Data-driven Prediction and Control Through the Lens of System Identification

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Paradigm shift in Engineering

- From component-oriented to system-level design (smart cities, intelligent transportation, industrial automation..)
- From first-principles modelling to data-driven







Paradigm shift in Engineering

- From component-oriented to system-level design (smart cities, intelligent transportation, industrial automation..)
- From first-principles modelling to data-driven
- Methods and tools must adapt, but not the foundational principles







 Standing on the shoulders of giants (optimal, robust, adaptive control, system identification, dynamical systems theory)..



- Standing on the shoulders of giants (optimal, robust, adaptive control, system identification, dynamical systems theory)..
- ..seeking new peaks (statistical learning, optimization, information theory)





Methods for simulating and controlling dynamical systems **directly** from data \rightarrow no knowledge of an explicit model is required

• Behavioral system theory (noise-free data)

(New) Direct data-driven methods through the lens of a(n old) giant

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- Behavioral system theory (noise-free data)
- Recent works towards a stochastic counterpart [1-2]

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¹Pan Ou Faulwasser, "On a Stochastic Fundamental Lemma and Its Use for Data-Driven MPC" 2021

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(New) Direct data-driven methods through the lens of a(n old) giant

Methods for simulating and controlling dynamical systems directly from data

 \rightarrow no knowledge of an explicit model is required

- Behavioral system theory (noise-free data)
- Recent works towards a stochastic counterpart [1-2]
- Today: System identification-based statistical reasoning
- Framework for simulation, filtering and control from noisy data

Joint work with

Mingzhou Yin



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1 A Bayesian perspective on the Fundamental Lemma

2 Confidence regions for noisy predictions

3 Informative data for simulation problems

Representation-free perspective on dynamical systems as sets of trajectories [Willems, 1987]

- The *Fundamental Lemma* [Willems, 2005] arguably a driving force behind recently proposed subspace-type data-driven analysis and control methods
- Non-parametric representation of an LTI system by the image of a Hankel data matrix

$$z_{[i,j]} o \mathcal{H}_L(z_{[i,j]}) := egin{bmatrix} z_i & z_{i+1} & \cdots & z_{N+i-L} \ z_{i+1} & z_{i+2} & \cdots & z_{N+i-L+1} \ dots & dots & dots & dots \ z_{i+L-1} & z_{i+L} & \cdots & z_{N+i-1} \end{bmatrix}$$

 $z_{[i,j]}$ is: **persistently exciting** (PE) of order L if $\mathcal{H}_L(z_{[i,j]})$ has full row rank

• Can we use raw data to span the I/O behavior of the system?

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Minimal linear time-invariant system

$$x_{t+1} = Ax_t + Bu_t$$
$$y_t = Cx_t + Du_t$$

 $x \in \mathbb{R}^{n_x}$ is the state, $u \in \mathbb{R}^{n_u}$ is the input, and $y \in \mathbb{R}^{n_y}$ is the output (the lag l is the smallest integer i such that the ext. observability matrix \mathcal{O}_i has rank n_x).

Direct prediction/simulation problem

Given: an input-output data trajectory $(u_{d [0,N-1]}, y_{d [0,N-1]})$.

Goal: for any *input* simulation trajectory $u_{s [0,L_s-1]}$, and any initial condition, find the (unique) *output* simulation trajectory $y_{s [0,L_s-1]}$.

Fundamental lemma

[Willems, 2005]

Controllable LTI system with McMillan degree n_x , I/O trajectory ($u_{d [0,N-1]}, y_{d [0,N-1]}$). If $u_{d [0,N-1]}$ is PE of order $L + n_x$, then ($u_{t [0,L-1]}, y_{t [0,L-1]}$) is an I/O trajectory **iff** there exists g s.t.

$$\begin{bmatrix} u_{t \ [0,L-1]} \\ y_{t \ [0,L-1]} \end{bmatrix} = \begin{bmatrix} \mathcal{H}_L(u_{d \ [0,N-1]}) \\ \mathcal{H}_L(y_{d \ [0,N-1]}) \end{bmatrix} g$$

Fundamental lemma & direct simulation

[Willems, 2005]

