Sensitivity Analysis in Variational Data Assimilation and Applications

DACIAN N. DAESCU

Dept. Mathematics & Statistics

Portland State University, Portland, Oregon, USA

Workshop on Diagnostics of data assimilation system performance

ECMWF, June 15-17, 2009

Outline

Goals:

1. Sensitivity to $\boldsymbol{\sigma}_b^2, \boldsymbol{\sigma}_o^2$ is feasible in data assimilation
2. A tool for DAS diagnosis and estimation of $\boldsymbol{\sigma}_b^2, \boldsymbol{\sigma}_o^2$

Elements:

1. Sensitivity equations of VDA: $[\mathbf{x}_b, \boldsymbol{\sigma}_b^2]$, $[\mathbf{y}, \boldsymbol{\sigma}_o^2]$
2. Estimation of DAS input parameters
3. Adjoint-based observation impact estimation
4. Illustrative numerical experiments
   - Diagnosis using error-variance sensitivity
   - Estimation of input error-variances

Sensitivity analysis: $\delta e = e(\mathbf{u}+\delta\mathbf{u}) - e(\mathbf{u}) \approx \nabla_{\mathbf{u}} e(\mathbf{u}) \cdot \delta\mathbf{u}$

1. **Model sensitivity:** Estimate the variations in the model output due to the variations in the model input

   - Model: $\mathbf{x}^f = \mathcal{M}(\mathbf{x})$
   - Forecast aspect: $e(\mathbf{x}) = (\mathbf{x}^f - \mathbf{x}^v)^{\mathrm{T}}\mathbf{C}(\mathbf{x}^f - \mathbf{x}^v)$
   - Sensitivity: $\nabla_{\mathbf{x}} e(\mathbf{x}) = 2\mathbf{M}^{\mathrm{T}}(\mathbf{x})\mathbf{C}(\mathbf{x}^f - \mathbf{x}^v)$

2. **DAS sensitivity:** Estimate the variations in the model output due to the variations in the DAS input

$$
\begin{aligned}
J(\mathbf{x}) &= \frac{1}{2}(\mathbf{x}-\mathbf{x}_b)^{\mathrm{T}}\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b) + \frac{1}{2}\left[\mathbf{h}(\mathbf{x})-\mathbf{y}\right]^{\mathrm{T}}\mathbf{R}^{-1}\left[\mathbf{h}(\mathbf{x})-\mathbf{y}\right] \\
\mathbf{x}_a &= \text{Arg } \min J \\
\mathbf{x}_a &= \mathbf{x}_a(\mathbf{u}), \qquad \mathbf{u} = [\mathbf{x}_b, \mathbf{B}, \mathbf{y}, \mathbf{R}]
\end{aligned}
$$

Sensitivity: $\nabla_{\mathbf{u}} e(\mathbf{x}_a) = \nabla_{\mathbf{u}}\mathbf{x}_a \nabla_{\mathbf{x}} e(\mathbf{x}_a)$

Sensitivity to parameters and impact estimates

- Derived from the first-order optimality conditions

$$\min_{\mathbf{x}} J(\mathbf{x}, \mathbf{u}) \Rightarrow \nabla_{\mathbf{x}} J(\mathbf{x}, \mathbf{u}) = \mathbf{0}$$

- Analysis sensitivity (implicit function theorem)

$$\nabla_{\mathbf{u}} \mathbf{x}(\mathbf{u}) = -\nabla^2_{\mathbf{ux}} J \left[\nabla^2_{\mathbf{xx}} J\right]^{-1}$$

- Sensitivity of a model functional output $e(\mathbf{x}(\mathbf{u}))$:

$$\nabla_{\mathbf{u}} e = \nabla_{\mathbf{u}} \mathbf{x} \nabla_{\mathbf{x}} e = -\nabla^2_{\mathbf{ux}} J \left[\nabla^2_{\mathbf{xx}} J\right]^{-1} \nabla_{\mathbf{x}} e$$

- Estimate the impact of variations in parameters:
  - first order accurate

$$\delta e \approx (\delta \mathbf{u})^T \nabla_{\mathbf{u}} e(\mathbf{x}(\mathbf{u}))$$

