Fitting models for Numerical Inversion of the Laplace Transform

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Overview

- Introduction to Numerical Inversion of the Laplace Transform (ILT)
- Inverting Laplace Transform in a discrete data framework
- Some Inversion scheme (Pike and Gaver methods)
- Numerical Experiments
- Conclusions

The Laplace Transform (LT) and its inversion

- The Laplace Transform F of a function f, is a complex function obtained by the integral map:

$$F(s) = \int_0^{\infty} e^{-st} f(t) dt, \quad Re(s) > \sigma_0 \quad , \tag{1}$$

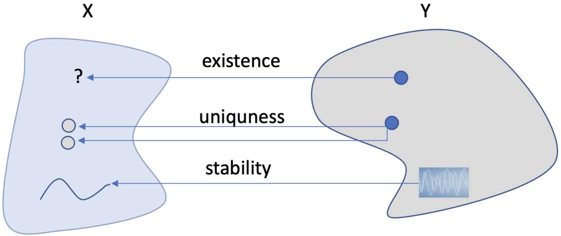
where σ_0 is the abscissa of convergence of Laplace Transform, a value that guarantees existence of F, and s is a complex variable.

- We focus on the real numerical inversion of the Laplace Transform, i.e. on the design and the implementation of a numerical method which computes $f(t)$, under the hypothesis that F is known on the real axis only.

Well-posed problems (Hadamard)

A problem is well-posed if the following three properties hold.

- Existence: For all suitable data, a solution exists.
- Uniqueness:For all suitable data, the solution is unique.
- Stability:The solution depends continuously on the data.



A problem that violates any of the three properties of well-posedness is called an ill-posed problem.

Real inversion of LT

The *real* numerical inversion of the Laplace Transform

$$f = \mathcal{L}^{-1}[F] \qquad s.t. \qquad F(s) = \int_0^{+\infty} e^{-st} f(t)dt = \mathcal{L}[f]$$

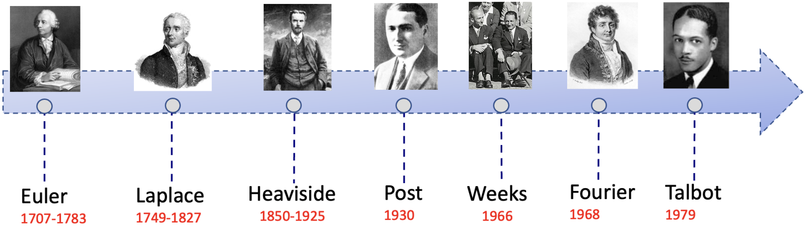
is an *inverse ill-posed problem* (according to Hadamard definition), since $\mathcal{L}^{-1}$ it insn't a continuous functional operator.

Numerical inversion methods require *regularization techniques* to deal with the *strong ill-conditioning.*

Numerical algorithms and related software elements exist, based on:

1. **sensitivity analysis** for the conditioning evaluation of inversion formulas;
2. **stopping rules** for automatic algorithms;
3. **theoretical and computable estimates** of approximation errors on the $f(t)$ computation.

The development of accurate numerical inversion LT is a long standing problem.



- Based on asymptotic expansion (Laplace's method) of the forward integral.

  Post (1930),Gaver (1966), Valko-Abate (2004),Weeks Methods (1966)

- Laguerre polynomial expansion method.

  Ward (1954), Weeks (1966), Weideman (1999), Talbot's Method (1979)

- Deformed contour methods:

  Talbot (1979), Weideman Trefethen (2007)

Numerical Inversion of LT: the main issue

Numerical Methods for the inversion of the Laplace Transform require the evaluation of the LT in some (prefixed) points.

In many the applications nothing is known about the LT function and /or *only* a finite data set of LT-values is generally available.

Example (Approximations of series expansions)

$$f(t) = sin^5(t)cos^5(t); \quad F(s) = \sum_{n=0}^{\infty} \frac{(-1)^n}{512} \left(\frac{5}{2^{2n}} - \frac{5}{6^{2n+1}} + \frac{1}{10^{2n+1}} \right) s^{2n}$$

Approximation on F introduces: truncation and/or discretization errors.

Example (Integration)

- $f(t+T) = f(t), \qquad F(s) = \frac{1}{1-e^{Ts}} \int_0^T f(t)e^{-px}dx$
- $g(t) = \frac{1}{t} f(t) \qquad G(s) = \int_s^{\infty} F(x)dx$

Quadrature rules give *only* a tabulated form for the LT.

