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SMR.1403 - 6

Spring Colloquium on
the Physics of Weather and Climate:
REGIONAL WEATHER PREDICTION
MODELLING AND PREDICTABILITY
(8 – 19 April 2002)

"Estimation Theory and Data Assimilation: Theoretical Foundation"

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These are preliminary lecture notes, intended only for distribution to participants

Estimation Theory and Data Assimilation: Theoretical Foundation

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OUTLINE

- DATA ASSIMILATION PROBLEM
  - State of the atmosphere

- GENERAL PRINCIPLES
  - Markov process and the general causality principle
  - Stochastic differential equations
  - Kolmogorov (Fokker-Planck) equation

- KALMAN FILTER
  - Error covariances
  - Observability and Controllability

- PROBABILISTIC VIEW
  - Bayes formula: conditional probability

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OUTLINE (cont.)

- **VARIATIONAL PRINCIPLES**
  - **Norms and vector spaces (Hilbert and Banach spaces)**
  - **First Variation**

- **CONTROL THEORY (optimization)**
  - **Unconstrained and Constrained optimization**

- **COST FUNCTION**
  - **Probability distribution: Gaussian error statistics**
  - ***Three*-dimensional variational data assimilation**
  - ***Four*-dimensional variational data assimilation**

- **ENSEMBLE DATA ASSIMILATION**
  - **Ensemble Kalman Filter and Smoother**
  - **Ensemble forecasting and data assimilation**

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DATA ASSIMILATION PROBLEM

- *Deterministic* NWP Problem: **Initial state of the atmosphere**
- *Probabilistic* NWP Problem: **Initial probability distribution**
- *"Forgotten"* NWP Problem: **Model errors (probability distribution)**

❑ OBSERVATIONS

- **Irregular distribution in *space* and *time***
- **Insufficient information**
- **Quality control**
- **Observation operators**

❑ NWP MODELS

- **Wide range of spatial and temporal scales**
- **Highly non-linear physical processes**
- **Coupled models (atmosphere-land-ocean)**

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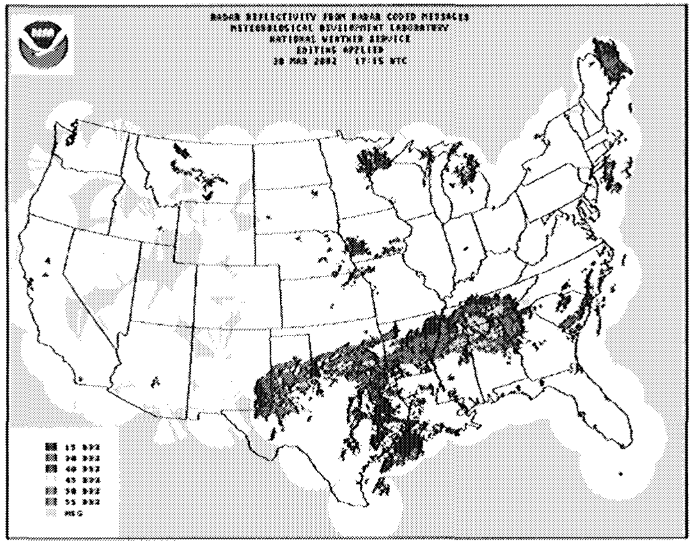
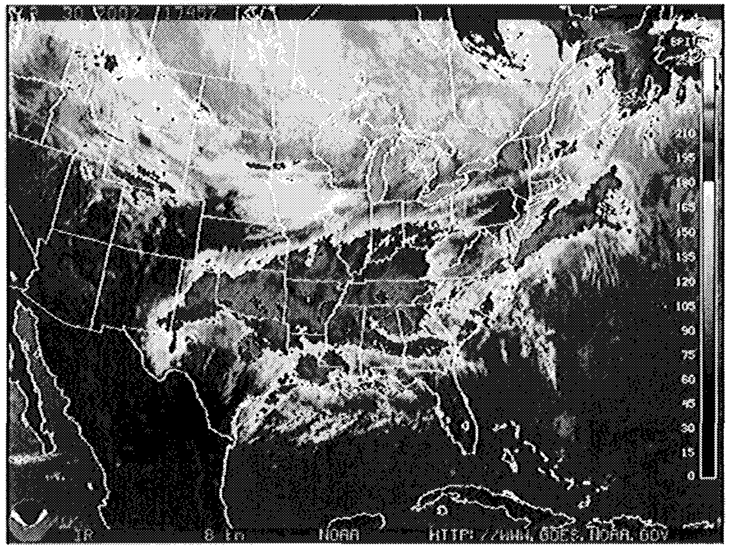
DATA COVERAGE

