Computing Special Functions via Inverse Laplace Transforms

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Outline

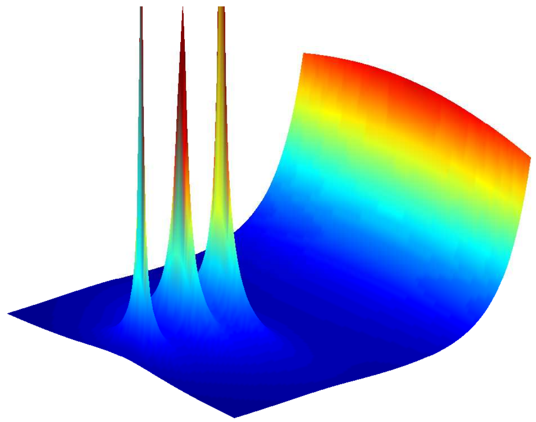
Part 1. Numerical inversion of the Laplace Transform

- Talbot's method on new contours
- Rational approximation to the exponential

$$f(t) = \frac{1}{2\pi i}\int_\Gamma e^{tz}F(z)\,dz$$

Part 2. Application to the Computation of Special Functions

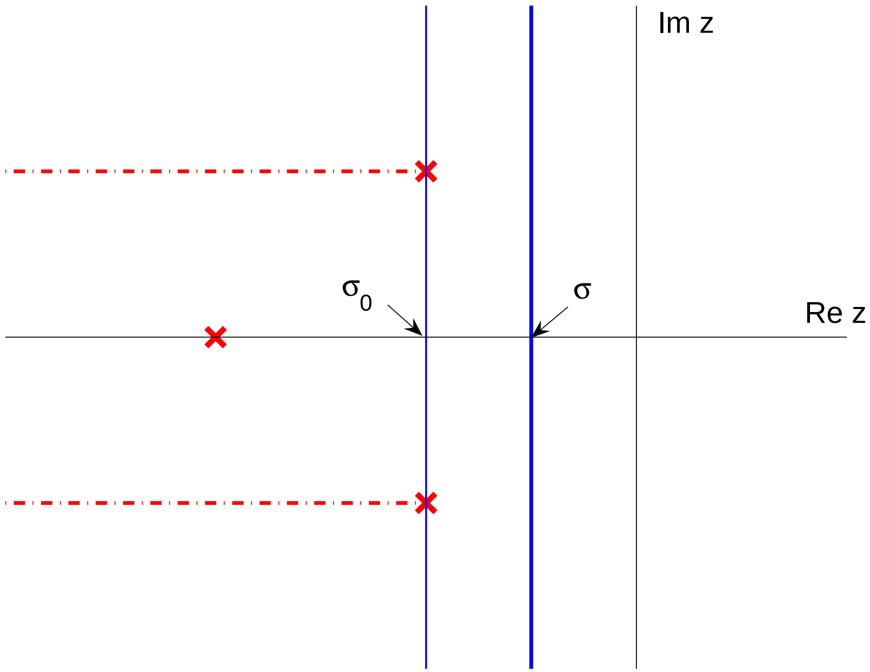
- The exponential function
- The Mittag-Leffler functions
- The gamma function
- The exponential integral
- Application to PDEs



Part 1. Inversion of the Laplace Transform

Laplace Transform and Inverse Formula (Bromwich)

$$F(z) = \int_0^\infty e^{-zt} f(t)\, dt, \quad f(t) = \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} e^{tz} F(z)\, dz, \quad \sigma > \sigma_0$$



Bromwich Integral:

$$f(t) = \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} e^{tz} F(z)\, dz, \quad \sigma > \sigma_0$$

Efficient quadrature rules for this integral? Will consider

- Talbot's method (= trapezoidal rule on deformed contour)
- Rational approximation to $\exp(z)$

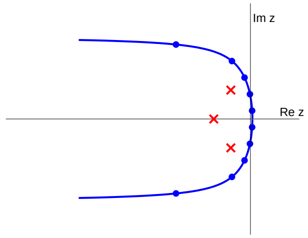
Several details are in fact NEW!

For example,

- In Talbot's method, new contours and improved parameters, and
- In the rational approximant method, the use of best approximation rather than Padé.

Method 1: Talbot [1979]

Deform Bromwich line to:



$$z(\theta) = \sigma + \mu\Big(\theta \cot\theta + \nu\, i\, \theta\Big), \quad -\pi \leq \theta \leq \pi$$

This converts Bromwich integral into:

$$f(t) = \frac{1}{2\pi i} \int_{-\pi}^{\pi} e^{z(\theta)t} F\big(z(\theta)\big) z'(\theta)\, d\theta.$$

Discretize by trapezoidal/midpoint rule, on uniform grid of $[-\pi, \pi]$

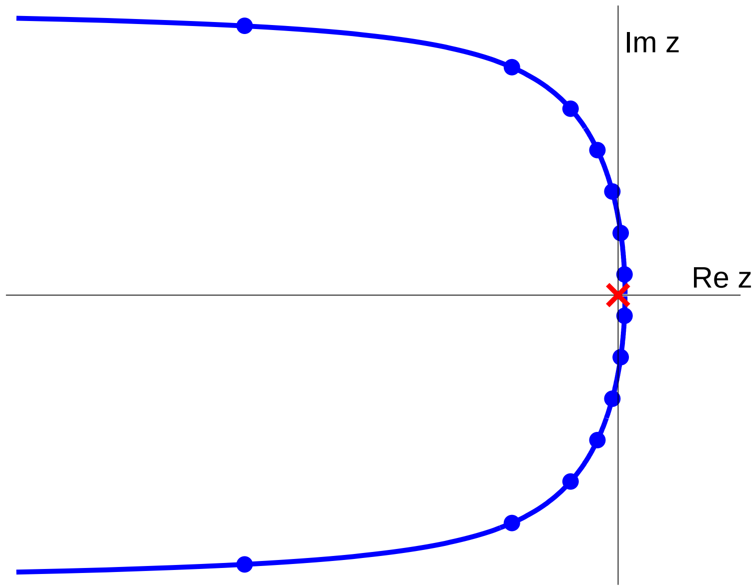
$$f(t) \approx \frac{h}{2\pi i} \sum_{k=1}^{N} e^{z(\theta_k)t} F\big(z(\theta_k)\big) z'(\theta_k).$$

