# Variational Data Assimilation Current Status 

Yannick Trémolet with contributions from Mike Fisher

ECMWF

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## Outline

(1) The Maximum Likelihood Approach
(2) 4D-Var (and 3D-Var)
(3) Minimization and Incremental 4D-Var

4 Preconditioning
(5) Operational 4D-Var Setup
(6) Summary

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## Maximum Likelihood

- We define the analysis $\mathbf{x}_{a}$ as the most probable state of the system given a background state $\mathbf{x}_{b}$ and observations $\mathbf{y}$ :

$$
\mathbf{x}_{a}=\arg \max _{\mathbf{x}} p\left(\mathbf{x} \mid \mathbf{y} \text { and } \mathbf{x}_{b}\right)
$$

- It will be convenient to define a cost function:

$$
J(\mathbf{x})=-\log p\left(\mathbf{x} \mid \mathbf{y} \text { and } \mathbf{x}_{b}\right)+K
$$

where $K$ is a constant.

- Since $\log$ is a monotonic function, $\mathbf{x}_{a}$ is also:

$$
\mathbf{x}_{a}=\arg \min _{\mathbf{x}} J(\mathbf{x})
$$

- Variational data assimilation comprises minimizing the cost function $J(\mathbf{x})$.


## Maximum Likelihood and Bayes' Theorem

- Applying Bayes' theorem gives:

$$
p\left(\mathbf{x} \mid \mathbf{y} \text { and } \mathbf{x}_{b}\right)=\frac{p\left(\mathbf{y} \text { and } \mathbf{x}_{b} \mid \mathbf{x}\right) p(\mathbf{x})}{p\left(\mathbf{y} \text { and } \mathbf{x}_{b}\right)}
$$

- $p\left(\mathbf{y}\right.$ and $\left.\mathbf{x}_{b}\right)$ is independent of $\mathbf{x}$ and a priori we know nothing about $\mathbf{x}$ (all values of $\mathbf{x}$ are equally likely) thus $p(\mathbf{x})$ is also independent of $\mathbf{x}$.
- Hence:

$$
p\left(\mathbf{x} \mid \mathbf{y} \text { and } \mathbf{x}_{b}\right) \propto p\left(\mathbf{y} \text { and } \mathbf{x}_{b} \mid \mathbf{x}\right)
$$

- Finally, if observation errors and backgound errors are uncorrelated:

$$
\begin{gathered}
p\left(\mathbf{y} \text { and } \mathbf{x}_{b} \mid \mathbf{x}\right)=p(\mathbf{y} \mid \mathbf{x}) p\left(\mathbf{x}_{b} \mid \mathbf{x}\right) \\
\Rightarrow J(\mathbf{x})=-\log p(\mathbf{y} \mid \mathbf{x})-\log p\left(\mathbf{x}_{b} \mid \mathbf{x}\right)+K
\end{gathered}
$$

## Maximum Likelihood and Cost Function

- The maximum likelihood approach is applicable to any probability density functions $p(\mathbf{y} \mid \mathbf{x})$ and $p\left(\mathbf{x}_{b} \mid \mathbf{x}\right)$.
- Consider the special case of Gaussian p.d.f's:

$$
\begin{aligned}
p\left(\mathbf{x}_{b} \mid \mathbf{x}\right) & =\frac{1}{(2 \pi)^{N / 2}|\mathbf{B}|^{1 / 2}} \exp \left[-\frac{1}{2}\left(\mathbf{x}-\mathbf{x}_{b}\right)^{T} \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}_{b}\right)\right] \\
p(\mathbf{y} \mid \mathbf{x}) & =\frac{1}{(2 \pi)^{M / 2}|\mathbf{R}|^{1 / 2}} \exp \left[-\frac{1}{2}[\mathcal{H}(\mathbf{x})-\mathbf{y}]^{T} \mathbf{R}^{-1}[\mathcal{H}(\mathbf{x})-\mathbf{y}]\right]
\end{aligned}
$$

where $\mathbf{B}$ and $\mathbf{R}$ are the background and observation error covariance matrices and $\mathcal{H}$ is the observation operator.

