Interval Interpolation with Exponential Sums

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Models with Exponential Sums

Let

$$f(x,t) = \sum_{j=1}^{p} x_{2j-1} e^{-x_{2j} t}, \quad n = 2p.$$

For a set of data measurements, $\tilde{y}_i$ at time t_i, $i = 1, \ldots, m$, we wish to determine *decay rates* x_{2j} and *amplitudes* x_{2j-1}, $j = 1, \ldots, p$, such that

$$f(x, t_i) = \tilde{y}_i, \quad i = 1, \ldots, m.$$

Such models appear in (e.g.) pharmocokinetics, compartment models, and radioactive decay.

Assume that each measurement $\tilde{y}_i$ approximates the exact value y_i, and obtain for each i an interval $[a_i, b_i]$ such that $y_i \in [a_i, b_i]$ is guaranteed.

Compute an enclosure or representation of the parameters x that are consistent, i.e.

$$f(x, t_i) \in [a_i, b_i], \quad i = 1, \ldots, m.$$

Case $p = 2$*:*

$$f(x, t) = x_1 e^{-x_2 t} + x_3 e^{-x_4 t}$$

Outline

- Prony's method
- Algorithm for an interval version of Prony's method
- Solution of linear interval systems of equations with special structure
- Combination of Prony's method with consistency techniques
- Conclusions and future work

Prony's Method - Overview

(R. Prony, 1795)

We require a minimum of 4 data points, which must be time equidistant, i.e. a set of observations $(\tilde{y}_i, t_i)$, $i = 1, \ldots, m$, with $m \geq 4$ and $t_i = t_0 + ih$ for some t_0 and stepsize h.

Let $\mu(t) = x_1 e^{x_2 t} + x_3 e^{x_4 t}$. This satisfies a linear difference equation

$$\zeta_1 \mu(t) + \zeta_2 \mu(t+h) + \mu(t+2h) = 0.$$

Setting $u_1 = e^{x_2 h}$ and $u_2 = e^{x_4 h}$ we obtain

$$x_1 e^{x_2 t}(\zeta_1 + \zeta_2 u_1 + u_1^2) + x_3 e^{x_4 t}(\zeta_1 + \zeta_2 u_2 + u_2^2) = 0.$$

Therefore u_1 and u_2 can be given as the roots of the quadratic

$$\zeta_1 + \zeta_2 u + u^2.$$

For each set of data points $y_j, y_{j+1}, y_{j+2}, y_{j+3}$, $j = 1, \ldots, m-3$, ζ_1 and ζ_2 must satisfy

$$\begin{aligned} \zeta_1 y_j + \zeta_2 y_{j+1} &= -y_{j+2}, \\ \zeta_1 y_{j+1} + \zeta_2 y_{j+2} &= -y_{j+3}. \end{aligned}$$

Prony's Method - An Interval Version

We now wish to transform the method to work with intervals, i.e. we are given interval data measurements $[y_1], \ldots, [y_m]$.

This requires us to:

- solve linear interval systems,
- find interval enclosures for the roots of a quadratic with interval coefficients.

Algorithm - Step a)

For $k = 1, \ldots, m-3$, solve the system(s)

$$\begin{pmatrix} [y_k] & [y_{k+1}] \\ [y_{k+1}] & [y_{k+2}] \end{pmatrix} \begin{pmatrix} \zeta_1 \\ \zeta_2 \end{pmatrix} = \begin{pmatrix} -[y_{k+2}] \\ -[y_{k+3}] \end{pmatrix}.$$

Let $[\zeta_1], [\zeta_2]$ be enclosures for the intersections of the solution sets.

It may be that these enclosures (and therefore the parameter set) are either empty or unbounded (in which case terminate).

Algorithm - Step b)

Compute interval enclosures $[u_1], [u_2]$ for the zero sets of the quadratic

$$[\zeta_1] + [\zeta_2]u + u^2.$$

If there are not two real (interval) roots which can be separated, terminate.