Inverting Laplace Transform in a discrete data framework

Definition (Discrete Data Problem)

Let be (t_i, F_i), $i = 1, \ldots, N$, a finite set of LT data, with *F unknown*, except a finite number of its values.

The Laplace Transform inversion procedure consists in:

1. *to represent the data by a functional form*: a **continuous fitting model**, s, **"performing" the LT properties**,
2. *to apply a LTI numerical method* to the continuous model.

The *approximation error on the computed inverse*, $f_s(t)$, depends on:

1. the **fitting error**, agreeable with the *conditioning* of the inversion formula;
2. the **conditioning and stability of the inversion formula**.

A RBF-based fitting model

Here we start from a scattered data interpolation problem: given the data F_i at location $\underline{x}_i \in \mathbb{R}^d$, $i = 1, 2, \ldots, n$, find a continuous function $s(\underline{x})$ (interpolant) satisfying $s(\underline{x}_i) = F_i$, $i = 1, \ldots, n$.

Definition (PHS+poly)

PHS interpolant augmented with polynomials
is the sum of a RBF interpolant, particularly a polyharmonic spline (PHS), and a polynomial term

$$s(x) = \sum_{j=1}^{n} \lambda_j \, |x - x_j|^m + \sum_{k=1}^{s} \beta_k \, p_k(x), \qquad (*)$$

with the matching conditions $\sum_{j=1}^{n} \lambda_j p_k(x_j) = 0, \quad k = 1, \ldots, s,.$
$\{p_k(\underline{x})\}_{k=1}^{s}$ is a basis for the multivariate polynomial space Π_l^d of total degree l in d dimensions with $s = \binom{l+d}{l}$.

PHS are *conditionally positive definite* RBFs; the **combination with polynomials guarantees a well-posed interpolation problem**, no matter how the nodes are scattered.

Theoretical remarks on the accuracy

Let $p^{(\alpha)}(\underline{x}) = x_1^{\alpha_1} \cdots x_d^{\alpha_d}$ be the *mth* element of total degree $\alpha = \alpha_1 + \cdots + \alpha_n$ from the augmented polynomial basis. Let F be a smooth multivariable function. The **approximation error** of the local RBF+poly interpolant $(*)$ of F can be bounded over the stencil as:

$$\|s(x) - F(x)\|_\infty \leq C\, h^{l+1} \max_{\underline{x} \in \Omega} |L_k[F(x)]|$$

where h is the internodal distance and L_k the differential operator

$$L^{(\alpha)} = \frac{1}{\alpha_1! \cdots \alpha_d!} \frac{\partial^\alpha}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}}$$

and such that each $\beta_k = L_k[F(x)] + O(h^{l+1})$, $k = 1, \ldots, s$. The model leads to an **accuracy** which convergence order is **determined by the degree l of augmented polynomial terms** [1].

[1] Bayona, V. (2019) *An insight into RBF-FD approximations augmented with polynomials.* Computers & Mathematics with Applications, 77(9), 2337-2353.

Numerical Inversion Methods

Inversion methods compute approximations of the *inverse* function taking information from the related LT at specific points , e.g.:

1. the Weeks' method computes the coefficients of a truncated series of the inverse function, based on Laguerre polynomials, by a Lagrange interpolation of F, on Chebyshev zeros [S.C. et al., 2007, Rosanna Campagna et al. 2013 & 2014];
2. the Fourier method gives the inverse function as a Fourier cosine series, deriving from the discretization of the Riemann inversion formula by trapezoidal quadrature [Dubner H., Abate J., 1968];
3. the Pike's method assumes the truncation expansion of the inverse function in terms of eigenfunctions and eigenvalues of the LT, to be computed in suitable points [Pike E.R., 1978];
4. the Gaver-Stehfest method is based on a linear combination of LT values, at uniformly distributed points; [Rosanna Campagna et al. 2018].

