



A Bayesian view of Data Assimilation

JCSDA Summer School.

Andrew Lorenc, Stevenson WA. July 2009.



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- Gaussian PDFs

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- Two gridpoints, one observation.

3. Issues in practical implementation

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- Solving the large matrix equation
- Estimating **B**.

4. Predicting the prior PDF

- a Bayesian view of 4D-Var v Ensemble KF



Bayes Theorem – adding information

Gaussian PDFs

(Non-Gaussian observational errors - Quality Control will be covered in another lecture.)



Met Office

Bayes' Theorem for Discrete Events

A B

events

$P(A)$

probability of A occurring, or
knowledge about A 's past occurrence

$P(A \cap B)$

probability that A and B both occur,

$P(A | B)$

conditional probability of A given B

We have two ways of expressing $P(A \cap B)$:

$$P(A \cap B) = P(B) P(A | B) = P(A) P(B | A)$$

\Rightarrow Bayes' Theorem:
$$P(A | B) = \frac{P(B | A) P(A)}{P(B)}$$

Can calculate $P(B)$ from:
$$P(B) = P(B | A)P(A) + P(B | \bar{A})P(\bar{A})$$



Bayes theorem in continuous form,
to estimate a value x given an observation y^o

$$p(x | y^o) = \frac{p(y^o | x)p(x)}{p(y^o)}$$

$p(x | y^o)$ is the **posterior** distribution,
 $p(x)$ is the **prior** distribution,
 $p(y^o | x)$ is the **likelihood** function for x

Can get $p(y^o)$ by integrating over all x : $p(y^o) = \int p(y^o | x)p(x)dx$



Assume Gaussian pdfs

Prior is Gaussian with mean x^b , variance V_b : $x \sim N(x^b, V_b)$

$$p(x) = (2\pi V_b)^{-\frac{1}{2}} \exp\left(-\frac{1}{2} \frac{(x - x^b)^2}{V_b}\right)$$

Ob y^o , Gaussian about true value x variance V_o : $y^o \sim N(x, V_o)$

$$p(y^o | x) = (2\pi V_o)^{-\frac{1}{2}} \exp\left(-\frac{1}{2} \frac{(y^o - x)^2}{V_o}\right)$$

Substituting gives a Gaussian posterior: $x \sim N(x^a, V_a)$

$$p(x) = (2\pi V_a)^{-\frac{1}{2}} \exp\left(-\frac{1}{2} \frac{(x - x^a)^2}{V_a}\right)$$



Advantages of Gaussian assumption

1. Best estimate is found by solving linear equations:

$$\frac{1}{V_a} = \frac{1}{V_o} + \frac{1}{V_b} \qquad \frac{1}{V_a} x^a = \frac{1}{V_o} y^o + \frac{1}{V_b} x^b$$

$$p(x) = (2\pi V_a)^{-\frac{1}{2}} \exp\left(-\frac{1}{2} \frac{(x - x^a)^2}{V_a}\right)$$

Taking logs gives quadratic equation; differentiating to find extremum gives linear equation.

2. Best estimate is a function of values & [co-]variances only.

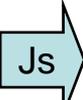
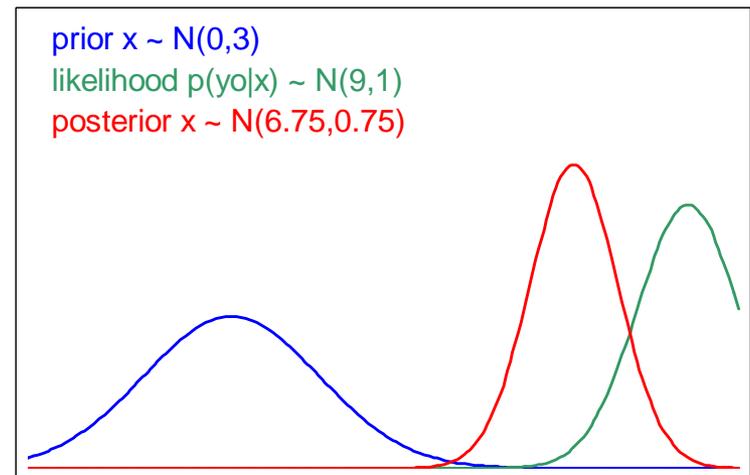
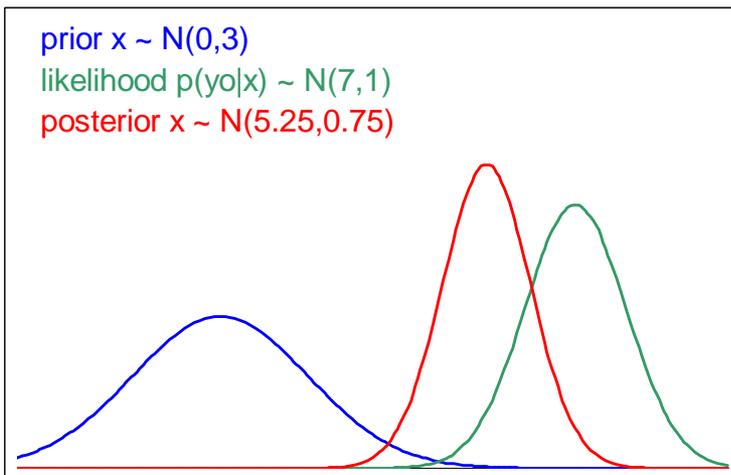
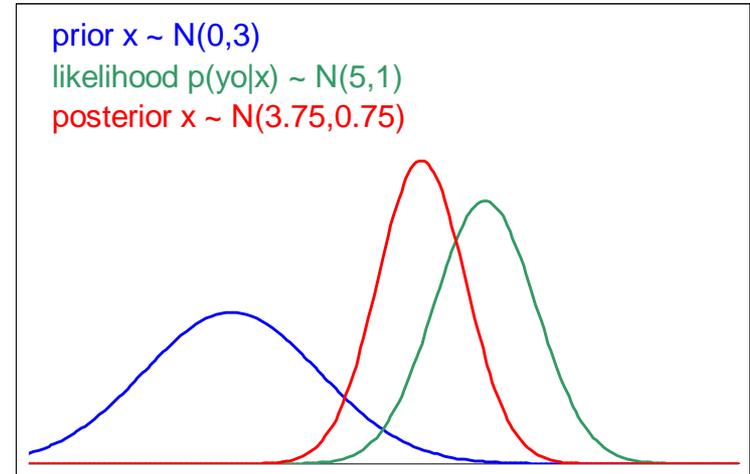
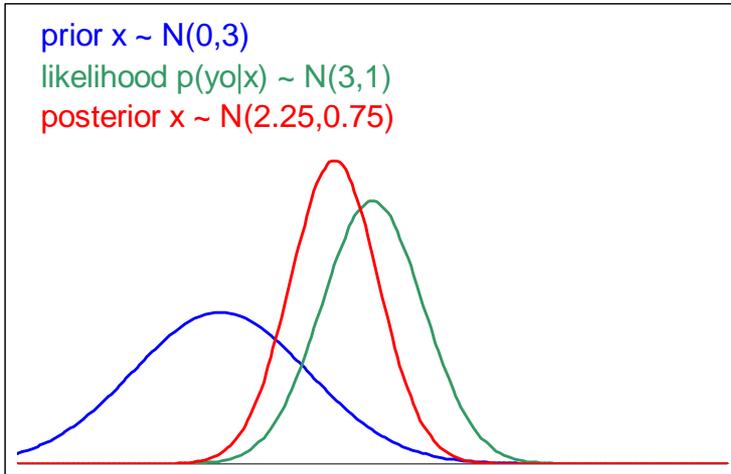
Often these are all we know.

3. Weights are independent of values.



Combination of Gaussian prior & observation

- Gaussian posterior,
- weights independent of values.



