Globally Optimal Parameter Estimation of Nonlinear Dynamical Models is an Eigenvalue Problem

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Overview

Overview

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Model Class

- Single output autonomous discrete–time polynomial state–space models of the form Σ

$$\Sigma : \begin{cases} \hat{\boldsymbol{x}}_{k+1} = \boldsymbol{f}(\hat{\boldsymbol{x}}_k, \boldsymbol{\theta}) \\ \hat{y}_k = g(\hat{\boldsymbol{x}}_k, \boldsymbol{\theta}) \end{cases} \tag{1}$$

where $\hat{\boldsymbol{x}}_k \in \mathbb{R}^n$ are the state variables at instant $k : k \in \mathbb{Z}^+$, $\boldsymbol{\theta} \in \mathbb{R}^\ell$ are the model parameters. $\boldsymbol{f} : \mathbb{R}^n \times \mathbb{R}^\ell \to \mathbb{R}^n$, $g : \mathbb{R}^n \times \mathbb{R}^\ell \to \mathbb{R}$ and $\boldsymbol{f}, g \in \mathbb{R}[\hat{\boldsymbol{x}}_k, \boldsymbol{\theta}]$ where $\boldsymbol{f}, g \in \mathbb{R}[\hat{\boldsymbol{x}}_k, \boldsymbol{\theta}]$ is a multivariate polynomial ring, $\hat{y} \in \mathbb{R}$ is the model output variable.

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  where $\hat{\boldsymbol{x}}_k \in \mathbb{R}^n$ are the state variables at instant $k : k \in \mathbb{Z}^+$, $\boldsymbol{\theta} \in \mathbb{R}^\ell$ are the model parameters. $\boldsymbol{f} : \mathbb{R}^n \times \mathbb{R}^\ell \rightarrow \mathbb{R}^n$, $g : \mathbb{R}^n \times \mathbb{R}^\ell \rightarrow \mathbb{R}$ and $\boldsymbol{f}, g \in \mathbb{R}[\hat{\boldsymbol{x}}_k, \boldsymbol{\theta}]$ where $\boldsymbol{f}, g \in \mathbb{R}[\hat{\boldsymbol{x}}_k, \boldsymbol{\theta}]$ is a multivariate polynomial ring, $\hat{y} \in \mathbb{R}$ is the model output variable.
- Σ is identifiable, i.e., a model compliant trajectory $\hat{\mathbf{y}} = \begin{bmatrix} \hat{y}_0 & \hat{y}_1 & \dots \hat{y}_{\mathsf{N}-1} \end{bmatrix}^{\mathsf{T}} \in \mathbb{R}^{\mathsf{N}}$ is generated uniquely by some $\boldsymbol{\theta}^* \in \Theta \subset \mathbb{R}^\ell$, where Θ is an open neighborhood of $\mathbb{R}^\ell$

Parameter Estimation

- Given observed output sequence $\mathbf{y} = \begin{bmatrix} y_0 & y_1 & \dots y_{N-1} \end{bmatrix}^T \in \mathbb{R}^N$, find a model compliant trajectory $\hat{\mathbf{y}}$ generated by some $\boldsymbol{\theta}^*$, such that the observed data is 'closely' approximated.

Parameter Estimation

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- Minimize

$$\begin{aligned} \min_{\boldsymbol{\theta},\hat{\mathbf{y}}} \quad & \|\mathbf{y} - \hat{\mathbf{y}}\|^2 \\ \text{s.t.} \quad & \boldsymbol{\Phi}(\boldsymbol{\theta}, \hat{\mathbf{y}}) = \mathbf{0} \end{aligned} \tag{2}$$

  where $\boldsymbol{\Phi}(\boldsymbol{\theta}, \hat{\mathbf{y}}) = \mathbf{0}$, is a system of polynomial equations, such that $\mathcal{V}(\boldsymbol{\Phi})$, forms a manifold in $\mathbb{R}^\ell \times \mathbb{R}^N$ on which the model-compliant trajectory $\hat{\mathbf{y}}$ and the corresponding model parameters $\boldsymbol{\theta}$ lie.
- Opt. problem in (2) is non-convex

