

Outline

Introduction: data, model class, approximation

Approximation error–model complexity trade-off

System identification \leftrightarrow low-rank approximation

Solution methods: variable projection

Exercises

Outline

Introduction: data, model class, approximation

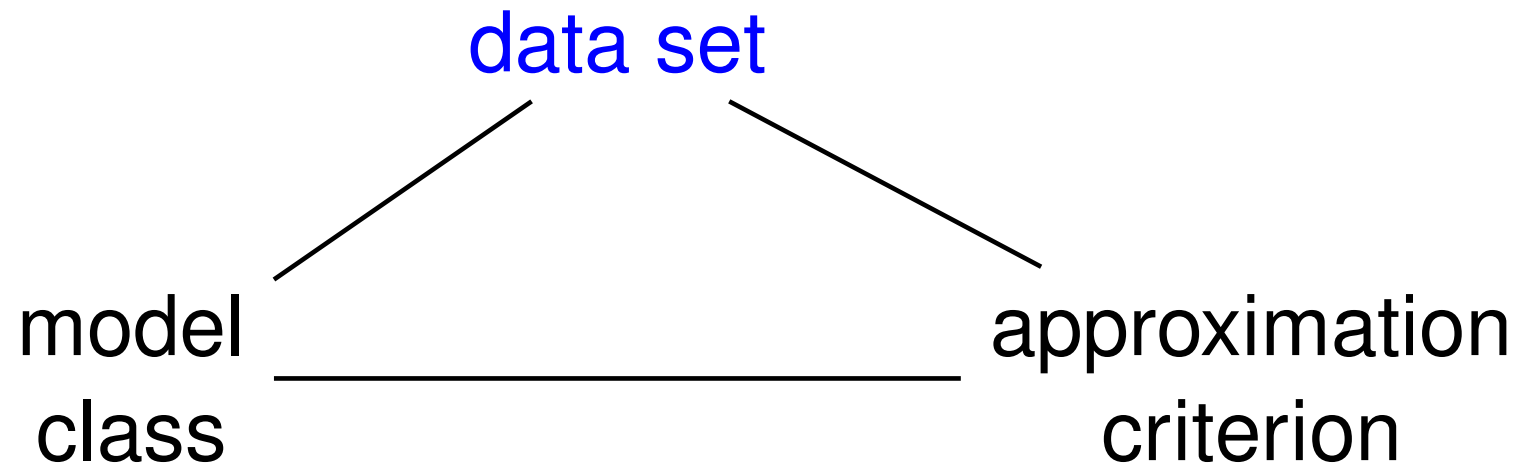
Approximation error–model complexity trade-off

System identification \leftrightarrow low-rank approximation

Solution methods: variable projection

Exercises

First is the data ...

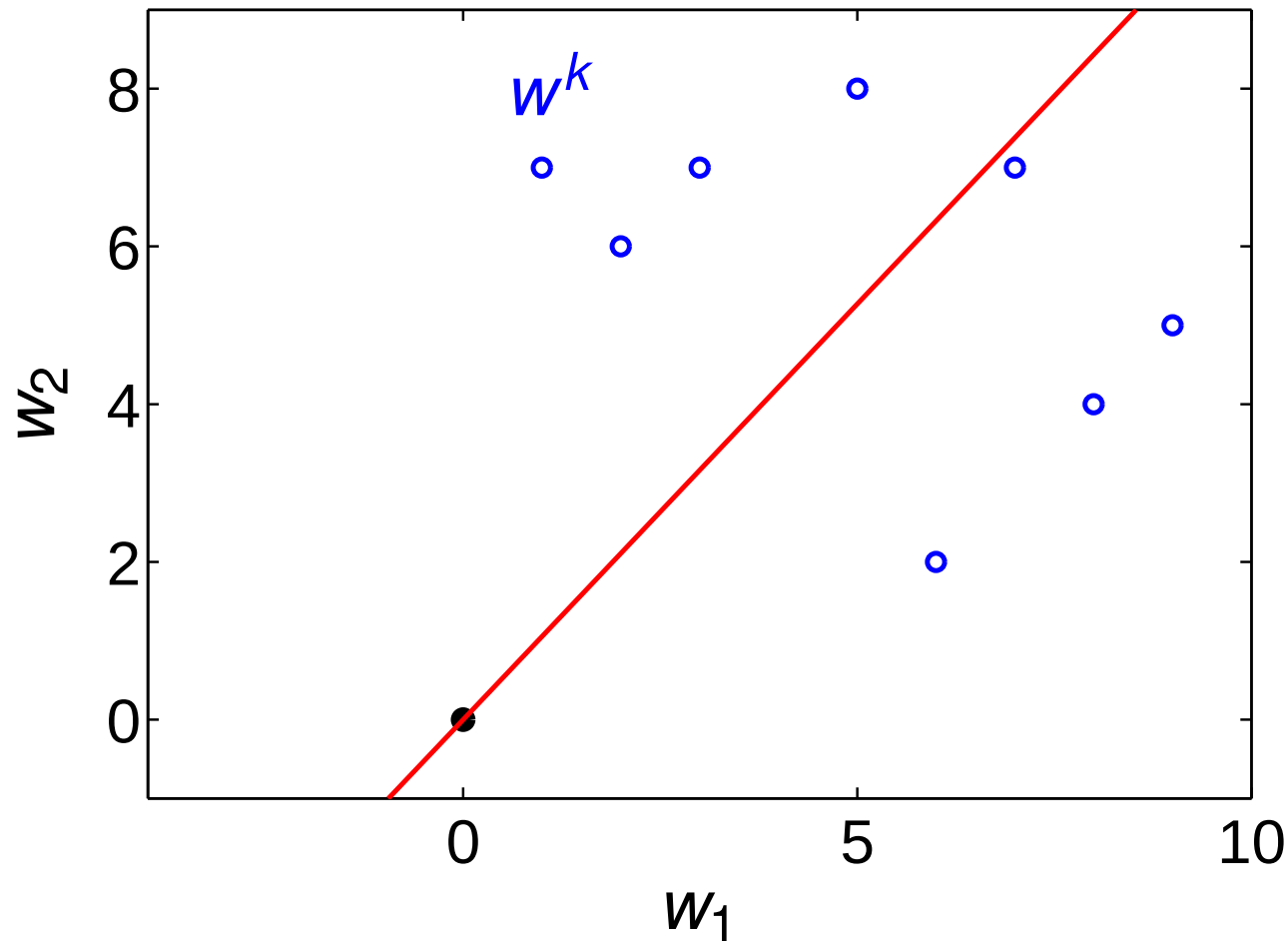


Line fitting (linear static model)

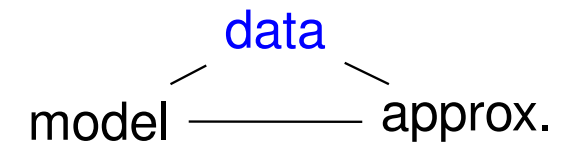
data
model ——— approx.

w^1, \dots, w^N — data points

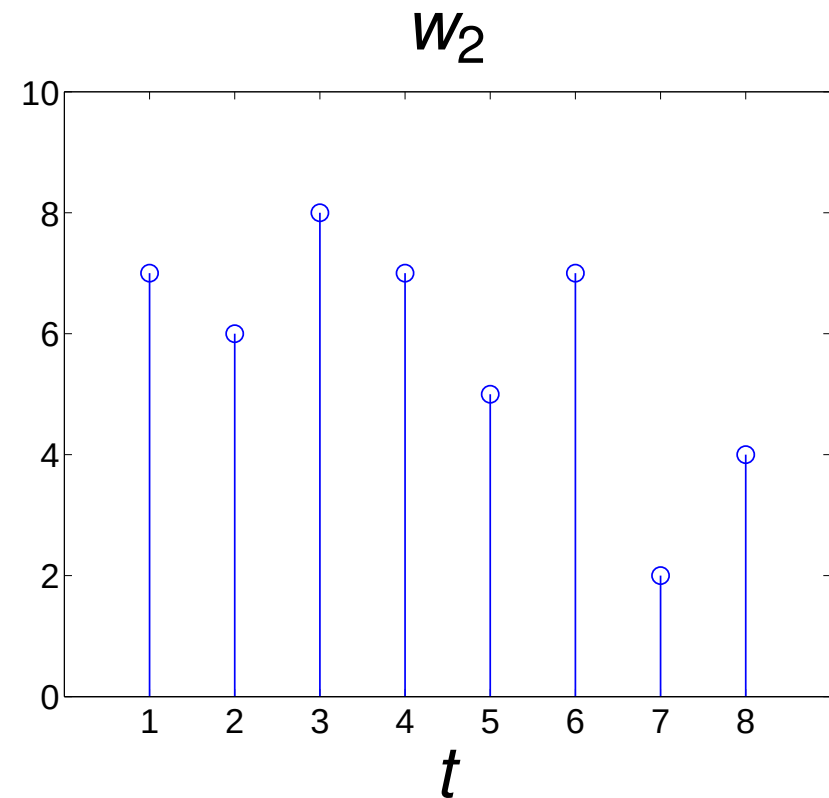
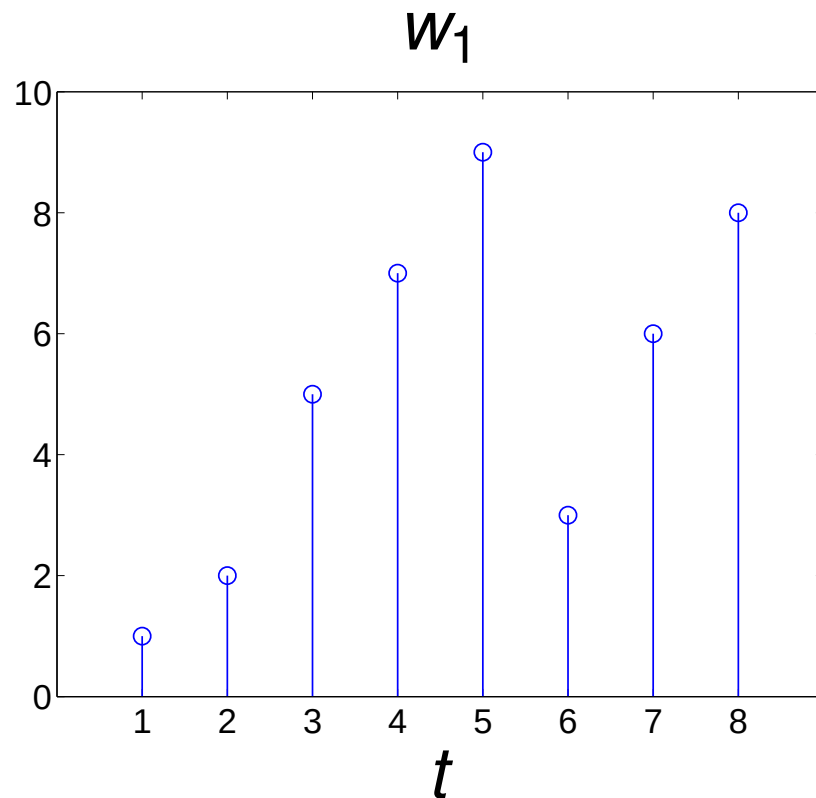
(the order is not important)



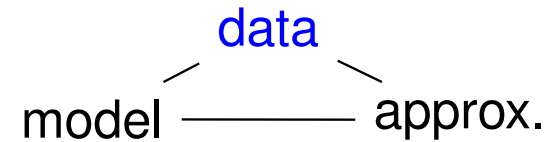
Time series data (dynamic model)



$w(1), \dots, w(T)$ — samples in time (the order is important)

