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Modélisation Numérique de l'Écoulement Atmosphérique et Assimilation de Données

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Variational Assimilation

Variational approach can easily be extended to time dimension.

Suppose for instance available data consist of

- Background estimate at time 0

  $x_0^b = x_0 + \zeta_0^b \qquad\qquad E(\zeta_0^b \zeta_0^{bT}) = P_0^b$

- Observations at times $k = 0, \ldots, K$

  $y_k = H_k x_k + \varepsilon_k \qquad\qquad E(\varepsilon_k \varepsilon_j^T) = R_k\, \delta_{kj}$

- Model (supposed for the time being to be exact)

  $x_{k+1} = M_k x_k \qquad\qquad k = 0, \ldots, K\text{-}1$

Errors assumed to be unbiased and uncorrelated in time, H_k and M_k linear

Then objective function

$$\xi_0 \in \mathcal{S} \rightarrow$$

$$\mathcal{J}(\xi_0) = (1/2)\,(x_0^b - \xi_0)^T [P_0^b]^{-1} (x_0^b - \xi_0) + (1/2)\,\Sigma_k [y_k - H_k \xi_k]^T R_k^{-1} [y_k - H_k \xi_k]$$

subject to $\xi_{k+1} = M_k \xi_k$, $\qquad\qquad k = 0, \ldots, K\text{-}1$

Strong Constraint 4D-Var is now used operationally at several meteorological centres (Météo-France, UK Meteorological Office, Canadian Meteorological Centre, Japan Meteorological Agency, ...) and, until recently, at ECMWF. The latter now has a 'weak constraint' component in its operational system.

Buehner *et al*. (*Mon. Wea. Rev*., 2010)

For the same numerical cost, and in meteorologically realistic situations, Ensemble Kalman Filter and Variational Assimilation produce results of similar quality.

Incremental Method

Variational assimilation, as it has been described, requires the use of the adjoint of the full model.

Simplifying the adjoint as such can be very dangerous. The computed gradient would not be exact, and experience shows that optimization algorithms (and especially efficient ones) are very sensitive to even slight misspecification of the gradient.

Principle of *Incremental Method* (Courtier *et al*., 1994, *Q. J. R. Meteorol. Soc*.) : simplify simultaneously the (local tangent linear) dynamics and the corresponding adjoint.

Incremental Method (continuation 1)

- Basic (nonlinear) model

$\xi_{k+1} = M_k(\xi_k)$

- Tangent linear model

$\delta\xi_{k+1} = M_k{}' \, \delta\xi_k$

where $M_k{}'$ is jacobian of M_k at point ξ_k.

- Adjoint model

$\lambda_k = M_k{}'^{\mathrm{T}} \lambda_{k+1} + \ldots$

Incremental Method. Simplify $M_k{}'$ and $M_k{}'^{\mathrm{T}}$.

Incremental Method (continuation 2)

More precisely, for given solution $\xi_k^{(0)}$ of nonlinear model, replace tangent linear and adjoint models respectively by

$$\delta\xi_{k+1} = L_k\, \delta\xi_k \qquad (2)$$

and

$$\lambda_k = L_k^{\mathrm{T}}\, \lambda_{k+1} + \dots$$

where L_k is an appropriate simplification of jacobian M_k'.

It is then necessary, in order to ensure that the result of the adjoint integration is the exact gradient of the objective function, to modify the basic model in such a way that the solution emanating from $\xi_0^{(0)} + \delta\xi_0$ is equal to $\xi_k^{(0)} + \delta\xi_k$, where $\delta\xi_k$ evolves according to (2). This makes the basic dynamics exactly linear.

Incremental Method (continuation 3)

As concerns the observation operators in the objective function, a similar procedure can be implemented if those operators are nonlinear. This leads to replacing $H_k(\xi_k)$ by $H_k(\xi_k^{(0)}) + N_k\delta\xi_k$, where N_k is an appropriate 'simple' linear operator (possibly, but not necessarily, the jacobian of H_k at point $\xi_k^{(0)}$). The objective function depends only on the initial $\delta\xi_0$ deviation from $\xi_0^{(0)}$, and reads

$$\mathcal{J}_\mathrm{I}(\delta\xi_0) = (1/2)\,(x_0^b - \xi_0^{(0)} - \delta\xi_0)^\mathrm{T}\,[P_0^b]^{-1}\,(x_0^b - \xi_0^{(0)} - \delta\xi_0) + (1/2)\,\Sigma_k[d_k - N_k\delta\xi_k]^\mathrm{T}\,R_k^{-1}\,[d_k - N_k\delta\xi_k]$$

where $d_k \equiv y_k - H_k(\xi_k^{(0)})$ is the innovation at time k, and the $\delta\xi_k$ evolve according to

$$\delta\xi_{k+1} = L_k\,\delta\xi_k \qquad (2)$$

With the choices made here, $\mathcal{J}_\mathrm{I}(\delta\xi_0)$ is an exactly quadratic function of $\delta\xi_0$. The minimizing perturbation $\delta\xi_{0,m}$ defines a new initial state $\xi_0^{(1)} \equiv \xi_0^{(0)} + \delta\xi_{0,m}$, from which a new solution $\xi_k^{(1)}$ of the basic nonlinear equation is determined. The process is restarted in the vicinity of that new solution.

