The ends and means of “data assimilation”

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What is data assimilation?

It's all about …

- making optimal use of,
- consistently extracting,
- or combining

information contained in observations and physical laws expressed through a model, and taking into account all uncertainties.

Outline … = Conclusions

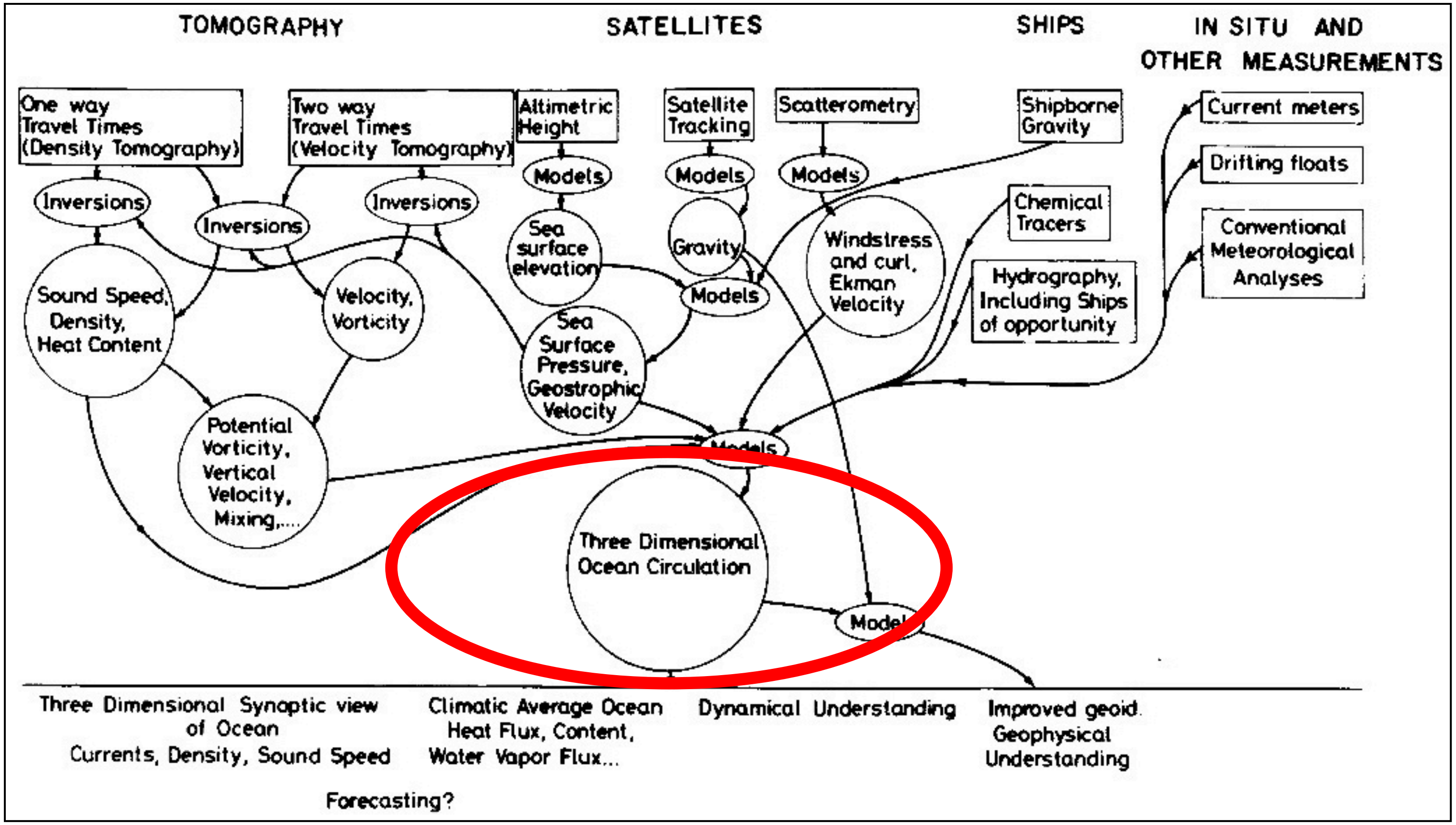
- DA seeks to optimally combine information content in observations, models, and their uncertainties(!)

- DA can mean different things to different people

- Depending on application, different methods:
  - forecasting: *filter methods* (e.g., Kalman filter)
  - reconstruction: *smoother / adjoint methods*

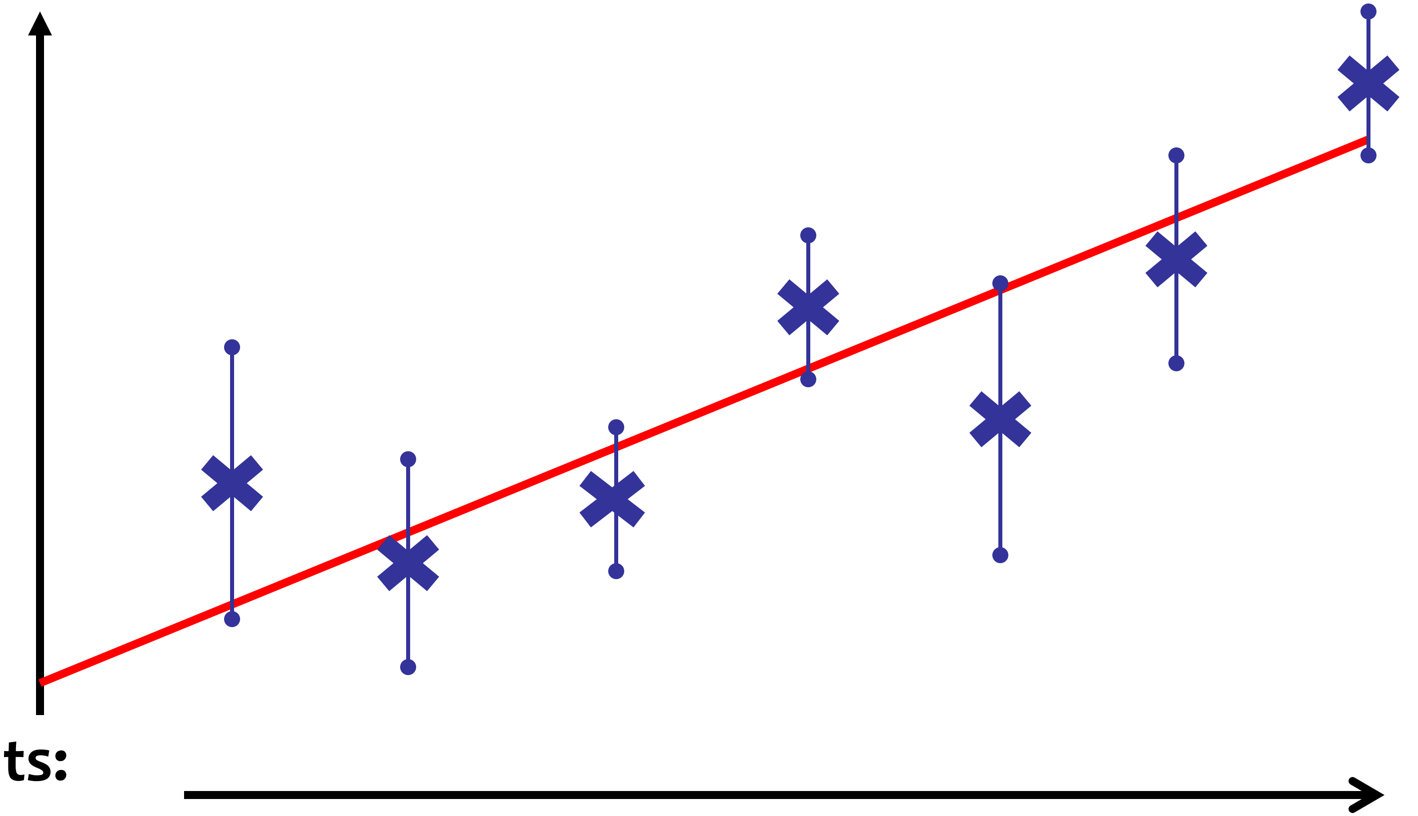
Combine two incomplete information sources

- Combine the heterogeneous streams of measured state variables with simulations of these same variables
- The way of how we combine is influenced by / takes into account the different sources of uncertainties!



***C. Wunsch**, in "A Celebration in Geophysics and Oceanography 1982. In Honor of Walter Munk on his 65th birthday."*

Formal framework – least-squares objective/cost function



Basic ingredients:

- observations (diverse types, sparse, inhomogeneously distributed in space & time)
- model (various levels of complexity)
- errors/uncertainties (of various kinds)

Least-squares objective/cost function

3 basic ingredients:

observations — model — errors

$$J = \sum_{i,j,k} \frac{1}{\sigma^2(i,j,k)} \left[y(i,j,k) - \mathbf{E}x(i,j,k) \right]^2$$

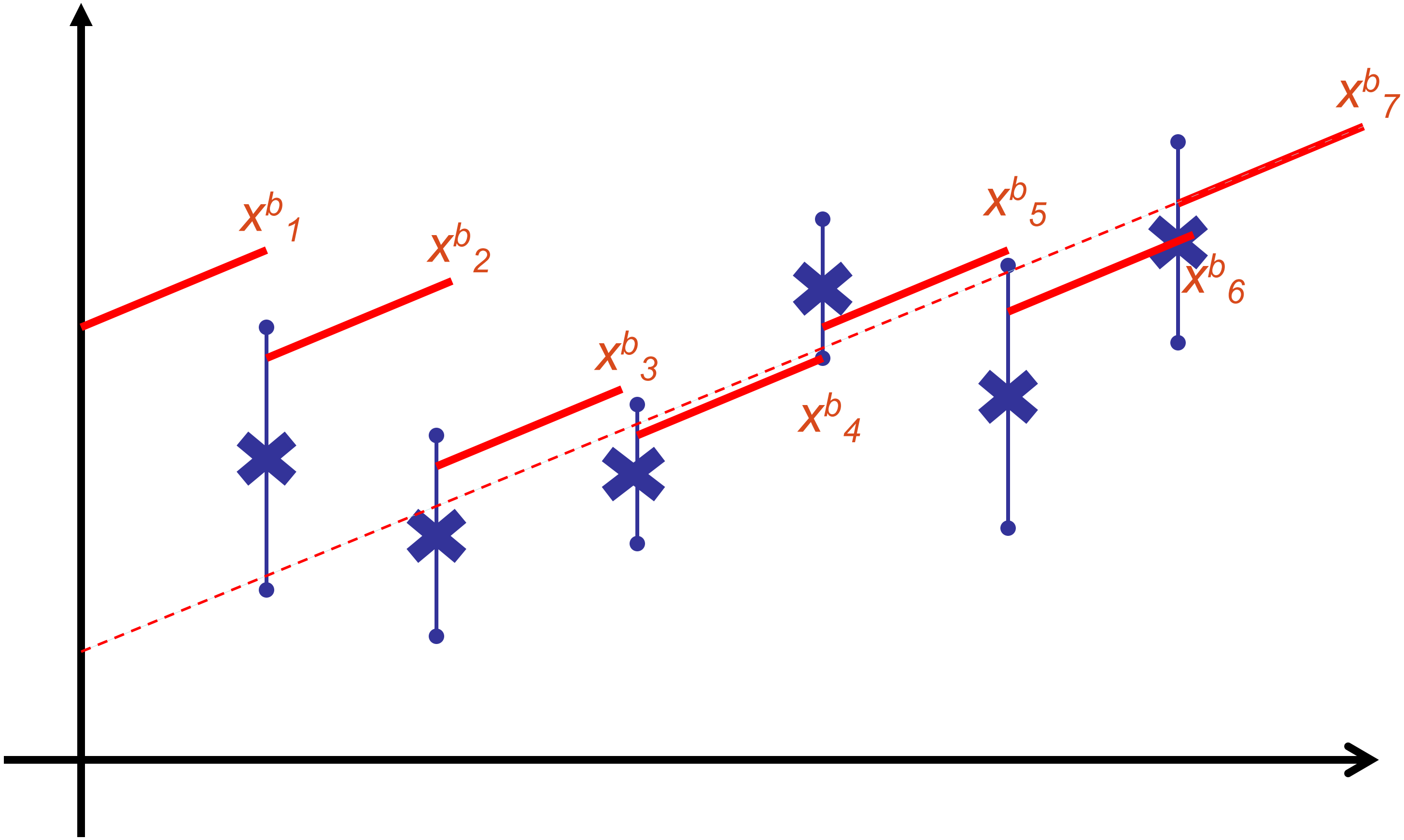
or, more generally (but dropping space indices i, j, k):

$$J = \left[y - \mathbf{E}x \right]^T \mathbf{R}^{-1} \left[y - \mathbf{E}x \right]$$

