Jet Propulsion Laboratory
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An Overview of State Estimation

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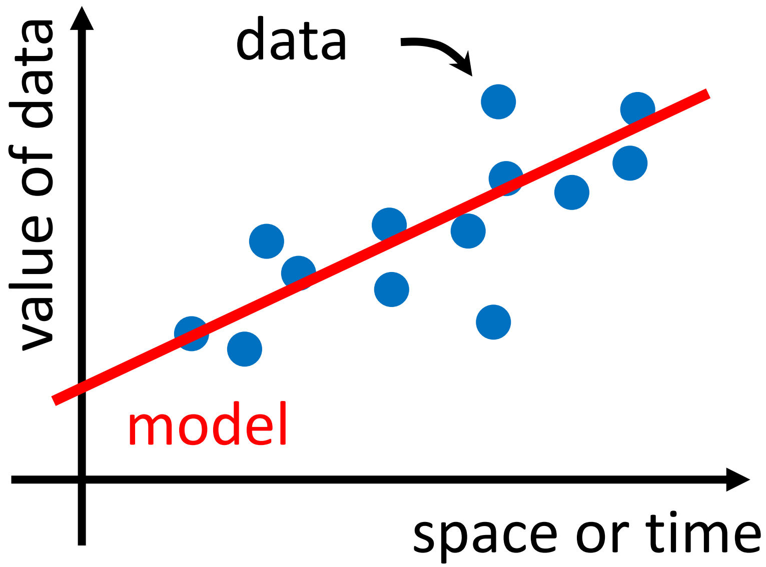
Scope of Lecture



"State Estimation" is
data analysis using a model.

- What is being solved?
- How is it being solved?

The Mathematical Problem (1/7)

Relation between model & data

model data

$$\mathbf{H}_t \mathbf{x}_t \approx \mathbf{y}_t \qquad t=1,2,\ldots,N$$

Observation matrix — state vector — data vector

model grid point

location of observation

$$\mathbf{x}_t \equiv \begin{pmatrix} \vdots \\ u_{ijk} \\ v_{ijk} \\ T_{ijk} \\ S_{ijk} \\ \eta_{ij} \\ \vdots \end{pmatrix}_t \qquad \mathbf{y}_t \equiv \begin{pmatrix} \vdots \\ \eta(x_n, y_n) \\ \vdots \\ T(x_n, y_n, z_n) \\ \vdots \end{pmatrix}_t$$

$$\left.\begin{array}{rl} u, v & \text{: zonal \& meridional velocity} \\ T, S & \text{: temperature \& salinity} \\ \eta & \text{: sea level} \end{array}\right\}$$

The Mathematical Problem (2/7)

Relation among model variables

$$\mathbf{x}_{t+1} = \mathbf{A}_t \mathbf{x}_t + \mathbf{G}_t \mathbf{u}_t \qquad t=1,2,\dots,N$$

State transition matrix

Forcing matrix

Control vector (forcing and other inhomogeneous terms, including errors of this relationship)

$$\mathbf{x}_t \equiv \begin{pmatrix} \vdots \\ u_{ijk} \\ v_{ijk} \\ T_{ijk} \\ S_{ijk} \\ \eta_{ij} \\ \vdots \end{pmatrix}_t \qquad \mathbf{u}_t \equiv \begin{pmatrix} \vdots \\ \tau^x_{ij} \\ \tau^y_{ij} \\ q_{ij} \\ e_{ij} \\ r_{ij} \\ \vdots \end{pmatrix}_t$$

model grid point

τ^x, τ^y : zonal & meridional wind stress

q : heat flux, e : evaporation

r : precipitation

The Mathematical Problem (3/7)

model state

data

model control

Observations $\quad \mathbf{H}_t \mathbf{x}_t \approx \mathbf{y}_t \qquad t=1,2,\dots,N$

Model $\quad \mathbf{x}_{t+1} = \mathbf{A}_t \mathbf{x}_t + \mathbf{G}_t \mathbf{u}_t \qquad t=1,2,\dots,N$

$$
\begin{pmatrix}
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 & \mathbf{H}_t & & & & & \\
 & & \mathbf{H}_{t+1} & & & & \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 & -\mathbf{A}_t & \mathbf{I} & & -\mathbf{G}_t & & \\
 & & -\mathbf{A}_{t+1} & \mathbf{I} & & -\mathbf{G}_{t+1} & \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots
\end{pmatrix}
\begin{pmatrix}
\vdots \\ \mathbf{x}_t \\ \mathbf{x}_{t+1} \\ \mathbf{x}_{t+2} \\ \mathbf{u}_t \\ \mathbf{u}_{t+1} \\ \vdots
\end{pmatrix}
\approx
\begin{pmatrix}
\vdots \\ \mathbf{y}_t \\ \mathbf{y}_{t+1} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \vdots
\end{pmatrix}
$$

$$\mathbf{E}\,\mathbf{a} \approx \mathbf{b}$$

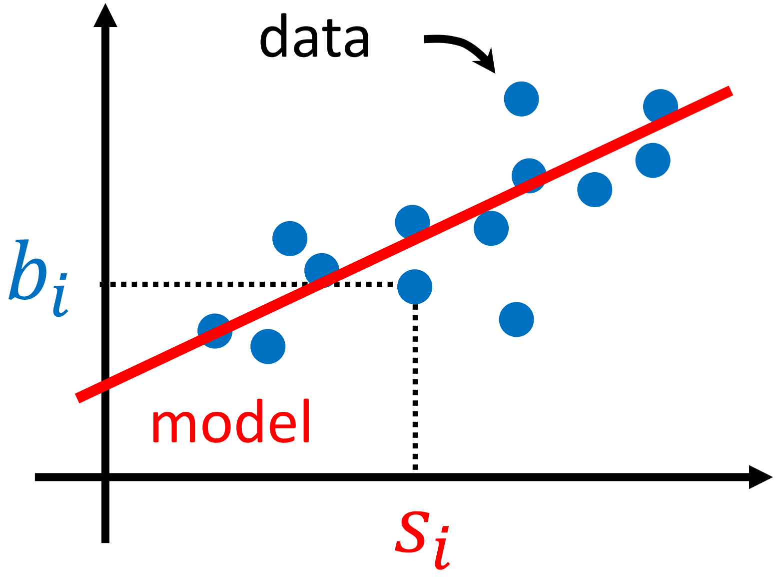
Combining model and data is an <u>inverse problem.</u>

The Mathematical Problem (4/7)

Linear Inverse Problem $\mathbf{E}\,\mathbf{a} \approx \mathbf{b}$

Given matrix $\mathbf{E}$ and vector $\mathbf{b}$ what is vector $\mathbf{a}$?

e.g., fitting a line through data $b = \alpha s + \beta$



$$\begin{pmatrix} s_1 & 1 \\ s_2 & 1 \\ \vdots & \vdots \\ s_n & 1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \approx \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

The Mathematical Problem (5/7)

$$
\begin{pmatrix}
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 & \mathbf{H}_t & & & & & \\
 & & \mathbf{H}_{t+1} & & & & \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 & -\mathbf{A}_t & \mathbf{I} & & -\mathbf{G}_t & & \\
 & & -\mathbf{A}_{t+1} & \mathbf{I} & & -\mathbf{G}_{t+1} & \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots
\end{pmatrix}
\begin{pmatrix}
\vdots \\ \mathbf{x}_t \\ \mathbf{x}_{t+1} \\ \mathbf{x}_{t+2} \\ \mathbf{u}_t \\ \mathbf{u}_{t+1} \\ \vdots
\end{pmatrix}
\approx
\begin{pmatrix}
\vdots \\ \mathbf{y}_t \\ \mathbf{y}_{t+1} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \vdots
\end{pmatrix}
\Rightarrow
\mathbf{E}\,\mathbf{a} \approx \mathbf{b}
$$

$$N \times M$$

$$N \ll M$$

Challenges

1) The large size of the problem,

2) Ill-posedness with more unknowns than knowns.

