CH X : OPTIMAL EXPERIMENTAL DESIGN

REVIEW : NONLINEAR PAR. ESTIM.

$$\hat{\theta} = \arg\min_{\theta} \quad \| M(\theta; u) - y \|_2^2$$

SIM. OUTPUT

$M : \mathbb{R}^d \times \mathbb{R}^N \to \mathbb{R}^N$

OUTP. MEASUREMENTS

$y \in \mathbb{R}^N$

(ASSUMING GAUSSIAN OUTPUT ERRORS)

$$\Sigma = \mathrm{cov}(\hat{\theta}) \approx \sigma_y^2 \cdot \left(J(\hat{\theta}; u)^T \cdot J(\hat{\theta}; u) \right)^{-1}$$

$$J(\theta; u) = \frac{\partial M}{\partial \theta}(\theta; u)$$

SO FAR, MEASUREMENTS WERE GIVEN (u, y FIXED)

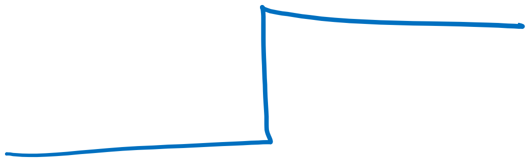
OFTEN, WE CAN <u>DECIDE</u> ON u AND <u>DESIGN</u> OUR EXPERIMENTS.

QUESTION: WHAT IS A "GOOD" EXPERIMENT?

"OBJECTIVE FUN" FOR EXP. DESIGN

EX:

JESUS' u

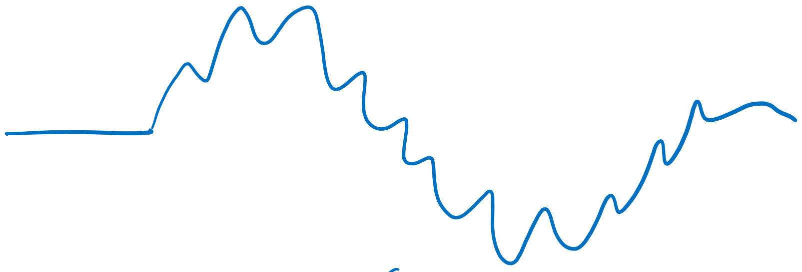


(u, y)

PAR. EST.

$\hat{\theta}_J, \Sigma_J$

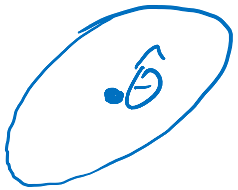
ROBIN'S u



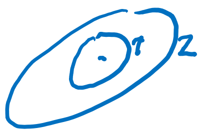
(u, y)

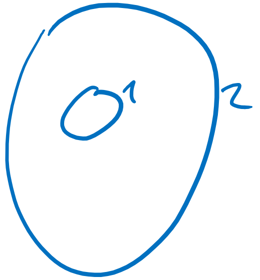
PAR. EST.

$\hat{\theta}_R, \Sigma_R$

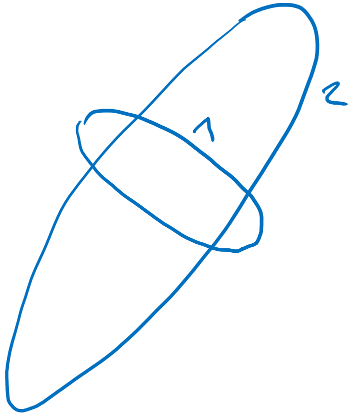


EXP. IS "BETTER" IF COV. MATRIX Σ IS "SMALLER"

Σ_1 IS "SMALLER" THAN Σ_2 IF "" $\iff \Sigma_1 < \Sigma_2 \iff 0 < \Sigma_2 - \Sigma_1$



1 IS BETTER



$\Sigma_i \in \mathbb{R}^{d \times d}$ IS POS. DEF. MATRIX,

1) CAN COMPARE TWO SUCH MATRICES WITH MATRIX INEQUALITIES ($\Sigma_1 < \Sigma_2$)

