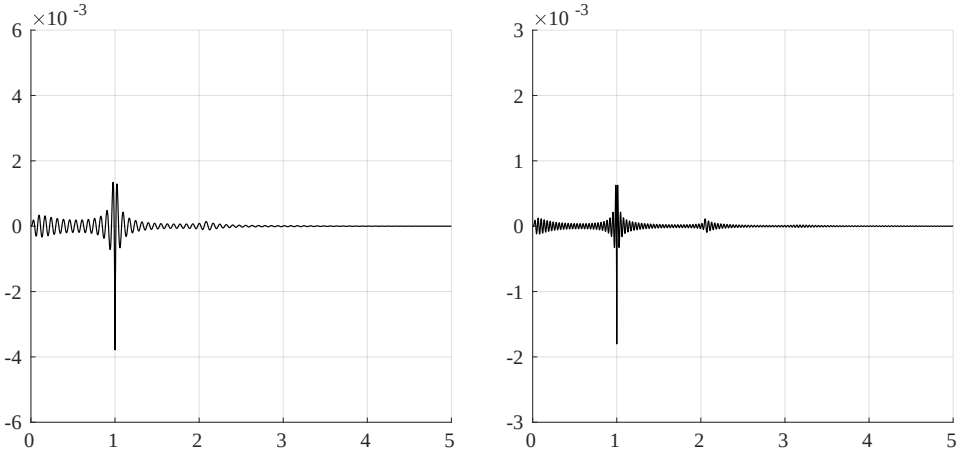
The updated results are shown in Figure 5.9. With $M = 30$, $n_\infty = 4$, increasing B from 78 to 83 reduced the maximum $|c_j|$ from 900 to about 56.4, while the L_1 error rose slightly from 3.4×10^{-4} to 3.8×10^{-4}. For $M = 60$, $n_\infty = 6$, increasing B from 160 to 175 reduced the maximum $|c_j|$ from 1.5×10^6 to about 97, while the L_1 error rose from 9.7×10^{-5} to 1.2×10^{-4}. These results appear superior to those obtained in [40] using the Beylkin-Monzón method: in our case, the error is more localized and the L_∞ errors are smaller.

Next, we consider the unit step function

$$H(x) := \mathbf{1}_{\{x \le 1\}}, \qquad x \ge 0.$$

Note that $H(x) = -h'(x)$, so exponential sum approximations to h yield approximations to H (as in Section 5.1). However, since $H(0+) \neq 0$, our algorithm can also be applied directly to H, which we do in the following experiments.

Figure 5.10a shows $H(x)$ together with a 15-term exponential sum approximation $\phi(x)$, and Figure 5.10b shows the error $H(x) - \phi(x)$. Figures 5.10c and 5.10d show the errors for approximations with 30 and 60 terms. In each case we set $A = 0$ and chose n_∞ and B to minimize the L_1 error while keeping all coefficients $|c_j| < 100$.



(a) $M = 30$, $n_\infty = 4$, $B = 83$ (b) $M = 60$, $n_\infty = 6$, $B = 175$

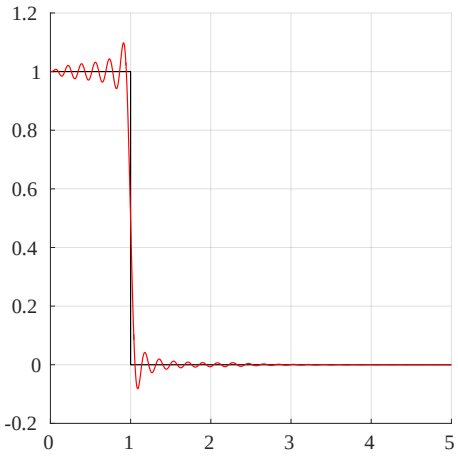
Figure 5.9: The graphs of $h(x) - \phi(x)$ for different values of M, n_∞, and B ($A = 0$ in all cases).

5.1.1 Approximating Completely Monotone Functions by Sums of Exponentials

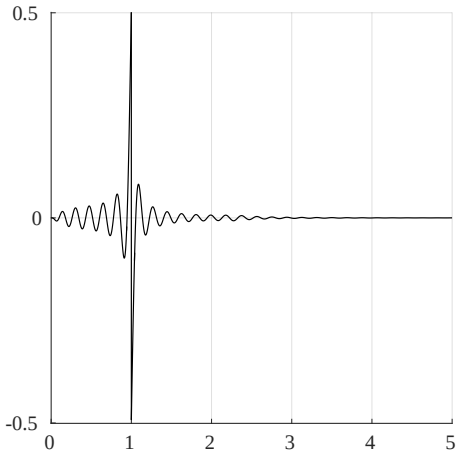
In this section, we illustrate through an example how one can improve the accuracy of approximating a $\mathcal{C}M$ function by a sum of exponentials when the maximum error over the entire interval $(0, \infty)$ is of interest. Here, unlike the previous section, we let all interpolation points as well as exponential sums coefficients take real number values.

It is known that the Laplace transform of a completely monotone function is a Stieltjes function. Therefore, such functions can be approximated using Padé approximations—either the classical single-point or the proposed multi-point versions. The resulting rational approximant can then be decomposed into partial fractions, which allows us to recover an approximation to the original completely monotone function as a sum of exponentials. Specifically, given a $\mathcal{C}M$ function h, we define its Laplace transform as

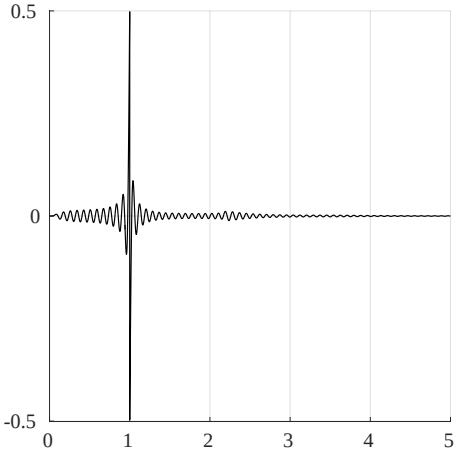
$$f(z) \coloneqq \int_0^\infty e^{-zx} h(x)\, dx,$$



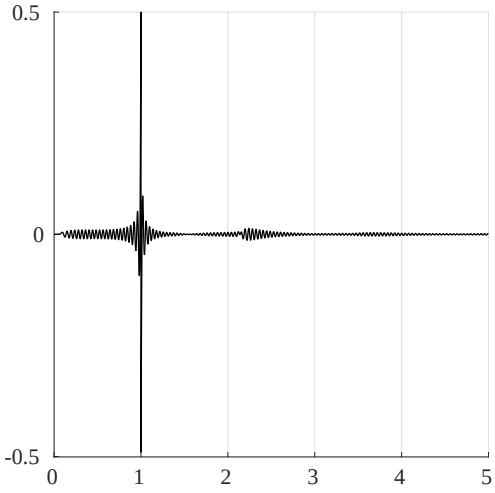
(a) $M = 15$, $n_\infty = 4$, $B = 34$



(b) $M = 15$, $n_\infty = 4$, $B = 34$



(c) $M = 30$, $n_\infty = 8$, $B = 75.5$



(d) $M = 60$, $n_\infty = 16$, $B = 158$

Figure 5.10: (a) The unit step function $H(x)$ (black) and its exponential sum approximation $\phi(x)$ (red). (b)–(d) The errors $H(x) - \phi(x)$ for different values of M, B, and n_∞. In all cases we set $A = 0$.

which is a Stieltjes function. Suppose that by our method f can be approximated as

$$f(z) \approx \sum_{i=1}^{M} \frac{w_i}{z + \alpha_i}.$$

Then, by taking the inverse Laplace transform, h can be approximated by a sum of exponentials:

$$h_M(x) = \sum_{i=1}^{M} w_i e^{-\alpha_i x}.$$

We measure the L_∞ error between h_M and h defined as $\sup_{x>0} |h(x) - h_M(x)|$.

By Theorem 21 and its notation, if $z_1, \ldots, z_N$ are the interpolation points with corresponding multiplicities $n_1, \ldots, n_N$, then the multi-point approximant is a Stieltjes function when $\sum_{i=1}^{N} n_i$ is even. (Note that the number of conditions is even for h and consequently for the Stieltjes function f, but odd for the Pick function $zf(z)$ with $n_0 = 1$, for which Theorem 20 applies.) If the last point $z_N = \infty$, then n_N represents the number of coefficients—from z^{-1} to z^{-n_i}—used in the expansion of f at infinity.

We next investigate how the choice of interpolation points $z_1, \ldots, z_N$ and corresponding $n_1, \ldots, n_N$ affects the error when $\sum_{i=0}^{N} n_i$ is fixed, and in particular, which arrangements yield smaller errors than those obtained using fewer points.

Matching the derivatives of the Stieltjes function

$$f(z) = \int_0^\infty e^{-zx} h(x)\, dx$$

with those of its rational approximation

$$\int_0^\infty e^{-zx} h_M(x)\, dx$$

at each interpolation point z_i is equivalent to

$$\int_0^\infty e^{-z_i x} x^j h(x)\, dx = \int_0^\infty e^{-z_i x} x^j h_M(x)\, dx, \qquad i = 1, \ldots, N,\ j = 0, \ldots, n_i - 1. \tag{5.16}$$

The goal is to minimize L_∞ error. Equation (5.16) can be written as

$$\int_0^\infty e^{-z_i x} x^j (h(x) - h_M(x))\, dx = 0.$$

For a fixed j, the function $e^{-z_i x} x^j$ attains its maximum at $x = j/z_i$ (found by setting the derivative of $e^{-z_i x + j \ln x}$ to zero, yielding $-z_i + j/x = 0$). Let $x^* = \operatorname{argmax} |h - h_M|$, then starting from $j = 1$ and choosing $z_{\text{new}} = j/x^*$ helps reduce $|h(x) - h_M(x)|$ near $x^* = j/z_{\text{new}}$. We then see which choice of j for $1 \leq j \leq n_i - 1$ reduces the new L_∞ errors the most.

In the computations below, Watson's Lemma (4.8) is used to determine the coefficients in the expansion of the function at infinity.

Table 5.1 illustrates how to choose the interpolation points and derivative multiplicities for the $\mathcal{C}M$ function $h(x) = e^{-\sqrt{x+1}}$ so as to reduce the error compared to the case with fewer points. Here, the total number of conditions is set to 20 ($M = 10$), though the method applies to any number of conditions.

Derivatives used	Interpolation points z_i	Error
$n_1 = 20$	$z_1 = 0.53$	3.4649×10^{-7}
$n_1 = 3, n_2 = 15, n_3 = 2$	$z_1 = 0.01, z_2 = 0.53, z_3 = \infty$	5.0224×10^{-8}
$(n_1, n_2, n_3, n_4) = (5, 11, 3, 1)$	$(z_1, z_2, z_3, z_4) = (0.05, 0.53, 5, \infty)$	1.8802×10^{-8}

Table 5.1: Exponential sums errors for $h(x) = e^{-\sqrt{x+1}}$.

In the first row, $z = 0.53$ provides the best single-point Padé approximation, yielding a minimum error of 3.4649×10^{-7}. As shown in Figure 5.11a, one maximum of the error function occurs around $x^* = 150$. To construct a two-point Padé approximation with smaller error near $x^* = 150$, $j/150$ for $1 \leq j \leq 19$ are candidates for z_{new}, where we start at $j = 1$ and check the L_∞ error. Setting $z_{\text{new}} = 0.01$ gives $\frac{1}{150} < z_{\text{new}} < \frac{2}{150}$, reducing the error near $x^* = 150$. If this would not sufficiently reduce the peak, a larger j could be used.

Using $z_1 = 0.01$, $z_2 = 0.53$, and $n_1 = 1$, $n_2 = 19$ keeps the total number of conditions unchanged while decreasing the error to 5.0389×10^{-7}. As shown in Figure 5.11b, the peak near $x = 150$ disappears, but a new maximum appears close to $x = 0$. To reduce this new peak, $z = \infty$ is added as an interpolation point. Choosing $z_1 = 0.01$, $z_2 = 0.53$, $z_3 = \infty$ with $n_1 = 1$, $n_2 = 18$, $n_3 = 1$ results in an error of 1.0829×10^{-7} (Figure 5.11c). The new maxima

near $x = 100$ and $x = 180$ suggest increasing n_1. Setting $n_1 = 2$, $n_2 = 17$, $n_3 = 1$ lowers the maximum error to 5.7036×10^{-8} (peak near $x = 130$). Using $n_1 = 3$, $n_2 = 16$, $n_3 = 1$ reduces the error at $x = 130$ but creates a new peak near zero, indicating a need to increase n_3. Setting $n_1 = 3$, $n_2 = 15$, $n_3 = 2$ yields a minimum error of 5.0224×10^{-8} (Figure 5.11d), which is optimal for this configuration.

To find a better four-point Padé approximation, in addition to $z_1 = 0.01$, $z_2 = 0.53$, and $z_3 = \infty$, we add $z_{\text{new}} = 5$ to improve accuracy for small x. Using $z_1 = 0.01$, $z_2 = 0.53$, $z_3 = 5$, $z_4 = \infty$ with $n_1 = 3$, $n_2 = 14$, $n_3 = 1$, $n_4 = 2$ gives an error of 7.0890×10^{-8} with a peak around $x = 100$. Adjusting to $n_1 = 4$, $n_2 = 13$, $n_3 = 1$, $n_4 = 2$ further reduces the error (Figure 5.11e). Two maxima occur for $x < 100$, while $z_1 = 0.01$ reduces the error for multiples of 100. To reduce the remaining peaks, we set $z_1 = 0.05$, improving the accuracy for multiples of 20. This change reduces the maximum error to 3.4542×10^{-8}, with a peak near $x = 200$, suggesting increasing n_1 to 5.

