Adjoint Estimation to Observing System Experiments Outcomes

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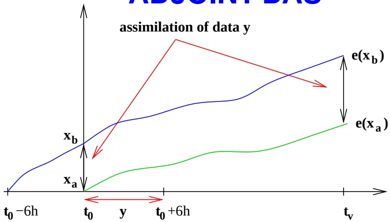
Outline

1. Problem formulation
   - The need for simplifying assumptions: 1-DA cycle OSEs
2. Sensitivity analysis in VDA: $[\mathbf{x}_b, \mathbf{B}]$, $[\mathbf{y}, \mathbf{R}]$
   - On the high-order ADJ-DAS OBSI measures
3. Adjoint estimation to 1-DA cycle OSEs
   - On the relevance of $\mathbf{y} - \mathbf{h}(\mathbf{x}_a)$ and $\mathbf{R}^{-1}$-sensitivity
4. Illustrative numerical experiments

Observation impact estimation: $e(\mathbf{x}) = \|\mathbf{x}^f - \mathbf{x}^v\|^2_{\mathbf{C}}$

ADJOINT-DAS



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

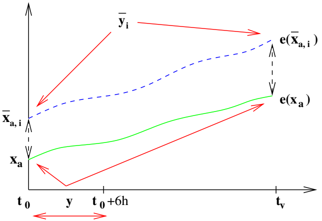
Observation impact (global)

$$\delta e = e(\mathbf{x}_a) - e(\mathbf{x}_b)$$

All-at-once OBSI estimation

$$\delta e \approx (\delta \mathbf{x}_a)^{\mathrm{T}} \mathbf{g} = \sum_i (\delta \mathbf{y}_i)^{\mathrm{T}} \left[\mathbf{K}^{\mathrm{T}} \mathbf{g}\right]_i$$

OSEs



Data denial $\bar{\mathbf{y}}_i = \mathbf{y} \setminus \{\mathbf{y}_i\}$

$$\bar{\mathbf{x}}_{a,i} = \bar{\mathbf{x}}_{b,i} + \bar{\mathbf{K}}_i[\bar{\mathbf{y}}_i - \bar{\mathbf{h}}_i(\bar{\mathbf{x}}_{b,i})]$$

$$\delta e(\mathbf{y}_i : \bar{\mathbf{y}}_i) = e(\mathbf{x}_a) - e(\bar{\mathbf{x}}_{a,i})$$

$$\boxed{\sum_i \delta e(\mathbf{y}_i : \bar{\mathbf{y}}_i) \neq \delta e}$$

Can ADJ-DAS techniques be used to estimate OSEs outcomes?

Adjoint estimation to OSEs outcomes

Problem formulation: For each data subset $\mathbf{y}_i$, a priori estimate

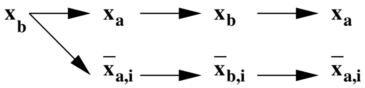
$$\delta e(\mathbf{y}_i : \bar{\mathbf{y}}_i) = e(\mathbf{x}_a) - e(\bar{\mathbf{x}}_{a,i})$$

Unresolved issues:

1. Estimation of data removal impact must rely on $\mathbf{x}_a$ only
2. Propagation of the background information in multi-cycles DA:

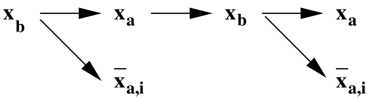
$$\boxed{\bar{\mathbf{x}}_{b,i} \neq \mathbf{x}_b, \quad \bar{\mathbf{B}}_i \neq \mathbf{B}}$$

MULTI–DA CYCLES OSEs



$$\bar{\mathbf{x}}_{a,i} = \bar{\mathbf{x}}_{b,i} + \bar{\mathbf{K}}_i[\bar{\mathbf{y}}_i - \bar{\mathbf{h}}_i(\bar{\mathbf{x}}_{b,i})]$$

SINGLE–DA CYCLE OSEs



$$\bar{\mathbf{x}}_{a,i} = \mathbf{x}_{b,i} + \bar{\mathbf{K}}_i[\bar{\mathbf{y}}_i - \bar{\mathbf{h}}_i(\mathbf{x}_{b,i})]$$

