Least-squares Globally Optimal Misfit Modelling for SISO Systems

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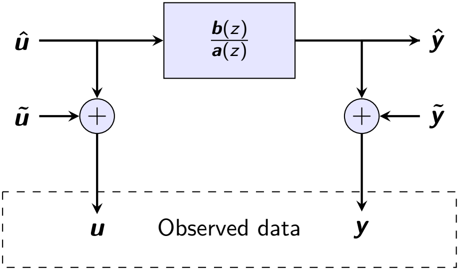
Misfit modelling



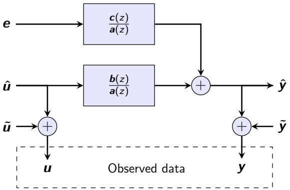
$$\min_{\tilde{\boldsymbol{u}},\tilde{\boldsymbol{y}},a_i,b_i} \quad \sigma^2 = ||\tilde{\boldsymbol{u}}||_2^2 + ||\tilde{\boldsymbol{y}}||_2^2 = \sum_{k=0}^{N-1}(u_k - \hat{u}_k)^2 + \sum_{k=0}^{N-1}(y_k - \hat{y}_k)^2,$$

$$\text{s.t.} \quad \hat{y}_{k+n} + a_1\hat{y}_{k+n-1} + \ldots + a_n\hat{y}_k = b_0\hat{u}_{k+n} + b_1\hat{u}_{k+n-1} + \ldots + b_n\hat{u}_k \quad \forall k \in \{0, \ldots, N-n-1\},$$

with $a_i, b_i \in \mathbb{R}, i = 1, \ldots, n$ the coefficients of $\boldsymbol{b}(z)/\boldsymbol{a}(z)$.

Misfit modelling: context

- Special case within misfit vs. latency framework *(Lemmerling and De Moor [4])*



- Subspace identification *(Van Overschee and De Moor [6])*
  - Linear algebra framework (QR, SVD)
  - Identification: Kalman state estimation + linear least-squares

- Behavioural systems theory *(Roorda [5], Willems [7])*
  - Set of difference equations $\rightarrow$ behaviour $\mathcal{B}$: $\hat{\boldsymbol{y}} \in \mathcal{B}$, $\tilde{\boldsymbol{y}} \in \mathcal{B}^{\perp}$
  - Identification: (Structured) total least squares *(De Moor [2])*

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Misfit modelling: methodology

- Inner problem: find optimal misfit $\tilde{\boldsymbol{y}}^*$ for given model and data
  - Linear problem $\rightarrow$ orthogonal projection
  - Optimal misfit is structured
- Outer problem: find optimal model $(\boldsymbol{a}, \boldsymbol{b})^*$ for given data
  - Substitute $\boldsymbol{y}^*$ in objective function
  - Characterise optima $\rightarrow$ system of multivariate polynomial eqs.
  - Solve the polynomial root-finding problem

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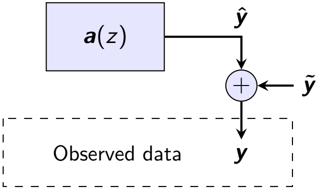
Autonomous misfit modelling[1]



$$\min_{\boldsymbol{a},\hat{\boldsymbol{y}}} \quad \sum_{k=0}^{N-1} (y_k - \hat{y}_k)^2,$$
$$\text{s.t.} \quad \hat{\boldsymbol{y}}\, a(z) = 0.$$

- LS-criterion implies orthogonality:

$$\sum_{k=0}^{N-1} (y_k - \hat{y}_k)^2 \text{ is minimal } \iff \hat{\boldsymbol{y}} \perp \tilde{\boldsymbol{y}}$$

[1] See *(De Moor [3])* for an in-depth discussion.

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Autonomous misfit modelling (inner)

- Canonical state-space realization $(\boldsymbol{A}, \boldsymbol{C})$ of $\boldsymbol{a}(z)$:

$$\boldsymbol{A} = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \dots \\ 0 & 0 & 0 & \dots & 1 \\ -a_n & -a_{n-1} & \dots & \dots & -a_1 \end{bmatrix}, \quad \text{and} \quad \boldsymbol{C} = \begin{bmatrix} 1 & 0 & \dots & 0 \end{bmatrix}$$

- $\mathcal{O} \in \mathbb{R}^{(N \times n)}$ is backward shift-invariant:

$$\underline{\mathcal{O}} \cdot \boldsymbol{A} = \overline{\mathcal{O}}$$

with $\mathcal{O} = \left[\boldsymbol{C}^T, (\boldsymbol{CA})^T, \dots, (\boldsymbol{CA}^{N-1})^T \right]^T$.

$$\Rightarrow \boxed{\hat{\boldsymbol{y}} \in \text{range}\,(\mathcal{O})}$$

Autonomous misfit modelling (inner)

$$
\boldsymbol{T_a} = \begin{bmatrix} a_n & 0 & \ddots & 0 \\ a_{n-1} & a_n & \ddots & 0 \\ \vdots & a_{n-1} & \ddots & \vdots \\ a_1 & \vdots & \ddots & a_n \\ 1 & a_1 & \ddots & a_{n-1} \\ 0 & 1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & a_1 \\ 0 & 0 & \ddots & 1 \end{bmatrix}
$$

- $\boldsymbol{T_a} \in \mathbb{R}^{(N \times N-n)}$
- $(\boldsymbol{T_a})^T \hat{\boldsymbol{y}} = 0$ and $\hat{\boldsymbol{y}} \in \text{range}\,(\mathcal{O})$