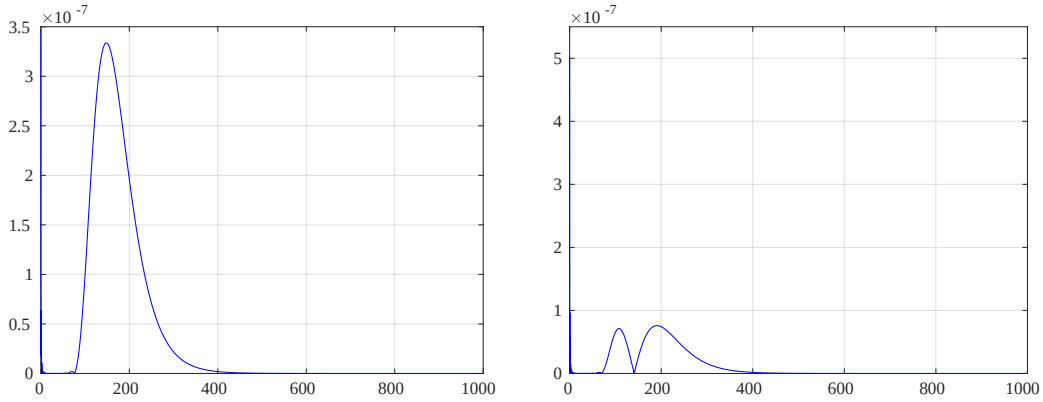
Repeating the above process with $z_1 = 0.05$, $z_2 = 0.53$, $z_3 = 5$, and $z_4 = \infty$ gives $n_1 = 5$, $n_2 = 11$, $n_3 = 3$, $n_4 = 1$, resulting in an error of 1.8802×10^{-8}—the best configuration for these points (Figure 5.11f).

5.2 Other applications of Padé approximation

5.2.1 Approximating GGCs via multi-point Padé approximation

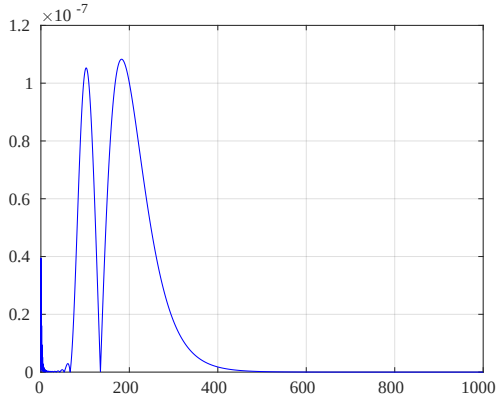
Now we are set to explain the main idea of our approach for approximating GGCs. In this section, we show how one can use the multi-point Padé approximation to find a sum of gamma r.v.s as approximation to any random variable following a GGC distribution. Our goal is to determine unique coefficients α_i and β_i, $i = 1, 2, \ldots, m$, as described in the following theorem, by using the algorithm for finding the unique rational approximation and the implementation method explained in Chapter 4.

Let X be a random variable with a distribution in the class of GGCs. We can approximate

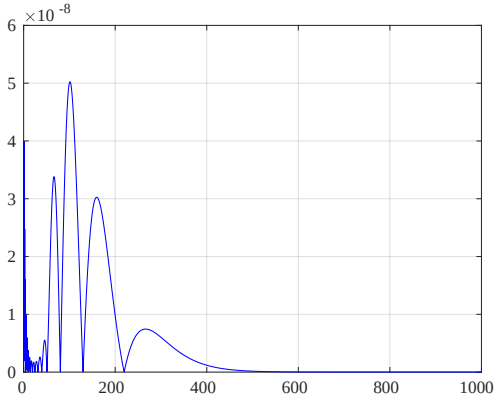


(a)

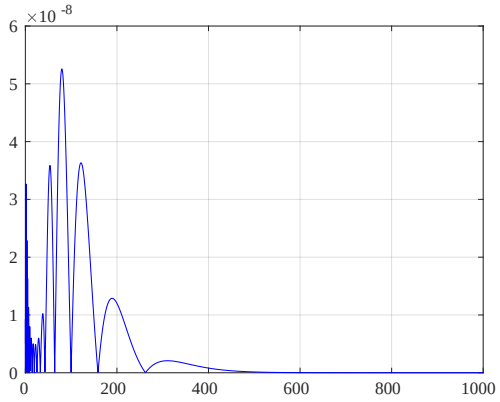
(b)



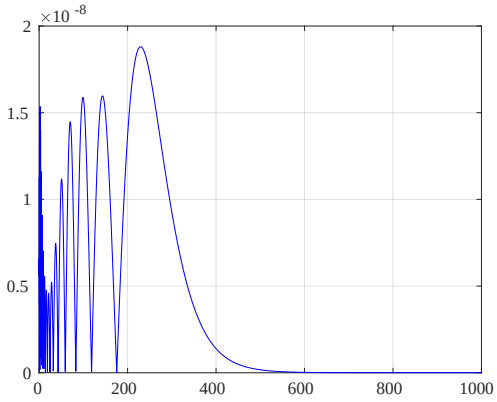
(c)



(d)



(e)



(f)

Figure 5.11: Error $|h(x) - h_M(x)|$ for $h(x) = e^{-\sqrt{x+1}}$: (a) $z_1 = 0.53$, $n_1 = 20$; (b) $z_1 = 0.01$, $z_2 = 0.53$, $n_1 = 1$, $n_2 = 19$; (c) $z_1 = 0.01$, $z_2 = 0.53$, $z_3 = \infty$, $n_1 = 1$, $n_2 = 18$, $n_3 = 1$; (d) $z_1 = 0.01$, $z_2 = 0.53$, $z_3 = \infty$, $n_1 = 3$, $n_2 = 15$, $n_3 = 2$; (e) $z_1 = 0.01$, $z_2 = 0.53$, $z_3 = 5$, $z_4 = \infty$, $n_1 = 4$, $n_2 = 13$, $n_3 = 1$, $n_4 = 2$; (f) $z_1 = 0.05$, $z_2 = 0.53$, $z_3 = 5$, $z_4 = \infty$, $n_1 = 5$, $n_2 = 11$, $n_3 = 3$, $n_4 = 1$.

the distribution of X arbitrarily well by distributions of finite sums of the form

$$Y := \sum_{i=1}^{m} \Gamma_i, \tag{5.17}$$

where $\Gamma_i \sim \text{Gamma}(\alpha_i, \beta_i)$ denote independent Gamma-distributed random variables with shape parameters $\alpha_i > 0$ and rate parameters $\beta_i > 0$.

Theorem 23. *Let the random variable X have a distribution in the class of GGCs. Fix $N, m, n_1, \ldots, n_N \in \mathbb{N}$ such that $n_1 + \cdots + n_N = 2m$, and let $z_1, z_2, \ldots, z_N > 0$ be a set of real points. Then, there exist positive numbers $\{\alpha_i\}_{1 \le i \le m}$ and $\{\beta_i\}_{1 \le i \le m}$ such that the random variable Y defined by (5.17) satisfies*

$$\frac{\mathbb{E}[Y^i e^{-z_j Y}]}{\mathbb{E}[e^{-z_j Y}]} = \frac{\mathbb{E}[X^i e^{-z_j X}]}{\mathbb{E}[e^{-z_j X}]}, \tag{5.18}$$

for $1 \le j \le N$ and $1 \le i \le n_j$. Moreover, the numbers $\{\alpha_i\}_{1 \le i \le m}$ and $\{\beta_i\}_{1 \le i \le m}$ are unique up to permutation.

Proof of Theorem 23. Since X is a GGC, its Laplace transform has the form (3.1). Note that if we prove the theorem when $a = 0$ in (3.1), then for the general case ($a \neq 0$), by writing Y and X as $Y - a + a$ and $X - a + a$ respectively, and using binomial theorem for Y^i and X^i as well as removing the extra term $e^{-z_j\, a}$ from both numerator and denominator of both left side and right side of (5.18) prove the theorem for $a \neq 0$. Hence, without loss of generality, we may assume that $a = 0$ in (3.1), that is,

$$\psi(z) = -\frac{d}{dz} \ln(\phi_X(z)) = \int_0^\infty \frac{U(dt)}{t + z}. \tag{5.19}$$

Thus, $\psi(z)$ is a Stieltjes function. As shown in Chapter 4, Stieltjes functions can be approximated arbitrarily well by multi-point Padé approximants. For a given set of points $z_1, z_2, \ldots, z_N$, the $[m - 1/m]$ Padé approximation to ψ at points $z_1, z_2, \ldots, z_N$ is a rational function of the form $R(z) = P(z)/Q(z)$, where

$$P(z) = a_0 + a_1 z + a_2 z^2 + \cdots + a_{m-1} z^{m-1}, \qquad Q(z) = b_0 + b_1 z + b_2 z^2 + \cdots + b_m z^m,$$

and they satisfy

$$\psi^{(i)}(z_j) = R^{(i)}(z_j), \qquad j = 1, 2, \ldots, N,\ i = 0, 1, \ldots, n_j - 1, \tag{5.20}$$

such that $n_1 + \cdots + n_N = 2m$.

By Theorem 21 there exists a unique $R(z) = P(z)/Q(z)$ satisfying conditions (5.20) and $R(z)$ has simple roots, denoted by $-\beta_i$, which lie on the negative real axis, and have positive residues, that is, $\alpha_i = P(-\beta_i)/Q'(-\beta_i) > 0$. Therefore, the rational function $R(z)$ can be written in partial fraction form as

$$R(z) = \sum_{i=1}^{m} \frac{\alpha_i}{z + \beta_i}, \tag{5.21}$$

where $\alpha_i, \beta_i > 0$.

We now claim that the random variable defined by (5.17), in which α_i and β_i are obtained via the multi-point Padé approximant process described above, satisfies the theorem statement. To see this, first note that

$$\phi_Y(z) = \prod_{i=1}^{m} (1 + z/\beta_i)^{-\alpha_i} = \exp\left(- \int_0^z R(w)\, dw \right). \tag{5.22}$$

In addition, we have

$$\psi(z) = -\frac{d}{dz} \ln(\phi_X(z)), \qquad R(z) = -\frac{d}{dz} \ln(\phi_Y(z)).$$

Therefore, by (5.20), we have

$$\phi_X^{(i)}(z_j)/\phi_X(z_j) = \phi_Y^{(i)}(z_j)/\phi_Y(z_j), \qquad j = 1, 2, \ldots, N,\ i = 1, 1, \ldots, n_j, \tag{5.23}$$

which is equivalent to equation (5.18) in the theorem.

To prove the uniqueness of α_i and β_i, note that if (5.18) holds, then, starting from the equivalent condition (5.23) backwards, we conclude that $R(z)$, given by (5.21), must be the unique Padé approximant to $\psi(z)$, yielding the uniqueness of α_i and β_i. □

Algorithm for finding α_i and β_i

Step 1: For $k = 0, 1, \ldots, 2m-1$ and $j = 1, \ldots, N$, compute numerically the following integrals:

$$g_{j,k} := (-1)^k \int_0^\infty x^k e^{-z_j x} f_X(x)\, dx, \tag{5.24}$$

where $f_X(x)$ is the density function of X.

Step 2: Set $s_{j,0} = -g_{j,1}/g_{j,0}$ for $j = 1, \ldots, N$, and then, for $k = 1, 2, \ldots, n_j - 1$, compute recursively

$$s_{j,k} = -\frac{1}{g_{j,0}} \left(\frac{g_{j,k+1}}{k!} + \sum_{i=0}^{k-1} s_{j,i} \frac{g_{j,k-i}}{(k-i)!} \right). \tag{5.25}$$

Step 3: Compute the multi-point Padé approximation $R(z) = P(z)/Q(z)$ via the steps 2 to 5 of the matrix approach explained in Section 4.2.

Step 4: Find the simple zeros $\{r_i\}_{1 \le i \le m}$ of $Q(z)$, which are all real and negative (as established in the theorem). Set

$$\beta_i = -r_i, \qquad \alpha_i = \frac{P(r_i)}{Q'(r_i)}, \tag{5.26}$$

for $i = 1, 2, \ldots, m$.

Remark 10. Recall that the method in the previous chapter computes the multi-point $[m-1/m]$ Padé approximation to the Stieltjes function $\psi(z) = -\frac{d}{dz}[\ln(\phi_X(z))]$, where $\phi_X(z)$ is the Laplace transform of X. In Step 1, we compute the coefficients $g_{j,k}$, which satisfy $g_{j,k} = \phi_X^{(k)}(z_j)$. Using the identity $\phi_X'(z) = -\psi(z)\phi_X(z)$ and expanding both sides in a Taylor series around each z_j, we get

$$\sum_{k \ge 0} \frac{g_{j,k+1}}{k!} z^k = -\left(\sum_{m \ge 0} s_{j,m} z^m \right) \left(\sum_{k \ge 0} \frac{g_{j,k}}{k!} z^k \right).$$

By comparing coefficients of z^k on both sides for $k = 1, 2, \ldots, n_j - 1$, we obtain the recursive identity (5.25) for computing $s_{j,k}$.

The subsequent steps determine the coefficients of the polynomials in the Padé approximation by solving a system of linear equations, leading to the coefficients α_i and β_i. As shown

in the proof above, these correspond to the parameters of the Gamma random variables in the approximating sum.

Numerical implementation for the Log-normal distribution

Log-normal distributions are widely used across various fields, ranging from finance—where they serve as the canonical model for stock price returns [69]—to insurance, where they model non-life insurance losses [52], and in many other disciplines [47].

A random variable X is said to follow a log-normal distribution with parameters $\mu \in (-\infty, \infty)$ and $\sigma > 0$, denoted by $X \sim LN(\mu, \sigma^2)$, if its probability density function is given by

$$f_X(x) = \frac{1}{x\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2}\left(\frac{\ln(x) - \mu}{\sigma}\right)^2\right), \quad x > 0. \tag{5.27}$$

The log-normal random variable X can be regarded as the exponential of a normal random variable with parameters (μ, σ^2). However, no explicit expression for its Laplace transform has been found to date. Asmussen et al. [5] derived an explicit approximation for the Laplace transform which performs well for small values of σ and is asymptotic to the true transform of the log-normal distribution. Miles [53] proposed an analytic continuation of the Laplace transform and presented efficient series approximations valid on $\mathbb{C} \setminus (-\infty, 0]$.

In this section, we aim to improve upon existing methods for approximating sums of log-normal distributions [32]. The convolution of log-normal distributions has numerous applications, spanning engineering, ecology, actuarial science, and finance (see, e.g., [25]).

So far, the methods proposed in the literature for approximating the sum of log-normal random variables can be broadly categorized into three main approaches: moment matching, series expansion of the Laplace transform of the convolution, and asymptotic approximations. Two common challenges associated with some of these methods arise when σ is large—resulting in a heavy-tailed log-normal distribution—and when only a small number of convolutions is considered, in which case the Central Limit Theorem does not apply [4].