Enclosures for the decay constants are given by

$$\{[x_2], [x_4]\} = \{\log([u_1])/h, \log([u_2])/h\}.$$

Algorithm - Step c)

We lastly obtain enclosures for the amplitudes $[x_1]$ and $[x_3]$ from the solution of a another system of two linear interval equations

$$\begin{pmatrix} 1 & 1 \\ [u_1] & [u_2] \end{pmatrix} \begin{pmatrix} z_1 \\ z_3 \end{pmatrix} = \begin{pmatrix} [y_1] \\ [y_2] \end{pmatrix}$$

with $x_1 = e^{-t_1 x_2} z_1$ and $x_3 = e^{-t_1 x_4} z_3$.

Solution of Linear Interval Systems

We wish to obtain the hull, i.e. the smallest bounding box, of the solution set of the interval system

$$\begin{pmatrix} [y_k] & [y_{k+1}] \\ [y_{k+1}] & [y_{k+2}] \end{pmatrix} \begin{pmatrix} \zeta_1 \\ \zeta_2 \end{pmatrix} = \begin{pmatrix} -[y_{k+2}] \\ -[y_{k+3}] \end{pmatrix}.$$

Solution set considering both dependencies $\subseteq$ Symmetric solution set $\subseteq$ General solution set.

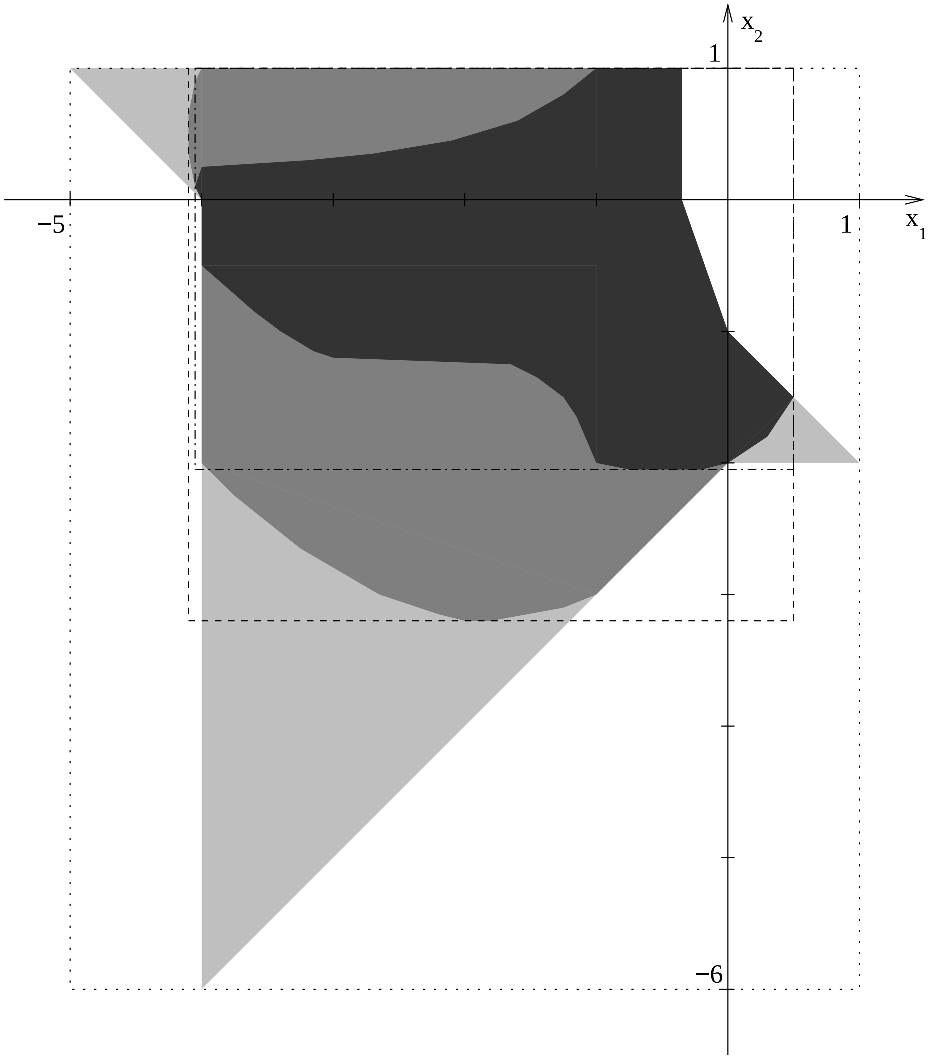
Methods exist to determine the hull of the general solution set *(Apostolatos/Kulisch 1968, Neumaier 1990)* and which describe the shape of the symmetric solution set *(Alefeld et al. 1997)*.