The Mathematical Problem (6/7)

Curve-fitting is also fundamentally ill-posed, as no solution exactly satisfies the equations.

$$\begin{pmatrix} s_1 & 1 \\ s_2 & 1 \\ \vdots & \vdots \\ s_n & 1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \approx \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

Explicitly writing the misfit of each equation $\gamma_1, \gamma_2, \cdots, \gamma_n$ where $\gamma_i = b_i - (\alpha s_i + \beta)$ the problem is mathematically,

$$\begin{pmatrix} s_1 & 1 & 1 & & & \\ s_2 & 1 & & 1 & & \\ \vdots & \vdots & & & \ddots & \\ s_n & 1 & & & & 1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma_1 \\ \gamma_2 \\ \vdots \\ \gamma_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

The Mathematical Problem (7/7)

The classic oceanographic inverse problem is that of determining reference level velocities in geostrophic calculations.

$$v(z) = v\left(z_{ref}\right) + \frac{g}{f\rho_0}\int_{z_{ref}}^{z} \frac{\partial\rho}{\partial x}\,dz$$

Wunsch (1977, Science)

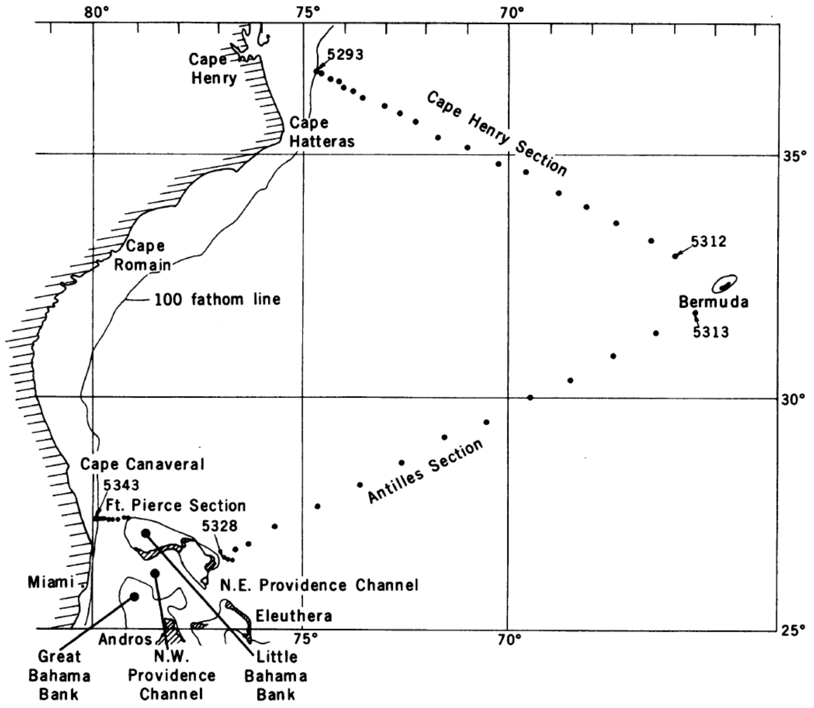


Fig. 1. Locations of *Atlantis* 215 stations used here.

range; then the statement that property C_k is conserved may be written

$$\sum_{j=1}^{M} (\bar{v}_{kj} + b_j)\,\Delta p_{kj}\Delta x_j = 0 \qquad (1)$$

and let there be $k = 1, \ldots, N$ such properties. Then we can combine Eq. 1 into matrix form

$$\mathbf{Ab} = -\Gamma \qquad (2)$$

where A is the $N \times M$ matrix of elements

Singular Value Decomposition (SVD)

The inverse problem $\mathbf{E}\,\mathbf{a} \approx \mathbf{b}$ can be solved using

Singular Value Decomposition $\mathbf{E} = \sum_{i=1}^{r} \sigma_i \boldsymbol{u}_i\, \boldsymbol{v}_i{}^T = \mathbf{U}\, \Xi\, \mathbf{V}^T$

where $r \leq min(N, M)$ and $\boldsymbol{u}_i{}^T \boldsymbol{u}_j = \boldsymbol{v}_i{}^T \boldsymbol{v}_j = \delta_{ij}$

Given this decomposition, we can write

$\mathbf{a} = \sum_{i=1}^{M} \gamma_i \boldsymbol{v}_i$ where $\gamma_i = \dfrac{\boldsymbol{u}_i{}^T \mathbf{b}}{\sigma_i}$ for $i = 1,2, \ldots r$

By "Ockham's Razor" we set $\gamma_i = 0$ for $i = r + 1, \ldots M$

Since $||\mathbf{a}|| = \sqrt{\sum_{i=1}^{M} \gamma_i{}^2}$ this is a Minimum Length Solution.

Other Inverse Methods

$$\mathbf{H}\,\mathbf{x} \approx \hat{\mathbf{y}}$$

Solve $\mathbf{E}\,\mathbf{a} \approx \mathbf{b}$ incorporating prior statistical information

- Minimum Variance Estimate

  aka Gauss-Markov inverse, basis of objective mapping.
  Closely related to the Kalman filter and related smoothers in state estimation.

- Least-Squares

  Closely related to the Adjoint Method (4dVAR) in state estimation.

… which turn out to be the same.

Minimum Variance Estimate

Solve $\mathbf{H}\mathbf{x} \approx \hat{\mathbf{y}}$ by incorporating prior statistical information

$$\mathbf{H}\mathbf{x} + \mathbf{n} = \hat{\mathbf{y}} \qquad \langle \mathbf{x}\mathbf{x}^T \rangle \equiv \mathbf{P} \qquad \langle \mathbf{n}\mathbf{n}^T \rangle \equiv \mathbf{R}$$

$$\langle \mathbf{x} \rangle = \mathbf{0} \qquad \langle \mathbf{n} \rangle = \mathbf{0}$$

A linear solution $\hat{\mathbf{x}} = \mathbf{B}\hat{\mathbf{y}}$ that minimizes error variance

$$\begin{aligned} \widehat{\mathbf{P}} &\equiv \langle (\hat{\mathbf{x}} - \mathbf{x})(\hat{\mathbf{x}} - \mathbf{x})^T \rangle \\ &= \langle (\mathbf{B}\hat{\mathbf{y}} - \mathbf{x})(\mathbf{B}\hat{\mathbf{y}} - \mathbf{x})^T \rangle \\ &= \mathbf{B} \langle \hat{\mathbf{y}}\hat{\mathbf{y}}^T \rangle \mathbf{B}^T - \langle \mathbf{x}\hat{\mathbf{y}}^T \rangle \mathbf{B}^T - \mathbf{B} \langle \hat{\mathbf{y}}\mathbf{x}^T \rangle + \langle \mathbf{x}\mathbf{x}^T \rangle \end{aligned}$$

is given by

$$\boxed{\hat{\mathbf{x}} = \mathbf{P}\mathbf{H}^T(\mathbf{H}\mathbf{P}\mathbf{H}^T + \mathbf{R})^{-1}\hat{\mathbf{y}}}$$

with error

$$\widehat{\mathbf{P}} = \mathbf{P} - \mathbf{P}\mathbf{H}^T (\mathbf{H}\mathbf{P}\mathbf{H}^T + \mathbf{R})^{-1} \mathbf{H}\mathbf{P}$$

Least-Squares Estimate (1/4)

Solve $\mathbf{Hx} \approx \hat{\mathbf{y}}$ that minimizes

$$\boxed{J = (\hat{\mathbf{y}} - \mathbf{Hx})^T \mathbf{R}^{-1} (\hat{\mathbf{y}} - \mathbf{Hx}) + \mathbf{x}^T \mathbf{P}^{-1} \mathbf{x}}$$

where $\mathbf{R} = \left\langle (\hat{\mathbf{y}} - \mathbf{Hx})(\hat{\mathbf{y}} - \mathbf{Hx})^T \right\rangle = \langle \mathbf{nn}^T \rangle$ and $\mathbf{P} = \langle \mathbf{xx}^T \rangle$

Why scale by inverse covariance?

Using Cholesky decomposition $\mathbf{R} = \mathbf{R}^{T/2}\, \mathbf{R}^{1/2}$

$$\begin{pmatrix} r_{11} & r_{12} & \cdots & r_{1N} \\ 0 & r_{22} & \cdots & r_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{NN} \end{pmatrix}$$

define $\mathbf{n}' \equiv \mathbf{R}^{-T/2} (\hat{\mathbf{y}} - \mathbf{Hx})$

then $(\hat{\mathbf{y}} - \mathbf{Hx})^T \mathbf{R}^{-1} (\hat{\mathbf{y}} - \mathbf{Hx}) = \mathbf{n}'^T \mathbf{n}'$ Notably $\langle \mathbf{n}' \mathbf{n}'^T \rangle = \mathrm{I}$

Least-Squares Estimate (2/4)

Example of de-correlating variables

$$\mathbf{R} = \begin{pmatrix} 1 & 0.99 \\ 0.99 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0.99 & 0.14 \end{pmatrix} \begin{pmatrix} 1 & 0.99 \\ 0 & 1 \end{pmatrix} = \mathbf{R}^{T/2}\, \mathbf{R}^{1/2}$$

$$\mathbf{R}^{-T/2} = \begin{pmatrix} 1 & 0 \\ 0.99 & 0.14 \end{pmatrix}^{-1} = \begin{pmatrix} 1 & 0 \\ -7.0 & 7.1 \end{pmatrix}$$

$$\mathbf{n}' = \mathbf{R}^{-T/2}\mathbf{n} = \begin{pmatrix} 1 & 0 \\ -7.0 & 7.1 \end{pmatrix} \begin{pmatrix} n_1 \\ n_1 \end{pmatrix}$$

Instead of having two of the same, the scaled version has just one of them and the scaled difference between them.