Our proposed method proceeds as follows. We approximate a log-normally distributed random variable X by a sum of independent gamma random variables, each with rate

parameter $\beta_i > 0$ and shape parameter $\alpha_i > 0$, that is,

$$X \approx \sum_{i=1}^{n} X_i,$$

such that $X_i \sim \text{Gamma}(\alpha_i, \beta_i)$. Once such an approximation is established for an arbitrary log-normal random variable, the convolution of log-normals becomes straightforward: the Laplace transform of the convolution equals the product of the individual Laplace transforms, which, in the case of sums of independent gamma random variables, is easily computable. Since $X \in GGC$, Theorem 23 and the subsequent discussion guarantee that X can indeed be approximated by a sum of independent gamma variables.

Without loss of generality, we may assume $X \sim LN(0, \sigma^2)$, because the Laplace transform of a log-normal random variable $Y \sim LN(\mu, \sigma^2)$ is related to the Laplace transform of X by

$$\phi_Y(z) = \phi_X(ze^{\mu}), \quad \text{Re}(z) > 0,$$

which implies that an approximation of X immediately yields an approximation of Y.

For numerical implementation, we select positive numbers $z_1, \ldots, z_k$ and corresponding nonnegative integers $n_1, \ldots, n_k$, and proceed as described in Steps 1–4 of Section 5.2.1. Specifically, we first compute $g_{j,k}$ and $s_{j,k}$ using $f_X(x)$ given in (5.27). Next, we obtain the Padé approximant to $-\frac{d}{dz}\ln(\phi_X(z))$, where $\phi_X(z)$ denotes the Laplace transform of the log-normal random variable X. Finally, using relation (5.26), we determine the parameters α_i and β_i from the multi-point Padé approximant.

To ensure sufficient numerical accuracy when subtracting alternating large values of $g_{j,k}$ and when locating the roots of the denominator polynomial of the Padé approximant, all computations are performed with high precision. Specifically, we use `Fortran90` together with the `MPFUN` multi-precision package at a precision level of 200 digits. In addition, to compute the coefficients $g_{j,k}$ accurately—which all subsequent calculations depend upon—we employ the double exponential quadrature method (5.6).

Finally, after obtaining the parameters α_i and β_i, we recover the corresponding density function using the well-known inverse Laplace transform technique of the Gaver–Stehfest algorithm. The algorithm was first developed by Gaver [35] in 1966 and subsequently improved

by Stehfest [71] in 1970. This approach is preferred because the density of the convolution of gamma random variables requires multiple integrations and lacks a closed-form expression, making direct computation difficult, especially when many gamma components are used in the approximation.

Given that $F(z) = \int_0^\infty e^{-zx} f(x)\,dx$ is known, the Gaver–Stehfest algorithm recovers $f(x)$ via

$$f_n(x) = \frac{\ln(2)}{x} \sum_{k=1}^{2n} a_k(n)\, F(k\ln(2)/x), \quad n \geq 1,\ x > 0, \tag{5.28}$$

where

$$a_k(n) = \frac{(-1)^{n+k}}{n!} \sum_{j=[(k+1)/2]}^{\min(k,n)} j^{n+1} \binom{n}{j} \binom{2j}{j} \binom{j}{k-j}, \quad 1 \leq n,\ 1 \leq k \leq 2n.$$

For numerical illustration, we set $\sigma = 0.83$, both to match empirical data from collision claim payments involving 30–40 year-old drivers [56] and to facilitate comparison with the single-point Padé approximation method in [32]. We choose $n = 10$, approximating X as a sum of ten independent gamma random variables. Using the single-point Padé method, we find that $z = 2.83$ yields the smallest L_∞ error of 7.53×10^{-6} relative to the log-normal density function. In contrast, employing the two-point Padé method with $z_1 = 0.6$, $z_2 = 17.8$ and corresponding integers $n_1 = 11$, $n_2 = 9$, the maximum error decreases to 9.2794×10^{-7}—an eightfold improvement over the best single-point Padé result.

5.2.2 Mixture of exponentials approximation

Let the random variable X follow a mixture of exponential distributions. Its probability density function can then be expressed as

$$f_X(x) = \int_0^\infty e^{-\lambda x}\, \mu(d\lambda), \quad x > 0, \tag{5.29}$$

for some measure μ on $(0, \infty)$. Consequently, the Laplace transform of X is given by

$$\phi_X(z) = \int_0^\infty e^{-zx} f(x)\,dx = \int_0^\infty \frac{\mu(d\lambda)}{z + \lambda}. \tag{5.30}$$

Observe that $\phi_X(z)$ is a Stieltjes function. Therefore, under similar conditions as in Theorem 23 and by analogous reasoning, $\phi_X(z)$ can be approximated by

$$R(z) = \sum_{i=1}^{m} \frac{\alpha_i}{z + \beta_i},$$

where $\alpha_i, \beta_i > 0$.

We define the hyperexponential random variable $\tilde{X}$ with pdf

$$\tilde{f}(x) = \sum_{i=1}^{m} \alpha_i e^{-\beta_i x}, \tag{5.31}$$

for which the Laplace transform is

$$\phi_{\tilde{X}}(z) = \int_0^\infty e^{-zx} \tilde{f}(x)\, dx = \sum_{i=1}^{m} \frac{\alpha_i}{z + \beta_i} = R(z). \tag{5.32}$$

To be able to approximate X with a hyperexponential random variable we impose the initial interpolation condition $R(0) = \phi_X(0) = 1$, resulting in $\sum_{i=1}^{m} \alpha_i/\beta_i = 1$. Hence, we can set conditions

$$\phi_X^{(i)}(z_j) = \phi_{\tilde{X}}^{(i)}(z_j), \quad j = 1, 2, \ldots, N,\ i = 0, 1, 2, \ldots, n_j - 1,$$

as well as $\phi_X(0) = \phi_{\tilde{X}}(0)$. Using an argument similar to that in Theorem 23, we establish the following result.

Theorem 24. *Let the random variable X have a distribution belonging to the class of mixture of exponential. Fix $N, m, n_1, \ldots, n_N \in \mathbb{N}$ such that $n_1 + \cdots + n_N = 2m - 1$, and let $z_1, z_2, \ldots, z_N > 0$. Then, there exist positive numbers $\{\alpha_i\}_{1 \le i \le m}$ and $\{\beta_i\}_{1 \le i \le m}$ such that the random variable $\tilde{X}$ defined by (5.31) satisfies*

$$\mathbb{E}[\tilde{X}^i e^{-z_j \tilde{X}}] = \mathbb{E}[X^i e^{-z_j X}] \tag{5.33}$$

for $1 \le j \le N$ and $0 \le i \le n_j - 1$. Furthermore, the numbers $\{\alpha_i\}_{1 \le i \le m}$ and $\{\beta_i\}_{1 \le i \le m}$ are unique up to permutation.

5.2.3 Approximating the cumulative distribution function via the Laplace transform

One useful application of exponential-sum approximations to $H(x)$ arises in the inversion of Laplace transforms. A relevant example in probability theory is the computation of the cumulative distribution function (cdf) of a positive random variable X when only its Laplace transform $\mathcal{L}_X(z) = \mathbb{E}[\exp(-zX)]$ is known. This situation frequently occurs, for instance, when determining the cdf of a sum of independent random variables.

The existing approaches primarily rely on inversion formulas that recover distribution functions from characteristic functions (see [78] and references therein). In general, the cdf of a distribution can be obtained through the inversion relation

$$F_X(x) = \mathcal{L}^{-1}\left[\frac{\mathcal{L}_X(s)}{s}\right](x). \tag{5.34}$$

Here, we propose an alternative approximation method for distributions supported on $[0, \infty)$. From the discussion in subsection 5.1, for any $M > 1$, one can find coefficients c_i and λ_i, $1 \le i \le M$, such that the unit step function $H(x)$ is approximated by

$$H_M(x) = \sum_{i=1}^{M} c_i e^{-\lambda_i x}.$$

Using this, the cdf of X can be approximated as

$$\mathbb{P}(X \le u) = \mathbb{E}[\mathbf{1}_{\{X/u \le 1\}}] = \mathbb{E}[H(X/u)] \approx \mathbb{E}\left[\sum_{j=1}^{M} c_j e^{-\lambda_j X/u}\right] = \sum_{j=1}^{M} c_j \mathcal{L}_X(\lambda_j/u), \qquad u \ge 0. \tag{5.35}$$

Figure 5.12 illustrates this approximation for the exponential, inverse Gaussian, and gamma distributions when $M = 60$, where the coefficients c_i and λ_i are obtained from Section 5.1. The figures demonstrate that the maximum L_∞ error among the three examples is at most 5×10^{-4}.

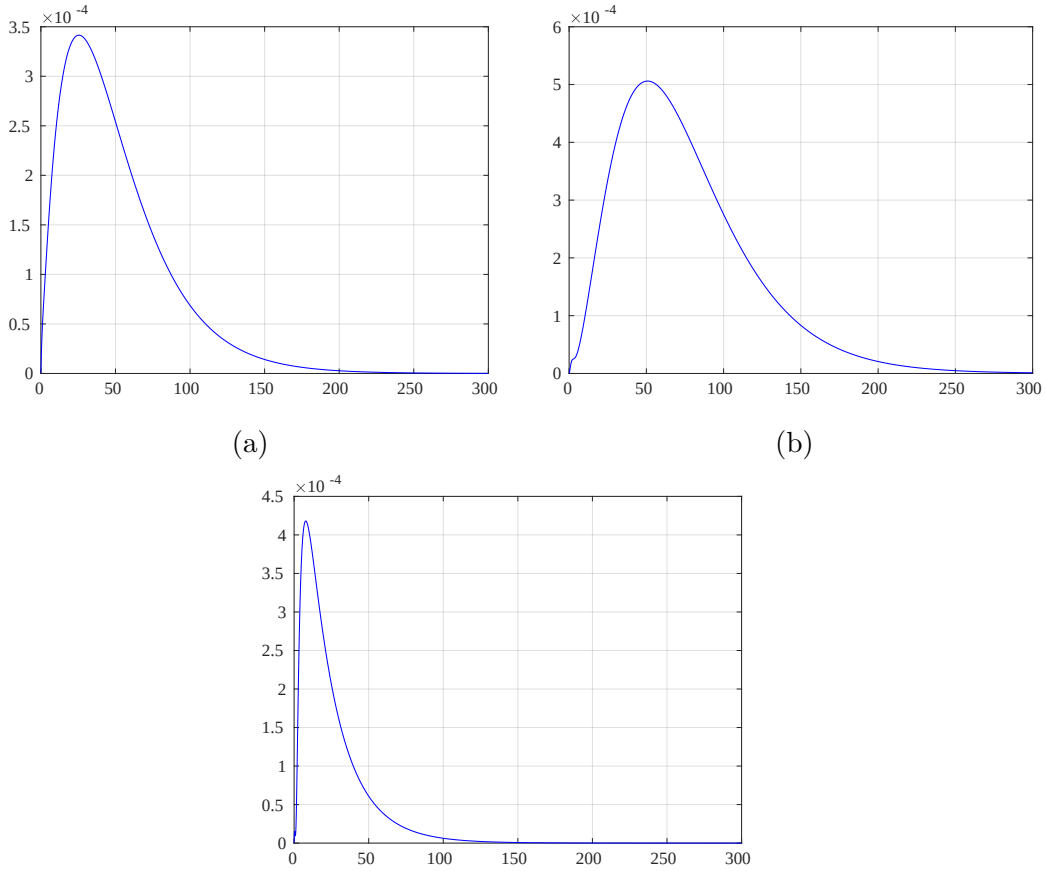


Figure 5.12: The error for the cdf and its approximation using relation (5.35) with $M = 60$ for: (a) exponential distribution with rate parameter 0.5, (b) gamma distribution with shape parameter 2 and rate parameter 0.5, and (c) inverse Gaussian distribution with mean and shape parameter equal to 1.

5.2.4 Gamma process approximation

A gamma process is a stochastic process that measures the cumulative occurrence of independent gamma-distributed increments over time. The gamma process at time t is denoted by $\Gamma(t;\gamma,\lambda)$, where γ and $\lambda > 0$ represent the shape and rate parameters, respectively. The marginal distribution of $\Gamma(t;\gamma,\lambda)$ at time t has the probability density function

$$f(x) = \frac{\lambda^{\gamma t}}{\Gamma(\gamma t)} e^{-\lambda x} x^{\gamma t - 1},$$

where $\Gamma(\cdot)$ in the denominator denotes the gamma function. Throughout this section, we restrict our attention to the case $\gamma = \lambda = 1$. This simplification is justified by the scaling and summation properties of gamma processes: for any constant $a > 0$, we have

$$a\Gamma(t; \gamma, \lambda) \sim \Gamma(t; \gamma, \lambda/a),$$

and for two independent gamma processes Γ_1 and Γ_2, it holds that

$$\Gamma_1(t; \gamma_1, \lambda) + \Gamma_2(t; \gamma_2, \lambda) \sim \Gamma_3(t; \gamma_1 + \gamma_2, \lambda).$$

The Laplace exponent of $\Gamma(t; 1, 1)$ is defined as the function $\psi(z)$ in

$$\phi_{\Gamma_t}(z) = \exp(-t\psi(z)), \tag{5.36}$$

where ϕ_{Γ_t} is the Laplace transform of the gamma process $\Gamma(t; 1, 1)$. Consequently, $\psi(z) = \ln(1 + z)$. To approximate the gamma process with a hyper-exponential process, we approximate $\psi(z)/z$ by a rational function using the multi-point Padé method.

Let the interpolation points $z_1, \ldots, z_N$ and corresponding integers $n_1, \ldots, n_N$ be given as in the definition of the multi-point Padé approximation, the multi-point Padé continued fraction approach can be applied to determine coefficients a_i and b_i such that

$$\frac{\psi(z)}{z} \approx \sum_{i=1}^{M} \frac{a_i}{z + b_i}.$$

To approximate the cdf of $\Gamma(t; 1, 1)$ at a given time t using the cdf of a hyper-exponential process, note that

$$-\frac{\ln(\phi(z))}{t} \approx \sum_{i=1}^{M} \frac{a_i z}{z + b_i},$$

which leads to

$$\phi(z) \approx \exp\left(-\sum_{i=1}^{M} \frac{t a_i z}{z + b_i}\right).$$

Finally, the cdf can be recovered from the inverse Laplace transform

$$F_1(x) = \mathcal{L}^{-1}\left\{\frac{\phi(z)}{z}\right\}(x), \tag{5.37}$$

which we approximate numerically using the Gaver–Stehfest inversion formula (5.28).