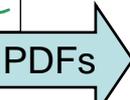
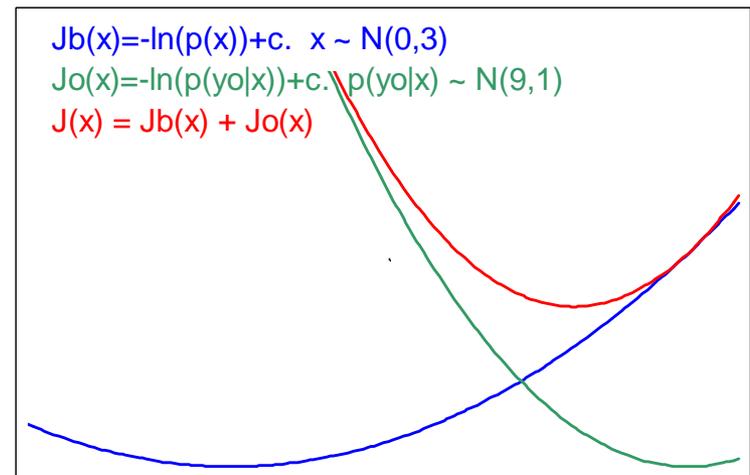
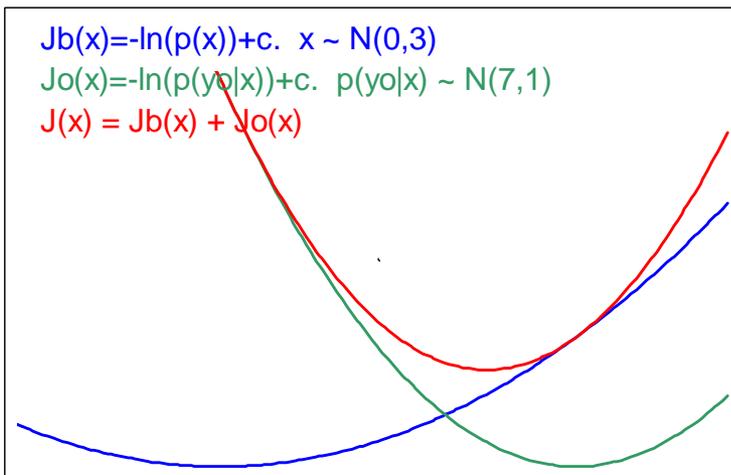
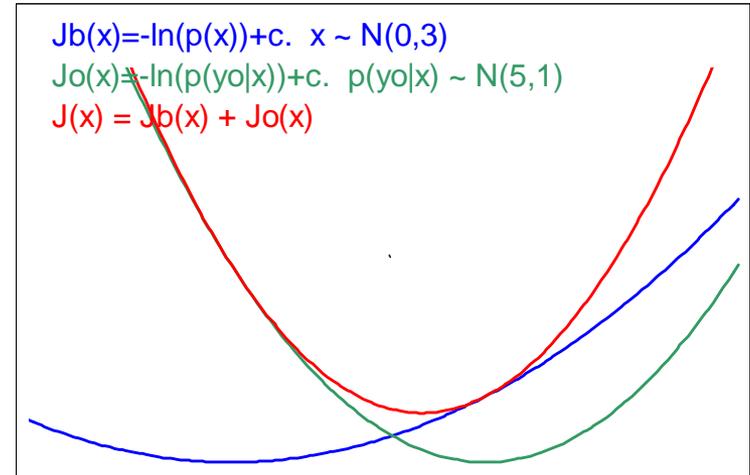
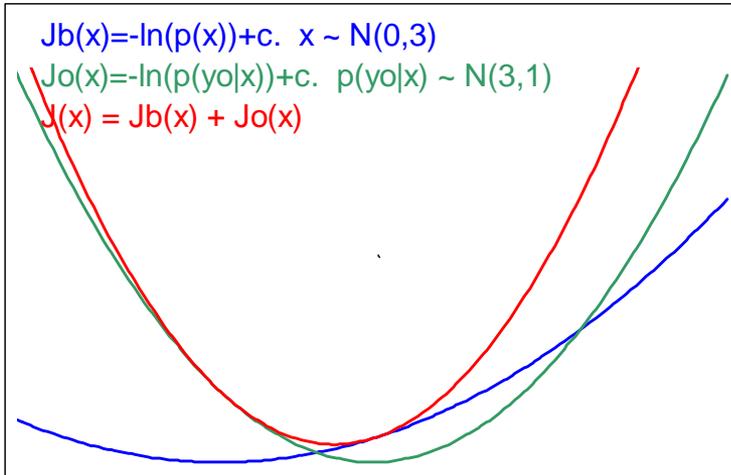


Variational Penalty Functions

- Finding the most probable posterior value involves maximising a product [of Gaussians]
- By taking $-\ln$ of the posterior PDF, we can instead minimise a sum [of quadratics]
- This is often called the “Penalty Function” J
- Additive constants can be ignored



Penalty functions: $J(x) = -\ln(p(x)) + c$ p Gaussian $\Rightarrow J$ quadratic





Simplest possible Bayesian NWP analysis



Simplest possible example – 2 grid-points, 1 observation. Standard notation:

Ide, K., Courtier, P., Ghil, M., and Lorenc, A.C. 1997: "Unified notation for data assimilation: Operational, Sequential and Variational" *J. Met. Soc. Japan*, Special issue "Data Assimilation in Meteorology and Oceanography: Theory and Practice." **75**, No. 1B, 181—189

Model is two grid points:

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

1 observed value y^o midway (but use notation for >1):

$$\mathbf{y}^o = (y^o)$$

Can interpolate an estimate y of the observed value:

$$\mathbf{y} = H(\mathbf{x}) = \frac{1}{2}x_1 + \frac{1}{2}x_2 = \mathbf{H}\mathbf{x} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

This example H is linear, so we can use matrix notation for fields as well as increments.



Met Office

background pdf

We have prior estimate x_1^b with error variance V_b :

$$p(x_1) = (2\pi V_b)^{-\frac{1}{2}} \exp\left(-\frac{1}{2} (x_1 - x_1^b)^2 / V_b\right)$$

$$p(x_2) = (2\pi V_b)^{-\frac{1}{2}} \exp\left(-\frac{1}{2} (x_2 - x_2^b)^2 / V_b\right)$$

But errors in x_1 and x_2 are usually correlated
 \Rightarrow must use a multi-dimensional Gaussian:

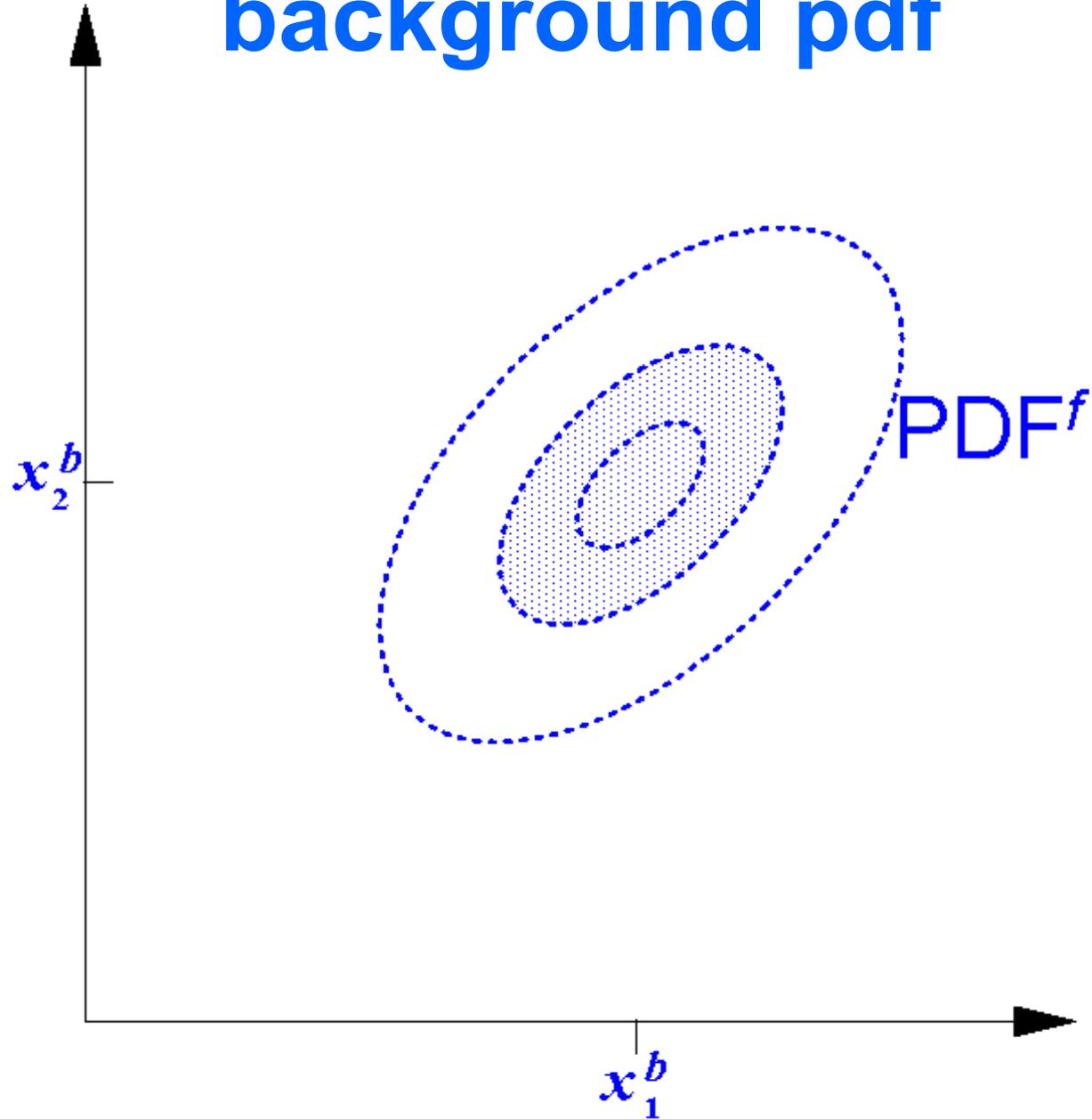
$$\mathbf{x} \sim N(\mathbf{x} : \mathbf{x}^b, \mathbf{B})$$

$$p(x_1 \cap x_2) = p(\mathbf{x}) = \left((2\pi)^2 |\mathbf{B}| \right)^{-\frac{1}{2}} \exp\left(-\frac{1}{2} (\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}^b) \right)$$

where \mathbf{B} is the covariance matrix:

$$\mathbf{B} = V_b \begin{pmatrix} 1 & \mu \\ \mu & 1 \end{pmatrix}$$

background pdf





Observational errors

Lorenc, A.C. 1986: "Analysis methods for numerical weather prediction."
Quart. J. Roy. Met. Soc., **112**, 1177-1194.