Parameter Estimation some history

Parameter Estimation some history

- In continuous-time models
  - polynomial state-space model $\rightarrow$ output equation $\rightarrow$ least squares cost function $\rightarrow$ iterative gradient based solver (sub-optimal solution) [Denis-Vidal et al., 2003, Verdiere, 2005]

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Globally Optimal Parameter Estimation

polynomial state-space model $\rightarrow$ **output equation** $\rightarrow$ least-squares cost function $\rightarrow$ **system of polynomial equations** $\rightarrow$ **eigenvalue problem**

Overview

Output difference equation

The output difference equation

$$\Phi(\boldsymbol{\theta}, \hat{y}_{k+n}, \ldots, \hat{y}_k) = 0 \tag{3}$$

relates the consecutive samples of a model compatible output sequence, and is a multivariate polynomial equation, such that

$$\Phi \in I_\Sigma \cap \mathbb{R}\left[\boldsymbol{\theta}, \hat{y}_{k+n}, \ldots, \hat{y}_k\right] \tag{4}$$

where

$$\begin{aligned} I_\Sigma = \langle & \hat{y}_k - g(\hat{\boldsymbol{x}}_k, \boldsymbol{\theta}), \\ & \hat{y}_{k+1} - g(\boldsymbol{f}(\hat{\boldsymbol{x}}_k, \boldsymbol{\theta}), \boldsymbol{\theta}), \\ & \vdots \\ & \hat{y}_{k+n} - g(\boldsymbol{f}^n(\hat{\boldsymbol{x}}_k, \boldsymbol{\theta}), \boldsymbol{\theta}) > . \end{aligned} \tag{5}$$

note that $I_\Sigma \in \mathbb{R}\left[\hat{\boldsymbol{x}}_k, \boldsymbol{\theta}, \hat{y}_k, \ldots, \hat{y}_{k+n}\right]$

Output difference equation

Construction of Φ

Given a single-output autonomous discrete-time (DT) polynomial state-space model Σ of order n (as in (1)), there exists a unique polynomial output difference equation of minimal degree, denoted by $\Phi(\boldsymbol{\theta}, \hat{y}_{k+n}, \ldots, \hat{y}_k) = 0$, which is the generator of the elimination ideal $I_\Sigma|_n \in \mathbb{R}[\boldsymbol{\theta}, \hat{y}_{k+n}, \ldots, \hat{y}_k]$ where

$$\Phi \in \underbrace{I_\Sigma \cap \mathbb{R}\left[\boldsymbol{\theta}, \hat{y}_{k+n}, \ldots, \hat{y}_k\right]}_{I_\Sigma|_n}$$

Moreover, Φ is of the same model order n and encapsulates the dynamical behavior of Σ in a single equation.

Output difference equation
Example

Consider the discretized Lotka–Volterra model

$$\Sigma_{\mathrm{LV}} : \begin{cases} \hat{x}^{(1)}_{k+1} = \hat{x}^{(1)}_k (1 + b - p\hat{x}^{(2)}_k) \\ \hat{x}^{(2)}_{k+1} = \hat{x}^{(2)}_k (1 - d + p\hat{x}^{(1)}_k) \\ \hat{y}_k = \hat{x}^{(2)}_k \end{cases} \tag{6}$$

where the superscript over $\hat{x}^{(.)}_k$ indicates the component of the state-variable.