  $\Rightarrow \text{null}\,\left((\boldsymbol{T_a})^T\right) = \text{range}\,(\mathcal{O})$
- $\text{range}\,(\boldsymbol{T_a}) \perp \text{null}\,\left((\boldsymbol{T_a})^T\right)$

$$
\text{range}\,(\boldsymbol{T_a}) \oplus \text{range}\,(\mathcal{O}) = \mathbb{R}^N \quad \text{with} \quad \text{range}\,(\boldsymbol{T_a}) \perp \text{range}\,(\mathcal{O})
$$

$$
\Rightarrow \boxed{\tilde{\boldsymbol{y}} = \boldsymbol{T_a}\left((\boldsymbol{T_a})^T \boldsymbol{T_a}\right)^{-1} (\boldsymbol{T_a})^T \boldsymbol{y}}
$$

Autonomous misfit modelling (inner)

- For $N \to \infty$: discrete Beurling–Lax theorem[2]:

$$\text{range}\,(\boldsymbol{T_a}) \oplus \text{range}\,(\mathcal{O}) = \ell_2$$

  - range $(\boldsymbol{T_a})$ a forward shift-invariant subspace $\mathcal{M}$ of ℓ_2
  - range $(\mathcal{O})$ a backward shift-invariant subspace $\mathcal{M}^\perp$ of ℓ_2

- Continuous Beurling–Lax via isometric misfit model[3]:
  - Orthogonal decomposition of $\mathcal{H}_2$
  - *All-pass* completion of $\boldsymbol{a}(z)$ as inner-function:

$$H(z) = \frac{\boldsymbol{a_r}(z)}{\boldsymbol{a}(z)} = \frac{1 + a_1 z + \ldots + a_n z^n}{z^n + \cdots + a_{n-1} z + a_n}$$

[2] The original paper by Beurling *(Beurling [1])* derives the theorem for continuous functions in $\mathcal{H}_2$.

[3] $Y(z)$ denotes the Z-transform of $\boldsymbol{y}$, $\tilde{Y}(z)$ and $\hat{Y}(z)$ are defined similarly.

Autonomous misfit modelling (outer)

- First-order necessary conditions for optimality:

$$\min_{\boldsymbol{a}} \quad \sigma^2 = ||\tilde{\boldsymbol{y}}||_2^2 = \boldsymbol{y}^T \boldsymbol{T_a}(\boldsymbol{T_a}^T \boldsymbol{T_a})^{-1} \boldsymbol{T_a} \boldsymbol{y}$$
$$\Rightarrow \quad \frac{\partial \sigma^2}{\partial a_i} = 0, \quad \forall i = 1, \ldots, n,$$

  is a system of n polynomial equations in n variables.

- Common roots characterize all the stationary points

  $\longrightarrow$ select globally optimal solution(s)

- Walsh's theorem

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SISO misfit modelling

$$\underbrace{\begin{bmatrix} a_n & -b_n & a_{n-1} & -b_{n-1} & \dots & a_1 & -b_1 & 1 & -b_0 & 0 & \dots & 0 & 0 \\ 0 & 0 & a_n & -b_n & a_{n-1} & -b_{n-1} & \dots & a_1 & -b_1 & 1 & b_0 & \dots & 0 \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ 0 & 0 & \dots & & a_n & -b_n & a_{n-1} & -b_{n-1} & \dots & a_1 & -b_1 & 1 & b_0 \end{bmatrix}}_{\boldsymbol{T_{a,b}}} \underbrace{\begin{bmatrix} \hat{w}_0 \\ \hat{w}_1 \\ \vdots \\ \hat{w}_{N-1} \end{bmatrix}}_{\hat{\boldsymbol{w}}} = \mathbf{0},$$

where:

$$\hat{\boldsymbol{w}} = \begin{bmatrix} \hat{y}_0 & \hat{u}_0 & \hat{y}_1 & \hat{u}_1 & \dots & \hat{y}_N & \hat{u}_N \end{bmatrix}.$$

- $\boldsymbol{T_{a,b}} \in \mathbb{R}^{(2N-2n \times 2N)}$
- Treat as autonomous model of order $2n$?
  - Optimal misfit: $\tilde{\boldsymbol{w}} = \boldsymbol{T_{a,b}} \left((\boldsymbol{T_{a,b}})^T \boldsymbol{T_{a,b}} \right)^{-1} (\boldsymbol{T_{a,b}})^T \boldsymbol{w}$
  - Optimal model: $\sigma^2 = ||\tilde{\boldsymbol{w}}||_2^2 = \boldsymbol{w}^T \boldsymbol{T_{a,b}} (\boldsymbol{T_{a,b}^T} \boldsymbol{T_{a,b}})^{-1} \boldsymbol{T_{a,b}} \boldsymbol{w}$

Questions?

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[1] A. Beurling. On two problems concerning linear transformations in Hilbert space. *Acta Mathematica*, 81:239 – 255, 1949.

[2] B. De Moor. Total least squares for affinely structured matrices and the noisy realization problem. *IEEE Transactions on Signal Processing*, 42(11):3104 – 3113, 1994.

[3] B. De Moor. Least squares optimal realisation of autonomous LTI systems is an eigenvalue problem. *Communications in Information and Systems*, 20(2):163 – 207, 2020.

[4] P. Lemmerling and B. De Moor. Misfit versus latency. *Automatica*, 37:2057 – 2067, 2001.

[5] B. Roorda. Algorithms for global total least square modelling of finite multivariable time series. *Automatica*, 1995.

[6] P. Van Overschee and B. De Moor. *Subspace Identification for Linear Systems: Theory – Implementation – Applications*. Kluwer Academic Publishers, 1996.

[7] J. C. Willems. From time series to linear system, Part I: Finite dimensional linear time invariant systems; Part II: Exact modelling; Part III: Approximate modelling. *Automatica*, 22/23(5,6,1):561 – 580, 675 – 694, 87 – 115, 1986, 1987.

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