instrumental error

$$\mathbf{y}^o \sim N(\mathbf{y}^t, \mathbf{E})$$

$$p(\mathbf{y}^o | \mathbf{y}) = (2\pi |\mathbf{E}|)^{-\frac{1}{2}} \exp\left(-\frac{1}{2} (\mathbf{y}^o - \mathbf{y})^T \mathbf{E}^{-1} (\mathbf{y}^o - \mathbf{y})\right)$$

error of representativeness

$$\mathbf{y} \sim N(H(\mathbf{x}^t), \mathbf{F})$$

$$p_t(\mathbf{y} | \mathbf{x}^t) = (2\pi |\mathbf{F}|)^{-\frac{1}{2}} \exp\left(-\frac{1}{2} (\mathbf{y} - H(\mathbf{x}^t))^T \mathbf{F}^{-1} (\mathbf{y} - H(\mathbf{x}^t))\right)$$

Observational error

$$\mathbf{y}^o \sim N(H(\mathbf{x}^t), \mathbf{E} + \mathbf{F})$$

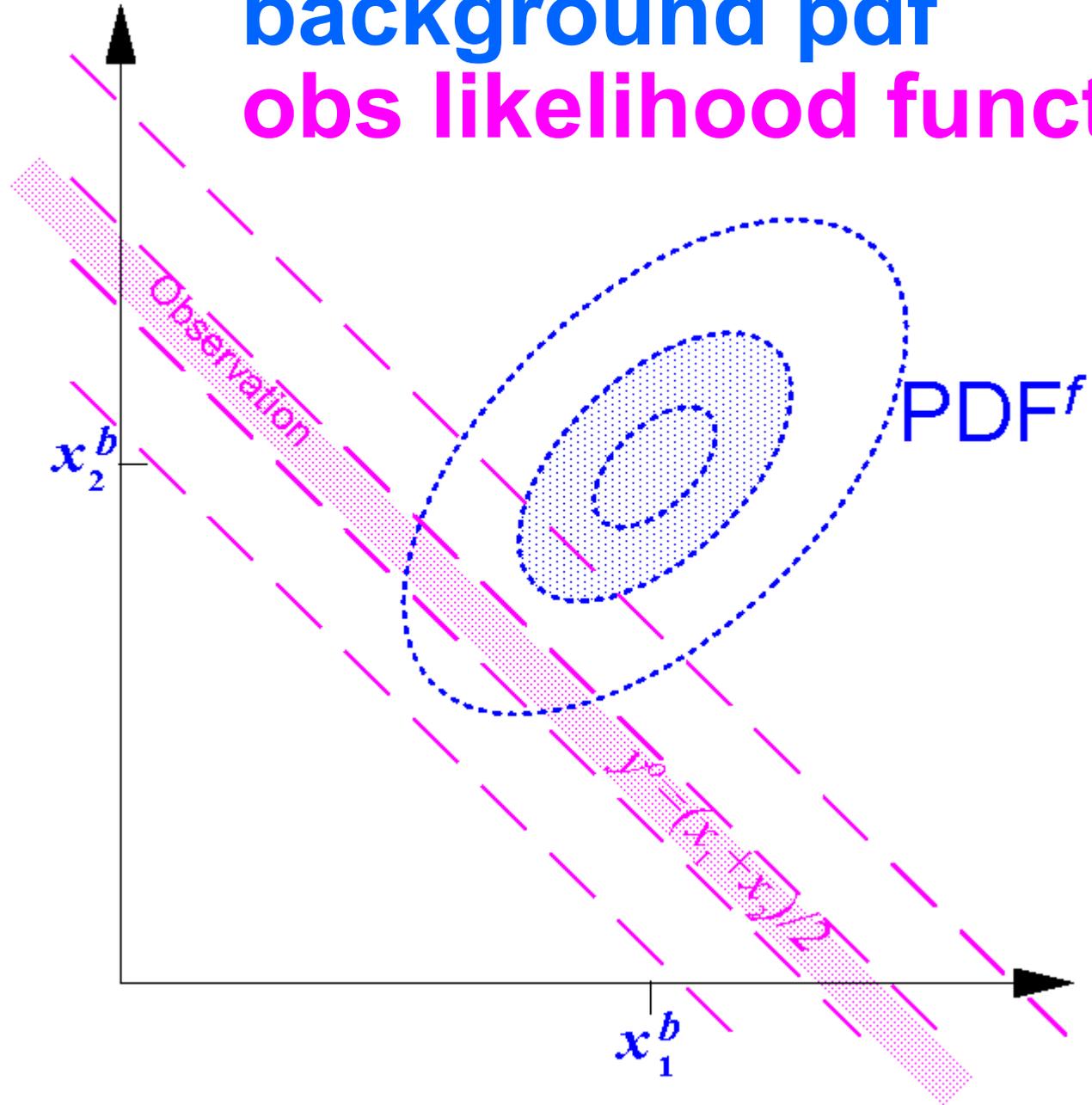
combines these 2 :

$$p(\mathbf{y}^o | \mathbf{x}^t) = \int p(\mathbf{y}^o | \mathbf{y}) p_t(\mathbf{y} | \mathbf{x}^t) d\mathbf{y}$$

$$= (2\pi |\mathbf{E} + \mathbf{F}|)^{-\frac{1}{2}} \exp\left(-\frac{1}{2} (\mathbf{y}^o - H(\mathbf{x}^t))^T (\mathbf{E} + \mathbf{F})^{-1} (\mathbf{y}^o - H(\mathbf{x}^t))\right)$$

background pdf

obs likelihood function





Bayesian analysis equation

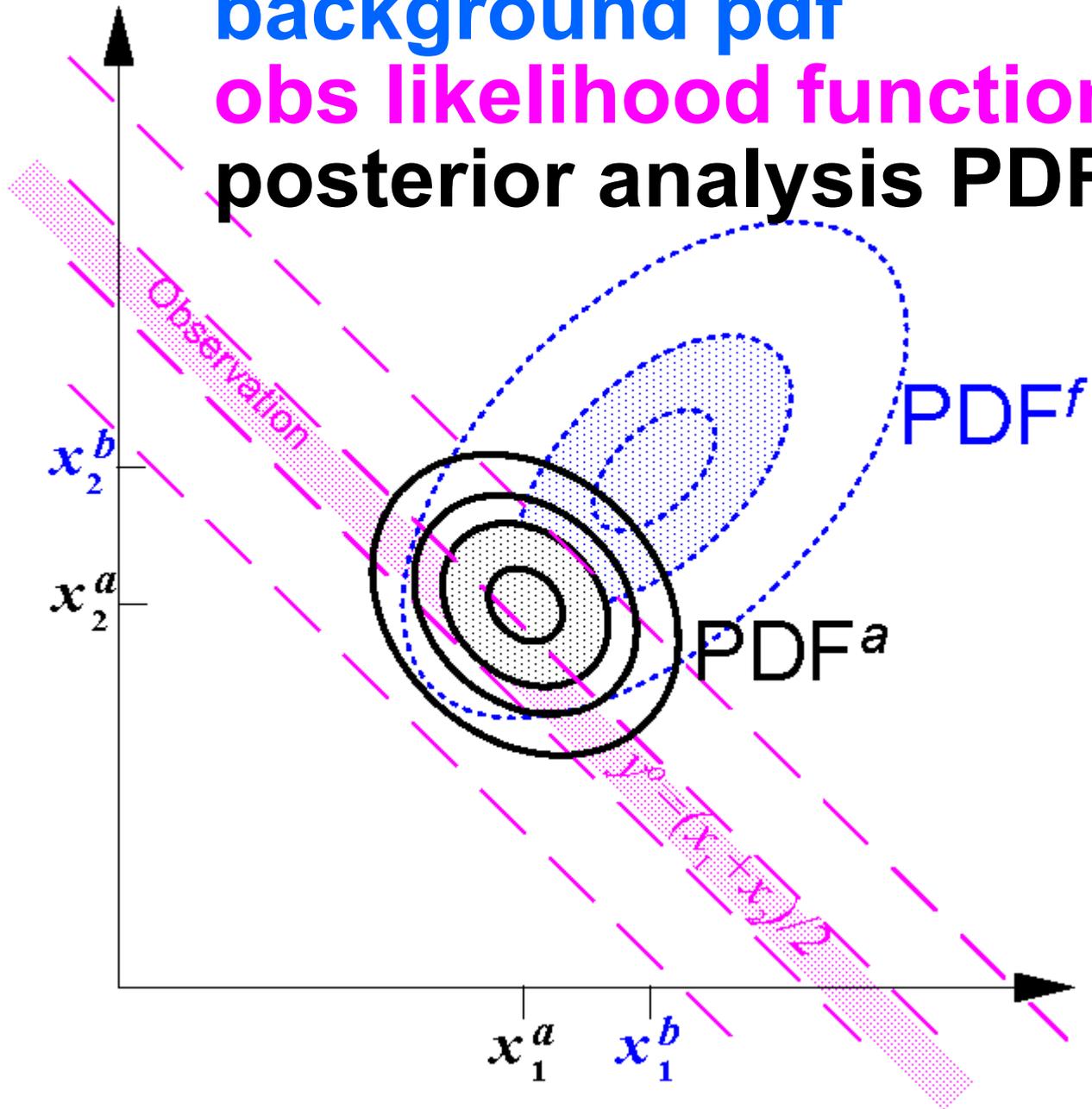
$$p(\mathbf{x}|\mathbf{y}^o) = \frac{p(\mathbf{y}^o|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y}^o)}$$