Least-Squares Estimate (3/4)

To minimizes $$J = (\hat{\mathbf{y}} - \mathbf{H}\mathbf{x})^T \mathbf{R}^{-1} (\hat{\mathbf{y}} - \mathbf{H}\mathbf{x}) + \mathbf{x}^T \mathbf{P}^{-1} \mathbf{x}$$

Solve $$\frac{\partial J}{\partial \mathbf{x}} = \mathbf{0}$$

Basic notation of vector differentiation

$$\frac{\partial s}{\partial \mathbf{x}} \equiv \begin{pmatrix} \frac{\partial s}{\partial x_1} & \cdots & \frac{\partial s}{\partial x_N} \end{pmatrix}^T \quad \Rightarrow \quad \frac{\partial (\boldsymbol{q}^T \mathbf{x})}{\partial \mathbf{x}} = \frac{\partial (\mathbf{x}^T \boldsymbol{q})}{\partial \mathbf{x}} = \boldsymbol{q}$$

$$\frac{\partial \boldsymbol{q}}{\partial \mathbf{x}} \equiv \begin{pmatrix} \frac{\partial q_1}{\partial x_1} & \cdots & \frac{\partial q_M}{\partial x_1} \\ \vdots & \cdots & \vdots \\ \frac{\partial q_1}{\partial x_N} & \cdots & \frac{\partial q_M}{\partial x_N} \end{pmatrix} \quad \Rightarrow \quad \frac{\partial (\mathbf{B}\mathbf{x})}{\partial \mathbf{x}} = \mathbf{B}^T \qquad \frac{\partial (\mathbf{x}^T \mathbf{B})}{\partial \mathbf{x}} = \mathbf{B}$$

Least-Squares Estimate (4/4)

To minimizes $$\boxed{J = (\hat{\mathbf{y}} - \mathbf{H}\mathbf{x})^T \mathbf{R}^{-1} (\hat{\mathbf{y}} - \mathbf{H}\mathbf{x}) + \mathbf{x}^T \mathbf{P}^{-1} \mathbf{x}}$$

Solve $$\frac{\partial J}{\partial \mathbf{x}} = \mathbf{0}$$

$$\frac{1}{2}\frac{\partial J}{\partial \mathbf{x}} = \frac{1}{2}\frac{\partial (\hat{\mathbf{y}} - \mathbf{H}\mathbf{x})}{\partial \mathbf{x}} \frac{\partial}{\partial (\hat{\mathbf{y}} - \mathbf{H}\mathbf{x})} (\hat{\mathbf{y}} - \mathbf{H}\mathbf{x})^T \mathbf{R}^{-1} (\hat{\mathbf{y}} - \mathbf{H}\mathbf{x}) + \frac{1}{2}\frac{\partial}{\partial \mathbf{x}} \mathbf{x}^T \mathbf{P}^{-1} \mathbf{x}$$

$$= -\mathbf{H}^T \mathbf{R}^{-1} (\hat{\mathbf{y}} - \mathbf{H}\mathbf{x}) + \mathbf{P}^{-1} \mathbf{x}$$

$$= (\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} + \mathbf{P}^{-1}) \mathbf{x} - \mathbf{H}^T \mathbf{R}^{-1} \hat{\mathbf{y}}$$

Therefore, $$\boxed{\hat{\mathbf{x}} = (\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} + \mathbf{P}^{-1})^{-1} \mathbf{H}^T \mathbf{R}^{-1} \hat{\mathbf{y}}}$$

Comparing Solutions

Solve $\mathbf{Hx} \approx \hat{\mathbf{y}}$ by incorporating prior statistical information

Least-Squares $\boxed{\hat{\mathbf{x}} = (\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H} + \mathbf{P}^{-1})^{-1}\ \mathbf{H}^T\mathbf{R}^{-1}\,\hat{\mathbf{y}}}$

Minimum Variance $\boxed{\hat{\mathbf{x}} = \mathbf{P}\mathbf{H}^T(\mathbf{H}\mathbf{P}\mathbf{H}^T + \mathbf{R})^{-1}\,\hat{\mathbf{y}}}$

The two are identical based on the “Matrix Inversion Lemma”

$$\mathbf{P}\mathbf{H}^T(\mathbf{H}\mathbf{P}\mathbf{H}^T + \mathbf{R})^{-1} = (\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H} + \mathbf{P}^{-1})^{-\mathbf{1}}\ \mathbf{H}^T\mathbf{R}^{-1}$$

Recap

1. State estimation is an inverse problem,

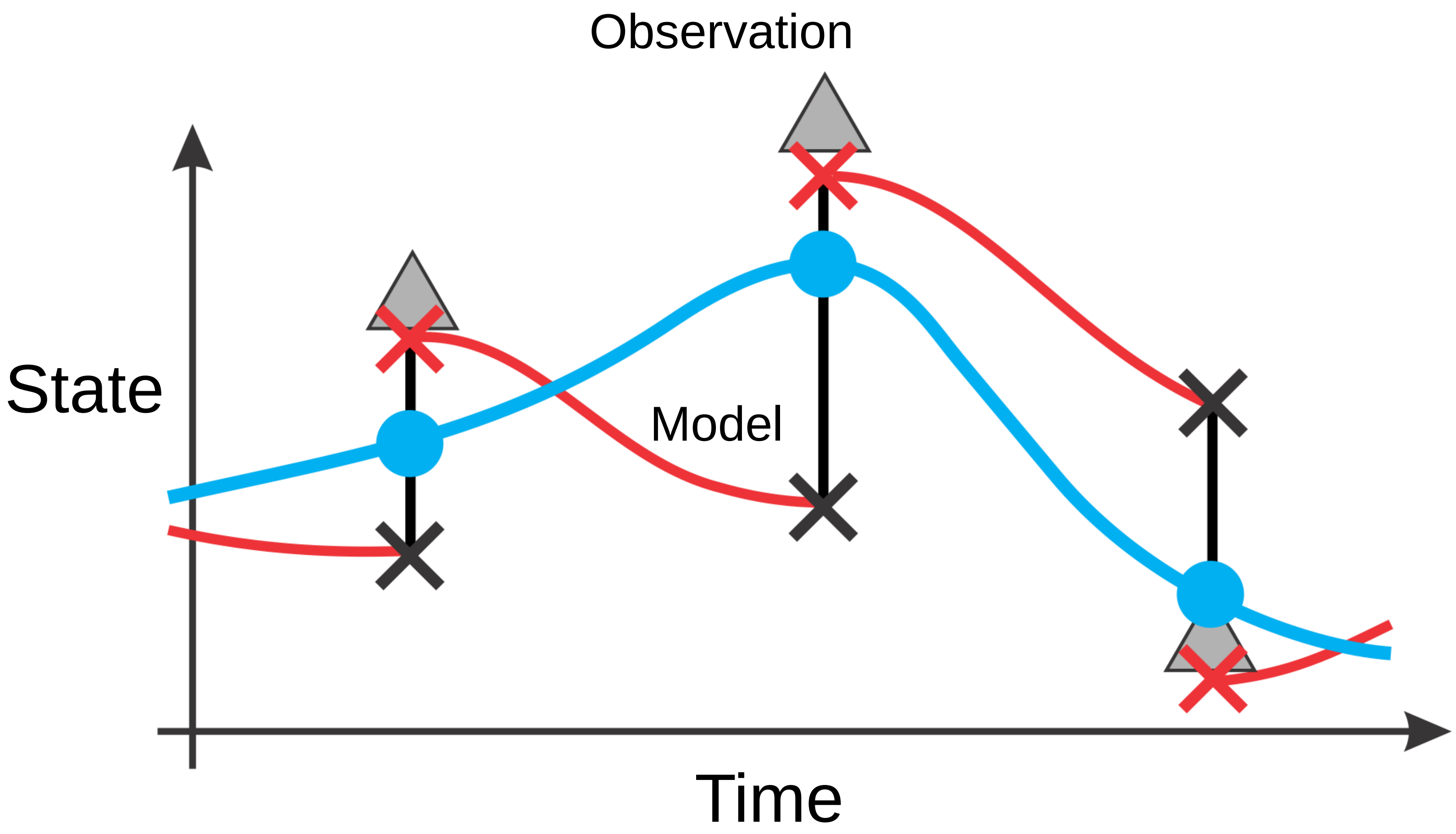
2. Various inverse methods are available;
    - Minimum length
    - Minimum Variance
    - Least-Squares
    - Maximum likelihood
    - Bayesian

Motivation for State Estimation (3/3)