  - second order accurate

$$\delta e \approx (\delta \mathbf{u})^T \nabla_{\mathbf{u}} e(\mathbf{x}(\mathbf{u})) + \frac{1}{2} (\delta \mathbf{u})^T \nabla^2_{\mathbf{uu}} e(\mathbf{x}(\mathbf{u})) (\delta \mathbf{u})$$

Sensitivity analysis in VDA: implicit is easier

$$J = \frac{1}{2}\frac{(x - x_b)^2}{\sigma_b^2} + \frac{1}{2}\frac{(x - y)^2}{\sigma_o^2} \Rightarrow x_a = x_b + \frac{\sigma_o^{-2}}{\sigma_b^{-2} + \sigma_o^{-2}}(y - x_b)$$

Optimality condition:

$$\begin{aligned} J'(x_a) &= \sigma_b^{-2}(x_a - x_b) + \sigma_o^{-2}(x_a - y) = 0 \\ J''(x_a) &= \sigma_b^{-2} + \sigma_o^{-2} \end{aligned}$$

Implicit function theorem: $J'(x_a, u) = 0 \Rightarrow \frac{\partial x_a}{\partial u} = -\left[J''(x_a, u)\right]^{-1} J'_u(x_a, u)$

$$\frac{\partial x_a}{\partial y} = \frac{\sigma_o^{-2}}{\sigma_b^{-2} + \sigma_o^{-2}} \qquad \frac{\partial x_a}{\partial x_b} = \frac{\sigma_b^{-2}}{\sigma_b^{-2} + \sigma_o^{-2}}$$

$$\frac{\partial x_a}{\partial \sigma_o^{-2}} = \frac{(y - x_a)}{\sigma_b^{-2} + \sigma_o^{-2}} \qquad \frac{\partial x_a}{\partial \sigma_b^{-2}} = \frac{(x_b - x_a)}{\sigma_b^{-2} + \sigma_o^{-2}}$$

Sensitivity equations of VDA

Daescu, MWR 2008

$$\nabla_{\mathbf{x}} J(\mathbf{x}_a) = 0 \iff \mathbf{B}^{-1}(\mathbf{x}_a - \mathbf{x}_b) + \mathbf{H}^T\mathbf{R}^{-1}[\mathbf{h}(\mathbf{x}_a) - \mathbf{y}] = 0$$

DAS input	Sensitivity	Equation
Observations	$\nabla_{\mathbf{y}} e(\mathbf{x}_a)$	$\mathbf{R}^{-1}\mathbf{H}\mathbf{A}\nabla_{\mathbf{x}} e(\mathbf{x}_a)$
Obs. error variance	$\nabla_{\boldsymbol{\sigma}_o^2} e(\mathbf{x}_a)$	$\{\mathbf{R}^{-1}[\mathbf{h}(\mathbf{x}_a) - \mathbf{y}]\} \odot \nabla_{\mathbf{y}} e(\mathbf{x}_a)$
Background	$\nabla_{\mathbf{x}_b} e(\mathbf{x}_a)$	$\mathbf{B}^{-1}\mathbf{A}\nabla_{\mathbf{x}} e(\mathbf{x}_a)$
Back. error variance	$\nabla_{\boldsymbol{\sigma}_b^2} e(\mathbf{x}_a)$	$[\mathbf{B}^{-1}(\mathbf{x}_a - \mathbf{x}_b)] \odot \nabla_{\mathbf{x}_b} e(\mathbf{x}_a)$

In particular, if $\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}[\mathbf{y} - \mathbf{H}\mathbf{x}_b]$ then

$$\nabla_{\mathbf{y}} e(\mathbf{x}_a) = \mathbf{K}^T\nabla_{\mathbf{x}} e(\mathbf{x}_a), \quad \nabla_{\mathbf{x}_b} e(\mathbf{x}_a) = \left[\mathbf{I} - \mathbf{H}^T\mathbf{K}^T\right] \nabla_{\mathbf{x}} e(\mathbf{x}_a)$$