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

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

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	$\nabla_{\boldsymbol{\sigma}_b^2} e(\mathbf{x}_a)$	$[\mathbf{B}^{-1}(\mathbf{x}_a - \mathbf{x}_b)] \odot \nabla_{\mathbf{x}_b} e(\mathbf{x}_a)$

If the observation errors are uncorrelated:

$$\boxed{\boldsymbol{\sigma}_o^{-2} \odot \nabla_{\boldsymbol{\sigma}_o^{-2}} e(\mathbf{x}_a) = [\mathbf{y} - \mathbf{h}(\mathbf{x}_a)] \odot \nabla_{\mathbf{y}} e(\mathbf{x}_a)}$$

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

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

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:

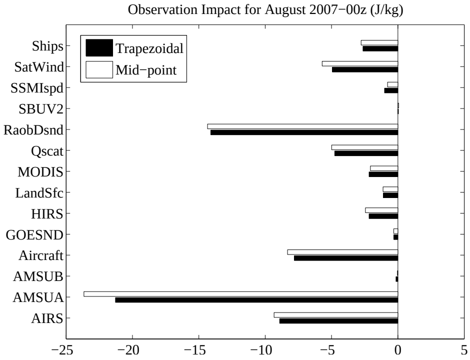
$$\delta e_2^{(a+b)/2} = (\delta\mathbf{x}_a)^{\mathrm{T}} \nabla_{\mathbf{x}} e(\mathbf{x}_{(a+b)/2}) = (\delta\mathbf{y})^{\mathrm{T}} \mathbf{K}^{\mathrm{T}} \nabla_{\mathbf{x}} e(\mathbf{x}_{(a+b)/2})$$

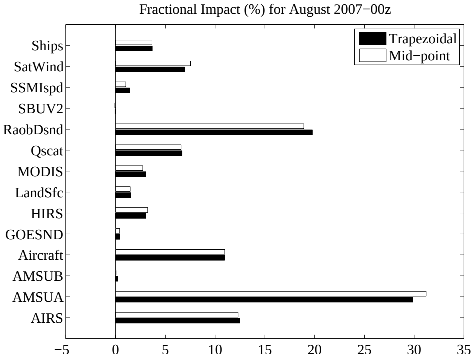
- Simpson's rule:

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

Adjoint-based estimation of the observation impact

GEOS-5 data impact on 24h forecast error valid for August 2007-00z
Daescu and Todling, MWR 2009





Modeling the data removal: 1-DA cycle OSEs

Control $$\sum_j \sigma_j^{-2}(x_a - y_j) = 0 \Rightarrow \frac{\partial x_a}{\partial \sigma_i^{-2}} = \frac{y_i - x_a}{\sum_j \sigma_j^{-2}}$$

Experiment $$\sum_{j\neq i} \sigma_j^{-2}(\bar{x}_{a,i} - y_j) = 0$$

y_i removal $$\begin{cases} \sum_{j\neq i} \sigma_j^{-2}[x_a(s) - y_j] + s\sigma_i^{-2}[x_a(s) - y_i] = 0 \\ x_a(1) = x_a,\ x_a(0) = \bar{x}_{a,i},\ x_a'(s) = \dfrac{\sigma_i^{-2}[y_i - x_a(s)]}{\sum_{j\neq i} \sigma_j^{-2} + s\sigma_i^{-2}} \end{cases}$$

Analysis impact: $\delta x_{a,i} = x_a(1) - x_a(0) \approx x_a'(1) = \sigma_i^{-2} \dfrac{\partial x_a}{\partial \sigma_i^{-2}}$

Forecast impact: $e(x_a) - e(\bar{x}_{a,i}) \approx (\delta x_{a,i}) e'(x_a) = \sigma_i^{-2} \dfrac{\partial x_a}{\partial \sigma_i^{-2}} e'(x_a)$

General formulation using a continuation approach

First order optimality condition and implicit differentiation

$$J_i(\mathbf{x}, s) = \bar{J}_i(\mathbf{x}) + sJ_i^o \Rightarrow \nabla \bar{J}_i(\mathbf{x}) + s\mathbf{H}_i^{\mathrm{T}}\mathbf{R}_i^{-1}[\mathbf{h}_i(\mathbf{x}) - \mathbf{y}_i] = 0$$

