Insights on observation residual approaches for model and observation error estimation

Ricardo Todling

Global Modeling and Assimilation Office, NASA

10th Adjoint Workshop
1-5 June 2015
Roanoke, West Virginia

In collaboration with: Yannick Trémolet
Discussions with: S. E. Cohn, D. P. Dee, M. Fisher, & M. Leutbecher

Outline

1. Introduction
2. Residual Estimation of System Error
3. Curiosities of Estimates from Residual Statistics
4. What do we get from 4d-Var Residual Diagnostics?
5. Recast Sequential Approach for **Q** into Variational Language
6. Closing Remarks

Introduction

Residual Statistics from Sequential Filtering Approach

Observation-minus-Background (OmB) residiuals

$$\mathbf{d}_o^b = \mathbf{y}^o - \mathbf{H}\mathbf{x}^b$$

OmB error covariance matrix

$$< \mathbf{d}_o^b (\mathbf{d}_o^b)^T > = \mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R}$$

- Sample error covariances of OmB residuals have traditionally been used to estimate and model time-independent background error covariances (Schlatter 1974, Hollingsworth & Lönnberg 1986, Dee & da Silva 1999, Franke 1999, and others, going back to the work of T. Kailath in the 70s).
- The expression above holds independently of optimality (though it relies on assumptions about background and observation errors).

Residual Statistics from Sequential Filtering Approach

Other available residuals:

$$\mathbf{d}_o^a = \mathbf{y}^o - \mathbf{H}\mathbf{x}^a \qquad \mathbf{d}_b^a = \mathbf{H}\mathbf{x}^b - \mathbf{H}\mathbf{x}^a$$

which lead to the following cross-covariances:

$$\begin{aligned}
< \mathbf{d}_o^a(\mathbf{d}_o^b)^T > &= \mathbf{R} + O(\Delta\mathbf{K}) \\
< \mathbf{d}_b^a(\mathbf{d}_o^b)^T > &= \mathbf{H}\mathbf{B}\mathbf{H}^T + O(\Delta\mathbf{K}) \\
< \mathbf{d}_b^a(\mathbf{d}_o^a)^T > &= \mathbf{H}\mathbf{A}\mathbf{H}^T + O(\Delta\mathbf{K})
\end{aligned}$$

where $\Delta\mathbf{K}$ is the deviation of the sequential *filter* gain from optimality.

General Remarks on Residual Statistics

- Only under the assumption of optimality, $\Delta\mathbf{K} = \mathbf{0}$, the cross-covariances become covariances and the expressions above can be used to estimate observation, background, and analysis error without concerns (Desroziers et al. 2005).
- The validity of replacing the expectation operator, $< \bullet >$, with the typical time average operator might not always be justifiable.
- Derivation of residual cross-covariances corresponding to those of the variational approach must be inferred carefully to try minimizing, if not possibly avoiding altogether, introducing time correlations.

Residual Estimation of System Error

Residual Statistics from Sequential Smoothing Approach

Residuals from a sequential lag-1 smoother can be used to derive an estimate of the model error covariance*:

$$\mathbf{d}_o^s = \mathbf{y}^o - \mathbf{HMx}^s \qquad \mathbf{d}_a^s = \mathbf{Hx}^a - \mathbf{HMx}^s$$

which lead to the following cross-covariances:

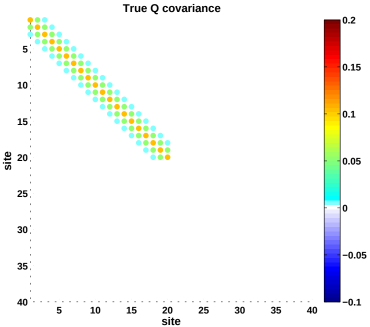
$$\begin{aligned} < \mathbf{d}_o^s(\mathbf{d}_o^b)^T > &= \mathbf{HQH}^T + \mathbf{R} + O(\Delta\mathbf{G}) \\ < \mathbf{d}_a^s(\mathbf{d}_o^s)^T > &= \mathbf{HQH}^T + O(\Delta\mathbf{K}) + O(\Delta\mathbf{G}) \end{aligned}$$

where $\Delta\mathbf{G}$ is the deviation of the sequential *smoother* gain from optimality.

* see Todling (2014; QJRMS).