$$f(t) = \int_0^\infty \frac{< F(\cdot), \psi^+(\omega, \cdot) >}{\lambda^+(\omega)} \psi^+(\omega, t) d\omega + \int_0^\infty \frac{< F(\cdot), \psi^-(\omega, \cdot) >}{\lambda^-(\omega)} \psi^-(\omega, t) d\omega \quad (2)$$

where $\psi^\pm$ and $\lambda^\pm$ are eigenfunctions and eigenvalues of the operator Laplace integral, following [Pike, 1978], the f in (2) is approximated by a truncated series:

$$f_M(t) = \sum_{k=0}^{M} \frac{c_k^+}{\lambda^+(k\Delta\omega)} \psi^+(k\Delta\omega, t) + \sum_{k=1}^{M} \frac{c_k^-}{\lambda^-(k\Delta\omega)} \psi^-(k\Delta\omega, t) \quad (3)$$

where $\Delta\omega = 2\pi/(\ln(L_2) - \ln(L_1))$, and

$$c_k^\pm = \begin{cases} \Delta\omega \int_{L_1}^{L_2} F(s) \psi^\pm(k\Delta\omega, s) ds & \text{if } k \neq 0 \\ \frac{\Delta\omega}{2} \int_{L_1}^{L_2} F(s) \psi^\pm(0, s) ds & \text{if } k = 0 \end{cases} . \quad (4)$$

The solution requires to compute the coefficients c_k, by solving the integrals:

$$c_k^{\pm} = \begin{cases} \Delta\omega \int_{L_1}^{L_2} F(s)\psi^{\pm}(k\Delta\omega, s)ds & \textit{if } \; k \neq 0 \\ \\ \frac{\Delta\omega}{2} \int_{L_1}^{L_2} F(s)\psi^{\pm}(0, s)ds & \textit{if } \; k = 0 \end{cases} .$$

$\Delta\omega$ is an amplification factor for the fitting error:

$$\|c_k^{\pm} - \tilde{c}_k^{\pm}\| \leq \begin{cases} |\Delta\omega| \int_{L_1}^{L_2} |F(x) - s(x)| \cdot |\psi^{\pm}(k\Delta\omega, x)|dx & \textit{if } \; k \neq 0 \\ \\ \left|\frac{\Delta\omega}{2}\right| \int_{L_1}^{L_2} |F(x) - s(x)| \cdot |\psi^{\pm}(0, x)|dx & \textit{if } \; k = 0 \end{cases} .$$

Following [Pike, 1978], we set $\Delta\omega = 2\pi/(10^5 - 10^{-15}) = 6.2832e - 05$, granting a contained growth of the fitting error.

Gaver's LTI formula

The LT inverse function is approximated by a linear combination of $F - values$:

$$f_M(t) = \gamma(t) \sum_{i=1}^{M} V_i F\left(i\gamma(t)\right), \qquad \gamma(t) = \ln 2/t \tag{5}$$

and

$$V_i = (-1)^{i+M/2} \sum_{k=[(i+1)/2]}^{min(i,M/2)} \frac{k^{M/2}(2k)!}{(M/2-k)!k!(k-1)!(i-k)!(2k-i)!} \tag{6}$$

An upper bound for the approximation error is computed:

$$\begin{aligned} |f_M(t) - f_s(t)| &\leq \gamma(t) \sum_{i=1}^{M} |V_i| |F\left(i\,\gamma(t)\right) - s\left(i\,\gamma(t)\right)| \leq \\ &\leq \left(\gamma(t) M \sum_{i=1}^{M} |V_i|\right) \|F - s\|_\infty \\ &\leq \theta(t, M) \|F - s\|_\infty := \Theta(t, M, \Delta, s) \end{aligned}$$

Numerical Experiments

The fitting model has to approximate the F-values, required by the inversion formula.

Numerical experiments highlight:

- the accuracy of the fitting model;
- the impact of the fitting error introduced and its extrapolation feature, on the inverse solution.
- **Test 1** (from 1.1 to 1.3): LTI by Pike's method applied to the PHS+poly model;
- **Test 2** (from 2.1 to 2.2): LTI by Gaver-Stehfest (GS)'s method applied to the PHS+poly model.

Data:

- $(x_i, y_i)_{i=1}^N$, with $\{x_i\}_{i=1}^N$ uniformly distributed in a subset $[a, b] = [1, 10]$ and $y_i = F(x_i)$ with

$$F(x) = e^{-x}/(1 + x), \qquad f(t) = e^{-(t-1)}u(t-1), \; t > 1, \; u(t) \text{ step function.}$$

Output:

