


# CO2 inversion as a system and its uncertainty quantification

Lin Wu

Marc Bocquet, Frédéric Chevallier, Thomas Lauvaux, Peter Rayer, Ken Davis

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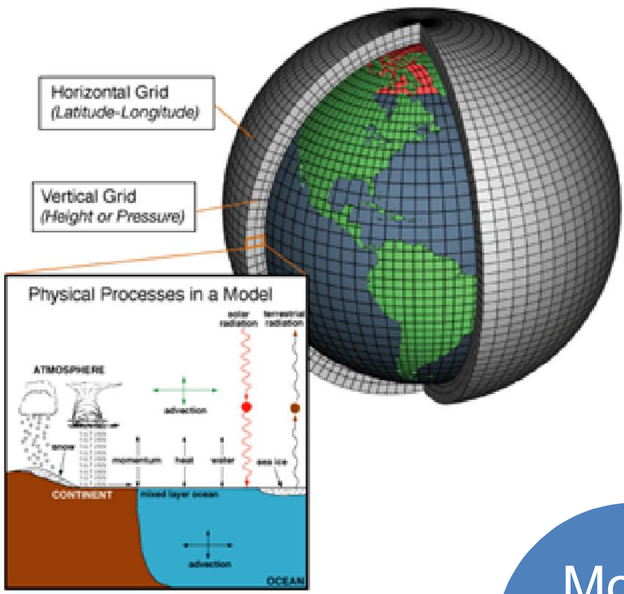
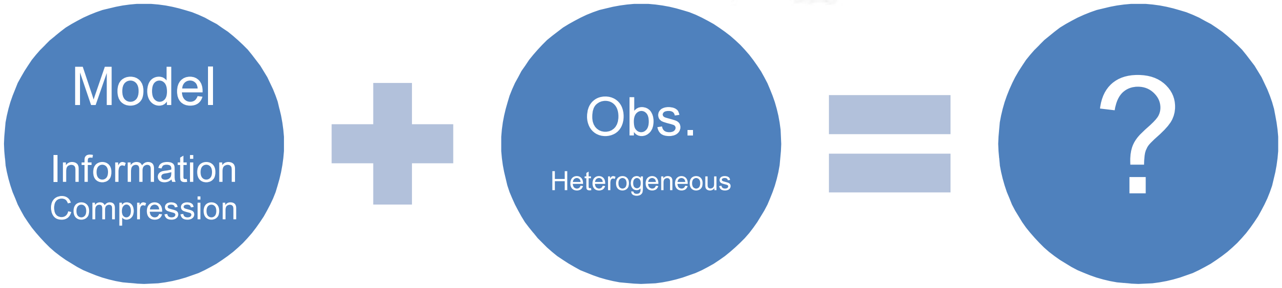
BridGES VEOLIA ENVIRONNEMENT ThalesAlenia Space cea UNIVERSITÉ DE VERSAILLES ST-QUENTIN-EN-YVELINES LSCE

# CO2 story: one carbon cycle to understand

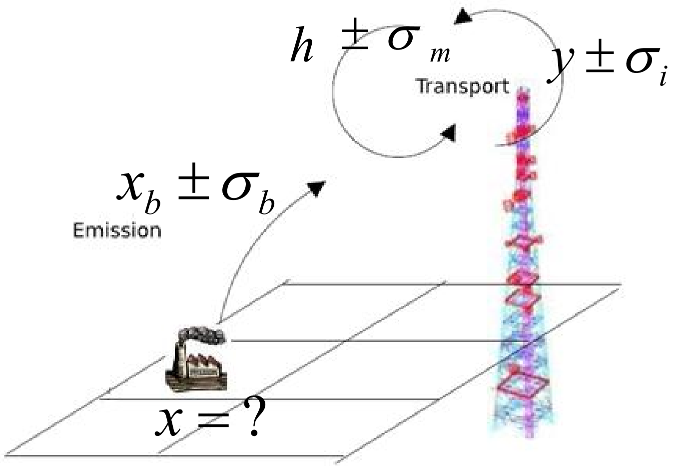



Fusion of informtion from diverse sources

# Simplest scalar case

Bouttier & Courtier 1999, Jacob 2007




Observation Eq.

$$y = hx + \varepsilon_o$$

$$\varepsilon_o = \varepsilon_i + \varepsilon_m$$

Information 1: first guess $x_b$

Information 2: observation $y$

Information? Probability distribution

First guess:

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma_b} \exp[-\frac{1}{2\sigma_b^2}(x - x_b)^2]$$

Observation conditioned by emission:

$$p(y|x) = \frac{1}{\sqrt{2\pi}\sigma_o} \exp[-\frac{1}{2\sigma_o^2}(y - hx)^2]$$

Information fusion? Production rule of proba.

$$p(x, y) = p(x)p(y|x) = p(y)p(x|y)$$

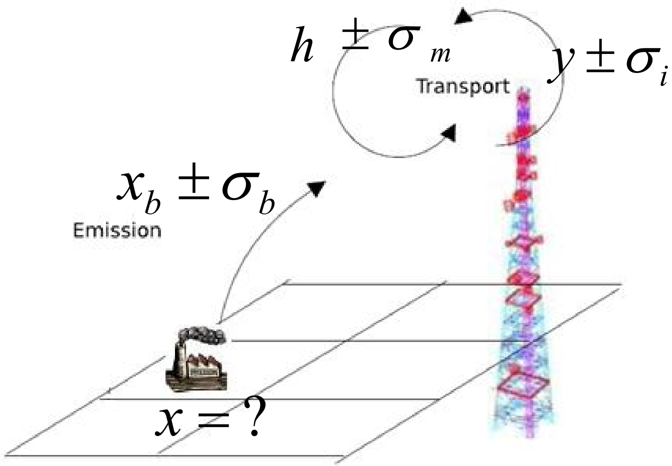
Inference? Bayes theorem/rule.

$$\underbrace{p(x|y)}_{\text{posterior}} = \frac{\overbrace{p(x)}^{\text{prior}}\,\overbrace{p(y|x)}^{\text{likelihood}}}{\underbrace{p(y)}_{\text{evidence}}}$$

*posterior ∝ likelihood × prior*

# Simplest scalar case

Bouttier & Courtier 1999, Jacob 2007




Bayesian calculus

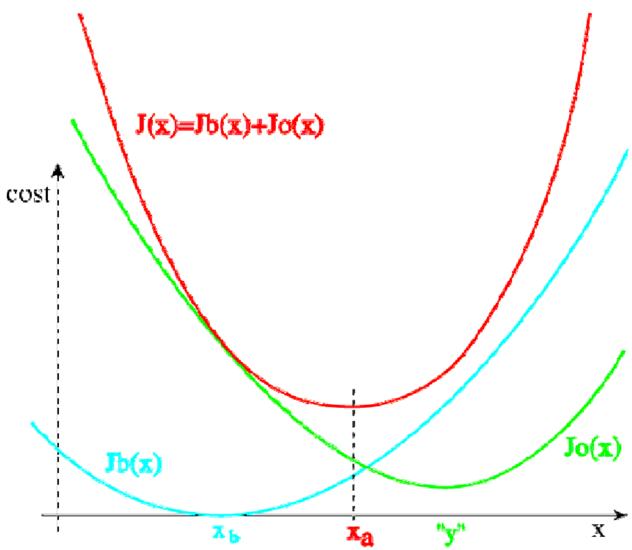
$$p(x|y) \propto \exp[-\frac{1}{2}(\frac{(x-x_b)^2}{\sigma_b^2} + \frac{(y-hx)^2}{\sigma_o^2})]$$

Estimation with posterior: find a criteria (MAP)

$$x_a = \arg\max_x p(x|y)$$

Calculus: minimization of a $\chi^2$ cost function

$$J(x) = \frac{1}{2}[\frac{(x-x_b)^2}{\sigma_b^2} + \frac{(y-hx)^2}{\sigma_o^2}]$$




Estimation:

$$x_a = x_b + k(y - hx_b)$$

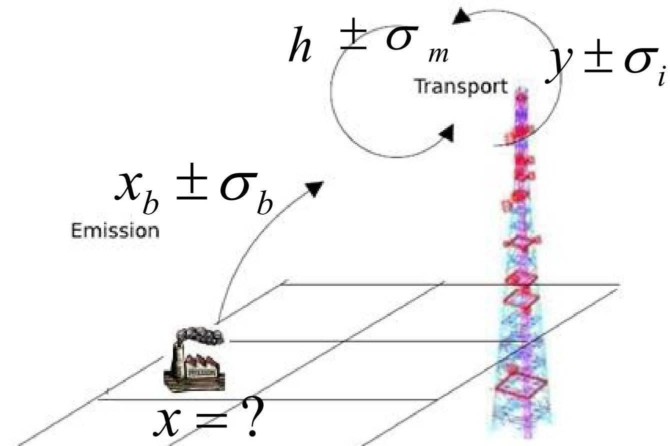
$$k = \sigma_b^2 h(h^2\sigma_b^2 + \sigma_o^2)^{-1}$$

(Kalman) gain $k = \frac{\partial x_a}{\partial y}$

- Sensitivity of analysis to obs
- Weighted by error statistics

# Simplest scalar case

Bouttier & Courtier 1999, Jacob 2007




Estimation: $$x_a = x_b + k(y - hx_b)$$

$$k = \sigma_b^2 h (h^2 \sigma_b^2 + \sigma_o^2)^{-1}$$

$$J(x) = \frac{1}{2}\left[\frac{(x - x_b)^2}{\sigma_b^2} + \frac{(y - hx)^2}{\sigma_o^2}\right]$$

Degree of freedom for signal (DFS)

$\sigma_o \ll \sigma_b$ $\quad \frac{(y - hx)^2}{\sigma_o^2} \uparrow$ **in** $J(x)$

$k \to 1/h \qquad x_a \to y/h$

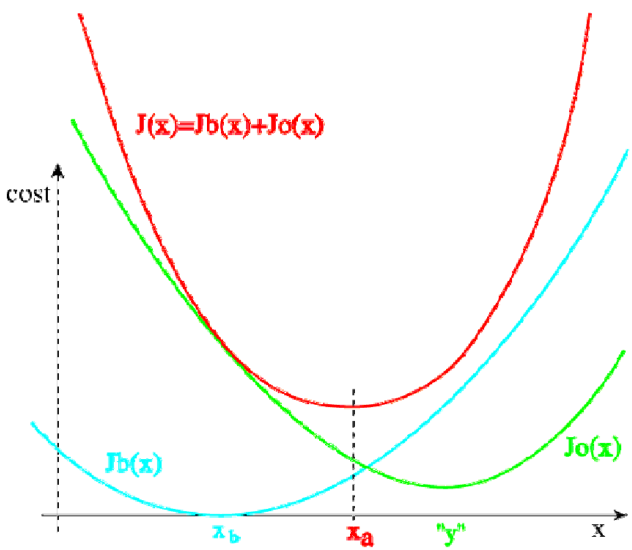
$y$ provides information on $x$

Degree of freedom for noise

$\sigma_o \gg \sigma_b$ $\quad \frac{(x - x_b)^2}{\sigma_b^2} \uparrow$ **in** $J(x)$

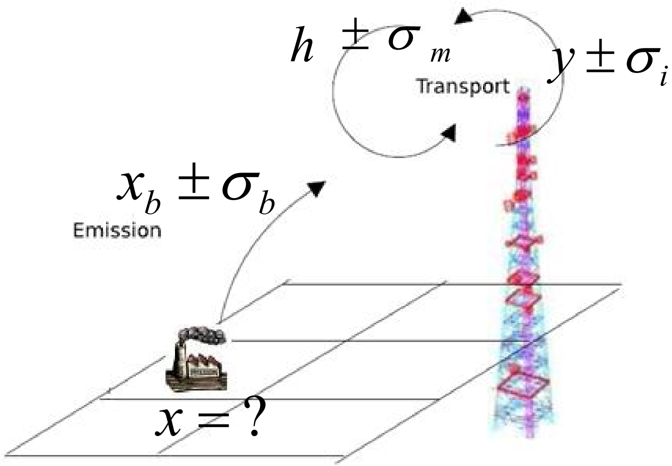
$k \to 0 \qquad x_a \to x_b$

$y$ provides only noise



# Simplest scalar case

Bouttier & Courtier 1999, Jacob 2007




Posterior uncertainty

$$p(x|y) \propto \exp[-\frac{1}{2}(\frac{(x-x_b)^2}{\sigma_b^2} + \frac{(y-hx)^2}{\sigma_o^2})]$$

$$= \exp(-\frac{1}{2}\frac{(x-x_a)^2}{\sigma_a^2})$$

$$(\sigma_a^2)^{-1} = (\sigma_b^2)^{-1} + h^2(\sigma_o^2)^{-1}$$

Sum of precision

Fisher info. matrix

Observation Eq.

$$y = hx + \varepsilon_o$$

$$\varepsilon_o = \varepsilon_i + \varepsilon_m$$

Information 1: first guess $x_b$

Information 2: observation $y$

Estimation:

$$y = hx \pm \sigma^o$$

$$x_a = x_b + k(y - hx_b)$$

$$x_a = ax + (1-a)x_b + k\varepsilon_o$$

Averaging kernel: $a = kh = \frac{\partial x_a}{\partial x}$

- Sensitivity of analysis to true emission
- Ideally 1

# A language of inversion: Bayesian synthesis

- Bayes' Theorem: uncertainty computation (information propagation) converting a prior probability to a posterior probability by assimilating Information from observations.

$$\underbrace{p(x|y)}_{\text{posterior}} = \frac{\overbrace{p(x)}^{\text{prior}}\,\overbrace{p(y|x)}^{\text{likelihood}}}{\underbrace{p(y)}_{\text{evidence}}}$$

  - y : observation
  - x : unknown parameter (source)

- Bayesian analysis in plain words

posterior ∝ likelihood × prior

# Bayesian inversion: vectorial case of linear dynamics and Gaussian error

Inverse modelling of sources $\mathbf{x}$ (2D+T); Gaussian assumption + linear observation operator.

- $\mathbf{H}$ Jacobian matrix of the problem (observation + model):

$$\mathbf{y} = \mathbf{H}\mathbf{x} + \varepsilon$$

- $\mathbf{x} - \mathbf{x}_b \propto \mathrm{N}(\mathbf{0}, \mathbf{B})$ $\mathbf{x}_b$ prior fluxes, $\mathbf{B}$ background error covariance matrix.

- $\varepsilon \propto \mathrm{N}(\mathbf{0}, \mathbf{R})$ $\mathbf{R}$ observation error covariance matrix.

# Bayesian inversion: vectorial case of linear dynamics and Gaussian error

- Bayes' Theorem: $$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{x})\,p(\mathbf{y}|\mathbf{x})}{p(\mathbf{y})} \quad \mathbf{x} \in \Re^n \quad \mathbf{y} \in \Re^d$$

  - Prior: $$p(\mathbf{x}) = \frac{\exp(-\frac{1}{2}(\mathbf{x}-\mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b))}{2\pi^{\frac{n}{2}}|\mathbf{B}|^{\frac{1}{2}}}$$

  - Likelihood $$p(\mathbf{y}|\mathbf{x}) = p(\overbrace{\mathbf{y}-\mathbf{H}\mathbf{x}}^{\varepsilon}) = \frac{\exp(-\frac{1}{2}\varepsilon^T \mathbf{R}^{-1}\varepsilon)}{2\pi^{\frac{d}{2}}|\mathbf{R}|^{\frac{1}{2}}}$$

  - Evidence $$p(\mathbf{y}) = \int p(\mathbf{x})\,p(\mathbf{y}-\mathbf{H}\mathbf{x})\,d\mathbf{x}$$
$$= \frac{\exp(-\frac{1}{2}(\mathbf{x}-\mathbf{x}_b)^T (\mathbf{R}+\mathbf{H}\mathbf{B}\mathbf{H}^T)^{-1}(\mathbf{x}-\mathbf{x}_b))}{2\pi^{\frac{d}{2}}|\mathbf{R}+\mathbf{H}\mathbf{B}\mathbf{H}^T|^{\frac{1}{2}}}$$

  - Posterior: $$p(\mathbf{x}|\mathbf{y}) = \frac{\exp(-\frac{1}{2}(\mathbf{x}-\mathbf{x}_a)^T \mathbf{P}_a^{-1}(\mathbf{x}-\mathbf{x}_a))}{2\pi^{\frac{n}{2}}|\mathbf{P}_a|^{\frac{1}{2}}}$$

