MATHEMATICAL PROBLEMS ASSOCIATED WITH ATMOSPHERIC DATA ASSIMILATION AND WEATHER PREDICTION

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Outline

- **Introduction of the variational data assimilation problem**
- **Lorenc (1986), Courtier (1997)**
  - The dual form of 3D-Var
    - → *Physical Space Statistical Analysis System* (**PSAS**): Cohn *et al.* (1998), GMAO, NASA;
    - → Daley and Barker (2001) (**NAVDAS** at NRL)
  - Equivalence between the primal (3D-Var) and dual (3D-PSAS) formulation of the statistical estimation problem
- **Modular representation of both algorithms**
  - Implementation based on the same operators of the variational assimilation system
- **Convergence of the minimization and preconditioning**
  - Significance of the two cost functions and impact on the results
- **Applications of the dual approach**
  - Sensitivity of observations with respect to observations (Langland, 2004)
  - Information content (Cardinali)
  - The weak-constraint 4D-Var and its dual formulation

The variational problem

Bayes' Theorem: $$p(\mathbf{x}\,|\,\mathbf{y}) = \frac{p(\mathbf{y}\,|\,\mathbf{x})P(\mathbf{x})}{P(\mathbf{y})}$$

- **Example:**
  - Observation and background error have Gaussian distributions

$$p(\mathbf{y}\,|\,\mathbf{x}) = \frac{1}{C_3}\exp\left\{-\frac{1}{2}(\mathbf{y}-\mathbf{H}(\mathbf{x}))^T\mathbf{R}^{-1}(\mathbf{y}-\mathbf{H}(\mathbf{x}))\right\}$$

$$P(\mathbf{x}) = \frac{1}{C}\exp\left\{-\tfrac{1}{2}(\mathbf{x}-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b)\right\}$$

  - $p(\mathbf{y}|\mathbf{x})$ is Gaussian only if **H** is linear
  - Maximum likelihood estimate (mode of the distribution):

$$J(\mathbf{x}) = -\ln p(\mathbf{x}\,|\,\mathbf{y})$$
$$= \tfrac{1}{2}(\mathbf{x}-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b) + \tfrac{1}{2}(\mathbf{H}(\mathbf{x})-\mathbf{y})^T\mathbf{R}^{-1}(\mathbf{H}(\mathbf{x})-\mathbf{y})$$

- Reducing $J(\mathbf{x})$ implies an increase in the probability of **x** being the true value

Incremental approach

Successive linearizations with respect to full model state obtained

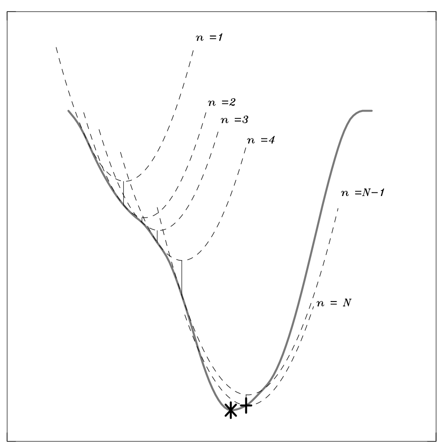
- Minimization of quadratic problems

$$J(\xi) = \tfrac{1}{2}\delta\mathbf{x}^T\mathbf{B}^{-1}\delta\mathbf{x} + \tfrac{1}{2}(\mathbf{H}'\delta\mathbf{x}-\mathbf{y}')^T\mathbf{R}^{-1}(\mathbf{H}'\delta\mathbf{x}-\mathbf{y}')$$
$$\equiv \tfrac{1}{2}\xi^T\xi + \tfrac{1}{2}(\mathbf{H}'\mathbf{G}\xi-\mathbf{y}')^T\mathbf{R}^{-1}(\mathbf{H}'\mathbf{G}\xi-\mathbf{y}')$$

where

$\delta\mathbf{x} = \mathbf{x} - \mathbf{x}_b$	:	increment
$\mathbf{H}' = \partial\mathbf{H}/\partial\mathbf{x}$	:	tangent-linear of the observation operator