- With an appropriate choice of the constant:

$$
J(\mathbf{x})=\frac{1}{2}\left(\mathbf{x}-\mathbf{x}_{b}\right)^{T} \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}_{b}\right)+\frac{1}{2}[\mathcal{H}(\mathbf{x})-\mathbf{y}]^{T} \mathbf{R}^{-1}[\mathcal{H}(\mathbf{x})-\mathbf{y}]
$$

- This is the variational data assimilation cost function.


## Maximum Likelihood: Remarks

- The maximum-likelihood approach is general: as long as we know the p.d.f's, we can define the cost function.
- Finding the global minimum may not be easy for non-Gaussian p.d.f's.
- In practice, background errors are usually assumed to be Gaussian (or a nonlinear transformation is applied to make them Gaussian).
- Non-Gaussian observation errors are taken into account.
- Directionally-ambiguous wind observations from scatterometers,
- Observations contaminated by occasional gross errors, which make outliers much more likely than implied by a Gaussian model.
- For Gaussian errors and linear observation operators, the maximum likelihood analysis coincides with the minimum variance solution. This is not the case in general:



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## 3D-Var and 4D-Var

$$
J(\mathbf{x})=\frac{1}{2}\left(\mathbf{x}-\mathbf{x}_{b}\right)^{T} \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}_{b}\right)+\frac{1}{2}[\mathcal{H}(\mathbf{x})-\mathbf{y}]^{\top} \mathbf{R}^{-1}[\mathcal{H}(\mathbf{x})-\mathbf{y}]
$$

- We have not precisely defined the space over which the state variable $\mathbf{x}$ is defined or the observation operator $\mathcal{H}$.
- Depending on the choice of $\mathbf{x}$ and $\mathcal{H}$, the general approach described earlier will lead to different variational data assimilation methods.
- The simplest approach is to consider $\mathbf{x}$ as the state over the 3D spatial domain at analysis time, while $\mathcal{H}$ spatially interpolates this state and converts model variables to observed quantities: this is 3D-Var.
- Another more common approach is to consider $\mathbf{x}$ as the state over the 3D spatial domain and over the period for which observations are available, while $\mathcal{H}$ spatially and temporally interpolates this state and converts model variables to observed quantities: this is 4D-Var.


## 4D-Var

- We now discretize the assimilation window in time and define $\mathbf{x}=\left\{\mathbf{x}_{i}\right\}_{i=0, n}$ and $\mathbf{y}=\left\{\mathbf{y}_{i}\right\}_{i=0, n}$ where $\mathbf{x}_{i}$ and $\mathbf{y}_{i}$ are the state and observations at time $t_{i}$ for $i=0, \ldots, n$.
- Assuming that observation errors are uncorrelated in time, $\mathbf{R}$ is block diagonal, with blocks $\mathbf{R}_{i}$ corresponding to the observations at time $t_{i}$.
- The 4D-Var cost function is:

$$
J(\mathbf{x})=\frac{1}{2}\left(\mathbf{x}_{0}-\mathbf{x}_{b}\right)^{T} \mathbf{B}^{-1}\left(\mathbf{x}_{0}-\mathbf{x}_{b}\right)+\frac{1}{2} \sum_{i=0}^{n}\left[\mathcal{H}_{i}\left(\mathbf{x}_{i}\right)-\mathbf{y}_{i}\right]^{T} \mathbf{R}_{i}^{-1}\left[\mathcal{H}_{i}\left(\mathbf{x}_{i}\right)-\mathbf{y}_{i}\right]
$$

- $\mathcal{H}_{i}$ represents a spatial interpolation and transformation from model variables to observed variables (i.e. a 3D-Var-style observation operator).