Illustration in L96

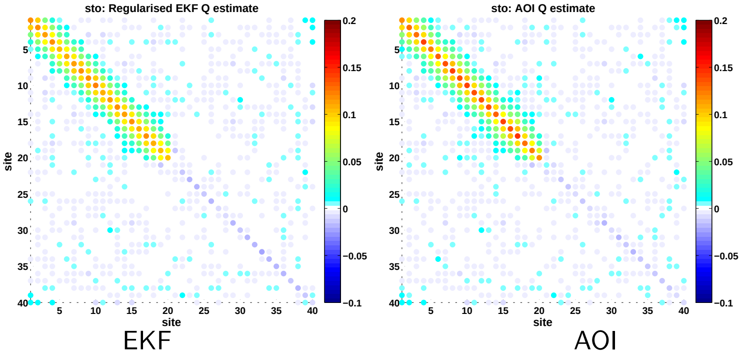
Examples for simple linear and nonlinear models serve as illustration of the method. For L96, with stochastically random Gaussian noise with covariance of the form below . . .



Specified model error covariance

Illustration in L96

Residual statistics from lag-1 smoothers implemented for two assimilation methodologies, namely the EKF and an adaptive OI, is shown to obtain reasonable estimates of **Q**.

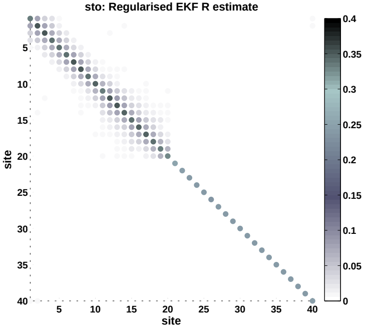


From Todling (2014; QJRMS)

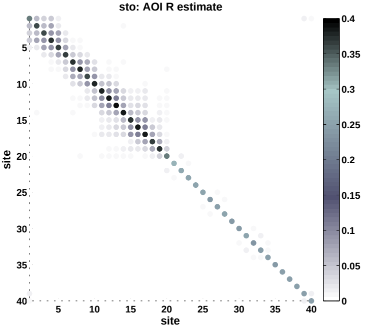
Curiosities of Estimates from Residual Statistics

Model or Observation Error?

Still examining the L96 application, when the residual diagnostic is used to estimate $\mathbf{R} \approx < \mathbf{d}_o^a(\mathbf{d}_o^b)^T >$, the derived estimates have a considerable signature of the model error.



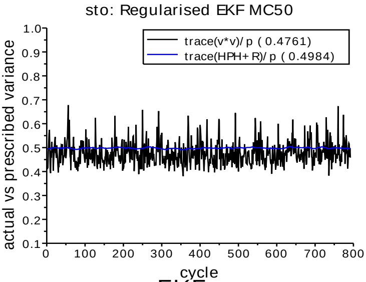
EKF



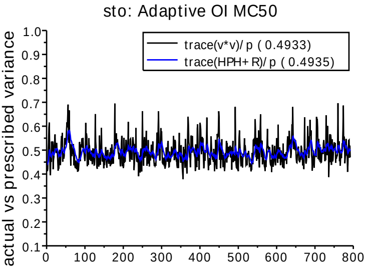
AOI

From Todling (2015; QJRMS)

Actual vs Prescribed OmB Residual Statistics: Original

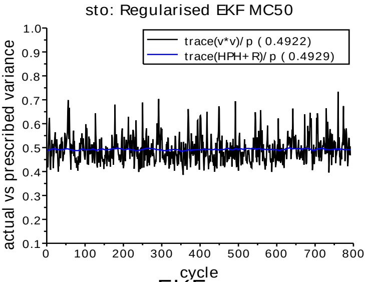


EKF

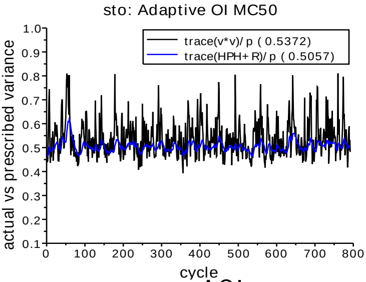


AOI

Actual vs Prescribed OmB Residual Statistics: Second Pass



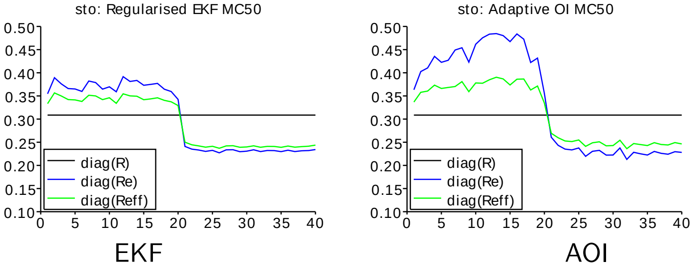
EKF



AOI

Model or Observation Error?