$\mathbf{y}' = \mathbf{y} - \mathbf{H}(\mathbf{x}_b)$:
innovation vector (observation departure with respect to the high resolution background state)
$\mathbf{G} = \mathbf{B}^{1/2}$



From Laroche and Gauthier (1998)

The dual formulation

- Explicit solution when H' is *linear*

$$\delta \mathbf{x}_a = \mathbf{BH}'^T (\mathbf{R} + \mathbf{H}'\mathbf{B}\mathbf{H}'^T)^{-1} \mathbf{y}'$$

- Solving a large matrix problem

$$\mathbf{w}^* = (\mathbf{R} + \mathbf{H}'\mathbf{BH}'^T)^{-1} \mathbf{y}'$$

  - **The PSAS minimization problem**

$$J_P(\mathbf{w}) = \tfrac{1}{2} \mathbf{w}^\mathbf{T} (\mathbf{R} + \mathbf{H}'\mathbf{BH}'^\mathbf{T}) \mathbf{w} - \mathbf{y}'^T \mathbf{w}$$

$$\nabla J_P(\mathbf{w}) = (\mathbf{H}'\mathbf{BH}'^T + \mathbf{R}) \mathbf{w} - \mathbf{y}'$$

$$\delta \mathbf{x}_a = \mathbf{BH}'^\mathbf{T} \mathbf{w}^*$$

- 3D-Var and PSAS should then give the same solution *at convergence*
- Control variable: **x** is in model space for 3D-Var
  w is in observation space for PSAS

3D-Var: variational formulation of the statistical estimation problem

Minimization of the cost function

$$J(\xi) = \frac{1}{2} \xi^T \xi + \frac{1}{2} (\mathbf{H}'\mathbf{G}\xi - \mathbf{y}')^T \mathbf{R}^{-1} (\mathbf{H}'\mathbf{G}\xi - \mathbf{y}')$$

$$\delta x = \mathbf{B}^{1/2} \xi \equiv \mathbf{G}\, \xi$$

where $\delta\mathbf{x} = \mathbf{x} - \mathbf{x}_b$: increment
$\mathbf{H}' = \partial\mathbf{H}/\partial\mathbf{x}$: tangent-linear of the observation operator
$\mathbf{y}' = \mathbf{y} - \mathbf{H}(\mathbf{x}_b)$: innovation vector (observation departure) (computed with respect to the high resolution background state)

Preconditioning the minimization

- Condition of the minimization relates to the ratio of the highest to the lowest eigenvalues of the Hessian matrices
- Courtier (1997): preconditioning with respect to $\mathbf{B}^{-1/2}$ for 3D-Var and with respect to $\mathbf{R}^{1/2}$ for PSAS

3D-Var	PSAS
$\xi = \mathbf{B}^{-1/2}\delta\mathbf{x}$	$\mathbf{u} = \mathbf{R}^{1/2}\mathbf{w}$
$J'' = \mathbf{I} + \mathbf{B}^{1/2^T}\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}\mathbf{B}^{1/2}$	$J''_P = \mathbf{I} + \mathbf{R}^{-1/2}\mathbf{H}\mathbf{B}\mathbf{H}^T\mathbf{R}^{-1/2^T}$

- The two problems have *exactly* the same condition number (Courtier, 1997) and should therefore have similar convergence rates.
- The argument extends to 4D-Var if **H'** includes the integration of the tangent linear model.