## Strong Constraint 4D-Var

- The states at various times are not independent: they are related through the forecast model:

$$
\mathbf{x}_{i}=\mathcal{M}_{i}\left(\mathbf{x}_{i-1}\right)
$$

where $\mathcal{M}_{i}$ is the forecast model integrated from time $t_{i-1}$ to time $t_{i}$.

- By introducing the vectors $\mathbf{x}_{i}$, the unconstrained minimization problem:

$$
\mathbf{x}_{a}=\arg \min _{\mathbf{x}} J(\mathbf{x})
$$

became a strong constraints minimization problem:

$$
\begin{aligned}
\mathbf{x}_{a} & =\arg \min _{\mathbf{x}_{0}} J\left(\mathbf{x}_{0}, \mathbf{x}_{1}, \cdots, \mathbf{x}_{k}\right) \\
\text { subject to } \mathbf{x}_{i} & =\mathcal{M}_{i}\left(\mathbf{x}_{i-1}\right) \text { for } i=1, \ldots, n
\end{aligned}
$$

- This form of 4D-Var is called strong constraint 4D-Var.


## Strong Constraint 4D-Var

- The 4D-Var cost function is:

$$
\begin{aligned}
J\left(\mathbf{x}_{0}, \mathbf{x}_{1}, \ldots, \mathbf{x}_{k}\right) & =\frac{1}{2}\left(\mathbf{x}_{0}-\mathbf{x}_{b}\right)^{T} \mathbf{B}^{-1}\left(\mathbf{x}_{0}-\mathbf{x}_{b}\right) \\
& +\frac{1}{2} \sum_{i=0}^{n}\left[\mathcal{H}_{i}\left(\mathbf{x}_{i}\right)-\mathbf{y}_{i}\right]^{T} \mathbf{R}_{i}^{-1}\left[\mathcal{H}_{i}\left(\mathbf{x}_{i}\right)-\mathbf{y}_{i}\right]
\end{aligned}
$$

- 4D-Var determines the analysis state at every gridpoint and at every time within the analysis window i.e. a four-dimensional analysis of the available asynoptic data.
- In deriving strong constraint 4D-Var, we have assumed that the observation operators and the model are perfect.
- As a consequence of the perfect model assumption, the analysis corresponds to a trajectory (i.e. an integration) of the forecast model.
- We will remove this assumption in the next lecture.


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## Minimizing the cost function

- We want to minimize the cost function:

$$
J(\mathbf{x})=\frac{1}{2}\left(\mathbf{x}-\mathbf{x}_{b}\right)^{T} \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}_{b}\right)+\frac{1}{2}[\mathcal{H}(\mathbf{x})-\mathbf{y}]^{T} \mathbf{R}^{-1}[\mathcal{H}(\mathbf{x})-\mathbf{y}]
$$

- This is a very large-scale minimization problem $\left(\operatorname{dim}(\mathbf{x}) \approx 300 \times 10^{6}\right.$ for the operational system at ECMWF.)
- Derivative-free algorithms are too slow (because each function evaluation gives very limited information about the shape of the cost function and in which direction the minimum might be).
- Practical algorithms for minimizing the cost function require its gradient.
- The simplest gradient-based minimization algorithm is called steepest descent:
- Repeat until the gradient is sufficiently small:
- Define a descent direction: $\mathbf{d}_{k}=-\nabla J\left(\mathbf{x}_{k}\right)$.
- Find a step $\alpha_{k}$, (line search) for which $J\left(\mathbf{x}_{k}+\alpha \mathbf{d}_{k}\right)<J\left(\mathbf{x}_{k}\right)$.
- Set $\mathbf{x}_{k+1}=\mathbf{x}_{k}+\alpha \mathbf{d}_{k}$.