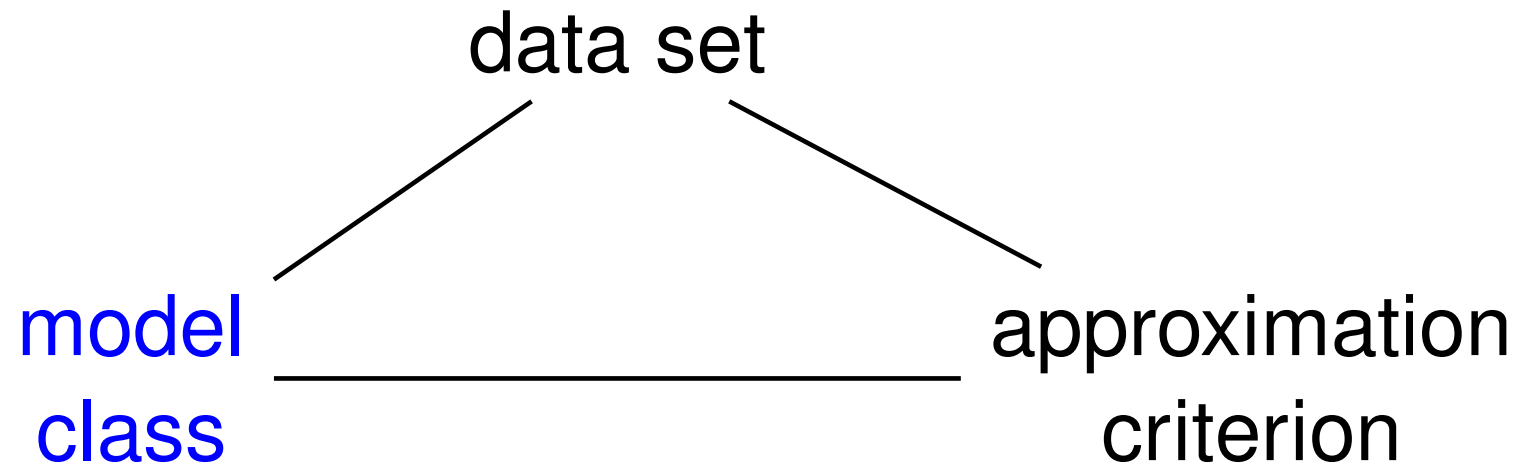


Summary: data



- ▶ the data is a set $w = \{ w^1, \dots, w^N \}$
- ▶ of vector valued $w^k = \begin{bmatrix} w_1^k \\ \vdots \\ w_q^k \end{bmatrix}$
- ▶ time series $w_i^k = (w_i^k(1), \dots, w_i^k(T_k))$
 - N — # of repeated experiments
 - q — # of variables
 - T_k — # of time samples in the k th exp.
- ▶ in static problems, $T_1 = \dots = T_N = 1$

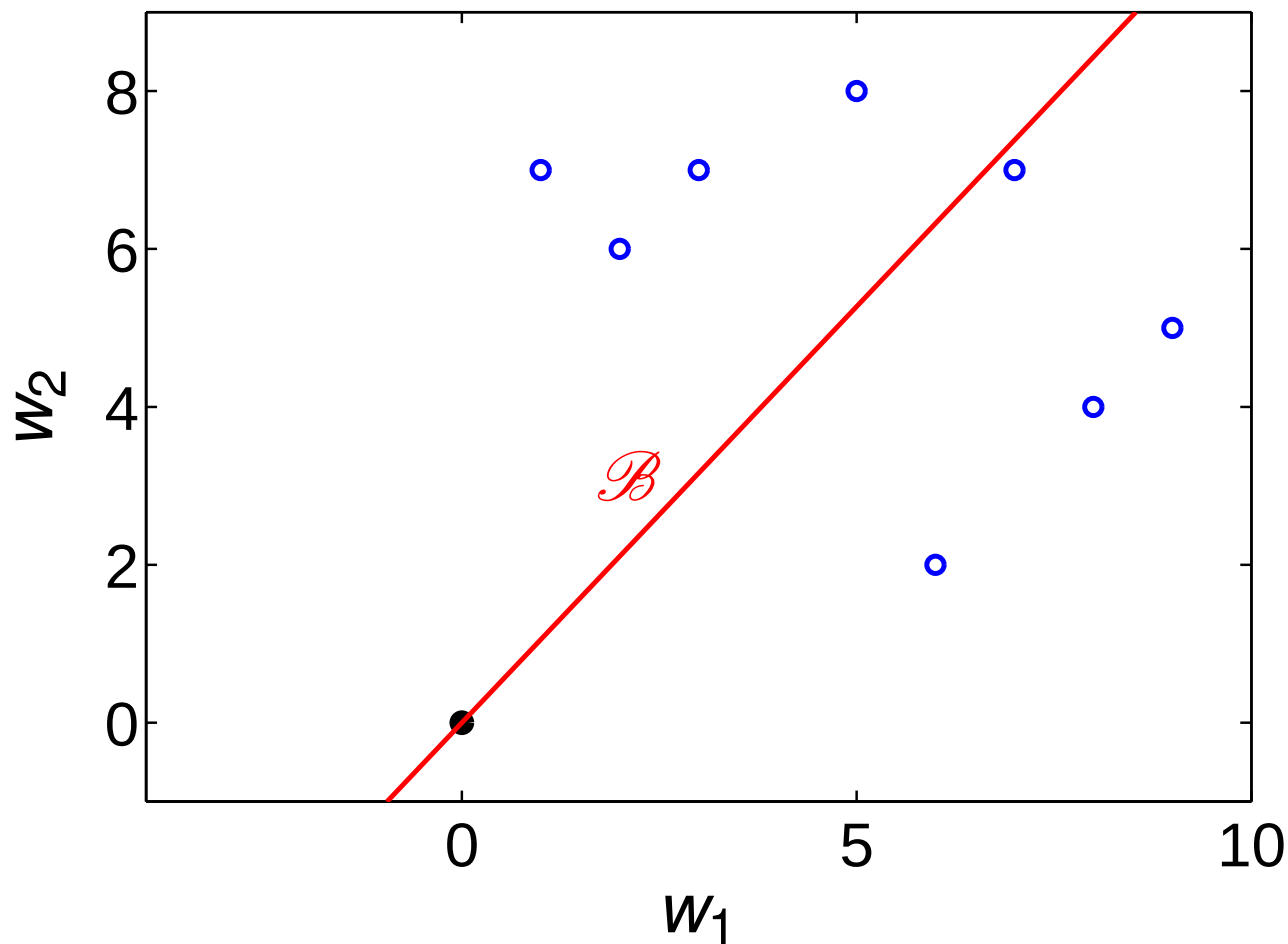
Next is the model class . . .



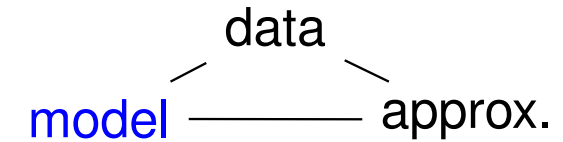
Line fitting (linear static model)

data
model ——— approx.

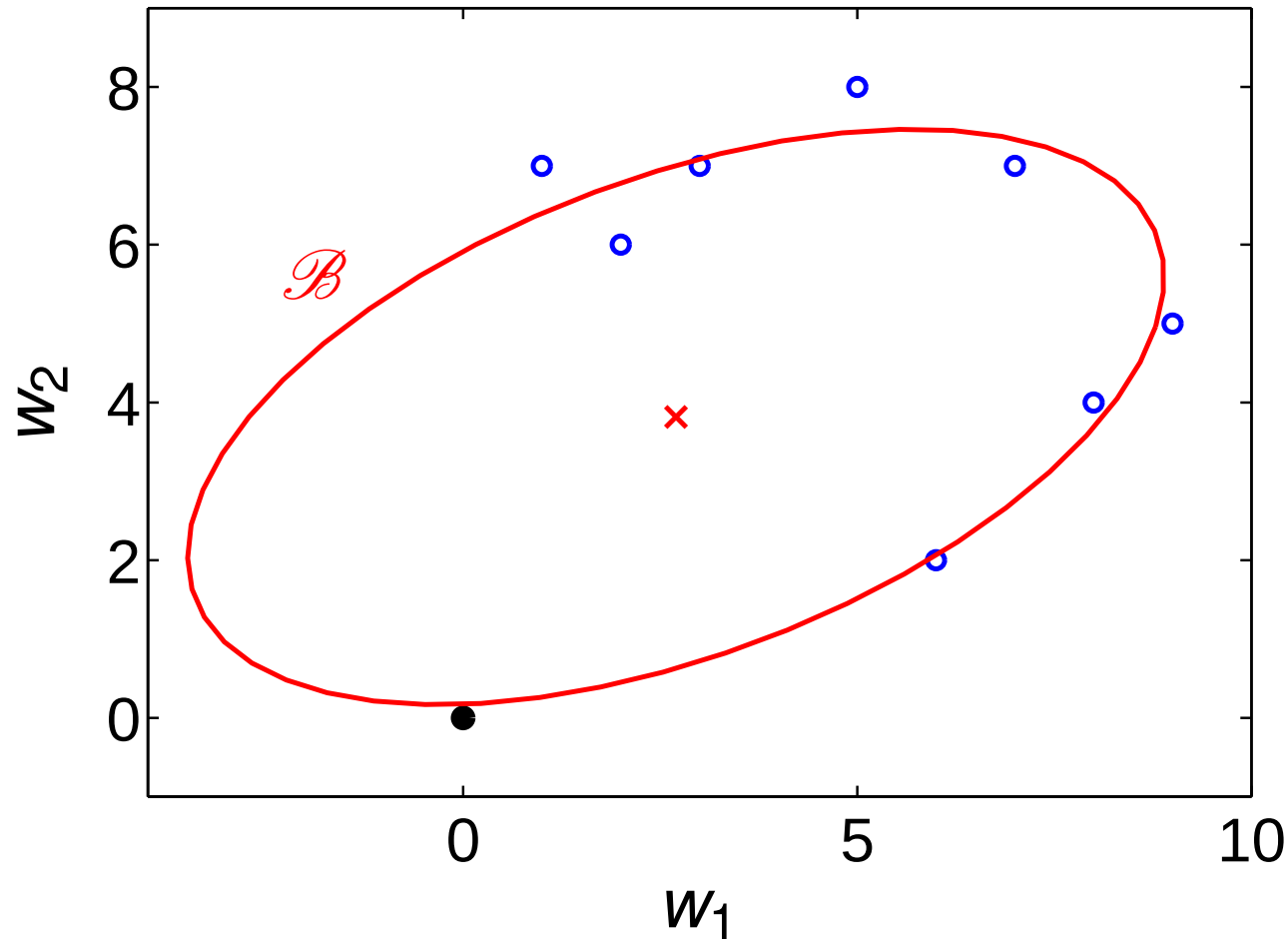
- \mathcal{B} — model: line through the origin
- \mathcal{M} — model class: all lines through the origin



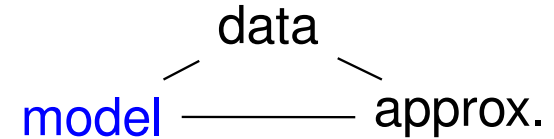
Conic section fitting (quadratic static model)



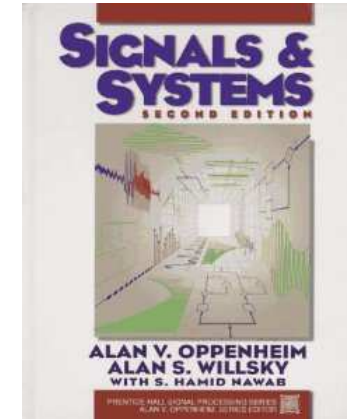
- \mathcal{B} — model: conic section
- \mathcal{M} — model class: all conic sections

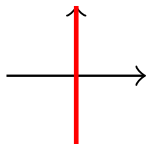
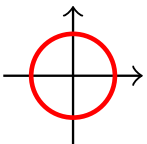


Classical definition of dynamical model

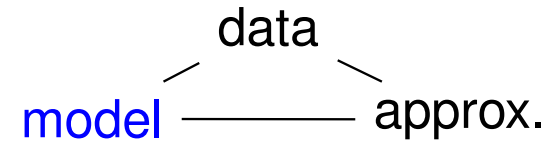


- ▶ dynamical model is **signal processor**



- ▶ specified by a **map** $\hat{y} = f(\hat{u})$
- ▶ "state space model", "transfer function model", . . .
- ▶ however, lines and conic sections may not be graphs
- ▶ *e.g.*,  ,  can't be represented by $f : \hat{u} \mapsto \hat{y}$