From Monday

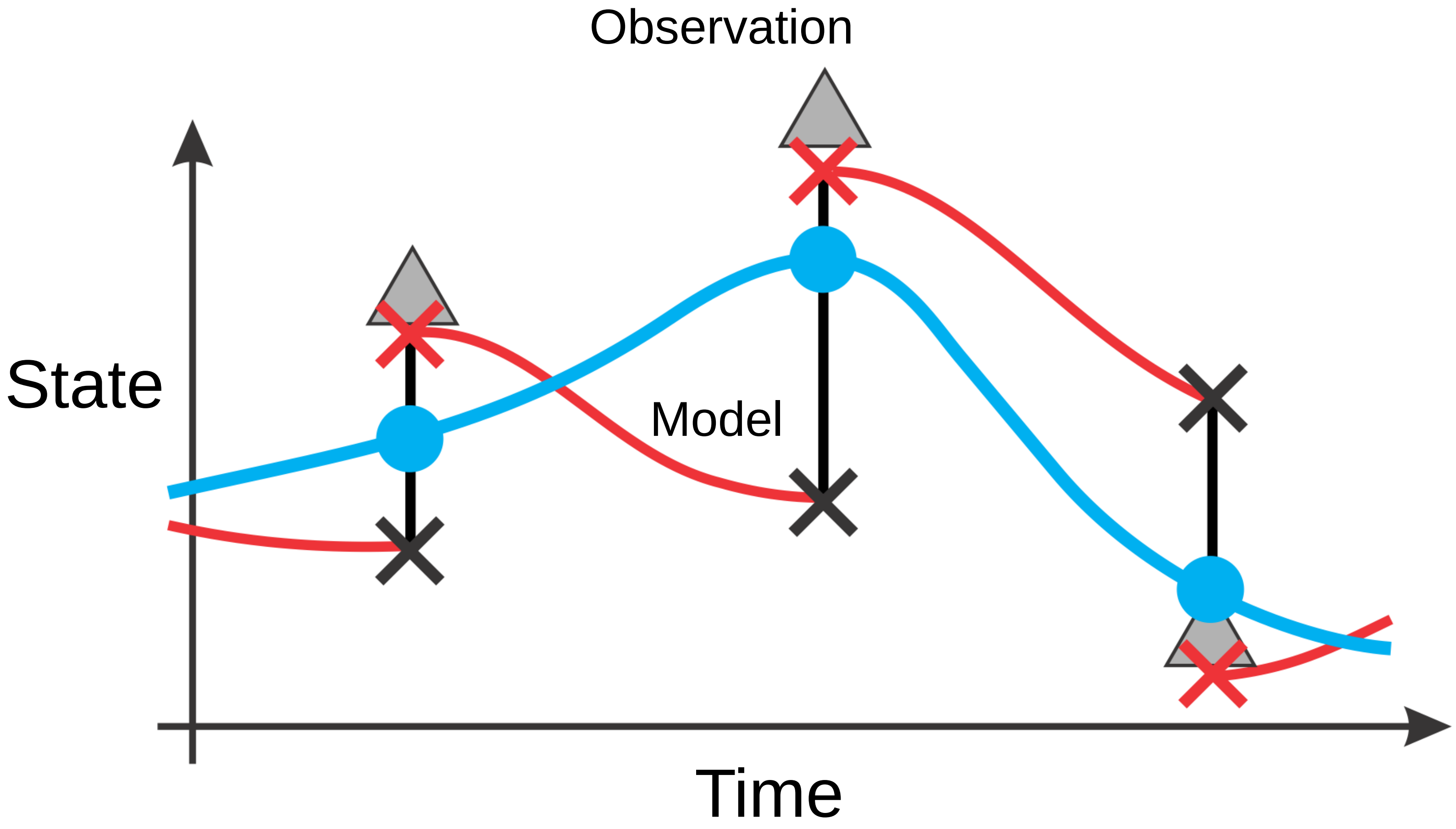
Data Assimilation vs State Estimation

From Monday



Kalman Filter (1/2)

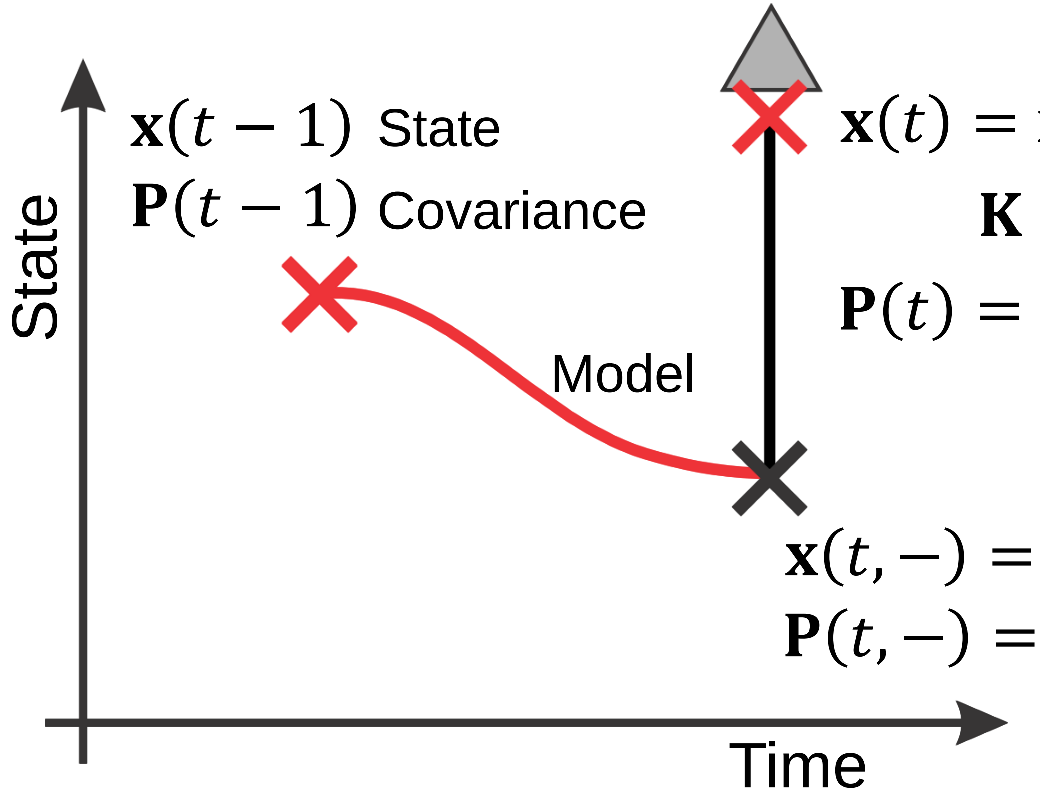
A recursive Minimum Variance Estimate



Kalman Filter (2/2)

A recursive Minimum Variance Estimate

Observation $\mathbf{y}(t)$ $\quad$ $\mathbf{Hx} \approx \mathbf{y}$ $\quad \Rightarrow \quad$ $\mathbf{H}\big(\mathbf{x} - \mathbf{x}(-)\big) \approx \mathbf{y} - \mathbf{Hx}(-)$



$$\mathbf{x}(t) = \mathbf{x}(t,-) + \mathbf{K}\big(\mathbf{y}(t) - \mathbf{Hx}(t,-)\big)$$

$$\mathbf{K} \equiv \mathbf{P}(t,-)\mathbf{H}^T\left(\mathbf{HP}(t,-)\mathbf{H}^T + \mathbf{R}\right)^{-1} \quad \text{Kalman Gain}$$

$$\mathbf{P}(t) = \mathbf{P}(t,-) - \mathbf{P}(t,-)\mathbf{H}^T\left(\mathbf{HP}(t,-)\mathbf{H}^T + \mathbf{R}\right)^{-1}\mathbf{HP}(t,-)$$

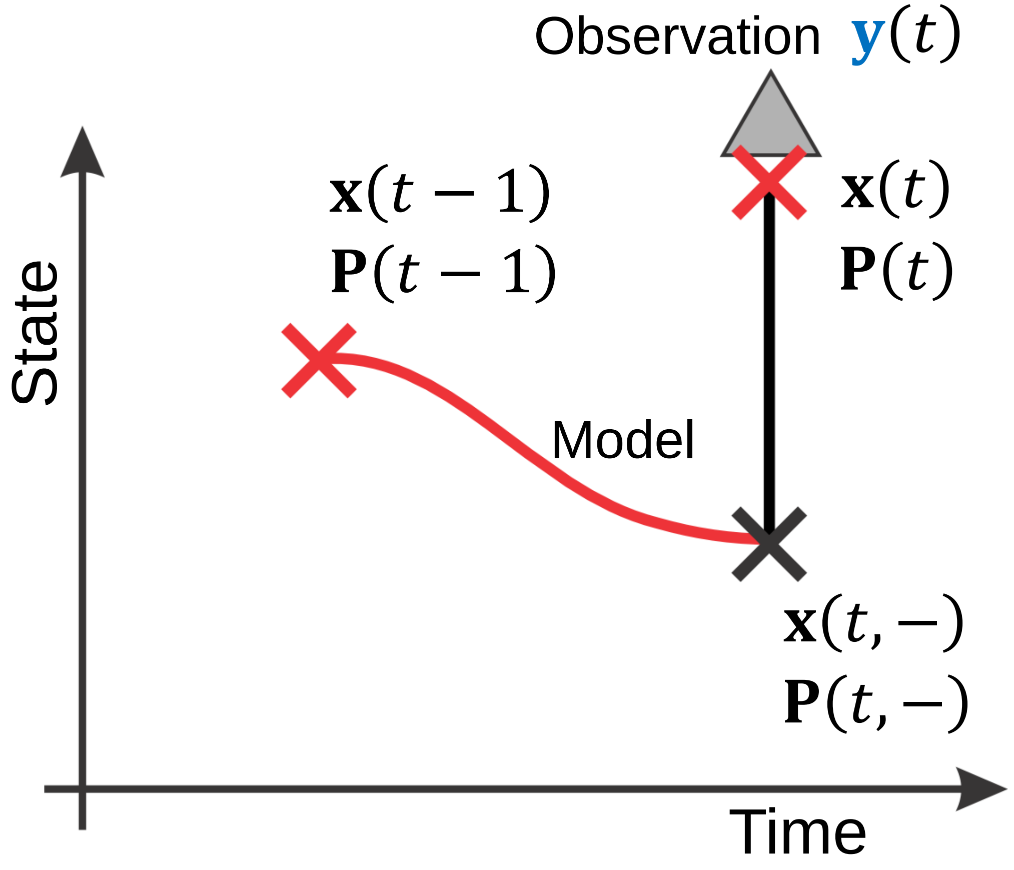
$$\mathbf{x}(t,-) = \mathbf{Ax}(t-1) + \mathbf{Gu}(t-1)$$

$$\mathbf{P}(t,-) = \mathbf{AP}(t-1)\mathbf{A}^T + \mathbf{GQG}^T$$

$$\mathbf{Q} \equiv \langle \mathbf{uu}^T \rangle$$

Kalman Filter (2/2)