## Minimizing the cost function

- Steepest descent can work well on very well conditioned problems in which the iso-surfaces of the cost function are nearly spherical.
- In this case, the steepest descent direction points towards the minimum.
- For poorly conditioned problems, with ellipsoidal iso-surfaces, steepest descent is not efficient.



## Minimizing the cost function

- Steepest Descent is inefficient because it does not use information about the curvature (i.e. the second derivatives) of the cost function.
- The simplest algorithm that uses curvature is Newton's method.
- Newton's method uses a local quadratic approximation:

$$
J(\mathbf{x}+\delta \mathbf{x}) \approx J(\mathbf{x})+\delta \mathbf{x}^{T} \nabla J(\mathbf{x})+\frac{1}{2} \delta \mathbf{x}^{T} J^{\prime \prime} \delta \mathbf{x}
$$

- Taking the gradient gives:

$$
\nabla J(\mathbf{x}+\delta \mathbf{x}) \approx \nabla J(\mathbf{x})+J^{\prime \prime} \delta \mathbf{x}
$$

- Since the gradient is zero at the minimum, Newton's method chooses the step at each iteration by solving:

$$
J^{\prime \prime} \delta \mathbf{x}=-\nabla J(\mathbf{x})
$$

- Newton's method works well for cost functions that are well approximated by a quadratic function (i.e. for quasi-linear observation operators).


## Minimizing the cost function

- Newton's method requires us to solve $J^{\prime \prime} \delta \mathbf{x}_{k}=-\nabla J\left(\mathbf{x}_{k}\right)$ at every iteration.
- $\mathrm{J}^{\prime \prime}$ is a $\sim 10^{8} \times 10^{8}$ matrix! Clearly, we cannot explicilty construct the matrix, or use direct methods to invert it.
- However, if we have a code that calculates Hessian-vector products, then we can use an iterative method (e.g. conjugate gradients) to solve for $\delta \mathbf{x}_{k}$.
- Such a code is called a second order adjoint. (See Wang, Navon, Le Dimet and Zou, 1992, Meteor. and Atmos. Phys.)
- Alternatively, some methods construct an approximation to $J^{\prime \prime}$ or $\left(J^{\prime \prime}\right)^{-1}$ : these methods are called quasi-Newton methods.
- The most popular quasi-Newton method are the BFGS algorithm, (named after its creators Broyden, Fletcher, Goldfarb and Shanno) and its variant, the limited memory BFGS method.


## Minimizing the cost function

- The methods presented so far apply to general nonlinear functions.
- An important special case occurs if the observation operator $\mathcal{H}$ is linear. In this case, the cost function is strictly quadratic, and the gradient is linear.
- In this case, it makes sense to determine the analysis by solving the linear equation $\nabla J(\mathbf{x})=0$.
- Since the matrix $J^{\prime \prime}=\mathbf{B}^{-1}+\mathbf{H}^{T} \mathbf{R}^{-1} \mathbf{H}$ is symmetric and positive definite, the best algorithm to use is conjugate gradients.
- A good introduction to the method can be found online: An Introduction to the Conjugate Gradient Method Without the Agonizing pain, Shewchuk (1994).
- This will be useful in the incremental 4D-Var.


## The Incremental Method

- A variant of the Newton method can be used: the nonlinear cost function is approximated by a quadratic cost function around the current guess. This quadratic cost function is minimized to provide an updated guess and the process is repeated.
- One complex problem is replaced by a series of (slightly) easier problems.

- The conjugate gradient algorithm can be used to solve efficiently the quadratic minimization problems.