We now compare our cdf approximations to those proposed in Proposition 1 of [38], where by a different definition of the Laplace exponent, it is given by $\psi_2(z) = -\ln(1-z)$, and its $[n/n]$ Padé approximation is $\psi_2^{[n/n]}(z) = p_{n,0}(z)/q_{n,0}(z)$, with

$$p_{n,0}(z) = 2\sum_{j=0}^{n} \binom{n}{j}^2 \Big(H_{n-j} - H_j\Big)(1-z)^j,$$

where $H_0 = 0$ and $H_j = 1 + \frac{1}{2} + \cdots + \frac{1}{j}$. Moreover,

$$q_{n,0}(z) = z^n P_n^{\{0,0\}}(2/z - 1),$$

with Jacobi polynomials $P_n^{\{0,0\}}(z)$ given by

$$P_n^{\{0,0\}}(z) = \sum_{j=0}^{n} \binom{n}{n-j}\binom{n+j}{j}\left(\frac{z-1}{2}\right)^j.$$

To compare our approach for approximating the cdf of the gamma process X_t at times $t = 1, 2$ with the method based on the Padé approximation introduced above, first take r_0 as the coefficient in asymptotic expansion

$$\psi_2^{[n/n]}(z) = r_0 + O(1/z), \quad \text{as } z \to \infty.$$

Observe that $X_t^{(n)}$ has an atom at zero ($\mathbb{P}(X_t^{(n)} = 0) = \exp(tr_0)$), implying the measure

$$\mu_t(dx) = \mathbb{P}(X_t^{(n)} \in dx) - e^{tr_0}\delta_0(dx),$$

is absolutely continuous with Fourier transform $\int_0^\infty \exp(itz)\mu_t(dx) = e^{t\psi_2^{[n/n]}(z)} - e^{tr_0}$. Hence, via the inverse Fourier transform the cdf corresponding to $\mu_t(dx)$ would be

$$v_t((0,x)) = 1 - e^{tr_0} - \frac{e^{-cx}}{\pi}\,\mathrm{Re}\left[\int_0^\infty \phi_n(c+iu)\,e^{-iux}\frac{du}{c+iu}\right],$$

where we set $\phi_n(z) = e^{t\psi_2^{[n/n]}(z)} - e^{tr_0}$. This expressions above lead to the following approximation for the cdf of $X_t^{(n)}$, obtained via Fourier inversion:

$$\mathbb{P}(X_t^{(n)} \le x) = 1 - \frac{e^{-cx}}{\pi}\,\mathrm{Re}\left[\int_0^\infty \phi_n(c+iu)\,e^{-iux}\frac{du}{c+iu}\right], \tag{5.38}$$

valid for $x > 0$ and any $c \in (0,1)$.

As benchmarks, the exact cdfs of X_t for $t = 1, 2$ are given by

$$\mathbb{P}(X_1 \le x) = 1 - e^{-x}, \qquad \mathbb{P}(X_2 \le x) = 1 - (x+1)e^{-x}.$$

Table 5.2 reports the L_∞ errors for both approaches at $t = 1, 2$. The first column at each time corresponds to the values from Table 1 of [38], which employs the single-point Padé approximation at time 0. The second column lists the errors from our two-point Padé approach, where the cdf is computed using (5.37) and the Gaver–Stehfest inversion method. The interpolation points and corresponding integers used in $\varepsilon_n^2(1)$ for $n = 5, 10, 15, 20$ are: $(z_1, z_2) = (5, 14)$, $(n_1, n_2) = (5, 5)$; $(z_1, z_2) = (10, 40)$, $(n_1, n_2) = (15, 5)$; $(z_1, z_2) = (5, 40)$, $(n_1, n_2) = (18, 12)$; $(z_1, z_2) = (15, 50)$, $(n_1, n_2) = (24, 16)$. The corresponding pairs for $\varepsilon_n^2(2)$ are: $(z_1, z_2) = (1, 14)$, $(n_1, n_2) = (6, 4)$; $(z_1, z_2) = (5, 20)$, $(n_1, n_2) = (14, 6)$; $(z_1, z_2) = (8, 20)$, $(n_1, n_2) = (21, 9)$; $(z_1, z_2) = (12, 20)$, $(n_1, n_2) = (24, 16)$.

$t = 1$	$\varepsilon_n^1(1)$	$\varepsilon_n^2(1)$	$t = 2$	$\varepsilon_n^1(2)$	$\varepsilon_n^2(2)$
$n = 5$	1.1×10^{-2}	4.05×10^{-4}	$n = 5$	3.3×10^{-4}	1.69×10^{-5}
$n = 10$	2.8×10^{-3}	6.23×10^{-6}	$n = 10$	2.6×10^{-5}	2.15×10^{-7}
$n = 15$	1.3×10^{-3}	5.89×10^{-7}	$n = 15$	5.4×10^{-6}	6.01×10^{-9}
$n = 20$	7.5×10^{-4}	1.47×10^{-8}	$n = 20$	1.8×10^{-6}	4.8×10^{-10}

Table 5.2: L_∞ errors for approximations of cdf $F(t, x)$, where X_t is the gamma process $\Gamma(t; 1, 1)$. The first column at each time reports $\varepsilon_n^1(t) = \max_{x>0} |\mathbb{P}(X_t \le x) - \mathbb{P}(X_t^n \le x)|$, while the second gives $\varepsilon_n^2(t) = \max_{x>0} |F(t, x) - F_1(x)|$ for the two-point Padé method.

5.2.5 Mean squared errors through multi-point Padé method

The error in L_2 norm of a function $f \in H$, where H denotes a Hilbert space equipped with the inner product $\langle f, g \rangle = \int_0^\infty f(x)g(x)\, d\mu(x)$, is defined by the norm

$$\|f\|_2 = \langle f, f \rangle^{\frac{1}{2}}.$$

We take μ to be the Borel measure on the positive real line, i.e., $d\mu(t) = dt$.

The problem of finding the best approximation to a completely monotone function $f(x)$ in L_2 by real-valued exponential sums of order n—that is, a sum of n exponential terms—can be formulated as follows: for a given n, find

$$Y(x) = \sum_{i=1}^{n} \alpha_i e^{-\lambda_i x}, \tag{5.39}$$

such that

$$\|f - Y\|_2^2 = \int_0^\infty (f(x) - Y(x))^2 \, dx \tag{5.40}$$

is minimized.

In [43], it is shown that any best approximation to a completely monotone function $f \in H$, where f is not in the form of exponential sum, is of the form $Y(x) = \sum_{i=1}^{n} \alpha_i \exp(-\lambda_i x)$, where $0 < \lambda_1 < \cdots < \lambda_n$ and $0 < \alpha_j$ for $1 \leq j \leq n$, in such a way that Y satisfies the generalized Aigrain–Williams equations:

$$\begin{aligned} \mathcal{L}(Y, \lambda_i) &= \mathcal{L}(f, \lambda_i), \quad i = 1, \ldots, n, \\ \mathcal{L}'(Y, \lambda_i) &= \mathcal{L}'(f, \lambda_i), \quad i = 1, \ldots, n, \end{aligned} \tag{5.41}$$

where $\mathcal{L}$ denotes the Laplace transform.

The existence of a best approximation has been proved, for instance, in [18] and [49]. When f is completely monotone, the existence and a constructive method to determine the best exponential sums are discussed in [43]. Moreover, the same reference shows that for a given f, multiple best or locally optimal approximations may exist.

Table 5.3 compares the mean squared errors for the function $f(z) = 1/(1+z)$ on $(0, \infty)$, and its approximation by a sum of exponentials obtained via the multi-point Padé method, against the best errors reported in Table 1 of [43] for a given number of exponential terms. The method used to determine the interpolation points and corresponding integers in the last two columns of Table 5.3 follows the same procedure described in Section 5.1 for efficiently obtaining better approximations in the L_∞ sense. We can see that our results are comparable to the optimal results in L_2 space.

n	Best L_2 error	L_2 error (multi-point Padé)	Interpolation points	Derivatives
1	3.18e−1	3.90e−1	$z_1 = 1.2$	$n_1 = 2$
2	1.31e−1	1.84e−1	$z_1 = 0.045$	$n_1 = 1$
			$z_2 = 0.8$	$n_2 = 2$
			$z_3 = \infty$	$n_3 = 1$
3	6.14e−2	8.46e−2	$z_1 = 0.018$	$n_1 = 1$
			$z_2 = 0.04$	$n_2 = 1$
			$z_3 = 0.6$	$n_3 = 3$
			$z_4 = \infty$	$n_4 = 1$
6	9.73e−3	2.66e−2	$z_1 = 0.0005$	$n_1 = 3$
			$z_2 = 0.01$	$n_2 = 3$
			$z_3 = 0.5$	$n_3 = 5$
			$z_4 = \infty$	$n_4 = 1$

Table 5.3: L_2 errors for approximations of $1/(1+z)$ by sums of exponentials. The first column shows the best least-squares errors, while the second column lists the L_2 errors for the approximations obtained via the multi-point Padé method.

Chapter 6

Applications of multi-point Padé approximation in risk measures

In this chapter, we investigate several well-known risk measures that can be efficiently approximated using our exponential sum approximation of the hockey stick function. Throughout this chapter, the random variable X represents risk, and positive values correspond to financial losses.

Before discussing the specific risk measures and their corresponding approximation methods introduced in the following sections, we first elaborate on an application of the hockey stick function (h) approximation from subsection 5.1, which will be used frequently throughout this chapter.

Assume we have a pool of independent non-negative losses X_i and define the aggregate loss $X = \sum_{i=1}^{n} X_i$. Suppose we are interested in approximating $\mathbb{E}[h(X)]$. A common approach in the literature relies on the linearity of h and the computation of the distribution of X to evaluate this expectation (see [41] and references therein). However, when the distribution of X is difficult to obtain, this approach becomes inefficient.

Instead, if we approximate by $\mathbb{E}[h_M(X)]$, where h_M is sum of M exponentials approxima-

tion to h, then, by independence of the X_i, we have

$$\mathbb{E}[h_M(X)] = \mathbb{E}\Big[\sum_{i=1}^{M} w_i e^{-r_i X}\Big] = \sum_{i=1}^{M} w_i \mathbb{E}[e^{-r_i X}] = \sum_{i=1}^{M} w_i \mathbb{E}\Big[e^{-r_i \sum_{j=1}^{n} X_j}\Big] = \sum_{i=1}^{M} w_i \prod_{j=1}^{n} \mathbb{E}[e^{-r_i X_j}].$$

The last term depends only on the Laplace transforms of the individual random variables X_j. When these Laplace transforms are not available in closed form, we can employ the double exponential quadrature method (5.6) to compute the desired approximation.

6.1 Expected Shortfall Approximation

Expected shortfall (ES) has long been used as a measure of market and credit risk in portfolios. It is also known as conditional value at risk (CVaR) or tail conditional expectation (TCE). In simple terms, the expected shortfall at level $p\%$ represents the expected loss in the worst $p\%$ of cases.

Following the 2008 financial crisis, which exposed fundamental limitations in the estimation of Value at Risk (VaR), the Basel Committee on Banking Supervision (BCBS), through the Fundamental Review of the Trading Book (FRTB), shifted the standard risk measure from VaR to expected shortfall. The rationale lies in the fact that ES captures losses occurring in the fat tails of the distribution, whereas VaR does not and therefore tends to underestimate market risk and the corresponding required capital. In fact, VaR fails to effectively capture extreme losses.

There are also other reasons why ES is preferred over VaR. For instance, VaR is typically computed using historical data and therefore fails to account for potential future crises. The FRTB framework, in contrast, requires stressed ES to be calculated during stressed periods.

In addition, ES is a *coherent* risk measure, meaning that it satisfies the properties of monotonicity, subadditivity, positive homogeneity, and translation invariance which are listed respectively as follows:

$$\mathrm{ES}_p(X_1) \leq \mathrm{ES}_p(X_2) \text{ if } X_1 \leq X_2,$$

$$\mathrm{ES}_p(X_1 + X_2) \leq \mathrm{ES}_p(X_1) + \mathrm{ES}_p(X_2),$$

$$\text{for } a \geq 0: \quad \text{ES}_p(aX) = a\text{ES}_p(X),$$

$$\text{for } a \geq 0: \quad \text{ES}_p(a + X) = \text{ES}_p(X) - a.$$

For a random variable X, for $0 < p < 1$, the expected shortfall is defined as

$$\text{ES}_p(X) = \frac{1}{1-p} \int_p^1 \text{VaR}_y(X)\, dy,$$

where $\text{VaR}_y(X)$ denotes the Value at Risk corresponding to confidence level y. The Value at Risk (the y-th quantile) of X is defined by

$$\text{VaR}_y(X) = \inf\{x \in \mathbb{R} : \mathbb{P}(X \leq x) \geq y\}.$$

Assuming X has a continuous distribution, the expected shortfall equals the tail conditional expectation:

$$TCE_p(X) = \mathbb{E}[X \mid X \geq \text{VaR}_p(X)]. \tag{6.1}$$

From this relation, it is evident that for any given random variable X and confidence level p, we have $\text{ES}_p(X) \geq \text{VaR}_p(X)$.

Rockafellar and Uryasev [62] introduced a technique that simultaneously computes VaR and TCE. Their approach can also be integrated into scenario-based optimization methods for portfolios with many instruments. Their main result is summarized in the theorem below.

Theorem 25 (Theorem 1 in [62])**.** *Define*

$$F_p(X, \lambda) = \lambda + \frac{1}{1-p}\mathbb{E}[(X - \lambda)^+],$$

where $0 < p < 1$*,* X *denotes the loss function, and*

$$(x)^+ = \begin{cases} x, & \text{if } x > 0, \\ 0, & \text{if } x \leq 0. \end{cases}$$

Then $F_p(X, \lambda)$ *is a convex and continuously differentiable function of* λ*. Moreover, for a random variable* X*,*

$$TCE_p(X) = \min_{\lambda \in \mathbb{R}} F_p(X, \lambda),$$

and

$$\text{VaR}_p(X) = \arg\min_{\lambda} F_p(X, \lambda).$$

Next, we illustrate the application of the multi-point Padé approximation using the exponential sum approximant to the hockey stick function for $M = 15$ from Section 5.1.