# Vectorial analog of the simplest scalar case

| | | |
|---|---|---|
| **Cost function** | $J(x)=\frac{1}{2}[\frac{(x-x_b)^2}{\sigma_b^2}+\frac{(y-hx)^2}{\sigma_o^2}]$ | $J(\mathbf{x})=\frac{1}{2}(\mathbf{x}-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b)+(\mathbf{y}-H(\mathbf{x}))^T\mathbf{R}^{-1}(\mathbf{y}-H(\mathbf{x}))$ |
| **Inversion** | $x_a=x_b+k(y-hx_b)$ | $\mathbf{x}_a=\mathbf{x}_b+\mathbf{K}(\mathbf{y}-\mathbf{H}\mathbf{x}_b)$ |
| **Kalman gain** | $k=\sigma_b^2h(h^2\sigma_b^2+\sigma_o^2)^{-1}$ | $\mathbf{K}=\mathbf{B}\mathbf{H}^T(\mathbf{H}\mathbf{B}\mathbf{H}^T+\mathbf{R})^{-1}$ |
| | or equivalently | $\mathbf{K}=(\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}+\mathbf{B}^{-1})\mathbf{H}^T\mathbf{R}^{-1}$ |
| **Aver. Kernel** | $a=kh$ | $\mathbf{A}=\mathbf{K}\mathbf{H}$ |
| **DFS** | $\frac{(y-hx)^2}{\sigma_o^2}\uparrow$ **in** $J(x)$ | $E[(\mathbf{x}_a-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}_a-\mathbf{x}_b)]$ |
| **DoF Noise** | $\frac{(x-x_b)^2}{\sigma_b^2}\uparrow$ **in** $J(x)$ | $E(\varepsilon^T\mathbf{R}^{-1}\varepsilon)$ |
| **Fisher Info. Mat. (precision)** | $(\sigma_a^2)^{-1}=(\sigma_b^2)^{-1}+h^2(\sigma_o^2)^{-1}$ | $\mathbf{P}_a^{-1}=\mathbf{B}^{-1}+\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}$ |
| **Posterior Err. Cov. Mat.** | $\sigma_a^2=(1-kh)\sigma_b^2$ | $\mathbf{P}_a=(\mathbf{I}-\mathbf{K}\mathbf{H})\mathbf{B}$ |

# More on DFS

$$\mathbf{DFS} = E[(\mathbf{x}_a - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}_a - \mathbf{x}_b)]$$

$$= E\left\{\mathbf{tr}\left[(\mathbf{x}_a - \mathbf{x}_b)(\mathbf{x}_a - \mathbf{x}_b)^T\right]\mathbf{B}^{-1}\right\}$$

$$= \mathbf{tr}\left\{E\left[(\mathbf{x}_a - \mathbf{x}_b)(\mathbf{x}_a - \mathbf{x}_b)^T\right]\mathbf{B}^{-1}\right\}$$

$$= \mathbf{tr}\left\{\mathbf{K}E\left[(\mathbf{y} - \mathbf{H}\mathbf{x}_b)(\mathbf{y} - \mathbf{H}\mathbf{x}_b)^T\right]\mathbf{K}^T\mathbf{B}^{-1}\right\}$$

$$= \mathbf{tr}\left\{\mathbf{K}(\mathbf{HBH}^T + \mathbf{R})\mathbf{K}^T\mathbf{B}^{-1}\right\}$$

$$= \mathbf{tr}(\mathbf{KH}) = \mathbf{tr}(\mathbf{A})$$

Trace of averaging kernel

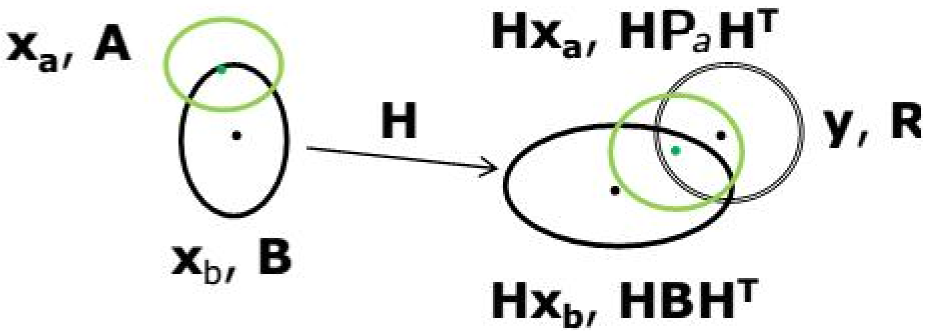
$$= \mathbf{tr}\left[(\mathbf{B} - \mathbf{P_a})\mathbf{B}^{-1}\right]$$

Reduction of uncertainty

$$= \mathbf{tr}\left(\overbrace{\mathbf{BH}^T\underbrace{(\mathbf{HBH}^T + \mathbf{R})^{-1}}_{\text{Info. from obs.}}}^{\mathbf{K}}\mathbf{H}\right)$$

Propagation of informatioin

# Inversion methods




Analytical inversion: linear algebra, maximal 5000-10000 parameters

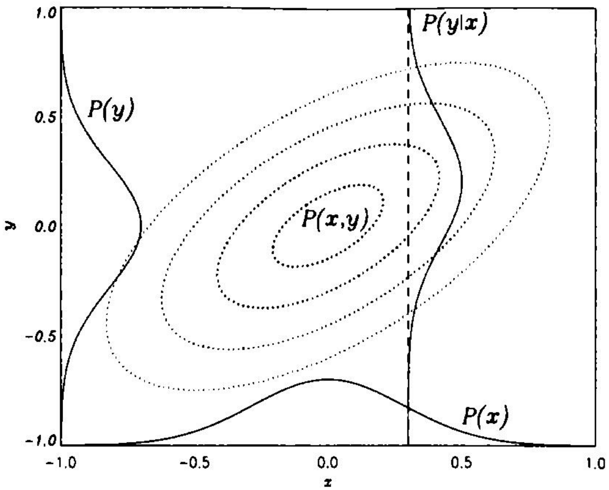
$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}(\mathbf{y} - \mathbf{H}\mathbf{x}_b)$$
$$\mathbf{P}_a = (\mathbf{I} - \mathbf{KH})\mathbf{B}$$

Variational Analysis: Gaussian assumptions + MAP ⇒ least square errors (Gauss' result)
Numerical optimization; easily dealing with a million parameters; adjoint techniques

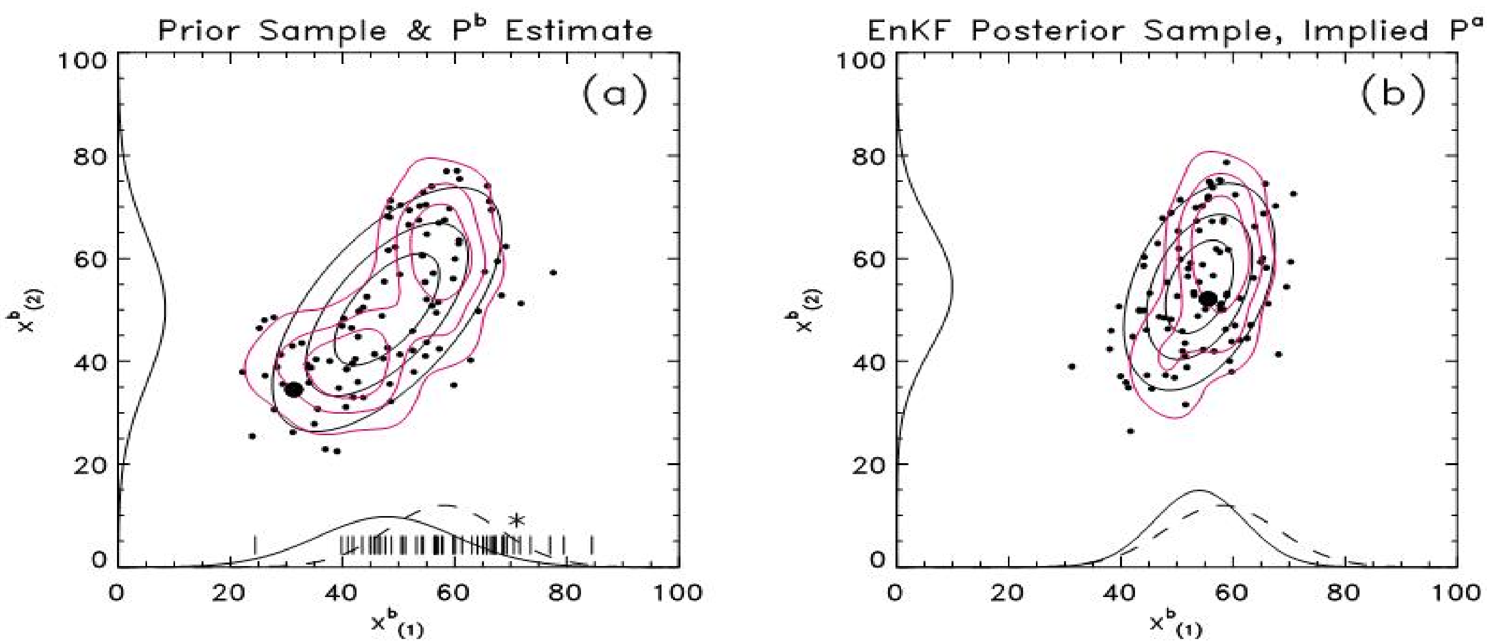
$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + (\mathbf{y} - H(\mathbf{x}))^T \mathbf{R}^{-1}(\mathbf{y} - H(\mathbf{x}))$$
$$\mathbf{P}_a = \left(\frac{1}{2}J''\right)^{-1}$$

Ensemble approach: representing PDFs with samples of manageable size

# Sketch of Bayesian Synthesis




- Red: true prior and posterior
- Points: samples
- Contours: Gaussian prior and posterior
- Obs for $x_1$




Hamil 2006

# Imporatant roles of $\mathbf{B}$ and $\mathbf{R}$

Fundamental role of $\mathbf{B}$ : corrections only in the column space of $\mathbf{B}$ !

Kalnay 2003

$\mathbf{B}$ spanned by a single vector $\mathbf{b}$

$$\mathbf{B} = \mathbf{b}\mathbf{b}^T$$

Suppose $\mathbf{H} = \mathbf{I}, \quad \mathbf{R} = \alpha^2 \mathbf{I}$

$$\begin{aligned}\delta \mathbf{x}_a &= \mathbf{x}_a - \mathbf{x}_b \\ &= \mathbf{B}\mathbf{H}^T \, [\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R}]^{-1} \, [\mathbf{y}_o - H(\mathbf{x}_b)] \\ &= \mathbf{b} \, \mathbf{b}^T \delta \mathbf{y}_o / (\mathbf{b}^T \mathbf{b} + \alpha^2)\end{aligned}$$

Correction Direction; Information spreading

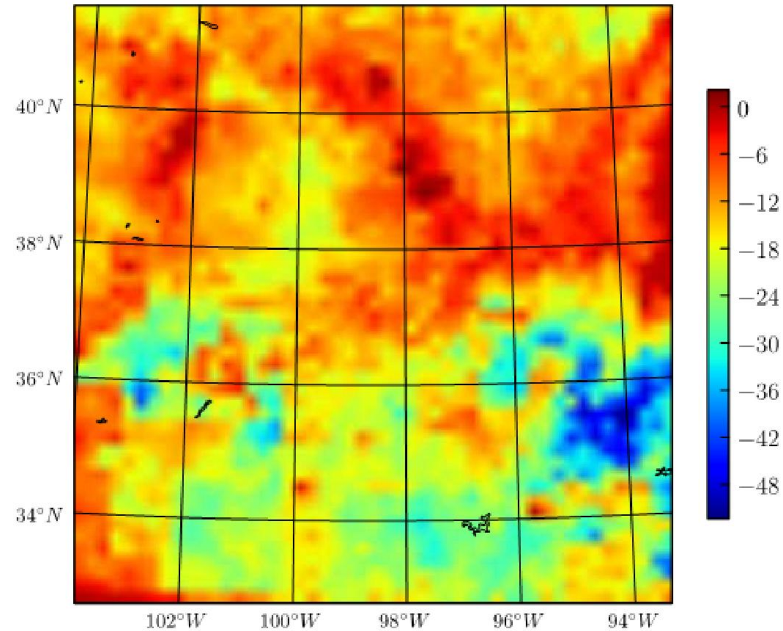
Projection of obs increment in (subspace) $\mathbf{b}$ info smoothing

Total error budget

Realistic $\mathbf{B}$ : difficult issue

Physical consistency: balanced $\mathbf{B}$

Sum of prior SiBcrop fluxes
Over 1-15 June 2007
Center USA 980km x 980 km




Balgovind correlation model

$$C(h) = \kappa^2 (1 + \frac{h}{L}) \exp(-\frac{h}{L})$$

# Diagnostics of error

Desroziers et al 2005

$$\mathbf{d}_b^o = \mathbf{y}^o - H(\mathbf{x}^b)$$
$$= \mathbf{y}^o - H(\mathbf{x}^t) + H(\mathbf{x}^t) - H(\mathbf{x}^b)$$
$$\simeq \boldsymbol{\epsilon}^o - \mathbf{H}\boldsymbol{\epsilon}^b$$

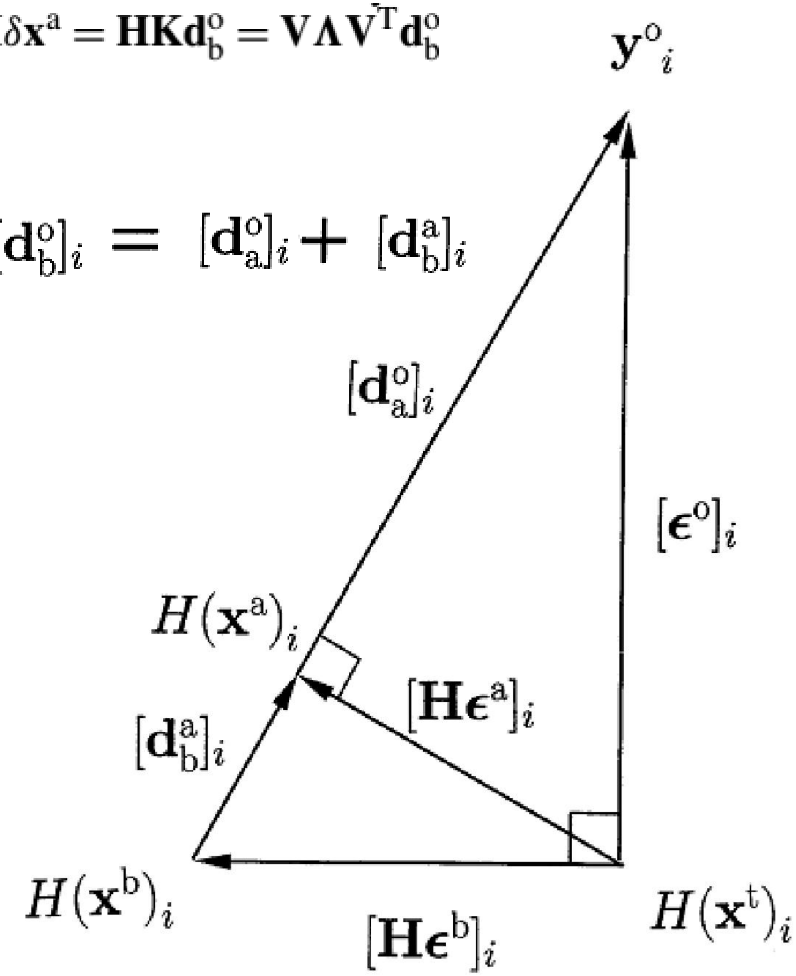
$$\mathbf{d}_b^a = \mathbf{H}\delta\mathbf{x}^a = \mathbf{HK}\mathbf{d}_b^o = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^T\mathbf{d}_b^o$$

$$E[\mathbf{d}_b^o(\mathbf{d}_b^o)^T]$$
$$= E[\boldsymbol{\epsilon}^o(\boldsymbol{\epsilon}^o)^T] + \mathbf{H}E[\boldsymbol{\epsilon}^b(\boldsymbol{\epsilon}^b)^T]\mathbf{H}^T$$
$$= \mathbf{R} + \mathbf{HBH}^T$$

$$[\mathbf{d}_b^o]_i = [\mathbf{d}_a^o]_i + [\mathbf{d}_b^a]_i$$

$$\mathbf{d}_a^o = \mathbf{y}^o - H(\mathbf{x}^b + \delta\mathbf{x}^a)$$
$$\simeq \mathbf{y}^o - H(\mathbf{x}^b) - \mathbf{HK}\mathbf{d}_b^o$$
$$= (\mathbf{I} - \mathbf{HK})\mathbf{d}_b^o$$
$$= \mathbf{R}(\mathbf{HBH}^T + \mathbf{R})^{-1}\mathbf{d}_b^o,$$

$$E[\mathbf{d}_a^o(\mathbf{d}_a^o)^T] = \mathbf{R} + \mathbf{H}\mathrm{P}_a^{-1}\mathbf{H}^T$$




$$E[\mathbf{d}_b^a(\mathbf{d}_b^o)^T] = \mathbf{HBH}^T$$
$$E[\mathbf{d}_a^o(\mathbf{d}_b^o)^T] = \mathbf{R}$$
$$E[\mathbf{d}_b^a(\mathbf{d}_a^o)^T] = \mathbf{H}\mathrm{P}_a^{-1}\mathbf{H}^T$$

# Optimality System (O.S. Le Dimet 90s) and SOI

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

Dynamic context

Control theory for high-dimensional system

$$\begin{cases} \frac{dX}{dt} = F(X) + B.V \\ X(0) = U \\ \frac{dP}{dt} + \left[\frac{\partial F}{\partial X}\right]^t P = C^t(CX - X_{obs}) \\ P(T) = 0 \\ \nabla_U J = -P(0) + (U - U_0) = 0 \\ \nabla_V J = -B^t.P = 0 \end{cases}$$

Backward propagation

obs impulse

Adjoint variable: sensitivity to obs impulse

O.S. as a general model

All information contained in O.S.

Optimization based on O.S.