## The Incremental Method

- The cost function is written as a function of the correction to the first guess (the increment) $\delta \mathbf{x}=\mathbf{x}-\mathbf{x}_{g}$ :

$$
\begin{aligned}
J\left(\mathbf{x}_{g}+\delta \mathbf{x}\right) & =\frac{1}{2}\left(\mathbf{x}_{g}+\delta \mathbf{x}-\mathbf{x}_{b}\right)^{T} \mathbf{B}^{-1}\left(\mathbf{x}_{g}+\delta \mathbf{x}-\mathbf{x}_{b}\right) \\
& +\frac{1}{2}\left[\mathcal{H}\left(\mathbf{x}_{g}+\delta \mathbf{x}\right)-\mathbf{y}\right]^{T} \mathbf{R}^{-1}\left[\mathcal{H}\left(\mathbf{x}_{g}+\delta \mathbf{x}\right)-\mathbf{y}\right]
\end{aligned}
$$

- The quadratic approximation of the cost function is obtained by linearizing around the curent guess:

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

where $\mathbf{b}=\mathbf{x}_{g}-\mathbf{x}_{b}, \mathbf{d}=\mathcal{H}\left(\mathbf{x}_{g}\right)-\mathbf{y}$ and $\mathbf{H}$ is the Jacobian of $\mathcal{H}$.

- The gradient is:

$$
\nabla J(\delta \mathbf{x})=\mathbf{B}^{-1}(\delta \mathbf{x}+\mathbf{b})+\mathbf{H}^{T} \mathbf{R}^{-1}(\mathbf{H} \delta \mathbf{x}+\mathbf{d})
$$

## Calculating the Gradient: Tangent Linear and Adjoint

- To minimize the cost function, we must be able to calculate its gradient:

$$
\nabla J(\delta \mathbf{x})=\mathbf{B}^{-1}(\delta \mathbf{x}+\mathbf{b})+\mathbf{H}^{T} \mathbf{R}^{-1}(\mathbf{H} \delta \mathbf{x}+\mathbf{d})
$$

- The Jacobians $\mathbf{H}$ and $\mathbf{H}^{T}$ are much too large to be represented explicitly: we can only represent these as operators (subroutines) that calculate matrix-vector products.
- These codes are called the tangent linear code for $\mathbf{H}$ and the adjoint code for $\mathbf{H}^{T}$.
- For a good introduction about writing adjoints, see: X. Y. Huang and X. Yang, 1996, Variational Data Assimilation with the Lorenz model, HIRLAM Technical Report 26.


## Writing the Adjoint Code

- Each line of the subroutine that applies $\mathcal{H}$ (including the forecast model) can be considered as a function $h_{k}$, so that

$$
\mathcal{H}(\mathbf{x}) \equiv h_{K} \circ h_{K-1} \circ \cdots \circ h_{1}(\mathbf{x})
$$

- Each of the functions $h_{k}$ can be linearized, to give the corresponding linear function $\mathbf{h}_{k}$. Each of these is extremely simple, and can be represented by one or two lines of code.
- The resulting code is called the tangent linear of $\mathcal{H}$ and:

$$
\mathbf{H} \delta \mathbf{x} \equiv \mathbf{h}_{K} \mathbf{h}_{K-1} \cdots \mathbf{h}_{1} \delta \mathbf{x}
$$

- The transpose, $\mathbf{H}^{T} \delta \mathbf{x} \equiv \mathbf{h}_{1}^{T} \mathbf{h}_{2}^{T} \cdots \mathbf{h}_{K}^{T} \delta \mathbf{x}$, is called the adjoint of $\mathcal{H}$.
- Again, each $\mathbf{h}_{k}^{T}$ is extremely simple - just a few lines of code.
- The difficulties in writing an adjoint can come from:
- Non differentiable functions in the nonlinear cost function (model physics),
- The length of the code (automatic tools can help).


## The Incremental Method

- The 4D-Var cost function and its gradient can be evaluated for the cost of:
- one integration of the forecast model,
- one integration of the adjoint model.
- This cost is still prohibitive:
- A typical minimization requires between 10 and 100 iterations,
- The cost of the adjoint is typically 3 times that of the forward model.
- The cost of the analysis would be roughly equivalent to between 20 and 200 days of model integration (with a 12 h window).
- The incremental algorithm reduces the cost of 4D-Var by reducing the resolution of the model and using simplified physics (or by using a perturbation forecast model).
- The analysis increments are calculated at reduced resolution and must be interpolated to the high-resolution model's grid.
- The departures $\mathbf{d}$ are always evaluated using the full-resolution versions of $\mathcal{H}(\operatorname{and} \mathcal{M})$ i.e. the observations are always compared with the full resolution state.