Suppose the non-negative loss random variable X is the sum of three independent lognormal random variables X_i with parameters $(0, \sigma_i^2)$ for $i = 1, 2, 3$. For any real number x, the identity $(x)^+ = x + (-x)^+$ holds. From definition of F in the theorem above, we can simplify:

$$F_p(X, \lambda) = \lambda + \frac{1}{1-p}\mathbb{E}[(X-\lambda)^+] = \lambda + \frac{1}{1-p}\mathbb{E}[X-\lambda] + \frac{1}{1-p}\mathbb{E}[(\lambda - X)^+]. \tag{6.2}$$

We can also write

$$\mathbb{E}[X-\lambda] = \mathbb{E}(X_1) + \mathbb{E}(X_2) + \mathbb{E}(X_3) - \lambda = e^{\sigma_1^2/2} + e^{\sigma_2^2/2} + e^{\sigma_3^2/2} - \lambda,$$

where the last equality follows from the lognormality of X_i. Using the exponential sum approximation of the hockey stick function, we obtain

$$\mathbb{E}[(\lambda - X)^+] = \lambda\,\mathbb{E}\left[\left(1 - \frac{X}{\lambda}\right)^+\right] \approx \lambda \sum_{i=1}^{15} w_i \mathbb{E}\left[e^{-r_i \frac{X}{\lambda}}\right] = \lambda \sum_{i=1}^{15} w_i \prod_{j=1}^{3} \mathbb{E}\left[e^{-r_i \frac{X_j}{\lambda}}\right],$$

where the last equality follows from independence of the X_i.

To compute the final term, we require the Laplace transform of each X_i, or an approximation thereof. Since each X_i is lognormal, it belongs to the class of generalized gamma convolutions (GGCs) and can therefore be approximated by a sum of independent gamma random variables via single-point Padé approximation [32].

If we use a 20-term gamma approximation with parameters (α_i, β_i), $1 \le i \le 20$, for each of X_1, X_2, and X_3, then the final term can be approximated by the Laplace transform of the sum of 20 independent gamma distributions:

$$\mathbb{E}\left[e^{-\frac{r_i}{\lambda}X}\right] \approx \prod_{k=1}^{20} \left(1 + \frac{r_i}{\lambda \beta_k}\right)^{-\alpha_k},$$

which completes the computation of $F_p(\lambda)$ for a given p and λ.

For $\sigma_1 = 0.15$, $\sigma_2 = 0.48$, $\sigma_3 = 1.10$, and $p = 0.99$, applying the method described above and, by Theorem 25, taking the minimum of $F_p(\lambda)$ yields an approximation of $\mathrm{ES}_p(L) = 22.3185$ and $\mathrm{VaR}_p(L) = 15.1221$ with a runtime of 0.5 seconds.

For validation, we also estimate $\mathrm{ES}_p(L)$ and $\mathrm{VaR}_p(L)$ via Monte Carlo simulation. Using relation (6.1), we first compute $\mathrm{VaR}_p(L)$, then calculate the mean of losses exceeding $\mathrm{VaR}_p(L)$. Specifically, we simulate L for a large number of samples N_{MC} (say $N_{MC} = 2 \times 10^6$). To find $\mathrm{VaR}_p(L)$, we sort the simulated losses in increasing order; the $\lfloor N_{MC} \times p \rfloor$-th order statistic corresponds to $\mathrm{VaR}_p(L)$. We then repeat the simulation N_{MC} times and take the mean of losses greater than this value to obtain an estimate of $\mathrm{ES}_p(L)$.

Since this Monte Carlo method involves sampling variability, we repeat the entire procedure 1000 times and take the average of all $\mathrm{VaR}_p(L)$ and $\mathrm{ES}_p(L)$ estimates. This yields $\mathrm{VaR}_p(L) = 15.1015$, $\mathrm{ES}_p(L) = 22.3205$ with a 99.73% confidence interval of $(22.3126, 22.3287)$ with a runtime of 244.61 seconds.

6.2 Individual Economic Capital Allocation

Given that the aggregate risk is $X = \sum_1^n X_i$, a more complicated problem than computing the total economic capital (EC) requirement via expected shortfall is the allocation of this EC among the constituent risks X_i. In other words, it is often of interest to assess the risk contribution of each summand X_i in an EC computation. Here, we aim to approximate the allocation problem of the shortfall risk measure, that is, to approximate

$$TCE_p(X_i, X) = \mathbb{E}[X_i | X > \mathrm{VaR}_p(X)].$$

By definition of conditional expectation, we can write

$$TCE_p(X_i, X) = \frac{\mathbb{E}[X_i 1_{\{X > \mathrm{VaR}_p(X)\}}]}{P(X > \mathrm{VaR}_p(X))} = \frac{\mathbb{E}[X_i] - \mathbb{E}[X_i 1_{\{X/\mathrm{VaR}_p(X) < 1\}}]}{1 - p}.$$

Now, using the unit step function approximation discussed in Section 5.1, $H(X) \approx \sum_{j=1}^M c_j e^{-\lambda_j X}$, we obtain

$$\mathbb{E}[X_i 1_{\{X/\mathrm{VaR}_p(X) < 1\}}] \approx \sum_{j=1}^{M} c_j \mathbb{E}[X_i e^{-\lambda_j X/\mathrm{VaR}_p(X)}].$$

Moreover, by assuming independence among the X_i, we can further simplify the last term:

$$\mathbb{E}[X_i e^{-\lambda_j X/\mathrm{VaR}_p(X)}] = \mathbb{E}[X_i e^{-\lambda_j X_i/\mathrm{VaR}_p(X)}] \prod_{\substack{k=1 \\ k \neq i}}^{n} \mathbb{E}[e^{-\lambda_j X_k/\mathrm{VaR}_p(X)}].$$

Therefore, since $\text{VaR}_p(X)$ and the coefficients λ_j are easily computable, the individual allocation approximation problem reduces to approximating the Laplace transform of each r.v. X_k at point $\lambda_j/\text{VaR}_p(X)$, as well as the expectation $\mathbb{E}[X_i e^{-\lambda_j X_i/\text{VaR}_p(X)}]$, both of which can be computed using the double exponential quadrature method (5.6).

We have illustrated an example of this method by taking X to be the sum of six independent r.v.s, two lognormal r.v.s with scale parameters 2.5 and 1.5 ($\mu = 0$), two Pareto r.v.s with scale parameter 1 and shape parameters 1.3 and 1.8, and two Weibull r.v.s with scale parameter 1 and shape parameters 0.3 and 0.5 respectively. We set the prudence level $p = 0.99$. Then this approach with $M = 60$ yields $TCE_p(X_1, X) \approx 1203.1$ with a runtime of 0.08 seconds in MATLAB. If we approximate $TCE_p(X_1, X)$ via Monte Carlo, we get 1204.5 for 20 times simulating 10^7 samples of X and then taking their average with a 99.73% confidence interval of $(1196.3, 1212.7)$ with a runtime of 707.34 seconds. We observe that in this case the relative error of our method is less than 0.0079 or 0.79% with probability 99.73%.

6.3 Tail Standard Deviation Approximation

Although expected shortfall captures the mean of a risk r.v. beyond the p-th quantile (i.e., VaR_p for a fixed prudence level p), it fails to account for the variability of the risk beyond VaR_p. To capture this variability in the tail, Furman and Landsman [33] introduced the tail standard deviation (TSD) risk measure with prudence level p and loading parameter λ, defined as

$$TSD_p^{\lambda}(X) = TCE_p(X) + \lambda SD_p(X), \tag{6.3}$$

where the tail standard deviation measure is given by

$$SD_p(X) = \sqrt{\mathbb{E}[(X - TCE_p(X))^2 | X \geq \text{VaR}_p]}. \tag{6.4}$$

If the cdf of the r.v. X is continuous, TCE in equations (6.3) and (6.4) can be replaced by ES, in which case the risk measure is referred to as the standard deviation shortfall.

Despite the ability of TSD to capture tail variability, it lacks several key properties desirable in a coherent risk measure. First, it is defined only when the second moment of the

risk variable is finite, whereas in insurance and finance, risks often have infinite variance but finite mean (see [68] and [60]). Second, it lacks monotonicity; that is, a smaller risk does not necessarily imply a smaller capital requirement, contradicting the intuition behind economic capital regulation. Finally, for co-monotonic random variables, TSD is not additive, whereas practical measures such as value at risk and expected shortfall are co-monotone additive. Two r.v.s X, Y defined on a probability space (Ω, A, P) are called co-monotone if, for every $(w, w') \in \Omega \times \Omega$, we have

$$(X(w) - X(w'))(Y(w) - Y(w')) \geq 0, \quad (P \times P)\text{-almost surely.}$$

Moreover, a risk measure ρ is called co-monotone additive if, for every co-monotone pair X, Y, it satisfies

$$\rho(X + Y) = \rho(X) + \rho(Y).$$

Since we have already approximated TCE_p in the previous section, we now focus on approximating SD_p to obtain an approximation for TSD. Furthermore, our approximation method applies to arbitrary sums of independent random variables, thereby addressing the additivity issue inherent in the tail standard deviation.

To compute the tail standard deviation measure $SD_p(X)$ with prudence level $p \in (0, 1)$, we evaluate $\mathbb{E}[(X - \mathrm{ES}_p(X))^2 | X > \mathrm{VaR}_p(X)]$ under the assumption of a continuous cdf. We can write

$$\begin{aligned}\mathbb{E}[(X - \mathrm{ES}_p(X))^2 | X > \mathrm{VaR}_p(X)] &= \mathbb{E}[X^2 - 2X\ \mathrm{ES}_p(X) | X > \mathrm{VaR}_p(X)] + \mathrm{ES}_p^2(X) \\ &= \mathbb{E}[X^2 | X > \mathrm{VaR}_p(X)] - 2\mathrm{ES}_p^2(X) + \mathrm{ES}_p^2(X).\end{aligned}$$

The above equations follow from the definitions of ES and the linearity of expectation. Note also that from the continuity assumption of the cdf, we have $\mathbb{P}(X > \mathrm{VaR}_p(X)) = 1 - p$.

Substituting $(X - \mathrm{VaR}_p(X))^2 + \mathrm{VaR}_p^2(X) + 2\mathrm{VaR}_p(X)(X - \mathrm{VaR}_p(X))$ for X^2, the first term in the last equation becomes

$$\frac{1}{1-p}\Big(\mathbb{E}\Big[\Big((X - \mathrm{VaR}_p(X))^+\Big)^2\Big] + \mathrm{VaR}_p^2(X)(1-p) + 2\mathrm{VaR}_p(X)\mathbb{E}[(X - \mathrm{VaR}_p(X))^+]\Big). \quad (6.5)$$

In general, for any positive constant a, we have

$$\begin{aligned}\mathbb{E}[((X-a)^+)^2] &= \mathbb{E}[(X-a+(a-X)^+)^2] = \mathbb{E}[(X-a)^2] + \mathbb{E}[((a-X)^+)^2] + 2\mathbb{E}[-((a-X)^+)^2] \\ &= \mathbb{E}[(X-a)^2] - a^2\mathbb{E}[((1-X/a)^+)^2].\end{aligned}$$

We can also rewrite the last term of equation (6.5) as

$$\begin{aligned}&2\mathrm{VaR}_p(X)\mathbb{E}[X - \mathrm{VaR}_p(X) + (\mathrm{VaR}_p(X) - X)^+] = \\ &2\mathrm{VaR}_p(X)\mathbb{E}[X] - 2\mathrm{VaR}_p^2(X) + 2\mathrm{VaR}_p^2(X)\mathbb{E}[(1 - X/\mathrm{VaR}_p(X))^+].\end{aligned}$$

Combining these results, we obtain

$$\begin{aligned}SD_p^2(X) = -\mathrm{ES}_p^2(X) + \frac{1}{1-p}\Big(&\mathbb{E}[X^2] - p\mathrm{VaR}_p^2(X) - \mathrm{VaR}_p^2(X)\mathbb{E}[((1 - X/\mathrm{VaR}_p(X))^+)^2] \\ &+ 2\mathrm{VaR}_p^2(X)\mathbb{E}[(1 - X/\mathrm{VaR}_p(X))^+]\Big).\end{aligned}$$

Next, we approximate the function $g(x) = ((1-x)^+)^2$ by a sum of exponential functions:

$$g(x) \approx 2\ \mathrm{Re}\Big[\sum_{j=1}^{M} \beta_j e^{-\gamma_j x}\Big].$$

As a result, we obtain

$$\mathbb{E}[((1 - X/\mathrm{VaR}_p(X))^+)^2] \approx 2\ \mathrm{Re}\sum_{j=1}^{M} \beta_j \mathbb{E}\Big[e^{-\gamma_j X/\mathrm{VaR}_p(X)}\Big] = 2\ \mathrm{Re}\sum_{j=1}^{M} \beta_j L_X(\gamma_j/\mathrm{VaR}_p(X)).$$

Also note that $\mathbb{E}[(1-X/\mathrm{VaR}_p(X))^+]$ can be approximated via the hockey stick approximation coefficients w_i, r_i as in the previous section:

$$\mathbb{E}[(1 - X/\mathrm{VaR}_p(X))^+] \approx \sum_{i=1}^{2M} w_i \mathbb{E}[e^{-r_i X/\mathrm{VaR}_p(X)}] = 2\ \mathrm{Re}\sum_{i=1}^{M} w_i L_X(r_i/\mathrm{VaR}_p(X)).$$

Finally, if X is a sum of independent r.v.s, its Laplace transform equals the product of the Laplace transforms of its components. Each individual Laplace transform at any point is approximated using the double exponential quadrature method (5.6). Thus, we are able to approximate $SD_p^2(X)$.

For a numerical illustration, consider the case where the risk r.v. X is the sum of six independent r.v.s: two lognormal r.v.s with scale parameters 1.5 and 2.5 ($\mu = 0$), two Pareto

r.v.s with scale parameter 1 and shape parameters 2.3 and 2.8, and two Weibull r.v.s with scale parameter 1 and shape parameters 0.3 and 0.5. We set the prudence level $p = 0.99$ and approximate the squared hockey stick function with a 20-term exponential sum ($M = 10$). This yields $SD_\alpha(X) \approx 4997.7$ with a runtime of 0.2 seconds in MATLAB on a Core-i7 PC.