The value added by $\mathbf{y}_i$ to $\bar{\mathbf{y}}_i$ may be interpreted as the forecast impact due to a change in the DAS of the observation error inverse covariance from $\mathbf{0}$ to $\mathbf{R}_i^{-1}$

$$\nabla_{\mathbf{x}} J_i(\mathbf{x}, s) = \mathbf{0} \Rightarrow \nabla_s \mathbf{x}_a^{i,s} = [\mathbf{y}_i - \mathbf{h}_i(\mathbf{x}_a^{i,s})]^{\mathrm{T}}\mathbf{R}_i^{-1}\mathbf{H}_i \left[\nabla^2 J_i\right]^{-1}_{|(\mathbf{x}_a^{i,s}, s)}$$

Linearization around $s = 1$

$$\delta e(\mathbf{y}_i : \bar{\mathbf{y}}_i) = e(\mathbf{x}_a^{i,1}) - e(\mathbf{x}_a^{i,0}) \approx \nabla_s \mathbf{x}_a^{i,s} \nabla_{\mathbf{x}} e(\mathbf{x}_a^{i,s})\Big|_{s=1} = [\mathbf{y}_i - \mathbf{h}_i(\mathbf{x}_a)]^{\mathrm{T}} \nabla_{\mathbf{y}_i} e(\mathbf{x}_a)$$

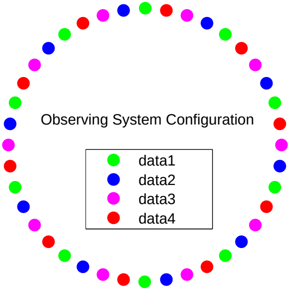
All-at-once f. o. a.: $\boxed{\delta e(\mathbf{y}_i : \bar{\mathbf{y}}_i) \approx [\mathbf{y}_i - \mathbf{h}_i(\mathbf{x}_a)]^{\mathrm{T}} \nabla_{\mathbf{y}_i} e(\mathbf{x}_a)}$

- Depends on the data set
- Depends on the specification of e

Experimental Setup: Lorenz 40-variable model

Lorenz and Emanuel, JAS 1998

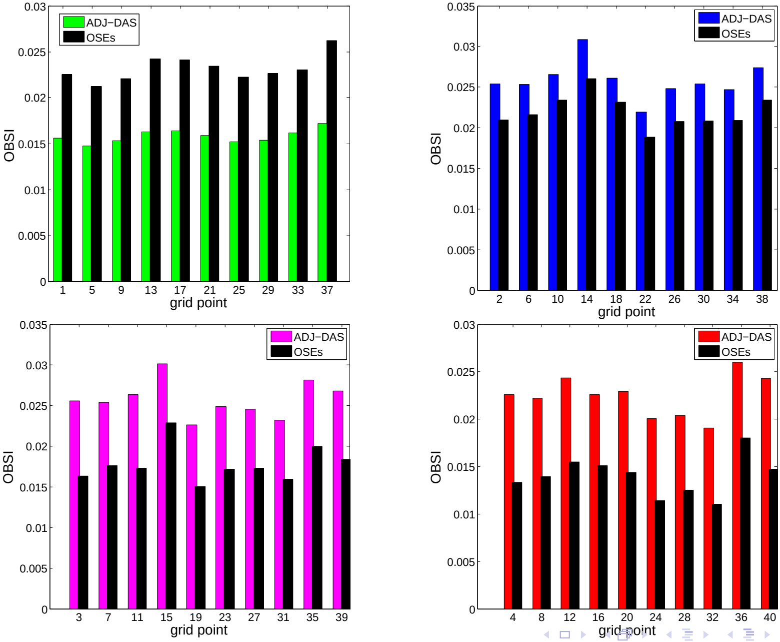
$$
\begin{aligned}
\frac{\mathrm{d}x_j}{\mathrm{d}\,t} &= (x_{j+1} - x_{j-2})x_{j-1} - x_j + F \\
\mathbf{x}_a(t_i) &= \mathbf{x}_b(t_i) + \mathbf{K}(t_i)[\mathbf{y}(t_i) - \mathbf{h}(\mathbf{x}_b(t_i))] \\
\mathbf{A}(t_i) &= [\mathbf{I} - \mathbf{K}(t_i)\mathbf{H}(t_i)]\mathbf{B}(t_i) \\
\mathbf{x}_b(t_{i+1}) &= \mathcal{M}_{t_i \to t_{i+1}}(\mathbf{x}_a(t_i)) \\
\mathbf{B}(t_{i+1}) &= \mathbf{M}_{t_i \to t_{i+1}} \mathbf{A}(t_i) \mathbf{M}^{\mathrm{T}}_{t_i \to t_{i+1}} + \mathbf{Q}(t_i)
\end{aligned}
$$