Operations involved in both algorithms

Direct operators

Input	Operator	Output
ξ	$\mathbf{G} = \mathbf{B}^{1/2}$	$\delta\mathbf{x}_0$
$\delta\mathbf{x}_k$	$\boldsymbol{L}(t_k, t_{k+L})$	$\delta\mathbf{x}_{k+L}$
$\delta\mathbf{x}_k$	$\mathbf{H}_k'$	$\mathbf{w}_k$
$\mathbf{w}_k$	$\mathbf{R}^{-1/2}$	$\mathbf{u}_k$

Adjoint operators

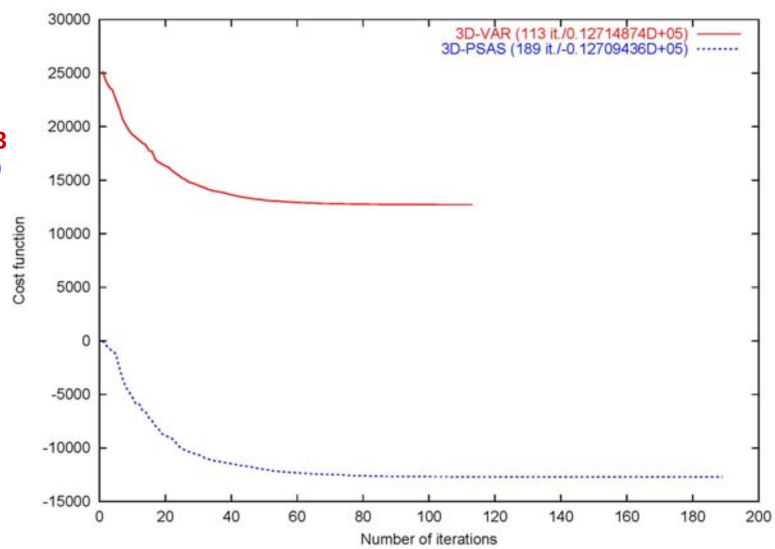
Input	Operator	Output
$\delta\mathbf{x}_0^*$	$\mathbf{G}^* = \mathbf{B}^{1/2^T}$	ξ^*
$\delta\mathbf{x}^*_{k+L}$	$\mathbf{L}^*(t_k, t_{k+L})$	$\delta\mathbf{x}^*_k$
$\mathbf{w}^*_k$	$\mathbf{H}'^*_k$	$\delta\mathbf{x}^*_k$
$\mathbf{u}_k^*$	$\mathbf{R}^{-1/2^T}$	$\mathbf{w}^*_k$

Modularisation of MSC's variational system

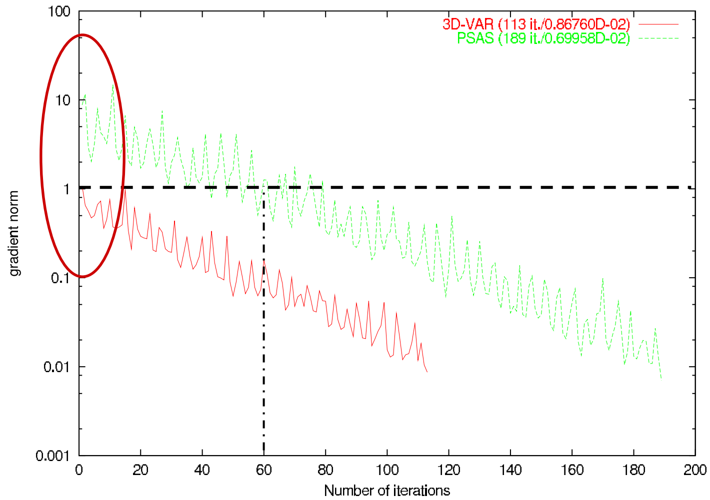
- **Decomposition of the 3D/4D-Var into its basic units**
  - Including the TLM and adjoint operators
  - 3D-Var and PSAS could be built and compared within a quasi-operational framework
    - → Extension to 4D-PSAS has been done also (without the outer iterations)

Cost function of PSAS (blue) and 3D-Var (red)