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Given $L_0 \ge I$ (define $L_s = L - L_0$), $y_{s [0, L_s - 1]}$ (y_s) is the unique output trajectory with past trajectory $(u_{ini \ [0, L_0 - 1]}, y_{ini \ [0, L_0 - 1]})$ (u_{ini}, y_{ini}) and input trajectory $u_{s \ [0, L_s - 1]}$ (u_s), iff there exists g s.t.

$$\begin{bmatrix} \mathbf{u}_{\text{ini}} \\ \mathbf{u}_{\text{s}} \\ \hline \mathbf{y}_{\text{ini}} \\ \mathbf{y}_{\text{s}} \end{bmatrix} = \begin{bmatrix} U \\ Y \end{bmatrix} g = \begin{bmatrix} U_{p} \\ U_{f} \\ \hline Y_{p} \\ Y_{f} \end{bmatrix} g = \begin{bmatrix} \mathcal{H}_{L}(u_{\text{d}} [0, N-1]) \\ \mathcal{H}_{L}(y_{\text{d}} [0, N-1]) \end{bmatrix} g$$

Noise-free case abstraction

The trajectory can be partitioned into a known and unknown part

$$\frac{\begin{bmatrix} \hat{z} \\ z \end{bmatrix}}{\begin{bmatrix} z \end{bmatrix}} = \frac{\begin{bmatrix} u \\ y \end{bmatrix}}{\begin{bmatrix} y \end{bmatrix}}, \quad Z = \begin{bmatrix} U \\ Y \end{bmatrix}, \quad \left(e.g. \ \hat{z} = \begin{bmatrix} u_{ini} \\ u_s \\ y_{ini} \end{bmatrix}, z = \begin{bmatrix} y_s \end{bmatrix} \right)$$

 $\hat{z} = Z_1 g \rightarrow g^*(\hat{z}, Z_1)$, from: known and data, to g $z = Z_2 g^* = Z_2 g^*(\hat{z}, Z_1)$ from: g and data, to unknown The trajectory can be partitioned into a known and unknown part

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 $z = \mathcal{F}_{Z}(\hat{z}), \quad (y_{s} = \mathcal{F}_{Z}(u_{ini}, u_{s}, y_{ini}) \text{ input-output mapping})$

Noisy case *regression* viewpoint

$$\begin{split} \tilde{y}_i^{d} &= y_i^{d} + w_i^{d}, \qquad w_i^{d} \sim \mathcal{N}(0, \sigma_y^2 I_p) \\ \tilde{u}_i^{d} &= u_i^{d} + v_i^{d}, \qquad v_i^{d} \sim \mathcal{N}(0, \sigma_u^2 I_m) \\ \tilde{y}_i^{ini} &= y_i^{ini} + w_i^{ini}, \qquad w_i^{ini} \sim \mathcal{N}(0, \sigma_{p,y}^2 I_p) \\ \tilde{u}_i^{ini} &= u_i^{ini} + v_i^{ini}, \qquad v_i^{ini} \sim \mathcal{N}(0, \sigma_{p,u}^2 I_m) \end{split}$$

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The Signal Matrix Model (SMM)

z

The maximum-a-posteriori (MAP) estimate of the trajectory is

$$f^{*}(g) = \arg \max_{z} \underbrace{p(z|\hat{z})}_{\propto p(\hat{z}|z)p(z)} = \sum_{z}(g) \left(\sum_{z}(g) + \sum_{w}\right)^{-1} \hat{z} + \sum_{w} \left(\sum_{z}(g) + \sum_{w}\right)^{-1} Zg$$

(MAP)

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where g is obtained through maximum marginal-likelihood (ML)

$$g^* \in \arg\min_{g} \underbrace{-p(\hat{z}|g)}_{\log \det (\Sigma_z(g) + \Sigma_w) + (\hat{z} - Zg)^\top (\Sigma_z(g) + \Sigma_w)^{-1} (\hat{z} - Zg)}$$
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ML: from known and data, to $g \rightarrow MAP$: from g and data, to unknown.