Incremental Method (continuation 4)

This defines a system of two-level nested loops for minimization. Advantage is that many degrees of freedom are available for defining the simplified operators L_k and N_k, and for defining an appropriate trade-off between practical implementability and physical usefulness and accuracy. It is the incremental method which, together with the adjoint method, makes variational assimilation possible.

First-Guess-At-the-right-Time 3D-Var (*FGAT 3D-Var*). Corresponds to $L_k = I_n$. Assimilation is four-dimensional in that observations are compared to a first-guess which evolves in time, but is three-dimensional in that no dynamics other than the trivial dynamics expressed by the unit operator is present in the minimization.

Weak constraint variational assimilation allows for errors in the assimilating model

- Data

  - Background estimate at time 0

  $$x_0^b = x_0 + \zeta_0^b \qquad E(\zeta_0^b \zeta_0^{bT}) = P_0^b$$

  - Observations at times $k = 0, \ldots, K$

  $$y_k = H_k x_k + \varepsilon_k \qquad E(\varepsilon_k \varepsilon_k^T) = R_k$$

  - Evolution equation

  $$x_{k+1} = M_k x_k + \eta_k \qquad E(\eta_k \eta_k^T) = Q_k \qquad k = 0, \ldots, K\text{-}1$$

  Errors assumed to be unbiased and uncorrelated in time, H_k and M_k linear

Then objective function

$$(\xi_0, \xi_1, \ldots, \xi_K) \rightarrow$$

$$\mathcal{J}(\xi_0, \xi_1, \ldots, \xi_K)$$

$$= (1/2)\,(x_0^{\,b} - \xi_0)^{\mathrm{T}}\,[P_0^{\,b}]^{-1}\,(x_0^{\,b} - \xi_0)$$

$$+ (1/2)\,\Sigma_{k=0,\ldots,K}[y_k - H_k\xi_k]^{\mathrm{T}}\,R_k^{-1}\,[y_k - H_k\xi_k]$$

$$+ (1/2)\,\Sigma_{k=0,\ldots,K-1}[\xi_{k+1} - M_k\xi_k]^{\mathrm{T}}\,Q_k^{-1}\,[\xi_{k+1} - M_k\xi_k]$$

Can include nonlinear M_k and/or H_k.

Time-correlated Errors

Example of time-correlated observation errors

$z_1 = x + \zeta_1$

$z_2 = x + \zeta_2$

$E(\zeta_1) = E(\zeta_2) = 0$; $E(\zeta_1{}^2) = E(\zeta_2{}^2) = s$; $E(\zeta_1 \zeta_2) = 0$

BLUE of x from z_1 and z_2 gives equal weights to z_1 and z_2.

Additional observation then becomes available

$z_3 = x + \zeta_3$

$E(\zeta_3) = 0$; $E(\zeta_3{}^2) = s$; $E(\zeta_1 \zeta_3) = cs$; $E(\zeta_2 \zeta_3) = 0$

BLUE of x from (z_1, z_2, z_3) has weights in the proportion $(1, 1+c, 1)$

Time-correlated Errors (continuation 1)

Example of time-correlated model errors

Evolution equation

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$x_{k+1} = x_k + \eta_k$ $\qquad$ $E(\eta_k^{\,2}) = q$

Observations

$y_k = x_k + \varepsilon_k$, $\qquad$ $k = 0, 1, 2$ $\qquad$ $E(\varepsilon_k^{\,2}) = r$, errors uncorrelated in time

Sequential assimilation. Weights given to y_0 and y_1 in analysis at time 1 are in the ratio $r/(r+q)$. That ratio will be conserved in sequential assimilation. All right if model errors are uncorrelated in time.

Assume $E(\eta_0\eta_1) = cq$

Weights given to y_0 and y_1 in estimation of x_2 are in the ratio

$$\rho = \frac{r - qc}{r + q + qc}$$

Variational assimilation has been extended to non Gaussian probability distributions (lognormal distributions), the unknown being the mode of the conditional distribution (M. Zupanski, Fletcher).

Bayesian character of variational assimilation ?

- If everything is linear and gaussian, ready recipe for obtaining bayesian sample

Perturb data (background, observations and model) according to their error probability distributions, do variational assimilation, and repeat process

Sample of system orbits thus obtained is bayesian

- If not, very little can be said at present

Conclusion on Sequential Assimilation

Pros

'Natural', and well adapted to many practical situations

Provides, at least relatively easily, explicit estimate of estimation error

Cons

Carries information only forward in time (of no importance if one is interested only in doing forecast)

In present form, optimality is possible only if errors are independent in time

Conclusion on Variational Assimilation

Pros

Carries information both forward and backward in time (important for reassimilation of past data).