Sensitivity equations of VDA

DAS input	Sensitivity	Equation
Observations	$\nabla_{\mathbf{y}} e(\mathbf{x}_a)$	$\mathbf{R}^{-1}\mathbf{H}\mathbf{A}\nabla_{\mathbf{x}} e(\mathbf{x}_a)$
Obs. error variance	$\nabla_{\boldsymbol{\sigma}_o^2} e(\mathbf{x}_a)$	$\{\mathbf{R}^{-1}[\mathbf{h}(\mathbf{x}_a) - \mathbf{y}]\} \odot \nabla_{\mathbf{y}} e(\mathbf{x}_a)$
Background	$\nabla_{\mathbf{x}_b} e(\mathbf{x}_a)$	$\mathbf{B}^{-1}\mathbf{A}\nabla_{\mathbf{x}} e(\mathbf{x}_a)$
Back. error variance	$\nabla_{\boldsymbol{\sigma}_b^2} e(\mathbf{x}_a)$	$\{\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}[\mathbf{y} - \mathbf{h}(\mathbf{x}_a)]\} \odot \nabla_{\mathbf{x}_b} e(\mathbf{x}_a)$

Insight: If $\mathbf{H} = \mathbf{I}$ and $\mathbf{B}$ and $\mathbf{R}$ are diagonal then

$$\nabla_{\boldsymbol{\sigma}_o^2} e(\mathbf{x}_a) \odot \nabla_{\boldsymbol{\sigma}_b^2} e(\mathbf{x}_a) \leq \mathbf{0}$$

Tuning $\neq$ Estimation

Parameter estimation

Data assimilation

$$\min_{\mathbf{x}} J(\mathbf{x},\mathbf{u}) \Rightarrow \nabla_{\mathbf{x}} J(\mathbf{x},\mathbf{u}) = \mathbf{0} \Rightarrow \mathbf{x} = \mathbf{x}(\mathbf{u})$$

Optimal parameter estimate

$$\min_{\mathbf{u}} e[\mathbf{x}(\mathbf{u})] \Rightarrow \nabla_{\mathbf{u}} e[\mathbf{x}(\mathbf{u})] = \mathbf{0}$$

$$\mathbf{u}_\star = \text{Arg } \min e$$

The steepest descent direction $-\nabla_{\mathbf{u}} e[\mathbf{x}(\mathbf{u})]$ *identifies the direction where small variations in the specification of the DAS input parameters, from the current DAS configuration, will be of largest forecast benefit*.

Parameter estimation requires:

1. an objective forecast error measure
2. statistical significance
3. a complete description of the DAS input parameters

High-order adjoint-DAS OBSI measures

Daescu and Todling, MWR 2009

1. Fundamental Theorem of Line Integrals (continuation framework)

$$\delta e = e(\mathbf{x}_a) - e(\mathbf{x}_b) = \int_{[\mathbf{x}_b,\, \mathbf{x}_a]} \nabla_{\mathbf{x}} e(\mathbf{x}) \cdot d\,\mathbf{x} \;\; \underset{\uparrow}{=} \;\; \int_0^1 (\delta \mathbf{x}_a)^{\mathrm{T}} \nabla_{\mathbf{x}} e(\mathbf{x}_s)\, ds$$

$$\mathbf{x} = \mathbf{x}_b + s\delta\mathbf{x}_a, \quad d\,\mathbf{x} = \delta\mathbf{x}_a\, ds$$

2. Approximation by numerical integration schemes
   - Trapezoidal rule:

$$\delta e_2^{a,b} = \frac{1}{2}(\delta\mathbf{x}_a)^{\mathrm{T}} \left[\nabla_{\mathbf{x}} e(\mathbf{x}_b) + \nabla_{\mathbf{x}} e(\mathbf{x}_a)\right] = (\delta\mathbf{y})^{\mathrm{T}} \frac{1}{2} \mathbf{K}^{\mathrm{T}} \left[\nabla_{\mathbf{x}} e(\mathbf{x}_b) + \nabla_{\mathbf{x}} e(\mathbf{x}_a)\right]$$