(MAP)

(ML)

Example 1: Direct data-driven simulation

$$\hat{z} = \begin{bmatrix} u_{\text{ini}} \\ u_{\text{s}} \\ y_{\text{ini}} \\ 0 \end{bmatrix}, \ z = \begin{bmatrix} 0 \\ 0 \\ 0 \\ y_{\text{s}} \end{bmatrix}, \ \Sigma_{w} = \begin{bmatrix} \Sigma_{u_{i}} & 0 & 0 & 0 \\ 0 & \Sigma_{u_{s}} & 0 & 0 \\ 0 & 0 & \Sigma_{y_{i}} & 0 \\ 0 & 0 & 0 & \Sigma_{y_{s}} \end{bmatrix}, \ \Sigma_{u_{i}} = \Sigma_{u_{s}} = \Sigma_{y_{i}} = 0, \ \Sigma_{y_{s}} = \infty \rightarrow \qquad y_{\text{s}} = Y_{f}g^{*}$$

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Truncated Infinite Impulse Response (IIR) estimation, comparison with Least-Squares



Estimates within two standard deviations Magenta: noisy data; blue: noise-free data

Example 2: Direct data-driven control

$$\begin{split} \min_{\hat{\mathbf{u}},\hat{\mathbf{y}}} & \sum_{k=0}^{L_{g}-1} \left(\left\| \hat{y}_{k} - y_{k}^{\text{ref}} \right\|_{Q}^{2} + \left\| \hat{u}_{k} - u_{k}^{\text{ref}} \right\|_{R}^{2} \right) \\ \text{s.t.} & \left(\begin{bmatrix} \mathsf{u}_{\text{ini}} \\ \hat{\mathbf{u}} \end{bmatrix}, \begin{bmatrix} \mathsf{y}_{\text{ini}} \\ \hat{\mathbf{y}} \end{bmatrix} \right) \text{ is a trajectory,} \\ & \hat{\mathbf{u}} \in \mathcal{U}, \hat{\mathbf{y}} \in \mathcal{Y}, \end{split}$$

$$\hat{z} = \begin{bmatrix} u_{\text{ini}} \\ u^{\text{ref}} \\ y_{\text{ini}} \\ y^{\text{ref}} \end{bmatrix}, \quad z = \begin{bmatrix} 0 \\ \hat{u} \\ 0 \\ \hat{y} \end{bmatrix}, \quad z = \begin{bmatrix} 0 \\ \hat{u} \\ 0 \\ \hat{y} \end{bmatrix}, \quad \sum_{u_s} = R^{-1} \otimes I_{L_s} \\ \sum_{y_i} = \sigma_{p,y}^2 I_p \otimes I_{L_s} \\ \sum_{y_s} = Q^{-1} \otimes I_{L_s} \end{bmatrix}$$

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CL cost comparison with competitors

$$\hat{z} = \begin{bmatrix} u_{\text{ini}} \\ u^{\text{ref}} \\ y_{\text{ini}} \\ y^{\text{ref}} \end{bmatrix}, \quad z = \begin{bmatrix} 0 \\ \hat{u} \\ 0 \\ \hat{y} \end{bmatrix}, \quad \sum_{i,j \in \mathcal{T}} \frac{z_{i,j}}{z_{i,j}} = \sigma_{p,y}^2 I_m \otimes I_{L_s} \\ \sum_{i,j \in \mathcal{T}} \frac{z_{i,j}}{z_{i,j}} = \sigma_{p,y}^2 I_p \otimes I_{L_s} \\ \sum_{i,j \in \mathcal{T}} \frac{z_{i,j}}{z_{i,j}} = \sigma_{p,y}^2 I_p \otimes I_{L_s} \end{bmatrix}$$



Adaptation using online data

Confidence regions for data-driven prediction

What is the error associated with predicting y_s from noisy data?

Confidence regions for data-driven prediction

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Prototype of stochastic data-driven predictors

Existing algorithms ^a can be expressed as

where λ is algorithm-dependent.