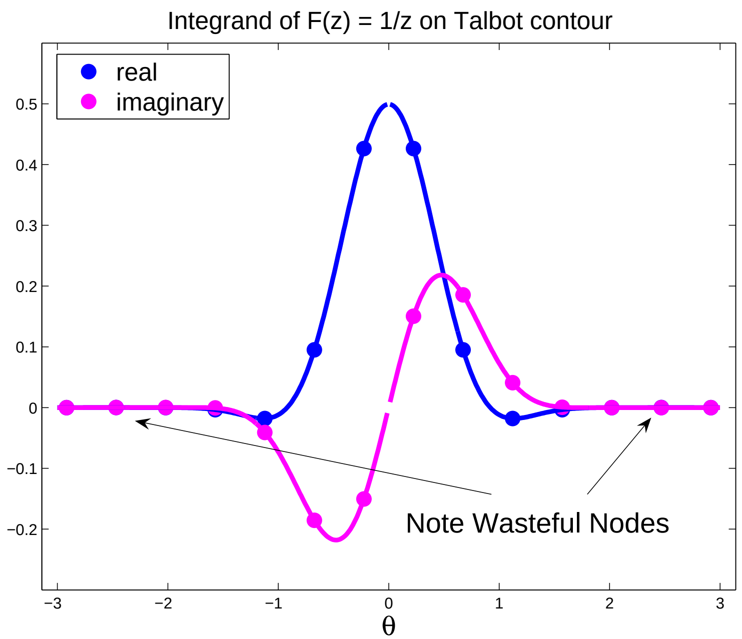
Reason for success? Use partial fraction expansion

$$\theta \cot\theta = 1 + 2\theta^2\Big(\frac{1}{\theta^2-\pi^2} + \frac{1}{\theta^2-4\pi^2} + \dots\Big)$$

to deduce that integrand decays rapidly on Talbot contour:

$$\exp\big(z(\theta)t\big) = O\Big(\exp\Big(\frac{2\mu t\theta^2}{\theta^2-\pi^2}\Big)\Big), \qquad |\theta| \to \pi^-.$$





To eliminate wasteful nodes, we propose a

Modified Talbot Method Trefethen & JACW [2005]

$$z(\theta) = \sigma + \mu\Big(\theta \cot \alpha\theta + \nu\, i\, \theta\Big), \quad -\pi \leq \theta \leq \pi$$

with

$$0 < \alpha < 1.$$

Optimal parameters σ, μ, ν, α for the two Talbot contours?

Analyze with the help of model problem

$$F(z) = \frac{1}{z-\lambda} \quad \Longleftrightarrow \quad f(t) = e^{\lambda t}, \quad \lambda < 0$$

(Motivation $\lambda \rightsquigarrow A \in \mathbb{R}^{n\times n}$,

$$F(z) = (zI - A)^{-1}, \qquad f(t) = \exp(At)$$)

By balancing various error terms, the following formulas for optimal contours have been derived JACW [2005]

Original Talbot method:

$$z = \frac{N}{t}\Big(0.3221\,\theta\cot(\theta) - 0.2407 + 0.2827\,i\,\theta\Big)$$

Modified Talbot method:

$$z = \frac{N}{t}\Big(0.5017\,\theta\cot(0.6407\,\theta) - 0.6122 + 0.2645\,i\,\theta\Big)$$

For the model problem

$$F(z) = (z-\lambda)^{-1},\ f(t) = e^{\lambda t},$$

these parameter choices achieve convergence rates

$$\text{Abs. Error.} = O\Big(2.6^{-N}\Big), \qquad \text{Abs. Error.} = O\Big(3.9^{-N}\Big),$$

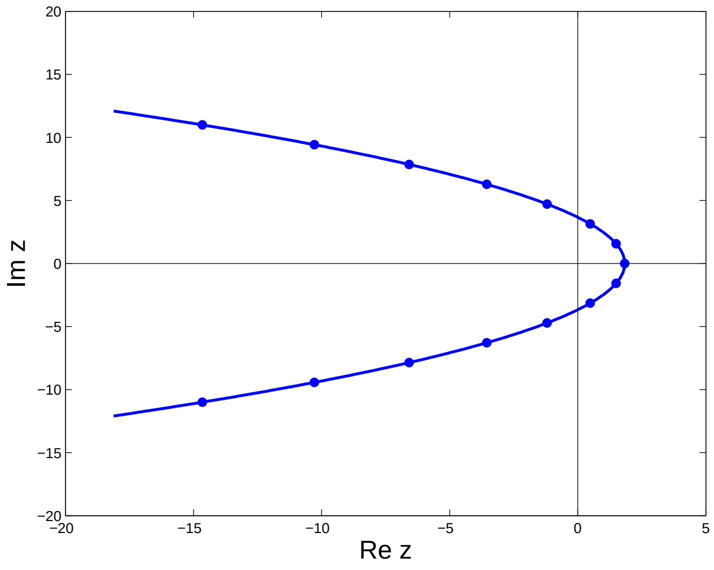
respectively, for the original and modified Talbot contours.

Two recently proposed alternatives to Talbot's contour:

Parabolic

Gavrilyuk/Makarov [2000]

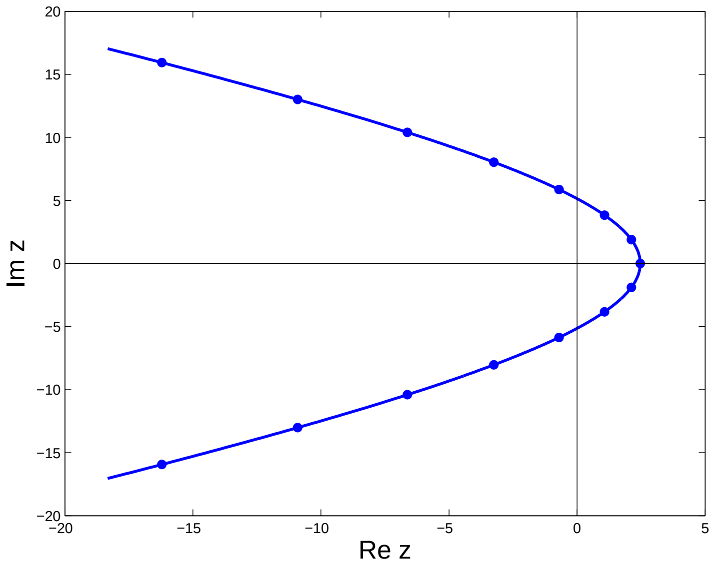
$$z = \mu\left(iw + 1\right)^2$$
$$-\infty < w < \infty$$