   - Midpoint rule:

$$\delta e_2^{(a+b)/2} = (\delta\mathbf{x}_a)^{\mathrm{T}} \nabla_{\mathbf{x}} e(\mathbf{x}_{(a+b)/2}) = (\delta\mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}} e(\mathbf{x}_{(a+b)/2})$$

   - Simpson's rule:

$$\delta e_4^{a,b,(a+b)/2} = (\delta\mathbf{y})^{\mathrm{T}} \frac{1}{6} \mathbf{K}^{\mathrm{T}} \left[\nabla_{\mathbf{x}} e(\mathbf{x}_b) + 4\nabla_{\mathbf{x}} e(\mathbf{x}_{(a+b)/2}) + \nabla_{\mathbf{x}} e(\mathbf{x}_a)\right]$$

Illustrative numerical results: Lorenz 40-variable model

Lorenz and Emanuel, JAS 1998

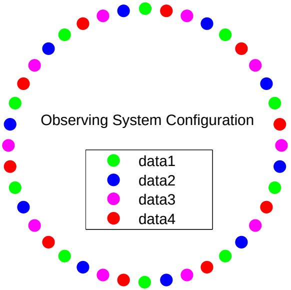
$$\frac{\mathrm{d}x_j}{\mathrm{d}\,t} = (x_{j+1} - x_{j-2})x_{j-1} - x_j + F$$

$$\mathbf{x}_a(t_i) = \mathbf{x}_b(t_i) + \mathbf{K}(t_i)[\mathbf{y}(t_i) - \mathbf{h}(\mathbf{x}_b(t_i))]$$

$$\mathbf{A}(t_i) = [\mathbf{I} - \mathbf{K}(t_i)\mathbf{H}(t_i)]\mathbf{B}(t_i)$$

$$\mathbf{x}_b(t_{i+1}) = \mathcal{M}_{t_i \to t_{i+1}}(\mathbf{x}_a(t_i))$$

$$\mathbf{B}(t_{i+1}) = \mathbf{M}_{t_i \to t_{i+1}}\mathbf{A}(t_i)\mathbf{M}^{\mathrm{T}}_{t_i \to t_{i+1}} + \mathbf{Q}(t_i)$$

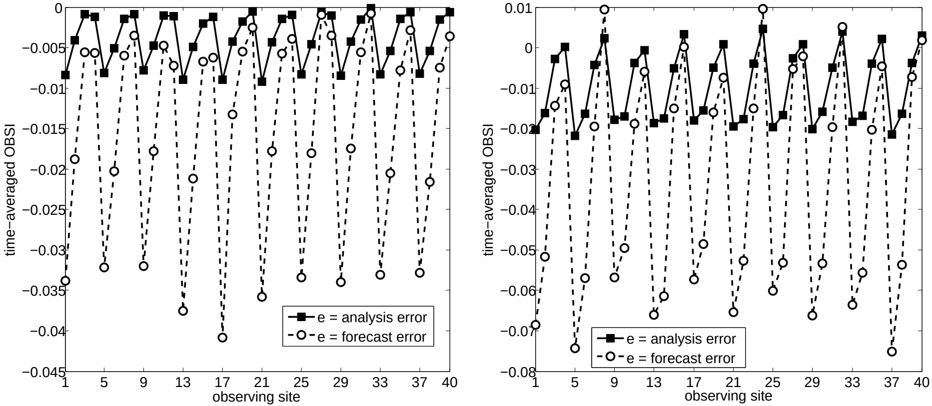


$$\Delta t = 0.05, F = 8, F^f = 7.6, t_v = t_0 + 4\Delta t, 2880 \text{ DAS cycles}$$

$$\sigma_o^{(1)} = 0.1, \quad \sigma_o^{(2)} = 0.2, \quad \sigma_o^{(3)} = 0.6, \quad \sigma_o^{(4)} = 0.8, \sigma_q = 0.1$$

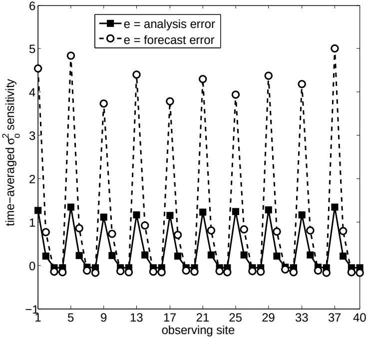
1. DAS-1: σ_o statistically consistent
2. DAS-2: $\sigma_o = 0.4$