$$RK4, \Delta t = 0.05, F = 8, F^f = 7.6, \sigma_q = 0.1, t_v = t_0 + 4\Delta t$$

$$\sigma_o^{(1)} = 0.1, \quad \sigma_o^{(2)} = 0.2, \quad \sigma_o^{(3)} = 0.3, \quad \sigma_o^{(4)} = 0.4$$

ADJ-DAS estimation to OSEs: $e(x) = \|x^f - x_b^f\|^2$



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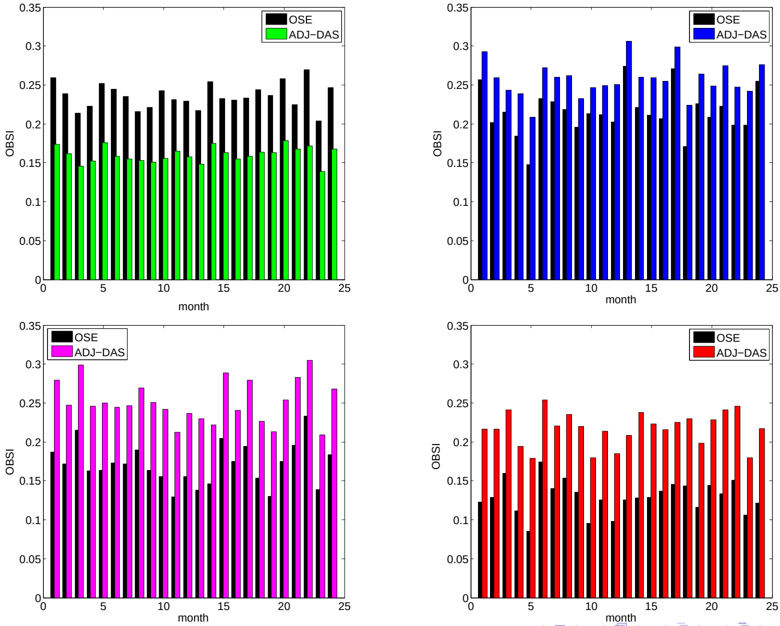
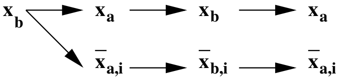


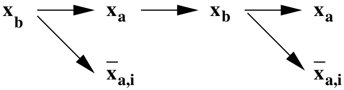
Concluding Remarks

- Adjoint-DAS approach provides
  1. high-order OBSI measures (numerical quadrature)
  2. sensitivity to any DAS input e.g., σ_o^2 and σ_b^2
  3. first-order estimates to certain 1-DA cycle OSEs outcomes
- Novel techniques needed to propagate background information.

MULTI–DA CYCLES OSEs



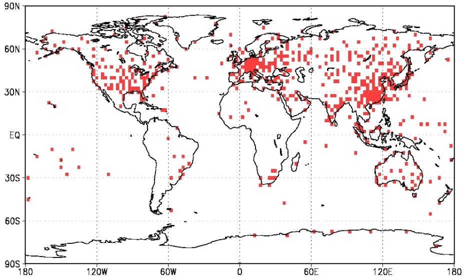
SINGLE–DA CYCLE OSEs



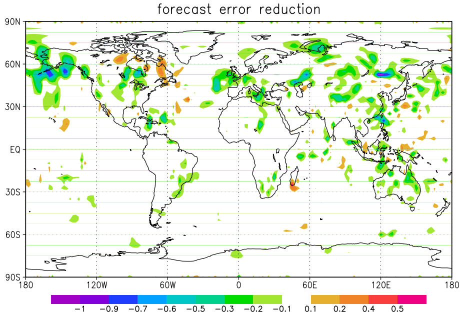
Idealized 4DVAR experiments with a SW model