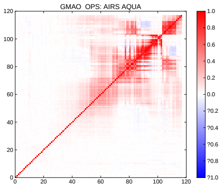
Not knowing any better - that is, that the error in the L96 application is due to errors in the model - using the **R** estimate as a "correction" to the specified observation error covariance leads to undesirable consequences. For example, re-estimation of **R** brings new estimates further away from true value.



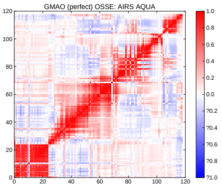
From Todling (2015; QJRMS)

Lesson from OSSEs

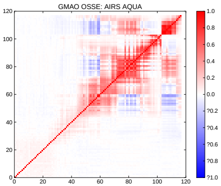
Somewhat analogous to what we just seen are various estimates of inter-channel correlations obtained from operational systems and OSSE's build off these systems. Funny enough, OSSE residual statistics might suggest observations to be largely correlated when in fact they are not. Examples from GEOS-5 are given below.



From GEOS-5 OPS



From early OSSE (perfect obs)



From tuned OSSE

Inspired by comment make by Anna Shlayeva at the Workshop on Correlated Obs. Errors, Reading U.K., 2014.
OSSE results from exps in Errico et al. (2013; QJRMS)
Results here from Todling (2015; QJRMS)

What do we get from 4d-Var Residual Diagnostics?

4d-Residuals

Consider SC 4d-Var in its 4d-PSAS form:

$$J(\delta \mathbf{x}_0) = \frac{1}{2}\delta \mathbf{x}_0^T \mathbf{B}^{-1}\delta \mathbf{x}_0 + \frac{1}{2}(\underline{\mathbf{d}}^b - \underline{\mathbf{H}}\delta \mathbf{x}_0)^T \underline{\mathbf{R}}^{-1}(\underline{\mathbf{d}}^b - \underline{\mathbf{H}}\delta \mathbf{x}_0)\,,$$

For

$$\begin{aligned} \underline{\mathbf{d}}^b &\equiv [(\mathbf{d}_0^b)^T\,(\mathbf{d}_1^b)^T\,\cdots\,(\mathbf{d}_K^b)^T]^T \\ \underline{\mathbf{d}}^a &\equiv [(\mathbf{d}_{0|0}^a)^T\,(\mathbf{d}_{1|0}^a)^T\,\cdots\,(\mathbf{d}_{K|0}^a)^T]^T \\ \underline{\mathbf{d}}^{ba} &\equiv \underline{\mathbf{d}}^b - \underline{\mathbf{d}}^a \end{aligned}$$

it is simple to show that

$$\begin{aligned} < \underline{\mathbf{d}}^{ba}(\underline{\mathbf{d}}^b)^T > &= \underline{\mathbf{H}}\mathbf{B}\underline{\mathbf{H}}^T(\underline{\mathbf{H}}\mathbf{B}\underline{\mathbf{H}} + \underline{\mathbf{R}})^{-1} < \underline{\mathbf{d}}^b(\underline{\mathbf{d}}^b)^T > \\ &\overset{\text{"opt"}}{=} \underline{\mathbf{H}}\mathbf{B}\underline{\mathbf{H}}^T\,. \end{aligned}$$