Property of Gaussians that, if H is linearisable : $\mathbf{x} \sim N(\mathbf{x}^a, \mathbf{A})$

where \mathbf{x}^a and \mathbf{A} are defined by:

$$\mathbf{A}^{-1} = \mathbf{B}^{-1} + \mathbf{H}^T (\mathbf{E} + \mathbf{F})^{-1} \mathbf{H}$$
$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{A} \mathbf{H}^T (\mathbf{E} + \mathbf{F})^{-1} (\mathbf{y}^o - H(\mathbf{x}^b))$$

background pdf
obs likelihood function
posterior analysis PDF





Analysis equation

For our simple example the algebra is easily done by hand, without manipulating matrices, giving:

$$\mathbf{x}^a = \begin{pmatrix} x_1^a \\ x_2^a \end{pmatrix} = \begin{pmatrix} x_1^b \\ x_2^b \end{pmatrix} + \frac{\left(V^b \left(\frac{1+\mu}{2} \right) \right)^2}{\mathbf{E} + \mathbf{F} + V^b \left(\frac{1+\mu}{2} \right)} \left[y^o - \frac{x_1^b + x_2^b}{2} \right] \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$



Practical implementation of the Bayesian Analysis Equation



Issues in practical implementation

“The devil is in the details”

There are significantly different choices possible for each of the following options. The combinations of these choices make up a very wide range and large number of analysis schemes, all implementing the same Bayesian equation!

- Modelling and representing prior background error covariances **B**.
- Expressing the equations in a form amenable to solution.
- Computing the solution.
- Estimating **B**.



Michael Ghil on OI & Kalman Filter

Reprinted from Preprint Volume: Fifth
Conference on Numerical Weather Prediction,
Nov. 2-6, 1981; Monterey, Calif. Published
by the American Meteorological Society,
Boston, Mass.

OPTIMAL INTERPOLATION AND THE KALMAN FILTER

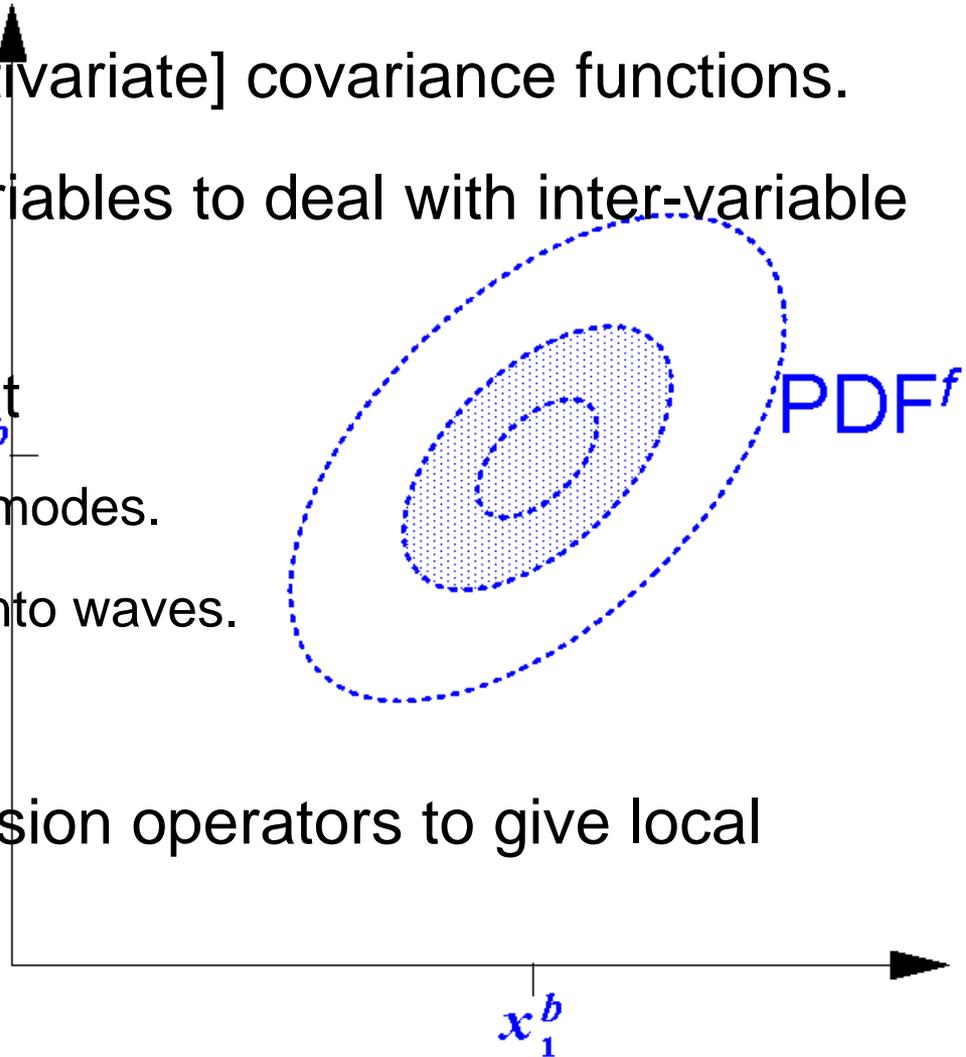
*are similar,
but the fun is in the difference.*

S. Cohn, M. Ghil* and E. Isaacson

Courant Institute of Mathematical Sciences
New York University, New York, New York 10012

Modelling and representing prior background error covariances **B**.

- Explicit point-point [multivariate] covariance functions.
- Transformed control variables to deal with inter-variable covariances.
- Vertical – horizontal split
 - EOF decomposition into modes.
 - Spectral decomposition into waves.
 - Wavelets.
- Recursive filters or diffusion operators to give local variations.
- Ensemble members.



Schlatter's (1975) multivariate

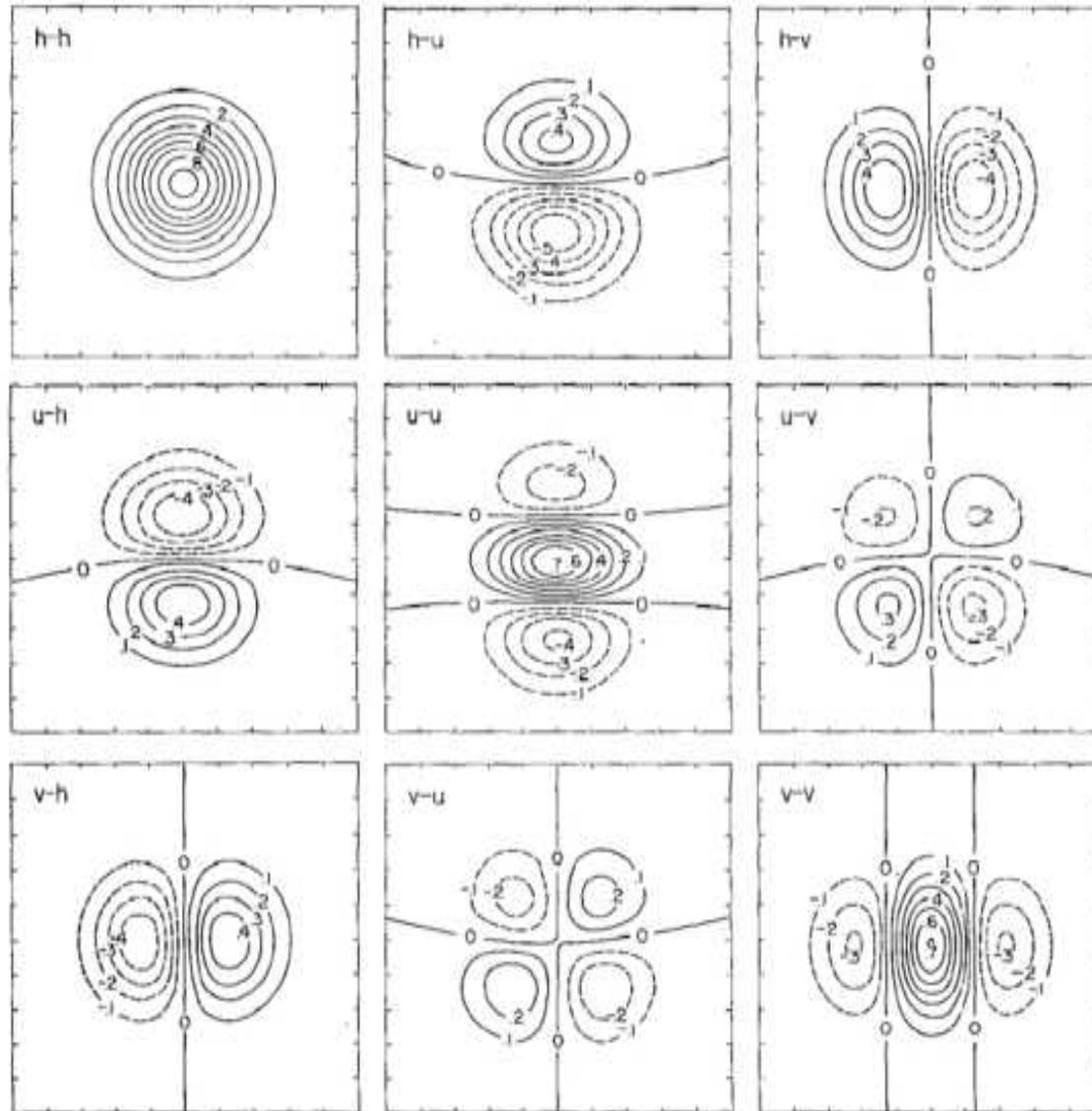


FIG. 3. Correlations among the variables h , u , and v based upon the expression $\mu = 0.95 \exp(-1.24r^2)$ for height-height correlation and the geostrophic relations. Diagrams centered at 110°W , 35°N . Tick marks 500 km apart.