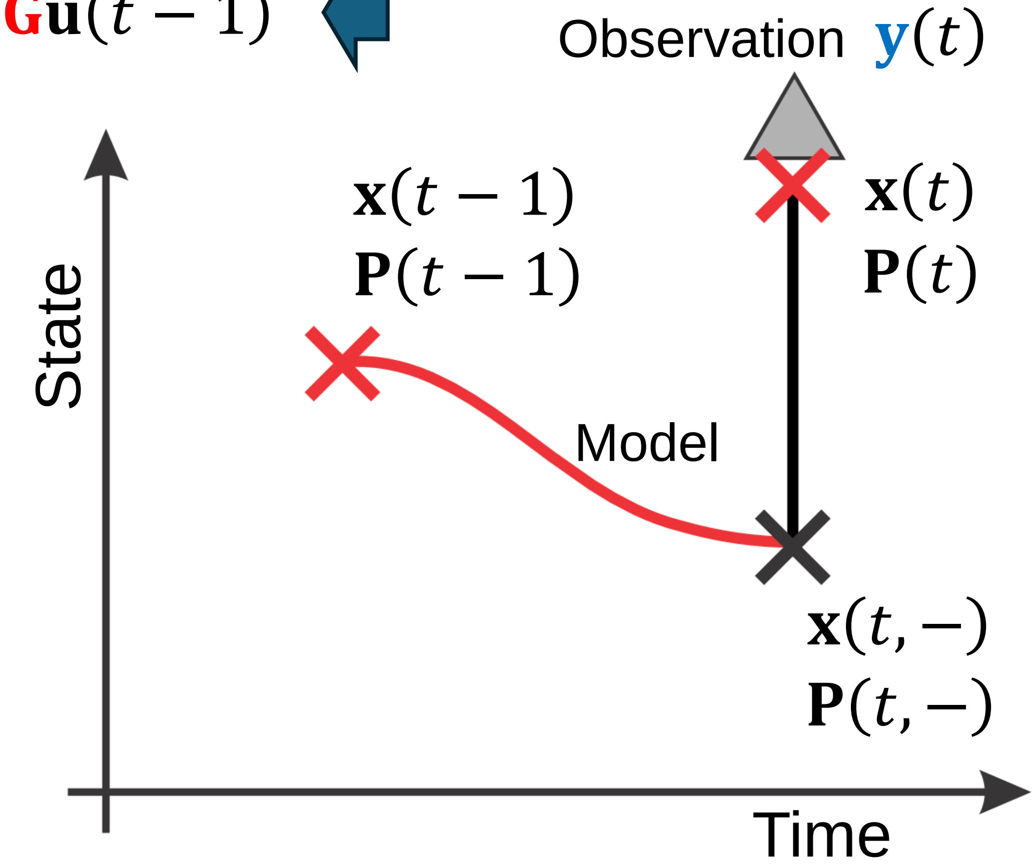
A recursive Minimum Variance Estimate



Rauch-Tung-Striebel Smoother (1/2)

A recursive Minimum Variance Estimate

$$\mathbf{x}(t) = \mathbf{A}\mathbf{x}(t-1) + \mathbf{G}\mathbf{u}(t-1)$$



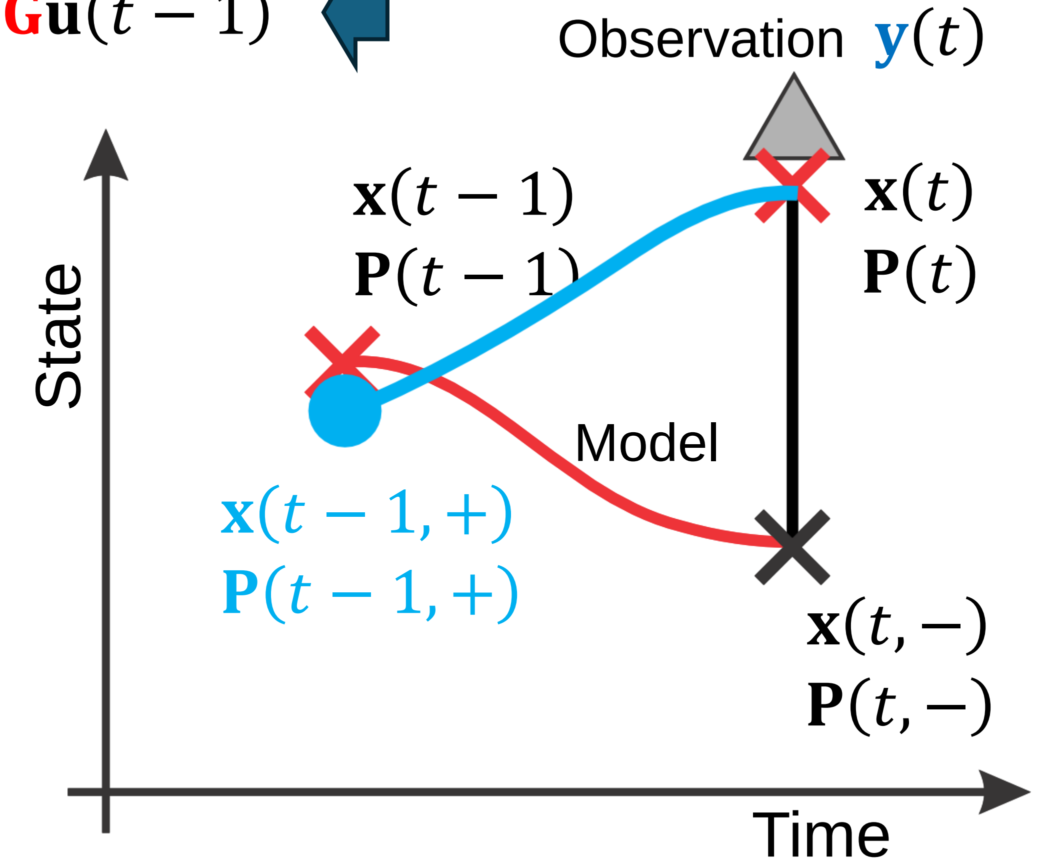
Rauch-Tung-Striebel Smoother (1/2)

A recursive Minimum Variance Estimate

$$\mathbf{x}(t) = \mathbf{A}\mathbf{x}(t-1) + \mathbf{G}\mathbf{u}(t-1)$$

$$\left.\begin{aligned} \mathbf{x}(t-1,+) &= \mathbf{x}(t-1) + \mathbf{S}[\mathbf{x}(t) - \mathbf{x}(t,-)] \\ \mathbf{S} &\equiv \mathbf{P}(t-1)\,\mathbf{A}^T\,\mathbf{P}(t,-)^{-1} \\ \mathbf{P}(t-1,+) &= \mathbf{P}(t-1) + \mathbf{S}[\mathbf{P}(t) - \mathbf{P}(t,-)]\mathbf{S}^T \end{aligned}\right\}$$

$$\left.\begin{aligned} \mathbf{u}(t-1,+) &= \mathbf{u}(t-1) + \mathbf{M}[\mathbf{x}(t) - \mathbf{x}(t,-)] \\ \mathbf{M} &\equiv \mathbf{Q}(t-1)\,\mathbf{G}^T\,\mathbf{P}(t,-)^{-1} \\ \mathbf{Q}(t-1,+) &= \mathbf{Q}(t-1) + \mathbf{M}[\mathbf{P}(t) - \mathbf{P}(t,-)]\mathbf{M}^T \end{aligned}\right\}$$