Number of iterations
3D-Var: 113
PSAS: 189



Norm of gradient as a function of iteration

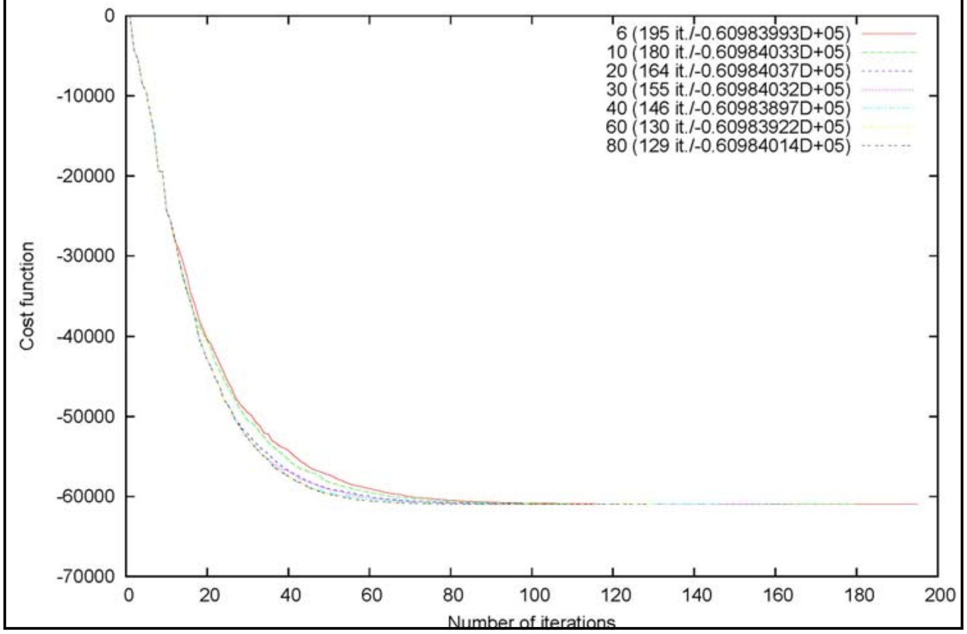


Impact of the dimension of the Hessian used in the BFGS approximation

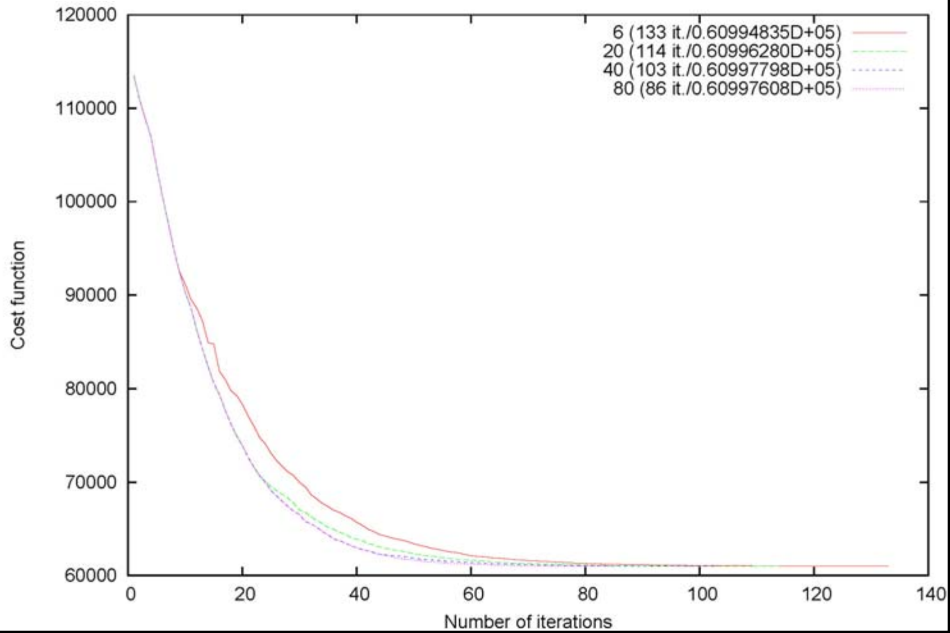
- **Quasi-Newton builds an approximation of the Hessian in the course of the minimization**
  - Limited-memory imposes a limit on the dimension of the approximate of the Hessian
  - Tests in M1QN3 (INRIA) with 6, 10, …, up to 80 pairs of

$$\left(\mathbf{x}_k - \mathbf{x}_{k-1}\right) \; and \; \left(\nabla J\left(\mathbf{x}_k\right) - \nabla J(\mathbf{x}_{k-1}\right)$$