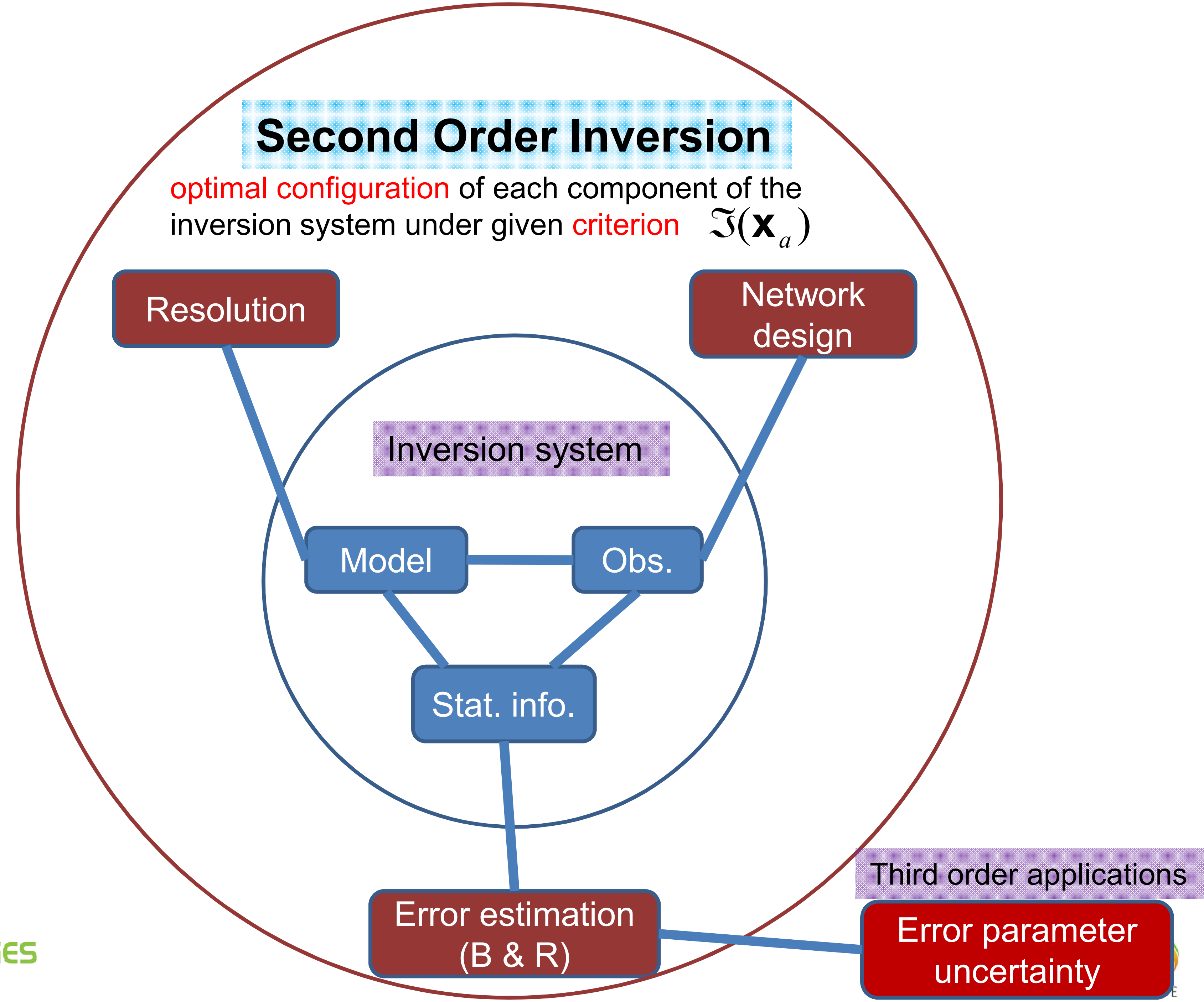
**Second order inversion (SOI)**

$$\Im(\mathbf{x}_a)$$

$\Im$ Performance of inversion system; not necessarily RMSE

$\mathbf{x}_a$ Solution given by O.S.

| | |
|---|---|
| Direct modeling | Cost 1 |
| Inversion/assim. | Cost 10 |
| SOI | Cost 100 |


Second Order Inversion
optimal configuration of each component of the inversion system under given criterion $\Im(\mathbf{x}_a)$
Resolution
Network design
Inversion system
Model
Obs.
Stat. info.
Error estimation (B & R)
Third order applications
Error parameter uncertainty

# Bayesian inversion: vectorial case of linear dynamics and Gaussian error

- Context: Inverse modelling of sources σ (2D+T); Gaussian assumption + linear observation operator.

  - H Jacobian matrix of the problem (observation + model):

$$\mu = \mathbf{H}\sigma + \varepsilon$$

  - $\sigma^b - \sigma \sim \mathcal{N}(\mathbf{0}, \mathbf{B})$; $\sigma^b$ prior fluxes, B background error covariance matrix.
  - $\varepsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{R})$; $\mathbf{R}$ observation error covariance matrix.

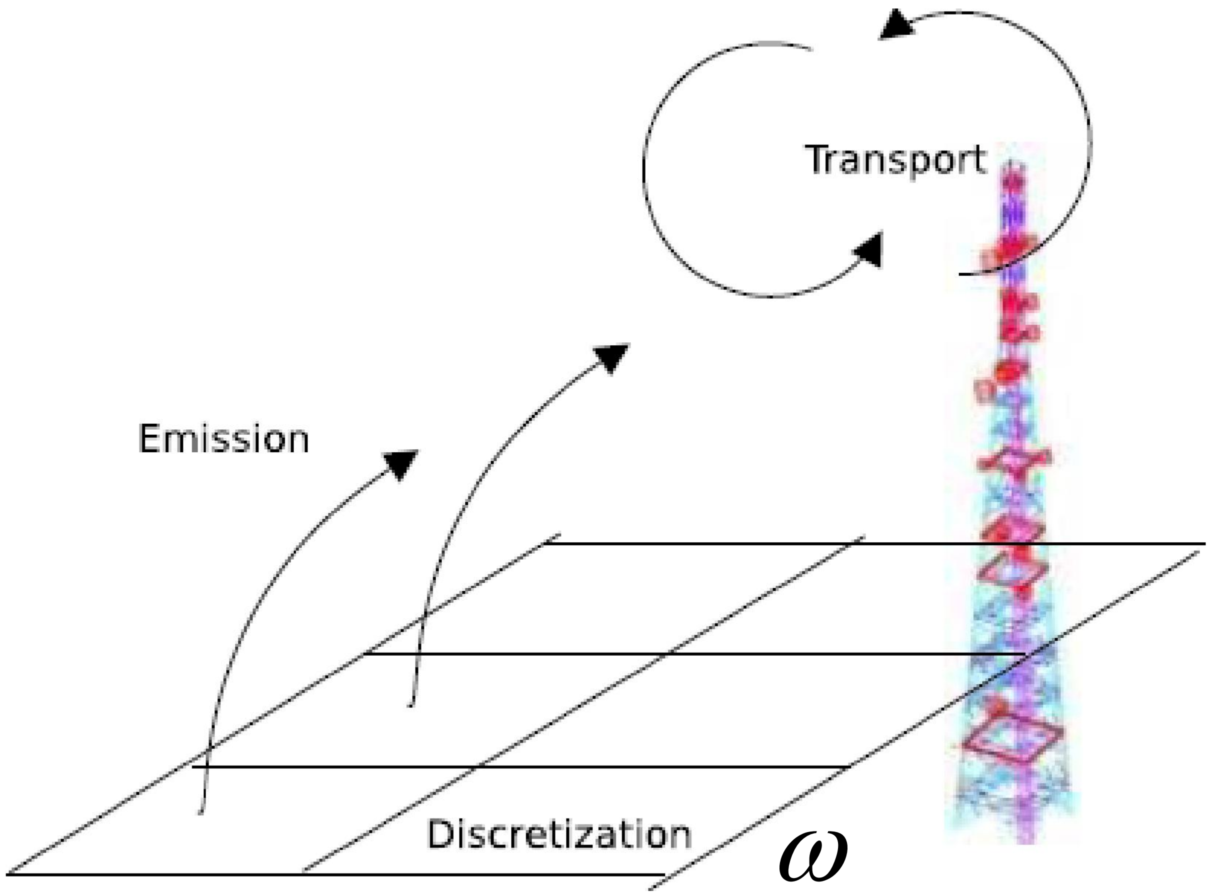
- BLUE analysis:

$$\sigma^a = \sigma^b + \mathbf{B}\mathbf{H}^{\mathrm{T}}\left(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}\right)^{-1}\left(\mu - \mathbf{H}\sigma^b\right),$$

$$\mathbf{P}^a = \mathbf{B} - \mathbf{B}\mathbf{H}^{\mathrm{T}}\left(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}\right)^{-1}\mathbf{H}\mathbf{B}.$$

- A representation ω is a discretization of the space-time domain of control (parameter) space Ω.

# Bayesian inversion: vectorial case of linear dynamics and Gaussian error




Decomposition of observation error: $\varepsilon_{\omega} = \varepsilon + \varepsilon_{\omega}^{c} + \varepsilon_{\omega}^{m}$

# $CO_2$ flux inversion

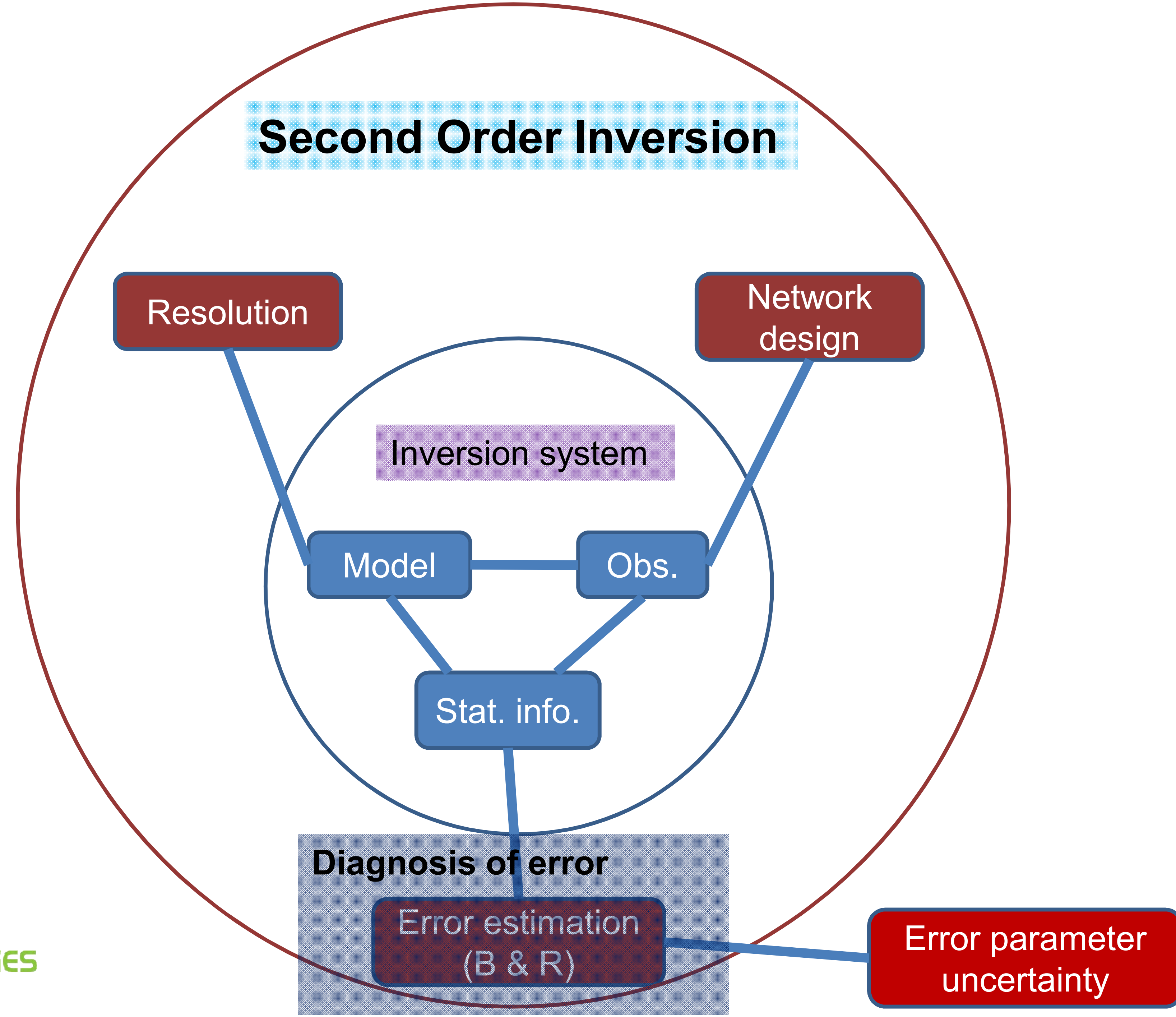
- $CO_2$ Inversion: Using concentration observations to retrieve surface $CO_2$ fluxes.

- Ill-posed problem due to the flux-observation mismatch (e.g. diffusive atmospheric transport that links fluxes with observations)

  - Aggregation of flux variables, e.g. eco-regions or coarser regular grid => aggregation error
  - Bayesian inversion: regularized by prior information (correlation in prior flux errors)

- Plan

  - Error diagnosis
  - Aggregation error: multiscale inversion (resolution optimization) & direct aggregation.
  - Estimates parameters of the prior and observation errors (hyper-parameter estimation)


Second Order Inversion
Resolution
Network design
Inversion system
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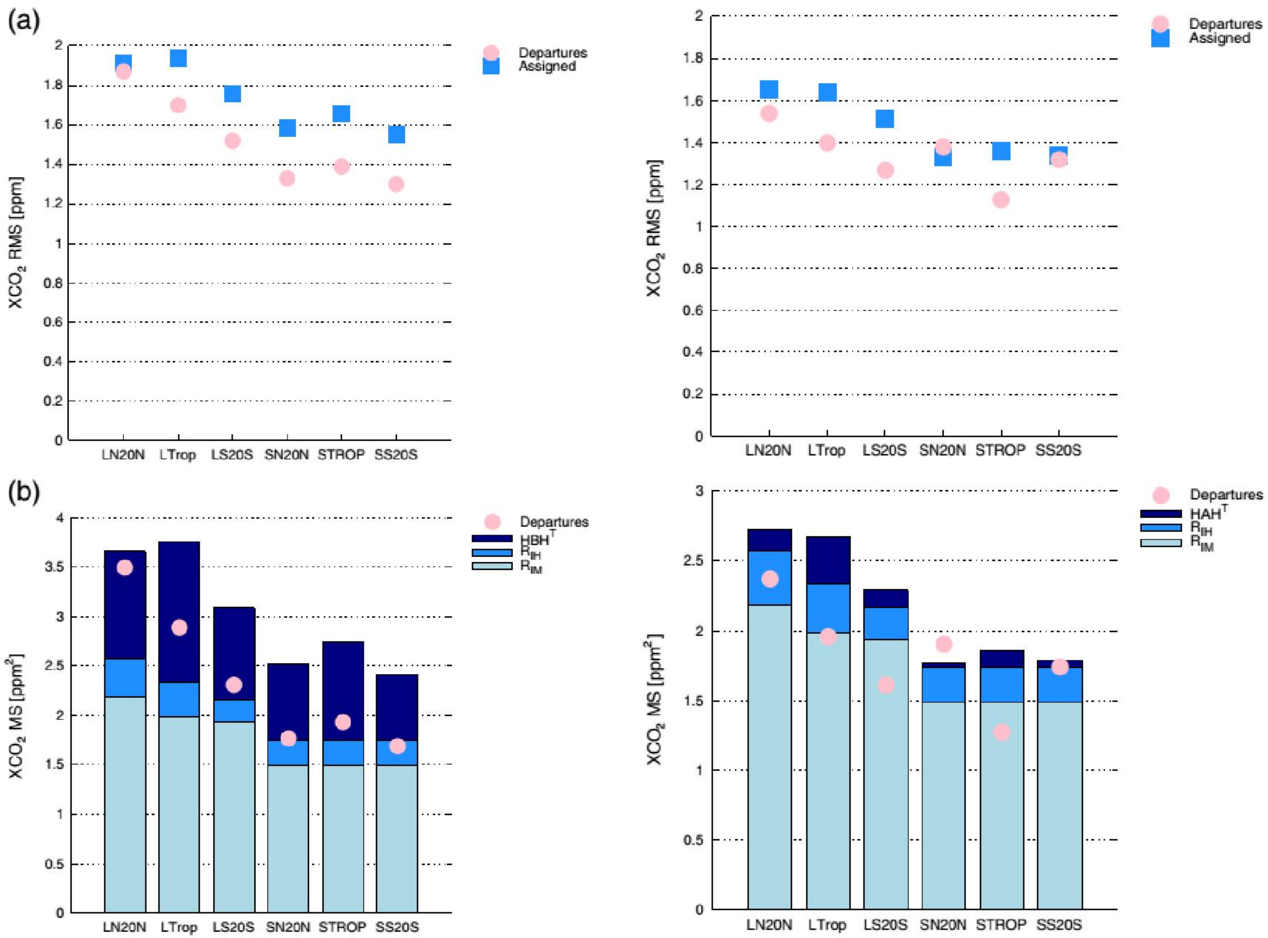
Stat. info.
Diagnosis of error
Error estimation (B & R)
Error parameter uncertainty

# Diagnosis of error

Chevallier & O'Dell 2013

- Variational inversion, Monte Carlo simulations for error statistics
- Compare  with GOSAT data