E: operator mapping from model space (x) to obs space (y)

R: error covariance matrix (with error variances σ^2)

The filtering (forecasting) problem



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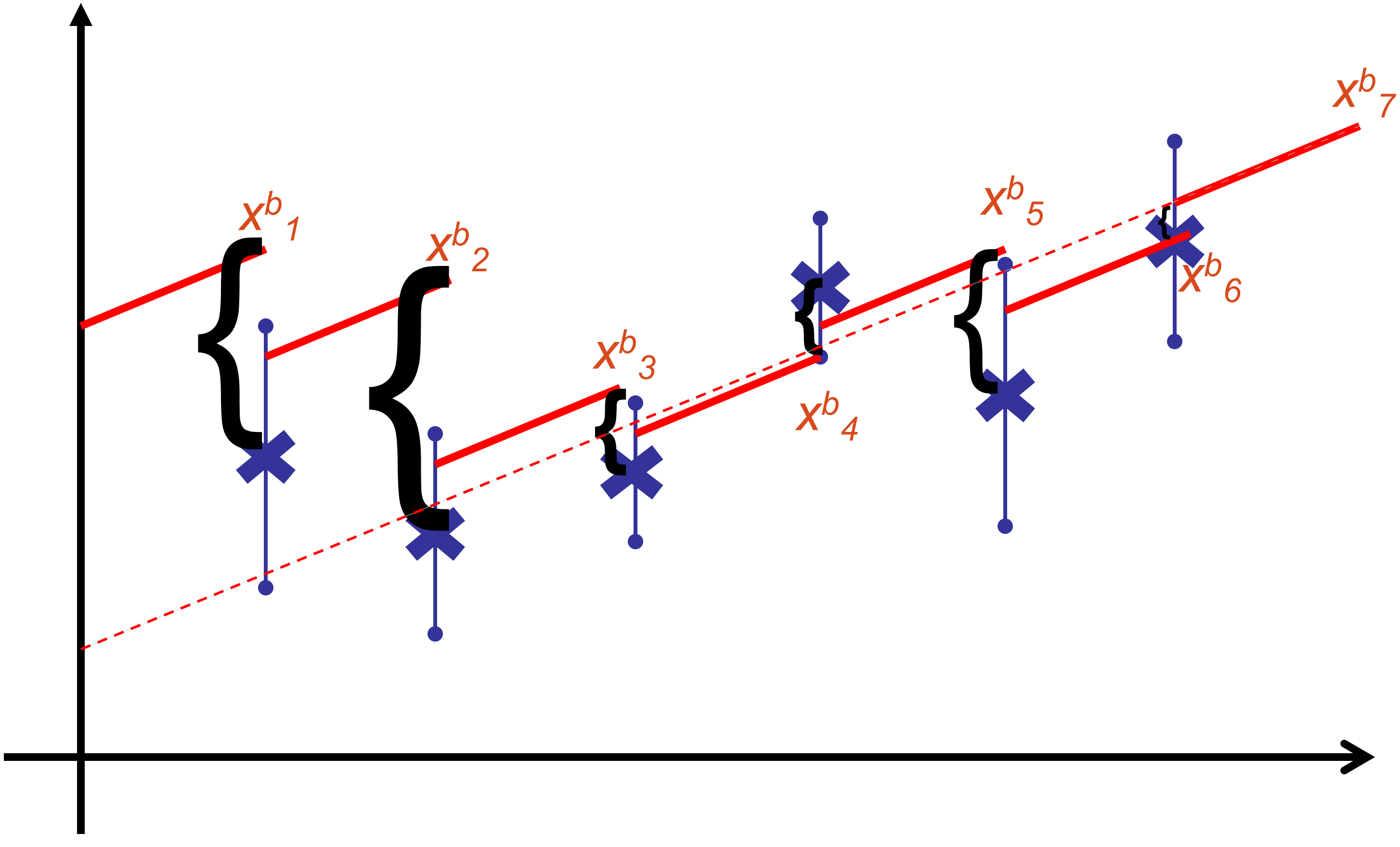

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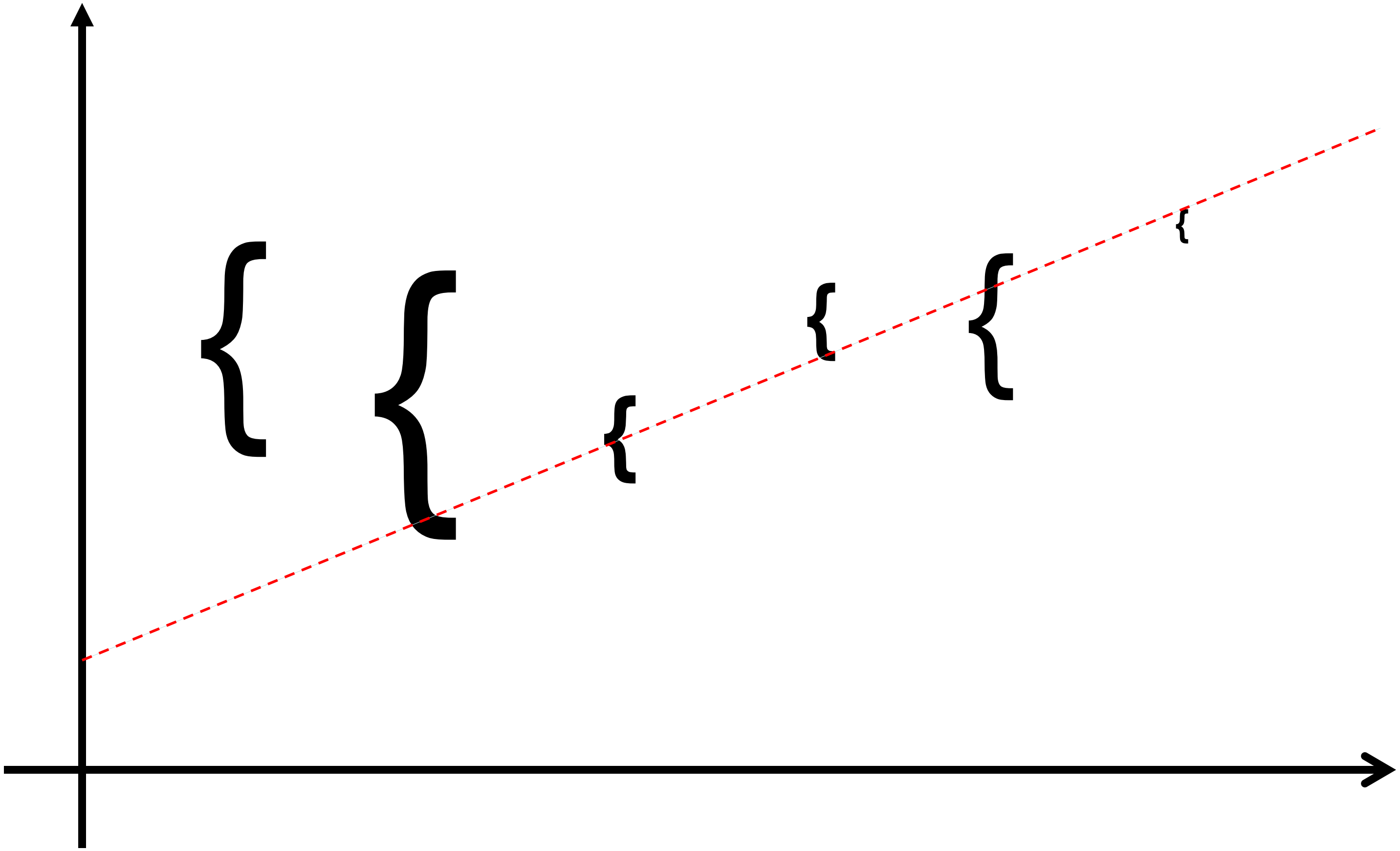
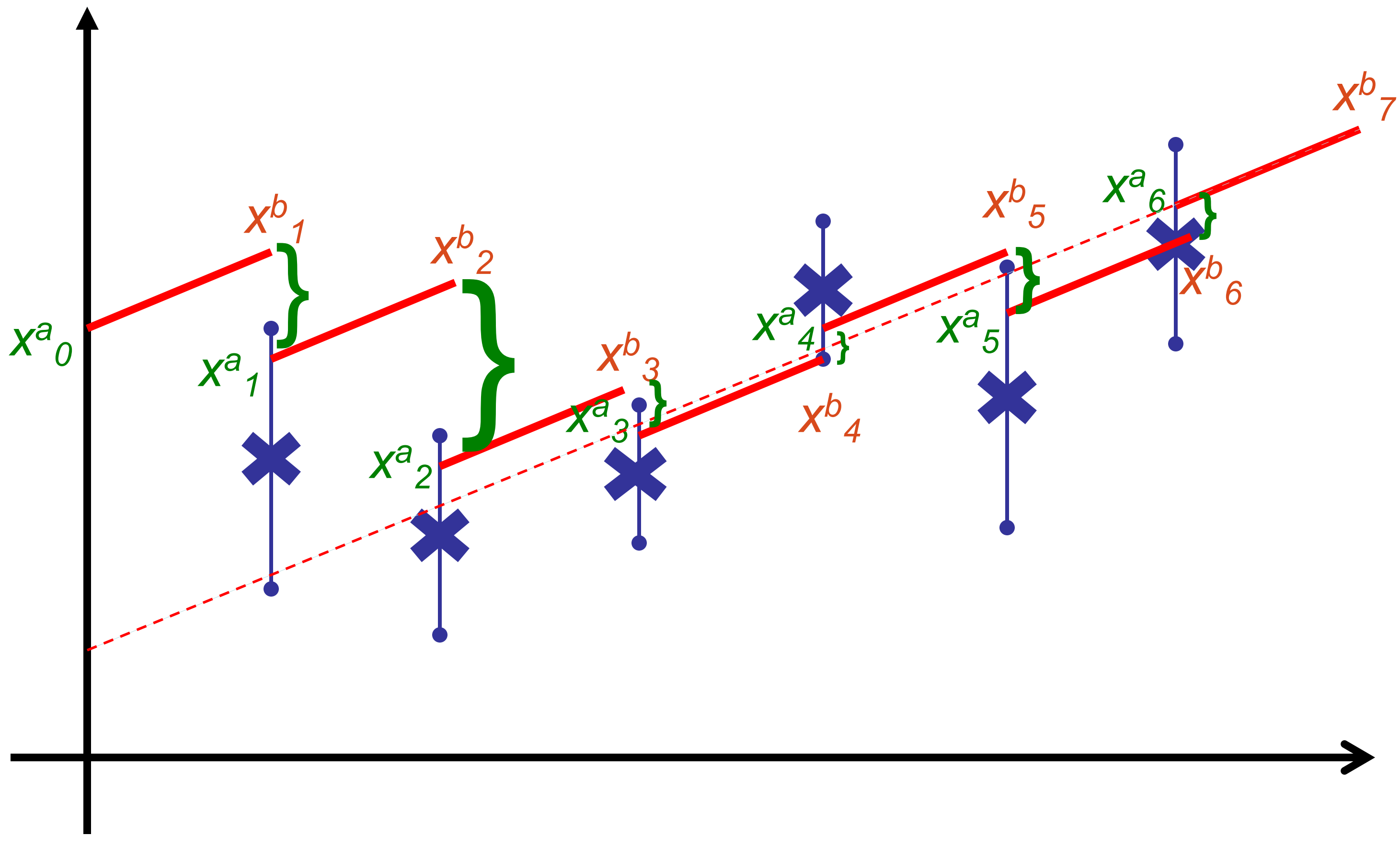