- ECMWF ERA-40 to provide $\mathbf{x}_a^{ref} = (h, u, v)$ at $2.5°$ resolution
- Twin experiments using model generated data 0-6h.
- Observation error $N(0, \sigma_o^2)$; Background error $N(0, \sigma_b^2)$, $\sigma_b^2/\sigma_o^2 = 4$

Observation location

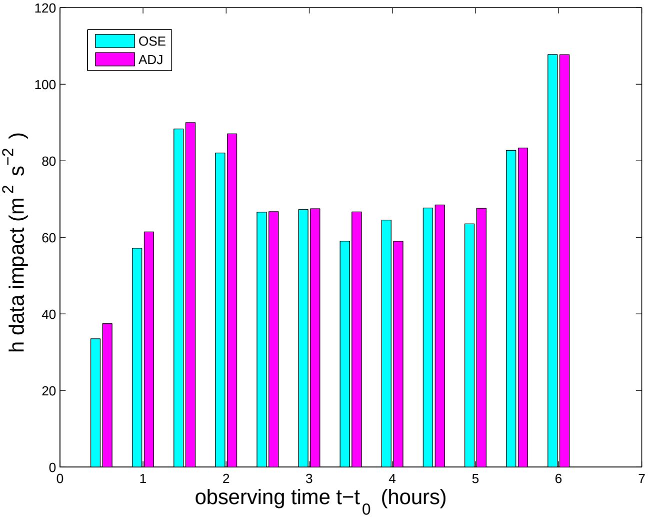


Forecast error reduction (m^2 s^{-2})



Adjoint estimation to OSE's outcomes: $e(x) = \|x - x_b\|^2$

h-data results



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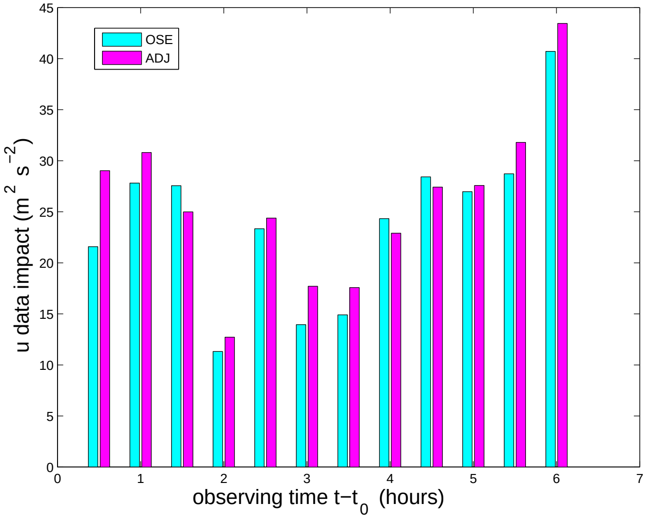
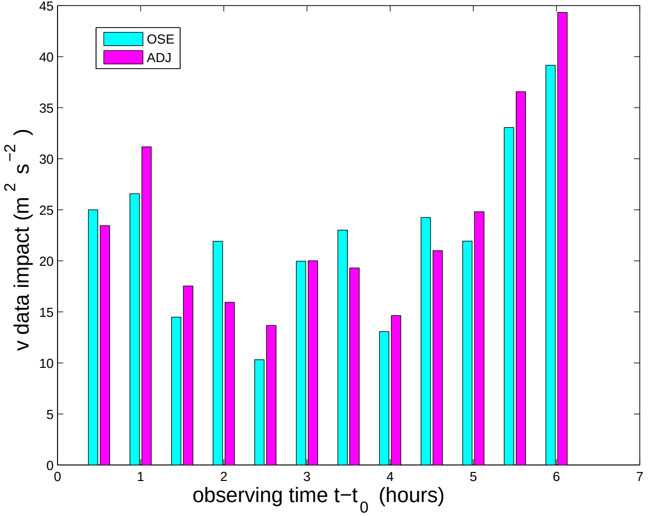
u-data results



Adjoint estimation to OSE's outcomes: $e(x) = \|x - x_b\|^2$

v-data results



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