Hyperbolic

López-Fernández/Palencia [2004]

$$z = \mu\left(1 + \sin\left(iw - \alpha\right)\right)$$
$$-\infty < w < \infty$$



With optimal parameter choices, the convergence rates are

Parabolic

Abs. Error $= O(2.8^{-N})$

Hyperbolic

Abs. Error $= O(3.2^{-N})$

Summary

Contour	Orig Talbot	Parabola	Hyperbola	Mod Talbot
Conv Rate	$O(2.6^{-N})$	$O(2.8^{-N})$	$O(3.2^{-N})$	$O(3.9^{-N})$

(Applies to model problem

$$F(z) = \frac{1}{z-\lambda} \quad \Longleftrightarrow \quad f(t) = e^{\lambda t}, \quad \lambda < 0 \ )$$

Estimation of Optimal Parameters?

Consider simpler problem: integrals on $\mathbb{R}$

$$I(f) = \int_{-\infty}^{\infty} f(x)\,dx.$$

Approximate by trapezoidal sum, with spacing h

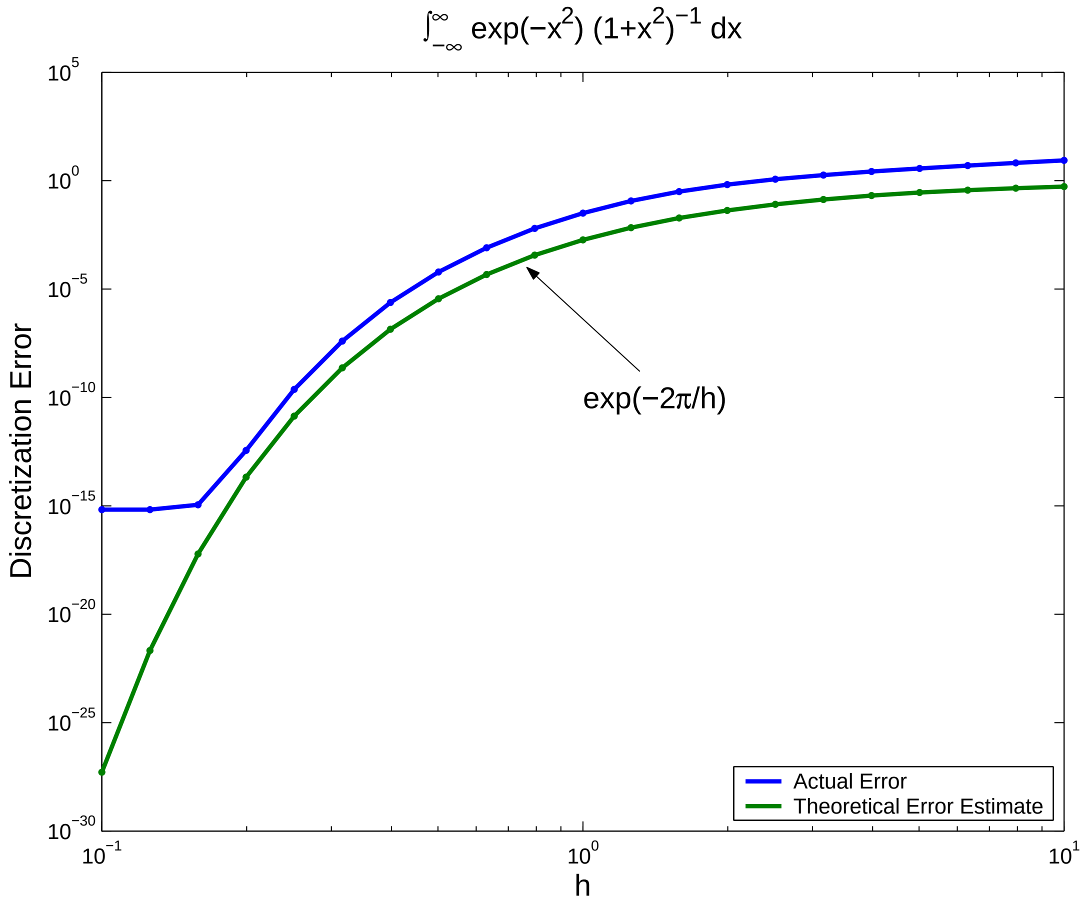
$$I_h(f) = h \sum_{k=-\infty}^{\infty} f(kh).$$

Discretization error,

$$DE_h(f) = I(f) - I_h(f),$$

often unexpectedly small:

Example: $$\int_{-\infty}^{\infty} \frac{e^{-x^2}}{1+x^2}\,dx = \pi e(1 - \operatorname{erf} 1)$$



Error Estimate Based on Contour Integrals [Martensen, 1968]

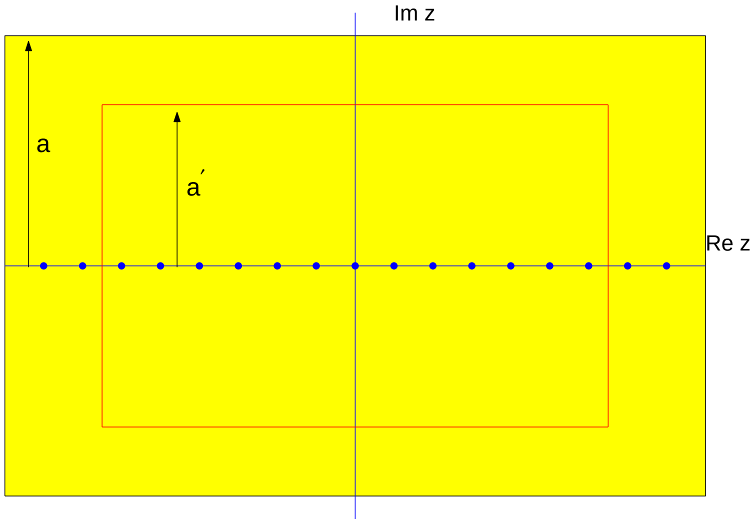
$$\frac{1}{2\pi i}\int_{\square_N} f(z)\cot\frac{\pi z}{h}\,dz = \frac{h}{\pi}\sum_{k=-N}^{N} f(kh)$$