## Incremental 4D-Var



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## Preconditioning

- We noted that the steepest descent method works best if the iso-surfaces of the cost function are approximately spherical. This is generally true of all minimization algorithms.
- The degree of sphericity of the cost function can be measured by the eigenvalues of the Hessian. (Each eigenvalue corresponds to the curvature in the direction of the corresponding eigenvector.)
- In particular, the convergence rate will depend on the condition number:

$$
\kappa=\lambda_{\max } / \lambda_{\min }
$$

- The convergence can be accelerated by reducing the condition number of the Hessian.
- The Hessian of the 4D-Var cost function is $J^{\prime \prime}=\mathbf{B}^{-1}+\mathbf{H}^{T} \mathbf{R}^{-1} \mathbf{H}$ (plus higher order terms).


## Preconditioning

- We can speed up the convergence of the minimization by a change of variables $\chi=\mathbf{L}^{-1} \delta \mathbf{x}$ (i.e. $\delta \mathbf{x}=\mathbf{L} \chi$ ), where $\mathbf{L}$ is chosen to make the cost function more spherical.
- A common choice is $\mathbf{L}=\mathbf{B}^{1 / 2}$.
- The 4D-Var cost function becomes:

$$
J(\chi)=\frac{1}{2} \chi^{T} \chi+\frac{1}{2}(\mathbf{H} \mathbf{L} \chi-\mathbf{d})^{T} \mathbf{R}^{-1}(\mathbf{H} \mathbf{L} \chi-\mathbf{d})
$$

- With this change of variables, the Hessian becomes:

$$
J_{\chi}^{\prime \prime}=\mathbf{I}+\mathbf{L}^{\top} \mathbf{H}^{\top} \mathbf{R}^{-1} \mathbf{H} \mathbf{L}
$$

- The presence of the identity matrix in this expression guarantees that all eigenvalues are $\geq 1$.
- There are no small eigenvalues to destroy the conditioning of the problem.


## A case of poor convergence

- First experiments with direct assimilation of Meteosat radiance data showed significant analysis differences far away from observations.
- Differences disappeared when the number of iterations was increased: they were the result of insufficiant convergence.
- The conditioning of 4D-Var had been degraded by the inclusion of Meteosat radiance data.


## Theoretical example

- Analysis of one variable at two locations.
- Background error $\sigma_{b}$ with correlation $\alpha$ between the two points.
- $n$ observations at each point with observation error $\sigma_{o}\left(\mathbf{R}=\sigma_{o}^{2} \mathbf{I}\right)$.
- Observation operator $\mathbf{H}$ is a $2 n \times 2$ matrix with $n$ rows equal to (10) and $n$ rows equal to ( 011 ). This gives $\mathbf{H}^{T} \mathbf{R}^{-1} \mathbf{H}=n \mathbf{I} / \sigma_{o}^{2}$.
- The condition number is:

$$
\kappa=\frac{\sigma_{b}^{2}(1+\alpha)+\sigma_{o}^{2} / n}{\sigma_{b}^{2}(1-\alpha)+\sigma_{o}^{2} / n}
$$

- If the grid points are close, $\alpha \approx 1$ and $\kappa=2 n\left(\sigma_{b} / \sigma_{o}\right)^{2}+1$.
- The conditioning of the problem deteriorates with:
- increasing data density (larger n),
- larger background error $\left(\sigma_{b}\right)$,
- more accurate data (smaller $\sigma_{o}$ ).