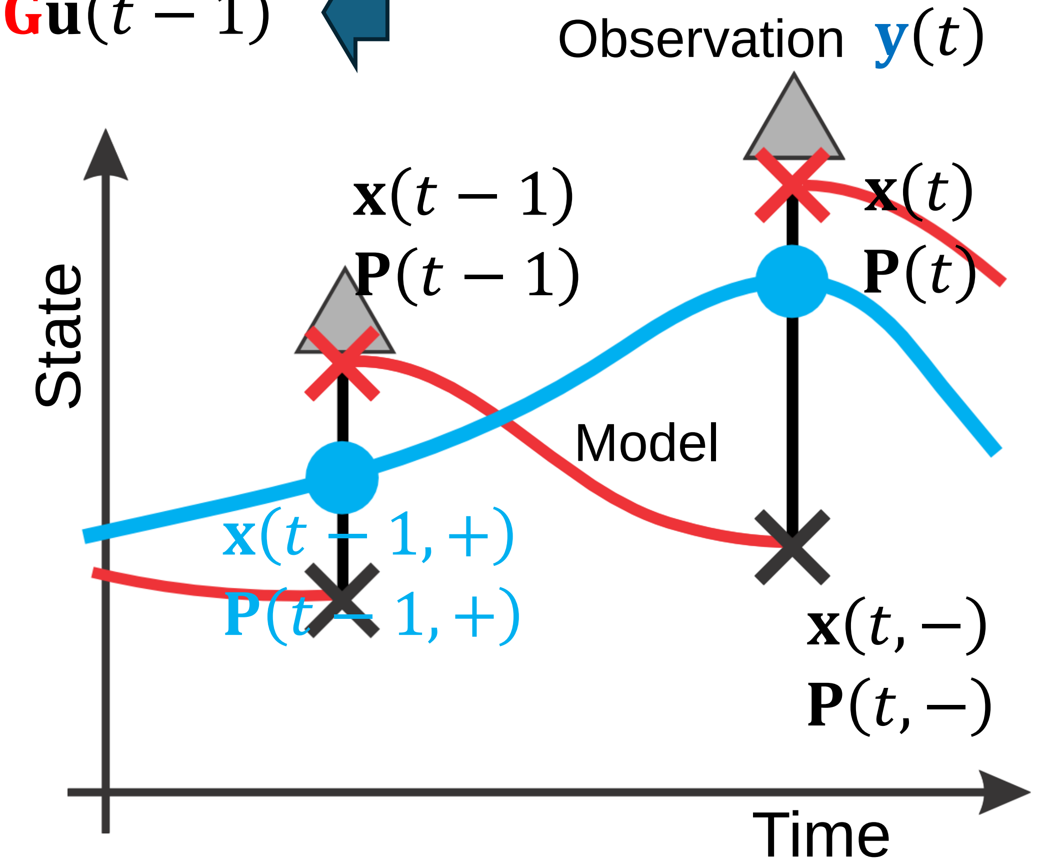
Rauch-Tung-Striebel Smoother (2/2)

A recursive Minimum Variance Estimate

$$\mathbf{x}(t) = \mathbf{A}\mathbf{x}(t-1) + \mathbf{G}\mathbf{u}(t-1)$$

$$\left.\begin{aligned} \mathbf{x}(t-1,+) &= \mathbf{x}(t-1) + \mathbf{S}[\mathbf{x}(t,+) - \mathbf{x}(t,-)] \\ \mathbf{S} &\equiv \mathbf{P}(t-1)\,\mathbf{A}^T\,\mathbf{P}(t,-)^{-1} \\ \mathbf{P}(t-1,+) &= \mathbf{P}(t-1) + \mathbf{S}[\mathbf{P}(t,+) - \mathbf{P}(t,-)]\mathbf{S}^T \end{aligned}\right\}$$

$$\left.\begin{aligned} \mathbf{u}(t-1,+) &= \mathbf{u}(t-1) + \mathbf{M}[\mathbf{x}(t,+) - \mathbf{x}(t,-)] \\ \mathbf{M} &\equiv \mathbf{Q}(t-1)\,\mathbf{G}^T\,\mathbf{P}(t,-)^{-1} \\ \mathbf{Q}(t-1,+) &= \mathbf{Q}(t-1) + \mathbf{M}[\mathbf{P}(t,+) - \mathbf{P}(t,-)]\mathbf{M}^T \end{aligned}\right\}$$



Adjoint Method (4D-var) (1/9)

A least-squares method that solves the problem iteratively by descent optimization.

Solve $\mathbf{Hx} \approx \mathbf{y}$ that minimizes

$$\boxed{J = (\mathbf{y} - \mathbf{Hx})^T \mathbf{R}^{-1} (\mathbf{y} - \mathbf{Hx}) + \mathbf{x}^T \mathbf{P}^{-1} \mathbf{x}}$$

analytically

$$\boxed{\hat{\mathbf{x}} = (\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} + \mathbf{P}^{-1})^{-1} \; \mathbf{H}^T \mathbf{R}^{-1} \, \mathbf{y}}$$

Adjoint Method (4D-var) (2/9)

$$\begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ & \mathbf{H}_t & & & & & \\ & & \mathbf{H}_{t+1} & & & & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ & -\mathbf{A} & \mathbf{I} & & -\mathbf{G} & & \\ & & -\mathbf{A} & \mathbf{I} & & -\mathbf{G} & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} \vdots \\ \mathbf{x}_t \\ \mathbf{x}_{t+1} \\ \mathbf{x}_{t+2} \\ \mathbf{u}_t \\ \mathbf{u}_{t+1} \\ \vdots \end{pmatrix} \approx \begin{pmatrix} \vdots \\ \mathbf{y}_t \\ \mathbf{y}_{t+1} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \vdots \end{pmatrix}$$

In terms of least-squares, the problem is to minimize

$$J \equiv \sum_{t=1}^{M} (\mathbf{y}_t - \mathbf{H}_t \mathbf{x}_t)^T \mathbf{R}_t^{-1} (\mathbf{y}_t - \mathbf{H}_t \mathbf{x}_t)$$

$$+ (\mathbf{x}_0 - \hat{\mathbf{x}}_0)^T \mathbf{P}_0^{-1} (\mathbf{x}_0 - \hat{\mathbf{x}}_0)$$

$$+ \sum_{t=0}^{M-1} (\mathbf{u}_t - \hat{\mathbf{u}}_t)^T \mathbf{Q}_t^{-1} (\mathbf{u}_t - \hat{\mathbf{u}}_t)$$

$$- 2\sum_{t=1}^{M} \boldsymbol{\lambda}_t^T [\mathbf{x}_t - \mathbf{A}\mathbf{x}_{t-1} - \mathbf{G}\mathbf{u}_{t-1}]$$

Lagrange multipliers

Adjoint Method (4D-var) (3/9)

$$J \equiv \sum_{t=1}^{M}(\mathbf{y}_t - \mathbf{H}_t\mathbf{x}_t)^T\mathbf{R}_t{}^{-1}(\mathbf{y}_t - \mathbf{H}_t\mathbf{x}_t)$$

$$+ (\mathbf{x}_0 - \hat{\mathbf{x}}_0)^T\mathbf{P}_0{}^{-1}(\mathbf{x}_0 - \hat{\mathbf{x}}_0)$$

$$+ \sum_{t=0}^{M-1}(\mathbf{u}_t - \hat{\mathbf{u}}_t)^T\mathbf{Q}_t{}^{-1}(\mathbf{u}_t - \hat{\mathbf{u}}_t)$$

$$- 2\sum_{t=1}^{M}\boldsymbol{\lambda}_t^T[\mathbf{x}_t - \mathbf{A}\mathbf{x}_{t-1} - \mathbf{G}\mathbf{u}_{t-1}]$$

Adjoint Method (4D-var) (4/9)

$$J \equiv \sum_{t=1}^{M}(\mathbf{y}_t - \mathbf{H}_t\mathbf{x}_t)^T \mathbf{R}_t{}^{-1}(\mathbf{y}_t - \mathbf{H}_t\mathbf{x}_t)$$
$$+ (\mathbf{x}_0 - \hat{\mathbf{x}}_0)^T \mathbf{P}_0{}^{-1}(\mathbf{x}_0 - \hat{\mathbf{x}}_0)$$
$$+ \sum_{t=0}^{M-1}(\mathbf{u}_t - \hat{\mathbf{u}}_t)^T \mathbf{Q}_t{}^{-1}(\mathbf{u}_t - \hat{\mathbf{u}}_t)$$
$$- 2\sum_{t=1}^{M} \boldsymbol{\lambda}_t^T[\mathbf{x}_t - \mathbf{A}\mathbf{x}_{t-1} - \mathbf{G}\mathbf{u}_{t-1}]$$

$$\left\{ \begin{array}{ll}
\frac{1}{2}\frac{\partial J}{\partial \mathbf{u}_t} = \mathbf{Q}^{-1}(\mathbf{u}_t - \hat{\mathbf{u}}_t) + \mathbf{G}^T\boldsymbol{\lambda}_{t+1} = \mathbf{0} & t = 0, 1, \ldots, M\text{-}1 \\
\frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_0} = \mathbf{P}_0{}^{-1}(\mathbf{x}_0 - \hat{\mathbf{x}}_0) + \mathbf{A}^T\boldsymbol{\lambda}_1 = \mathbf{0} & \\
\frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_t} = -\mathbf{H}_t\mathbf{R}_t{}^{-1}(\mathbf{y}_t - \mathbf{H}_t\mathbf{x}_t) - \boldsymbol{\lambda}_t + \mathbf{A}^T\boldsymbol{\lambda}_{t+1} = \mathbf{0} & t = 1, 2, \ldots, M\text{-}1 \\
\frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_M} = -\mathbf{H}_M\mathbf{R}_M{}^{-1}(\mathbf{y}_M - \mathbf{H}_M\mathbf{x}_M) - \boldsymbol{\lambda}_M = \mathbf{0} & \\
\frac{1}{2}\frac{\partial J}{\partial \boldsymbol{\lambda}_t} = \mathbf{x}_t - \mathbf{A}\mathbf{x}_{t-1} - \mathbf{G}\mathbf{u}_{t-1} = \mathbf{0} & t = 1, 2, \ldots, M
\end{array} \right.$$