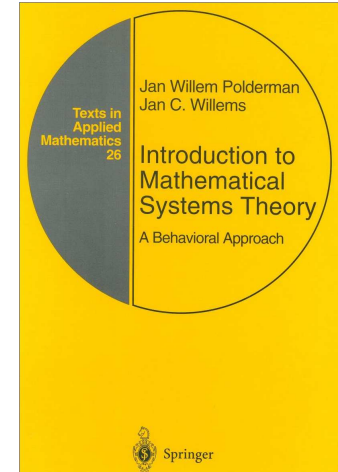
Behavioral definition of model



- ▶ a model is a **subset**

$$\mathcal{B} = \{ \hat{w} \mid g(\hat{w}) = 0 \text{ holds} \}$$

- ▶ represented by an **implicit function** g

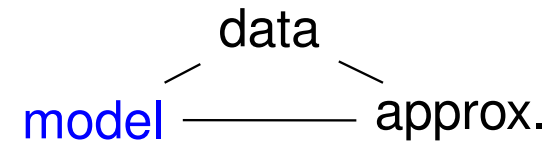


- ▶ in the static case, $g(\hat{w}) = 0$ is algebraic equation
- ▶ in the dynamic case, $g(\hat{w}) = 0$ is difference equation

- ▶ $\hat{w} = \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix}$, $\hat{y} = f(\hat{u})$ is a special case of $g(\hat{w}) = 0$

$$(g(\hat{u}, \hat{y}) = \hat{y} - f(\hat{u}))$$

Summary: model



- ▶ three data modeling examples:

problem

line fitting

conic section fitting

system identification

model

static linear

static nonlinear

dynamic

- ▶ two definitions of a model:

classical

map $\hat{y} = f(\hat{u})$

f — function

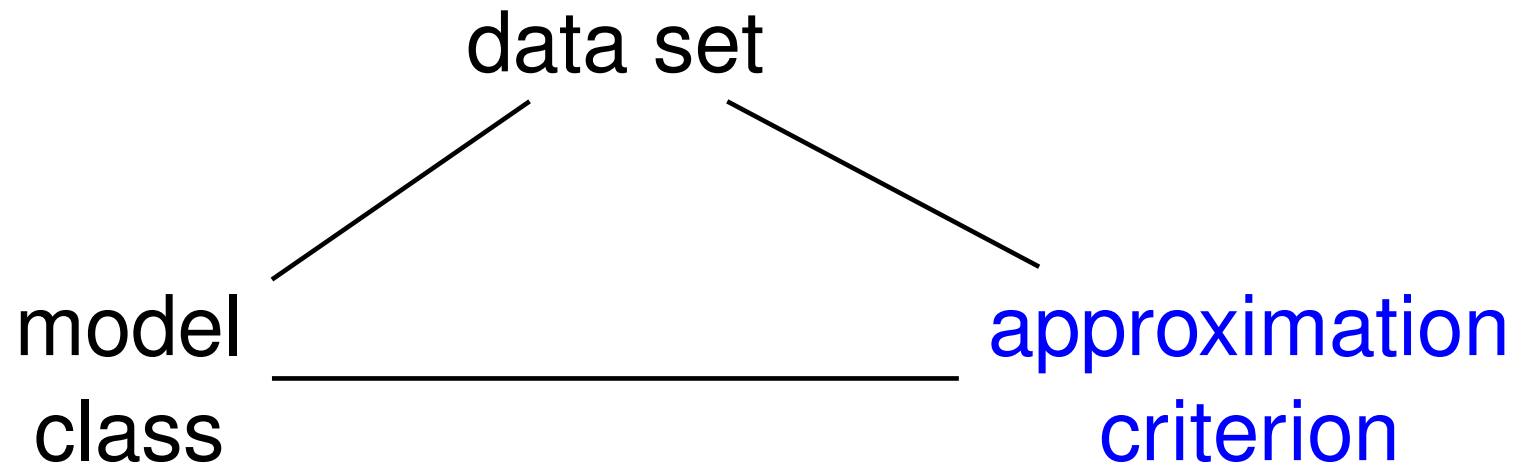
behavioral

set $\{ \hat{w} \mid g(\hat{w}) = 0 \}$

g — relation

- ▶ the classical one can not deal with all examples

Finally, the approximation criterion . . .

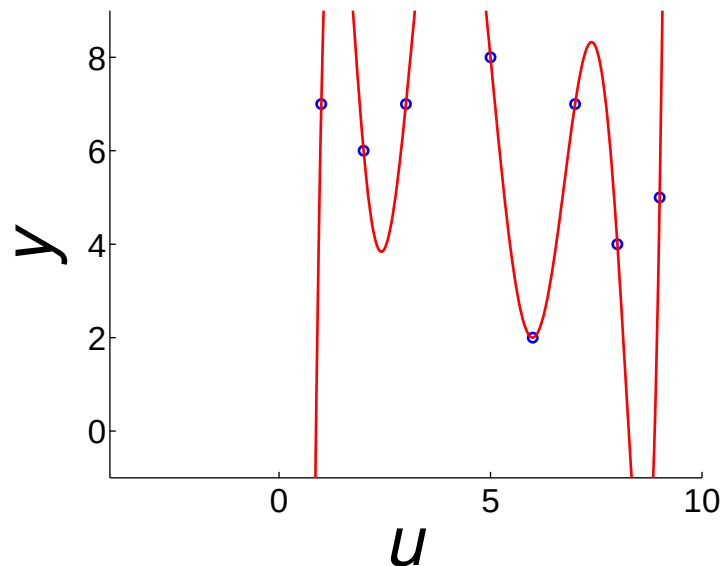


Exact model

$$w \subset \mathcal{B} \iff w^1, \dots, w^N \in \mathcal{B}$$
$$\iff : \text{"}w \text{ is exact data of } \mathcal{B}\text{"}$$

- ▶ two well known exact modeling problems
 - ▶ realization: LTI model class, impulse resp. data
 - ▶ interpolation: static nonlinear model class

polynomial interpolation



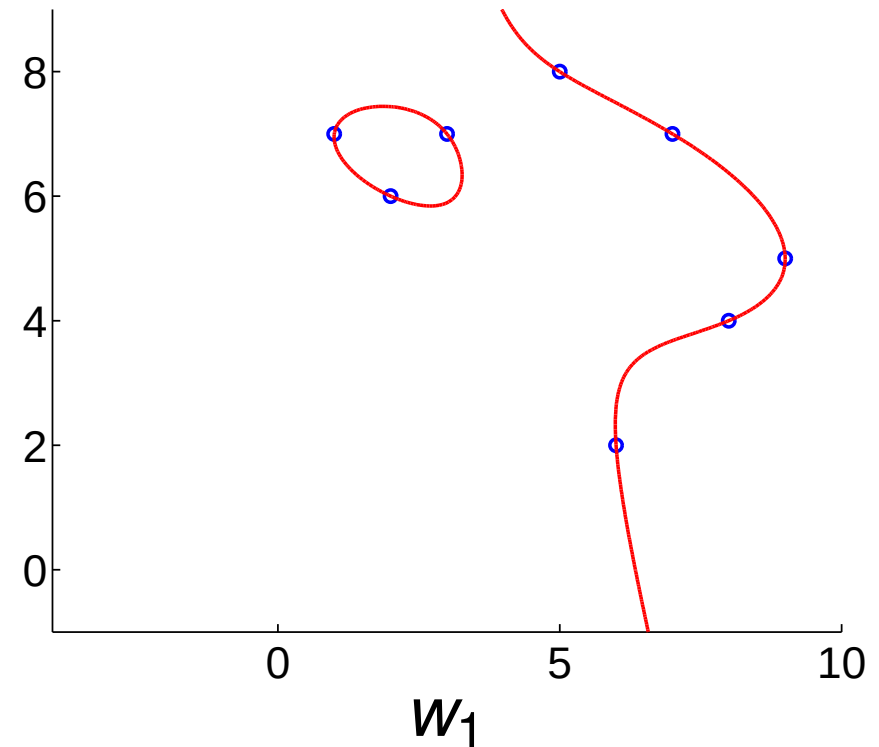
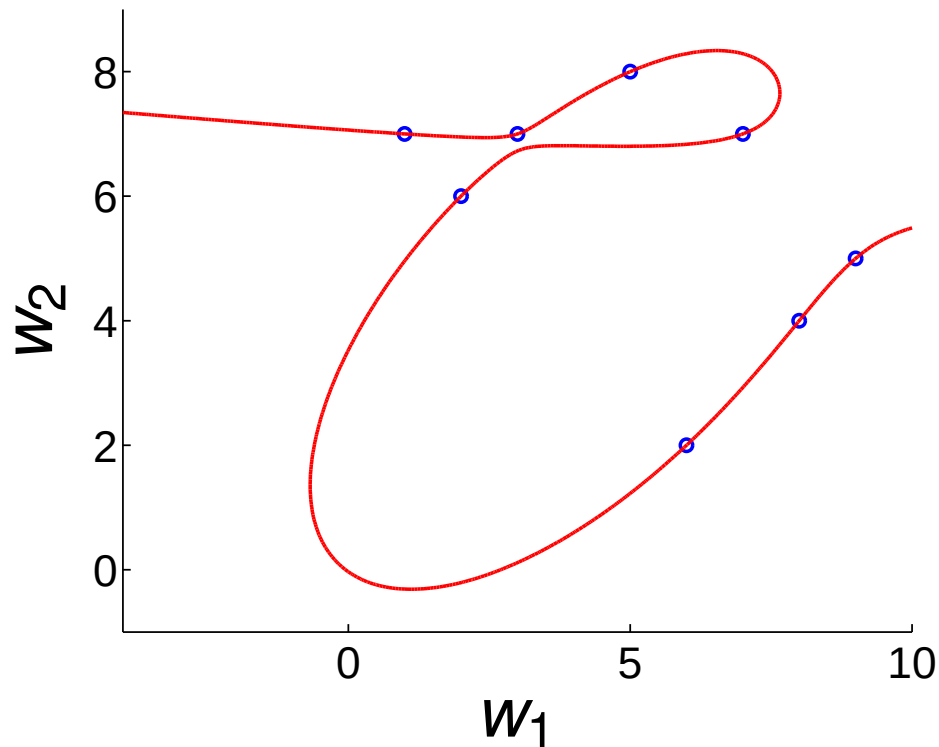
$$\mathcal{B} = \left\{ \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \mid \hat{y} = f(\hat{u}) \right\}$$