$\Longrightarrow$

$$DE_h(f) = \mathrm{Re}\int_{-\infty+ia'}^{\infty+ia'} f(z)\left(1 - i\cot\frac{\pi z}{h}\right)dz$$

$\Longrightarrow$

$$|DE_h(f)| \le \left(\coth\frac{\pi a'}{h} - 1\right)\int_{-\infty+ia'}^{\infty+ia'} |f(z)|\,dz$$



Often

$$|DE_h(f)| = O(e^{-2\pi a/h})$$

A question-and-answer session:

Q: What if $f(z)$ is entire?

A: Growth-rate of $f(z)$ as $z \to \pm i\infty$ comes into play.

Q: What if $f(x)$ is not real-valued?

A: Will have two error terms, one for upper half-plane, one for lower. Need to estimate separately. ($\Longrightarrow$ Discretization Error, Two Parts)

Q: How does one compute infinite trapezoidal sum?

A: Rapidly decaying terms, truncate ($\Longrightarrow$ Truncation Error)
(Slowly decaying terms, apply series acceleration.)

Apply the above ideas to the Bromwich integral:

Match two parts of discretization error to truncation error.
This gives two equations.

If contour contains only two parameters, solve.

If contour contains three parameters, solve for two of these.
Thus obtain error estimate involving only one free parameter.
Minimize error estimate with univariate routine.

Summary (reprise)

Contour	Orig Talbot	Parabola	Hyperbola	Mod Talbot
Conv Rate	$O(2.6^{-N})$	$O(2.8^{-N})$	$O(3.2^{-N})$	$O(3.9^{-N})$

Method 2: Rational Approximation to the Exponential

Vlach [1969], Luke [1972]

Recall the Bromwich integral

$$f(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{tz} F(z)\, dz.$$

Make the change of variables $s = zt$, i.e.,

$$f(t) = \frac{1}{2\pi t i} \int_{\Gamma'} e^{s} G(s)\, ds, \qquad G(s) = F(s/t).$$

Approximate e^s by a type $(N-1, N)$ rational function

$$r(s) = \sum_{k=1}^{N} \frac{c_k}{s - s_k}$$

and substitute into Bromwich integral. This yields

$$f(t) \approx \sum_{k=1}^{N} w_k G(s_k), \qquad w_k = c_k e^{s_k} t^{-1}$$

Note: This quadrature formula is closely related to Talbot quadrature

$$f(t) \approx \frac{h}{2\pi i} \sum_{k=1}^{N} e^{z(\theta_k)t} F\big(z(\theta_k)\big) z'(\theta_k)$$

Put

$$s = zt, \qquad s_k = z(\theta_k)t, \qquad c_k = z'(\theta_k)N^{-1};$$

then the two formulas are seen to be identical.

Conclusion: The Talbot method may be seen as a rational approximation method, with the nodes of the trapezoidal rule featuring as the poles in the rational approximation. Details in

Trefethen, Weideman, Schmelzer, “Talbot Quadratures and Rational Approximation”,

Tech. Rep. 05/20, Oxford University Computing Laboratory, 2005.

How to choose $r(s)$?

Padé approximation Vlach [1969], Luke [1972]

- Highly accurate, but only in small regions
- Coefficients c_k grow rapidly as $N \to \infty$ $\Longrightarrow$ ill-conditioned

Alternative choice of $r(s)$ (Trefethen, JACW, Schmelzer [2005])

Best approximation to e^s on $\mathbb{R}^-$ (Famous $1/9$ problem)

- Cody, Meinardus, Varga [1969]

Chebyshev rational approximations to e^{-z}, application to parabolic PDE

- Carpenter, Ruttan, Varga [1984]

Computation of (N, N) coefficients by Remes algorithm

- Magnus [1994], Aptekarev [2002] Sup-norm error estimate on $\mathbb{R}^-$

$$\|e^s - r^*(s)\| = \inf_r \|e^s - r(s)\| \sim 2(9.289\ldots)^{-(N+1/2)}, \quad N \to \infty$$

Technicality: Literature considers only (N, N), we need $(N-1, N)$

Define

$$r(s) = r^*(s) - r^*(\infty)$$

(Not quite optimal, but close for $N \gg 1$)

Compute $r^*(s)$ by

- Remes algorithm (expensive and cumbersome)
- Carathéodory-Fejér method (only approximate, but practical)

Will refer to this as the CMV-CF method

(Cody, Meinardus, Varga, Carathéodory, Fejér)