Cost function of PSAS vs. number of iterations



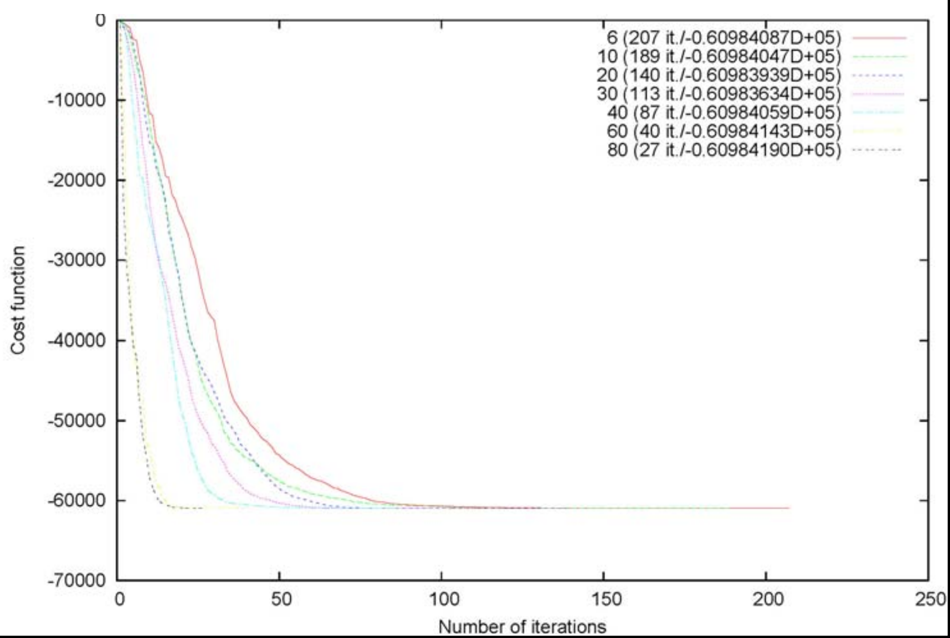
Cost function of 3D-Var vs. number of iterations



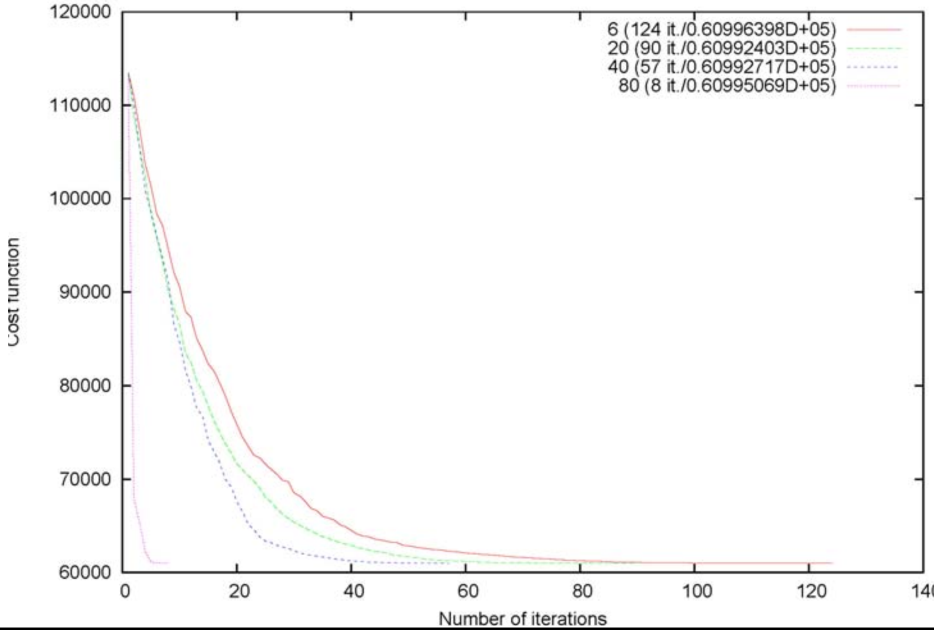
Cycling the Hessian

- **Experiment to test the quality of the approximate Hessian obtained from a limited memory quasi-Newton (M1QN3)**
  - o Use the Hessian of the previous experiment to precondition the *same* problem
  - o Impact of augmenting the dimension used for its representation