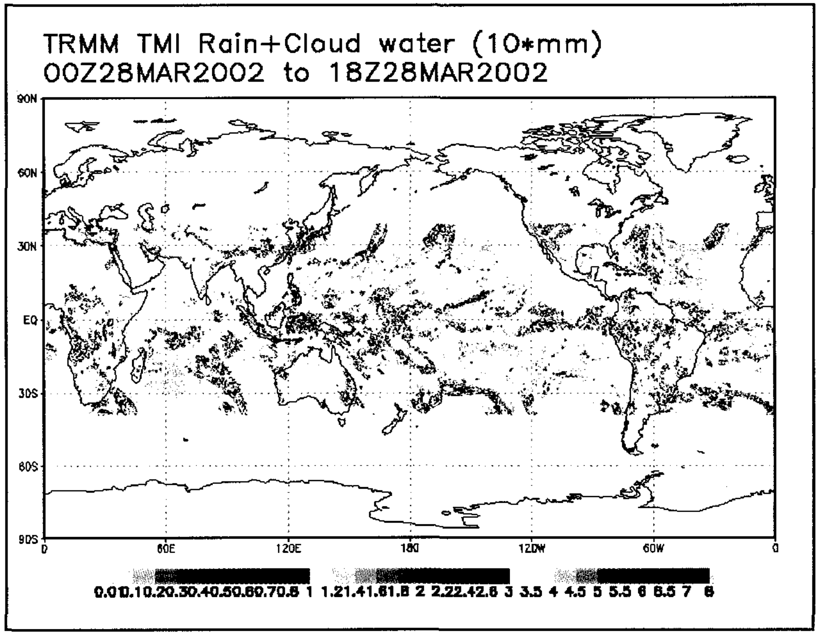
Radar Reflectivity



GOES IR



TRMM Rain + Cloud water



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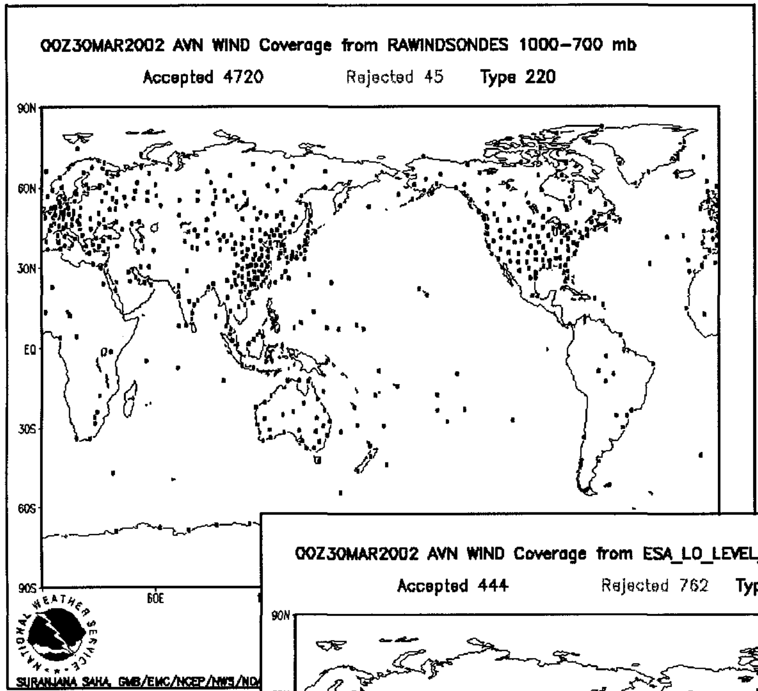
QUALITY CONTROL