Summary

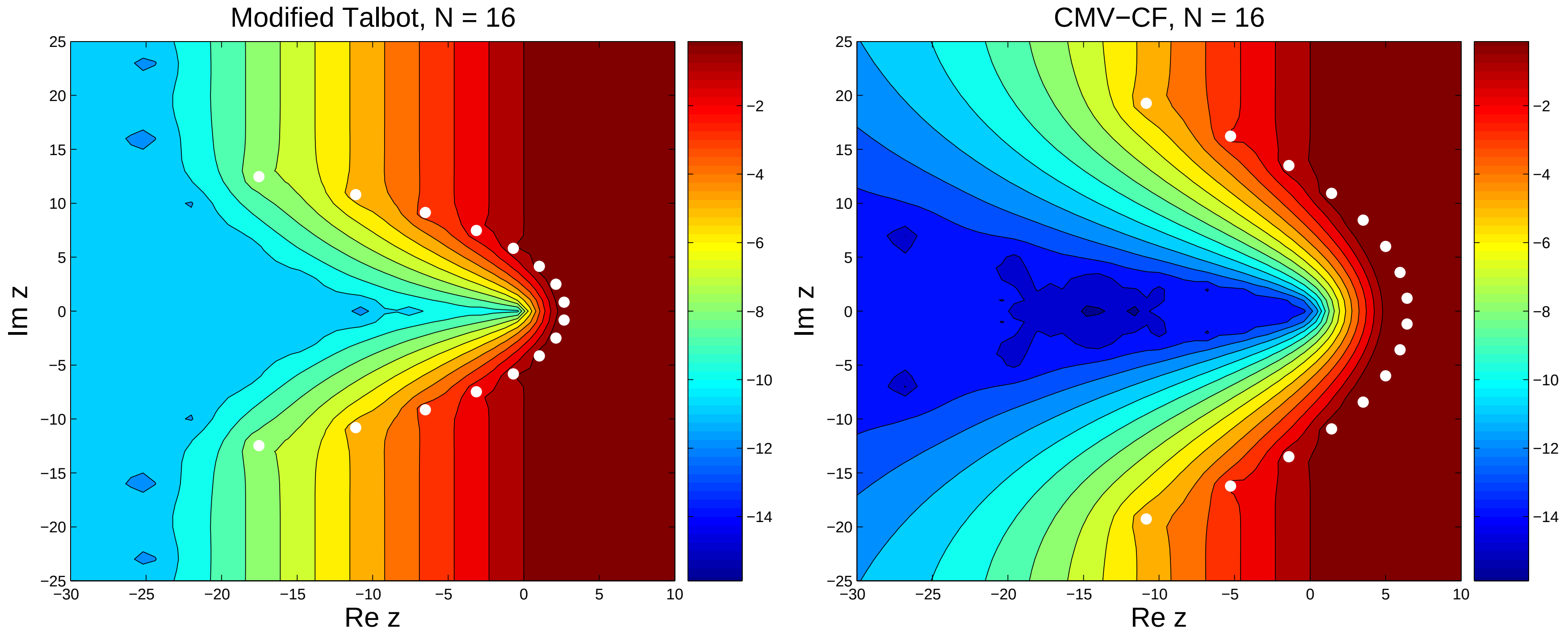
Contour	Mod Talbot	CMV-CF
Conv Rate	$O(3.9^{-N})$	$O(9.3^{-N})$

Numerical results were computed in MATLAB:
To achieve machine precision

$$2(9.289\ldots)^{-(N+1/2)} \sim 2^{-52} \qquad \Longrightarrow \qquad N \sim 16$$

Part 2. Computation of Special Functions

Exponential function: e^z



Application to Matrix Exponential: Recall scalar model problem

$$e^{\lambda t} = \frac{1}{2\pi i}\int_{\Gamma} e^{zt}\, F(z)\, dz, \qquad F(z) = \frac{1}{z-\lambda}, \qquad \lambda < 0$$

Formulas also valid when $\lambda \rightsquigarrow A \in \mathbb{R}^{n\times n}$, A s.p.d.

$$e^{At}\boldsymbol{v} = \frac{1}{2\pi i}\int_{\Gamma} e^{zt}\, \mathbf{F}(z)\, dz, \qquad \Big(z\,I - A\Big)\mathbf{F}(z) = \boldsymbol{v}$$

Note: Each function evaluation in quadrature rule

$\Longrightarrow$ one linear system solve

Linear systems can be solved efficiently:

- A single Hessenberg or Schur decomposition of A is required
- Can also be solved in parallel

Example: Heat equation in 2D

$$u_t = c\nabla^2 u, \quad (x, y) \in [-1, 1]^2$$

Dirichlet BCs $u = 0$ on boundary, and initial condition

$$u(x, y, 0) = e^x(1 - x^2)(1 - y^2)$$

Problem: To compute solution at $t = 1$, say.

Numerical procedure: Approximate Laplacian by discrete operator (e.g., 5-point finite difference stencil). This gives semi-discrete system

$$\mathbf{u}_t = D\,\mathbf{u}, \qquad \mathbf{u}(0) = \mathbf{u}_0.$$

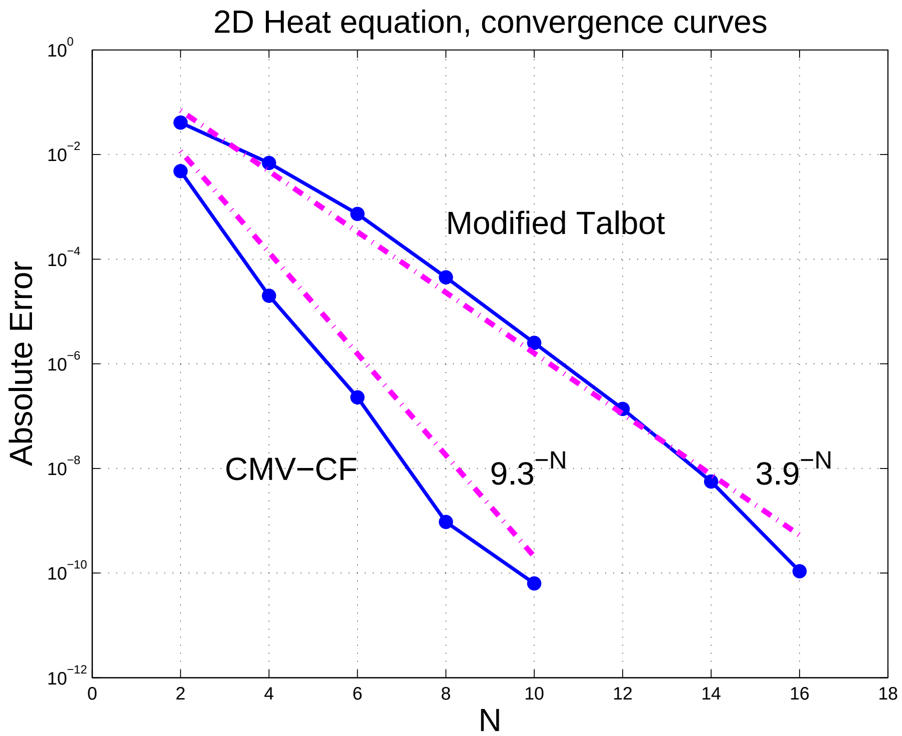
with solution

$$\mathbf{u}(t) = e^{Dt}\,\mathbf{u}_0.$$

Approximate as above by inverting Laplace Transform

$$e^{Dt}\,\mathbf{u}_0 = \frac{1}{2\pi i}\int_\Gamma e^{zt}\,\mathbf{F}(z)\,dz, \qquad \Big(zI - D\Big)\mathbf{F}(z) = \mathbf{u}_0$$

Errors at $(x,y,t) = (0, 0, 1)$ (with $c = 0.02$)



Conclusion:
To reach 10 digit accuracy elliptic problem (linear system) needs to be solved 5 times in case of CMV-CF method, and 8 times for Mod Talbot.