We also approximate $SD_\alpha(X)$ via the Monte Carlo method. We generate a vector of simulated X values of size 2×10^7 to approximate the expectation in (6.4). Due to the nature of tail expectations, we perform two additional loops of sizes 300 and 20 to obtain a more precise estimate, arriving at $SD_\alpha(X) \approx 4975.3$ via the Monte Carlo method, with a 99.73% confidence interval of $(4778.16, 5172.40)$ with a runtime of 4.5 hours in Fortran 90 on the same PC.

Comparing the result of our approximation with that of Monte Carlo simulation, we observe that the relative error of our method in this case is less than 0.0337 or 3.37% with probability 99.73%.

6.4 Expectile approximation

The concept of expectiles was introduced by Newey and Powell [55] as the minimizers of $\mathbb{E}[\rho_p(X - m) - \rho_p(X)]$ over m, where the expectation is taken with respect to a random variable X with cdf F_X (assumed to have a finite mean), $p \in (0, 1)$, and ρ_p is the asymmetric least squares loss function:

$$\rho_p(x) = x^2 \, |p - 1_{\{x<0\}}|.$$

In other words, analogous to the quantile at level p, Q_p, which minimizes a piecewise-linear loss function,

$$Q_p(X) = \text{argmin}_{x \in \mathbb{R}} \left[p \, \mathbb{E}[(X - x)^+] + (1 - p) \, \mathbb{E}[(X - x)^-] \right],$$

expectiles minimize an asymmetric quadratic loss:

$$T_p(X) = \text{argmin}_{x \in \mathbb{R}} \left[p \, \mathbb{E}\Big[((X - x)^+)^2\Big] + (1 - p) \, \mathbb{E}\Big[((X - x)^-)^2\Big] \right]. \tag{6.6}$$

It can be shown that the expectile is the value t satisfying

$$t - \mathbb{E}[X] = \frac{2p-1}{1-p} \int_t^\infty (x-t)\, dF_X(x). \tag{6.7}$$

It follows immediately from the equation above that when $p = 1/2$, the corresponding expectile equals the mean $\mathbb{E}[X]$. Alternatively, the expectile t satisfies

$$(1-p) \int_{-\infty}^t (t-x)\, dF_X(x) = p \int_t^\infty (x-t)\, dF_X(x). \tag{6.8}$$

By Theorem 1 in [55], the expectile T is a strictly monotone functional of p, and as a functional on random variables, it is linear. Bellini and Bignozzi [10] proved that the only elicitable coherent risk measures are expectiles with $p \geq 1/2$.

To approximate $T_p(X)$ for a random variable X that is the sum of independent components X_j, $1 \leq j \leq n$, we use equation (6.7) and rewrite it as

$$t - \mathbb{E}[X] = \frac{2p-1}{1-p}\, \mathbb{E}[(X-t)^+] = \frac{2p-1}{1-p} \Big(\mathbb{E}[X] - t + t\, \mathbb{E}[(1 - X/t)^+] \Big). \tag{6.9}$$

Using the hockey-stick function approximation, we obtain

$$\mathbb{E}[(1-X/t)^+] \approx \sum_{i=1}^M w_i \mathbb{E}\left[e^{-r_i X/t}\right] = \sum_{i=1}^M w_i L_X(r_i/t) = \sum_{i=1}^M w_i \prod_{j=1}^n L_{X_j}(r_i/t).$$

For a numerical example, consider r.v. X to be of uniform distribution on $(2, 5)$. Then the exact expectile when $p = 0.99$ is $T_p(X) = 4.7260$. The estimated expectile via the described method yields $t = 4.7324$, giving the relative error of 0.0013 or 0.13%.

Chapter 7

Dependence Structures of Multi-Dimensional GGC Models

In this chapter we first investigate the upper and lower tail dependence coefficients for dependent GGCs, seeking to find a better alternative than Gaussian copula. Then we introduce a new Laplace transform inversion for GGCs.

Prior to the 2007–2008 global financial crisis, Gaussian copulas were standard tools for pricing various complex derivatives (such as collateralized debt obligations) in multifactor models. After the crisis, however, it became apparent that these models were inadequate for this task [64]. The main issue lies in the weak tail dependence exhibited by Gaussian copulas.

For example, the upper tail dependence coefficient, defined for two random variables X and Y as

$$\lambda_U = \lim_{u \to 1^-} \frac{1}{1-u} \mathbb{P}(F_X(X) \geq u, F_Y(Y) \geq u), \tag{7.1}$$

becomes zero in the Gaussian copula case. Recall that the copula of two random variables X and Y is defined by

$$C(u, v) = \mathbb{P}(F_X(X) \leq u, F_Y(Y) \leq v),$$

where $F_X(x)$ and $F_Y(y)$ are the cdfs of X and Y, respectively, and $0 \leq u, v \leq 1$.

The Gaussian copula $C_\rho(u, v)$ is defined, for $0 \leq u, v \leq 1$, as

$$C_\rho(u, v) = \phi_2(\phi^{-1}(u), \phi^{-1}(v); \rho),$$

where $\phi(u)$ and $\phi^{-1}(u)$ denote cdf of the standard normal distribution function and its inverse, and $\phi_2(s, t; \rho)$ denotes the cdf of the bivariate normal distribution with correlation parameter ρ.

The Gaussian copula fails to capture tail dependence effectively. Specifically, if (X, Y) follows a bivariate normal distribution with any correlation $\rho \in (-1, 1)$, then X and Y are asymptotically independent, i.e.

$$\lim_{t\to\infty} \mathbb{P}(X > t \mid Y > t) = 0,$$

which is not realistic since risk variables in practice tend to exhibit asymptotic dependence. In other words, risk factors often display tail dependence.

Therefore, we propose using GGCs and investigate whether, through a suitable choice of parameters, they can exhibit non-zero tail dependence. We aim to study dependence structures arising from the multivariate GGC class. One alternative model of dependence that we propose to examine is defined as follows.

Let $\Gamma_t^{(1)}$ and $\Gamma_t^{(2)}$ be two independent gamma processes, and define

$$\Gamma_t := \Gamma_{ct}^{(1)} + \Gamma_{(1-c)t}^{(2)}.$$

We then define two dependent random variables:

$$X = \int_0^\infty h(t)\, d\Gamma_t^{(1)}, \qquad Y = \int_0^\infty g(t)\, d\Gamma_t.$$

Note that when functions $h(t)$ and $g(t)$ are step functions, X and Y are GGCs and by Theorem 8, it is also true for X, Y as weak limits of such random variables. Our goal is to investigate when these two random variables exhibit non-zero tail dependence.

7.1 Simple Cases to Investigate

Consider two simple piecewise constant functions, $h(t) = A\,\mathbf{1}_{\{0<t\le T_1\}}$ and $g(t) = B\,\mathbf{1}_{\{0<t\le\tau\}}$, where $A > 0$ and $T_1, \tau > 0$. By scaling, we can assume $B = 1$. Then,

$$X = A\,\Gamma^{(1)}_{T_1}, \qquad Y = \Gamma_\tau = \Gamma^{(1)}_{c\tau} + \Gamma^{(2)}_{(1-c)\tau}.$$

Let $T_2 = c\tau$ and $T_3 = (1-c)\tau$. With this notation, we have

$$X = A\,\Gamma^{(1)}_{T_1}, \qquad Y = \Gamma^{(1)}_{T_2} + \Gamma^{(2)}_{T_3}.$$

Our goal is to compute the upper tail dependence coefficient (7.1) and lower tail dependence coefficient

$$\lambda_L = \lim_{u\to 0^+} \frac{1}{u}\,\mathbb{P}(F_X(X) \le u, F_Y(Y) \le u) = \lim_{u\to 0^+} \frac{1}{u}\mathbb{P}(X \le F_X^{-1}(u),\, Y \le F_Y^{-1}(u)). \tag{7.2}$$

We now consider the case

$$X = \theta\Gamma^{(1)}_1, \qquad Y = \theta\Gamma^{(1)}_1 + \Gamma^{(2)}_1, \;\; \theta > 0. \tag{7.3}$$

We first compute the joint cumulative distribution function in order to calculate λ_L. We have:

(i) If $y \le x$, then

$$\begin{aligned}
\mathbb{P}(X < x, Y < y) &= \mathbb{P}\Big(\Gamma^{(1)}_1 < \tfrac{x}{\theta},\, \theta\Gamma^{(1)}_1 + \Gamma^{(2)}_1 < y\Big) = \mathbb{P}(\theta\Gamma^{(1)}_1 + \Gamma^{(2)}_1 < y) \\
&= \int_0^y e^{-u} \int_0^{\frac{y-u}{\theta}} e^{-v}\,dv\,du = \int_0^y e^{-u}\Big(1 - e^{\frac{u-y}{\theta}}\Big)\,du \\
&= 1 - \frac{e^{-y}}{1-\theta} + \frac{\theta}{1-\theta} e^{-\frac{y}{\theta}}.
\end{aligned}$$

(ii) If $y > x$, then

$$\begin{aligned}
\mathbb{P}(X < x, Y < y) &= \mathbb{P}\Big(\Gamma_1^{(1)} < \tfrac{x}{\theta},\, \theta\Gamma_1^{(1)} + \Gamma_1^{(2)} < y\Big) \\
&= \mathbb{P}\Big(\Gamma_1^{(1)} < \tfrac{x}{\theta},\, \Gamma_1^{(2)} < y - x\Big) + \mathbb{P}\Big(\Gamma_1^{(1)} < \tfrac{x}{\theta},\, y - x < \Gamma_1^{(2)} < y - \theta\Gamma_1^{(1)}\Big) \\
&= \int_0^{\frac{x}{\theta}} e^{-u} \int_0^{y-x} e^{-v}\, dv\, du + \int_0^{\frac{x}{\theta}} e^{-u} \int_{y-x}^{y-\theta u} e^{-v}\, dv\, du \\
&= (1 - e^{-\frac{x}{\theta}})(1 - e^{x-y}) + \int_0^{\frac{x}{\theta}} e^{-u}(e^{x-y} - e^{\theta u - y})\, du \\
&= 1 - e^{-\frac{x}{\theta}} - \frac{e^{-y}}{\theta - 1}\Big(e^{\frac{\theta-1}{\theta}x} - 1\Big).
\end{aligned}$$

Consequently, for the lower tail dependence in this case we have:

(i) If $F_Y^{-1}(u) \le F_X^{-1}(u)$, it implies

$$1 - e^{-\frac{y}{\theta}} \le 1 - \frac{e^{-y}}{1-\theta} + \frac{\theta}{1-\theta} e^{-\frac{y}{\theta}}.$$

Now if $1 > \theta$, it yields $e^{y/\theta} \le e^y$, which is impossible. Also, if $1 < \theta$, then $e^y \le e^{y/\theta}$. Therefore, this case cannot happen.

(ii) Therefore for every $0 < u < 1$, we have $F_Y^{-1}(u) > F_X^{-1}(u)$, then

$$\begin{aligned}
\lambda_L &= \lim_{u \to 0^+} \frac{1}{u}\, \mathbb{P}(F_X(X) \le u, F_Y(Y) \le u) \\
&= \lim_{u \to 0^+} \frac{1}{u}\, \mathbb{P}(X \le F_X^{-1}(u),\, Y \le F_Y^{-1}(u)) \\
&= \lim_{u \to 0^+} \frac{1 - e^{-\frac{x}{\theta}} - \frac{e^{-y}}{\theta-1}(e^{\frac{\theta-1}{\theta}x} - 1)}{u} \\
&= \lim_{u \to 0^+} \frac{u - \frac{e^{-y}}{\theta-1}(e^{\frac{\theta-1}{\theta}x} - 1)}{u} \\
&= 1 - \lim_{u \to 0^+} \frac{\frac{e^{-y}}{\theta-1}\Big((1-u)^{1-\theta} - 1\Big)}{u} \\
&= 1 - \lim_{u \to 0^+} \left[-\Big((1-u)^{1-\theta} - 1\Big) \frac{e^{-y}}{\theta - 1} \frac{dy}{du} + e^{-y}(1-u)^{-\theta} \right] \\
&= -\lim_{y \to 0^+} \frac{e^{-y}}{e^{-y} - e^{-\frac{y}{\theta}}} \left[\left(\frac{e^{-y} - \theta e^{-\frac{y}{\theta}}}{1-\theta} \right)^{1-\theta} - 1 \right] = 0,
\end{aligned}$$

where we used L'Hôpital's rule, the relation $y \to 0^+$ as $u \to 0^+$, and the identities $u = 1 - e^{-\frac{x}{\theta}}$, and

$$\frac{dy}{du} = \frac{1-\theta}{e^{-y} - e^{-\frac{y}{\theta}}}.$$

The final result $\lambda_L = 0$ was also confirmed numerically for both cases $\theta < 1$ and $\theta > 1$.