State estimation via filtering (sequential) methods



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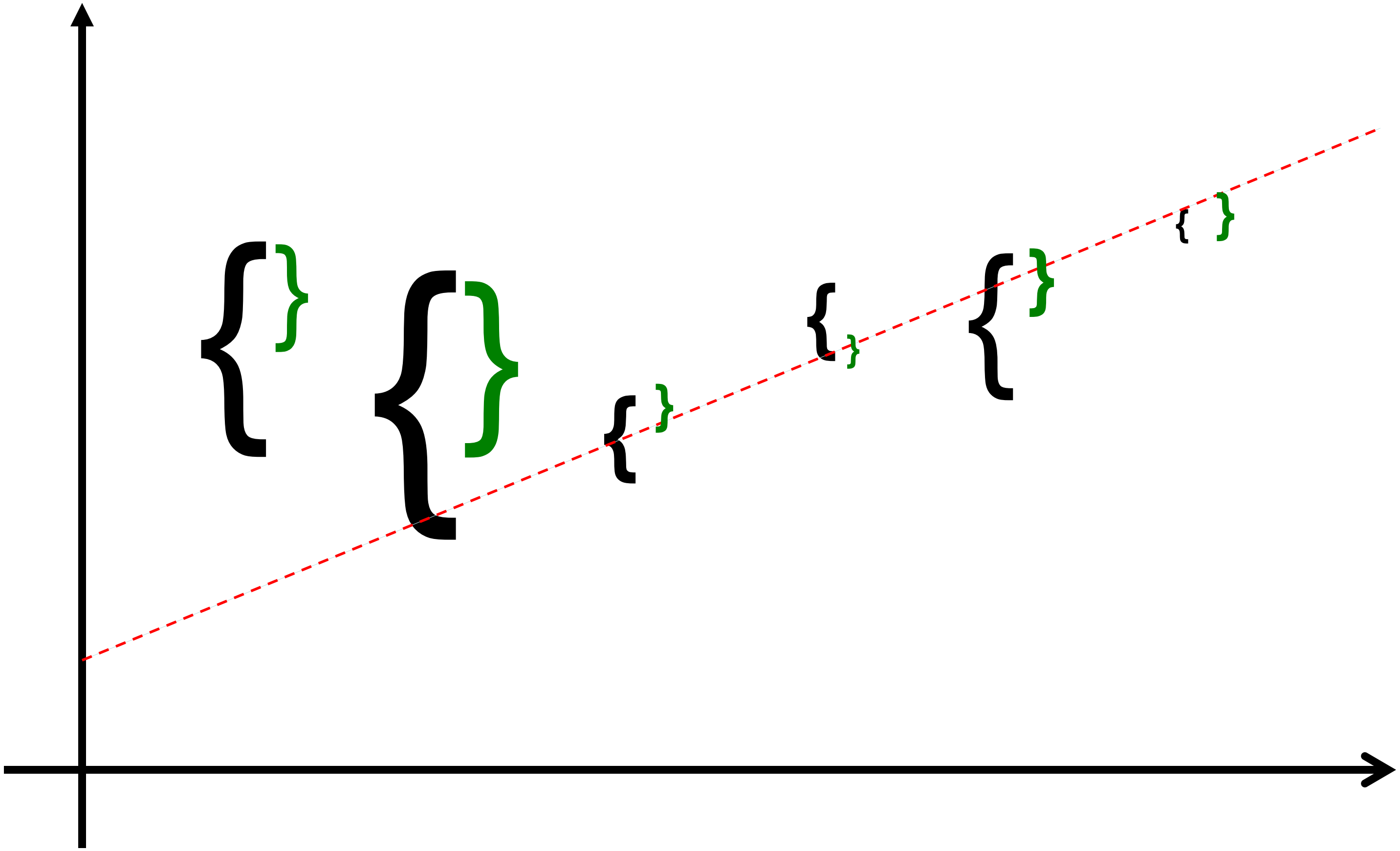
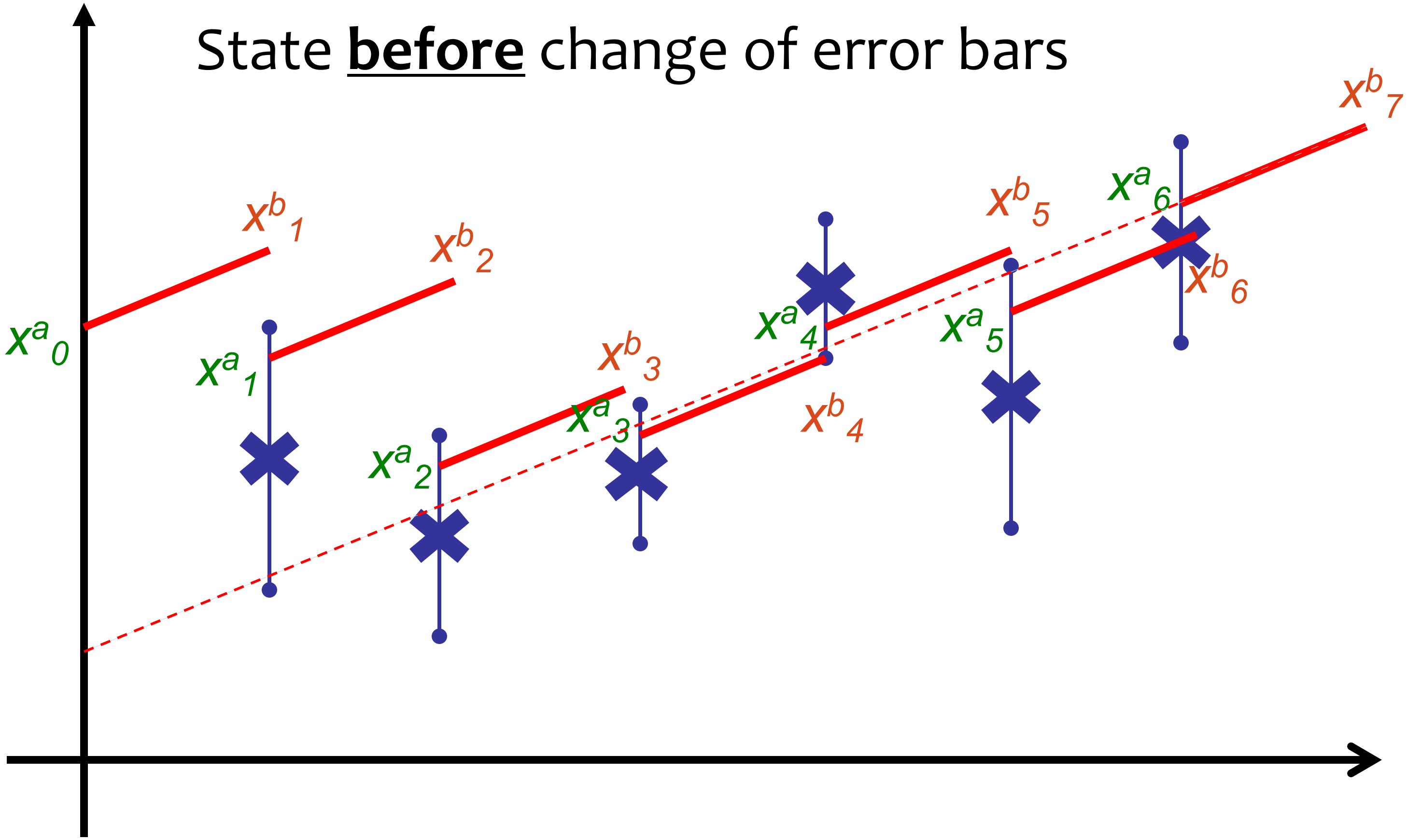


- Innovation vector (or residual)
- Analysis increment

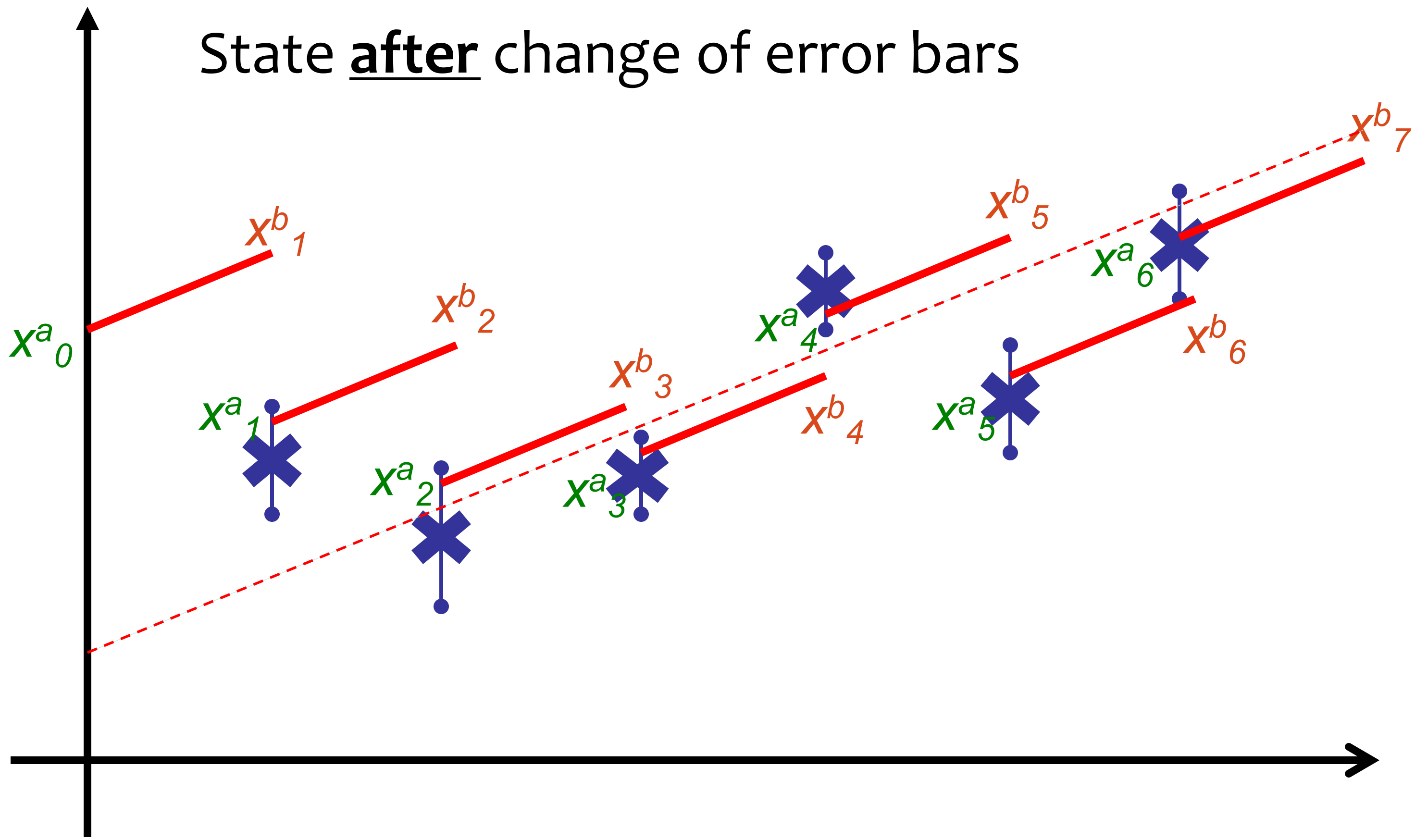
State estimation via filtering (sequential) methods



NOTE:

- <u>The role/importance of error/uncertainty estimates</u>!
- What if we reduce observation errors?