Adjoint-based OBSI estimation: DAS-1 vs. DAS-2



1. OBSI - no direct information on how to best make use of data
2. The sensitivity to observation error variance is necessary

Sensitivity to observation error variance in DAS-2



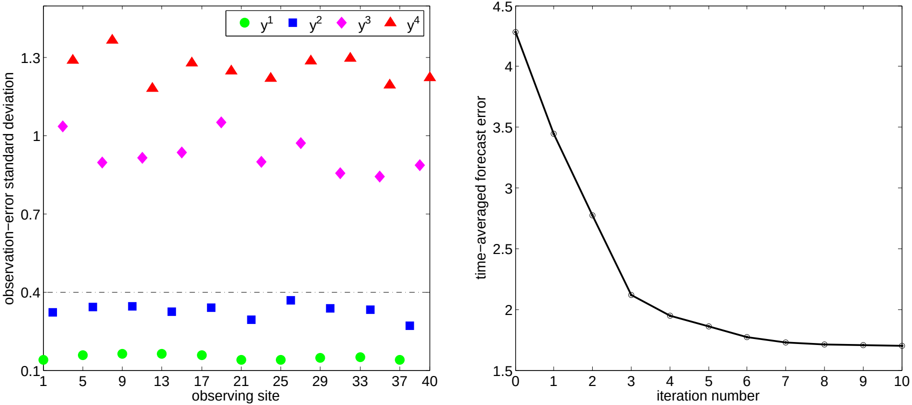
The steepest descent direction $-\nabla_{\boldsymbol{\sigma}_o^2} e(\mathbf{x}_a)$ identifies the direction where small variations in $\boldsymbol{\sigma}_o^2$, from the current DAS configuration, will be of largest analysis/forecast benefit.

Diagnosis:

1. $\boldsymbol{\sigma}_o^{(1)}, \boldsymbol{\sigma}_o^{(2)}$ are overestimated, large $\delta\boldsymbol{\sigma}_o^2$ impact
2. $\boldsymbol{\sigma}_o^{(3)}, \boldsymbol{\sigma}_o^{(4)}$ are underestimated, small $\delta\boldsymbol{\sigma}_o^2$ impact

Observation error variance estimation in DAS-2

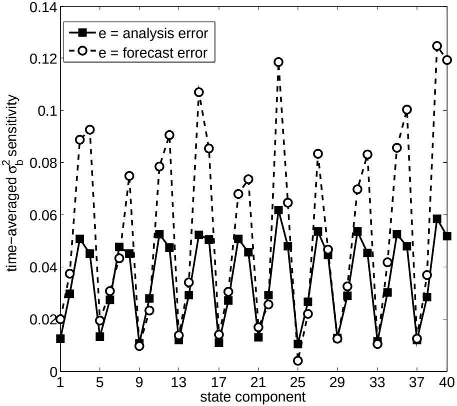
$$\min_{\boldsymbol{\sigma}_o^2} e(\mathbf{x}_a)$$

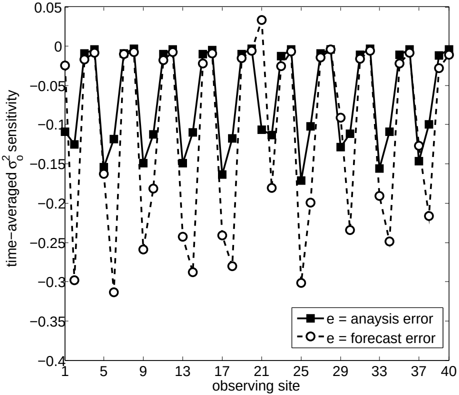


1. Accurate/improved estimation to high-impact data error variances
2. Overestimation to low-impact data error variances
3. Fast convergence (benefit from gradient information)