Also, for calculating the upper tail dependence, we first obtain the joint probabilities:

(i) If $y < x$, then

$$\begin{aligned}\mathbb{P}(X > x, Y > y) &= \mathbb{P}(\theta\Gamma_1^{(1)} > x,\ \theta\Gamma_1^{(1)} + \Gamma_1^{(2)} > y) \\ &= \mathbb{P}\left(\Gamma_1^{(1)} > \frac{x}{\theta}\right) = \int_{\frac{x}{\theta}}^{\infty} e^{-u} du = e^{-\frac{x}{\theta}}.\end{aligned}$$

(ii) If $y > x$, then

$$\begin{aligned}\mathbb{P}(X > x, Y > y) &= \mathbb{P}(\theta\Gamma_1^{(1)} > x,\ \theta\Gamma_1^{(1)} + \Gamma_1^{(2)} > y) \\ &= \mathbb{P}\left(\Gamma_1^{(1)} > \frac{x}{\theta},\ \Gamma_1^{(2)} > y - x\right) + \mathbb{P}\left(\Gamma_1^{(1)} > \frac{x}{\theta},\ y - x > \Gamma_1^{(2)} > y - \theta\Gamma_1^{(1)}\right) \\ &= \int_{\frac{x}{\theta}}^{\infty} e^{-u} \int_{y-x}^{\infty} e^{-v} dv\, du + \int_{\frac{x}{\theta}}^{\infty} e^{-u} \int_{\max(y-\theta u, 0)}^{y-x} e^{-v} dv\, du \\ &= e^{-\frac{x}{\theta}} e^{x-y} + \int_{\frac{x}{\theta}}^{\infty} e^{-u} \left(e^{\min(\theta u - y, 0)} - e^{x-y}\right) du \\ &= e^{x\frac{\theta-1}{\theta} - y} + \int_{\frac{x}{\theta}}^{\frac{y}{\theta}} e^{-u}(e^{\theta u - y}) du + \int_{\frac{y}{\theta}}^{\infty} e^{-u} du - e^{x-y} \int_{\frac{x}{\theta}}^{\infty} e^{-u} du \\ &= \frac{\theta}{\theta - 1} e^{-\frac{y}{\theta}} - \frac{e^{x\frac{\theta-1}{\theta} - y}}{\theta - 1}.\end{aligned}$$

Note that We have

$$F_X(x) = 1 - e^{-x/\theta}, \qquad F_Y(y) = 1 - \frac{e^{-y}}{1-\theta} + \frac{\theta e^{-y/\theta}}{1-\theta}.$$

It follows that $F_X^{-1}(u) = -\theta \ln(1-u)$, and for all $u \in (0,1)$, we have $F_Y^{-1}(u) > F_X^{-1}(u)$. Indeed, this inequality is equivalent to

$$u > F_Y(F_X^{-1}(u)) = 1 - \frac{(1-u)^\theta}{1-\theta} + \frac{\theta(1-u)}{1-\theta},$$

which simplifies to

$$\frac{(1-u)^\theta}{1-\theta} > \frac{1-u}{1-\theta},$$

true for all $u \in (0,1)$ and $\theta > 0$.

We then have

$$\begin{aligned}
\lambda_U &= \lim_{u\to 1^-} \frac{1}{1-u}\,\mathbb{P}(F_X(X) \geq u,\, F_Y(Y) \geq u) \\
&= \lim_{u\to 1^-} \frac{1}{1-u}\,\mathbb{P}(X \geq F_X^{-1}(u),\, Y \geq F_Y^{-1}(u)) \\
&= \frac{1}{\theta-1} \lim_{u\to 1^-} (1-u)^{-1}\Big[\theta e^{-y/\theta} - (1-u)^{1-\theta} e^{-y}\Big],
\end{aligned}$$

where $y = F_Y^{-1}(u)$, so that

$$1-u = \frac{e^{-y} - \theta e^{-y/\theta}}{1-\theta}.$$

Substituting this expression for $1-u$ and using that $y \to +\infty$ as $u \to 1^-$, we obtain:

$$\lambda_U = \lim_{y\to+\infty} \left[\frac{\theta e^{-y/\theta}}{\theta e^{-y/\theta} - e^{-y}} + e^{-y}(1-\theta)^{\theta-1}(e^{-y} - \theta e^{-y/\theta})^{-\theta}\right].$$

If $\theta \in (0,1)$, then

$$e^{-y} - \theta e^{-y/\theta} = e^{-y}(1+o(1)), \quad y \to +\infty.$$

It follows that

$$\lambda_U = \lim_{y\to+\infty} \left[-\frac{\theta e^{-y/\theta}}{e^{-y}} + e^{-y}(1-\theta)^{\theta-1} e^{\theta y}\right] = 0.$$

If instead $\theta > 1$, then

$$\lambda_U = \lim_{y\to+\infty} \left[\frac{\theta e^{-y/\theta}}{\theta e^{-y/\theta} - e^{-y}} - e^{-y}(\theta-1)^{\theta-1}(\theta e^{-y/\theta} - e^{-y})^{-\theta}\right].$$

In this case,

$$\theta e^{-y/\theta} - e^{-y} = \theta e^{-y/\theta}(1+o(1)), \quad y \to +\infty,$$

and thus

$$\lambda_U = \lim_{y\to+\infty} \left[\frac{\theta e^{-y/\theta}}{\theta e^{-y/\theta}} - e^{-y}(\theta-1)^{\theta-1}(\theta e^{-y/\theta})^{-\theta}\right] = 1 - \frac{(\theta-1)^{\theta-1}}{\theta^\theta}.$$

Hence, we conclude this section with the following theorem

Theorem 26. *For dependent random variables X and Y defined by (7.3), the upper tail dependence coefficient is equal to*

$$\lambda_U = \begin{cases} 0, & \text{if } \theta \in (0, 1], \\ 1 - \dfrac{(\theta - 1)^{\theta - 1}}{\theta^{\theta}}, & \text{if } \theta > 1. \end{cases} \tag{7.4}$$

This result is significant because the parameter $\theta > 1$ yields a strictly positive upper tail dependence coefficient. Consequently, extreme events of one component are accompanied by extreme events of the other with non-vanishing probability.

The explicit expression of the upper tail dependence coefficient provides a quantitative measure of extremal dependence and highlights the ability of the proposed dependence structure to capture clustering of large values. This distinguishes the model from classical Gaussian copula that enforces asymptotic independence.

From an applied perspective, the presence of non-zero upper tail dependence is particularly relevant in risk management, finance, and insurance, where joint extreme losses play a central role [77]. Models exhibiting positive upper tail dependence are better suited for stress testing [3], portfolio risk aggregation [17], and the assessment of systemic risk [48], as they account for the increased likelihood of simultaneous extreme outcomes.

This theorem also suggests some directions for future research. One direction is the development of statistical inference procedures for estimating the dependence parameter based on extreme-value data. Additionally, embedding the present dependence structure into higher-dimensional settings or time-dependent models may provide a tractable framework for studying extremal dependence in multivariate or dynamic systems.

7.2 Change of integration curve for inverse Laplace transform of a GGC

In many applications, quantities of interest are naturally expressed in terms of the Laplace transform rather than the density or distribution function itself. Consequently, the numerical

and analytical inversion of Laplace transforms plays an important role in the study and practical use of GGCs.

The standard inversion of the Laplace transform is given by the Bromwich integral, which represents the original function as a complex contour integral along a vertical line in the complex plane [20]. It states that if $f(x)$ has a continuous derivative and $|f(x)| < Ke^{\gamma x}$ for some positive constants K and γ, then

$$f(x) = \frac{1}{2\pi \mathrm{i}} \lim_{T\to\infty} \int_{c-\mathrm{i}T}^{c+\mathrm{i}T} \phi(z) e^{zx} \mathrm{d}z,$$

where $c > \gamma$ and ϕ is LT of f. While this representation is exact and theoretically well understood, it is often ill-suited for numerical computation. In particular, the integrand typically exhibits highly oscillatory behavior, slow decay at infinity, and sensitivity to numerical errors.

The aim of this section is to reformulate the inverse Laplace transform for GGCs by deforming the integration contour into a more favorable curve in the complex plane. By exploiting analyticity properties of the Laplace transform, we derive alternative integral representations that reduce oscillations and improve convergence. This change of integration curve provides a foundation for more robust numerical schemes and offers additional insight into the analytic structure of GGC distributions.

Here we prove an inversion relation between the density function f of a GGC and its LT ϕ. Before stating the main result, we prove to lemmas required to prove the theorem.

Lemma 1. *Fix $\epsilon \in (0, \pi/2)$ and assume that $|z| < 1/4$ and $\pi/2 \le \arg(z) \le \pi - \epsilon$. Then there exists a constant $M = M(\epsilon)$ such that for all $t \in (0, 1/2)$ we have*

$$\left| \frac{\ln(z+t)}{\ln(t)} \right| < M. \tag{7.5}$$

Proof. First of all, we note that

$$\ln(z+t) = \ln|z+t| + \mathrm{i}\arg(z+t).$$

Since $|\arg(z+t)| < \pi$ and $|\ln(t)| > \ln(2)$ for $t \in (0, 1/2)$, we conclude that the function

$$t \mapsto |\arg(z+t)/\ln(t)|$$

is bounded from above by $\pi/\ln(2)$ for $t \in (0, 1/2)$, thus

$$\left| \left| \frac{\ln(z+t)}{\ln(t)} \right| - \left| \frac{\ln|z+t|}{\ln(t)} \right| \right| \leq \left| \frac{\arg(z+t)}{\ln(t)} \right| < \frac{\pi}{\ln(2)}$$

for all $t \in (0, 1/2)$. Therefore, to prove (7.5), it is enough to show that

$$\left| \frac{\ln|z+t|}{\ln(t)} \right| < M, \quad t \in (0, 1/2), \tag{7.6}$$

for some constant $M = M(\epsilon)$.

Denote $|z| = r$ (so that $0 < r < 1/4$). Note that we have

$$|z+t| < |z| + t < 3/4.$$

For $0 < t \leq r/2$, we use the estimate

$$|z+t| \geq r - t \geq r/2$$

and obtain

$$\left| \frac{\ln|z+t|}{\ln(t)} \right| \leq \frac{|\ln(r/2)|}{|\ln(t)|} \leq \frac{|\ln(r/2)|}{|\ln(r/2)|} = 1.$$

For $r/2 < t < 2r$, we use the estimate

$$|z+t| \geq |\operatorname{Im}(z+t)| = |\operatorname{Im}(z)| > r\sin(\epsilon),$$

and obtain

$$\left| \frac{\ln|z+t|}{\ln(t)} \right| < \frac{|\ln(r\sin(\epsilon))|}{|\ln(t)|} < \frac{|\ln(r\sin(\epsilon))|}{|\ln(2r)|} \leq \left| \frac{\ln(r)}{\ln(2r)} \right| + \left| \frac{\ln(\sin(\epsilon))}{\ln(2r)} \right| < 2 + \frac{|\ln(\sin(\epsilon))|}{\ln(2)}.$$

For $2r \leq t < 1/2$, we have $|z/t| \leq 1/2$, so that $|1 + z/t| \geq 1 - |z/t| \geq 1/2$. Thus

$$\left| \ln|z+t| \right| \leq |\ln(t)| + \left| \ln|1+z/t| \right| \leq |\ln(t)| + \ln(2),$$

and

$$\left| \frac{\ln|z+t|}{\ln(t)} \right| \leq \frac{|\ln(t)| + \ln(2)}{|\ln(t)|} = 1 + \frac{\ln(2)}{|\ln(t)|} < 2.$$

Thus we have established (7.6) with

$$M = M(\epsilon) = 2 + \frac{|\ln(\sin(\epsilon))|}{\ln(2)}.$$

□

Lemma 2. *Let X be a GGC random variable and $\phi_X(z) = \mathbb{E}[\exp(-zX)]$ its Laplace transform. Fix $\epsilon \in (0, \pi/2)$. Then the function $\phi_X(z)$ is uniformly bounded in the set*

$$\mathcal{S}_\epsilon := \Big\{ |z| < 1/4,\ \pi/2 \le \arg(z) \le \pi - \epsilon \Big\}$$

and satisfies $\phi_X(z) \to 1$ as $z \to 0$ in this set.

Proof. Let $g(z) = -\ln \phi_X(z)$ be the Thorin-Bernstein function

$$g(z) = -az - \int_0^\infty \ln(1 + z/t) U(\mathrm{d}t).$$

Denote

$$C := \max\{ |\ln(1+w)/w| \ :\ |w| = 1/2 \}.$$

Then for $z \in \mathcal{S}_\epsilon$ we have

$$\begin{aligned} |\operatorname{Re} g(z)| \le |g(z)| &\le a/4 + \int_0^{1/2} |\ln(1+z/t)| U(\mathrm{d}t) + \int_{1/2}^\infty |\ln(1+z/t)| U(\mathrm{d}t) \\ &\le a/4 + \int_0^{1/2} |\ln(t)| U(\mathrm{d}t) + \int_0^{1/2} |\ln(z+t)| U(\mathrm{d}t) + \frac{C}{4} \int_{1/2}^\infty t^{-1} U(\mathrm{d}t) \\ &= a/4 + (1+M) \int_0^{1/2} |\ln(t)| U(\mathrm{d}t) + \frac{C}{4} \int_{1/2}^\infty t^{-1} U(\mathrm{d}t). \end{aligned}$$

In deriving this upper bound, we used the fact that $|z/t| < 1/2$ for $z \in \mathcal{S}_\epsilon$ and $t > 1/2$ (thus $|\ln(1+z/t)| \le C|z|/t \le (C/4)/t$), as well as Lemma 1. Given that $\int_0^{1/2} |\ln(t)| U(\mathrm{d}t) < \infty$ and $\int_{1/2}^\infty t^{-1} U(\mathrm{d}t) < \infty$ (true for any GGC random variable – see Definition 6), we conclude that $\operatorname{Re} f(z)$ is bounded in the set S_ϵ. This proves the first part of the statement of Lemma 2. To prove the second part (the fact that $\phi_X(z) \to 1$ as $z \to 0$), we use Lemma 1 and the Dominated Convergence Theorem. □

Now we are ready to prove our main result

Theorem 27. *Let X be a GGC random variable with finite Thorin measure and $\phi_X(z) = \mathbb{E}[\exp(-zX)]$ its Laplace transform. Then, for any $\theta \in [\pi/2, \pi)$, the probability density function $f_X(x)$ can be obtained via*

$$f_X(x) = \frac{1}{\pi} \operatorname{Im} \left[e^{\mathrm{i}\theta} \int_0^\infty \phi_X(e^{\mathrm{i}\theta} y) e^{e^{\mathrm{i}\theta} xy} \mathrm{d}y \right]. \tag{7.7}$$

Proof. First note that by Theorem 7, we can write $\phi(z) = \exp(-g(z))$ for some Thorin-Bernstein function g. Then by Definition 3.1 we obtain

$$\operatorname{Re} g(z) = \int_0^\infty \ln|1 + z/t| U(\mathrm{d}t),$$

where without loss of generality we assumed $a = 0$ in Definition 3.1. Denote by ξ the minimum of $|1 + w|$, where w lies in the sector $\pi/2 < \arg(w) < \theta$. Then for any $c > 0$ and z large enough we have

$$\begin{aligned}\operatorname{Re} g(z) &= \int_0^c \ln|1 + z/t| U(\mathrm{d}t) + \int_c^\infty \ln|1 + z/t| U(\mathrm{d}t) \\ &> \int_0^c \ln|1 + z/c| U(\mathrm{d}t) + \ln \xi U((c, \infty)) = \ln|1 + z/c| U((0, c)) + \ln \xi U((c, \infty)).\end{aligned}$$

Now choose c large enough so that $U((0, c)) > 0$ and set $U((0, c)) = d > 0$. Last inequality yields $\operatorname{Re} g(z) > d \ln|1 + z/c|$, resulting in

$$|\phi_X(z)| = e^{-\operatorname{Re} g(z)} < |1 + z/c|^{-d}. \tag{7.8}$$

By symetry, the same bound holds in the set $\pi/2 \leq -\arg(z) \leq \theta$. Thus we can write the inverse Laplace transform of $f_X(x)$ in the form

$$f_X(x) = \frac{1}{2\pi \mathrm{i}} \int_{\mathrm{i}\mathbb{R}} \phi_X(z) e^{zx} \mathrm{d}z. \tag{7.9}$$

Now, consider the contour $\gamma_{r,R}$, that is the boundary of the set $\pi/2 \leq \arg(z) \leq \theta$ and $r \leq |z| \leq R$ as shown in Figure 7.1.