State estimation via filtering (sequential) methods



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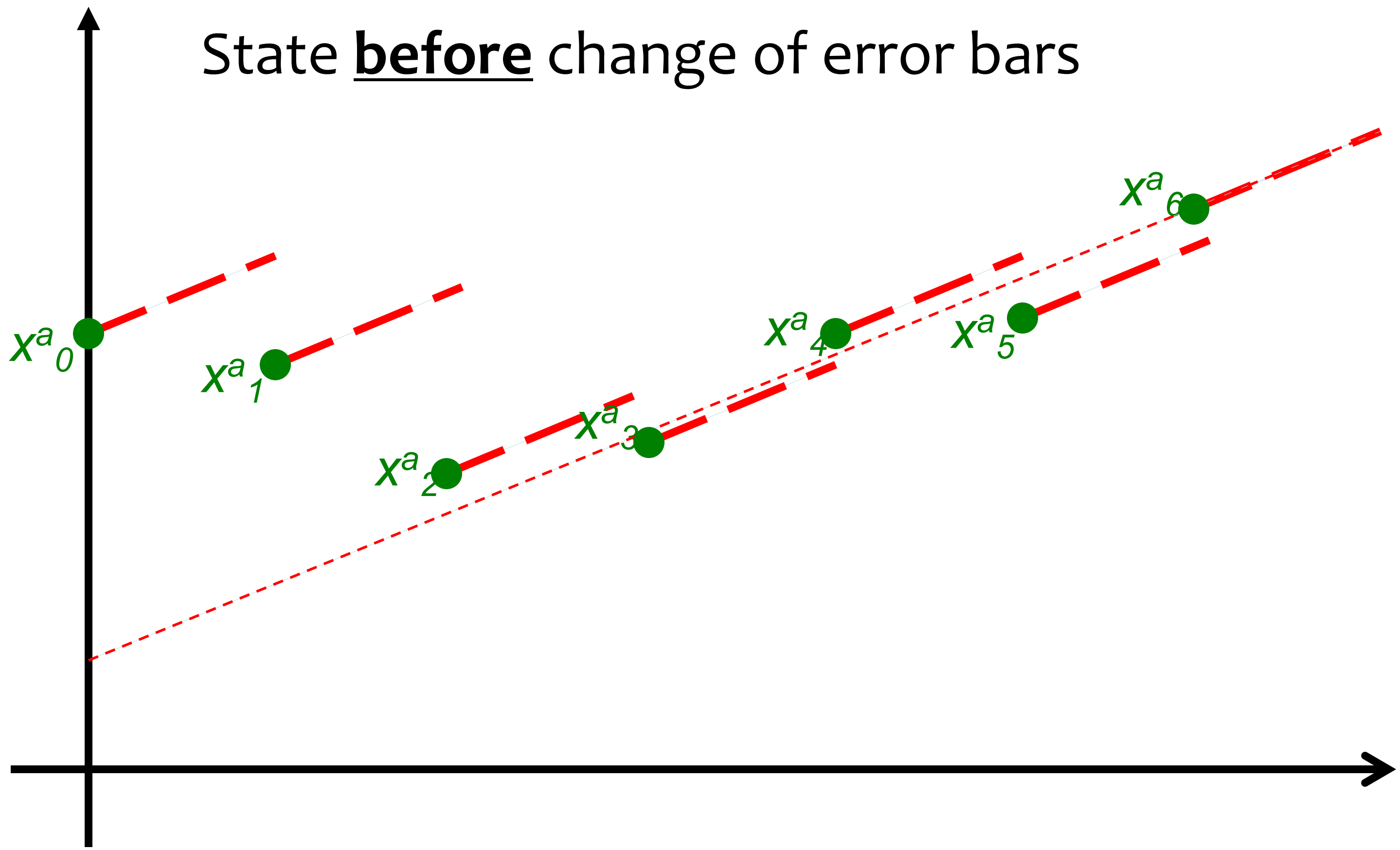

NOTE:

- It's *easy* to **over-fit the data** if error bars are unrealistically small!
- But is it *good*?

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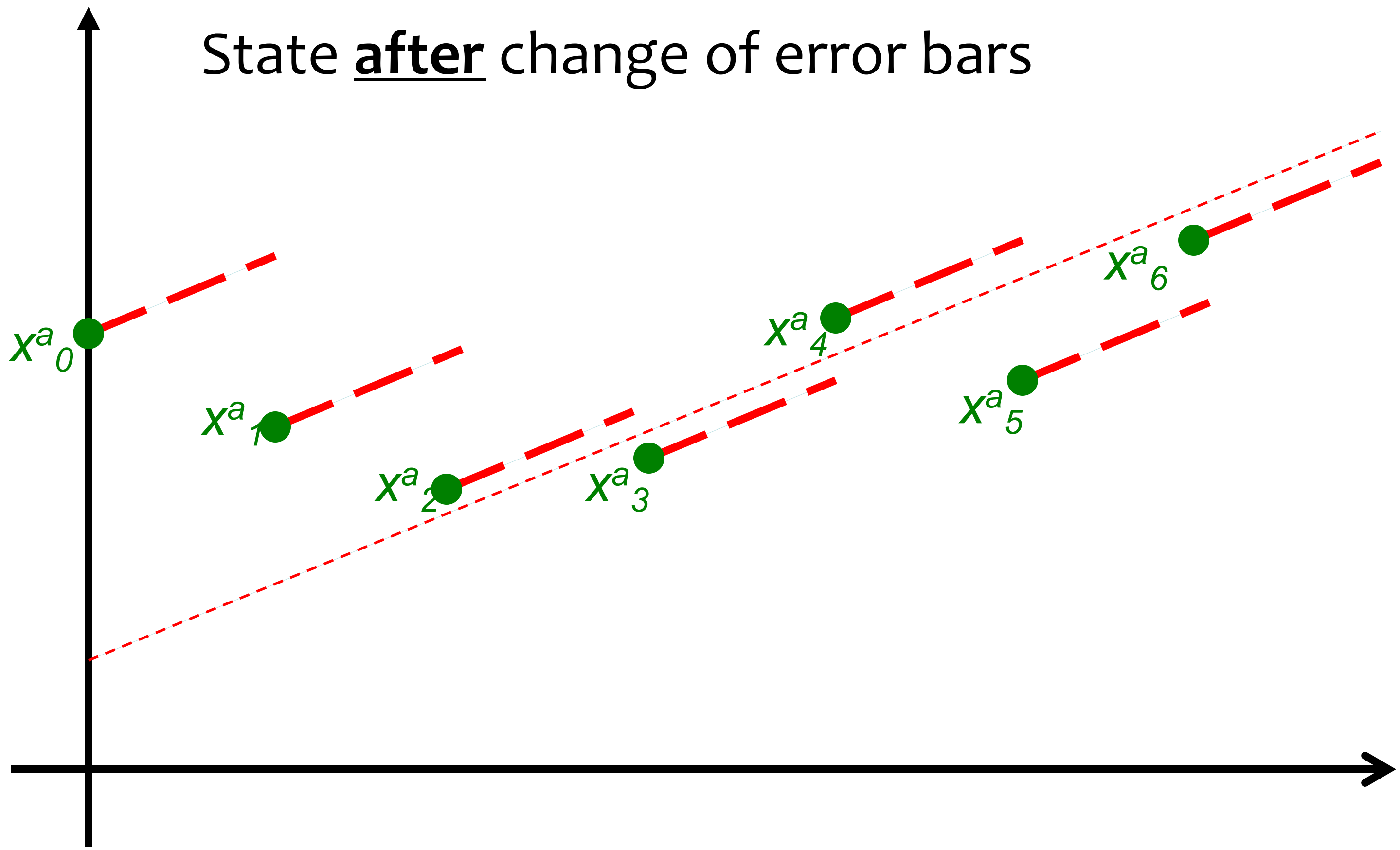

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"Analysis" and "re-analysis" in Numerical Weather Prediction

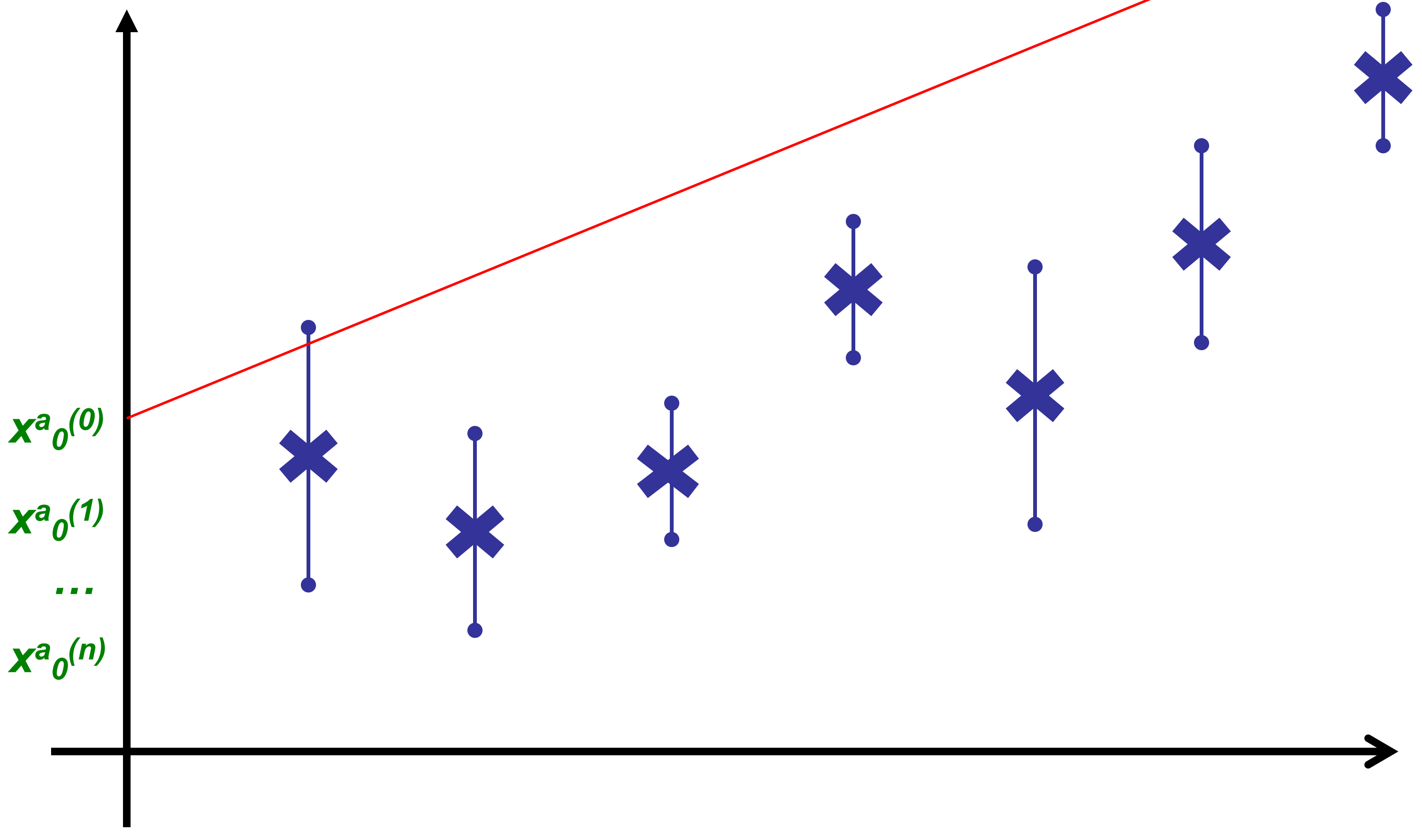
- **<u>"Analysis"</u>** is done in operational (real-time) mode
  - not all observations available in time (< 20%?)
  - forecast model changes over time (e.g., resolution, …)
- **<u>"Re-analysis"</u>** consists of:
  - redoing the forecast/analysis steps over extended period
  - use the same model
  - use all observations (incl. delayed-mode)
- Current global re-analyses:
  - ECMWF/ERA-Interim, NASA/MERRA, JRA-25/55, NCEP-CFSR, CMC-GDPS, NOAA/20CR, …
  - e.g.: *Lindsay et al.; Chaudhuri et al. (both J. Clim., 2014)*
- Regional Arctic high-res. re-analyses:
  - Arctic System Reanalysis (ASR), PIOMAS (ocean/ice), …

Various implementations & approximations:

- Nudging
- Relaxation
- Successive correction
- Optimal (or statistical) interpolation
- 3D-Var
- …