f is 8th order polynomial

Exact 3rd order nonlinear static models

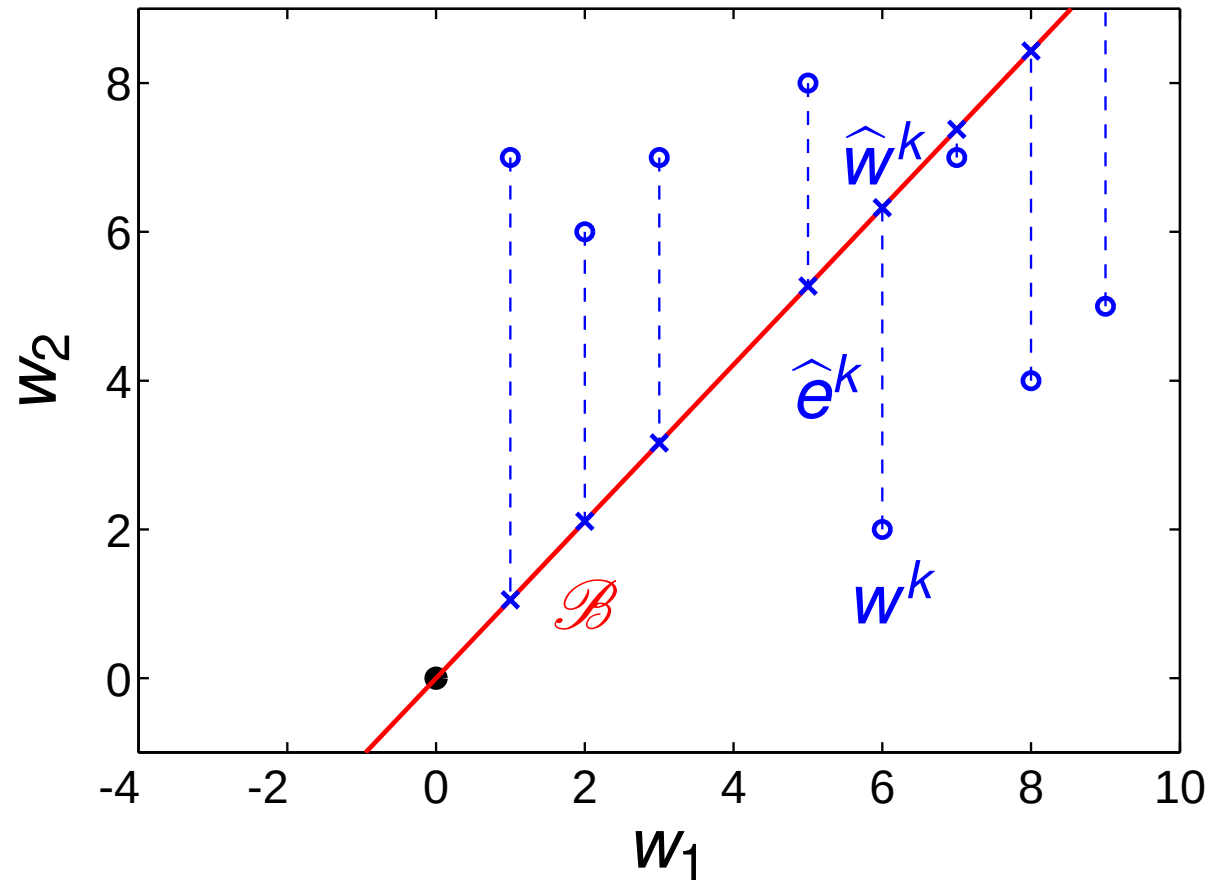
$$\mathcal{B} = \left\{ \begin{bmatrix} \hat{w}_1 \\ \hat{w}_2 \end{bmatrix} \mid g(\hat{w}_1, \hat{w}_2) = 0 \right\}$$

g is 3rd order polynomial in \hat{w}_1, \hat{w}_2

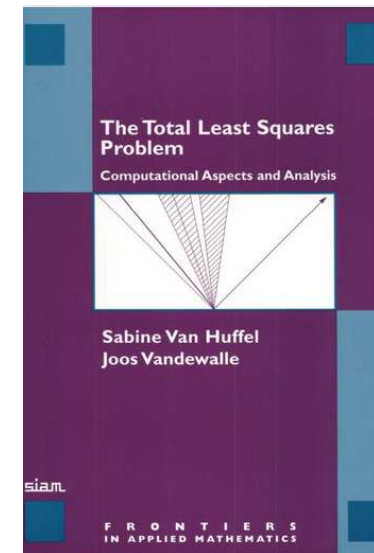
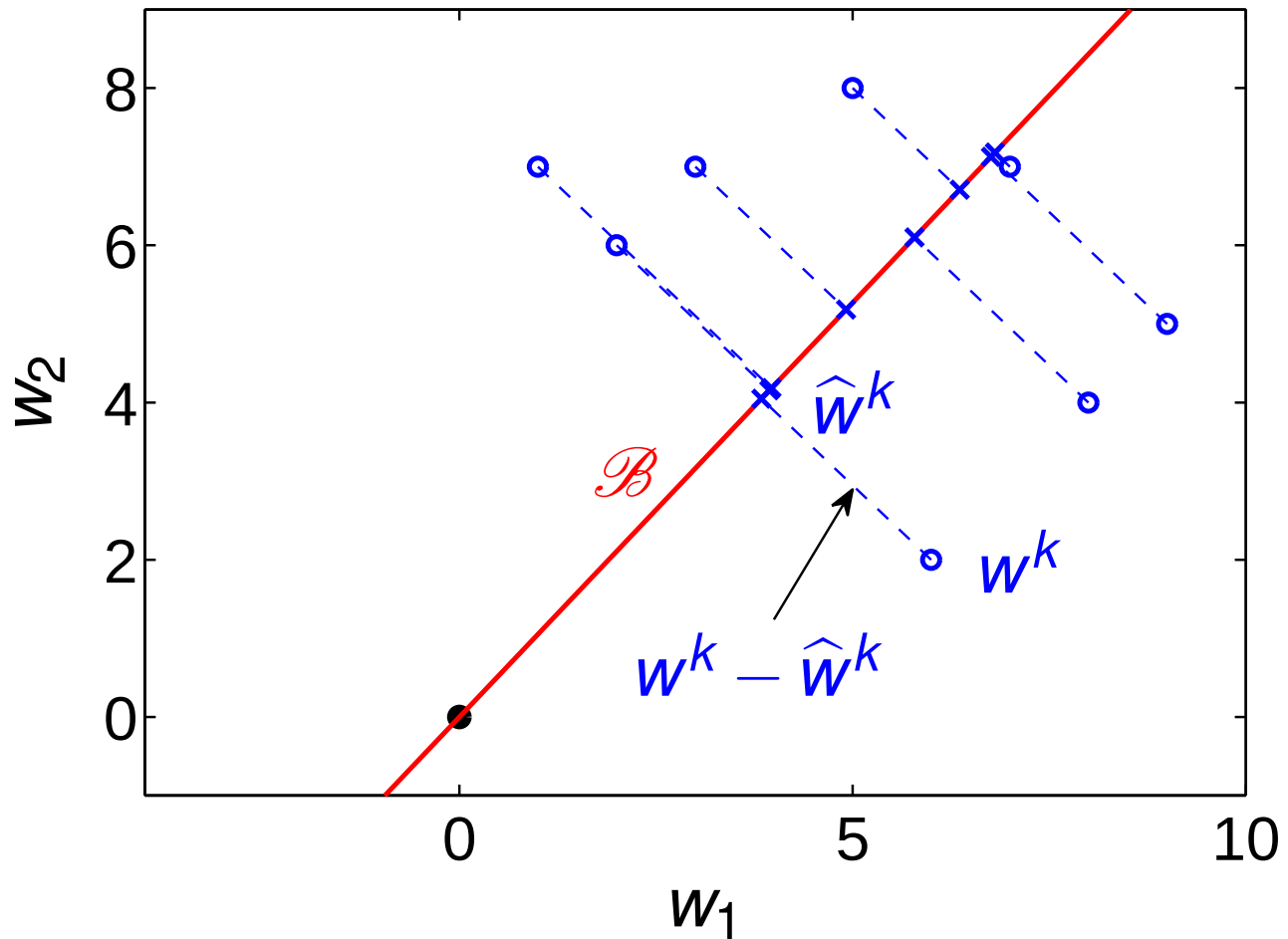
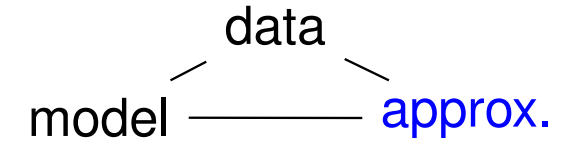


Ordinary least squares

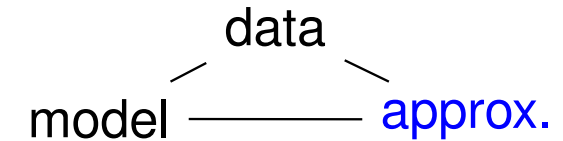
data
model ——— approx.



Total least squares



Linear static case



► total least squares

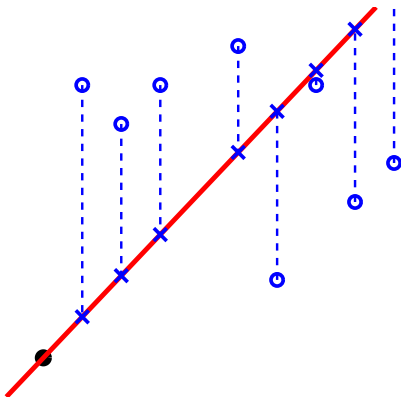
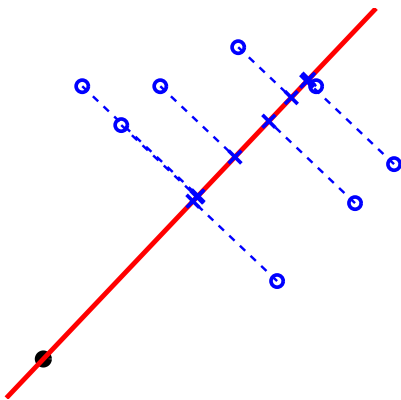
$$\min_{\hat{u}, \hat{y}, \theta} \left\| \begin{bmatrix} u - \hat{u} & y - \hat{y} \end{bmatrix} \right\|_F \quad \text{s.t.} \quad \underbrace{\hat{u}\theta = \hat{y}}_{(\hat{u}, \hat{y}) \in \mathcal{B}(\theta)}$$

$$\hat{w} = (\hat{u}, \hat{y}) \text{ approximates } w = (u, y)$$

► ordinary least squares

$$\min_{\hat{e}, \theta} \|\hat{e}\|_2 \quad \text{s.t.} \quad \underbrace{u\theta = y + \hat{e}}_{(\hat{e}, u, y) \in \mathcal{B}_{\text{ext}}(\theta)}$$

\hat{e} is unobserved (latent) input



Approximation criteria

- ▶ Misfit approach:

modify w as little as possible,
so that \hat{w} is exact

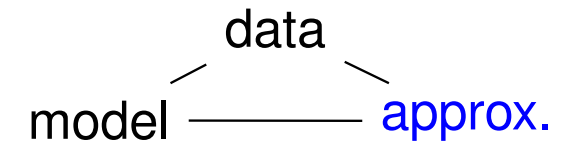
$\|w - \hat{w}\|$ is the misfit criterion

- ▶ Latency approach:

augment \mathcal{B} by as small as possible e ,
so that (e, w) is exact

$\|e\|$ is the latency criterion

Deterministic vs stochastic setting



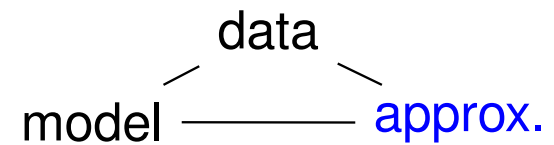
- ▶ stochastic estimation \Leftrightarrow deterministic approx.