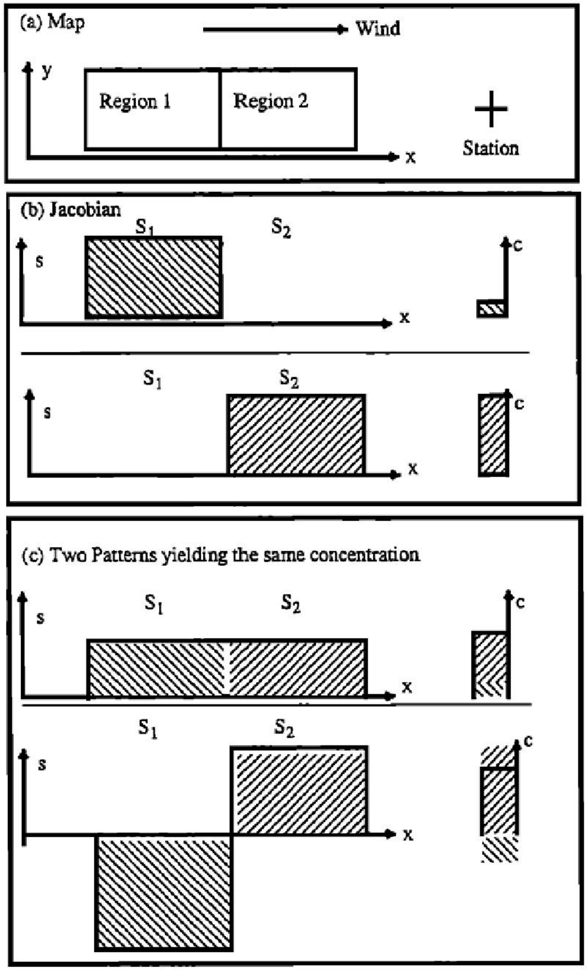



$$E\left[(\mathbf{Hx}_b - \mathbf{y})(\mathbf{Hx}_b - \mathbf{y})^T\right] = \mathbf{HBH}^T + \mathbf{R}$$

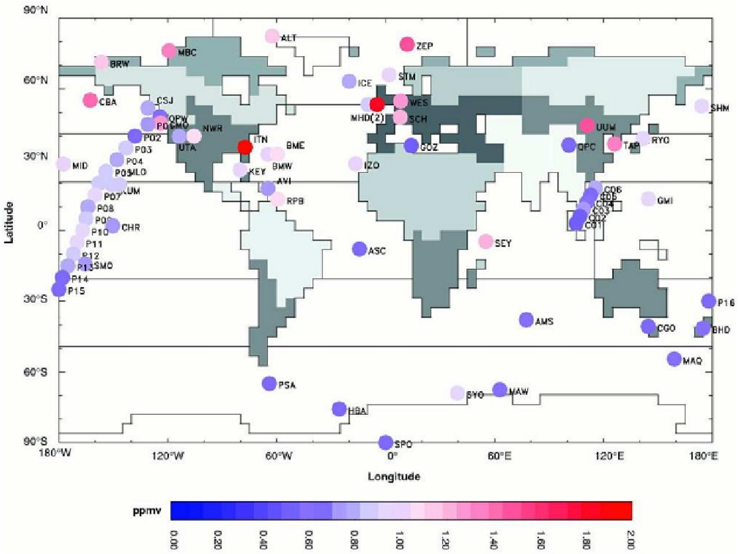
$$E\left[(\mathbf{Hx}_a - \mathbf{y})(\mathbf{Hx}_a - \mathbf{y})^T\right] = \mathbf{H}\,\mathbf{P}_a^{-1}\,\mathbf{H}^T + \mathbf{R}$$

# Aggregation error

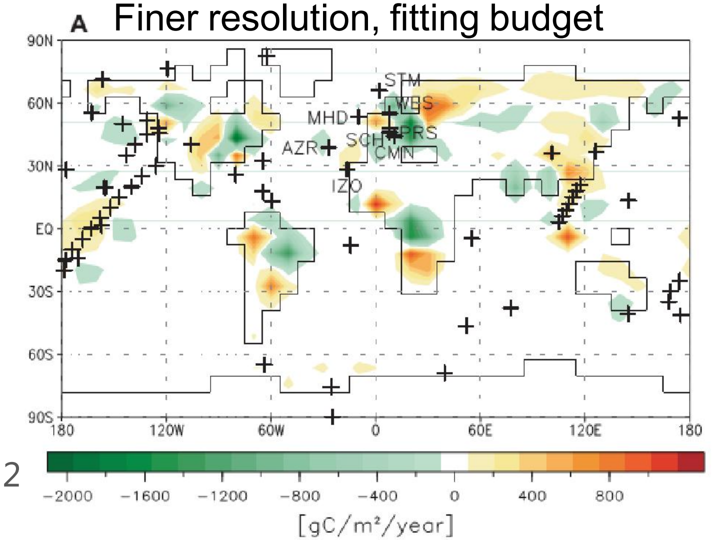
Kaminski et al 2011
Missing small scale details
(high frequency )

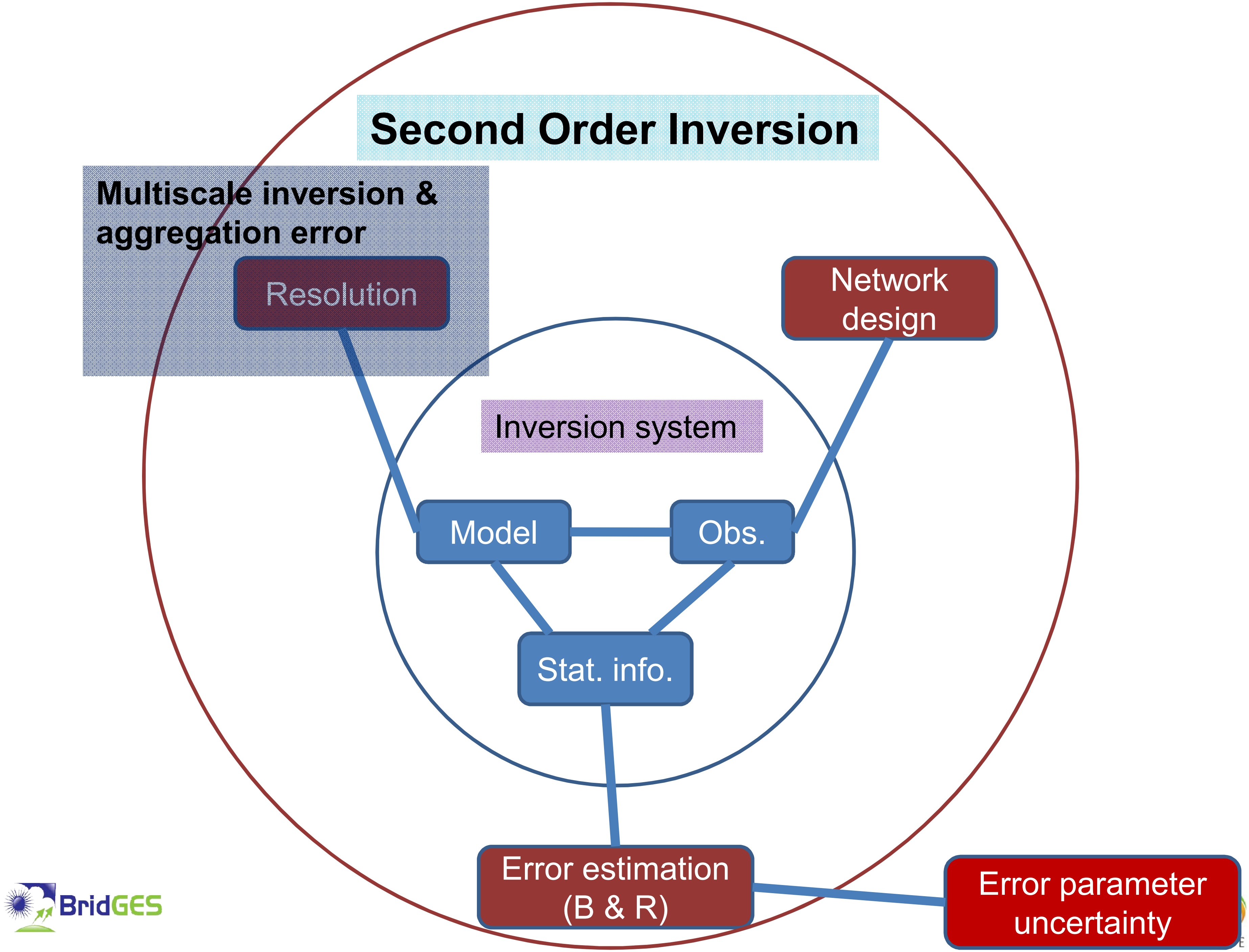



Bousquet et al 2000

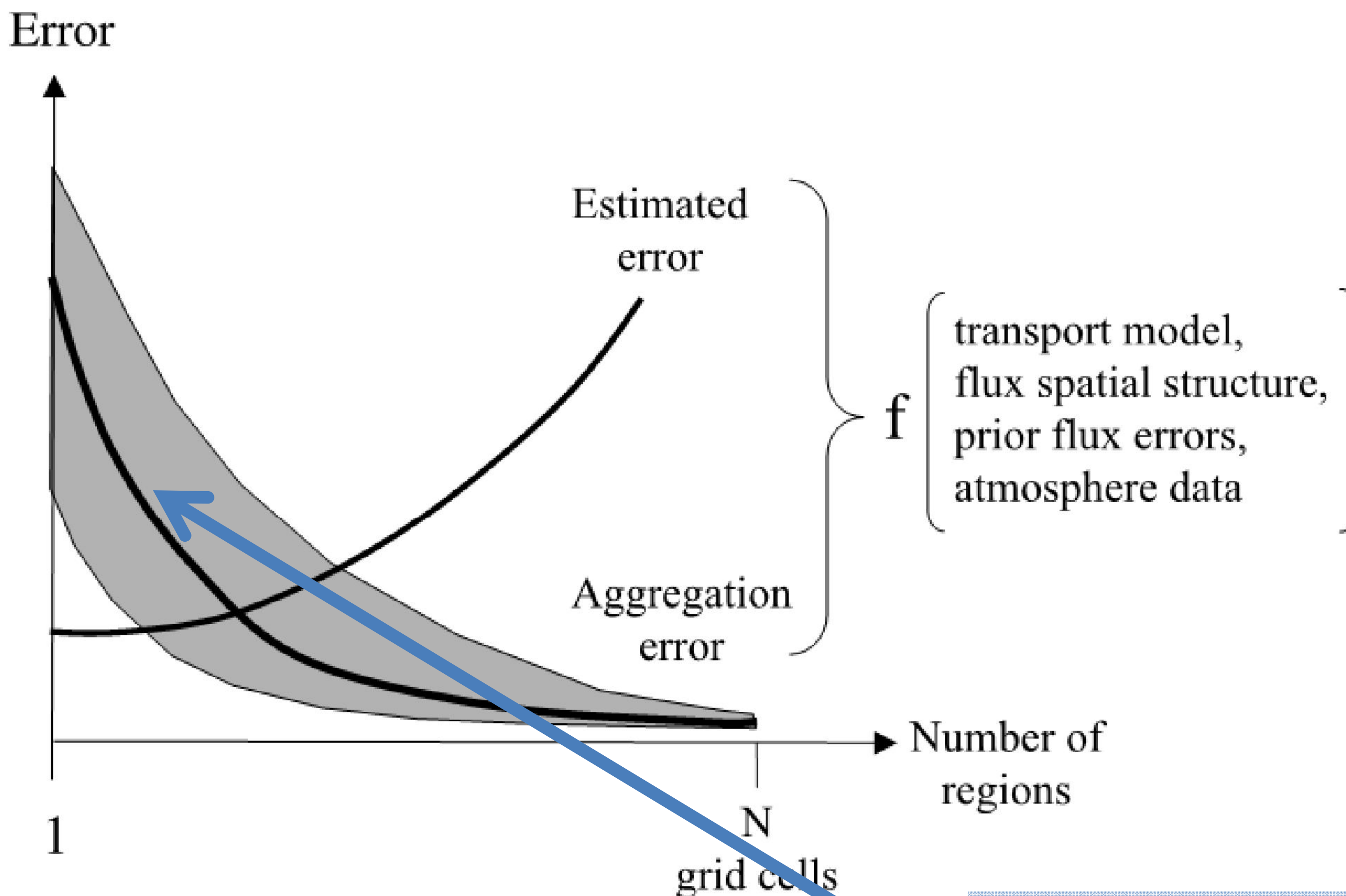



Kaminski & Heimann 2001
Finer resolution, fitting budget




Second Order Inversion
Multiscale inversion &
aggregation error
Resolution
Network
design
Inversion system
Model
Obs.
Stat. info.
Error estimation
(B & R)
Error parameter
uncertainty
BridGES

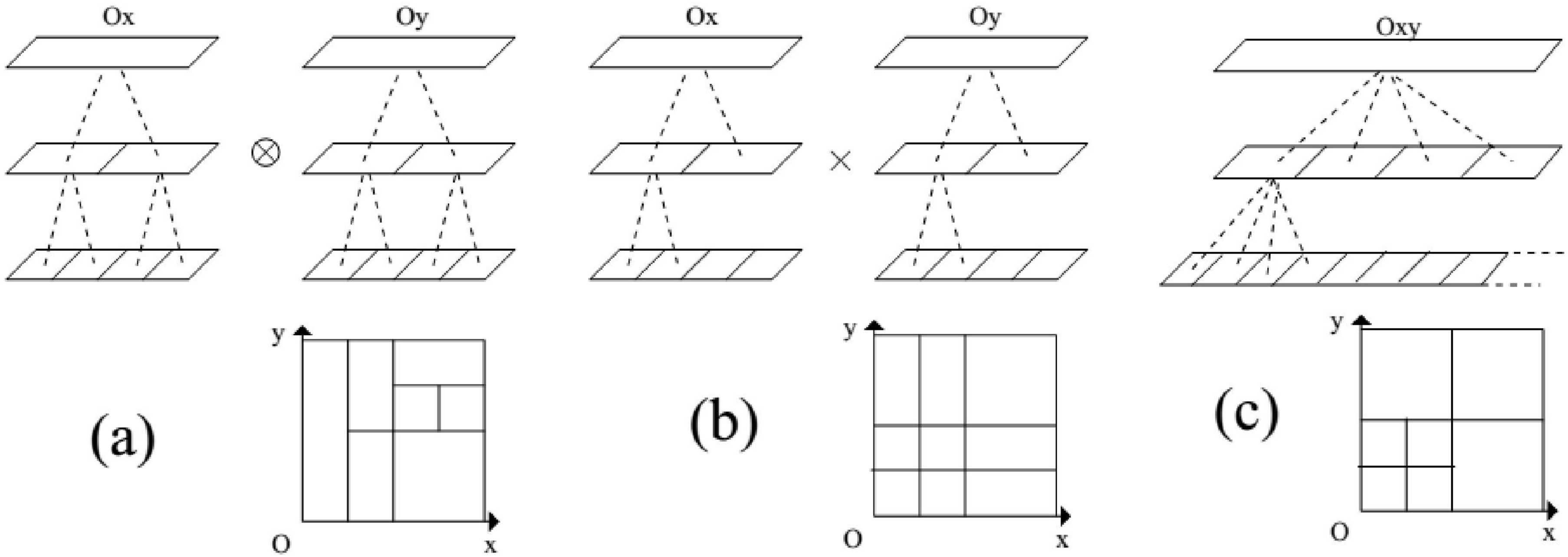
# Aggregation error




Peylin et al 2011

Ideal case:
- No model error
- Finest resolution offordable

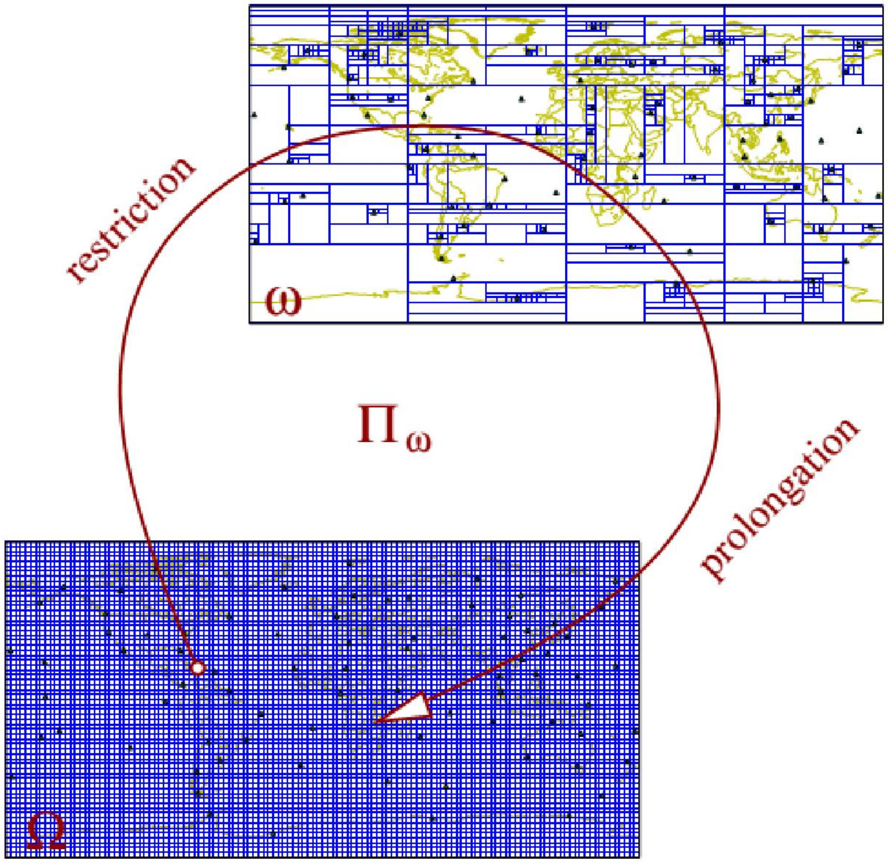
# Multiscale structure




- Memory costs for a 2D+T control space
  - Tilings: up to 8 times the size of the finest grid Jacobian
  - Qtrees: up to 8/3 times the size of the finest grid Jacobian.
- Empirically, optimisation on the qtrees is twice faster than on the tilings.