Can easily take into account temporal statistical dependence (Järvinen *et al.*)

Does not require explicit computation of temporal evolution of estimation error

Very well adapted to some specific problems (*e. g.*, identification of tracer sources)

Cons

Does not readily provide estimate of estimation error

Requires development and maintenance of adjoint codes. But the latter can have other uses (sensitivity studies).

- Dual approach seems most promising. But still needs further development for application in non exactly linear cases.

- Is ensemble variational assimilation possible ? Probably yes. But also needs development.

How to write the adjoint of a code ?

Operation $a = b \times c$

Input b, c Output a but also b, c

For clarity, we write

$a = b \times c$
$b' = b$
$c' = c$

$\partial J/\partial a$, $\partial J/\partial b'$, $\partial J/\partial c'$ available. We want to determine $\partial J/\partial b$, $\partial J/\partial c$

Chain rule

$$\partial J/\partial b = (\partial J/\partial a)(\partial a/\partial b) + (\partial J/\partial b')(\partial b'/\partial b) + (\partial J/\partial c')(\partial c'/\partial b)$$

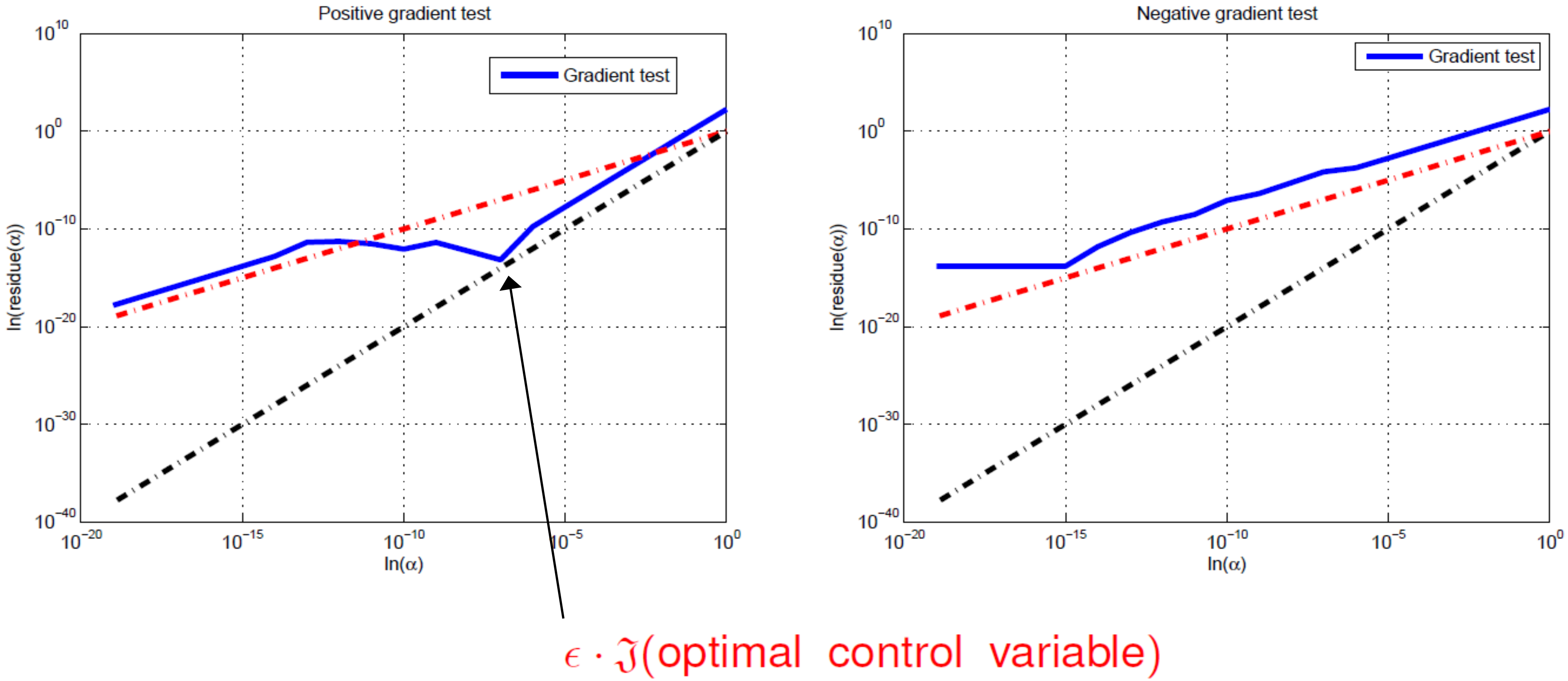
$$\qquad\qquad\quad c \qquad\qquad\qquad\qquad 1 \qquad\qquad\qquad\qquad 0$$

$$\partial J/\partial b = (\partial J/\partial a)\, c + \partial J/\partial b'$$

Similarly

$$\partial J/\partial c = (\partial J/\partial a)\, b + \partial J/\partial c'$$

Gradient test



$\epsilon = 2^{-53}$ zero machine

$residue(\alpha) = (\mathfrak{J}(x + \alpha dx) - \mathfrak{J}(x)) - \alpha \nabla \mathfrak{J}(x) dx$

M. Jardak