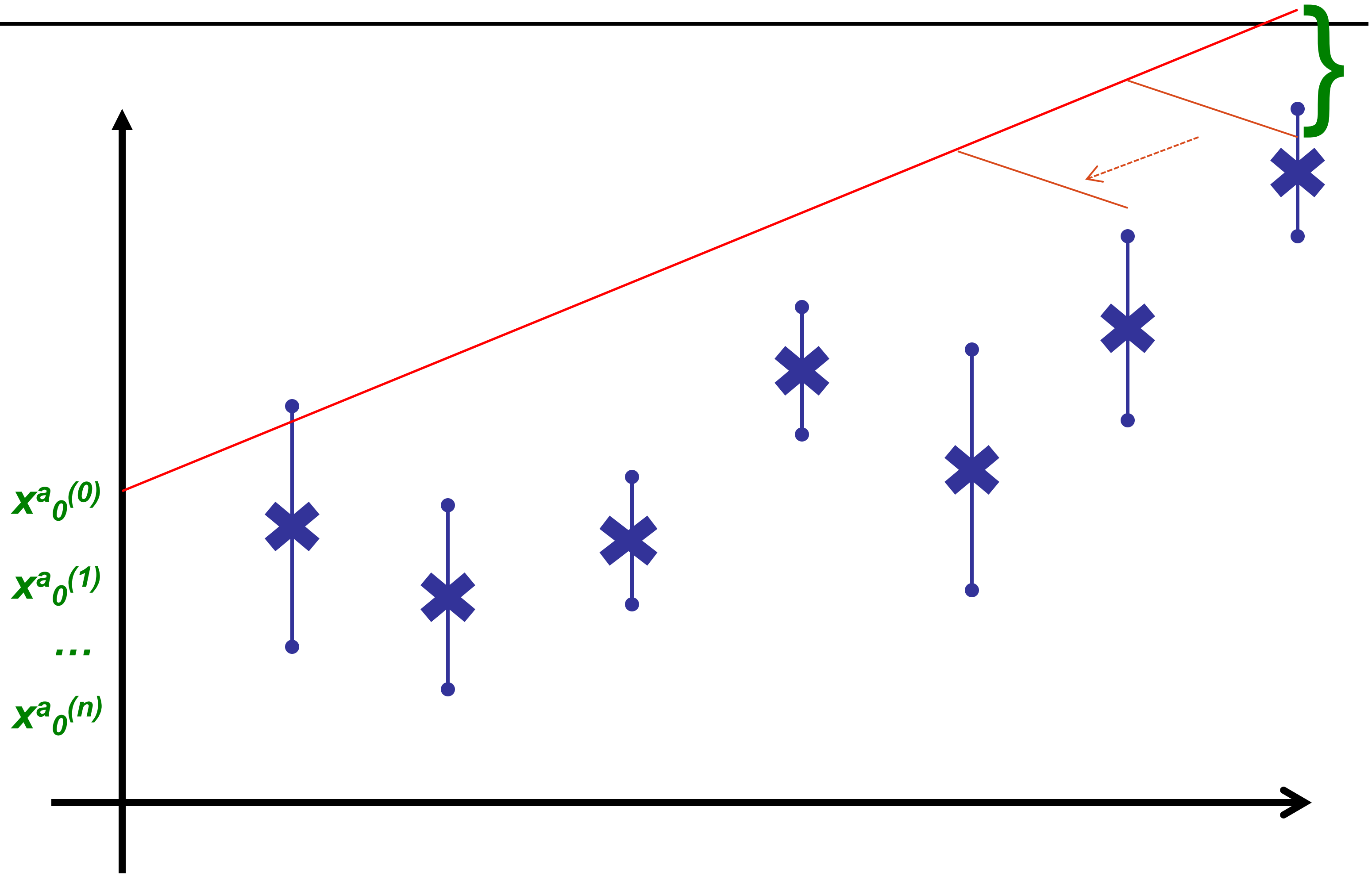
Lots of computational science & engineering involved to make it work

State estimation via smoother (adjoint) method



- Starting from first guess solution with initial condition: $x^a{}_0{}^{(0)}$, iteratively vary $x^a{}_0$, such as to minimize model data misfit
- Optimal solution obtained from initial condition $x^a{}_0{}^{(n)}$

State estimation via smoother (adjoint) methods



- Entire model trajectory is adjusted simultaneously
- Sensitivity of misfit cost function to previous states is carried (and accumulated) *backward in time* by the **adjoint model**

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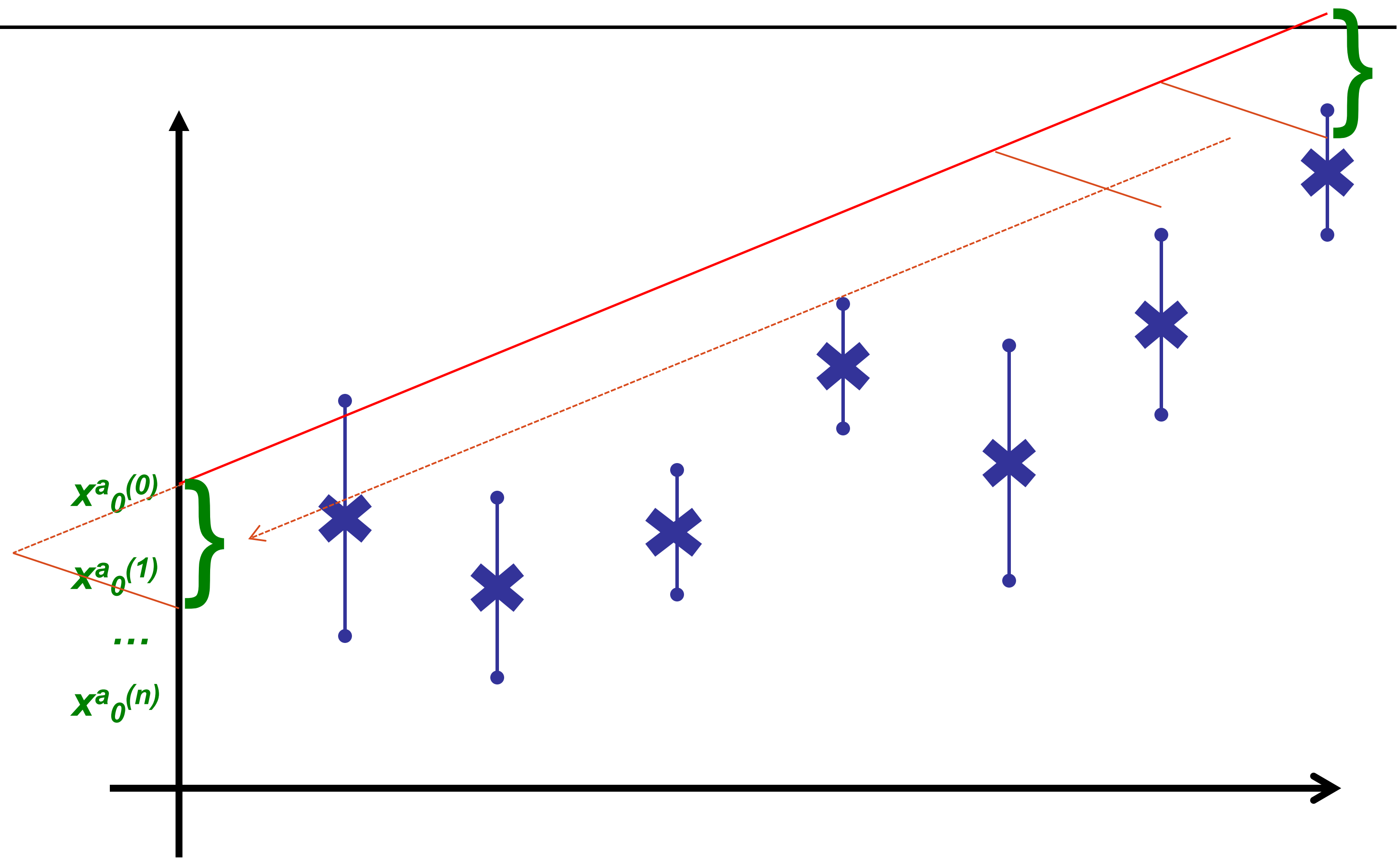

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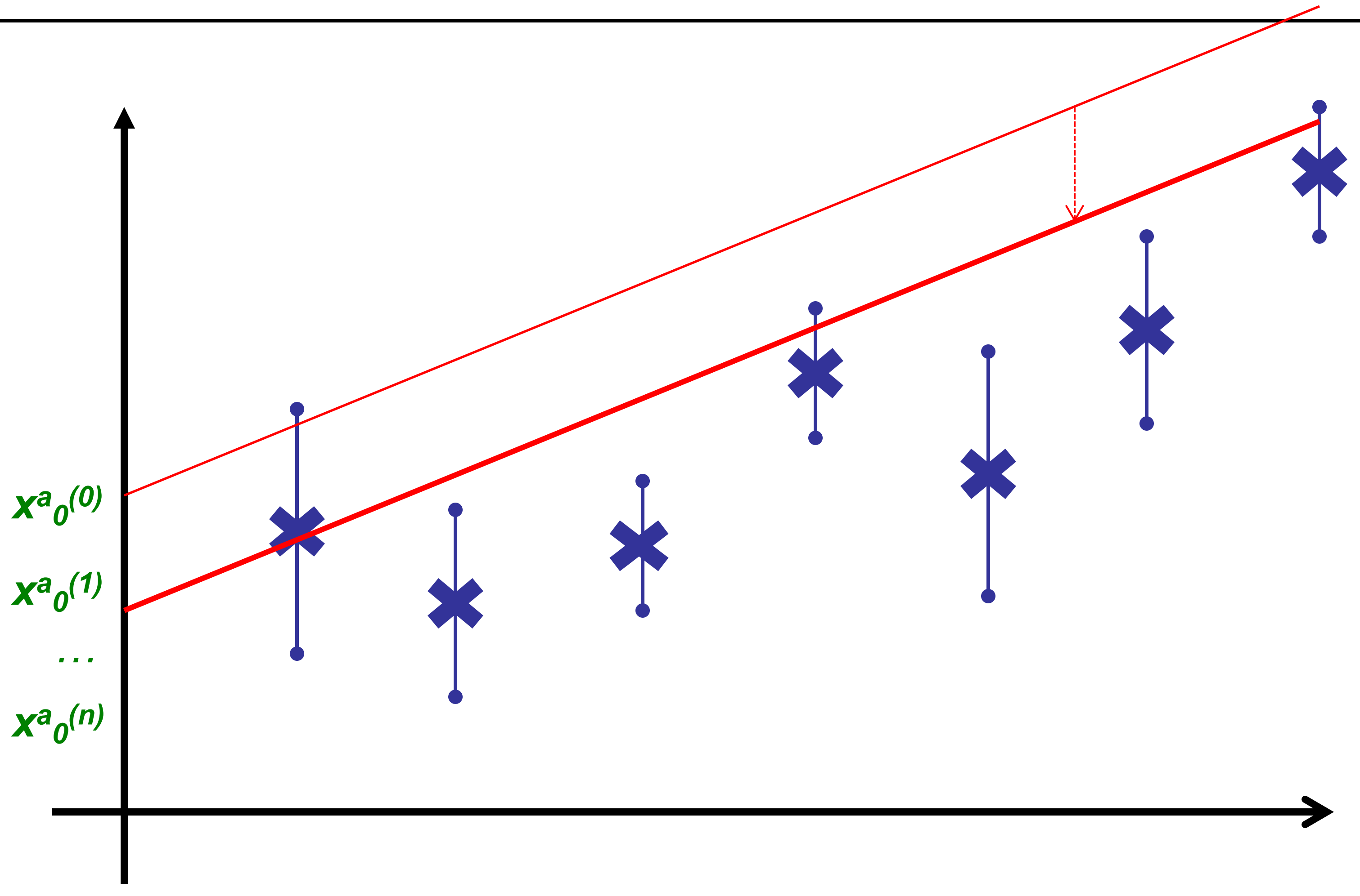
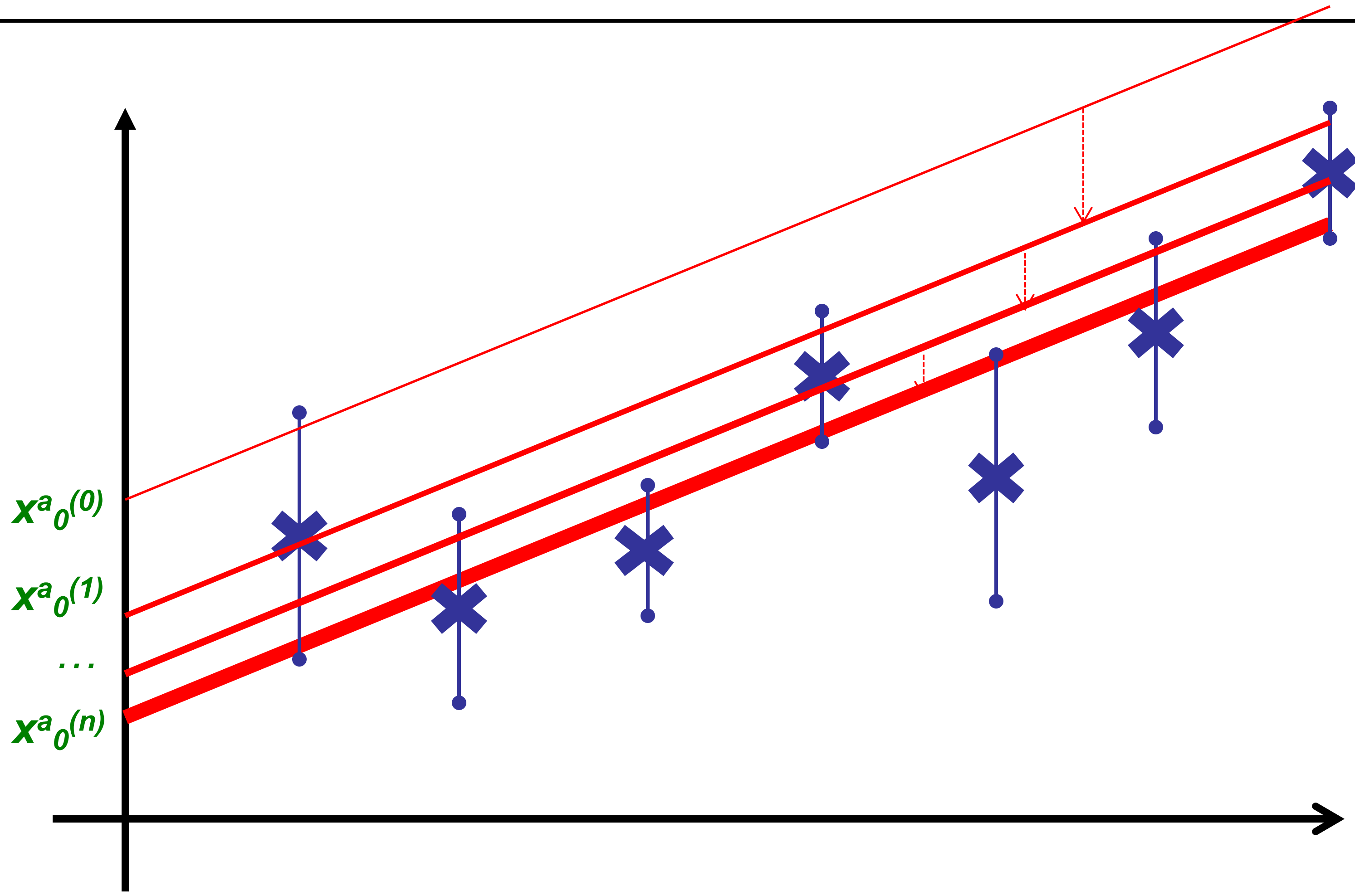