Comparisons with `expm` (built-in MATLAB routine for matrix exponentials, based on Padé approximation and scaling)

Mesh size $\Delta x = 2/M$, $\Delta y = 2/M$, matrix is of order $(M-1)^2 \times (M-1)^2$

Use $N = 16$ quadrature points:

M	CMV-CF	`expm`
20	0.10	0.36
40	0.33	20
60	0.73	780

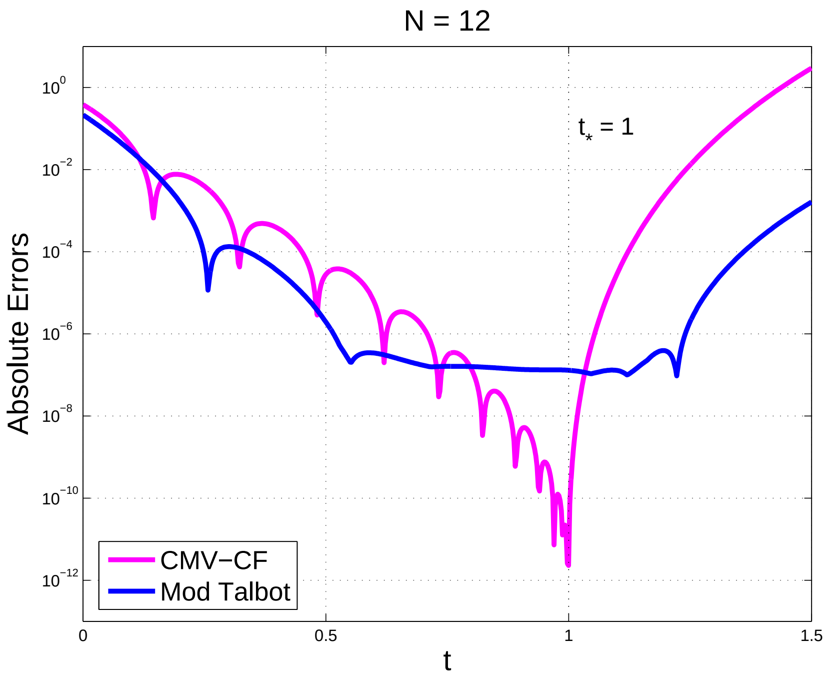
CPU time (in s) computed in MATLAB 7 on Pentium 4 (3.4 GHz)

Have also found that methods based on Talbot contours are numerically more stable than `expm`

An advantage of Talbot over CMV: Sols required at many values of t

New value of $t \implies$ new quadrature points $\implies$ new system solves

Can avoid additional system solves by fixing parameters at, say, $t = t_*$ and solve linear systems once. Then use solution vectors with t dependent coefficients to compute quadrature sum at nearby values of t.



The Mittag-Leffler Functions:

Recall scalar model problem:

$$\exp(\lambda t) = \frac{1}{2\pi i}\int_\Gamma e^{zt}\, F(z)\, dz, \qquad F(z) = \frac{1}{z-\lambda}$$

Generalize to:

$$E_\alpha(\lambda t^\alpha) = \frac{1}{2\pi i}\int_\Gamma e^{zt}\, F(z)\, dz, \qquad F(z) = \frac{1}{z - z^{1-\alpha}\lambda}$$

Series:

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)}$$

Special cases:

$$E_0(z) = \frac{1}{1-z}, \qquad E_{1/2}(z) = e^{z^2}\mathrm{erfc}(-z), \qquad E_1(z) = e^z$$

Application to (time)-fractional PDEs (sub-diffusion)

$$D_t^\alpha u = c\nabla^2 u$$

D_t^α is Caputo's fractional derivative

$$D_t^\alpha f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{f'(s)}{(t-s)^\alpha}\, ds, \qquad (0 < \alpha < 1).$$

As $\alpha \to 1$, fractional derivative $\rightsquigarrow$ ordinary derivative.

Semi-discretize $c\nabla^2 \rightsquigarrow D$, and take the Laplace Transform. Then

$$\mathbf{u}(t) = \frac{1}{2\pi i} \int_\Gamma e^{zt}\, \mathbf{F}(z)\, dz, \qquad \Big(z\, I - z^{1-\alpha} D\Big) \mathbf{F}(z) = \mathbf{u}_0$$