Sensitivity to input error variance in DAS-1

$$\nabla_{\boldsymbol{\sigma}_b^2} e(\mathbf{x}_a) \qquad\qquad \nabla_{\boldsymbol{\sigma}_o^2} e(\mathbf{x}_a)$$

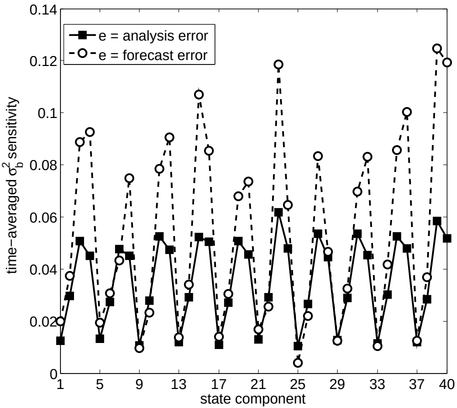


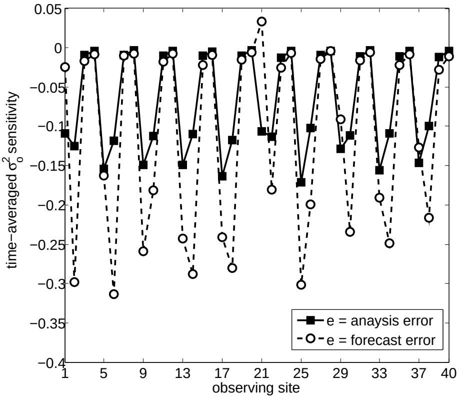


1. $\boldsymbol{\sigma}_o^2$ known to be statistically consistent to observation errors
2. **Diagnosis:**

Sensitivity to input error variance in DAS-1

$\nabla_{\sigma_b^2} e(\mathbf{x}_a)$ $\nabla_{\sigma_o^2} e(\mathbf{x}_a)$

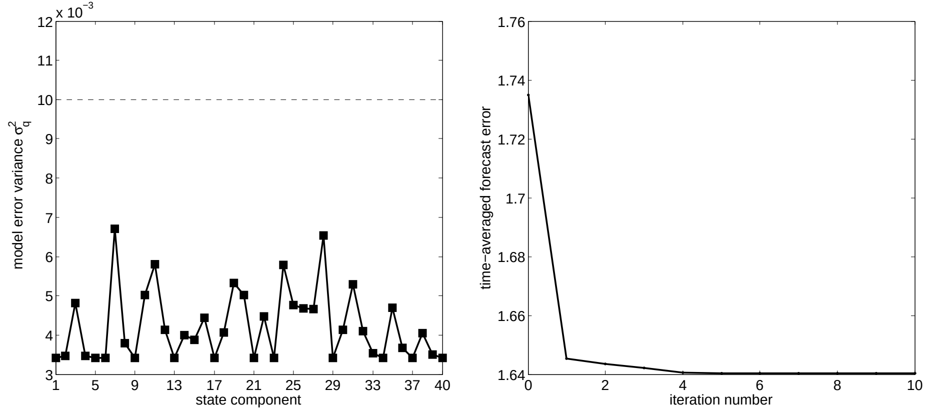




1. σ_o^2 known to be statistically consistent to observation errors
2. **Diagnosis:** σ_b^2 overestimated in DAS-1
3. **Solution:** improve σ_b^2 by estimating σ_q^2: $\nabla_{\sigma_q^2(t_i)} \sigma_b^2(t_{i+1}) = \mathbf{I}$

Model error variance estimation in DAS-1

$$\min_{\boldsymbol{\sigma}_q^2} e(\mathbf{x}_a)$$



1. Forecast error reduction of $\sim 5\%$
2. Fast convergence

Conclusions

1. Sensitivity to $\boldsymbol{\sigma}_b^2, \boldsymbol{\sigma}_o^2$ is feasible in data assimilation
2. Provides tools for DAS diagnosis and estimation of $\boldsymbol{\sigma}_b^2, \boldsymbol{\sigma}_o^2, \boldsymbol{\sigma}_q^2$
3. All the necessary tools are in place or are being developed
4. Need for objective forecast error measures
5. A proof of concept was presented