# Multiscale inversion

- The source variables (vector $\sigma$) can be discretised on an adaptive grid $\omega$.
- Restriction ($\mathbf{\Gamma}_\omega$) and prolongation ($\mathbf{\Gamma}^*_\omega$) operators can help to transfer $\sigma$ from the finest regular grid cell $\Omega$ to $\omega$.
- The composition of a restriction and a prolongation gives a projection operator $\mathbf{\Pi}_\omega$ which depends on the geometry of $\omega$.



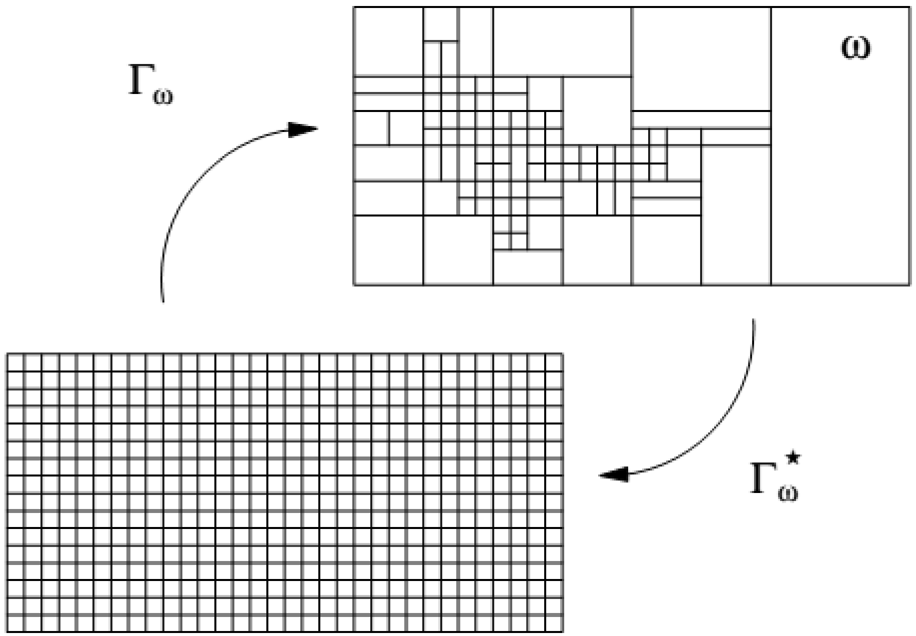
# Up and down the scale ladder (1/4)

## Restriction and prolongation

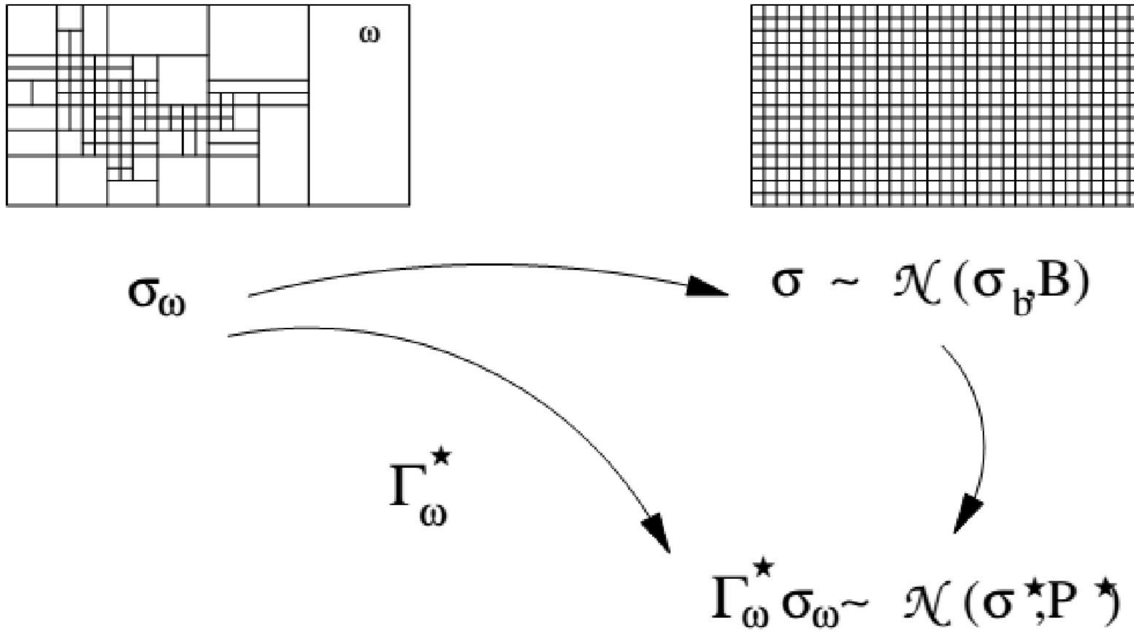
- Restriction operator : $\sigma \underset{\text{coarse graining}}{\longrightarrow} \sigma_\omega = \mathbf{\Gamma}_\omega \sigma$, where $\mathbf{\Gamma}_\omega : \mathbb{R}^{N_{\text{fg}}} \to \mathbb{R}^N$ defines the coarse graining operator (non-ambiguous).
- Prolongation operator : $\mathbf{\Gamma}^\star_\omega : \mathbb{R}^N \to \mathbb{R}^{N_{\text{fg}}}$ refines $\sigma_\omega$ into $\sigma$ (ambiguous).

## Scaling of errors

- Background error covariance matrix: $\mathbf{B}_\omega = \mathbf{\Gamma}_\omega \mathbf{B} \mathbf{\Gamma}^{\mathrm{T}}_\omega$,
- Observations/representativity/model errors: $\mathbf{R}_\omega$, to be discussed later.



# Up and down the scale ladder (2/4)




## Bayesian choice of a prolongation operator

- Idea: Use prior $\sigma \sim \mathcal{N}(\sigma_b, \mathbf{B})$ to refine the source. Knowing $\sigma_\omega$ in representation $\omega$, then from Bayes' rule, the most likely refined source is given by the mode of

$$q(\sigma|\sigma_\omega) = \frac{q(\sigma)}{q_\omega(\sigma_\omega)}\delta(\sigma_\omega - \mathbf{\Gamma}_\omega \sigma)$$

# Up and down the scale ladder (3/4)

## Bayesian choice of a prolongation operator

- Refinement is now a statistical process ! But the prolongation operator will be defined as the most likely refinement operation.
- Thus the (estimate of the) refined source is

$$\sigma^\star = \sigma_b + \mathbf{B}\mathbf{\Gamma}_\omega^{\mathrm{T}}\left(\mathbf{\Gamma}_\omega\mathbf{B}\mathbf{\Gamma}_\omega^{\mathrm{T}}\right)^{-1}(\sigma_\omega - \mathbf{\Gamma}_\omega\sigma_b)$$

which suggests the (affine) prolongation operator

$$\mathbf{\Gamma}_\omega^\star \equiv (\mathbf{I}_{N_{\mathrm{fg}}} - \mathbf{\Pi}_\omega)\sigma_b + \mathbf{\Lambda}_\omega^\star \,,$$

where the linear part of $\mathbf{\Gamma}_\omega^\star$ is

$$\mathbf{\Lambda}_\omega^\star \equiv \mathbf{B}\mathbf{\Gamma}_\omega^{\mathrm{T}}\left(\mathbf{\Gamma}_\omega\mathbf{B}\mathbf{\Gamma}_\omega^{\mathrm{T}}\right)^{-1}, \quad \text{and} \quad \mathbf{\Pi}_\omega \equiv \mathbf{\Lambda}_\omega^\star\mathbf{\Gamma}_\omega \,.$$

# Up and down the scale ladder (4/4)

## Up and down

- Must consistently satisfy $\mathbf{\Gamma}_\omega \mathbf{\Gamma}^\star_\omega = \mathbf{I}_N$.
- Down and up: $\mathbf{\Gamma}^\star_\omega \mathbf{\Gamma}_\omega = (\mathbf{I}_{N_{\mathrm{fg}}} - \mathbf{\Pi}_\omega)\sigma_b + \mathbf{\Pi}_\omega$

## Properties of $\mathbf{\Pi}_\omega$

- $\mathbf{\Pi}_\omega$ is a projector since $\mathbf{\Pi}^2_\omega = \mathbf{\Pi}_\omega$.
- It is also $\mathbf{B}^{-1}$-symmetric: $\mathbf{\Pi}_\omega \mathbf{B} = \mathbf{B}\mathbf{\Pi}^{\mathrm{T}}_\omega$.

## Observation equation in representation $\omega$

- Then $\mathbf{H}$ becomes $H_\omega = \mathbf{H}\mathbf{\Gamma}^\star_\omega$, and

$$\mu = H_\omega \sigma_\omega + \varepsilon_\omega = \mathbf{H}\mathbf{\Gamma}^\star_\omega \mathbf{\Gamma}_\omega \sigma + \varepsilon_\omega \,,$$

so that

$$\mu = \mathbf{H}\sigma_b + \mathbf{H}\mathbf{\Pi}_\omega(\sigma - \sigma_b) + \varepsilon_\omega \,.$$

# Accounting for aggregation errors

- Consistent observation equations:

$$\mu = \mathbf{H}\sigma + \varepsilon = \mathbf{H}_\omega \sigma_\omega + \varepsilon_\omega \,.$$

- Assuming aggregation is the only source of scale-dependent errors, one has $\mathbf{H}\sigma + \varepsilon = \mathbf{H}\sigma_b + \mathbf{H}\mathbf{\Pi}_\omega(\sigma - \sigma_b) + \varepsilon_\omega$, leading to the identification

$$\varepsilon_\omega = \varepsilon + \mathbf{H}\left(\mathbf{I}_{N_{\mathrm{fg}}} - \mathbf{\Pi}_\omega\right)(\sigma - \sigma_b) = \varepsilon + \varepsilon^c_\omega \,.$$

- Assuming independence of the error and source priors, the computation of the covariance matrix of these errors leads to

$$\mathbf{R}_\omega = \mathbf{R} + \mathbf{H}\left(\mathbf{I}_{N_{\mathrm{fg}}} - \mathbf{\Pi}_\omega\right)\mathbf{B}\mathbf{H}^{\mathrm{T}} \,.$$

- In that case, one checks that the innovation statistics $\mathbf{D} = \mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}$ are scale-independent $(\mathbf{R} + \mathbf{H}_\omega \mathbf{B}_\omega \mathbf{H}_\omega^{\mathrm{T}} \longrightarrow \mathbf{R}_\omega + \mathbf{H}_\omega \mathbf{B}_\omega \mathbf{H}_\omega^{\mathrm{T}} = \underline{\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}})$.

# Optimal representation mitigates aggregation effect

- $\omega$ maximizes DFS (bocquet et al., 2011): normalized uncertainty reduction $(\mathbf{B}-\mathbf{P}^a)\mathbf{B}^{-1} = \mathbf{B}\mathbf{H}^{\mathrm{T}}\mathbf{D}^{-1}\mathbf{H}$

$$\mathrm{DFS}_\omega = \mathrm{Tr}(\mathbf{\Pi}_\omega \mathbf{B}\mathbf{H}^{\mathrm{T}}\mathbf{D}^{-1}\mathbf{H}).$$

Optimal information propagation from observation sites to the whole domain

- The aggregation effect can be quantified by:

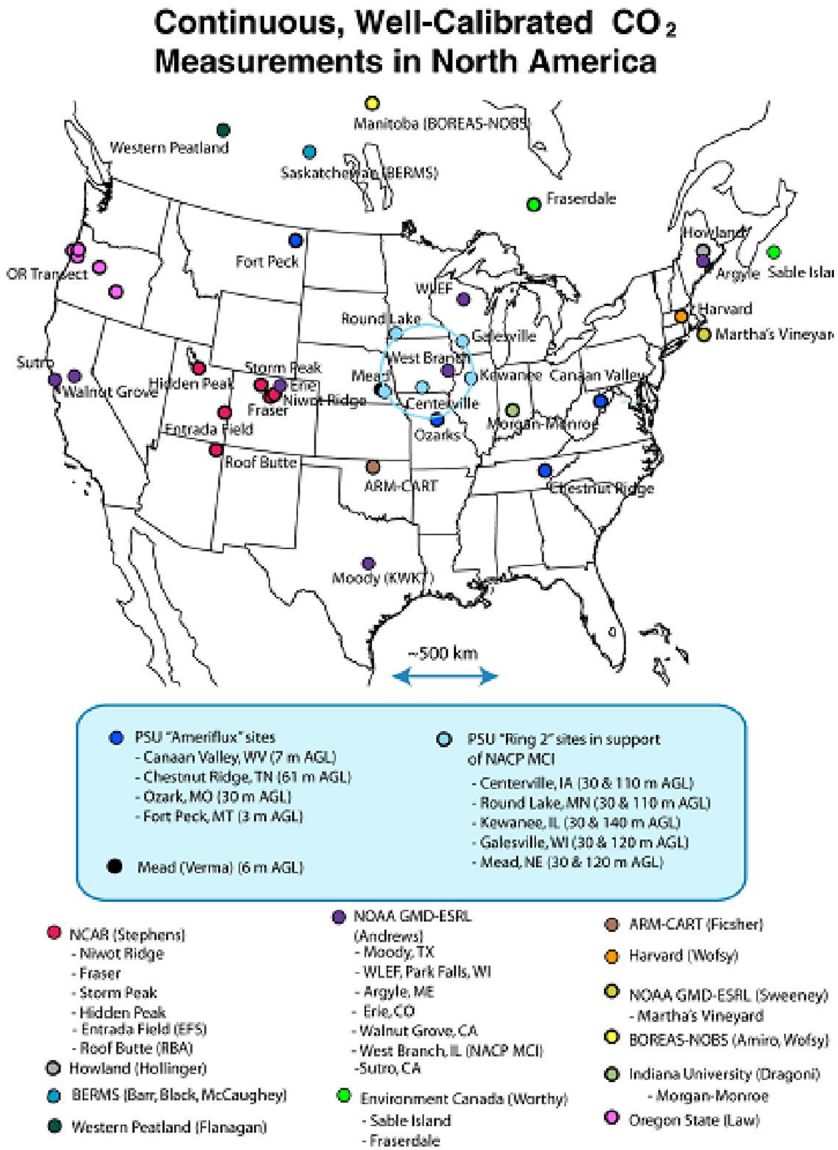
$$\widehat{\mathscr{I}_\omega} = \mathrm{Tr}\left[\mathbf{R}^{-1}(\mathbf{R}_\omega - \mathbf{R})\right] = \mathrm{Tr}\left(\mathbf{B}\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right) - \mathrm{Tr}\left(\mathbf{\Pi}_\omega \mathbf{B}\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right).$$

To minimize the aggregation effect is equivalent to the maximization of the Fisher criterion (Wu et al., 2011):

$$\mathrm{Tr}(\mathbf{\Pi}_\omega \mathbf{B}\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}).$$

which is the limiting case of the DFS criterion when **R** is inflated or when **B** vanishes.