Transformed control variable.

- Look for a “balanced” variable from which we can calculate balanced flow in all variables: streamfunction, PV.
- Define transforms from (\mathbf{U}) or to (\mathbf{T}) this variable and a residual variable, which by construction/hypothesis is uncorrelated making \mathbf{B} block diagonal. (Compare EOFs)
- Transformed variables still need spatial covariance model, but not multivariate. (Further transforms may be used to represent these.)

$$\delta \mathbf{x} = \mathbf{U}_p \begin{pmatrix} \psi \\ \chi \\ \mathbf{b} \end{pmatrix} = \mathbf{U}_p \mathbf{v}$$

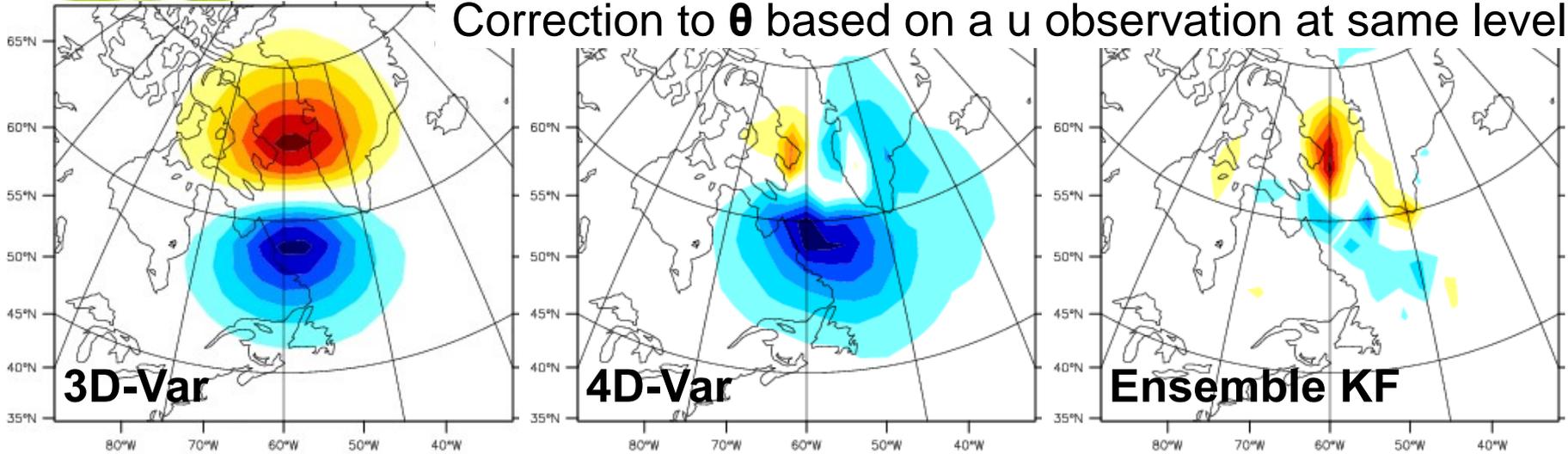
$$\mathbf{B}_{(\mathbf{v})} = \begin{pmatrix} \mathbf{B}_{(\psi)} & 0 & 0 \\ 0 & \mathbf{B}_{(\chi)} & 0 \\ 0 & 0 & \mathbf{B}_{(\mathbf{b})} \end{pmatrix}$$

$$\mathbf{B}_{(\mathbf{x})} = \mathbf{U}_p \mathbf{B}_{(\mathbf{v})} \mathbf{U}_p^T$$

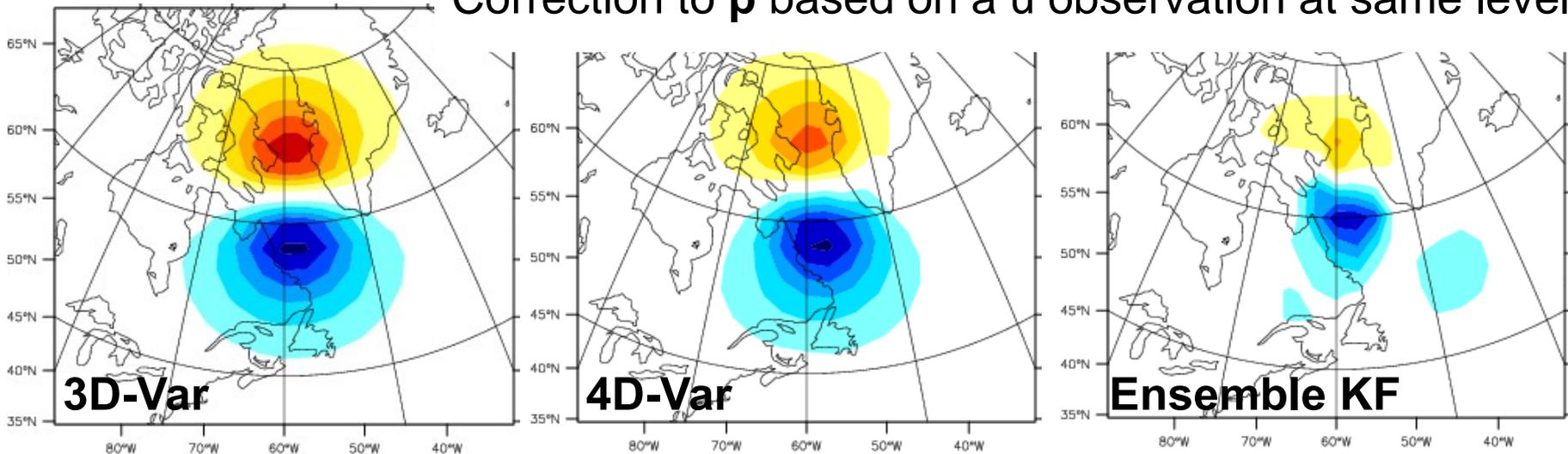


Comparison of covariance models

Correction to θ based on a u observation at same level



Correction to p based on a u observation at same level





Equations - all equivalent.

- Variational \mathbf{x}^a minimises $J(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}^b) + \frac{1}{2}(\mathbf{y}^o - H(\mathbf{x}))^T \mathbf{R}^{-1}(\mathbf{y}^o - H(\mathbf{x}))$

$$\mathbf{A}^{-1} = \left(\frac{\partial^2 J}{\partial \mathbf{x}^2} \right) = \mathbf{B}^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H}$$
- Kalman Filter. Kalman Gain= \mathbf{K} . $\mathbf{x}^a = \mathbf{x}^b + \mathbf{K}(\mathbf{y}^o - H(\mathbf{x}^b))$ $\mathbf{A} = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{B}$
- Observation space $\mathbf{K} = \mathbf{B}\mathbf{H}^T (\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R})^{-1}$
 Demonstrate equivalence using Sherman–Morrison–Woodbury formula
- Model space $\mathbf{K} = (\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} + \mathbf{B}^{-1})^{-1} \mathbf{H}^T \mathbf{R}^{-1}$
- Ensemble space Square-root Filters, e.g. ETKF

$$\mathbf{B} = \mathbf{Z}^f (\mathbf{Z}^f)^T$$

$$\mathbf{Z}^a = \mathbf{Z}^f \mathbf{T}$$

$$\mathbf{A} = \mathbf{Z}^a (\mathbf{Z}^a)^T$$



Estimating PDFs or covariances

- Even if we knew the “truth”, we could never run enough experiments in the lifetime of an NWP system to estimate its error PDF, or even its error covariance \mathbf{B} .
- Simplifying assumptions are essential (e.g. Gaussian, ...)
- Even a simplified error model has so many parameters that we cannot determine them by NWP trials to determine which give the best forecasts.
- In practice we can only measure innovations – cannot get separate estimates of \mathbf{B} & \mathbf{R} without assumptions (Talagrand).
- ***Need to understand physics!***