- Optimal initial condition $x^a_0{}^{(n)}$ obtained *iterative*ly
- Need to vary J with respect to x^a_o
  - **gradient-based optimization!**

State estimation via smoother (adjoint) method



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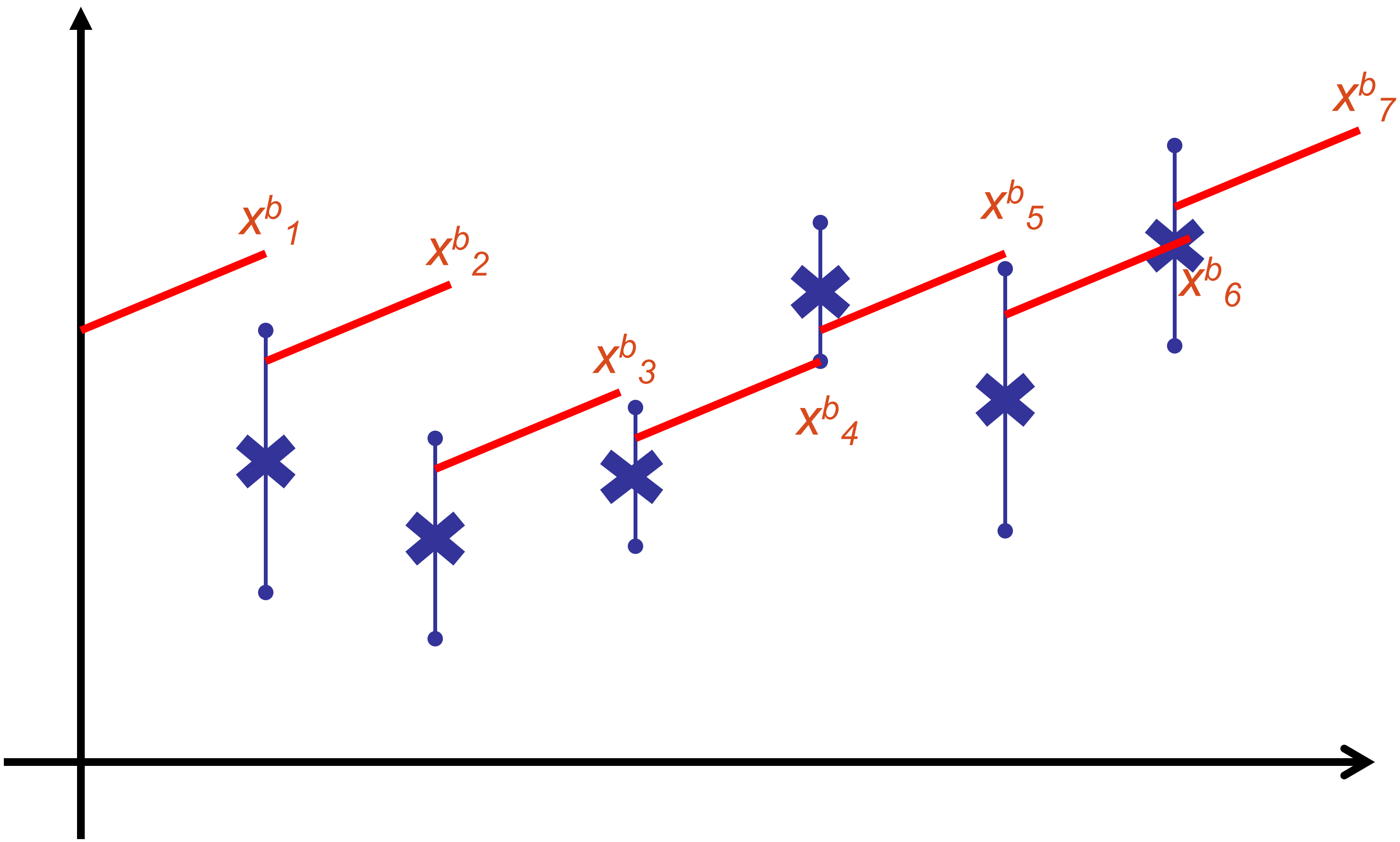
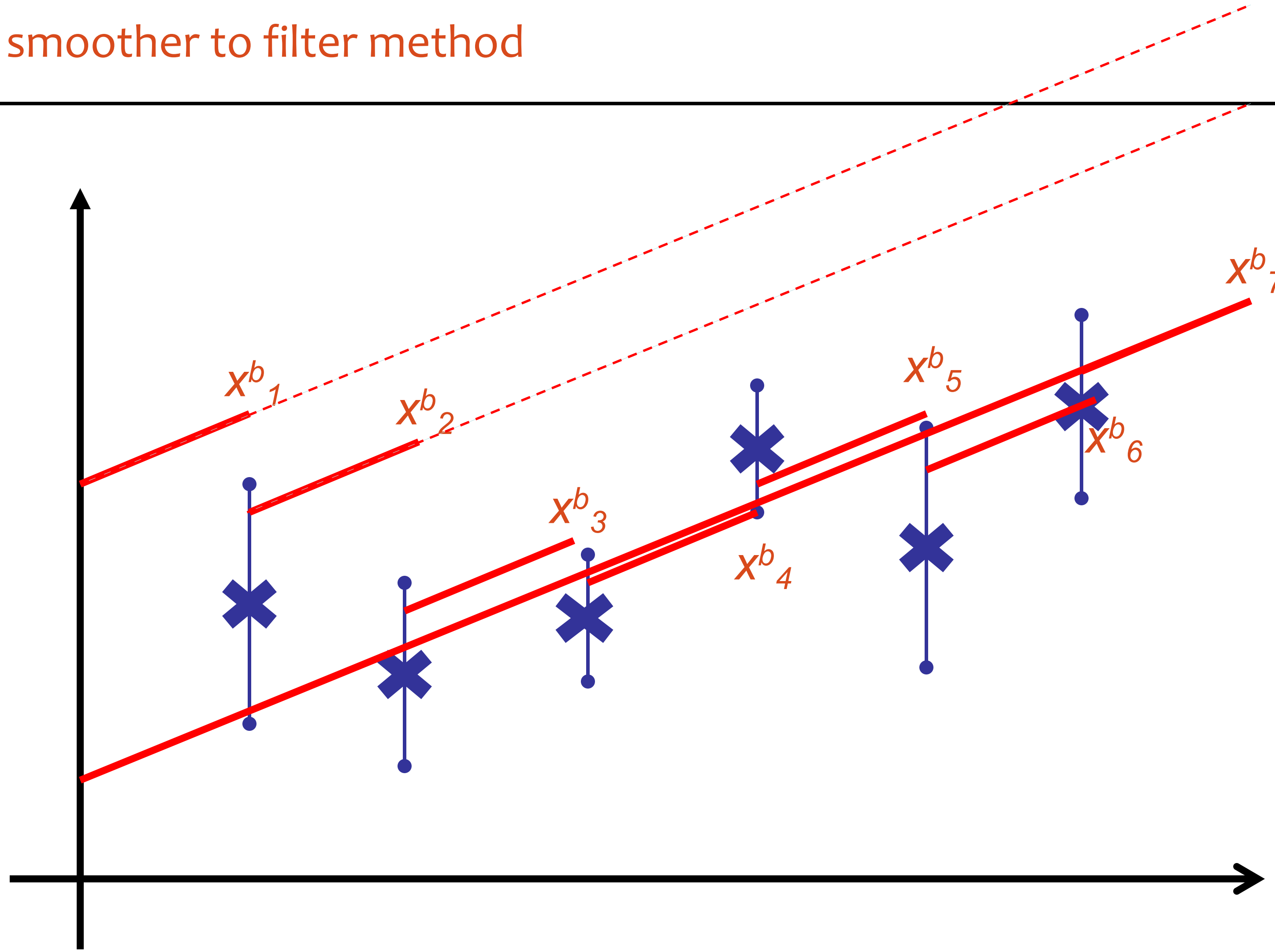
Compare smoother to filter method



- <u>Filter</u> can only propagate information content from observations *forward in time*
- <u>Smoother</u> uses *past, present, and future* observation combined!