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where the superscript over $\hat{x}^{(.)}_{k}$ indicates the component of the state-variable. Here, $I_{\Sigma_{\mathrm{LV}}}$ can be generated using,

$$I_{\Sigma_{\mathrm{LV}}} = \begin{array}{c} < \hat{y}_k - \hat{x}^{(2)}_{k}, \\ \hat{y}_{k+1} - \hat{x}^{(2)}_{k}(1 - d + p\hat{x}^{(1)}_{k}), \\ \hat{y}_{k+2} - \hat{x}^{(2)}_{k}(1 - d + p\hat{x}^{(1)}_{k})(1 - d + p\hat{x}^{(1)}_{k}(1 + b - p\hat{x}^{(2)}_{k})) > \end{array} \tag{7}$$

In order to eliminate $\boldsymbol{x}_k$ we will use consecutive Sylvester resultants

Sylvester Matrix and Resultants

Consider the system,

$$\begin{cases} f_1(x) = a_r x^r + a_{r-1}x^{r-1} + \ldots + a_0 = 0, \\ f_2(x) = b_s x^s + b_{s-1}x^{s-1} + \ldots + b_0 = 0 \end{cases}$$

which has common roots. Construct $\boldsymbol{Mk} = \mathbf{0}$ by multiplying $f_1(x)$ and $f_2(x)$ with powers of x s.t.,

$$\begin{matrix} s \text{ rows}: \\ \\ r \text{ rows}: \end{matrix} \left[\begin{array}{cccccccc} a_0 & a_1 & \ldots & a_r & & & & \\ & a_0 & a_1 & \ldots & a_r & & & \\ & & \ddots & \ddots & & \ddots & & \\ & & & a_0 & a_1 & \ldots & a_r & \\ \hline b_0 & b_1 & \ldots & b_s & & & & \\ & b_0 & b_1 & \ldots & b_s & & & \\ & & \ddots & \ddots & & \ddots & & \\ & & & b_0 & b_1 & \ldots & b_s & \end{array}\right] \begin{bmatrix} x^0 \\ x^1 \\ \vdots \\ x^{r+s-1} \end{bmatrix} = \left[\begin{array}{c} 0 \\ 0 \\ \vdots \\ 0 \\ \hline 0 \\ 0 \\ \vdots \\ 0 \end{array}\right].$$

$\boldsymbol{M} \in \mathbb{R}^{(r+s)\times(r+s)}$ is the **Sylvester matrix** [Cox et al., 2015]

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Sylvester Resultant

if $f_1(x)$ and $f_2(x)$ have a common root, then $\det \boldsymbol{M} = 0$

$$\mathrm{Res}(f_1, f_2, x) = \det(\mathrm{Syl}(f_1, f_2, x))$$

Output difference equation
Example

Let us first eliminate the state variable $\hat{x}_k^{(2)}$, First, lets consider

$$\text{Res} : \begin{cases} f_1(\hat{x}_k^{(2)}) = \hat{y}_k - \hat{x}_k^{(2)} \\ f_2(\hat{x}_k^{(2)}) = \hat{y}_{k+1} - (1 - d + p\hat{x}_k^{(1)})\hat{x}_k^{(2)} \end{cases}$$

we can construct the Sylvester matrix as,

$$\underbrace{\begin{bmatrix} \hat{y}_k & -1 \\ \hat{y}_{k+1} & -(1 - d + p\hat{x}_k^{(1)}) \end{bmatrix}}_{\text{Syl}(f_1, f_2, \hat{x}_k^{(2)})} \begin{bmatrix} 1 \\ \hat{x}_k^{(2)} \end{bmatrix} = \mathbf{0}$$

$$\text{Res}(f_1, f_2, \hat{x}_k^{(2)}) = \det(\text{Syl}(f_1, f_2, \hat{x}_k^{(2)})) = \hat{y}_k(1 - d + p\hat{x}_k^1) - \hat{y}_{k+1}$$