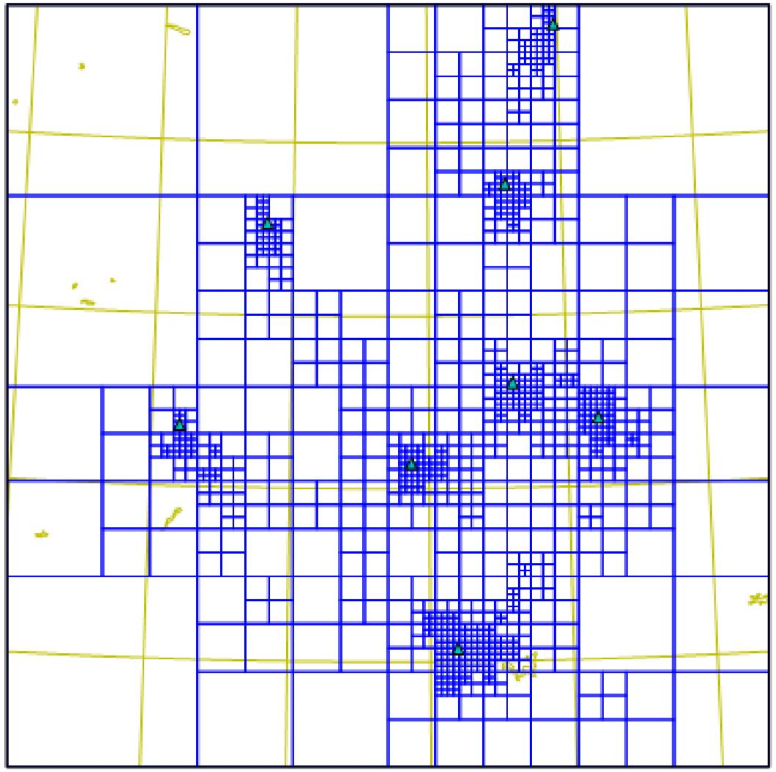
# Inversion system: Experimental setup

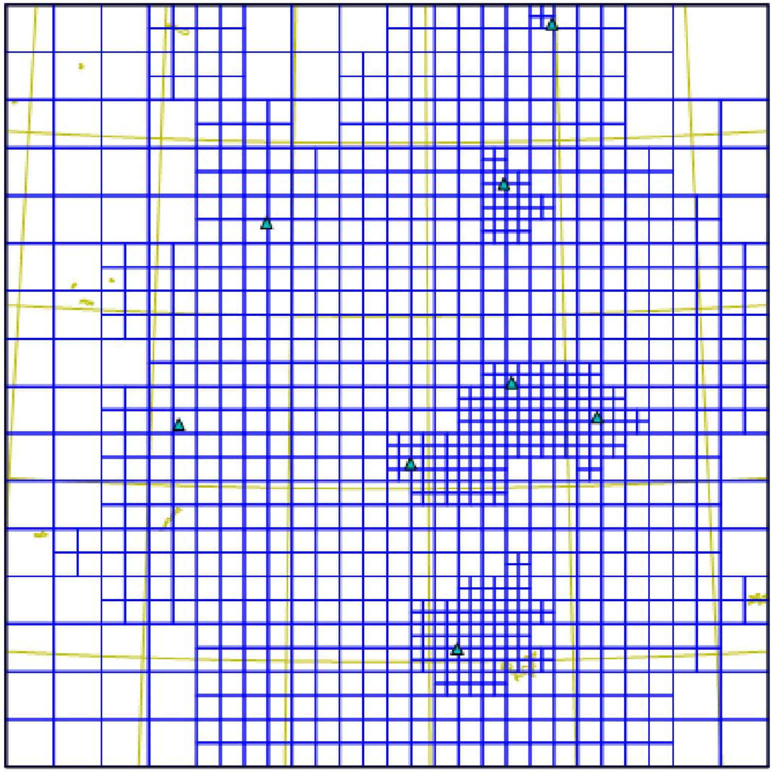



## Setup

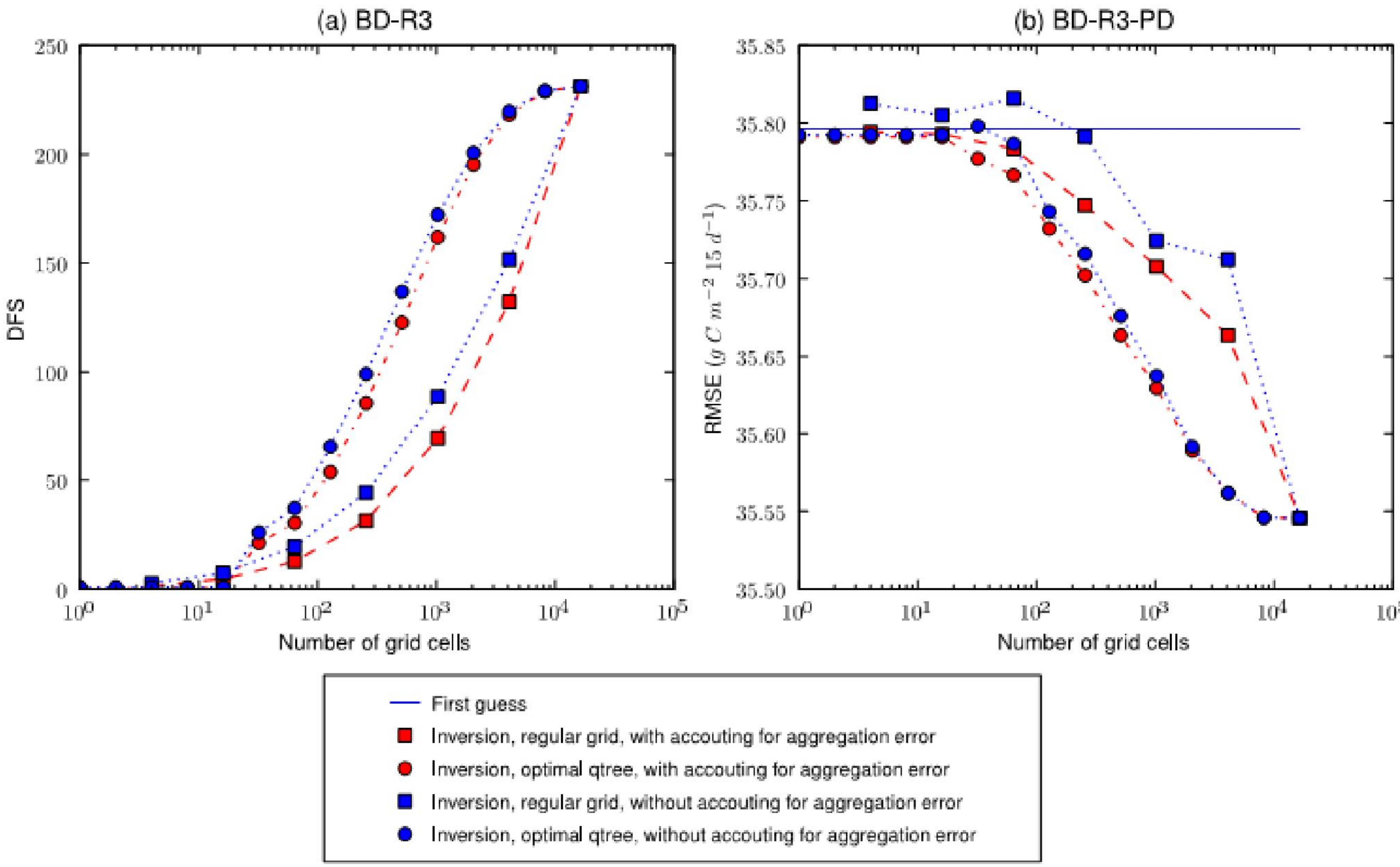
- **Domain**: 980km$\times$980km with 20km$\times$20km grid cell
- **Period**: 01$\sim$15 June 2007 or weekly inversions
- $\mu$: hourly synthetic or real observations from 8 towers
- $\sigma^b$: SiBcrop fluxes
- **H**: Computed from particles generated by Lagrangian model LPDM
- **R**: Diagonal or temporal correlations
- **B**: Diagonal or Balgovind parameterization

# Optimal representations with different settings

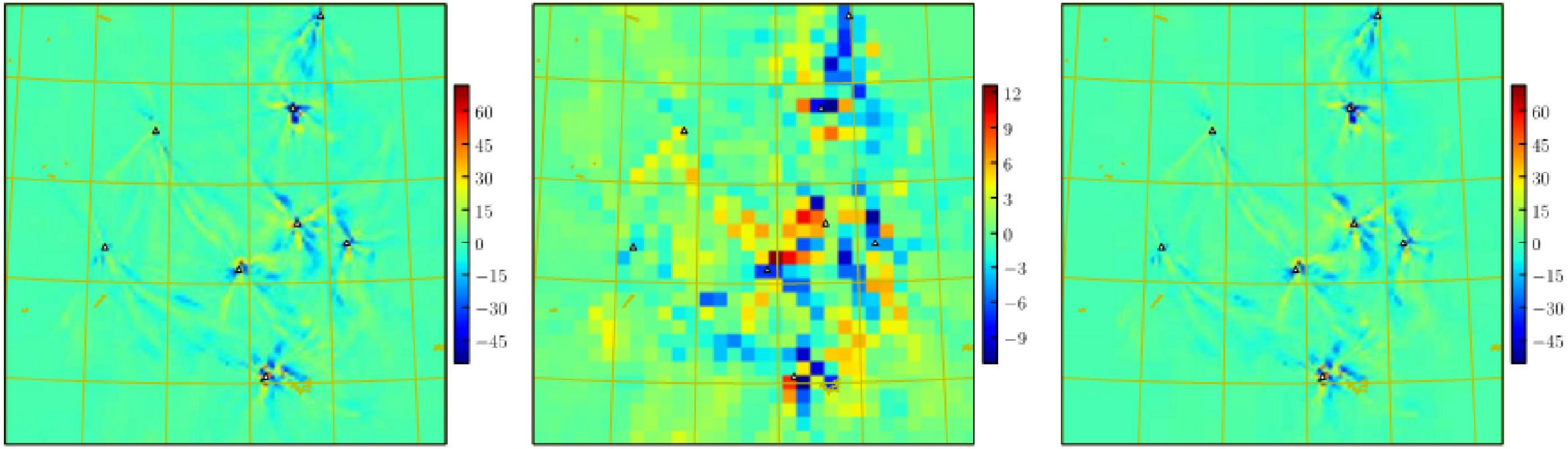

(a) BD-R3-N1024


(b) B50-R3-N1024

# Inversion on regular and optimal representations: diagonal B

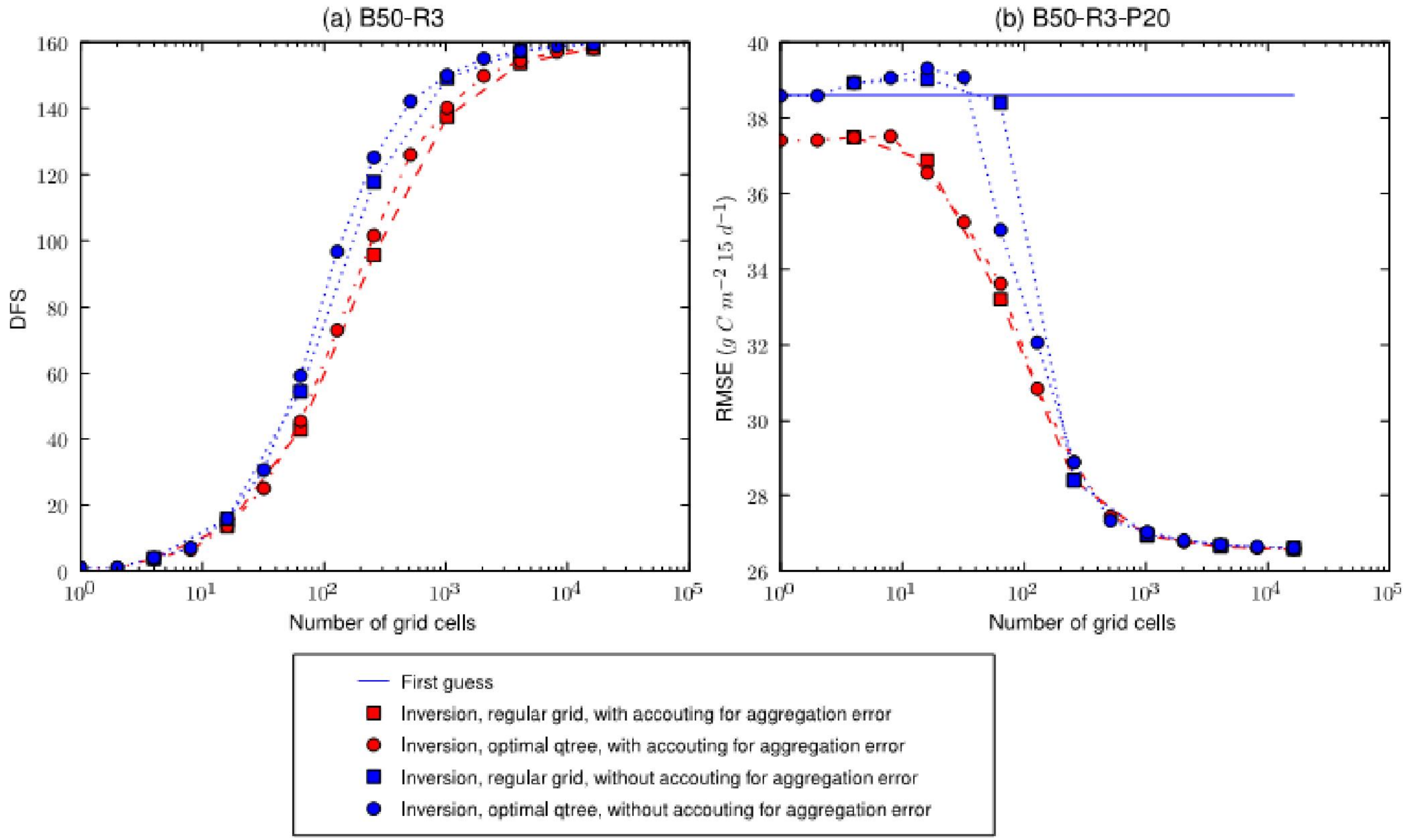


# Performance of optimal grid for diagonal B

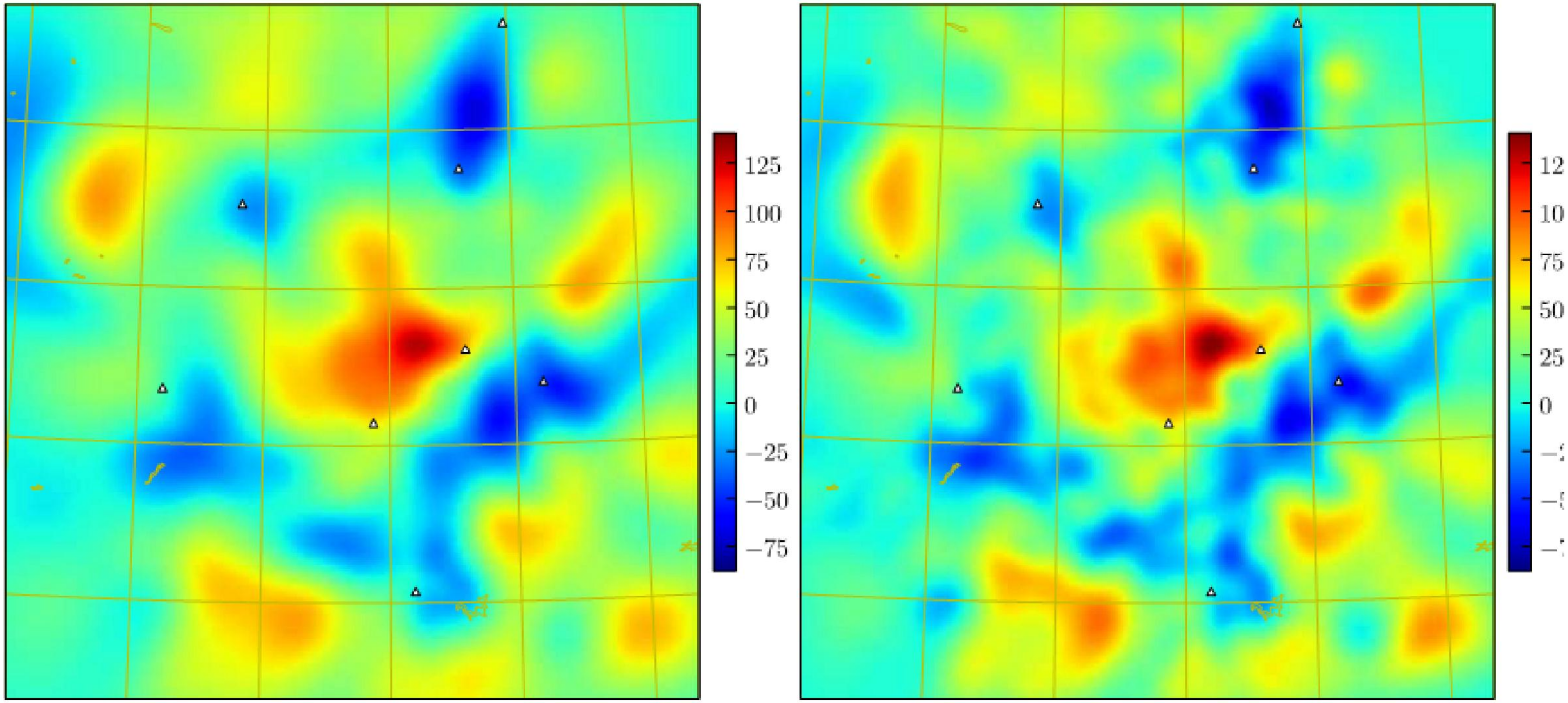



(a) BD-R3-PD, CORR (finest grid) (b) BD-R3-PD, CORR (regular grid) (c) BD-R3-PD, CORR (optimal grid)