^aSubspace predictor [Fiedler, 2021], SMM, Wasserstein distance minimization [Lian, 2021]

Goal: obtain **probabilistic** and **deterministic** confidence regions

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(PRED

SMM as data-driven predictor

- Output noise (y_{ini}, Y_p, Y_f)
- Specific matrix structure: *M* length-*L* input-output trajectories

$$z_i^d = \operatorname{col}\left(u_{t_i}^d, \cdots, u_{t_i+L-1}^d, y_{t_i}^d, \cdots, y_{t_i+L-1}^d\right) \in \mathbb{R}^{L(n_u+n_y)}, \quad i = 0, \cdots, M-1$$

Matrix $Z = \begin{bmatrix} z_0^d & \cdots & z_{M-1}^d \end{bmatrix}$ is mosaic Hankel $(t_{i+1} = t_i + 1)$ or Page $(t_{i+1} = t_i + L)$

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The ML estimate of g solves

$$\min_{g} \operatorname{logdet} \left(\begin{bmatrix} \Sigma_{Y_{p}}(g) & 0 \\ 0 & \Sigma_{Y_{f}}(g) \end{bmatrix} + \begin{bmatrix} \Sigma_{y_{i}} & 0 \\ 0 & 0 \end{bmatrix} \right) + \delta^{\top} \left(\begin{bmatrix} \Sigma_{Y_{p}}(g) & 0 \\ 0 & \Sigma_{Y_{f}}(g) \end{bmatrix} + \Sigma_{y_{i}} \right)^{-1} \underbrace{\delta}_{Y_{p}g - y_{ini}},$$

where $\Sigma_{y_i} = \sigma_{p,y}^2 I_{n_y L_0}$, $\Sigma_{Y_p}(g) = \sigma_{p,y}^2 \|g\|_2^2 I_{n_y L_0}$, $\Sigma_{Y_f}(g) = \sigma_y^2 \|g\|_2^2 I_{n_y L_s}$.

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The ML estimate of g solves

$$\min_{g} \text{ logdet} \left(\begin{bmatrix} \Sigma_{Y_{\rho}}(g) & 0 \\ 0 & \Sigma_{Y_{f}}(g) \end{bmatrix} + \begin{bmatrix} \Sigma_{y_{i}} & 0 \\ 0 & 0 \end{bmatrix} \right) + \delta^{\top} \left(\begin{bmatrix} \Sigma_{Y_{\rho}}(g) & 0 \\ 0 & \Sigma_{Y_{f}}(g) \end{bmatrix} + \Sigma_{y_{i}} \right)^{-1} \underbrace{\delta}_{Y_{\rho}g - y_{ini}},$$

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Quadratic approximation of the obj. about $g = \hat{g}$ gives (PRED) with $\lambda = n_y \left(L_0 \sigma_{p,y}^2 / \|\hat{g}\|_2^2 + L \sigma_y^2 \right)$.

Confidence regions for data-driven predictors

Probabilistic and robust (in probability) bounds for PRED

Consider prediction $y = \mathcal{F}_Z(\cdot)$ of true output y_0 . Then

$$\mathbf{y} - \mathbf{y}_{0} \mid \boldsymbol{g}, \delta \sim \mathcal{N} \left(\boldsymbol{\Gamma} \delta, \underbrace{\begin{bmatrix} -\boldsymbol{\Gamma} & \boldsymbol{I}_{n_{y}L'} \end{bmatrix} \begin{bmatrix} \boldsymbol{\Sigma}_{\boldsymbol{Y}_{p}}(\boldsymbol{g}) & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Sigma}_{\boldsymbol{Y}_{f}}(\boldsymbol{g}) \end{bmatrix} \begin{bmatrix} -\boldsymbol{\Gamma}^{\top} \\ \boldsymbol{I}_{n_{y}L'} \end{bmatrix} + \boldsymbol{\Gamma} \boldsymbol{\Sigma}_{\boldsymbol{y}_{i}} \boldsymbol{\Gamma}^{\top} \\ \underbrace{\boldsymbol{\Sigma}} \right)$$

where $\Gamma = \operatorname{col} \left(CA^{L_0}, \cdots, CA^{L-1} \right) \operatorname{col} \left(C, \cdots, CA^{L_0-1} \right)^{\dagger}$.

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where $\Gamma = \operatorname{col} \left(CA^{L_0}, \cdots, CA^{L-1} \right) \operatorname{col} \left(C, \cdots, CA^{L_0-1} \right)^{\dagger}$.