Adjoint Method (4D-var) (5/9)

$$\begin{cases} \frac{1}{2}\frac{\partial J}{\partial \mathbf{u}_t} = \mathbf{Q}^{-1}(\mathbf{u}_t - \hat{\mathbf{u}}_t) + \mathbf{G}^T \boldsymbol{\lambda}_{t+1} = \mathbf{0} & t = 0, 1, \ldots, M\text{-}1 \\ \frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_0} = \mathbf{P}_0{}^{-1}(\mathbf{x}_0 - \hat{\mathbf{x}}_0) + \mathbf{A}^T \boldsymbol{\lambda}_1 = \mathbf{0} & \\ \frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_t} = -\mathbf{H}_t \mathbf{R}_t{}^{-1}(\mathbf{y}_t - \mathbf{H}_t \mathbf{x}_t) - \boldsymbol{\lambda}_t + \mathbf{A}^T \boldsymbol{\lambda}_{t+1} = \mathbf{0} & t = 1, 2, \ldots, M\text{-}1 \\ \frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_M} = -\mathbf{H}_M \mathbf{R}_M{}^{-1}(\mathbf{y}_M - \mathbf{H}_M \mathbf{x}_M) - \boldsymbol{\lambda}_M = \mathbf{0} & \\ \frac{1}{2}\frac{\partial J}{\partial \boldsymbol{\lambda}_t} = \mathbf{x}_t - \mathbf{A}\mathbf{x}_{t-1} - \mathbf{G}\mathbf{u}_{t-1} = \mathbf{0} & t = 1, 2, \ldots, M \end{cases}$$

1) Integrate model from first guess controls.

$$\mathbf{x}_t = \mathbf{A}\mathbf{x}_{t-1} + \mathbf{G}\mathbf{u}_{t-1} \qquad t = 1, 2, \ldots, M$$

with $\mathbf{x}_0 = \hat{\mathbf{x}}_0$ $\quad \mathbf{u}_t = \hat{\mathbf{u}}_t$

Adjoint Method (4D-var) (6/9)

$$\frac{1}{2}\frac{\partial J}{\partial \mathbf{u}_t} = \mathbf{Q}^{-1}(\mathbf{u}_t - \hat{\mathbf{u}}_t) + \mathbf{G}^T \boldsymbol{\lambda}_{t+1} \qquad t = 0, 1, \ldots, M\text{-}1$$

$$\frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_0} = \mathbf{P}_0{}^{-1}(\mathbf{x}_0 - \hat{\mathbf{x}}_0) + \mathbf{A}^T \boldsymbol{\lambda}_1$$

$$\frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_t} = -\mathbf{H}_t \mathbf{R}_t{}^{-1}(\mathbf{y}_t - \mathbf{H}_t \mathbf{x}_t) - \boldsymbol{\lambda}_t + \mathbf{A}^T \boldsymbol{\lambda}_{t+1} \qquad t = 1, 2, \ldots, M\text{-}1$$

$$\frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_M} = -\mathbf{H}_M \mathbf{R}_M{}^{-1}(\mathbf{y}_M - \mathbf{H}_M \mathbf{x}_M) - \boldsymbol{\lambda}_M = \mathbf{0}$$

$$\frac{1}{2}\frac{\partial J}{\partial \boldsymbol{\lambda}_t} = \mathbf{x}_t - \mathbf{A}\mathbf{x}_{t-1} - \mathbf{G}\mathbf{u}_{t-1} = \mathbf{0} \qquad t = 1, 2, \ldots, M$$

2) Determine terminal Lagrange multiplier.

$$\boldsymbol{\lambda}_M = -\mathbf{H}_M \mathbf{R}_M{}^{-1}(\mathbf{y}_M - \mathbf{H}_M \mathbf{x}_M)$$

Adjoint Method (4D-var) (7/9)

$$\frac{1}{2}\frac{\partial J}{\partial \mathbf{u}_t} = \mathbf{Q}^{-1}(\mathbf{u}_t - \hat{\mathbf{u}}_t) + \mathbf{G}^T \boldsymbol{\lambda}_{t+1} \qquad t = 0, 1, \ldots, M\text{-}1$$

$$\frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_0} = \mathbf{P}_0^{-1}(\mathbf{x}_0 - \hat{\mathbf{x}}_0) + \mathbf{A}^T \boldsymbol{\lambda}_1$$

$$\frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_t} = -\mathbf{H}_t \mathbf{R}_t^{-1}(\mathbf{y}_t - \mathbf{H}_t \mathbf{x}_t) - \boldsymbol{\lambda}_t + \mathbf{A}^T \boldsymbol{\lambda}_{t+1} = \mathbf{0} \qquad t = 1, 2, \ldots, M\text{-}1$$

$$\frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_M} = -\mathbf{H}_M \mathbf{R}_M^{-1}(\mathbf{y}_M - \mathbf{H}_M \mathbf{x}_M) - \boldsymbol{\lambda}_M = \mathbf{0}$$

$$\frac{1}{2}\frac{\partial J}{\partial \boldsymbol{\lambda}_t} = \mathbf{x}_t - \mathbf{A}\mathbf{x}_{t-1} - \mathbf{G}\mathbf{u}_{t-1} = \mathbf{0} \qquad t = 1, 2, \ldots, M$$

3) Determine all other Lagrange multipliers by the adjoint model.

$$\boldsymbol{\lambda}_t = \mathbf{A}^T \boldsymbol{\lambda}_{t+1} - \mathbf{H}_M \mathbf{R}_M^{-1}(\mathbf{y}_M - \mathbf{H}_M \mathbf{x}_M) \qquad t = M-1, M-2, \ldots, 1$$

with $\boldsymbol{\lambda}_t = \boldsymbol{\lambda}_M$ at $t = M$

Adjoint Method (4D-var) (8/9)

$$\frac{1}{2}\frac{\partial J}{\partial \mathbf{u}_t} = \mathbf{Q}^{-1}(\mathbf{u}_t - \hat{\mathbf{u}}_t) + \mathbf{G}^T\boldsymbol{\lambda}_{t+1} \qquad t = 0, 1, \ldots, M\text{-}1$$

$$\frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_0} = \mathbf{P}_0{}^{-1}(\mathbf{x}_0 - \hat{\mathbf{x}}_0) + \mathbf{A}^T\boldsymbol{\lambda}_1$$

$$\frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_t} = -\mathbf{H}_t\mathbf{R}_t{}^{-1}(\mathbf{y}_t - \mathbf{H}_t\mathbf{x}_t) - \boldsymbol{\lambda}_t + \mathbf{A}^T\boldsymbol{\lambda}_{t+1} = \mathbf{0} \qquad t = 1, 2, \ldots, M\text{-}1$$

$$\frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_M} = -\mathbf{H}_M\mathbf{R}_M{}^{-1}(\mathbf{y}_M - \mathbf{H}_M\mathbf{x}_M) - \boldsymbol{\lambda}_M = \mathbf{0}$$

$$\frac{1}{2}\frac{\partial J}{\partial \boldsymbol{\lambda}_t} = \mathbf{x}_t - \mathbf{A}\mathbf{x}_{t-1} - \mathbf{G}\mathbf{u}_{t-1} = \mathbf{0} \qquad t = 1, 2, \ldots, M$$

4) Calculate cost function gradient for descent algorithm;

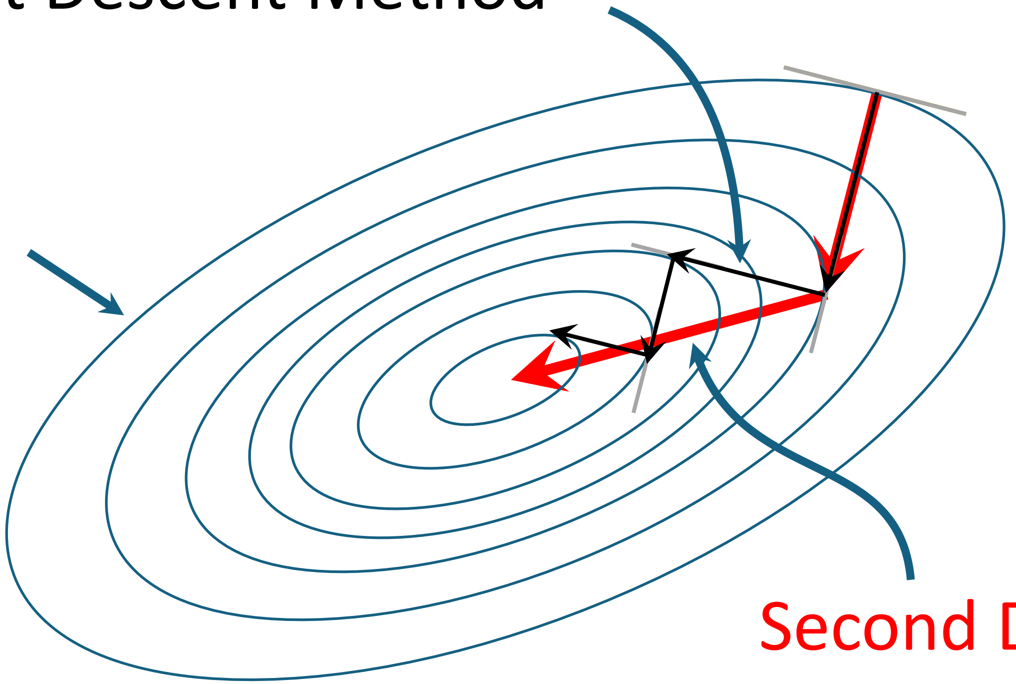
$$\frac{1}{2}\frac{\partial J}{\partial \mathbf{x}_0} = \mathbf{P}_0{}^{-1}(\mathbf{x}_0 - \hat{\mathbf{x}}_0) + \mathbf{A}^T\boldsymbol{\lambda}_1 \qquad \frac{1}{2}\frac{\partial J}{\partial \mathbf{u}_t} = \mathbf{Q}_t{}^{-1}(\mathbf{u}_t - \hat{\mathbf{u}}_t) + \mathbf{G}^T\boldsymbol{\lambda}_{t+1} \quad t = 0, 1, \ldots, M-1$$