Output difference equation
Example

Now, lets consider

$$\text{Res}: \begin{cases} f_2(\hat{x}_k^{(2)}) = \hat{y}_{k+1} - (1 - d + p\hat{x}_k^{(1)})\hat{x}_k^{(2)} \\ f_3(\hat{x}_k^{(2)}) = \hat{y}_{k+2} + f_{31}(b, d, p, \hat{x}_k^{(1)})\hat{x}_k^{(2)} + f_{32}(b, d, p, \hat{x}_k^{(1)})(x\hat{(2)}_k)^2 \end{cases}$$

we can construct the Sylvester matrix as,

$$\underbrace{\begin{bmatrix} \hat{y}_{k+1} & -(1 - d + p\hat{x}_k^{(1)}) & 0 \\ 0 & \hat{y}_{k+1} & -(1 - d + p\hat{x}_k^{(1)}) \\ \hat{y}_{k+2} & f_{31}(b, d, p, \hat{x}_k^{(1)}) & f_{32}(b, d, p, \hat{x}_k^{(1)}) \end{bmatrix}}_{\text{Syl}(f_2, f_3, \hat{x}_k^{(2)})} \begin{bmatrix} 1 \\ \hat{x}_k^{(2)} \\ (\hat{x}_k^{(2)})^2 \end{bmatrix} = \mathbf{0}$$

$$\text{Res}(f_2, f_3, \hat{x}_k^{(2)}) = \det(\text{Syl}(f_2, f_3, \hat{x}_k^{(2)}))$$

Output difference equation

Observe

$$\mathrm{Res}(f_1, f_2, \hat{x}_k^{(2)}), \mathrm{Res}(f_2, f_3, \hat{x}_k^{(2)}) \in \mathbb{R}[b, d, p, x_k^{(1)}, \hat{y}_k, \hat{y}_{k+1}, \hat{y}_{k+2}]$$

eliminate $\hat{x}_k^{(1)}$ by computing,

$$\Phi = \mathrm{Res}(\mathrm{Res}(f_1, f_2, \hat{x}_k^{(2)}), \mathrm{Res}(f_2, f_3, \hat{x}_k^{(2)}), \hat{x}_k^{(1)}) = 0$$

which is,

$$\hat{y}_k^2 \hat{y}_{k+1}(pd - p) + \hat{y}_k \hat{y}_{k+1}^2 p - \hat{y}_k \hat{y}_{k+1}(bd - b) - \hat{y}_{k+1}^2(b+1) + \hat{y}_k \hat{y}_{k+2} = 0$$

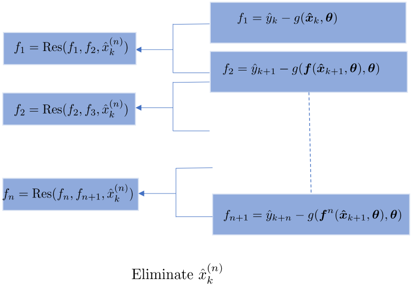
Summary: Output difference equation

$$f_1 = \hat{y}_k - g(\hat{\boldsymbol{x}}_k, \boldsymbol{\theta})$$

$$f_2 = \hat{y}_{k+1} - g(\boldsymbol{f}(\hat{\boldsymbol{x}}_{k+1}, \boldsymbol{\theta}), \boldsymbol{\theta})$$

$$f_{n+1} = \hat{y}_{k+n} - g(\boldsymbol{f}^n(\hat{\boldsymbol{x}}_{k+1}, \boldsymbol{\theta}), \boldsymbol{\theta})$$

Summary: Output difference equation



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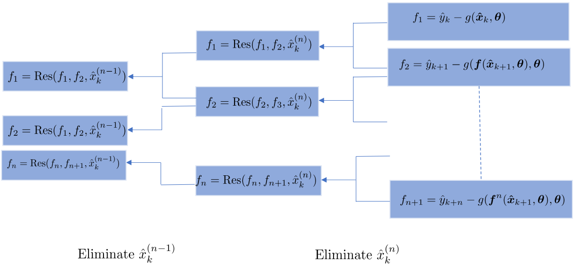