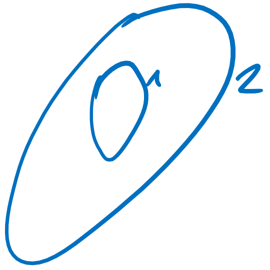
2) FOR MANY MATRIX PAIRS, NEITHER $\Sigma_1 < \Sigma_2$ NOR $\Sigma_2 < \Sigma_1$ HOLDS (UNDECIDED WHICH IS BETTER)

3) SPACE OF POS. DEF. MATRICES IS "HALF-ORDERED"

NEED "SCALAR" CRITERION $\phi(\Sigma)$ TO COMPARE, E.G. ELLIPSOID VOLUME $\in \mathbb{R}$

DEF. FOR GIVEN CRIT. $\phi : \mathbb{R}^{d \times d} \to \mathbb{R}$, WE SAY "$\Sigma_1$ BETTER Σ_2" IFF "$\phi(\Sigma_1) < \phi(\Sigma_2)$"

REASONABLE CRITERIA ϕ SATISFY:



$$\Sigma_1 < \Sigma_2 \Longrightarrow \phi(\Sigma_1) < \phi(\Sigma_2)$$

$$\not\Longleftarrow$$

SOME POSSIBILITIES FOR ϕ:

$$\Sigma = \begin{pmatrix} \cdot & & & & \\ & \cdot & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & \cdot \end{pmatrix}$$

A-CRITERION: $\phi_A(\Sigma) = \underline{\underline{\mathrm{trace}(\Sigma)}} = \sum_{i=1}^{d} \Sigma_{ii}$ = SUM OF EIGENVALUES

D-CRITERION: $\phi_D(\Sigma)$ = PRODUCT OF EIGENVALUES = VOLUME = $\underline{\underline{\det(\Sigma)}}$

$\vdots$

IN PRACTICE, NEED TO SCALE PARAMETERS, E.G. BY A SCALING MATRIX $S = \begin{pmatrix} s_1 & & \\ & \ddots & \\ & & s_d \end{pmatrix}$ WITH $s_i > 0$ OF APPR. UNITS. (FOR A-CRITERION, THIS IS NECESSARY).

$$\Sigma \longrightarrow \underline{\underline{S^{-1} \cdot \Sigma \cdot S^{-1}}}$$

IDEA OF OPT.EXP. DESIGN: MINIMIZE $\phi(\Sigma)$ BY CHOOSING u

$\phi(\Sigma)$ DEPENDS ON Σ. $\quad \Sigma = \sigma_y^2 \cdot (J^T J)^{-1}$

Σ DEP. ON σ_y^2 AND J. ASSUME σ_y^2 FIXED. E.G. $\sigma_y^2 = 1$

J DEP. ON θ AND u. $\quad J = \frac{\partial M}{\partial \theta}(\theta; u)$

ASSUME θ FIXED AT OUR BEST AVAILABLE GUESS, $\theta = \bar{\theta}$

$$\phi\left(\left(J(\bar{\theta};u)^T \cdot J(\bar{\theta};u)\right)^{-1}\right) =: f(u)$$

$$\boxed{J \text{ DOES } \underline{\text{NOT}} \text{ DEPEND ON } y!}$$

OPT. EXP.

$$\boxed{u = \arg\min_u f(u)}$$

AIM OF COMP. DEMO:

- COMP. JESUS' SIGNAL u WITH "OUR" u
- CHOOSE D-CRITERION (NO NEED FOR SCALING)

PLAN OF ATTACK:

WRITE $M(\theta; u)$

$$\boxed{J(\theta; u)}$$

$$\mathrm{cov}(\theta; u) \equiv \mathrm{cov}(u)$$

(ASS. θ FIXED AT BEST EST.)

$\cancel{\phi(\mathrm{cov}(\theta; u}$

$\phi(\mathrm{cov}(u))$