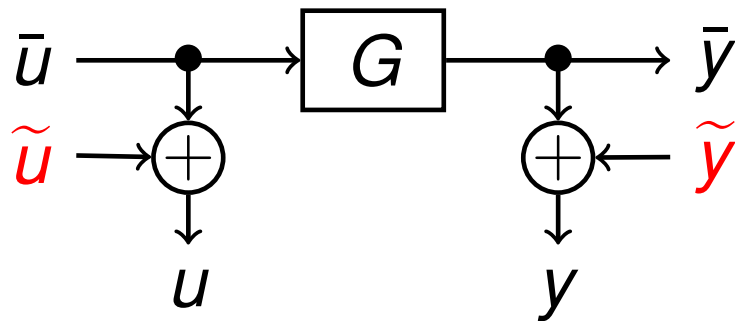
- ▶ also in control

LQG control $\Leftrightarrow H_2$ optimal control

Misfit and latency in the stochastic setting



EIV \leftrightarrow misfit

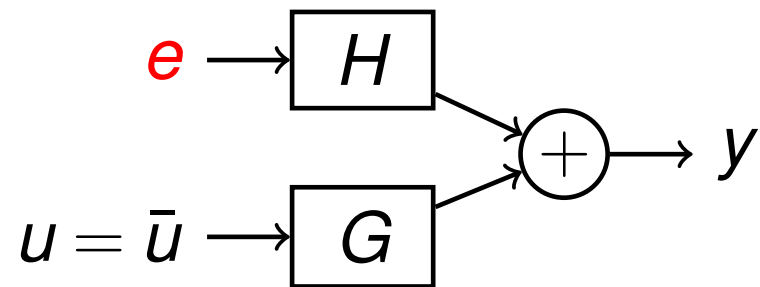


\tilde{u}, \tilde{y} — measurement errors

$$\min_{\hat{w} \in \mathcal{B}} \|w - \hat{w}\|$$

$$\mathcal{B} := \left\{ \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \mid \hat{y} = \hat{G}\hat{u} \right\}$$

ARMAX \leftrightarrow latency

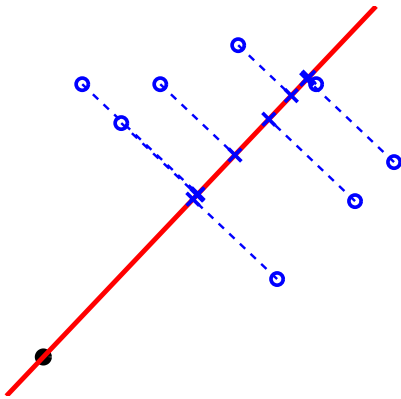
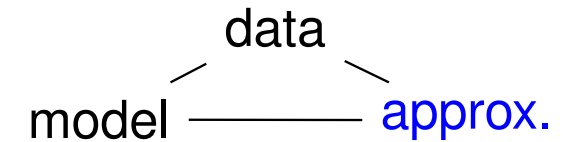


e — disturbance

$$\min_{(\hat{e}, w) \in \mathcal{B}_{\text{ext}}} \|\hat{e}\|$$

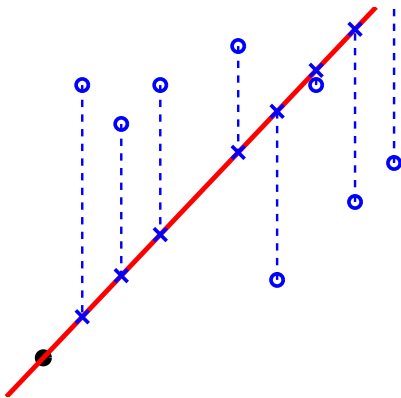
$$\mathcal{B}_{\text{ext}} := \left\{ \begin{bmatrix} \hat{e} \\ u \\ y \end{bmatrix} \mid y = [\hat{H} \ \hat{G}] \begin{bmatrix} \hat{e} \\ u \end{bmatrix} \right\}$$

Summary: approximation criterion



- ▶ TLS \leftrightarrow misfit \leftrightarrow errors-in-variables

$$\min_{\hat{w} \in \mathcal{B}} \|w - \hat{w}\| \quad \left(\begin{array}{l} \text{projection} \\ \text{of } w \text{ on } \mathcal{B} \end{array} \right)$$



- ▶ OLS \leftrightarrow latency \leftrightarrow ARMAX

$$\min_{(\hat{e}, w) \in \mathcal{B}_{\text{ext}}} \|\hat{e}\|$$

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Exercises

A general problem



the aim is to obtain "simple" and "accurate" model:

"accurate" \rightarrow min. error($w, \hat{\mathcal{B}}$) = misfit/latency

"simple" \rightarrow Occam's razor principle:
among equally accurate models,
choose the simplest

Model complexity

- ▶ simple models are small models

$$\mathcal{B}_1 \subset \mathcal{B}_2 \implies \mathcal{B}_1 \text{ is simpler than } \mathcal{B}_2$$

- ▶ nonlinear model complexity is an open problem
- ▶ in the linear time-invariant case, \mathcal{B} is a subspace

size of the model = dimension of \mathcal{B}

- ▶ however, models with inputs are infinite dimensional

Linear time-invariant model's complexity

- ▶ restriction of \mathcal{B} on an interval $[1, T]$

$$\mathcal{B}|_T = \{ w = (w(1), \dots, w(T)) \mid \exists w_p, w_f, \\ \text{such that } (w_p, w, w_f) \in \mathcal{B} \}$$

- ▶ for sufficiently large T

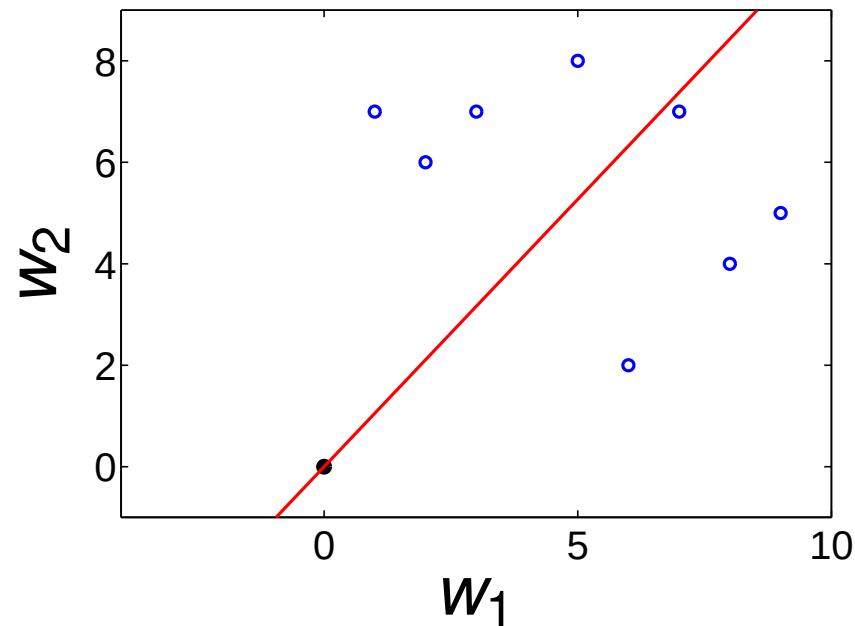
$$\dim(\mathcal{B}|_T) = (\# \text{ of inputs}) \cdot T + (\text{order})$$

$$\text{complexity}(\mathcal{B}) = \begin{bmatrix} m \\ l \end{bmatrix} \begin{array}{l} \rightarrow \# \text{ of inputs} \\ \rightarrow \text{order or lag} \end{array}$$

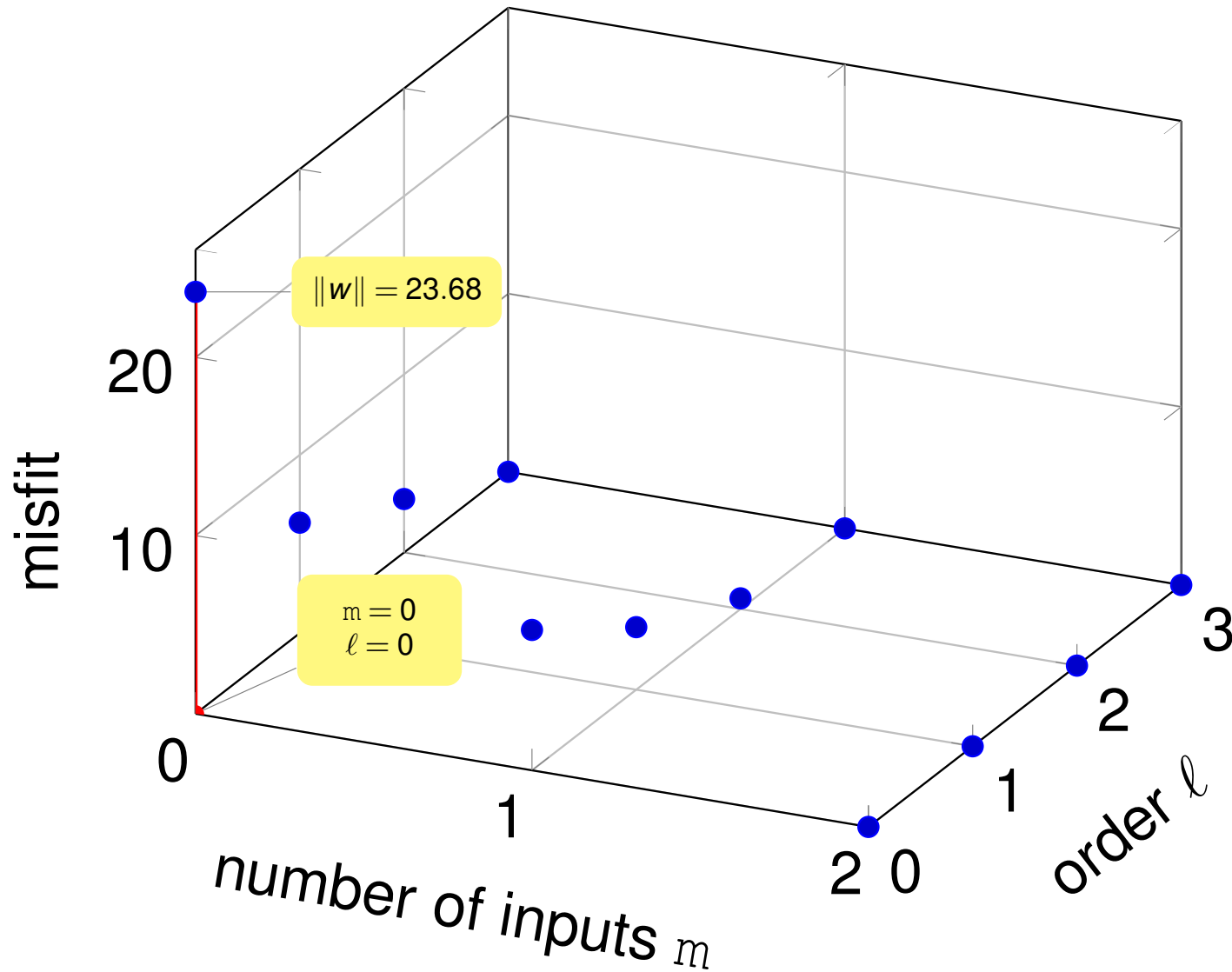
- ▶ $\mathcal{L}_{m,l}$ — set of LTI systems of bounded complexity

Complexity selection

- ▶ if m is given and fixed, choosing the complexity is an *order selection problem*
 - ▶ in general, choosing the complexity involves *order selection and input selection*
- illustrated next on the example from the introduction