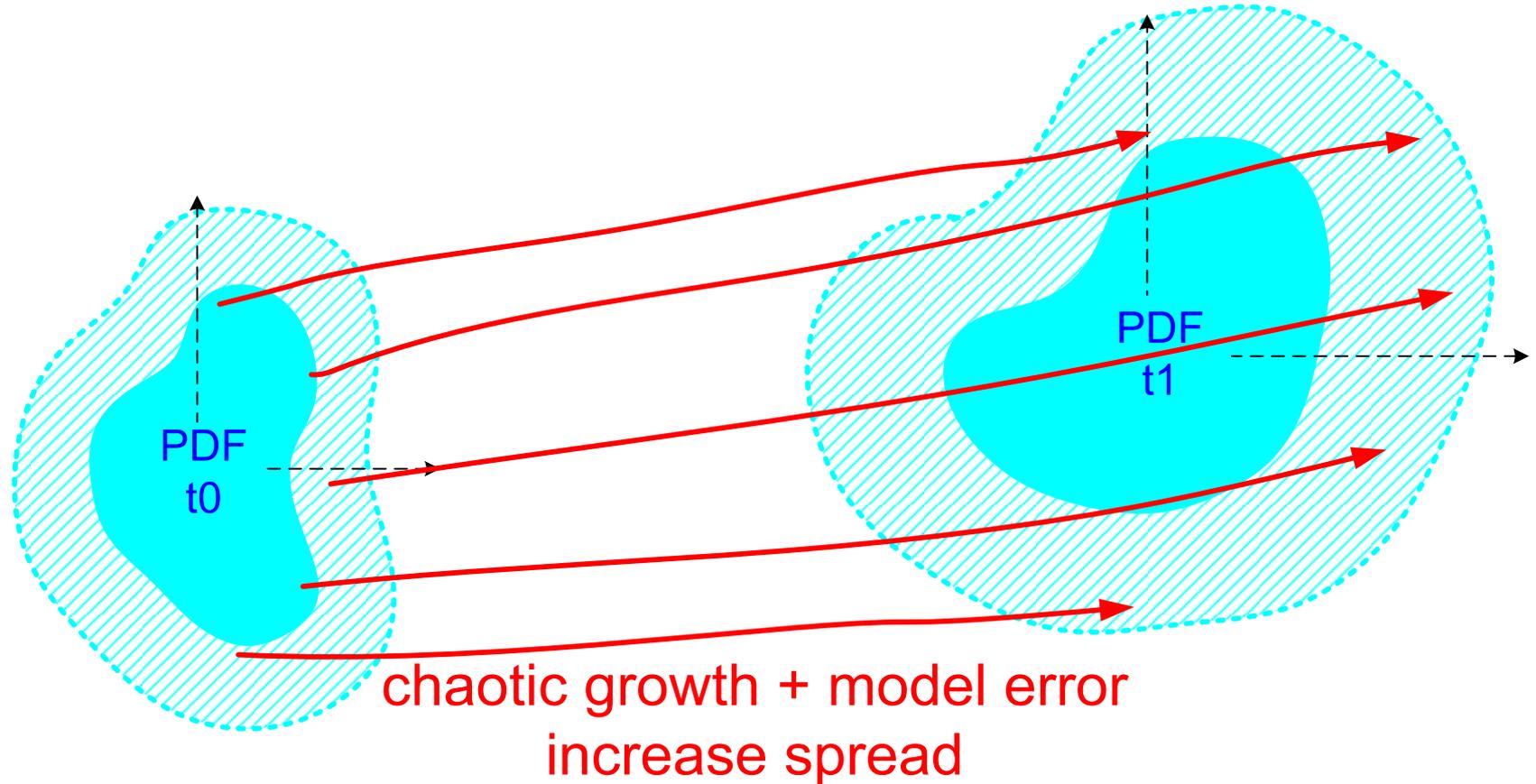


How to estimate the prior PDF?
How to calculate its time evolution?

i.e. 4D-Var versus Ensemble KF



Fokker-Planck Equation



Ensemble methods attempt to sample entire PDF.



Gaussian Probability Distribution Functions

- Easier to fit to sampled errors.
- Quadratic optimisation problems, with linear solution methods – much more efficient.
- The Kalman filter is optimal for linear models, but
 - it is not affordable for expensive models (despite the “easy” quadratic problem)
 - it is not optimal for nonlinear models.
- Advanced methods based on the Kalman filter can be made affordable:
 - Ensemble Kalman filter (EnKF, ETKF, ...)
 - Four-dimensional variational assimilation (4D-Var)



Extended Kalman Filter

\mathbf{x} is mean of PDF, \mathbf{P} is covariance.

Analysis step

$$\mathbf{x}^a(t_i) = \mathbf{x}^f(t_i) + \mathbf{P}^f(t_i) \mathbf{H}_i^T \left(\mathbf{H}_i \mathbf{P}^f(t_i) \mathbf{H}_i^T + \mathbf{R}_i \right)^{-1} \left(\mathbf{y}_i^o - H_i(\mathbf{x}^f(t_i)) \right)$$

$$\mathbf{P}^a(t_i) = \mathbf{P}^f(t_i) - \mathbf{P}^f(t_i) \mathbf{H}_i^T \left(\mathbf{H}_i \mathbf{P}^f(t_i) \mathbf{H}_i^T + \mathbf{R}_i \right)^{-1} \mathbf{H}_i \mathbf{P}^f(t_i)$$

Forecast step

$$\mathbf{x}^f(t_{i+1}) = M_i(\mathbf{x}^a(t_i))$$

True discretised dynamics \mathbf{x}^t assumed to differ by stochastic perturbations:

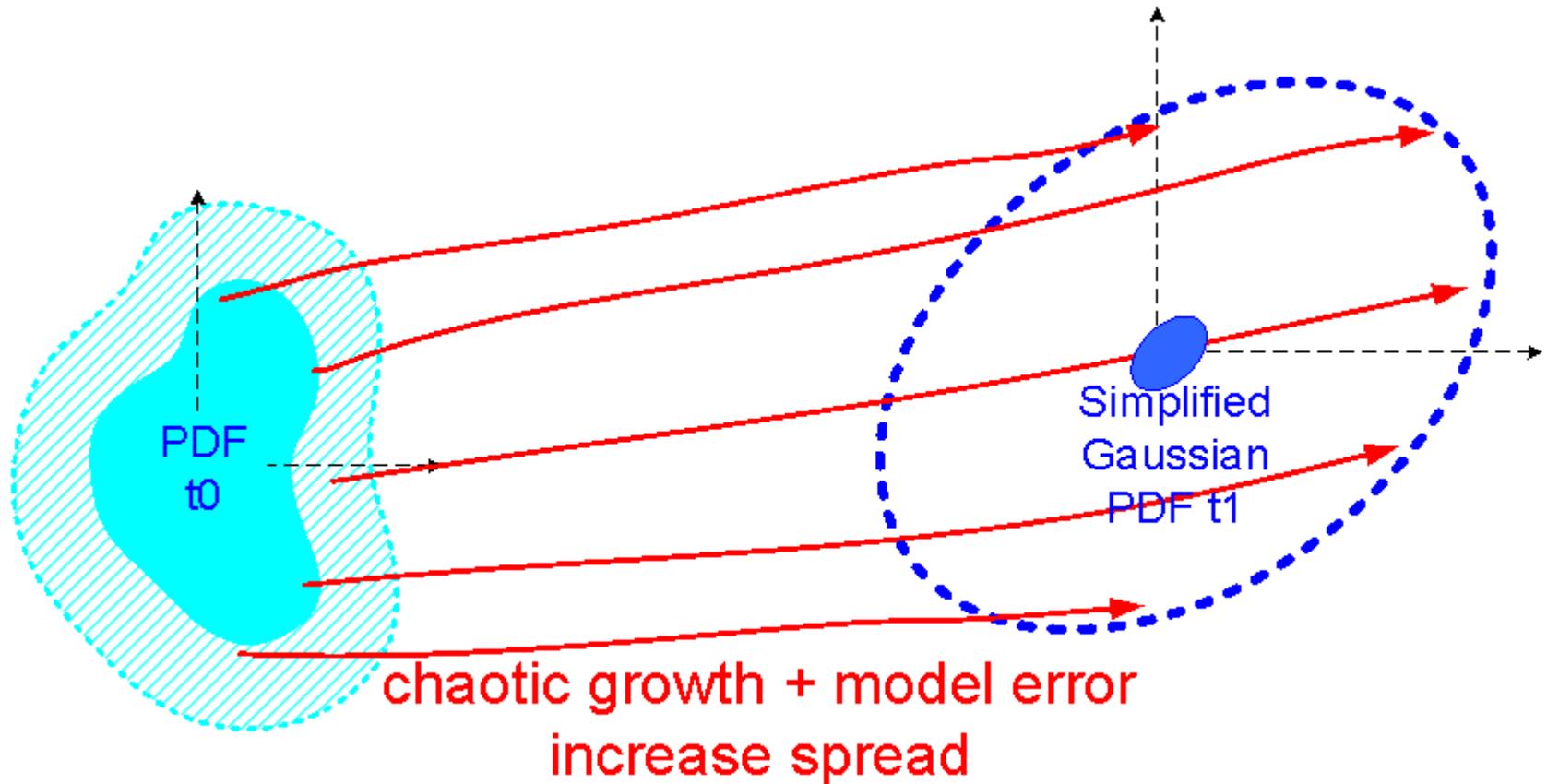
$$\mathbf{x}^t(t_{i+1}) = M_i(\mathbf{x}^t(t_i)) + \boldsymbol{\eta}(t_i)$$

where $\boldsymbol{\eta}$ is a noise process with zero mean and covariance matrix \mathbf{Q}_i .

$$\mathbf{P}^f(t_{i+1}) = \mathbf{M}_i \mathbf{P}^a(t_i) \mathbf{M}_i^T + \mathbf{Q}_i$$



Ensemble Kalman filter



Fit Gaussian to forecast ensemble.