Numerical experiment: Fractional 1D heat equation, with $\alpha = 1/2$

$$D_t^{1/2} u = u_{xx}, \qquad 0 \leq x \leq \pi,$$

subject to

$$u(x, 0) = \sin x, \qquad u(0, t) = 0, \quad u(\pi, t) = 0.$$

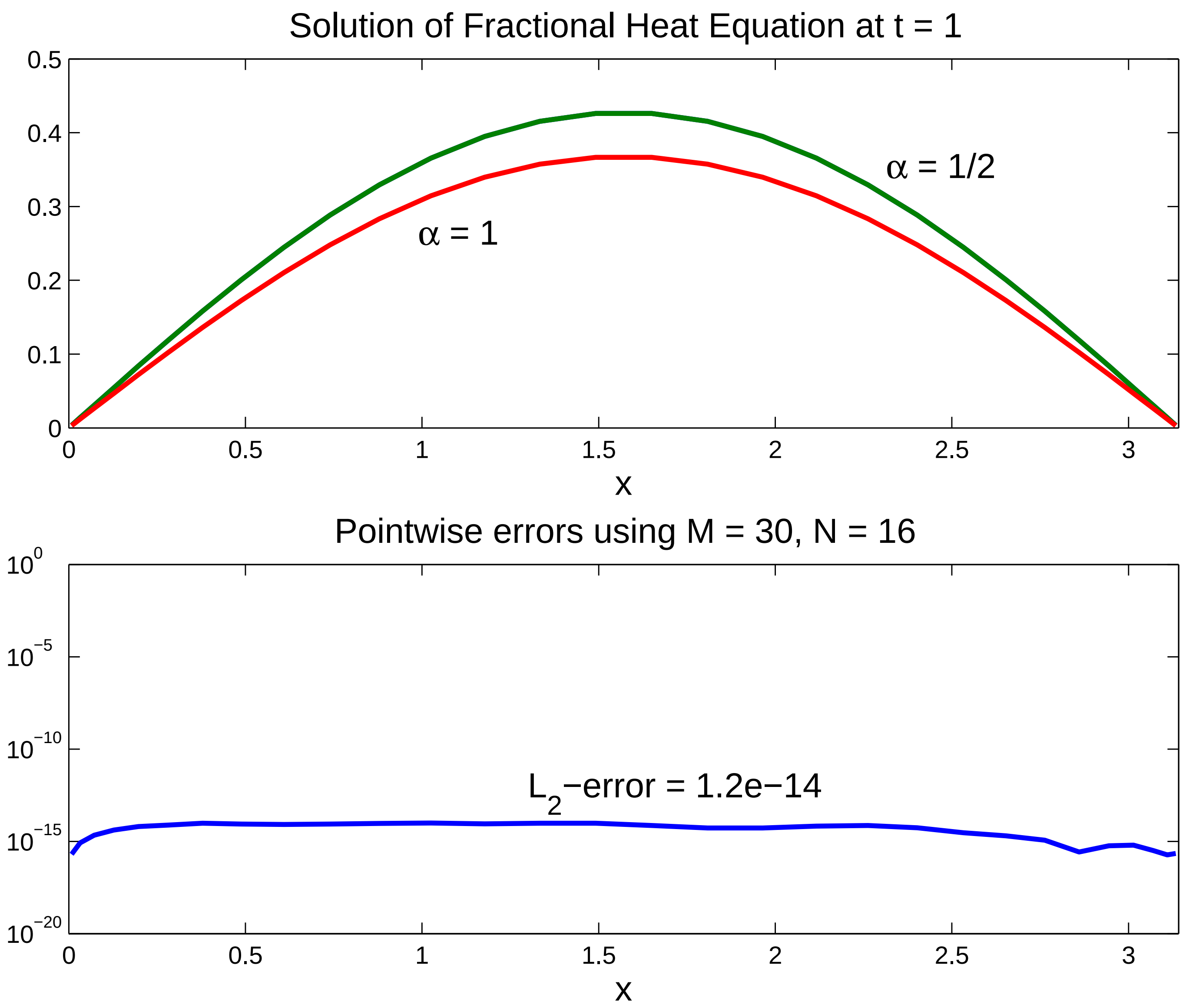
Analytical solution

$$u(x, t) = e^t \mathrm{erfc}(\sqrt{t}) \sin x.$$

Qualitative properties similar to

$$u(x, t) = e^{-t} \sin x$$

but steady state approached at slower rate.

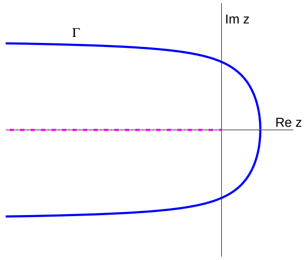


Solution of Fractional Heat Equation at t = 1
α = 1/2
α = 1
x
Pointwise errors using M = 30, N = 16
L2−error = 1.2e−14
x

Gamma Function (Schmelzer & Trefethen, [2005])

Hankel's contour integral for reciprocal of Gamma function

$$\frac{1}{\Gamma(\zeta)} = \frac{1}{2\pi i}\int_\Gamma e^z\, z^{-\zeta}\, dz$$



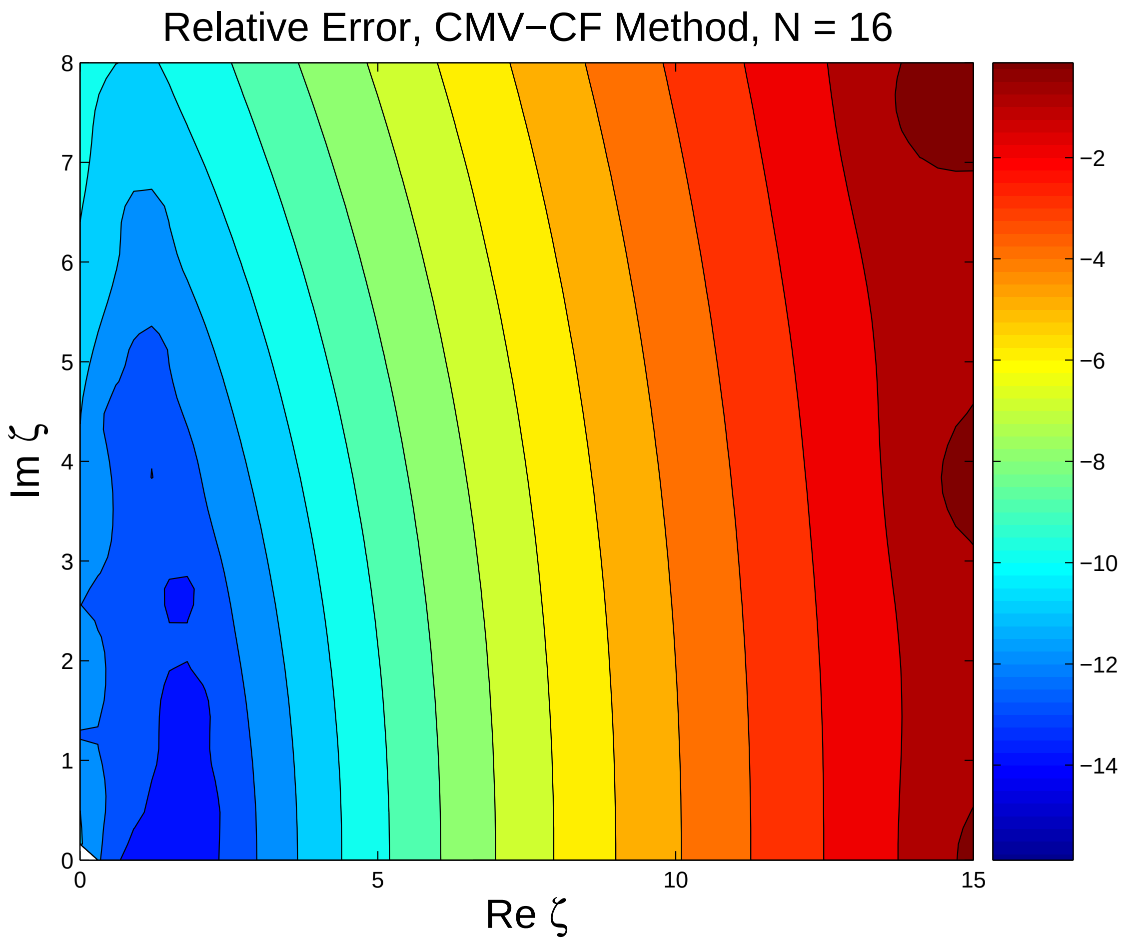
(Actually, well-known formula from tables of Laplace transforms