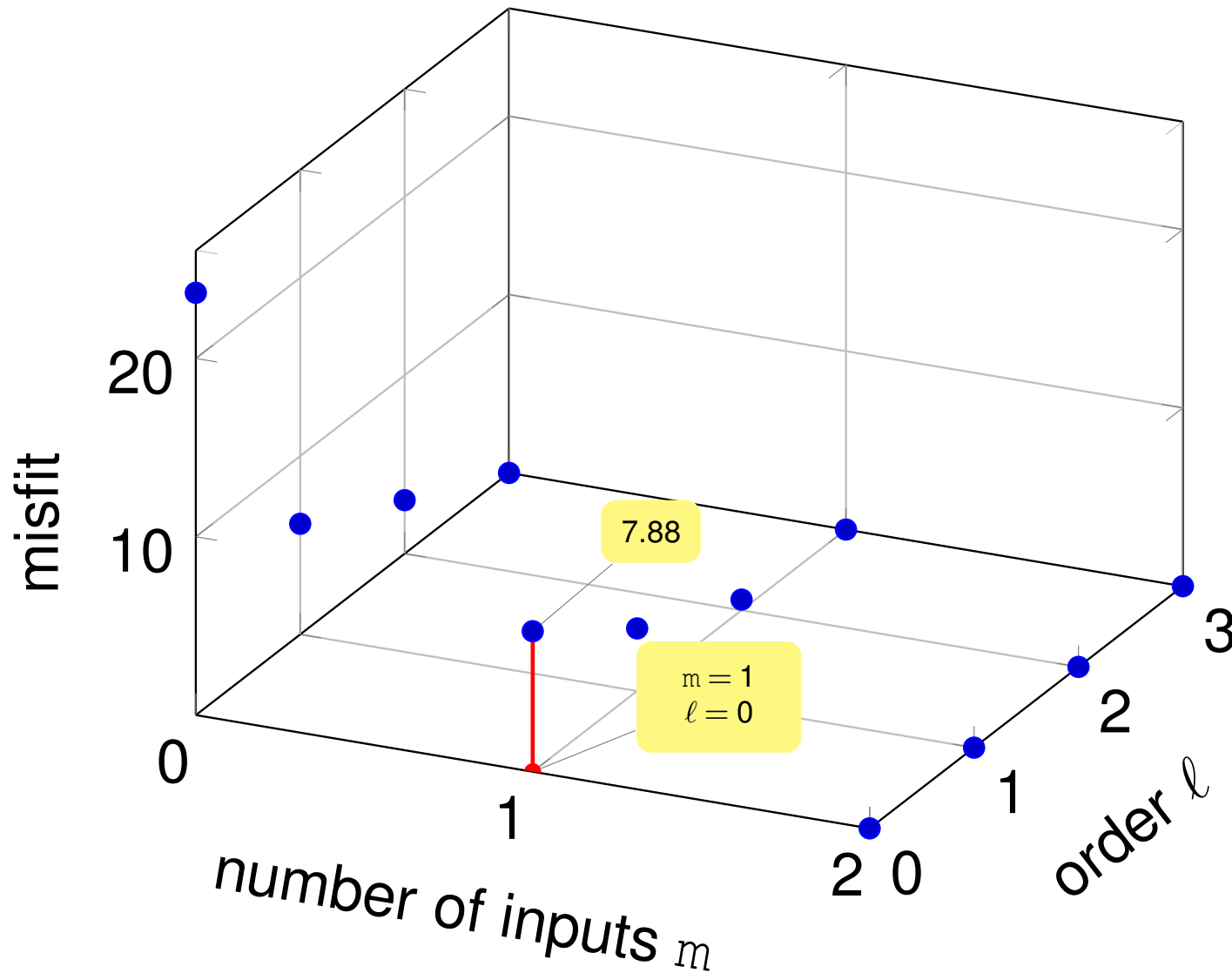


Example: misfit-complexity trade-off



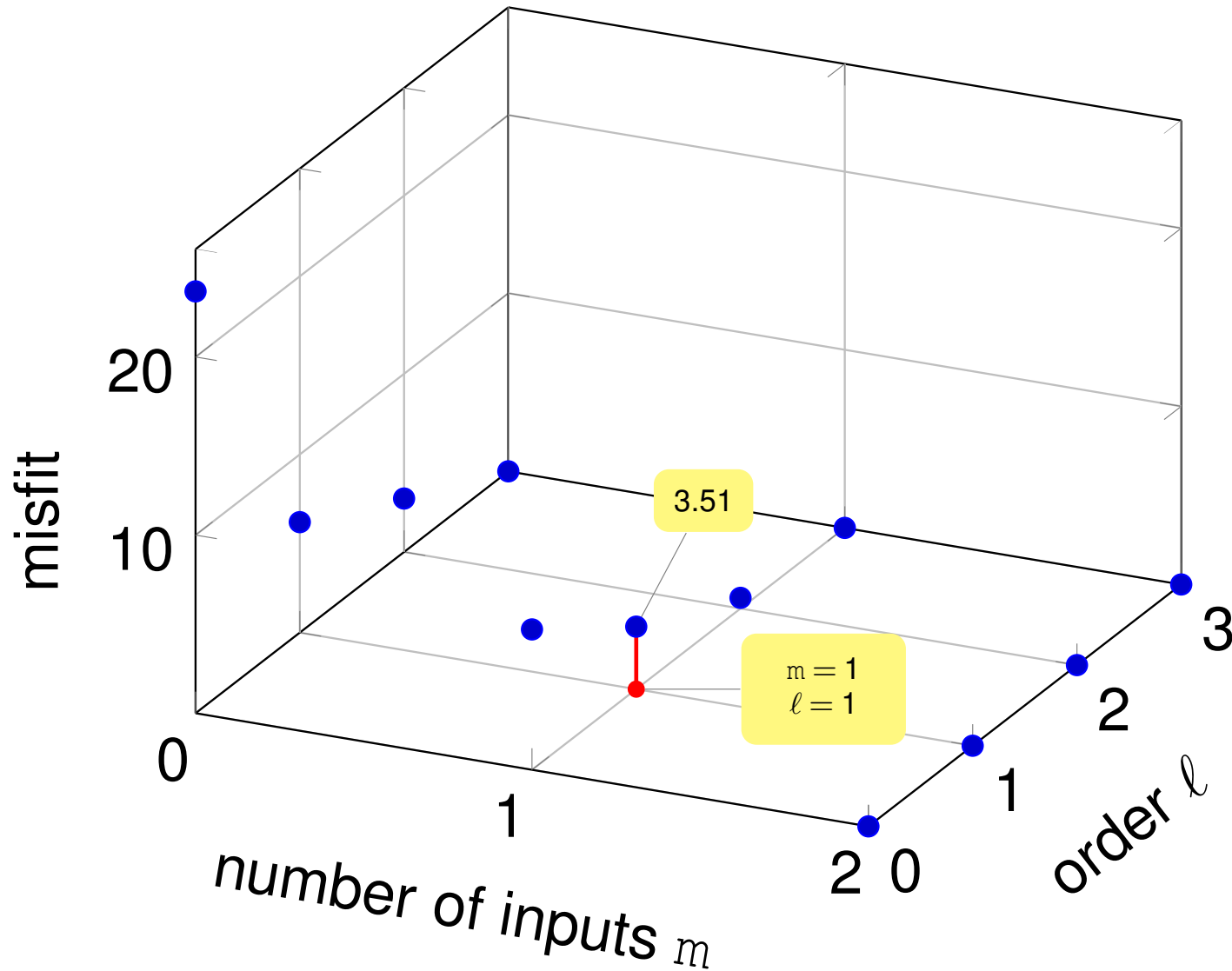
$m = 0, \ell = 0 \implies \mathcal{B} = \{0\}$ is the only model

Example: misfit-complexity trade-off



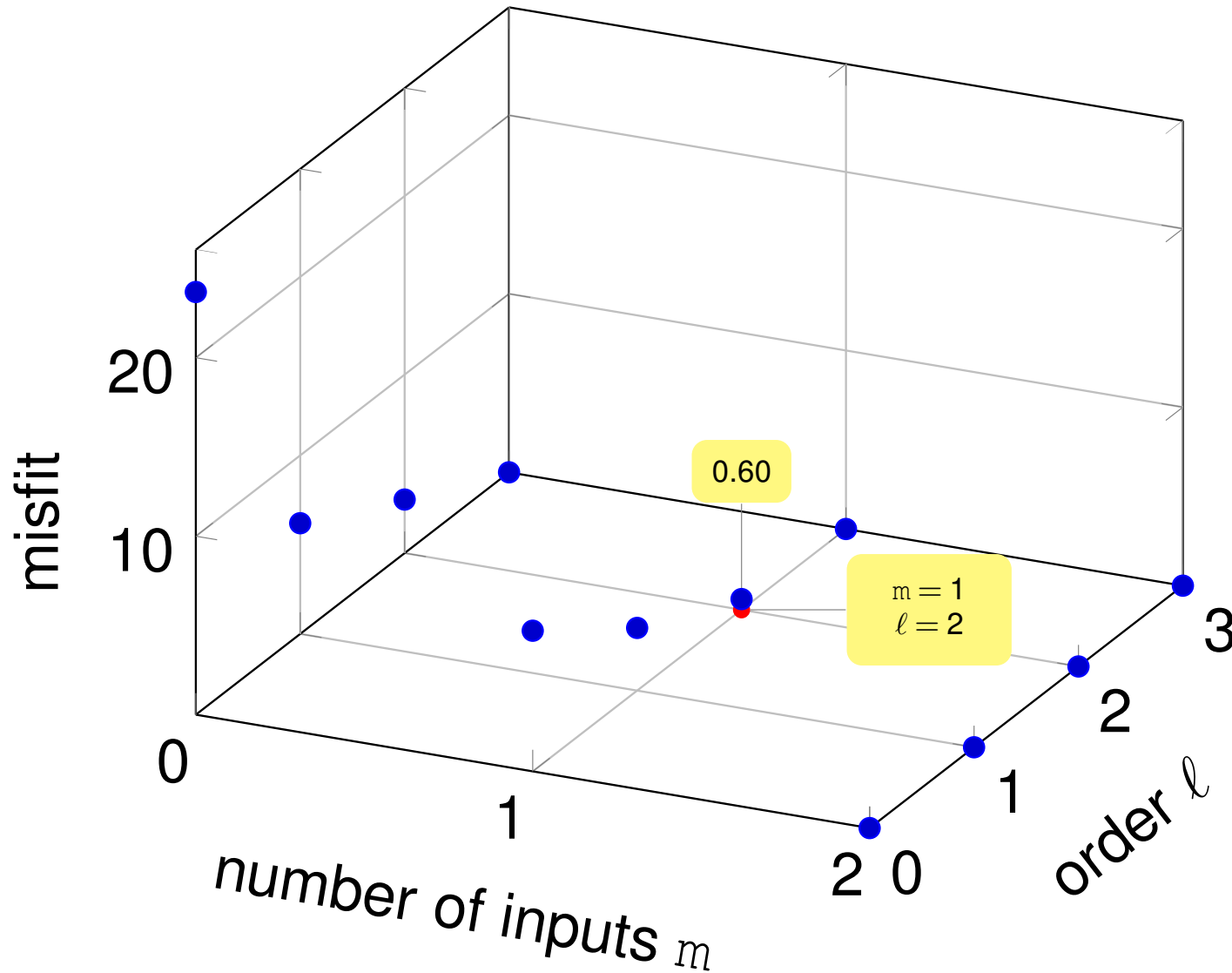
$m = 1, \ell = 0 \implies \mathcal{B}$ is a line through 0