Compare smoother to filter method



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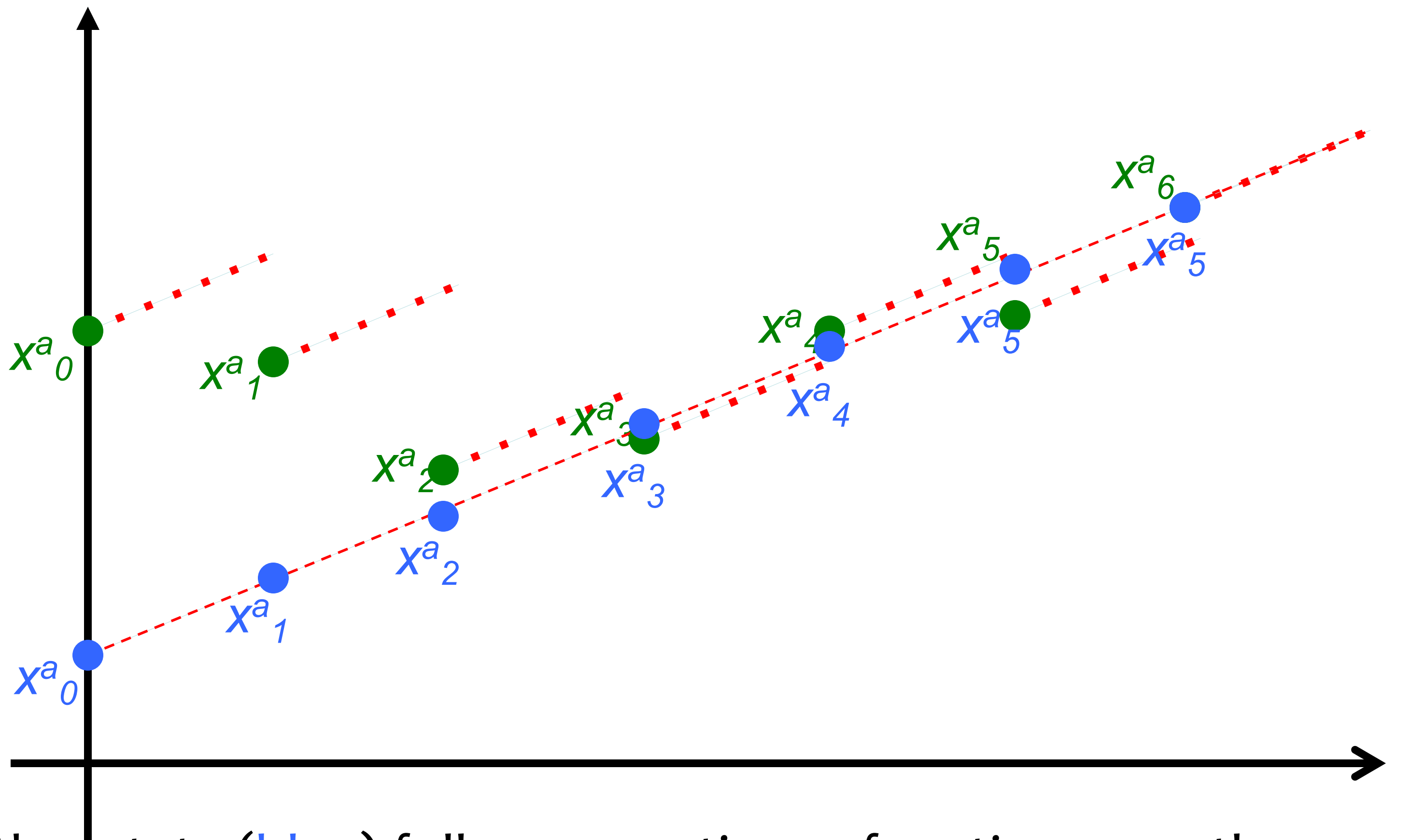
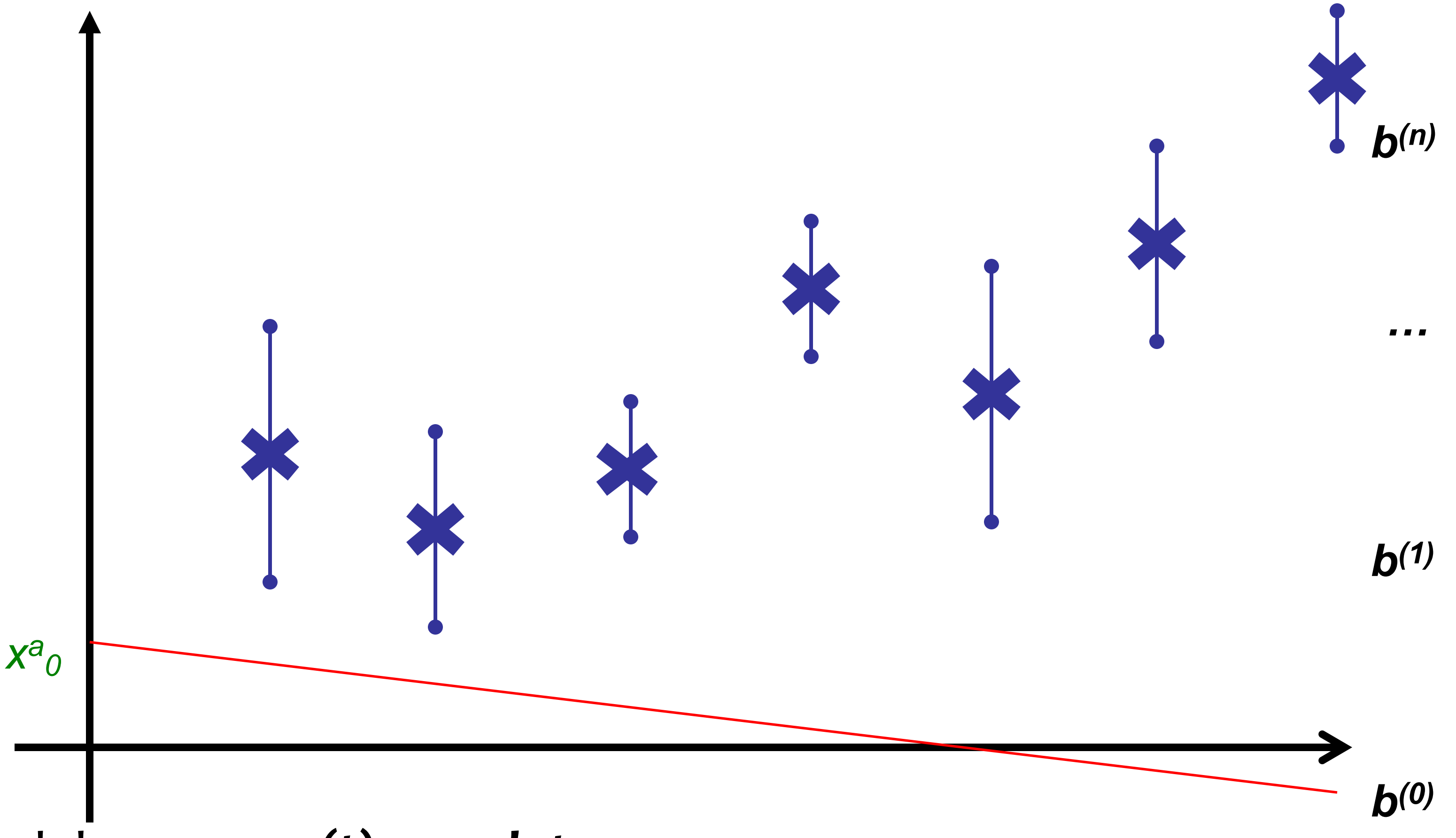


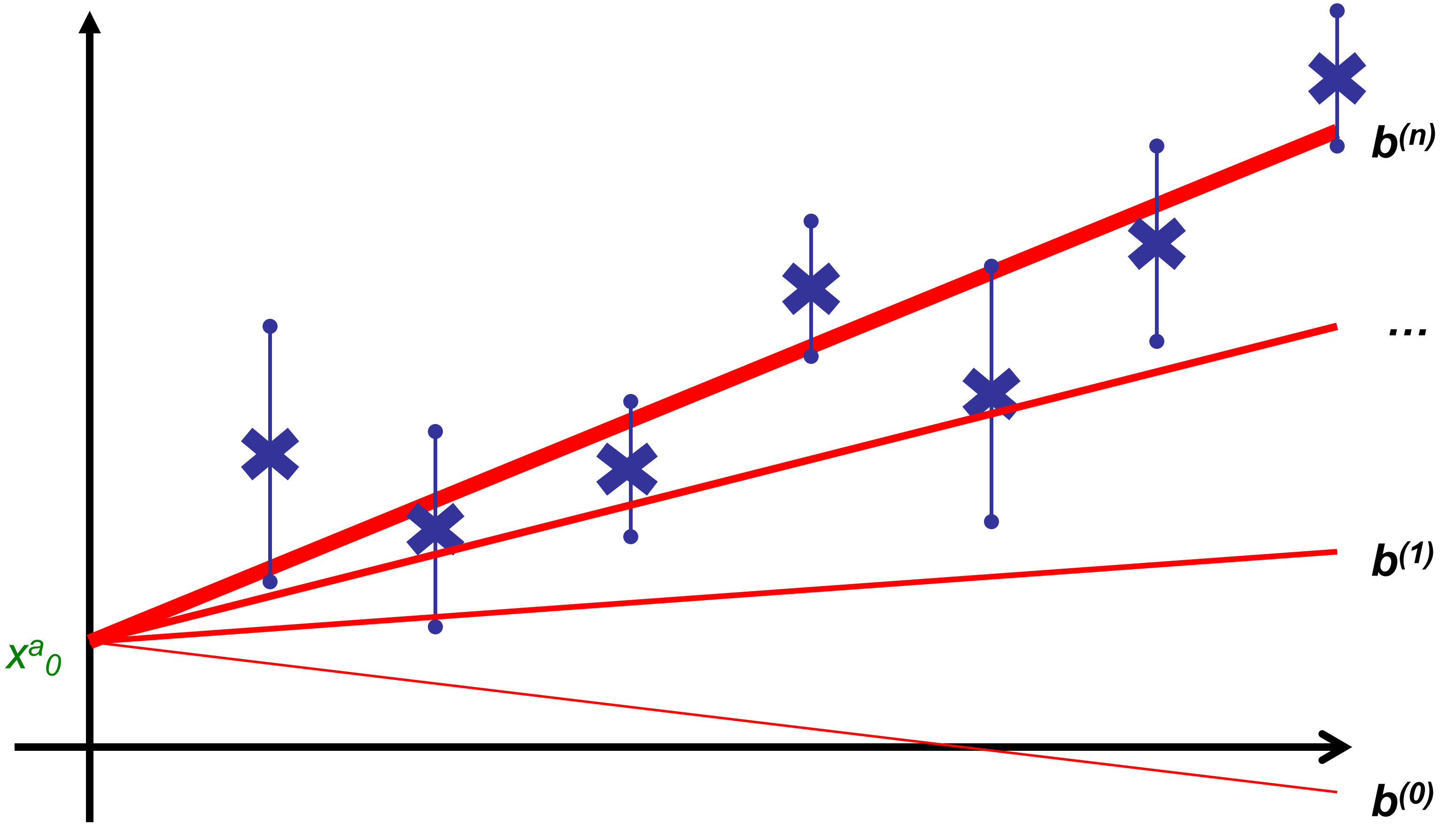
- <u>Smoother state </u>(blue) follows equations of motions exactly
  - tendency/trends (*dx/dt*) physically realistic
- <u>Filter state </u>(green) fits observations better
  - validity of tendency/trends unclear

Parameter estimation via smoother (adjoint) method



- for model $x(t) = a + b\,t$
  - instead of varying initial condition $x^a(0) = a$,
  - vary slope (i.e. "model parameter") b