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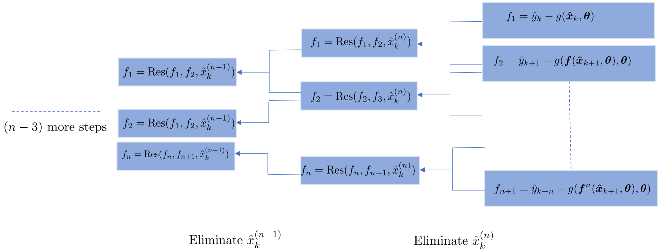

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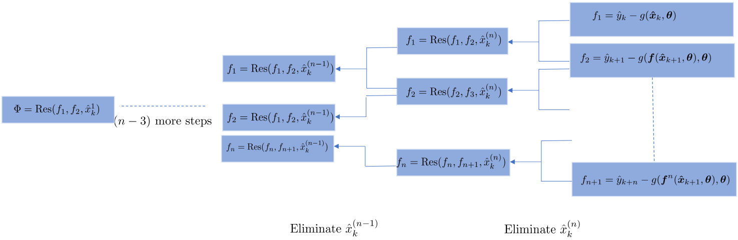

Manifold of the Model Compliant Data

Given model compliant data,

$$\hat{\mathbf{y}} = \left[\hat{y}_0, \ldots, \hat{y}_{\text{N-1}}\right]^{\mathsf{T}} \in \mathbb{R}^{\mathsf{N}}$$

the output equation $\Phi(\boldsymbol{\theta}, \hat{y}_{k+n}, \ldots, \hat{y}_k) = 0$ is satisfied by all $\hat{y}_k$ where $k \in \mathbb{Z}^+$.

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the output equation $\Phi(\boldsymbol{\theta}, \hat{y}_{k+n}, \ldots, \hat{y}_k) = 0$ is satisfied by all $\hat{y}_k$ where $k \in \mathbb{Z}^+$. Consider the system of equations,

$$\boldsymbol{\Phi}(\boldsymbol{\theta}, \hat{\mathbf{y}}) = \begin{bmatrix} \phi(\boldsymbol{\theta}, \hat{y}_0, \ldots, \hat{y}_n) \\ \phi(\boldsymbol{\theta}, \hat{y}_1, \ldots, \hat{y}_{n+1}) \\ \vdots \\ \phi(\boldsymbol{\theta}, \hat{y}_{\mathsf{N}-n-1}, \ldots, \hat{y}_{\mathsf{N}-1}) \end{bmatrix} = \mathbf{0}, \qquad (8)$$

where $\boldsymbol{\Phi} \in \mathbb{R}\left[\boldsymbol{\theta}, \hat{\mathbf{y}}\right]$ $\boldsymbol{\Phi} : \mathbb{R}^{\mathsf{N}+\ell} \rightarrow \mathbb{R}^{\mathsf{N}-n}$. $\mathcal{V}(\boldsymbol{\Phi})$ describes the positive dimensional variety over which the model compatible data and the associated model parameter lie.

Overview

Parameter Estimation as system of polynomial equations

Minimize the misfit as

$$\begin{aligned} \min_{\theta, \hat{\mathbf{y}}} \quad & \frac{1}{2}\|\tilde{\mathbf{y}}\|_2^2 = \frac{1}{2}\|\mathbf{y} - \hat{\mathbf{y}}\|_2^2 , \\ \text{s.t.} \quad & \boldsymbol{\Phi}(\boldsymbol{\theta}, \hat{\mathbf{y}}) = 0 \end{aligned}$$

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The Lagrangian is,

$$\mathcal{L}(\boldsymbol{\theta}, \hat{\mathbf{y}}) = \frac{1}{2} ||\mathbf{y} - \hat{\mathbf{y}}||_2^2 + \boldsymbol{\lambda}^\mathsf{T} \mathbf{\Phi} \tag{9}$$

Parameter Estimation as system of polynomial equations

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$$\text{s.t.} \quad \mathbf{\Phi}(\boldsymbol{\theta},\hat{\mathbf{y}}) = 0$$