Preconditioned PSAS with its own Hessian



Preconditioned 3D-Var with its own Hessian



Estimation of the Hessian

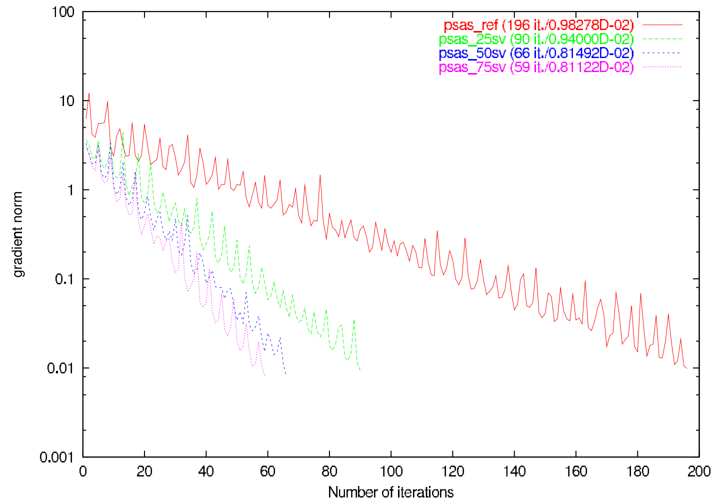
- **Hessian matrices**
  - Let $\mathbf{L} = \mathbf{R}^{-1/2}\mathbf{H}\mathbf{B}^{1/2}$
  - 3D-Var: $$J'' = \mathbf{I} + \left(\mathbf{R}^{-1/2}\mathbf{H}\mathbf{B}^{1/2}\right)^T\left(\mathbf{R}^{-1/2}\mathbf{H}\mathbf{B}^{1/2}\right)$$ $$= \mathbf{I}_n + \mathbf{L}^T\mathbf{L}$$
  - PSAS: $$J''_P = \mathbf{I} + \mathbf{R}^{-1/2}\mathbf{H}\mathbf{B}\mathbf{H}^T\mathbf{R}^{-1/2T} = \mathbf{I}_m + \mathbf{L}\mathbf{L}^T$$
- **Correspondence of eigenvectors**

3D-Var $J''_{3D}\mathbf{v} = \left(\mathbf{I}_n + \mathbf{L}^T\mathbf{L}\right)\mathbf{v} = \lambda\mathbf{v}$

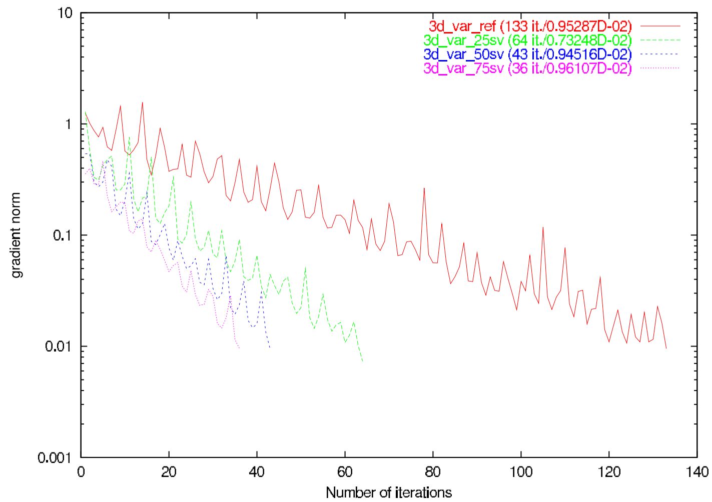
PSAS $J''_P\mathbf{u} = \left(\mathbf{I}_m + \mathbf{L}\mathbf{L}^T\right)\mathbf{u} = \lambda\mathbf{u}$

$$\mathbf{u} = \frac{1}{\sqrt{\lambda - 1}}\mathbf{L}\mathbf{v} \qquad \mathbf{v} = \frac{1}{\sqrt{\lambda - 1}}\mathbf{L}^T\mathbf{u}$$