$$\frac{t^{\zeta-1}}{\Gamma(\zeta)} = \frac{1}{2\pi i}\int_\Gamma e^{zt}\, z^{-\zeta}\, dz, \qquad \text{Re}\,\zeta > 0$$

Let $t = 1$.)

Approximate Hankel's formula with Talbot/CMV quadrature

$$\frac{1}{\Gamma(\zeta)} \approx \sum_{k=1}^{N} w_k\, z_k^{-\zeta}$$


Relative Error, CMV−CF Method, N = 16
Im ζ
Re ζ
0
1
2
3
4
5
6
7
8
0
5
10
15
−2
−4
−6
−8
−10
−12
−14

Exponential Integral:

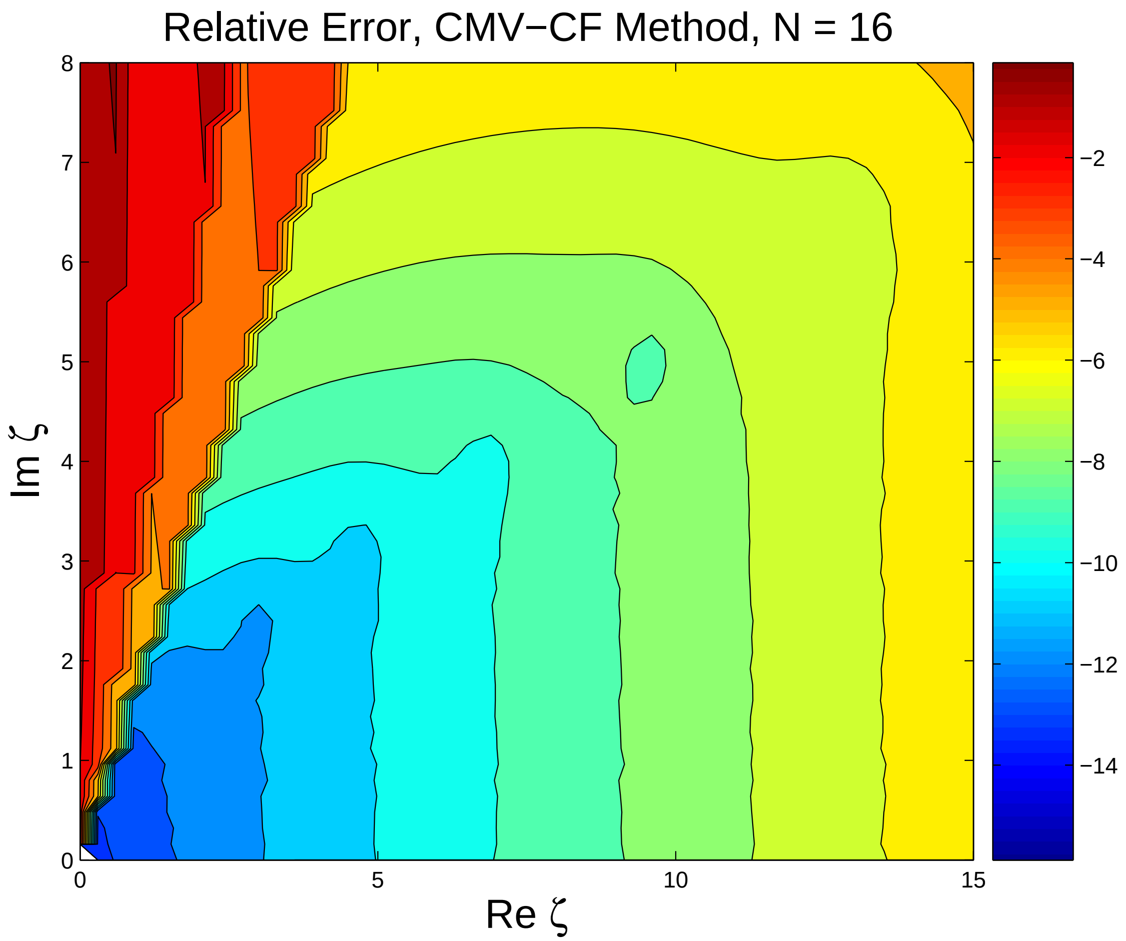
$$E_1(\zeta) = \int_\zeta^\infty \frac{e^{-t}}{t}\, dt, \qquad |\text{arg } \zeta| < \pi$$

From tables of Laplace Transforms:

$$E_1(\zeta t) = \frac{1}{2\pi i}\int_\Gamma e^{zt} \frac{\log(1 + z/\zeta)}{z}\, dz, \qquad \text{Re } z > \begin{cases} 0 \\ -\text{Re } \zeta \end{cases}$$

Put $t = 1$ and approximate by Talbot and/or CMV quadrature:

$$E_1(\zeta) \approx \sum_{k=1}^{N} w_k \frac{\log(1 + z_k/\zeta)}{z_k}$$



Relative Error, CMV−CF Method, N = 16
Im ζ
Re ζ
0
1
2
3
4
5
6
7
8
0
5
10
15
−2
−4
−6
−8
−10
−12
−14

Conclusions

Two new methods for ILTs were introduced, both work well:

- Method based on best approximation to e^z on $\mathbb{R}^-$ is more accurate, but
- Modified Talbot method more flexible and easier to implement

As tools for the computation of special functions:

- These methods seem to be competitive for functions of matrix argument (matrix exponential, Mittag-Leffler), but
- For functions of scalar argument (gamma, exponential integral) further investigation and fine tuning are required