The Lagrangian is,

$$\mathcal{L}(\boldsymbol{\theta},\hat{\mathbf{y}}) = \frac{1}{2}||\mathbf{y}-\hat{\mathbf{y}}||_2^2 + \boldsymbol{\lambda}^{\mathsf{T}}\mathbf{\Phi} \tag{9}$$

The associated FONCs are,

$$\partial\mathcal{L}/\partial\hat{\mathbf{y}} = -(\mathbf{y}-\hat{\mathbf{y}}) + \left(\frac{\partial\mathbf{\Phi}}{\partial\hat{\mathbf{y}}}\right)^{\mathsf{T}}\boldsymbol{\lambda} = 0, \tag{10}$$

$$\partial\mathcal{L}/\partial\boldsymbol{\theta} = \left(\frac{\partial\mathbf{\Phi}}{\partial\boldsymbol{\theta}}\right)^{\mathsf{T}}\boldsymbol{\lambda} = 0 \tag{11}$$

$$\partial\mathcal{L}/\partial\boldsymbol{\lambda} = \mathbf{\Phi} = 0 \tag{12}$$

Here, $\boldsymbol{\lambda}\in\mathbb{R}^{\mathsf{N}-n}$, and (10)- (12) is a square system of polynomial equations with $(\mathsf{N})+\ell+(\mathsf{N}-n)$ equations.

Parameter Estimation as system of polynomial equations

Consider the FONC in (11),

$$\left(\frac{\partial \mathbf{\Phi}}{\partial \boldsymbol{\theta}}\right)^{\mathsf{T}} \boldsymbol{\lambda} = 0$$

here, $\frac{\partial \mathbf{\Phi}}{\partial \boldsymbol{\theta}} \in \mathbb{R}^{(N-n)\times \ell}$

Parameter Estimation as system of polynomial equations

Consider the FONC in (11),

$$\left(\frac{\partial \mathbf{\Phi}}{\partial \boldsymbol{\theta}}\right)^{\mathsf{T}} \boldsymbol{\lambda} = 0$$

here, $\frac{\partial \mathbf{\Phi}}{\partial \boldsymbol{\theta}} \in \mathbb{R}^{(\mathsf{N}-n)\times \ell}$ we know from [Nõmm and Moog, 2016], if the model Σ is identifiable then,

$$\operatorname{rank}\left(\frac{\partial \mathbf{\Phi}}{\partial \boldsymbol{\theta}}\right) = \ell \tag{13}$$

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$$\text{rank}\left(\frac{\partial \mathbf{\Phi}}{\partial \boldsymbol{\theta}}\right) = \ell \tag{13}$$

and since $\boldsymbol{\lambda} \in \text{null}\left(\frac{\partial \phi}{\partial \boldsymbol{\theta}}\right)^{\mathsf{T}}$, we can write,

$$\boldsymbol{\lambda} = \boldsymbol{V}(\boldsymbol{\theta}, \hat{\mathbf{y}})\boldsymbol{c}$$

where, $\boldsymbol{V} \in \mathbb{R}^{(\mathsf{N}-n)\times(\mathsf{N}-n-\ell)}$ and $\boldsymbol{c} \in \mathbb{R}^{N-n-\ell}$. $\boldsymbol{V}$ is the basis of the nullspace of $\left(\frac{\partial \phi}{\partial \boldsymbol{\theta}}\right)^{\mathsf{T}}$ and the components of $\boldsymbol{V}$, $v_{ij} \in \mathbb{R}[\boldsymbol{\theta}, \hat{\mathbf{y}}]$

Parameter Estimation as system of polynomial equations

The FONCs can be re-written as,

$$-(\mathbf{y} - \hat{\mathbf{y}}) + \left(\frac{\partial \boldsymbol{\Phi}}{\partial \hat{\mathbf{y}}}\right)^{\mathsf{T}} \boldsymbol{V} \boldsymbol{c} = \mathbf{0} \quad (14)$$

$$\boldsymbol{\Phi} = 0 \quad (15)$$

Here, (14)- (15) is a square system with $\mathsf{N} + (\mathsf{N} - n)$ equations