# Inversion on regular and optimal representations: correlated B



# Irrealistic correlation length for Balgovind B

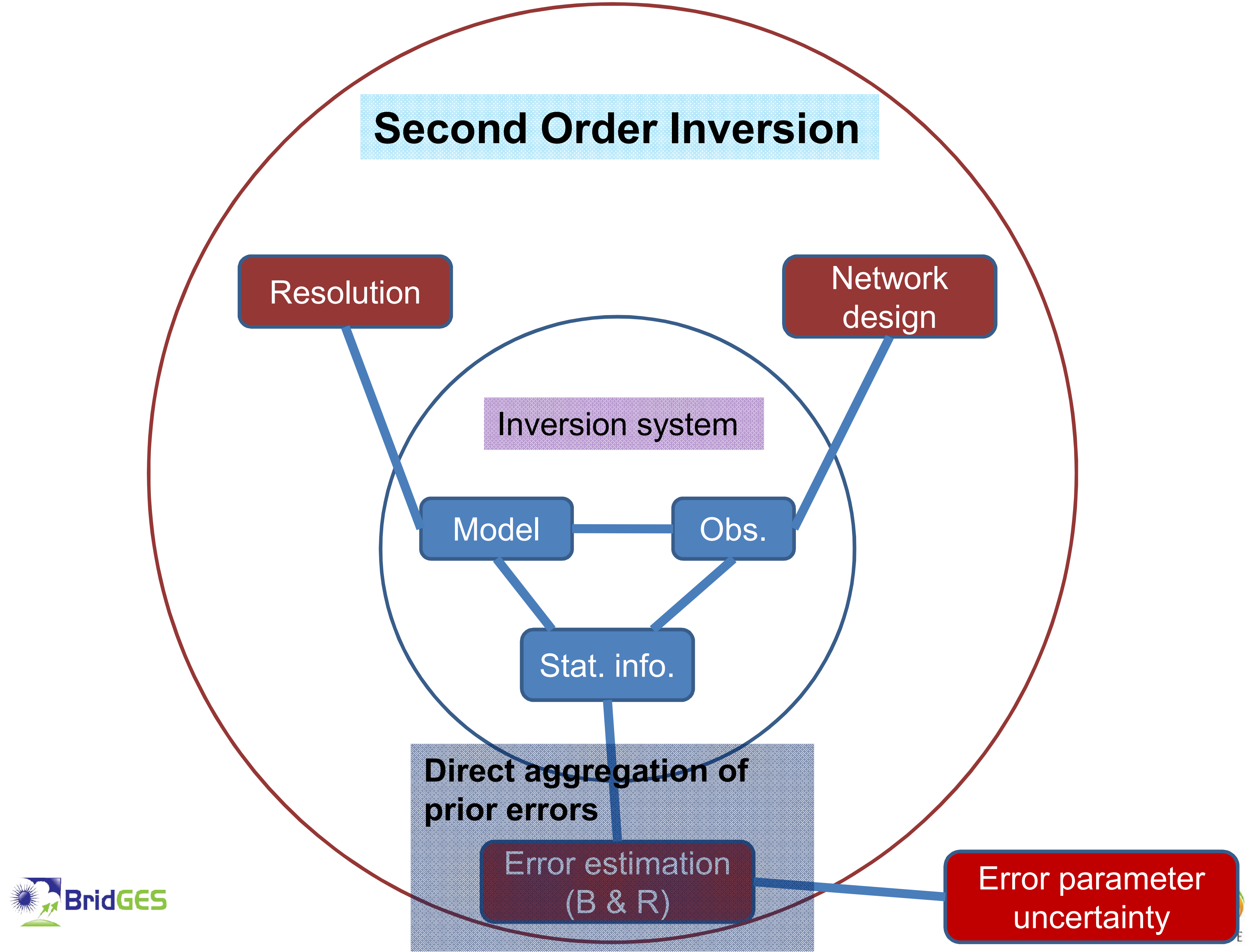



(a) B50-R3-P50, CORR (finest grid)

(b) B20-R3-P50, CORR (finest grid)

## Summary on mutiscale inversion & aggregation error

- A typical second order inversion problem
  - Critereia: e.g. DFS
  - Model configuration: resolution
- An ideal case: model-error-free + finest resolution available
- Explicit aggregation error + information flow map
- Maximizing Fisher criteria = minimizing aggregation error
- Future directions: model error and trade-off between aggregation and estimation error



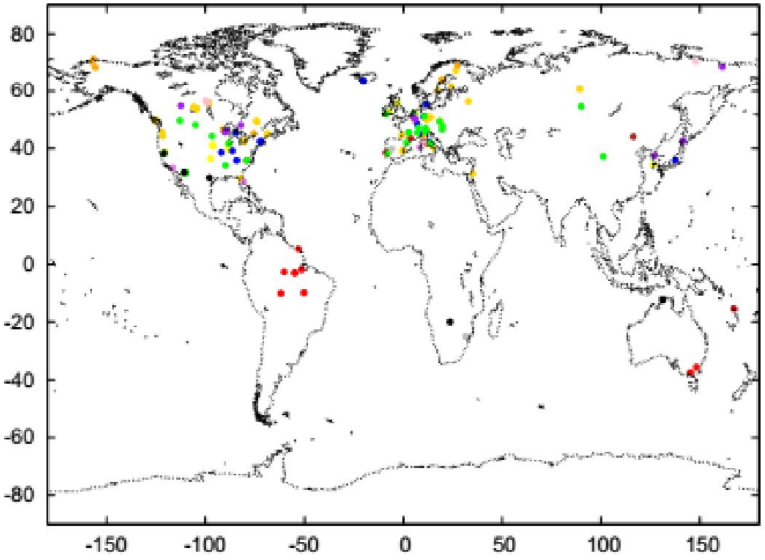
Second Order Inversion
Resolution
Network design
Inversion system
Model
Obs.
Stat. info.
Direct aggregation of prior errors
Error estimation (B & R)
Error parameter uncertainty
BridGES

# Structure of the prior CO2 flux errors

Chevallier et al 2012

Use daily-mean eddy-covariance flux measurements to assign the error statistics of the prior fluxes (Chevallier et al., 2012)

$i$-th day, $1 < i < T_d$, $T_d = 365$
$j$-th year, $1 < j < T_y$, $T_y = 17$
$s$-th site, $1 < s < N$, $N = 156$




Data courtesy from the FLUXNET PIs as part of a La Thuile project. 1991~2007, 156 sites

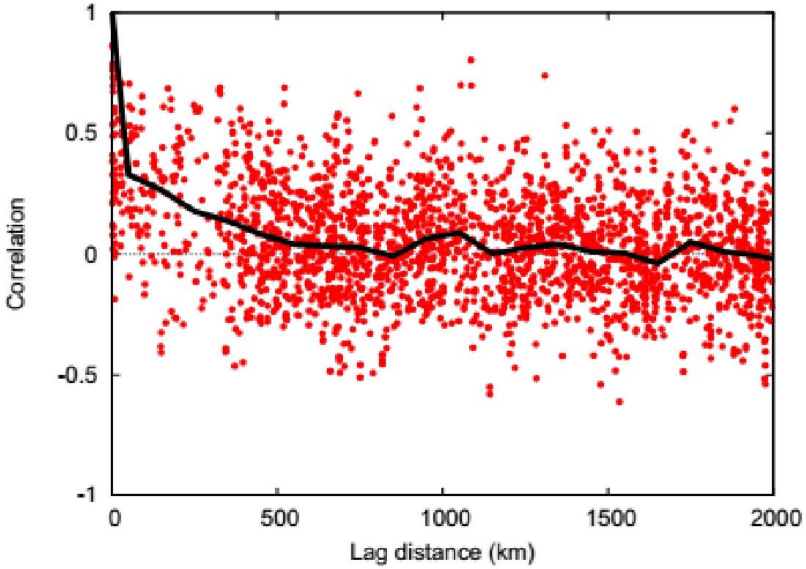
- FLUXNET Observations $[y^s_{i,j}]_{i,j,s}$;
- ORCHIDEE (a process-based terrestrial ecosystem model) simulations $[x^s_{i,j}]_{i,j,s}$.

**Statistics**

- Model-minus-observations
- Observation variability

# Structure of the prior $CO_2$ flux errors

Chevallier et al 2012




Small spatial correlations.

For a given day $i$, for all site pairs, Pearson correlation

$$r_i(s_p, s_q) = \frac{\sum_{j=1}^{T_y} (d_{i,j}^{s_p} - \bar{d}_i^{s_p})(d_{i,j}^{s_q} - \bar{d}_i^{s_q})}{\sqrt{\sum_{j=1}^{T_y} (d_{i,j}^{s_p} - \bar{d}_i^{s_p})^2} \sqrt{\sum_{j=1}^{T_y} (d_{i,j}^{s_q} - \bar{d}_i^{s_q})^2}}$$

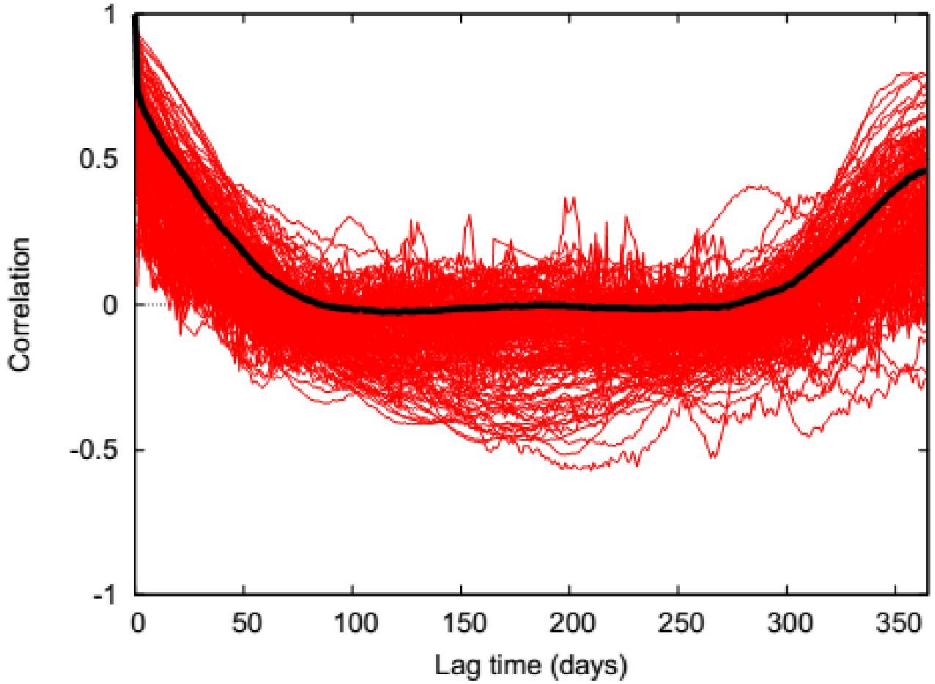
**Model-minus-observations**

$$d_{i,j}^{s} = y_{i,j}^{s} - x_{i,j}^{s}$$

- Short spatial correlation length of few hundred kilometers ($< 0.2$ after 200 km)
- Independent of plant functional types except for deciduous broad-leaved forests

# Structure of the prior CO2 flux errors

Chevallier et al 2012




Large temporal correlations.

For a given site $s$, for date lags in days, Pearson

$$\text{correlation } r_s(t_p, t_q) = \frac{\sum_{j=1}^{T_y} (d^s_{t_p,j} - \bar{d}^s_{t_p})(d^s_{t_q,j} - \bar{d}^s_{t_q})}{\sqrt{\sum_{j=1}^{T_y} (d^s_{t_p,j} - \bar{d}^s_{t_p})^2} \sqrt{\sum_{j=1}^{T_y} (d^s_{t_q,j} - \bar{d}^s_{t_q})^2}}$$

**Model-minus-observations**

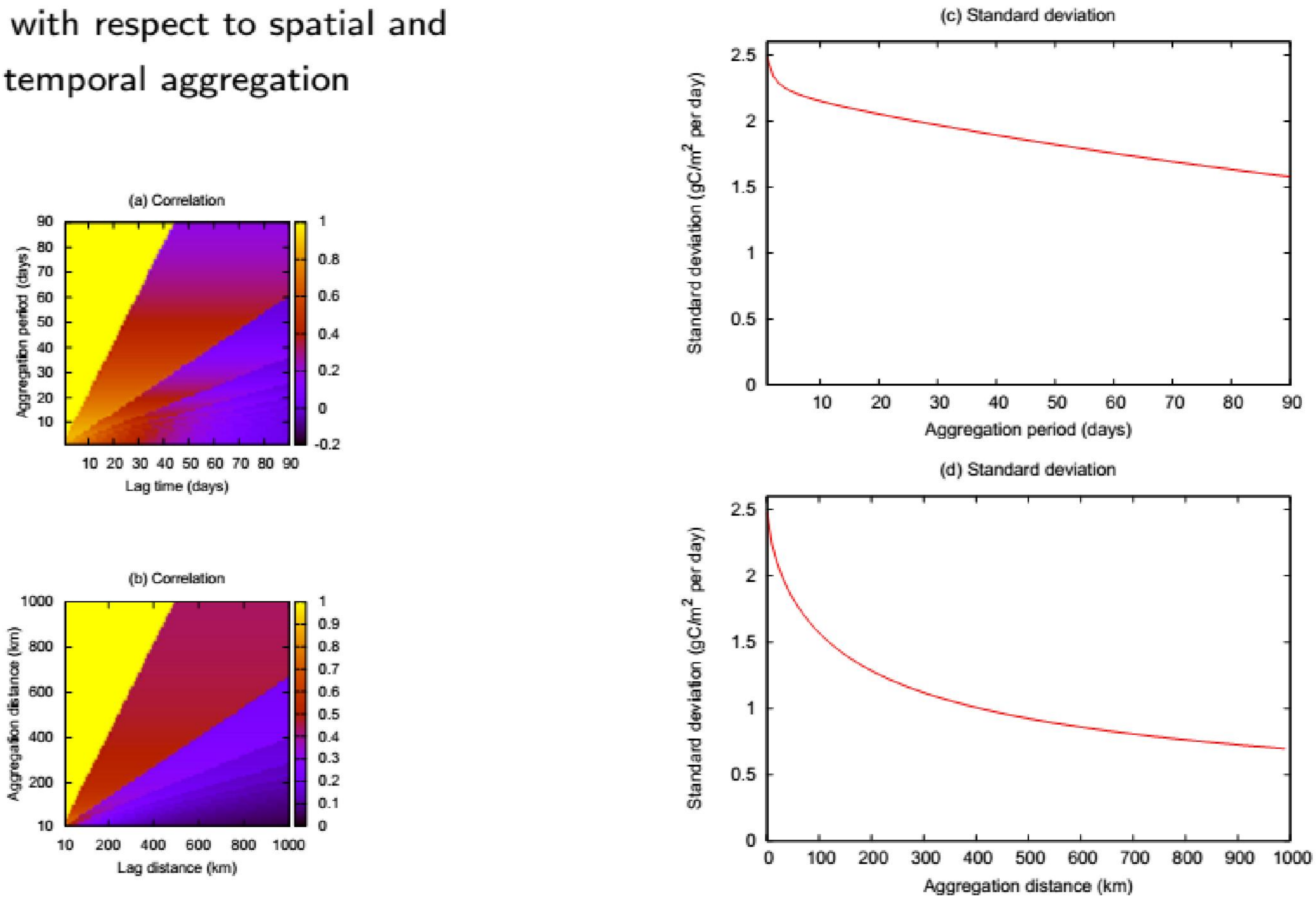
$$d^s_{i,j} = y^s_{i,j} - x^s_{i,j}$$

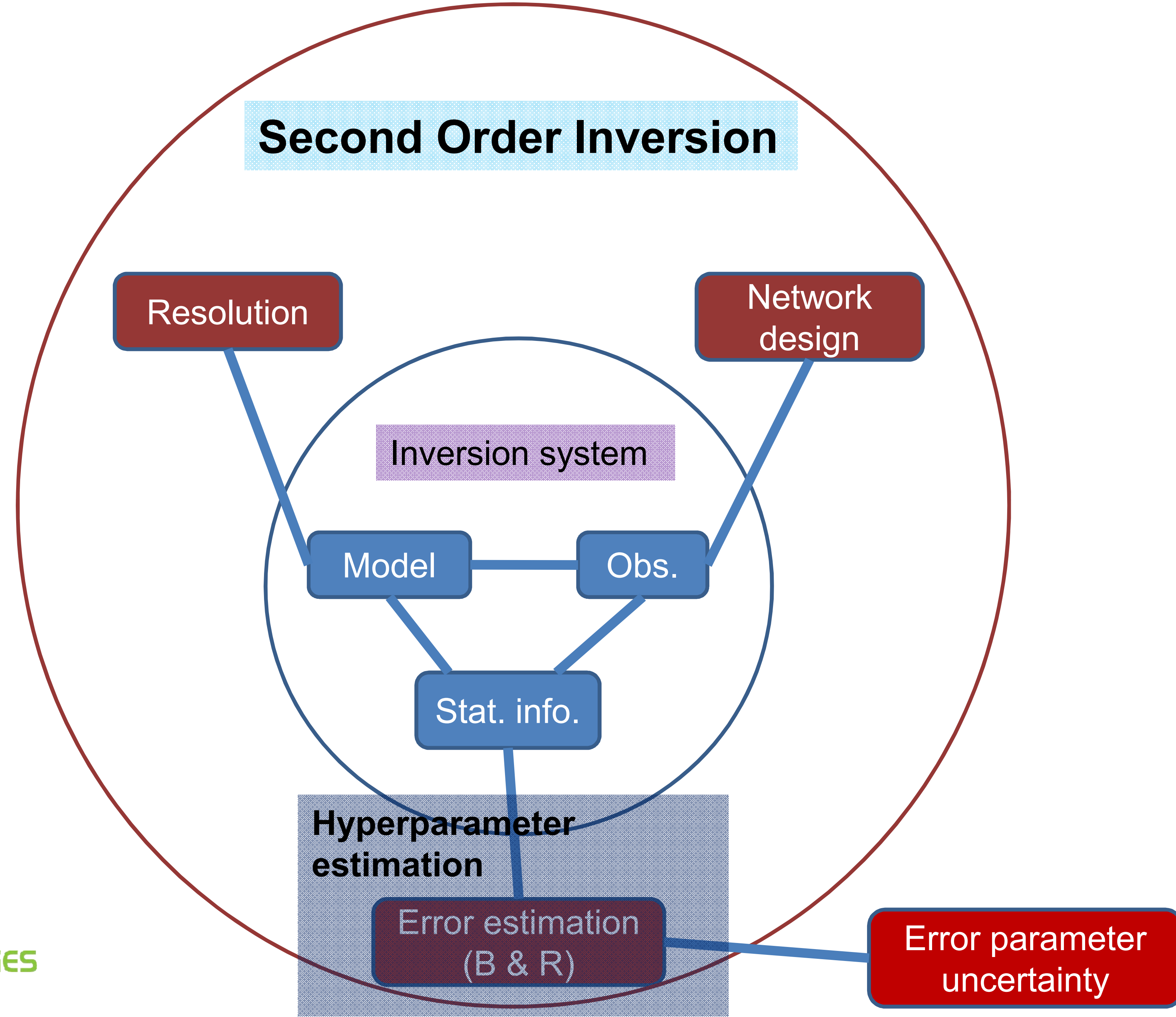
- Large temporal correlation length (positive for lags $< 85$ days and for lags $> 274$ days)
- Reflects systematic errors over weeks