The hull of the smallest solution set can be obtained with some elementary analysis and by solving a number of point systems.

Solution of Linear Interval Systems - Example

We show the three solution sets together with their hulls for the following system:

$$\begin{pmatrix} [1,3] & [0,1] \\ [0,1] & [-4,-1] \end{pmatrix} \begin{pmatrix} \zeta_1 \\ \zeta_2 \end{pmatrix} = \begin{pmatrix} [-4,-1] \\ [-1,2] \end{pmatrix}$$


x_2
1
−5
1
x_1
−6

Models with Exponential Sums - Example

$$\begin{array}{rcll}
x_1 e^{4.387 x_2} & + & x_3 e^{4.387 x_4} & \in & [-0.304, -0.298] \\
x_1 e^{12.069 x_2} & + & x_3 e^{12.069 x_4} & \in & [21.43, 21.86] \\
x_1 e^{19.751 x_2} & + & x_3 e^{19.751 x_4} & \in & [171.9, 175.3] \\
x_1 e^{27.434 x_2} & + & x_3 e^{27.434 x_4} & \in & [1257, 1282]
\end{array}$$

This can be easily formulated as a *constraint satisfaction problem*:

$$\begin{array}{rcccl}
-0.304 & \leq & x_1 e^{4.387 x_2} + x_3 e^{4.387 x_4} & \leq & -0.298 \\
21.43 & \leq & x_1 e^{12.069 x_2} + x_3 e^{12.069 x_4} & \leq & 21.86 \\
171.9 & \leq & x_1 e^{19.751 x_2} + x_3 e^{19.751 x_4} & \leq & 175.3 \\
1257 & \leq & x_1 e^{27.434 x_2} + x_3 e^{27.434 x_4} & \leq & 1282
\end{array}$$

Prony's method computes (in 0.01s) the following enclosures for the set of parameters x_1, x_2, x_3, x_4:
$[-6.673, -3.374], [-0.130, 0.014], [0.911, 1.344], [0.247, 0.266]$.

Starting with an initial box $[-100, 100], [-10, 10], [-100, 100], [-10, 10]$, the constraint satisfaction program *Realpaver* computes (in 12.8s):
$[-100, 100], [-3.33, 10], [-100, 100], [-3.33, 10]$.

Starting with the enclosures computed by Prony's method, *Realpaver* computes (with computation time limited to 12.8s):
$[-5.909, -3.800], [-0.125, 0.010], [0.990, 1.205], [0.253, 0.261]$.

Conclusions

Advantages of Prony's method: requires no initial box, very fast, delivers a guaranteed enclosure for the parameter set.

Disadvantages of Prony's method: very sensitive to data peturbations, requires fairly narrow data intervals, does not always deliver a (non-empty and finite) result.

We conclude that Prony's method may be a powerful preprocessing tool for parameter set estimation problems involving exponential sums.

Future Work

- Prony's method may be used more than once on the same problem, with different measurement data, with successive tightening of the enclosures, in the case that the input data was peturbed. E.g. put

  $$F(t) := [x_1]e^{-[x_2]t} + [x_3]e^{-[x_4]t}.$$

  If $[y_i] \setminus F(t_i)$ is large for some i then we have proven that certain measurements are not possible.

- Implement the method in the case p=3, p=4, ... This will require enclosures for the special solution sets of linear interval systems of p equations in p unknowns, plus enclosures for the roots of a degree p interval polynomial.