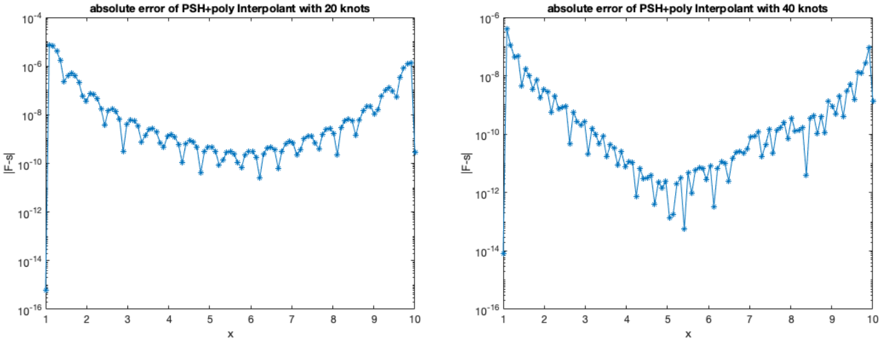
- an approximation of f at the points

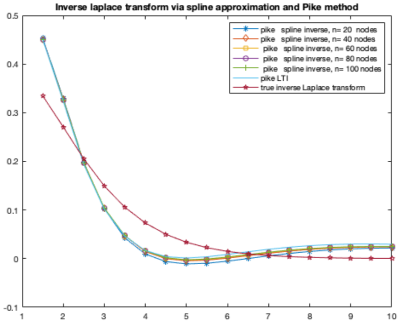
$$t_j \in [1.5, 10], \; t_1 = 1.5, \; t_{j+1} = t_j + 0.5, \; j = 1, ..., 17.$$

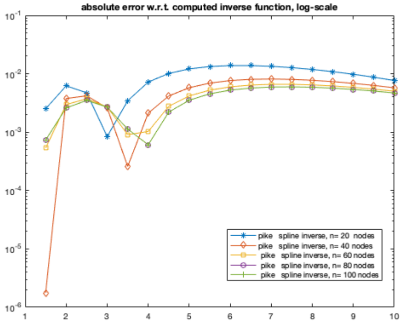
Procedure:

- define the PHS+poly model s on different sets of N knots (with $N = 20, 40, 60, 80, 100$);
- apply Pike's inversion formula to s, integrating s on $[L1, L2] \supset [a, b]$. The eigenfunctions number is set to $M = 25$.

Set PHS r^7 augmented with *17 degree polynomials*. Integration interval $[L1, L2] = [10^{-15}, 10] \supset [1, 10]$.
The fitting error decreases when the number of knots grows up:







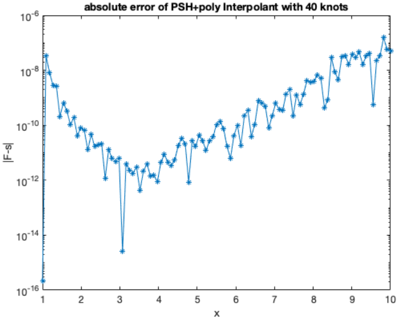
f_s

$(N = 20, \ldots, 100)$ vs f_F (left); Absolute errors $|f_s(t) - f_F(t)|$ (right).

The discrepancy w.r.t. the true f depends on the conditioning of the inversion formula.

	$N = 20$	$N = 40$	$N = 60$	$N = 80$	$N = 100$
$MSE = \frac{\|f_F - f_s\|_2^2}{18}$	9.8497e-05	3.4910e-05	2.3182e-05	1.8887e-05	1.8887e-05

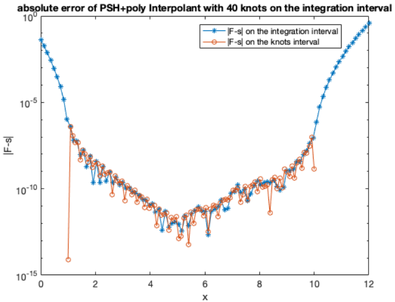
Set PHS r^7 augmented with **25 degree polynomials**. $[L1, L2] = [10^{-15}, 10]$. The *fitting* error decreases, according with the theoretical bound.

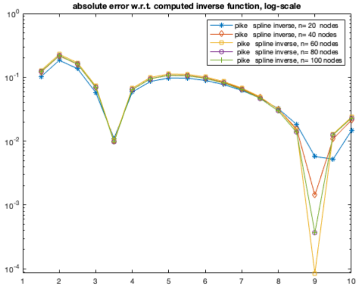


For each $t \in [1.5, 10]$ the accuracy on F reflects on the inverse computation.

	$N = 20$	$N = 40$	$N = 60$	$N = 80$	$N = 100$
$MSE = \frac{\|f_F - f_s\|_2^2}{18}$	1.4045e-01	4.8312e-06	7.1163e-06	6.6879e-06	6.6879e-06

In this test we highlight the accuracy in the **extrapolation**, when the PHS+poly is integrated on $[L1, L2] = [10^{-15}, \mathbf{12}] \supset [1, 10]$. Set PHS r^7 + 17 degree polynomials.