<u>Parameter</u> estimation via smoother (adjoint) method



- for model $x(t) = a + b\,t$
  - instead of varying initial condition $x^a(0) = a$,
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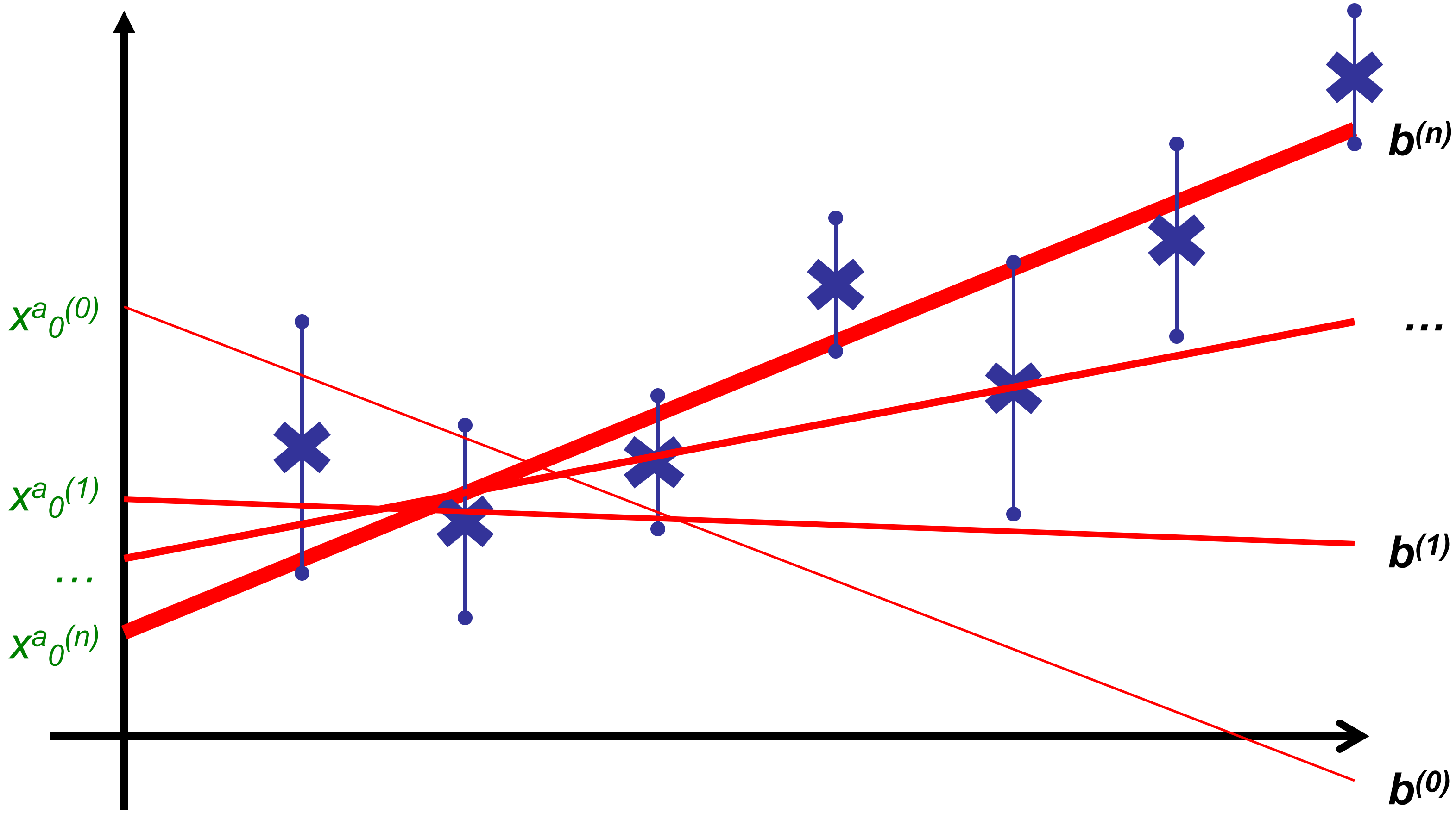
<u>**Joint state & parameter**</u> estimation via smoother (adjoint) method

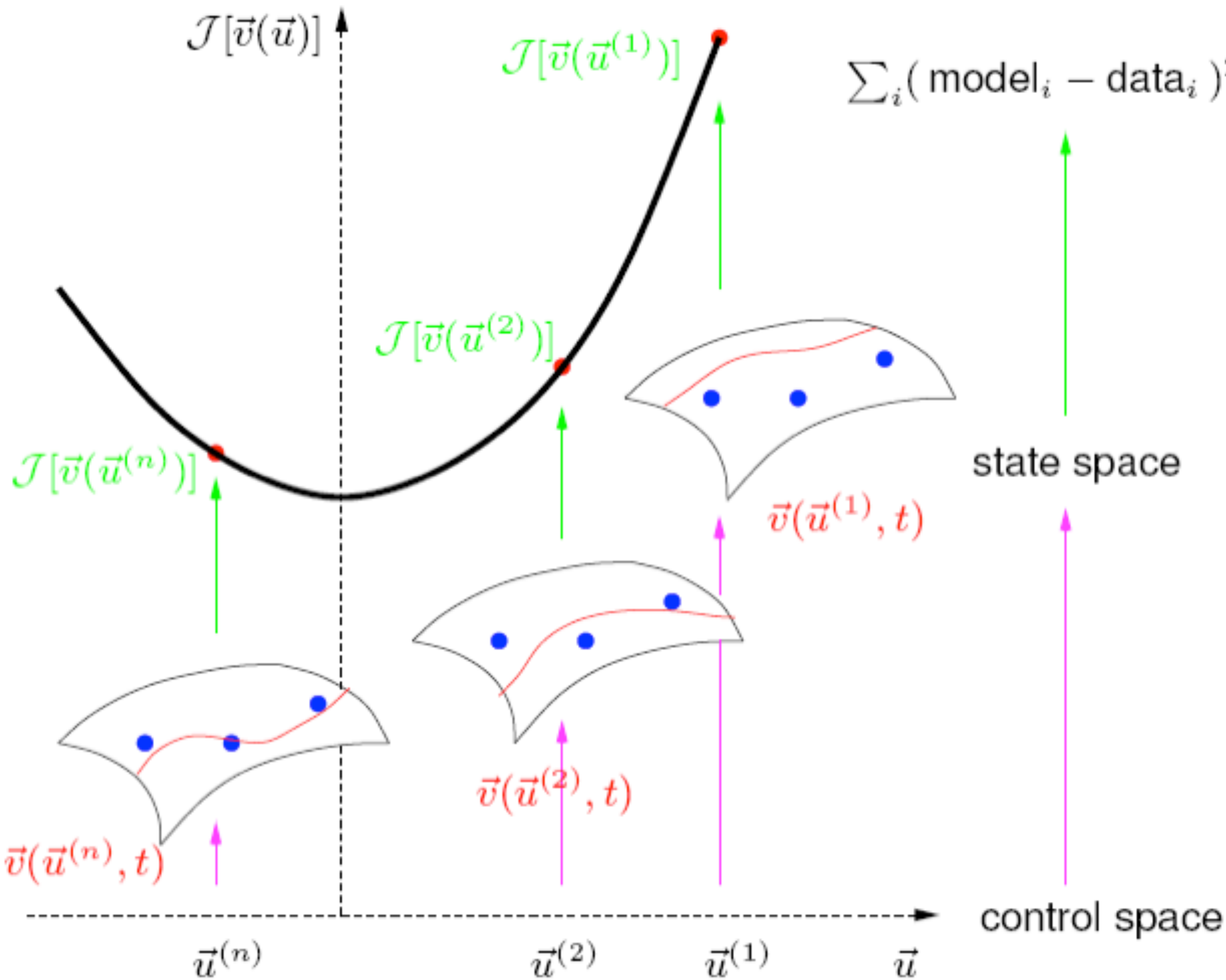


- for model $x(t) = a + b\,t$, <u>*simultaneously vary*</u>
  - initial condition (i.e. "model state") $x^a(0) = a$
  - and slope (i.e. "model parameter") b

END

An optimal estimation/control approach

Iterative optimization via ***gradient*** obtained from ***adjoint*** *model*



The smoother (reconstruction) problem

Consider *perfect* model **L** (i.e., $\eta = 0$), and obs. y with noise ϵ:

$$x_{k+1}^t = \mathbf{L} x_k^t$$
$$y_{k+1} = \mathbf{E} x_{k+1}^t + \epsilon_{k+1}$$

Variational form of least-squares estimation problem:

$$J(x) = \sum_{0 \le k \le N} [\mathbf{E} x_k - y_k]^T \mathbf{R}^{-1} [\mathbf{E} x_k - y_k]$$

Extend to Lagrange function $\mathcal{L}$, Lagrange multipliers μ_k:

$$\mathcal{L}(x, \mu) = J(x) + \sum_{0 \le k \le N} \mu_k^T [x_{k+1} - \mathbf{L} x_k]$$

The smoother (reconstruction) problem

Lagrange multiplier method:

Stationary point of $\mathcal{L}$ leads to set of normal equations:

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}(t)} = \mathbf{x}(t) - L\left[\mathbf{x}(t-1)\right] = 0 \qquad 1 \leq t \leq t_f$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}(t)} = \frac{\partial J_0}{\partial \mathbf{x}(t)} - \boldsymbol{\mu}(t) + \left[\frac{\partial L[\mathbf{x}(t)]}{\partial \mathbf{x}(t)}\right]^T \boldsymbol{\mu}(t+1) = 0 \qquad 0 < t < t_f$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}(t_f)} = \frac{\partial J}{\partial \mathbf{x}(t_f)} - \boldsymbol{\mu}(t_f) = 0 \qquad t = t_f$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}(0)} = \frac{\partial J}{\partial \mathbf{x}(0)} - \left[\frac{\partial L[\mathbf{x}(0)]}{\partial \mathbf{x}(0)}\right]^T \boldsymbol{\mu}(1) \qquad t_0 = 0$$

The smoother (reconstruction) problem

"Variational" hints that we need a gradient:

- gradient of J with respect to *independent* or *control* variables!
- Here: Vary initial conditions, x_0 such as to minimize J

BUT: J depends not just on x_0, but on all $x_k, \ k \geq 0$.

- consider *nonlinear model* $x_{k+1} = L(x_k)$
- linearized version is *state transition matrix* $\mathbf{L}$

$$\delta x_{k+1} = \frac{\partial x_{k+1}}{\partial x_k} \delta x_k = \mathbf{L} \, \delta x_k$$

Need chain rule of differentiation:

$$\begin{aligned} J &= J(x_0, x_1, x_2, \ldots, x_N) \\ &= J\Big(x_0, L(x_0), L(L(x_0)), \ldots, L^N(x_0)\Big) \end{aligned}$$

The smoother (reconstruction) problem

$$\mu_0 = \frac{\partial J}{\partial x_0} = \sum_{1 \le k \le N} \frac{\partial x_k}{\partial x_0} \left(\frac{\partial J}{\partial x_k} \right)$$

$$= \frac{\partial x_1}{\partial x_0} \left(\frac{\partial J}{\partial x_1} \right) + \frac{\partial x_1}{\partial x_0} \frac{\partial x_2}{\partial x_1} \left(\frac{\partial J}{\partial x_2} \right) + \ldots + \frac{\partial x_1}{\partial x_0} \cdots \frac{\partial x_N}{\partial x_{N-1}} \left(\frac{\partial J}{\partial x_N} \right)$$

$$= \mathbf{L}^T \frac{\partial J}{\partial x_1} + \mathbf{L}^T \mathbf{L}^T \frac{\partial J}{\partial x_2} + \ldots + \mathbf{L}^T \cdots \mathbf{L}^T \frac{\partial J}{\partial x_N}$$

$\mathbf{L}^T$: is the **adjoint model** (and $\mathbf{L}$ is the **tangent linear model**)

$\mu_k = \left(\frac{\partial J}{\partial x_k} \right)$: **Lagrange multipliers** or **gradients**

The smoother (reconstruction) problem

For intermediate step of the adjoint model integration one obtains:

$$
\begin{aligned}
\mu_k = \frac{\partial J}{\partial x_k} &= \mathbf{L}^T \frac{\partial J}{\partial x_{k+1}} + \mathbf{E}^T \mathbf{R}^{-1} \left[\mathbf{E} x_k - y_k \right] \\
&= \mathbf{L}^T \left(\mathbf{L}^T \frac{\partial J}{\partial x_{k+2}} + \mathbf{E}^T \mathbf{R}^{-1} \left[\mathbf{E} x_{k+1} - y_{k+1} \right] \right) \\
&\qquad + \mathbf{E}^T \mathbf{R}^{-1} \left[\mathbf{E} x_k - y_k \right]
\end{aligned}
$$

- The adjoint model $\mathbf{L}^T$ propagates μ_k (the sensitivity of J with respect to all earlier states x_k) backward in time to x_0;
- Each model–data misfit (i.e. innovation vector $\mathbf{E} x_k - y_k$) is a *source* of sensitivity;
- The gradient of J with respect to x_0 takes into account (and weighs) the size of *all* misfit terms, *all* (inverse) error covariances, and *all* (linearized) model dynamics.

Conclusions

- DA seeks to optimally combine information content in observations, models, and their uncertainties!
- DA can mean very(!) different things to different people
- Depending on application, different methods warranted:
  - forecasting: *filter methods* (e.g., Kalman filter)
  - reconstruction: *smoother methods* (adjoint method)
- formal estimation methods to synthesize the diverse & sparse observations seems important for climate reconstructions
  - it is feasible,
  - simply copying NWP approaches not always useful,
  - remains a challenge for the time to come