Example: misfit-complexity trade-off



$m = 1, \ell = 1 \implies \mathcal{B}$ is 1st order SISO

Example: misfit-complexity trade-off



$m = 1, \ell = 2 \implies \mathcal{B}$ is 2nd order SISO

Approximation error-complexity trade-off

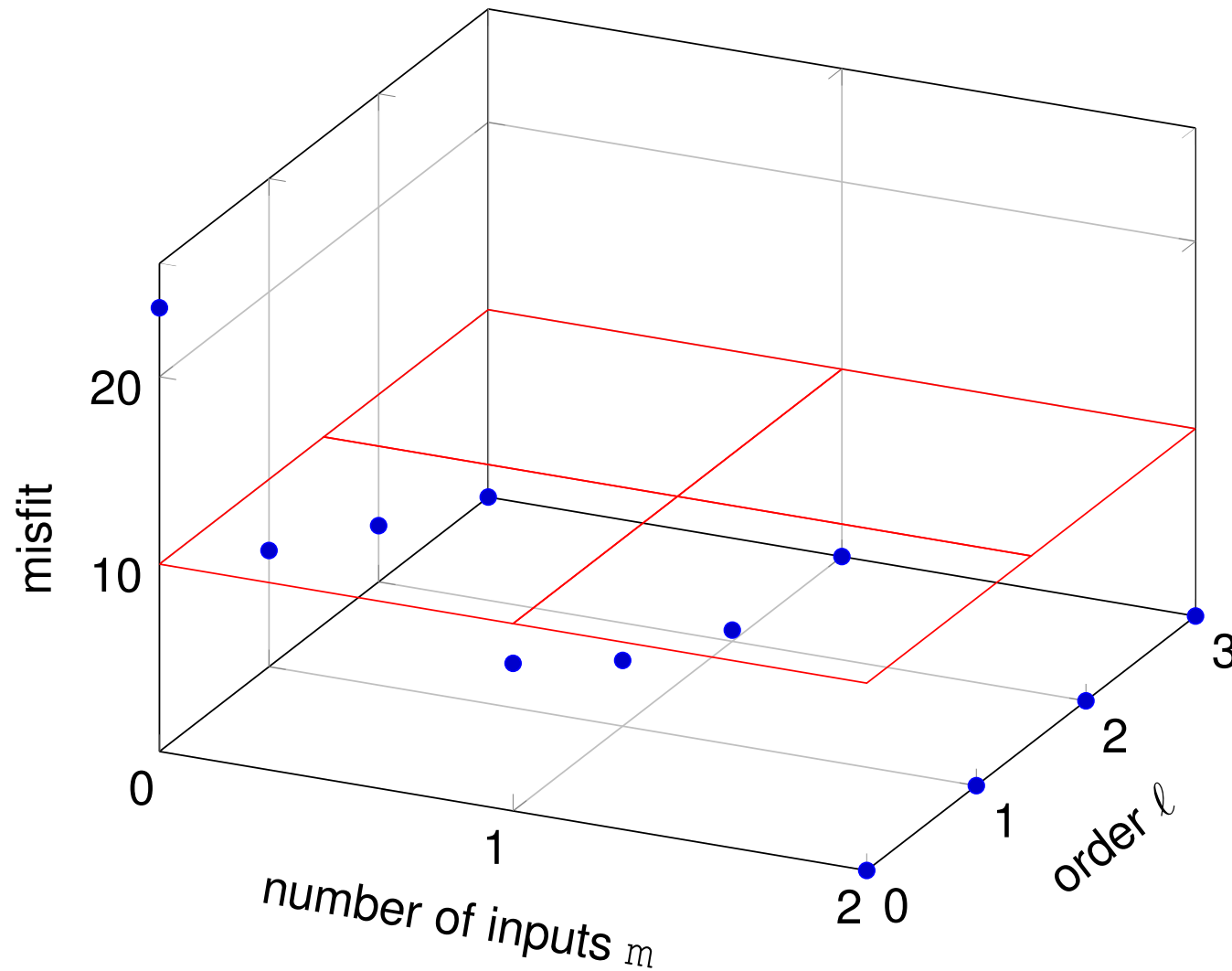
$$\text{minimize over } \hat{\mathcal{B}} \in \mathcal{L} \quad \begin{bmatrix} \text{error}(w, \hat{\mathcal{B}}) \\ \text{complexity}(\hat{\mathcal{B}}) \end{bmatrix}$$

three ways to "scalarize" the problem:

1. minimize over $\hat{\mathcal{B}} \in \mathcal{L}$ $\text{error}(w, \hat{\mathcal{B}}) + \lambda \text{complexity}(\hat{\mathcal{B}})$
2. minimize over $\hat{\mathcal{B}} \in \mathcal{L}$ $\text{complexity}(\hat{\mathcal{B}})$
subject to $\text{error}(w, \hat{\mathcal{B}}) \leq \mu$
3. minimize over $\hat{\mathcal{B}}$ $\text{error}(w, \hat{\mathcal{B}})$
subject to $\hat{\mathcal{B}} \in \mathcal{L}_{m,\ell}$

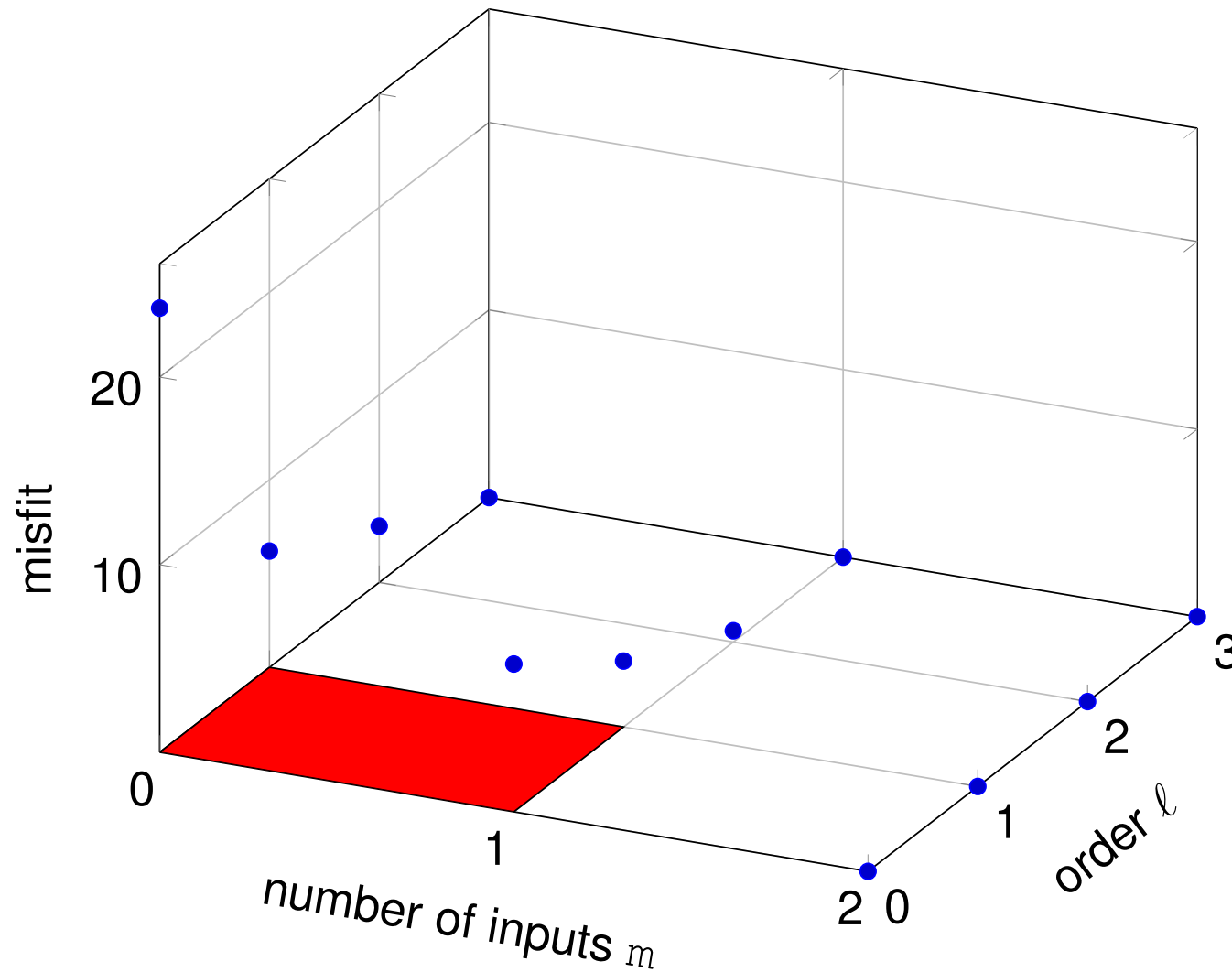
Complexity minimization with error bound

minimize over $\hat{\mathcal{B}} \in \mathcal{L}$ complexity($\hat{\mathcal{B}}$)
subject to error($w, \hat{\mathcal{B}}$) $\leq \mu$



Error minimization with complexity bound

minimize over $\hat{\mathcal{B}}$ error($w, \hat{\mathcal{B}}$)
subject to $\hat{\mathcal{B}} \in \mathcal{L}_{m,\ell}$



Summary: error-complexity trade-off

- ▶ LTI model complexity

$$\text{complexity}(\mathcal{B}) = \begin{bmatrix} m \\ \ell \end{bmatrix} \begin{array}{l} \rightarrow \text{\# of inputs} \\ \rightarrow \text{order or lag} \end{array}$$

- ▶ error-complexity trade-off

$$\text{minimize over } \hat{\mathcal{B}} \in \mathcal{L} \begin{bmatrix} \text{error}(w, \hat{\mathcal{B}}) \\ \text{complexity}(\hat{\mathcal{B}}) \end{bmatrix}$$

- ▶ tracing all optimal solutions requires hyper parameter
 1. λ — no physical meaning
 2. μ — bound on the error
 3. (m, ℓ) — bound on the complexity

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Approximate identification problem

$$\begin{array}{ll} \text{minimize} & \text{over } \hat{\mathcal{B}} \quad \text{error}(w, \hat{\mathcal{B}}) \\ \text{subject to} & \hat{\mathcal{B}} \in \mathcal{L}_{m,l} \end{array}$$

- ▶ in the case error = misfit

$$\text{error}(w, \hat{\mathcal{B}}) = \min_{\hat{w} \in \hat{\mathcal{B}}} \|w - \hat{w}\|$$

- ▶ the problem is

$$\begin{array}{ll} \text{minimize} & \text{over } \hat{\mathcal{B}}, \hat{w} \quad \|w - \hat{w}\| \\ \text{subject to} & \hat{w} \in \hat{\mathcal{B}} \in \mathcal{L}_{m,l} \end{array}$$

Exact, noisy, and missing data

- ▶ $v_i^k(t)$ — variance of the measurement noise on $w_i^k(t)$

$$\|\mathbf{w} - \widehat{\mathbf{w}}\|_{\alpha}^2 = \sum_{k=1}^N \sum_{i=1}^q \sum_{t=1}^T \alpha_i^k(t) (w_i^k(t) - \widehat{w}_i^k(t))^2$$

		exact data
noisy data	—	$v_i^k(t) = 0, \alpha_i^k(t) = \infty$
$\alpha_i^k(t) := \frac{1}{v_i^k(t)}$		missing data
		$v_i^k(t) = \infty, \alpha_i^k(t) = 0$

- ▶ $v_i^k(t) = \infty$ imposes equality constraint $\widehat{w}_i^k(t) = w_i^k(t)$
- ▶ $v_i^k(t) = 0$ makes $\|\mathbf{w} - \widehat{\mathbf{w}}\|_{\alpha}^2$ independent of $w_i^k(t)$

Summary: identification problem

- ▶ approximate identification in the misfit setting

$$\begin{array}{ll} \text{minimize} & \text{over } \hat{\mathcal{B}}, \hat{\mathbf{w}} \quad \|\mathbf{w} - \hat{\mathbf{w}}\|_{\alpha} \\ \text{subject to} & \hat{\mathbf{w}} \in \hat{\mathcal{B}} \in \mathcal{L}_{m,l} \end{array} \quad (\text{SYSID})$$

- ▶ element-wise weighted error criterion $\|\cdot\|_{\alpha}$

$$\begin{array}{ll} \text{exact} & w_i^k(t) \leftrightarrow \alpha_i^k(t) = \infty \\ \text{missing} & w_i^k(t) \leftrightarrow \alpha_i^k(t) = 0 \end{array}$$

Next: SYSID \leftrightarrow Hankel structured LRA

exact trajectory $w \in \mathcal{B} \in \mathcal{L}_{m,l}$

\Updownarrow

$$R_0 w(t) + R_1 w(t+1) + \dots + R_\ell w(t+\ell) = 0$$

\Updownarrow

rank deficient

$$\mathcal{H}_{\ell+1}(w) := \begin{bmatrix} w(1) & w(2) & \dots & w(T-\ell) \\ w(2) & w(3) & \dots & w(T-\ell+1) \\ w(3) & w(4) & \dots & w(T-\ell+2) \\ \vdots & \vdots & & \vdots \\ w(\ell+1) & w(\ell+2) & \dots & w(T) \end{bmatrix}$$

$w \in \mathcal{B} \iff \mathcal{H}_{\ell+1}(w)$ rank deficient

- ▶ relation at time $t = 1$

$$R_0 w(1) + R_1 w(2) + \dots + R_\ell w(\ell + 1) = 0$$

- ▶ in matrix form:

$$\begin{bmatrix} R_0 & R_1 & \dots & R_\ell \end{bmatrix} \begin{bmatrix} w(1) \\ w(2) \\ \vdots \\ w(\ell + 1) \end{bmatrix} = 0$$

$w \in \mathcal{B} \iff \mathcal{H}_{\ell+1}(w)$ rank deficient

- ▶ relation at time $t = 2$

$$R_0 w(2) + R_1 w(3) + \cdots + R_\ell w(\ell + 2) = 0$$

- ▶ in matrix form:

$$\begin{bmatrix} R_0 & R_1 & \cdots & R_\ell \end{bmatrix} \begin{bmatrix} w(2) \\ w(3) \\ \vdots \\ w(\ell + 2) \end{bmatrix} = 0$$