Adjoint Method (4D-var) (9/9)

Descent Optimization

Steepest Descent Method

isopleths of J



Second Derivative Methods

e.g., Conjugate-Gradient Method
Quasi-Newton Method

What are "data error" R & "state error" P?

$$J \equiv \sum_{t=1}^{M}(\mathbf{y}_t - \mathbf{H}_t\mathbf{x}_t)^T \mathbf{R}_t^{-1}(\mathbf{y}_t - \mathbf{H}_t\mathbf{x}_t)$$
$$+ (\mathbf{x}_0 - \hat{\mathbf{x}}_0)^T \mathbf{P}_0^{-1}(\mathbf{x}_0 - \hat{\mathbf{x}}_0)$$
$$+ \sum_{t=0}^{M-1}(\mathbf{u}_t - \hat{\mathbf{u}}_t)^T \mathbf{Q}_t^{-1}(\mathbf{u}_t - \hat{\mathbf{u}}_t)$$
$$- 2\sum_{t=1}^{M} \boldsymbol{\lambda}_t^T [\mathbf{x}_t - \mathbf{A}\mathbf{x}_{t-1} - \mathbf{G}\mathbf{u}_{t-1}]$$

$$\mathbf{P}(-) = \mathbf{A}\mathbf{P}(t-1)\mathbf{A}^T + \mathbf{G}\mathbf{Q}\mathbf{G}^T$$
$$\mathbf{P}(t) = \mathbf{P}(-) - \mathbf{P}(-)\mathbf{H}^T(\mathbf{H}\mathbf{P}(-)\mathbf{H}^T + \mathbf{R})^{-1}\,\mathbf{H}\mathbf{P}(-)$$

Data   True state of model

Data error $\hat{\mathbf{y}} - \mathbf{H}\mathbf{x}$

State Estimate

State error $\hat{\mathbf{x}} - \mathbf{x}$

Actual ocean

Representation error $\mathbf{x} - \mathbf{w}$

because $\mathbf{x} = \boldsymbol{\Gamma}\mathbf{w}$

Modeling

Example estimating $\mathbf{R}$

$\mathbf{R}$ can be estimated from observations and model simulation

$$\mathbf{y} = \mathbf{s} + \mathbf{n}$$

$$\mathbf{m} = \mathbf{s} + \mathbf{p}$$

Assuming signal and errors are mutually uncorrelated, i.e.,

$$\langle \mathbf{s}\mathbf{n}^T \rangle = \mathbf{0} \qquad \langle \mathbf{s}\mathbf{p}^T \rangle = \mathbf{0} \qquad \langle \mathbf{n}\mathbf{p}^T \rangle = \mathbf{0}$$

covariances among data and model simulation are,

$$\langle \boldsymbol{y}\boldsymbol{y}^T \rangle = \langle \mathbf{s}\mathbf{s}^T \rangle + \langle \mathbf{n}\mathbf{n}^T \rangle$$

$$\langle \mathbf{m}\mathbf{m}^T \rangle = \langle \mathbf{s}\mathbf{s}^T \rangle + \langle \mathbf{p}\mathbf{p}^T \rangle$$

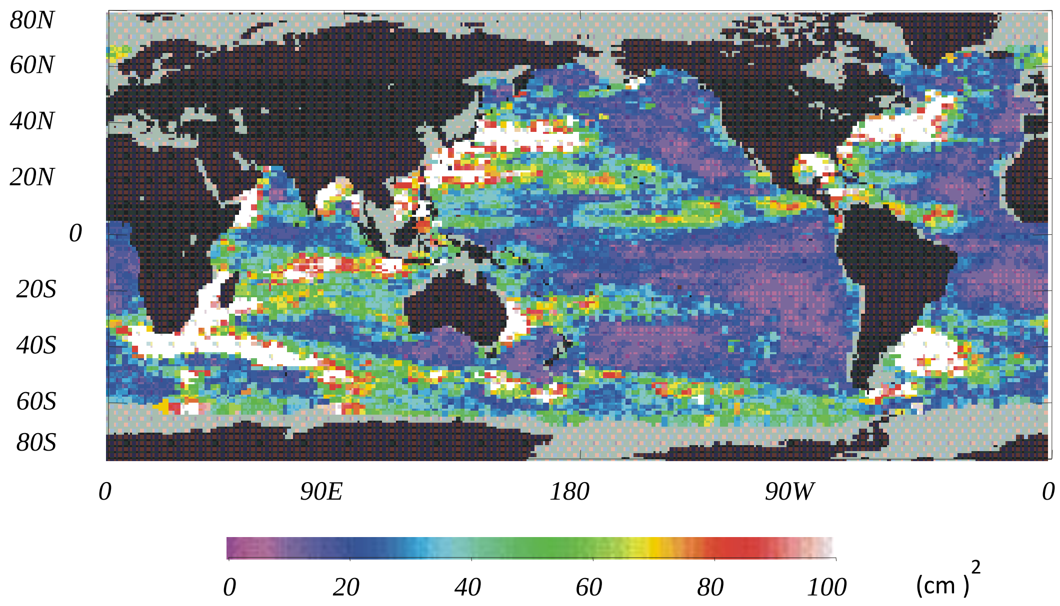
$$\langle \boldsymbol{y}\mathbf{m}^T \rangle = \langle \mathbf{s}\mathbf{s}^T \rangle$$

Which can be solved for $\langle \mathbf{n}\mathbf{n}^T \rangle \equiv \mathrm{R}$ and $\langle \mathbf{p}\mathbf{p}^T \rangle \equiv \mathbf{H}\mathbf{P}_{\boldsymbol{sim}}{}^T\ \mathbf{H}^T$

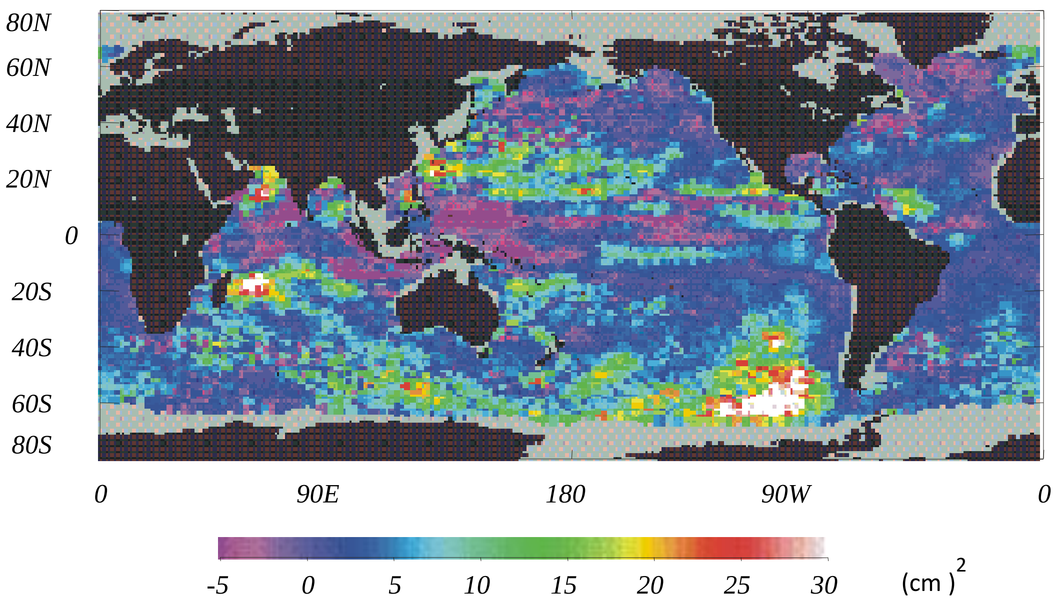
Example estimating $\mathbf{R}$

Error estimates comparing altimetry data with a coarse resolution OGCM.

$$\mathbf{R} \equiv \langle \mathbf{n}\mathbf{n}^T \rangle = \langle \boldsymbol{y}\boldsymbol{y}^T \rangle - \langle \boldsymbol{y}\mathbf{m}^T \rangle$$



$$\mathbf{H}\mathbf{P}_{sim}{}^{T}\,\mathbf{H}^T = \langle \mathbf{p}\mathbf{p}^T \rangle = \langle \mathbf{m}\mathbf{m}^T \rangle - \langle \boldsymbol{y}\mathbf{m}^T \rangle$$



[*Fukumori et al., 1999*]

Summary

1. State estimation is an inverse problem,
2. Various inverse methods are available,
   - Minimum Variance
   - Least-Squares
3. Kalman filter & RTS smoother are recursive minimum variance estimates,
4. Adjoint method is an iterative least-squares estimate,
5. Practical consideration of errors.

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