The Ensemble Kalman Filter (EnKF)

Construct an ensemble $\{\mathbf{x}_i^f\}$, ($i = 1, \dots, N$) :

$$\mathbf{P}^f = \mathbf{P}_e^f = \overline{(\mathbf{x}^f - \overline{\mathbf{x}^f})(\mathbf{x}^f - \overline{\mathbf{x}^f})^T},$$

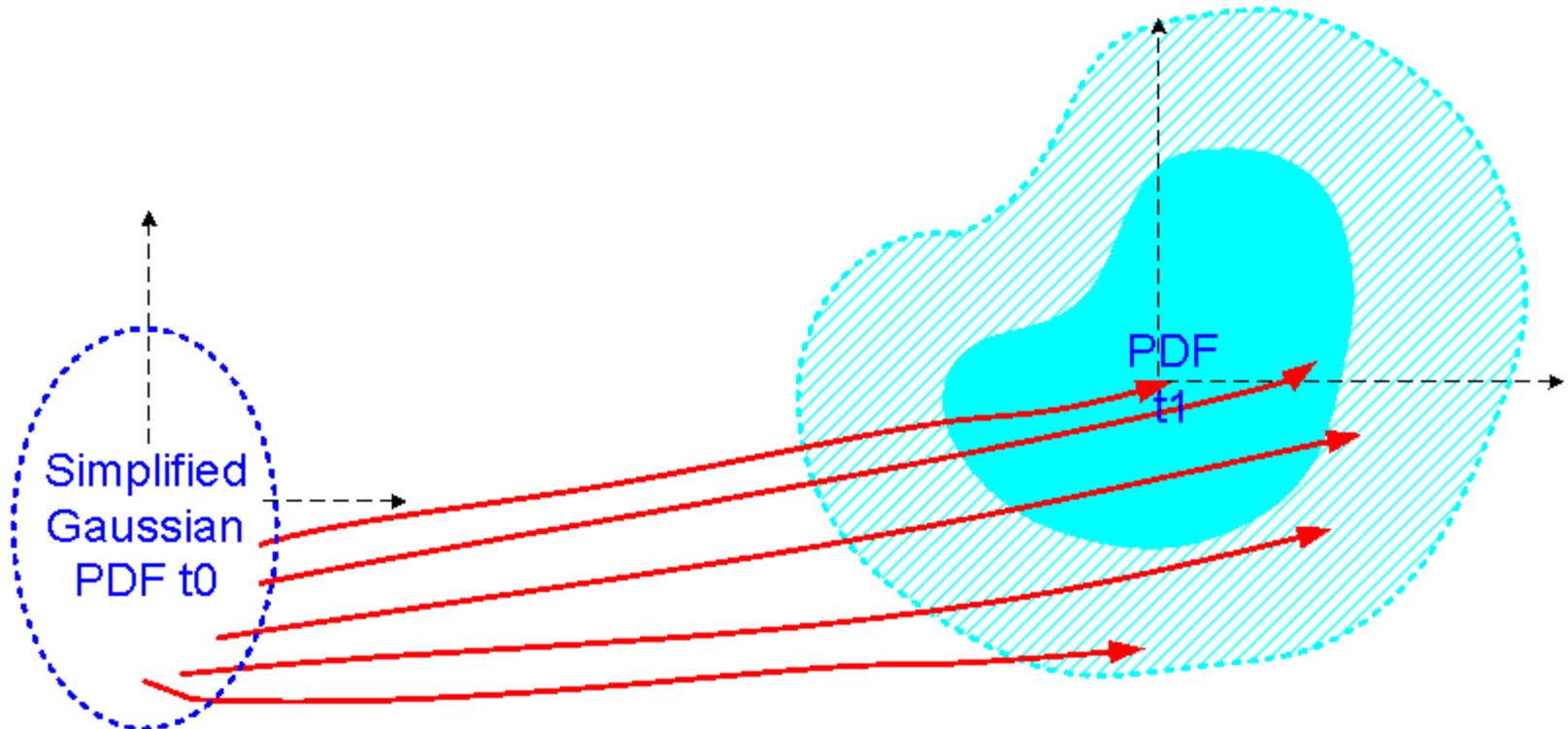
$$\mathbf{P}^f \mathbf{H}^T = \overline{(\mathbf{x}^f - \overline{\mathbf{x}^f})(H(\mathbf{x}^f) - \overline{H(\mathbf{x}^f)})^T},$$

$$\mathbf{H} \mathbf{P}^f \mathbf{H}^T = \overline{(H(\mathbf{x}^f) - \overline{H(\mathbf{x}^f)})(H(\mathbf{x}^f) - \overline{H(\mathbf{x}^f)})^T}$$

Use these in the standard KF equation to update the best estimate (ensemble mean):

$$\overline{\mathbf{x}}^a = \overline{\mathbf{x}}^f + \mathbf{P}^f \mathbf{H}^T (\mathbf{H} \mathbf{P}^f \mathbf{H}^T + \mathbf{R})^{-1} (\mathbf{y}^o - H(\overline{\mathbf{x}}^f)).$$

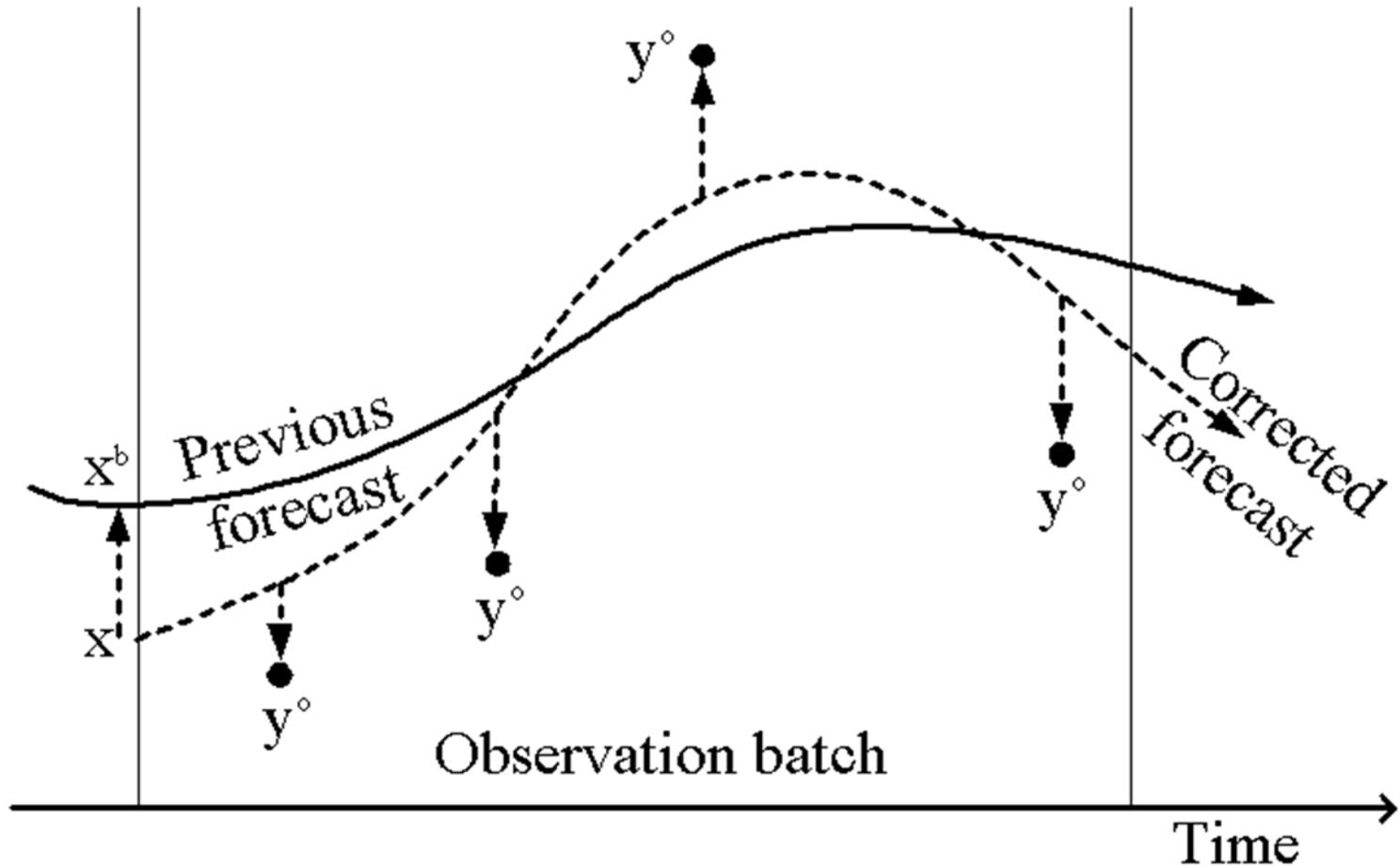
Deterministic 4D-Var



Initial PDF is approximated by a Gaussian.