The true output y_0 belongs w.p. p to

$$\mathcal{Y} = \left\{ \tilde{y} \mid \left(y - \tilde{y} - \Gamma \delta \right)^{\mathsf{T}} \Sigma^{-1} \left(y - \tilde{y} - \Gamma \delta \right) \leq \mu_{\mathsf{P}} \right\}, \quad \mathsf{F}_{\chi^{2}(L')}(\mu_{\mathsf{P}}) = \mathsf{P}$$

 $F_{\chi^2(d)}(\cdot)$ is the cumulative distribution function of the χ^2 -distribution with d degrees of freedom.

Insights from the proof



Insights from the proof

•
$$y - y_0 = \underbrace{E_f g}_{\text{noise in } Y_f} + \underbrace{y^-}_{\text{wrong initial condition}}$$

 $E_f = Y_f - Y_f^0; \quad y^- \text{ free response from I.C. } u_{\text{ini}}^- = 0, \ y_{\text{ini}}^- = Y_p^0 g - y_{\text{ini}}^0$
• $y_{\text{ini}}^- = \delta + (y_{\text{ini}} - y_{\text{ini}}^0) - E_p g$

$$\mathbf{y}^{-} = \begin{bmatrix} CA^{L_0} \\ \vdots \\ CA^{L-1} \end{bmatrix} \mathbf{x}^{-}, \ \mathbf{y}_{\mathsf{ini}}^{-} = \begin{bmatrix} C \\ \vdots \\ CA^{L_0-1} \end{bmatrix} \mathbf{x}^{-} \Rightarrow \mathbf{y}^{-} = \Gamma \mathbf{y}_{\mathsf{ini}}^{-}$$

Insights from the proof

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• Holds for general predictors

$$\mathcal{F}_{Z}(\cdot) = Y_{f}g, \quad \text{s.t.} \quad \begin{bmatrix} U_{p} \\ U_{f} \\ Y_{p} \end{bmatrix} g = \begin{bmatrix} u_{\text{ini}} \\ u_{s} \\ y_{\text{ini}} + \delta \end{bmatrix}$$

X Confidence regions depend on model's quantities (range space of observability); no closed form solution in more general (noise and matrix structures) cases

- X Confidence regions depend on model's quantities (range space of observability); no closed form solution in more general (noise and matrix structures) cases
 - Quantification of the prediction error due to noisy information; tool for designing new predictors

Minimum mean-squared error predictor

The minimum MSE predictor of the class (PRED) is

$$\mathcal{F}_{Z}(\cdot) = Y_{f} \operatorname{argmin}_{g(,\delta)} \underbrace{\delta^{\top} \Gamma^{\top} \Gamma \delta + \operatorname{tr}(\Sigma)}_{\mathsf{MSE}(g, \delta)} = \operatorname{argmin}_{g(,\delta)} \|\delta\|_{Q}^{2} + \lambda_{\mathsf{MSE}} \|g\|_{2}^{2}$$
s.t.
$$\begin{bmatrix} U_{p} \\ U_{f} \\ Y_{p} \end{bmatrix} g = \begin{bmatrix} u_{\mathsf{ini}} \\ u_{\mathsf{s}} \\ y_{\mathsf{ini}} + \delta \end{bmatrix}$$
(MSE-PRED)

Numerical experiments

Two-output 4th order system. L = 10, $L_0 = 8$, M = 80, $\sigma^2 = 0.1$, p = 0.90, unit Gaussian input.



CR of different predictors (based on true Γ).

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CR of different predictors (based on true Γ).

1000 randomly generated systems (states between 3 and 8). L = 20, $L_0 = 8$, L' = 12, M = 320, unit Gaussian input.

Comparison of the empirical MSE.

	$\sigma^2 = 0.1$	$\sigma^2 = 0.5$	$\sigma^2 = 1$
Sub	0.115	0.558	1.106
SMM	0.099	0.476	0.915
WD	0.113	0.548	1.091
MSE-SMM	0.096	0.460	0.897
MSE-MB	0.094	0.435	0.833

How to best choose u_d ?

- The Fundamental Lemma is effectively an experiment design result
- Goal: go beyond PRBS (Pseudo Random Binary Signals) and randomly selected input..
- Data informativity for the noisy given-input simulation problem
- Informativity encompasses both the selection of the input and the matrix structure (Hankel/Page)

Bayesian design of experiment (DOE)

Interpret the output trajectory y_s as a random variable.