Parameter Estimation: Example $n = 1$

Let's first consider a first order model with one model parameter

$$\Sigma_1 : \begin{cases} \hat{x}_{k+1} = \theta \hat{x}_k^3 \\ \hat{y}_k = \hat{x}_k \end{cases} \tag{16}$$

The output difference equation is given as,

$$\phi(\hat{y}_k, \hat{y}_{k+1}, \theta) = \hat{y}_{k+1} - \theta \hat{y}_k^3 = 0 \tag{17}$$

The parameter in θ is globally
identifiable [Nõmm and Moog, 2016], thus we can expect it to a find a unique minimizer

Parameter Estimation: Example $n = 1$

Given $\mathbf{y} = \begin{bmatrix} 1.00685 & 0.59511 & 0.02801 \end{bmatrix}^\mathsf{T}$ we can write (10)- (12) for Σ_1 as,

$$\begin{cases} \left(\begin{bmatrix} \hat{y}_0 \\ \hat{y}_1 \\ \hat{y}_2 \end{bmatrix} - \begin{bmatrix} 1.00685 \\ 0.59511 \\ 0.02801 \end{bmatrix} \right) + \begin{bmatrix} -3\theta \hat{y}_0^2 & 0 \\ 1 & -3\theta \hat{y}_1^2 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \\ \begin{bmatrix} -\hat{y}_0^3 & -\hat{y}_1^3 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \\ \begin{bmatrix} \hat{y}_1 - \theta \hat{y}_0^3 \\ \hat{y}_2 - \theta \hat{y}_1^3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \end{cases}$$

Parameter Estimation: Example $n = 1$

Given $\mathbf{y} = \begin{bmatrix} 1.00685 & 0.59511 & 0.02801 \end{bmatrix}^{\mathsf{T}}$ we can write (10)- (12) for Σ_1 as,

$$\begin{cases} \left(\begin{bmatrix} \hat{y}_0 \\ \hat{y}_1 \\ \hat{y}_2 \end{bmatrix} - \begin{bmatrix} 1.00685 \\ 0.59511 \\ 0.02801 \end{bmatrix} \right) + \begin{bmatrix} -3\theta\hat{y}_0^2 & 0 \\ 1 & -3\theta\hat{y}_1^2 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \\ \begin{bmatrix} -\hat{y}_0^3 & -\hat{y}_1^3 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \\ \begin{bmatrix} \hat{y}_1 - \theta\hat{y}_0^3 \\ \hat{y}_2 - \theta\hat{y}_1^3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \end{cases}$$

Solving (25) using `HomotopyContinuation.jl` [Breiding and Timme, 2018], we find the globally optimal solution $(\boldsymbol{\theta}, \hat{y}_0, \hat{y}_1, \hat{y}_2) = (0.5194, 1.0228, 0.5558, 0.0891)$

Parmeter Estimation: Example $n = 1$

There exists a partial linear structure in the system (25), such that the system can be written as a multiparameter eigenvalue problem (MEVP) of the form

$$\underbrace{\begin{bmatrix} \hat{y}_0 - 1.00685 & -3\theta\hat{y}_0^2 & 0 \\ \hat{y}_1 - 0.59511 & 1 & -3\theta\hat{y}_1^2 \\ \hat{y}_2 - 0.02801 & 0 & 1 \\ 0 & -\hat{y}_0^3 & -\hat{y}_1^3 \\ \hat{y}_1 \quad -\theta\hat{y}_0^3 & 0 & 0 \\ \hat{y}_2 \quad -\theta\hat{y}_1^3 & 0 & 0 \end{bmatrix}}_{\mathcal{M}(\theta,\hat{\mathbf{y}})} \begin{bmatrix} 1 \\ \lambda_1 \\ \lambda_2 \end{bmatrix} = \mathbf{0}$$

here, (23) is 4-parameter 4th degree MEVP. Using `MacaulayLab` [Vermeersch and De Moor, 2022] we find the same globally optimal solution.