The function $\phi_X(z)$ is analytic in the upper half-plane $\operatorname{Im}(z) > 0$, thus it is analytic inside $\gamma_{r,R}$ and on $\gamma_{r,R}$, thus we apply Cauchy Theorem and conclude that

$$\int_{\gamma_{r,R}} \phi_X(z) e^{zx} \mathrm{d}z = 0.$$

Then we will have

$$\int_{\gamma_{r,R}} \phi(z) e^{zx} dz = \int_{\gamma_1} \phi(z) e^{zx} dz + \int_{\gamma_2} \phi(z) e^{zx} dz + \int_{\gamma_3} \phi(z) e^{zx} dz + \int_{\gamma_4} \phi(z) e^{zx} dz = 0,$$

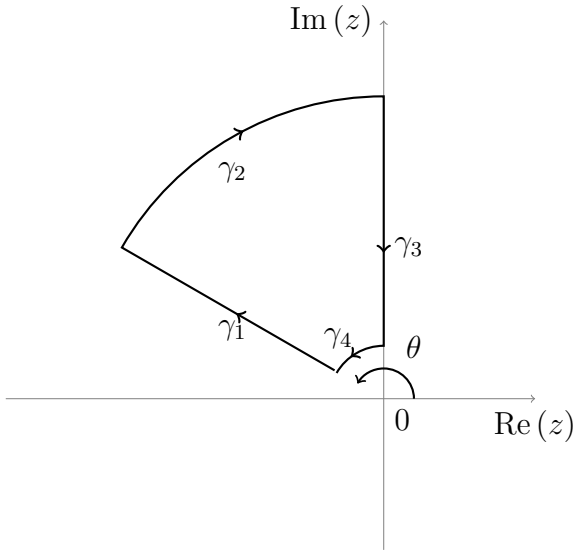


Figure 7.1: The contour $\gamma_{r,R} = \gamma_1 + \gamma_2 + \gamma_3 + \gamma_4$

resulting in

$$\int_{ir}^{iR} \phi(z)e^{zx}dz = \int_{\gamma_1} \phi(z)e^{zx}dz - \int\limits_{\substack{|z|=R,\\ \pi/2<arg(z)<\theta}} \phi(z)e^{zx}dz + \int\limits_{\substack{|z|=r,\\ \pi/2<arg(z)<\theta}} \phi(z)e^{zx}dz. \tag{7.10}$$

Now by Lemma 2, due to $\phi(z)e^{zx}$ being uniformly bounded as $|z| = r \to 0$, we can deduce $\int_{\gamma_4} \phi(z)e^{zx}dz \leq r\pi \max|\phi(z)e^{zx}|/2$. Consequently

$$\lim_{r\to 0^+} \int_{\gamma_4} \phi(z)e^{zx} = \lim_{r\to 0} \int\limits_{\substack{|z|=r,\\ \pi/2<arg(z)<\theta}} \phi(z)e^{zx}dz = 0. \tag{7.11}$$

Set $M_R = \max\limits_{\substack{|z|=R,\\ \pi/2<arg(z)<\theta}} \left|e^{-g(z)}\right|$. By change of variable $z = R\exp(i\beta)$, we can write

$$\Big| \int\limits_{\substack{|z|=R,\\ \pi/2<arg(z)<\theta}} e^{-g(z)+zx}dz \Big| \leq R\,M_R \int_{\pi/2}^{\theta} \left|e^{Rx\,\exp(i\beta)}e^{i\beta}\right|d\beta = R\,M_R \int_{\pi/2}^{\theta} e^{Rx\cos(\beta)}d\beta.$$

Additionally, for $\pi/2 < \beta < \theta$ the inequality $\cos(\beta) < 1 - 2\beta/\pi$ holds. Therefore, we conclude

$$\Big| \int\limits_{\substack{|z|=R,\\ \pi/2<arg(z)<\theta}} e^{-g(z)+zx}dz \Big| \leq R\,M_R \int_{\pi/2}^{\theta} e^{Rx(1-2\beta/\pi)}d\beta = R\,M_R \int_{0}^{\theta-\pi/2} e^{-2Rx\alpha/\pi}d\alpha,$$

where we used a change of variable $\beta = \pi/2 + \alpha$. Moreover,

$$\int_0^{\theta-\pi/2} e^{-2Rx\alpha/\pi} d\alpha < \int_0^{\infty} e^{-2Rx\alpha/\pi} d\alpha = \frac{\pi}{2Rx},$$

substituting in the last inequality yields

$$\Big| \int_{\substack{|z|=R,\\ \pi/2<arg(z)<\theta}} e^{-g(z)+zx} dz \Big| \leq \frac{\pi M_R}{2x},$$

but $M_R = \max_{\substack{|z|=R,\\ \pi/2<arg(z)<\theta}} \left| e^{-\operatorname{Re} g(z)} \right|$ and by (7.8) $\lim_{R\to\infty} M_R \to 0$, yielding

$$\lim_{R\to\infty} \int_{\gamma_2} \phi(z) e^{zx} = 0. \tag{7.12}$$

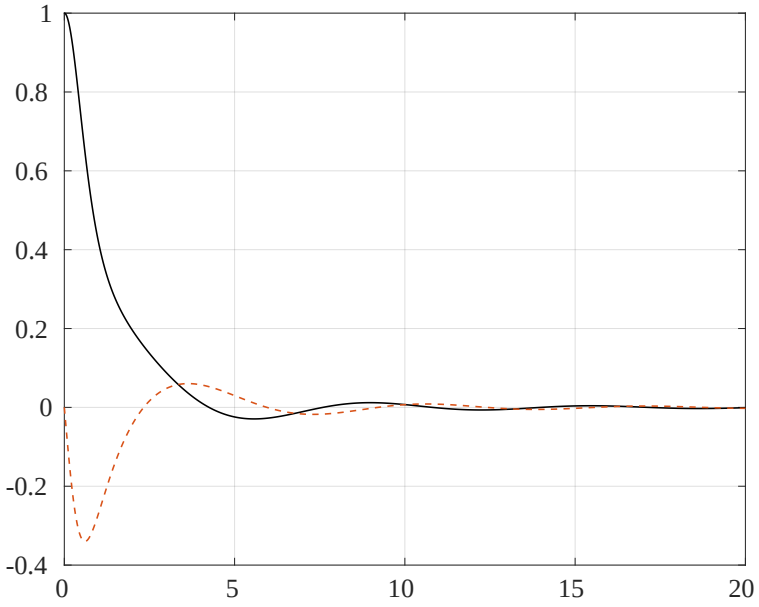
Now we take the limit of (7.10) as $r \to 0^+$ and the limit as $R \to +\infty$. Through (7.11) and (7.12) we obtain the result:

$$\int_0^{\mathrm{i}\infty} \phi_X(z) e^{zx} dz = \int_{\substack{z=r\,e^{i\theta},\\ 0<r<\infty}} \phi(z) e^{zx} dz = e^{\mathrm{i}\theta} \int_0^{\infty} \phi_X(e^{\mathrm{i}\theta} y) e^{e^{\mathrm{i}\theta} xy} \mathrm{d}y.$$

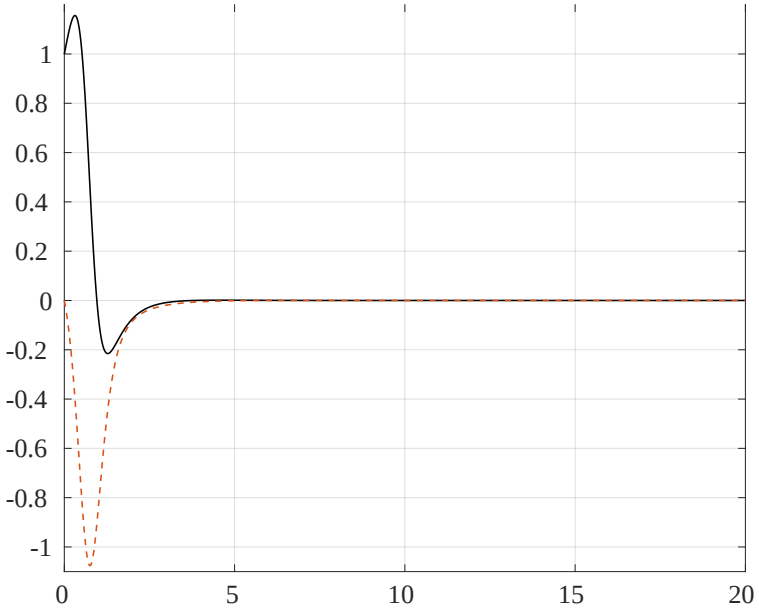
By symmetry, we have a similar result for an integral from $-\infty\mathrm{i}$ to 0. Combining these two results and the fact that $\int_{\substack{z=r\,e^{-i\theta},\\ -\infty<r<0}} \phi(z) e^{zx} dz$ is negative conjugate of $\int_{\substack{z=r\,e^{i\theta},\\ 0<r<\infty}} \phi(z) e^{zx} dz$ gives us (7.7). □

Now we illustrate through an example how Theorem 27 can help. Consider a gamma distribution with shape parameter 2 and rate parameter 1. Then its pdf would be $f(x) = xe^{-x}$ and it satisfies the conditions of Theorem 27. That is, it has total Thorin measure 2 and finite mean of 2. If we proceed with the common inverse relation (7.9), Figure 7.2a shows the rate of convergence of real and imaginary part of $\phi(z)e^{zx}$ to zero for z on the veritcal imaginary axis (with $x = 1$ and $dz = 0.0001$). Alternatively, if we use the relation (7.7), as Figure 7.2b shows, the convergence is quite faster along the lines $e^{i3\pi/4}$ and $e^{-i3\pi/4}$.

To exhibit accuracy improvement as a result of Theorem 27 application, consider the same example above. Here we set $0 < x < 10$ and $y = 10000y_1^3$, where y_1 are equally spaced

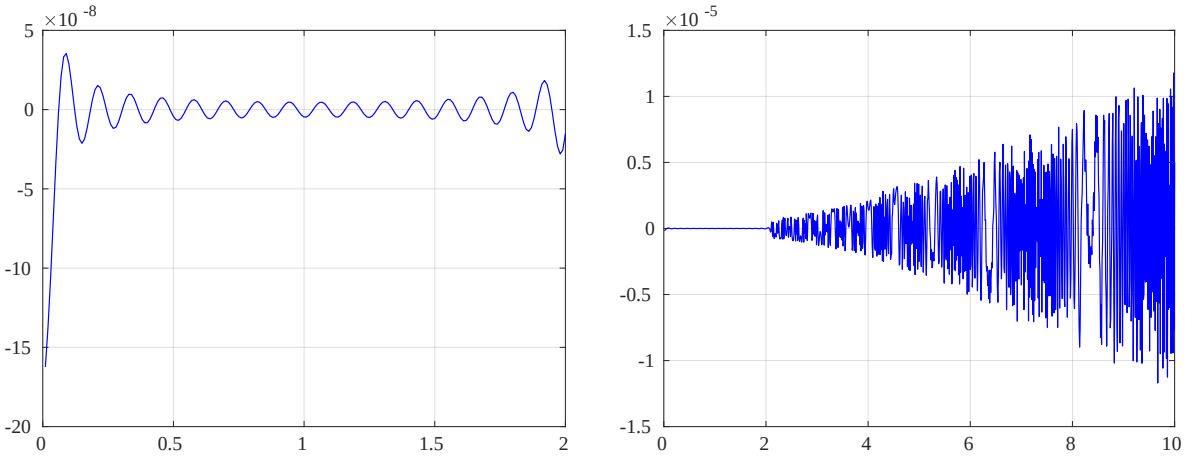


(a) Over the line $z = i\mathbb{R}^+$



(b) Over the line $z = \mathbb{R}\exp(i3\pi/4)$

Figure 7.2: The graphs of real part (black) and imaginary part (red) of integrand $\phi(z)e^{zx}$ for $x = 1$ and different integration formulas, where horizontal axis measures $|z|$.



(a) Over $(0, 2)$ (b) Over $(0, 10)$

Figure 7.3: The error of approximating $f(x)$ by (7.9).

points in $[0, 1]$ with step size 0.0001. The error of approximating f by relation (7.9) on the interval $(0, 2)$ is depicted in Figure 7.3a and over $(0, 10)$ in Figure 7.3b. On the other hand, if we use the relation (7.7) with $\theta = 2\pi/3$, the error as shown in Figure 7.4 is conspicuously smaller than that of Figure 7.3.

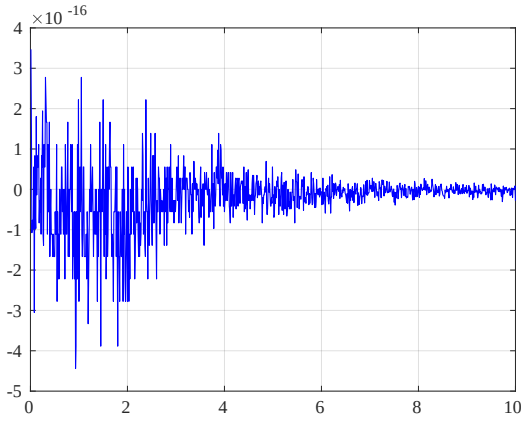


Figure 7.4: The error of approximating $f(x)$ by (7.7) with $\theta = 2\pi/3$ over $(0, 10)$.

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