## A case of poor convergence

- The lack of convergence with Meteosat data was traced back to too large humidity background error in very dry areas.


| Condition Number | Original bg error | Modified bg error |
| :---: | :---: | :---: |
| Without Meteosat data | 2229 | 2208 |
| With Meteosat data | 4495 | 2232 |

- Is there a more systematic way of achieving good preconditioning?


## Hessian Preconditioning

- The incremental cost function can be written as:

$$
J(\delta \mathbf{x})=\frac{1}{2} \delta \mathbf{x}^{T} J^{\prime \prime} \delta \mathbf{x}+\mathbf{g}^{T} \delta \mathbf{x}+c
$$

- Preconditioning replaces $J(\mathbf{x})$ by:

$$
J_{\chi}(\chi)=\frac{1}{2} \chi^{T} \mathbf{L}^{T} J^{\prime \prime} \mathbf{L} \chi+\mathbf{g}^{T} \mathbf{L} \chi+c
$$

- The difficulty is to find $\mathbf{L}$ such that $\kappa\left(\mathbf{L}^{T} J^{\prime \prime} \mathbf{L}\right) \ll \kappa\left(J^{\prime \prime}\right)$
- A perfect preconditioner would be $\mathbf{L}=\left(J^{\prime \prime}\right)^{-1 / 2}$. (If $\kappa\left(\mathbf{L}^{T} J^{\prime \prime} \mathbf{L}\right)=1$, the minimisation converges in one iteration.)
- Is there an approximation of the Hessian that can easily be inverted?


## Hessian Eigenvectors Preconditioning

- The Hessian can be written as: $J^{\prime \prime}=\sum_{k=1}^{N} \lambda_{k} \mathbf{v}_{k} \mathbf{v}_{k}^{T}$ where $\lambda_{k}$ and $\mathbf{v}_{k}$ are its eigenvalues and eigenvectors.
- Preconditioning based on the $K$ leading eigenvectors of $J^{\prime \prime}$ :

$$
\begin{gathered}
\mathbf{L}^{-1}=\mathbf{I}+\sum_{k=1}^{K}\left(\mu_{k}^{1 / 2}-1\right) \mathbf{v}_{k} \mathbf{v}_{k}^{T} \\
\text { gives } J_{\chi}^{\prime \prime}=\sum_{k=1}^{K} \mu_{k} \lambda_{k} \mathbf{v}_{k} \mathbf{v}_{k}^{T}+\sum_{k=K+1}^{N} \lambda_{k} \mathbf{v}_{k} \mathbf{v}_{k}^{T} .
\end{gathered}
$$

- Choose $\mu_{k}$ verifying $\mu_{k} \lambda_{k}<\lambda_{K+1}$, then

$$
\kappa\left(J_{\chi}^{\prime \prime}\right)=\lambda_{K+1} / \lambda_{N}=\lambda_{K+1} .
$$

- The eigenvectors can be computed using the Lanczos method, which is very closely related to the conjugate gradient algorithm.


## Conjugate Gradient and Lanczos Algorithm

- The relation between Conjugate Gradient and Lanczos Algorithms allows to simultaneously:
- Minimise the cost function,
- Compute the eigenvectors and eigenvalues of the Hessian.
- The connection can be exploited to improve the minimisation:
- At each outer loop iteration, the eigenvectors and eigenvalues of the Hessian can be computed,
- They are used to precondition the minimisation in the following outer loop iteration.
- The 4D-Var eigenvectors are large scale:
- They can be computed at low resolution and used to precondition a higher resolution miminization.
- This leads to multi-incremental algorithm.
- It only applies to strictly quadratic inner loop cost functions: Var QC, QuickScat ambiguous winds in outer loop.