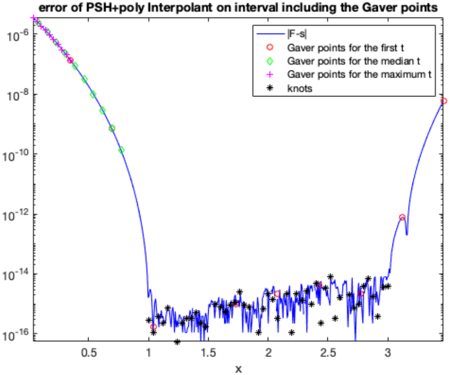




The fitting error **outside the knots interval**, reflects on the inverse accuracy:

	$N = 20$	$N = 40$	$N = 60$	$N = 80$	$N = 100$
$MSE = \frac{\|\|f_F - f_s\|\|_2^2}{18}$	6.5622e-03	8.5175e-03	9.3977e-03	8.5368e-03	8.5368e-03

The evaluation points change with t; figure describes their distribution w.r.t. the knots interval and the corresponding fitting errors.



Fitting error (blue continuos line, '-') between F and s on 500 points of a wide interval including all the GS points generating by the fixed t values. Fitting error at the GS points distribution for the minimum ($'\circ'$) for the median ($'\diamond'$) and for the maximum ($'+'$) t. Fitting error at the **Interpolating knots** ($'*'$).

We observe the good quality of the approximated inverse LT, also when the inversion formula requires the **extrapolation of information from data**, by evaluating the spline model outside the knots interval.

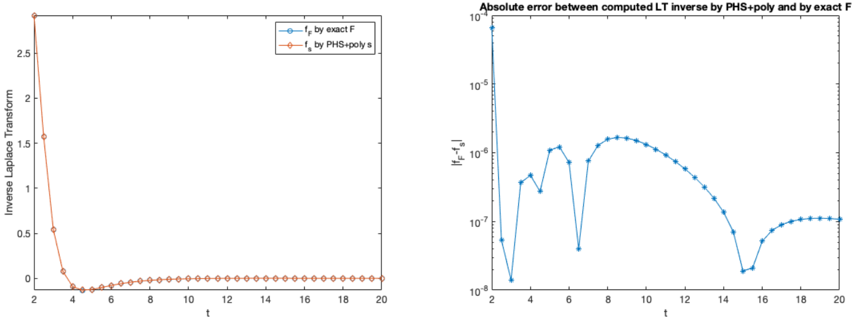


Figure 1: f_M vs f_s, obtained by applying the algorithm to F and s respectively (left). Pointwise absolute error $|f_M(t) - f_s(t)|$.

Set $F(x) = \frac{2ax}{(x^2+a^2)^2}$, $a = 2$, with $f(t) = tsin(at)$.

The amplification factor θ of the inversion formula gives information on the *possible* **fatal impact** of the fitting error on the solution.

- $\|F - s\|_\infty$ is the maximum discrepancy on the GS points for each t;
- $\theta(t, M)$ is the amplification factor due to the inversion formula;
- $\Theta(t, M, \Delta, s)$ is the computable upper bound for the approximation error.

t	$\lvert f_M(t) - f_s(t)\rvert$	$\|F - s\|_\infty$	$\theta(t, M)$	$\Theta(t, M, \Delta, s)$
2.0	8.97946e-11	4.43530e-11	1.50993e+05	6.69701e-06
3.0	8.00476e-09	1.65883e-09	1.00662e+05	1.66982e-04
4.0	5.30296e-10	6.83621e-10	7.54967e+04	5.16111e-05
5.0	2.20194e-08	4.83468e-09	6.03973e+04	2.92002e-04
8.0	1.45021e-08	3.16201e-09	3.77483e+04	1.19360e-04
9.0	1.57366e-06	7.90296e-09	3.35541e+04	2.65177e-04
10.0	2.23597e-07	1.22119e-08	3.01987e+04	3.68783e-04

Conclusions

- Laplace transform inversion formulas **work on continuous models**;
- fitting models can help to recover **missing information**;
- The results emphasize that a *good* fitting model is a **necessary requirement** for the application of the inversion method.

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Thanks to Florence colleagues for the gentle invitation :)

See you soon in Naples

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Credits. Rosario Cuomo (my uncle :))