$w \in \mathcal{B} \iff \mathcal{H}_{\ell+1}(w)$ rank deficient

- ▶ relation at time $t = T - \ell$

$$R_0 w(T - \ell) + R_1 w(T - \ell + 1) + \dots + R_\ell w(T) = 0$$

- ▶ in matrix form:

$$\begin{bmatrix} R_0 & R_1 & \dots & R_\ell \end{bmatrix} \begin{bmatrix} w(T - \ell) \\ w(T - \ell + 1) \\ w(T - \ell + 2) \\ \vdots \\ w(T) \end{bmatrix} = 0$$

Putting it all together

- ▶ relation for $t = 1, \dots, T - \ell$

$$R_0 w(t) + R_1 w(t+1) + \dots + R_\ell w(t+\ell) = 0$$

- ▶ in matrix form:

$$\underbrace{[R_0 \quad R_1 \quad \dots \quad R_\ell]}_R \underbrace{\begin{bmatrix} w(1) & w(2) & \dots & w(T-\ell) \\ w(2) & w(3) & \dots & w(T-\ell+1) \\ w(3) & w(4) & \dots & w(T-\ell+2) \\ \vdots & \vdots & & \vdots \\ w(\ell+1) & w(\ell+2) & \dots & w(T) \end{bmatrix}}_{\mathcal{H}_{\ell+1}(w)} = 0$$

$w \in \mathcal{B} \iff \mathcal{H}_{\ell+1}(w)$ rank deficient

- ▶ with $R \in \mathbb{R}^{(q-m) \times q(\ell+1)}$ full row rank,

$$\text{rank}(\mathcal{H}_{\ell+1}(w) = 0) \leq ql + m \quad (q - \# \text{ of variables})$$

$$w \in \mathcal{B} \in \mathcal{L}_{m,\ell} \iff \text{rank}(\mathcal{H}_{\ell+1}(w)) \leq ql + m$$

- ▶ multiple time-series \iff mosaic-Hankel matrix

$$\{w^1, \dots, w^N\} \subset \mathcal{B} \in \mathcal{L}_{m,\ell}$$

$$\iff \text{rank} \left(\underbrace{\begin{bmatrix} \mathcal{H}_{\ell+1}(w^1) & \cdots & \mathcal{H}_{\ell+1}(w^N) \end{bmatrix}}_{\mathcal{H}_{\ell+1}(w)} \right) \leq ql + m$$

Structured weighted low-rank approximation

$$\begin{array}{ll} \text{minimize} & \text{over } \hat{\mathcal{B}} \text{ and } \hat{\mathbf{w}} \quad \|\mathbf{w} - \hat{\mathbf{w}}\|_{\alpha} \\ \text{subject to} & \hat{\mathbf{w}} \subset \hat{\mathcal{B}} \in \mathcal{L}_{m,\ell} \end{array} \quad (\text{SYSID})$$



$$\begin{array}{ll} \text{minimize} & \text{over } \hat{\mathbf{w}} \quad \|\mathbf{w} - \hat{\mathbf{w}}\|_{\alpha} \\ \text{subject to} & \text{rank}(\mathcal{H}_{\ell+1}(\hat{\mathbf{w}})) \leq q\ell + m \end{array} \quad (\text{SLRA})$$

Summary: structured low-rank approximation

- ▶ (SYSID) \iff (SLRA)
- ▶ LTI model class \iff Hankel structure
- ▶ repeated experiments \iff mosaic-Hankel structure

$$\left[\mathcal{H}_{\ell+1}(w^1) \quad \cdots \quad \mathcal{H}_{\ell+1}(w^N) \right]$$

- ▶ bounded complexity \iff rank constraint

$$(m, \ell) \iff r = q\ell + m$$

Outline

Introduction: data, model class, approximation

Approximation error–model complexity trade-off

System identification \leftrightarrow low-rank approximation

Solution methods: variable projection

Exercises

Solution methods

- ▶ **given:** data w and complexity bound (m, ℓ)
- ▶ **find:** $\hat{\mathcal{B}}$ that solves (SYSID) or, equivalently, (SLRA)

1. choice of model representation

- ▶ transfer function
- ▶ input/state/output
- ▶ ...

2. choice of optimization method

- ▶ local optimization
- ▶ global optimization
- ▶ convex relaxations

Model vs model representation

- ▶ 1st order SISO model $\mathcal{B} \in \mathcal{L}_{1,1}$

$$\mathcal{B}_{\text{de}}(\theta) = \left\{ \hat{w} \mid \begin{bmatrix} \theta_1 & \theta_2 & \theta_3 & \theta_4 \end{bmatrix} \begin{bmatrix} \hat{w}_1(t) \\ \hat{w}_2(t) \\ \hat{w}_1(t+1) \\ \hat{w}_2(t+1) \end{bmatrix} = 0, \forall t \right\}$$

- ▶ transfer functions

$$G_{w_1 \mapsto w_2}(z) = -\frac{\theta_1 + \theta_3 z}{\theta_2 + \theta_4 z}, \quad G_{w_2 \mapsto w_1}(z) = -\frac{\theta_2 + \theta_4 z}{\theta_1 + \theta_3 z}$$

- ▶ state space, convolution, ..., **representations**

Problem formulation vs solution method

- ▶ in the classical setting, model = representation
- ▶ \implies problems are mixed with solution methods
- ▶ *e.g.*, "total least-squares" is both problem and method
- ▶ the behavioral setting distinguishes

	used for	involves
abstract	problem formulation	$\mathcal{B}, \mathcal{L}_{m,l}$
concrete	solution methods	$\mathcal{B}(\theta), \theta \in \Theta$

- ▶ low-rank approx. is abstract problem formulation

Parameter optimization problem

- ▶ model representation

$$\mathcal{B}(\theta) = \{ \hat{w} \mid g_{\theta}(\hat{w}) = 0 \}$$

- ▶ parameterized model class

$$\mathcal{M} = \{ \mathcal{B}(\theta) \mid \theta \in \Theta \}$$

- ▶ optimization problem

$$\begin{array}{ll} \text{minimize} & \text{over } \theta \in \Theta, \hat{w} \quad \|w - \hat{w}\|_{\alpha} \\ \text{subject to} & g_{\theta}(\hat{w}) = 0 \end{array} \quad (\text{SYSID}_{\theta})$$

Bilinear structure of the problem

- ▶ (SYSID $_{\theta}$) — constrained nonlinear least-squares
- ▶ \mathcal{B} linear
 - $\implies g_{\theta}(\hat{w})$ bilinear (in θ and \hat{w})
 - \implies (SYSID $_{\theta}$) can be solved globally for given θ
- ▶ variable projection (VARPRO)
for separable nonlinear least-squares problems
- ▶ if $T \gg \ell$, elimination of \hat{w} leads to big reduction

System theoretic view of VARPRO

solving (SYSID_θ) for given θ



misfit evaluation: $\text{error}(w, \mathcal{B}(\theta))$



likelihood evaluation



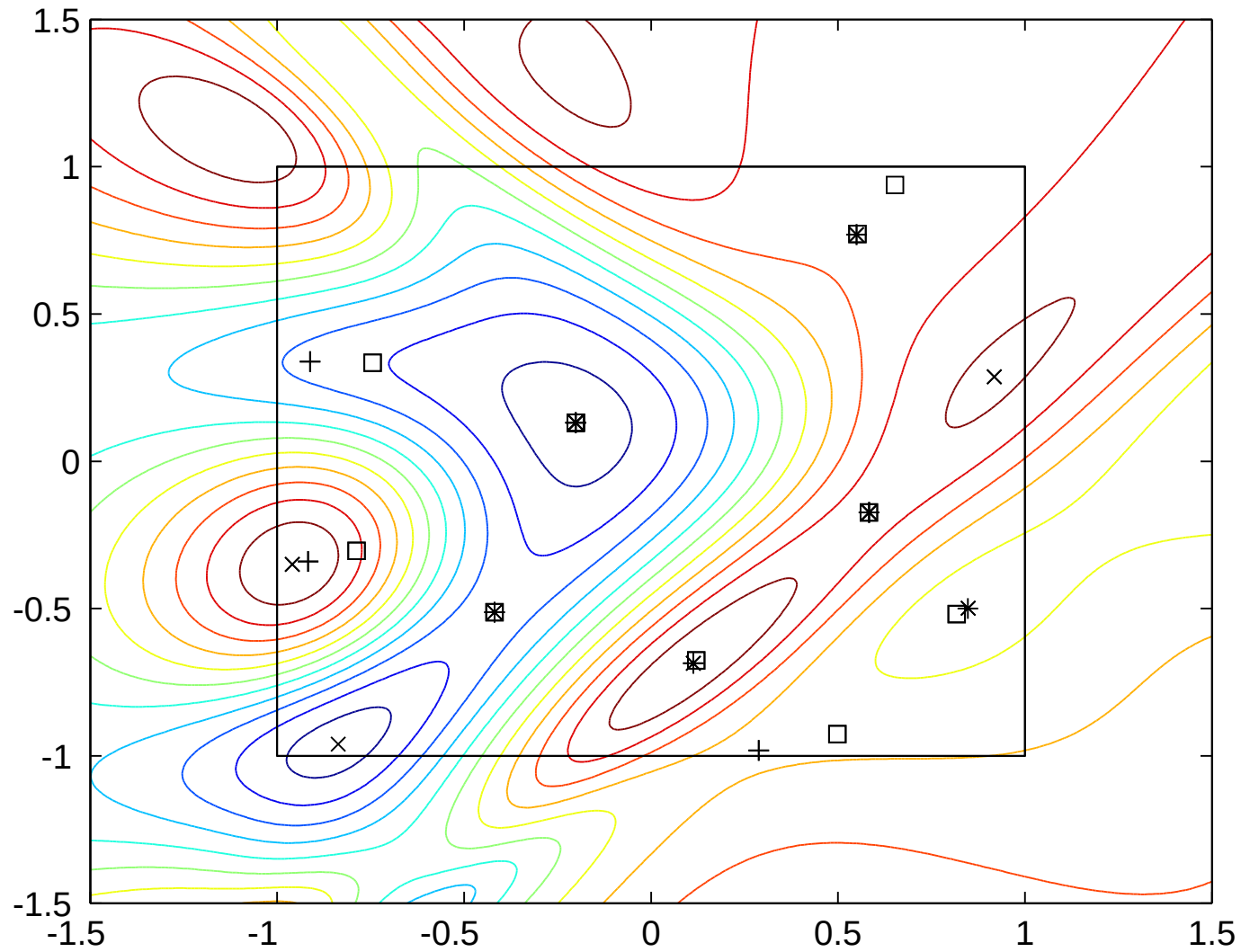
least-squares smoothing of w by $\mathcal{B}(\theta)$



fast algorithms:
Kalman smoothing
Cholesky factorization

...

Non-convexity of error($w, \mathcal{B}(\theta)$)



Computational details

- ▶ $O(T)$ evaluation of error $(w, \mathcal{B}(\theta))$ and its derivatives
 - ▶ using the Kalman smoother
 - ▶ Cholesky factorization of banded Toeplitz matrix
 - ▶ ...
- ▶ $\mathcal{B}(\theta) = \mathcal{B}(\alpha\theta)$, for all $\alpha \neq 0$
- ▶ $\Theta = \{ \theta \mid \|\theta\|_2 = 1 \} \implies$ optimization on a manifold
 - ▶ generic methods (optimization theory)
 - ▶ custom methods (system identification)
 - ▶ data driven local coordinates (McKelvey)
 - ▶ ...

Summary: solution methods

- ▶ solution methods involve two choices:
 1. model representation
 2. optimization method
- ▶ in the linear case, bilinear structure \rightsquigarrow VARPRO
- ▶ constraint nonlinear least-squares problem

$$\min_{\theta \in \Theta} \text{error}(w, \mathcal{B}(\theta))$$

- ▶ Θ is a manifold \rightsquigarrow optimization on a manifold