## Superlinear Convergence and Rounding Error

- When $\lambda_{\text {max }}$ or $\lambda_{\text {min }}$ has converged in the Lanczos process, $J(\mathbf{x})$ has been fully minimised in the direction of the eigenvector.
- The minimisation then behaves as if it were minimising a problem with a smaller condition number $\kappa=\lambda_{\text {max }} / \lambda_{\text {min }}$.
- Conjugate Gradients should converge superlinearly.
- In practice, rounding errors spoil things, making the convergence linear.
- Rounding error causes the Lanczos algorithm to produce spurious multiple copies of eigenvectors.
- The two effects are connected.
- A well-known method of preventing spurious multiple eigenvalues in the Lanczos algorithm is to explicitely orthogonalise the gradient vectors. This method also restores superlinear convergence in CG.


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## Operational 4D-Var Setup

- Strong constraint 4D-Var has been used in operations at ECMWF since 25 Nov. 1997.
- The current configuration uses a 12 h cycling window.
- The outer loop (and forecast) resolution is T799 ( 25 km ).
- The inner loops resolutions are T95, T159 and T255 (200, 125 and 80 km ).
- On average, 9 million observations are assimilated per 12 h cycle.
- $96 \%$ of assimilated data is from satellites.
- On average, 4D-Var runs on 1536 CPUs in 1h10.


## Observation Coverage



6 February 2009 00 UTC $\pm 3 h$

## Observation Sources



Assimilating new data types requires a lot of ressources (developments and computer time).

## Observation Numbers



Observation numbers have increased regularly and will increase even faster in the future.

## Observation Usage

Data count for one 12h 4D-Var cycle (0900-2100 UTC, 3 March 2008)

|  | Screened |  | Assimilated |  |
| :--- | ---: | ---: | ---: | ---: |
| Synop: | 450,000 | $0.3 \%$ | 64,000 | $0.7 \%$ |
| Aircraft: | 434,000 | $0.3 \%$ | 215,000 | $2.4 \%$ |
| Dribu: | 24,000 | $0.02 \%$ | 7,000 | $0.1 \%$ |
| Temp: | 153,000 | $0.1 \%$ | 76,000 | $0.8 \%$ |
| Pilot: | 86,000 | $0.1 \%$ | 39,000 | $0.4 \%$ |
| AMV's: | $2,535,000$ | $1.6 \%$ | 125,000 | $1.4 \%$ |
| Radiance data: | $150,663,000$ | $96.9 \%$ | $8,207,000$ | $91.0 \%$ |
| Scat: | 835,000 | $0.5 \%$ | 149,000 | $1.7 \%$ |
| GPS radio occult. | 271,000 | $0.2 \%$ | 137,000 | $1.5 \%$ |
| TOTAL: | $155,448,000$ | $100.0 \%$ | $9,018,000$ | $100.0 \%$ |

We are still far from using all available observations.

## Performance



Forecast performance has increased regularly over the years.

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## Summary

- The Maximum Likelihood approach is general and can be in principle be applied to non-Gaussian, nonlinear analysis.
- 3D-Var and 4D-Var derive from the maximum likelihood principle.
- 4D-Var is an extension of 3D-Var to the case where observations are distributed in time.
- The cost function is minimized using algorithms based on knowledge of its gradient.
- The incremental method with appropriate preconditioning allows the computational cost to be reduced to acceptable levels.
- In strong constraint 4D-Var the model is assumed to be perfect, so that the four-dimensional analysis state corresponds to an integration (trajectory) of the model.


## Summary

- Most (all?) of the main NWP centres run variational data assimilation schemes operationally.
- ECMWF, United Kingdom, France, Germany, Canada, USA (NCEP, NRL, GMAO), Japan, Korea, Taiwan, China, Australia, HIRLAM countries, ALADIN countries...
- Forecast performance has improved over the years, in particular because of the ability of variational systems to adapt to and benefit from the varying components of the global observing system.
- Other aspects are important but were not covered in this talk:
- Modelling of B and balance considerations,
- Definition of the observation operators,
- Observation variational bias correction.