Descent algorithm only explores a small part of the PDF, on the way to a local minimum.

Simple 4D-Var, as a least-squares best fit of a deterministic model trajectory to observations





Assumptions in deriving deterministic 4D-Var

Bayes Theorem - posterior PDF: $P(x|y^o) = P(y^o|x)P(x)/P(y^o)$

where the obs likelihood function is given by:

$$P(y^o|x) = f(y^o - y), \text{ where } y = H(x)$$

Impossible to evaluate the integrals necessary to find “best”.

Instead assume best x maximises PDF, and minimises $-\ln(\text{PDF})$:

$$J(x) = -\ln [P(y^o|x)] - \ln [P(x)]$$

Purser, R.J. 1984: "A new approach to the optimal assimilation of meteorological data by iterative Bayesian analysis". Preprints, 10th conference on weather forecasting and analysis. Am Met Soc. 102-105

Lorenc, A.C. 1986: "Analysis methods for numerical weather prediction." Quart. J. Roy. Met. Soc., 112, 1177-1194.



The deterministic 4D-Var equations

$$P(\mathbf{x} | \underline{\mathbf{y}}^o) \propto P(\mathbf{x}) P(\underline{\mathbf{y}}^o | \mathbf{x}) \quad \text{Bayesian posterior pdf.}$$

Assume
Gaussians

$$P(\mathbf{x}) \propto \exp\left(-\frac{1}{2}(\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}^b)\right)$$

$$P(\underline{\mathbf{y}}^o | \mathbf{x}) = P(\underline{\mathbf{y}}^o | \underline{\mathbf{y}}) \propto \exp\left(-\frac{1}{2}(\underline{\mathbf{y}} - \underline{\mathbf{y}}^o)^T \underline{\mathbf{R}}^{-1}(\underline{\mathbf{y}} - \underline{\mathbf{y}}^o)\right)$$

But nonlinear model makes pdf non-Gaussian:
full pdf is too complicated to be allowed for.

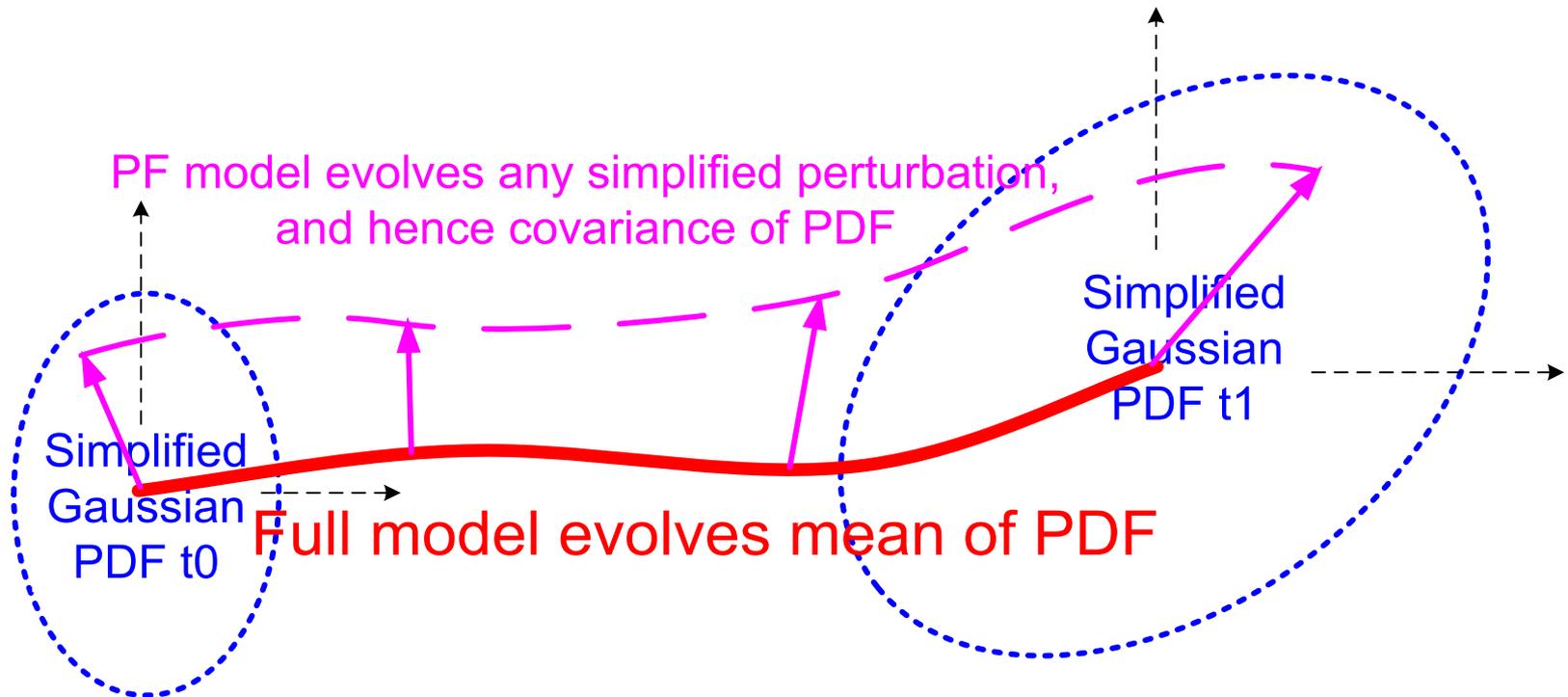
$$\underline{\mathbf{y}} = \underline{H}(\underline{M}(\mathbf{x}))$$

So seek mode of pdf by
finding minimum of
penalty function

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}^b) + \frac{1}{2}(\underline{\mathbf{y}} - \underline{\mathbf{y}}^o)^T \underline{\mathbf{R}}^{-1}(\underline{\mathbf{y}} - \underline{\mathbf{y}}^o)$$

$$\nabla_{\mathbf{x}} J(\mathbf{x}) = \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}^b) + \underline{\mathbf{M}}^* \underline{\mathbf{H}}^* \underline{\mathbf{R}}^{-1}(\underline{\mathbf{y}} - \underline{\mathbf{y}}^o)$$

Statistical, incremental 4D-Var



Statistical 4D-Var approximates entire PDF by a Gaussian.



Statistical 4D-Var - equations

Independent, Gaussian background and model errors \Rightarrow non-Gaussian pdf for general $\underline{\mathbf{y}}$:

$$P(\delta \underline{\mathbf{x}}, \delta \underline{\boldsymbol{\eta}} | \underline{\mathbf{y}}^o) \propto \exp\left(-\frac{1}{2}(\delta \underline{\mathbf{x}} - (\underline{\mathbf{x}}^b - \underline{\mathbf{x}}^g))^T \underline{\mathbf{B}}^{-1}(\delta \underline{\mathbf{x}} - (\underline{\mathbf{x}}^b - \underline{\mathbf{x}}^g))\right) \exp\left(-\frac{1}{2}(\delta \underline{\boldsymbol{\eta}} + \underline{\boldsymbol{\eta}}^g)^T \underline{\mathbf{Q}}^{-1}(\delta \underline{\boldsymbol{\eta}} + \underline{\boldsymbol{\eta}}^g)\right) \exp\left(-\frac{1}{2}(\underline{\mathbf{y}} - \underline{\mathbf{y}}^o)^T \underline{\mathbf{R}}^{-1}(\underline{\mathbf{y}} - \underline{\mathbf{y}}^o)\right)$$

Incremental linear approximations in forecasting model predictions of observed values converts this to an approximate Gaussian pdf:

$$\underline{\mathbf{y}} = \underline{\mathbf{H}} \underline{\mathbf{M}}^o(\delta \underline{\mathbf{x}}, \underline{\boldsymbol{\eta}}) + \underline{\mathbf{H}}(\underline{\mathbf{M}}(\underline{\mathbf{x}}^g, \underline{\boldsymbol{\eta}}^g))$$

The mean of this approximate pdf is identical to the mode, so it can be found by minimising:

$$J(\delta \underline{\mathbf{x}}, \delta \underline{\boldsymbol{\eta}}) = \frac{1}{2}(\delta \underline{\mathbf{x}} - (\underline{\mathbf{x}}^b - \underline{\mathbf{x}}^g))^T \underline{\mathbf{B}}^{-1}(\delta \underline{\mathbf{x}} - (\underline{\mathbf{x}}^b - \underline{\mathbf{x}}^g)) + \frac{1}{2}(\delta \underline{\boldsymbol{\eta}} + \underline{\boldsymbol{\eta}}^g)^T \underline{\mathbf{Q}}^{-1}(\delta \underline{\boldsymbol{\eta}} + \underline{\boldsymbol{\eta}}^g) + \frac{1}{2}(\underline{\mathbf{y}} - \underline{\mathbf{y}}^o)^T \underline{\mathbf{R}}^{-1}(\underline{\mathbf{y}} - \underline{\mathbf{y}}^o)$$



Questions and answers