Preconditioning the PSAS with 25, 50 and 75 singular vectors



Preconditioning the 3D-Var with 25, 50 and 75 singular vectors



Cycling the Hessian

- **3D-Var control variable is the model state and stays the same from one analysis to the next**
  - Approximation of the Hessian from one analysis can be easily used for the next one
- **PSAS control variable depends on the observations used and their distribution (in time and space)**
- **Cycling the Hessian for PSAS uses its mapping in model space**

$$\mathbf{u}_k(t_0) \quad \rightarrow \quad \mathbf{v}_k(t_0) = \frac{1}{\sqrt{\lambda_k - 1}} \mathbf{L}_0^T \mathbf{u}_k(t_0)$$

$$\mathbf{v}_k(t_0) = \frac{1}{\sqrt{\lambda_k - 1}} \mathbf{B}^{1/2^T} \mathbf{H}_0^T \mathbf{R}_0^{-1/2^T} \mathbf{u}_k(t_0)$$

Cycling the Hessian

- **3D-Var control variable is the model state and stays the same from one analysis to the next**
  - Approximation of the Hessian from one analysis can be easily used for the next one
- **PSAS control variable depends on the observations used and their distribution (in time and space)**
- **Cycling the Hessian for PSAS uses its mapping in model space**
  - Remapped according to the distribution of the new set of variables

$$\mathbf{u}_k(t_0 + T) = \frac{1}{\sqrt{\lambda_k - 1}} \mathbf{L}_1 \mathbf{v}_k(t_0)$$

$$= \frac{1}{\sqrt{\lambda_k - 1}} \mathbf{R}_1^{-1/2} \mathbf{H}_1 \mathbf{B}^{1/2} \mathbf{v}_k(t_0)$$

Conclusions

- **Equivalence of 3D/4D-PSAS and 3D/4D-Var**
  - Equivalence of the result at convergence *when the observation operator is linear and the pdfs are Gaussian*
    - → Incremental form extends the validity of this statement to nonlinear observation operators and non-Gaussian p.d.f.
  - Both approaches
    - → have similar convergence rates (Courtier, 1997)
    - → can be built by using the same basic operators common to both algorithms (the PALM approach)
  - PSAS cost function has no immediate significance
    - → Unrealistic values of the a posteriori p.d.f. at the beginning of the minimization
    - → Problematic for applications where the number of iterates is set to a fixed number

Summary (cont'd)

- **Preconditioning of the minimization**
  - o Both algorithms benefits similarly from preconditioning
  - o Cycling is more easily done in 3D/4D-Var as the dimension and topology of the control variable remains the same
    - → Control variable of PSAS changes with the observations used
  - o Equivalence between the eigenvectors of their respective Hessian matrices
    - → Permits cycling of the eigenvectors from the previous analysis to the next
    - → Preconditioning of PSAS is effective but requires solving for the eigenvectors of the Hessian (Lanczos algorithm)
      - – Minimization with a conjugate gradient enables to obtain the singular vectors from the iterates of the minimization

Conclusions

- **Application of the PSAS algorithm is useful for**
  - o the estimation of sensitivity with respect to observations
    - → Relationship between the eigenvectors of both Hessians
    - → Mapping forecast sensitivities into observation space
  - o Weak-constraint 4D-Var
    - → Dimension of the control variable is proportional to the number of observations used
  - o See El Akkraoui *et al.* (QJRMS, 2008) for details