# Direct aggregation of prior errors

Variations of the statistics of the prior errors with respect to spatial and temporal aggregation

Chevallier et al 2012




Second Order Inversion
Resolution
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Model
Obs.
Stat. info.
Hyperparameter estimation
Error estimation (B & R)
Error parameter uncertainty

BridGES

# Uncertainty quantification: hyper-parameter estimation (1/2)

$$C(h) = \kappa^2(1+\frac{h}{L})\exp(-\frac{h}{L})$$

- Hyper-parameters vector $\boldsymbol{\theta} = [\kappa^o, \kappa^b, L]^{\mathrm{T}})$
- Innovation vector $\mathbf{d} = \mu - \mathbf{H}\sigma^b$
- Innovation error covariance matrix $\mathbf{D}_{\boldsymbol{\theta}} = \mathbf{R}_{\boldsymbol{\theta}} + \mathbf{H}\mathbf{B}_{\boldsymbol{\theta}}\mathbf{H}^{\mathrm{T}}$

▶ Likelihood

$$p(\mu|\boldsymbol{\theta}) = \frac{\exp\left(-\frac{1}{2}(\mu - \mathbf{H}\sigma^b)^{\mathrm{T}}\mathbf{D}_{\boldsymbol{\theta}}^{-1}(\mu - \mathbf{H}\sigma^b)\right)}{(2\pi)^{\frac{d}{2}}|\mathbf{D}_{\boldsymbol{\theta}}|^{\frac{1}{2}}}$$

- Maximum likelihood estimation (MLE): minimizing negative log-likelihood

$$\mathscr{L}(\boldsymbol{\theta}) = \frac{1}{2}\ln|\mathbf{D}_{\boldsymbol{\theta}}| + \frac{1}{2}(\mu - \mathbf{H}\sigma^b)^{\mathrm{T}}\mathbf{D}_{\boldsymbol{\theta}}^{-1}(\mu - \mathbf{H}\sigma^b)$$

- Desroziers Scheme: given $L$, solve MLE iteratively for $[\kappa^o, \kappa^b]^{\mathrm{T}}$

# Uncertainty quantification: hyper-parameter estimation (2/2)

- $\chi^2$: Gaussian assumptions lead to $\chi^2$ probability density with number of degrees of freedom equal to the number of observations $d$:

$$\chi^2(\sigma^a) = (\mu - \mathbf{H}\sigma^a)^{\mathrm{T}}\mathbf{R}_{\boldsymbol{\theta}}^{-1}(\mu - \mathbf{H}\sigma^a) + (\sigma^a - \sigma^b)^{\mathrm{T}}\mathbf{B}_{\boldsymbol{\theta}}^{-1}(\sigma^a - \sigma^b)$$

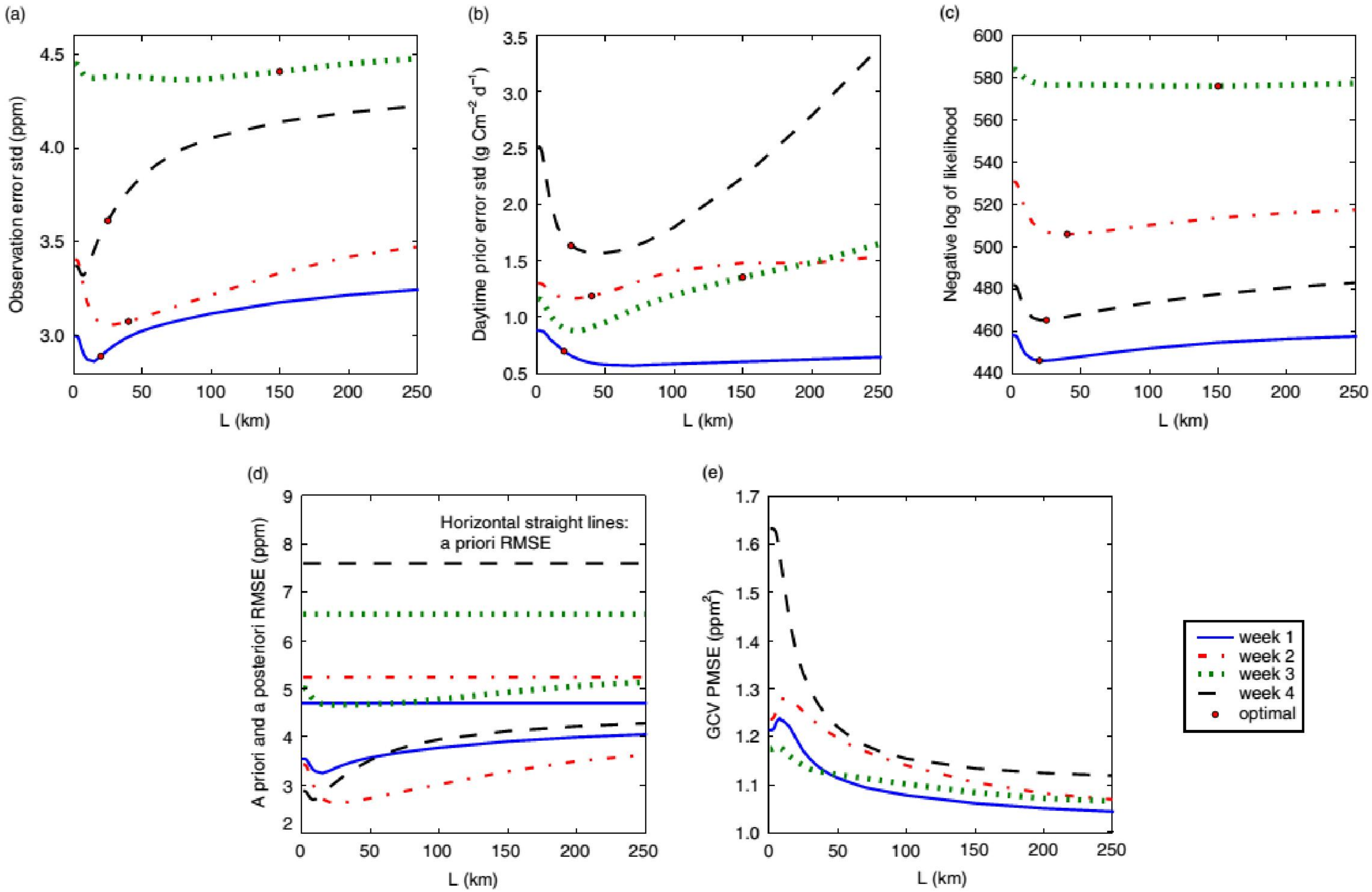
- Information propagation:

$$\mathrm{DFS} = \mathrm{Tr}\left(\mathbf{B}_{\boldsymbol{\theta}}\mathbf{H}^{\mathrm{T}}\mathbf{D}_{\boldsymbol{\theta}}^{-1}\mathbf{H}\right).$$

- General Cross Validation (GCV) minimizes the predictive mean-square error (PMSE) formulated in $\mathbf{R}^{-1}$-norm:

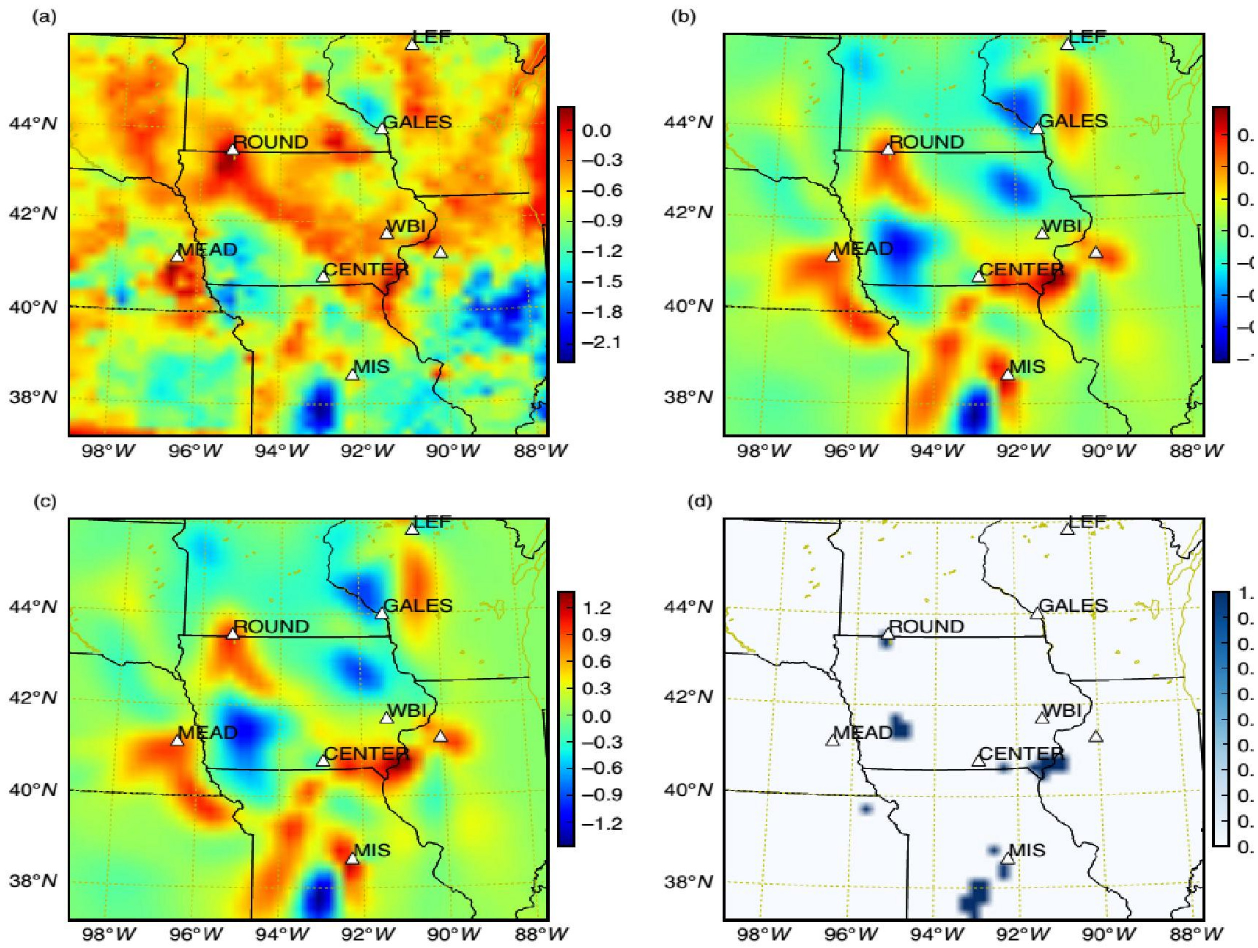
$$P(\boldsymbol{\theta}) = \frac{1}{d}\|\mathbf{H}\left(\sigma^t - \sigma^a\right)\|_{\mathbf{R}^{-1}}^2$$

# Results

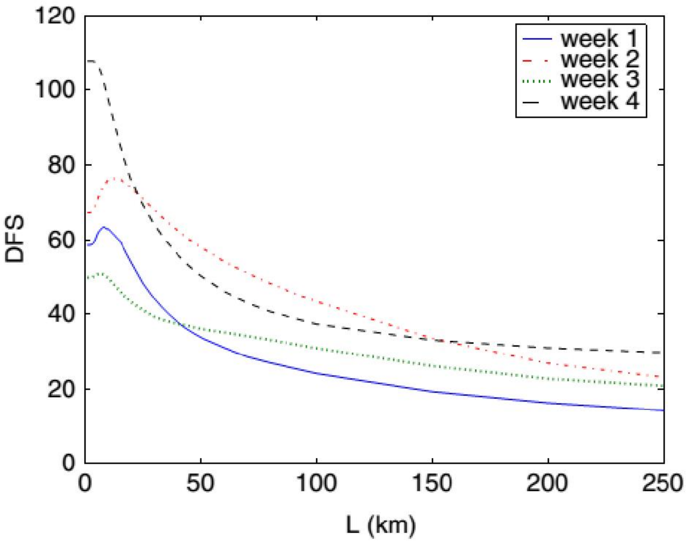


(a)
Observation error std (ppm)
L (km)
(b)
Daytime prior error std (g Cm$^{-2}$ d$^{-1}$)
L (km)
(c)
Negative log of likelihood
L (km)
(d)
Horizontal straight lines:
a priori RMSE
A priori and a posteriori RMSE (ppm)
L (km)
(e)
GCV PMSE (ppm$^2$)
L (km)
week 1
week 2
week 3
week 4
optimal

# Results



(a)
(b)
(c)
(d)
LEF
GALES
ROUND
WBI
MEAD
CENTER
MIS
44°N
42°N
40°N
38°N
98°W
96°W
94°W
92°W
90°W
88°W
0.0
−0.3
−0.6
−0.9
−1.2
−1.5
−1.8
−2.1
1.2
0.9
0.6
0.3
0.0
−0.3
−0.6
−0.9
−1.2




## Uncertainties for hyperparameter estimations

| | $\sigma_o$ | Daytime $\sigma_b$ | $\sigma_b L$ |
|---|---|---|---|
| Week 1 | $2.89 \pm 0.149$ | $3.21 \pm 1.13$ | $20 \pm 6.77$ |
| Week 2 | $3.08 \pm 0.181$ | $5.45 \pm 1.99$ | $40 \pm 13.6$ |
| Week 3 | – | – | – |
| Week 4 | $3.62 \pm 0.241$ | $7.51 \pm 3.48$ | $25 \pm 7.90$ |

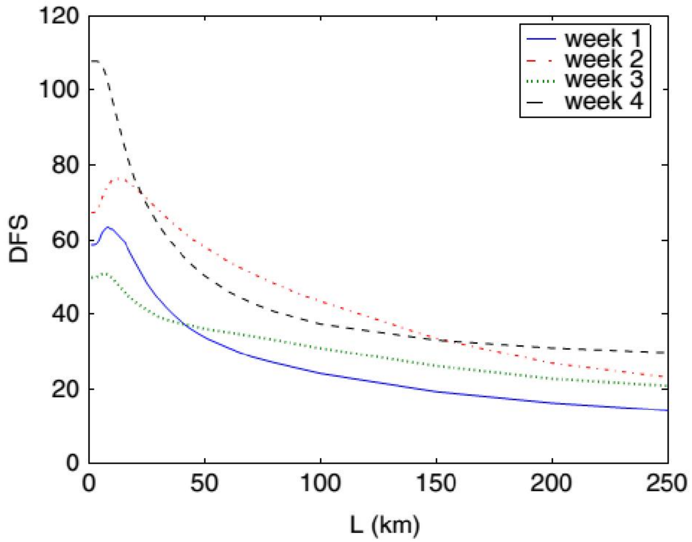
$$\mathcal{H}_{ij}(\boldsymbol{\theta}) = \frac{\partial^2 \mathcal{L}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}_i \partial \boldsymbol{\theta}_j}. \qquad \mathcal{H}(\boldsymbol{\theta}^*)^{-1}.$$

## Summary

Evaluates diiverse criteria: MLE, $\chi^2$, GCV using real data

Short correlation length: summer time mostly 15 -80 km, occasionally 100 km; confirms the results obtained by direct aggregation of background errors.

When atmospheric transport error is significant, difficult to identify a meaningful optimal L

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$$\mathcal{H}_{ij}(\boldsymbol{\theta}) = \frac{\partial^2 \mathcal{L}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}_i \partial \boldsymbol{\theta}_j}. \qquad \mathcal{H}(\boldsymbol{\theta}^*)^{-1}.$$

- **Why DFS is not a proper criterion for hyperparameter estimation?**
- **Why DFS decreases with respect to correlation length?**

# Few words

**Inversion as a system**: three components: model, obs, stat information,
Optimal control theory, success of variational methods (4DVar)
Other system concepts, e.g. observability?

**Inversion as an information machine**: information fusion and flow
relative entropy, entropy dynamics, maximum entropy principle

**Second order inversion**: optimal configuration of inversion system
& **Uncertainty quantification:**
Model resolution & aggregation error, error parameter estimation,

# References


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