Parameter Estimation: Example n=1

We can incorporate the identifiability rank condition which allows us to write $\begin{bmatrix}\lambda_1 & \lambda_2\end{bmatrix}^\mathsf{T} = \begin{bmatrix}\hat{y}_1^3 & -\hat{y}_0^3\end{bmatrix}^\mathsf{T} c$ such that the resulting system of equation is,

$$\begin{cases} \left(\begin{bmatrix}\hat{y}_0\\ \hat{y}_1\\ \hat{y}_2\end{bmatrix} - \begin{bmatrix}1.00685\\ 0.59511\\ 0.02801\end{bmatrix}\right) + \begin{bmatrix}-3\theta\hat{y}_0^2 & 0\\ 1 & -3\theta\hat{y}_1^2\\ 0 & 1\end{bmatrix} \begin{bmatrix}\hat{y}_1^3\\ -\hat{y}_0^3\end{bmatrix} c = \begin{bmatrix}0\\ 0\\ 0\end{bmatrix} \\ \begin{bmatrix}\hat{y}_1 - \theta\hat{y}_0^3\\ \hat{y}_2 - \theta\hat{y}_1^3\end{bmatrix} = \begin{bmatrix}0\\ 0\end{bmatrix} \end{cases}$$

`HomotopyContinuation.jl` yields the same globally optimal solution, however the equivalent MEVP is of degree 6 which makes solving the EP using `MacaulayLab` inefficient

Parameter Estimation: Example n=1

We will now consider a special case where $\mathrm{N} = 2n + l$. Since we can write $\hat{\mathbf{y}} = \boldsymbol{f}_{\text{comp}}(\boldsymbol{x}_0, \boldsymbol{\theta})$, satisfies (15), we can substitute it in (14), resulting in a smaller system of equations $2n + \ell$ equations in $2n + \ell$ variables. For the cubic model we are already in the situation where $\mathrm{N} = 2n + \ell = 3$, the FONCs reduce to,

$$\left\{ \left(\begin{bmatrix} \hat{x}_0 \\ \theta \hat{x}_0^3 \\ \theta^4 \hat{x}_0^9 \end{bmatrix} - \begin{bmatrix} 1.00685 \\ 0.59511 \\ 0.02801 \end{bmatrix} \right) + \begin{bmatrix} -3\theta \hat{x}_0^2 & 0 \\ 1 & -3\theta^2 \hat{x}_0^6 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \theta^3 \hat{x}_0^9 \\ -\hat{x}_0^3 \end{bmatrix} c = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \right.$$

The solution is $(0.5194, 1.0228)$. Note, that the resulting system of equations is of degree 16. The final question is a Numerical one, is it better to work with more equations of lower degree OR less equations of higher degree.

Parameter Estimation: Lotka–Volterra ($n = 2$)

Consider we are given $\mathrm{N} = 6$ measured sequence from the Lotka–Volterra model (6).

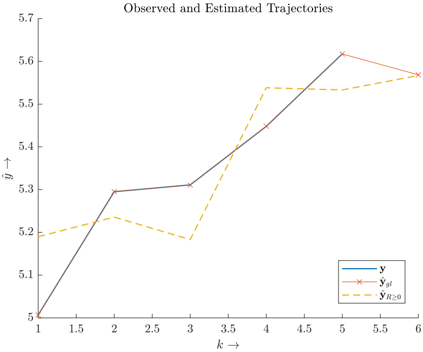

Figure: Estimation of $\mathrm{N} = 6$ datapoints where $\ell = 3$ requires a maximum 13 equations, which are of degree 5.

Overview

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