 $y^1_{s} \sim \mathcal{N}(0, \Sigma_{\mathsf{K}}) \quad
ightarrow extsf{Prior} extsf{distribution}$

$$y_{s}^{2} \sim \mathcal{N}(Y_{f}g^{*}, \underbrace{\Sigma_{Y_{f}}(g^{*})}_{\text{sub-matrix of } \Sigma_{z}(g^{*})}) \rightarrow Data-based \ estimate \ (via \ SMM)$$

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Combine prior and data-based estimates to provide the posterior

$$(y_{\mathsf{s}}|(u_{\mathsf{d}},y_{\mathsf{d}})) \sim \mathcal{N}(\mathcal{K}(Y_{f}g^{*}),\Sigma_{\mathsf{post}}) \quad o \quad \textit{Posterior} ext{ of } y_{\mathsf{s}}$$

where $K = \Sigma_{K} (\Sigma_{K} + \Sigma_{Y_{f}})^{-1}$ is the Kalman gain and $\Sigma_{post} = \Sigma_{K} - \Sigma_{K} (\Sigma_{K} + \Sigma_{Y_{f}})^{-1} \Sigma_{K}$ is the posterior covariance.

The experiment is **meaningful** when the *difference* between prior and posterior distributions is **maximized**.

Mutual information and information criterion

Mutual information [Cover, 1991] of two multivariate random variables x and y

$$I(x; y) = H(x) + H(y) - H(x, y) = H(x) - H(x|y)$$

$$\Rightarrow I(y_{s}; (u_{d}, y_{d})) = \mathbb{E} \left[\underbrace{D(y_{s}|(u_{d}, y_{d})||p(y_{s}))}_{KL \text{ divergence between prior and posterior trajectory}} \right]$$

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Information criterion for SMM

If $\Sigma_{Y_f}(g) = \sigma_y^2 \|g\|_2^2 I_{n_y L_s}$, then there exists a function f such that

$$I(y_{s}; (u_{d}, y_{d})) = f(||g||_{2}^{2}, \Sigma_{K})$$

where $f(||g||_2^2, \cdot)$ is monotonically decreasing.

Bi-level input design problem

The input data trajectory can be designed to maximize the information: $u_{\rm d~[0,N-1]}\to U,\,Y\to g^*\to I$

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$$\begin{split} & \min_{g,u_{d}} \|g\|_{2}^{2} \rightarrow \quad information \ criterion \\ & \text{s.t.} \quad u_{d} \in \mathcal{U} \quad \rightarrow \quad input \ constraints \\ & g \in \underset{g \in \mathcal{G}, u_{d}}{\text{srg min}} \quad \text{logdet}(\Sigma_{y}(g)) + \begin{bmatrix} Y_{p}g - y_{\text{ini}} \\ 0 \end{bmatrix}^{\top} \Sigma_{y}^{-1}(g) \begin{bmatrix} Y_{p}g - y_{\text{ini}} \\ 0 \end{bmatrix} \rightarrow \quad ML \ estimator \end{split}$$

Two **challenges** associated with the bi-level program:

- Inner-problem depends on Y_p (implicitly function of u_d)
- Dealing with the bi-level program

A. lannelli (ETH)

Truncated IIR estimation with Hankel matrices

Fit metric:
$$W = 100 \left(1 - \left[\frac{\sum_{i=0}^{L_s-1} (y_{s,i} - \hat{y}_{s,i})^2}{\sum_{i=0}^{L_s-1} (y_{s,i} - \overline{y}_s)^2} \right]^{1/2} \right)$$



- Optimally designed input perform better than standard PE inputs
- Informativity key to achieve the improvement

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• Informativity key to achieve the improvement



- Optimal input do not have "intuitive" shape
- Impact of DOE is a function of the SNR

- Statistical framework for the direct prediction and control problems
- First prediction error bounds and data informativity studies in this implicit non-parametric setting
- Towards a principled way to reason about robustness in data-driven problems

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- Stochastic MPC formulation based on prediction error-bounds
- Informative input for control (dual control in direct problems)**
- Adaptive signal matrices: when and why?

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Thank you for your attention!