4d-Residuals

When the evolution of forecast errors within the var-window is taken into account (i.e., considering how model error also propagates in the window), we really have

$$< \underline{\mathbf{d}}^b(\underline{\mathbf{d}}^b)^T >= \underline{\mathbf{H}}\mathbf{P}^f_{0|-1}\underline{\mathbf{H}}^T + \underline{\tilde{\mathbf{R}}}$$

where $\underline{\tilde{\mathbf{R}}}$ is given by

$$\underline{\tilde{\mathbf{R}}}_{\ell,m} \equiv \mathbf{R}_\ell \delta_{\ell,m} + \mathbf{H}_{\ell|-1} \left(\sum_{i=0}^{\ell-1} \sum_{j=0}^{m-1} \mathbf{M}_{\ell,\ell-i|-1} \mathbf{Q}_{\ell-i,m-j} \mathbf{M}^T_{m,m-j|-1} \right) \mathbf{H}^T_{m|-1} \, ,$$

When $\mathbf{B} = \mathbf{P}^f_{0|1}$, somewhat unsurprisingly, one finds that

$$< \underline{\mathbf{d}}^a(\underline{\mathbf{d}}^b)^T > \approx \underline{\tilde{\mathbf{R}}}$$

This means:

- The cross covariance of “OmA” and “OmB” from 4d-Var give an estimate of an *effective* observation error covariance.
- Indeed, only at initial time do we the sought out observation error covariance, i.e., $< \mathbf{d}^a_0(\mathbf{d}^b_0)^T > \approx \mathbf{R}$.

Recast Sequential Approach for **Q** into Variational Language

Residual **Q** estimation: sequential to variational

Motivated by the sequential approach, we consider two loosely connected 4d-Var problems:

- one being double the window size of the other
- think of the short-window as the filter
- think of the long-window as the smoother
- furthermore, each long window cycle is started from the short-window analysis

and derive expressions that relate the two problems to allow extracting information on the model error covariance:

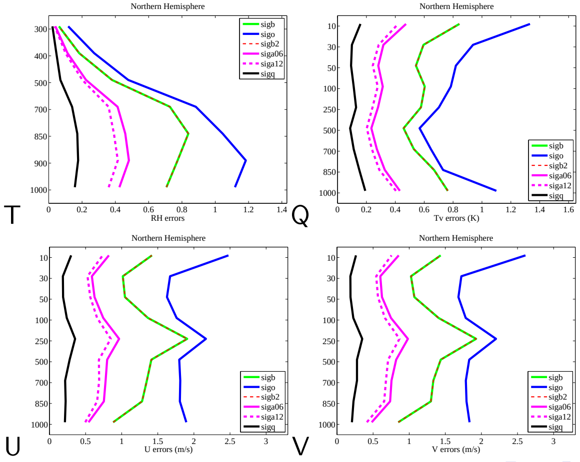
$$\left(< \underline{\mathbf{w}}_{\mathcal{I}_1} (\mathbf{d}^b_{\mathcal{I}_1})^T > \right)_{\ell,m} \overset{opt}{=} \sum_{i=k_s}^{-1} \sum_{j=k_s}^{-1} \mathbf{H}_\ell \mathbf{M}_{\ell,\ell-i|k_s-1} \mathbf{Q}_{\ell-i,m-j} \mathbf{M}^T_{m,m-j|k_s-1} \mathbf{H}^T_m + O(\Delta \mathbf{M}_{\ell,m})$$

$$\overline{< \underline{\mathbf{w}}_{\mathcal{I}_1} (\mathbf{d}^b_{\mathcal{I}_1})^T >} \overset{opt}{=} \underline{\mathbf{HQH}}^T$$

where

- $\mathbf{d}^b_{\mathcal{I}_1}$ is the OmB residual in the first half of the short or long-window problems
- $\underline{\mathbf{w}}_{\mathcal{I}_1}$ is an incremental residual differencing the OmA of the short-window with that of the long-window problem within the first half of the long-window

Residual **Q** estimation: sequential to variational



Closing Remarks

Closing Remarks

- Many of the insights on residual diagnostics presented here have been appreciated by others - largely in this audience.
- However, I hope to have provided a few illustrations highlighting what we know from theory: that in actuality, background, model and observations errors are inseparable.
- It is possible to estimate model error covariances from residual statistics using smoother ideas, but the entanglement with background and observations errors, particularly in variational approaches, make it really hard to obtain conclusive results.

Remark related to words on "Historical Overview":

- Recently, Grewal & Andrews (2010: IEEE Control Systems Magazine, 69-78) provides a nice review of the use of Kalman filtering in Aerospace. It seems unfortunate, though, that these authors are not aware of the earlier review of McGee & Schmidt (1985: NASA TM 86847).