RAWINSONDES



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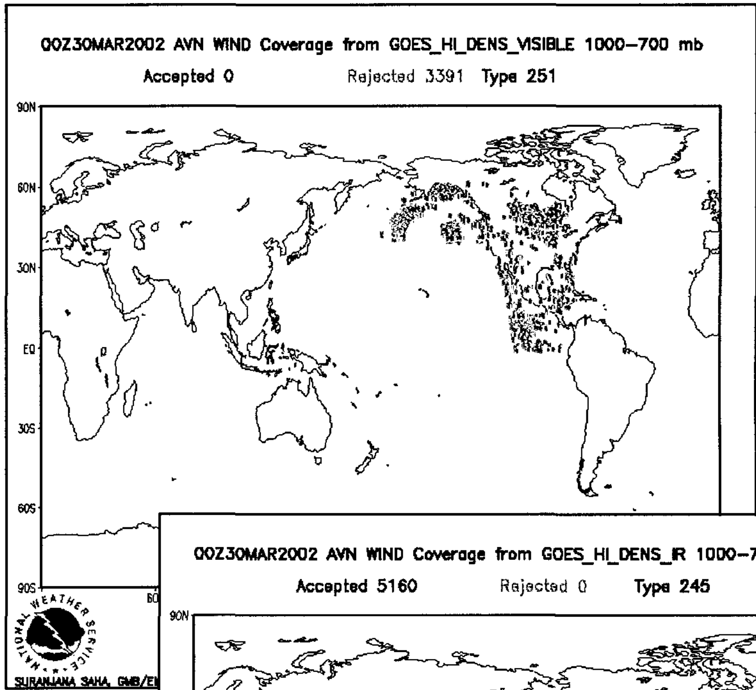
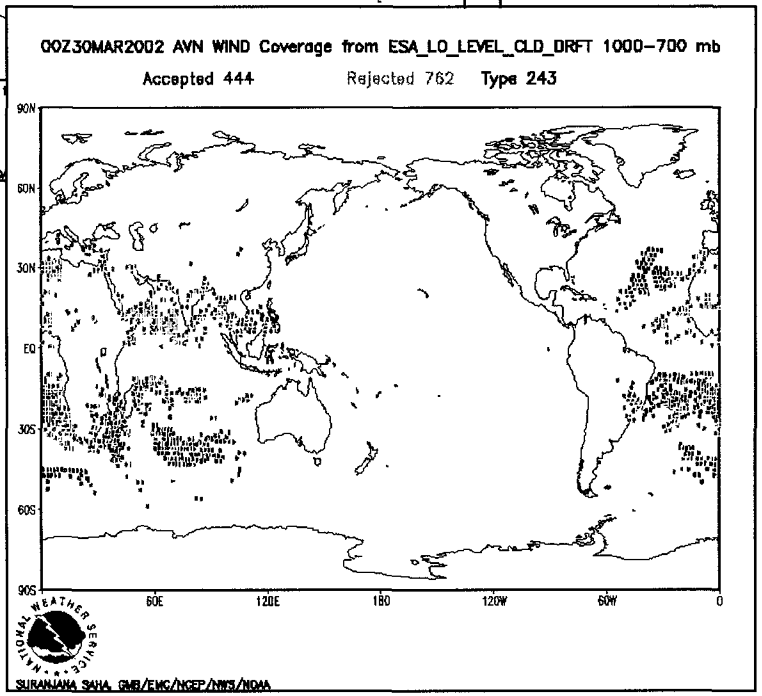
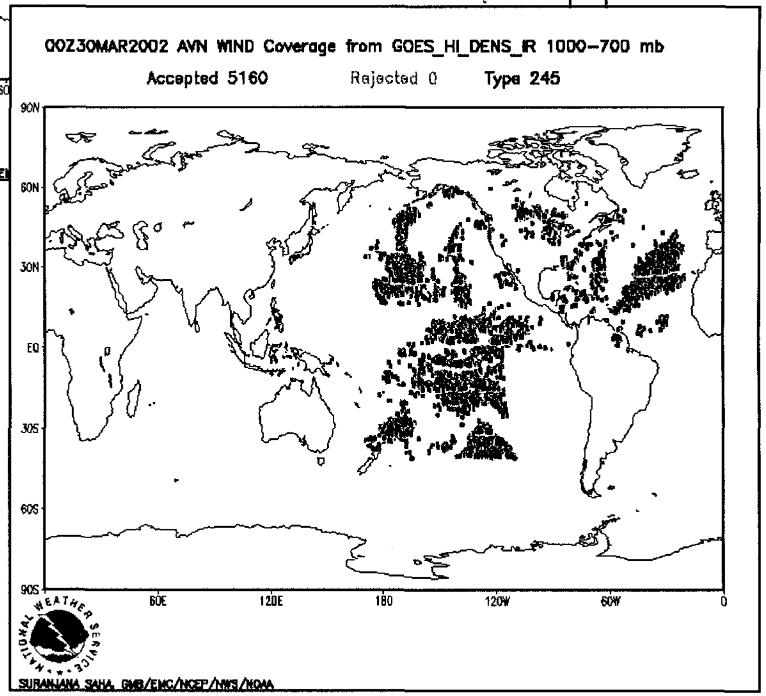




ESA LOW-LEVEL WIND



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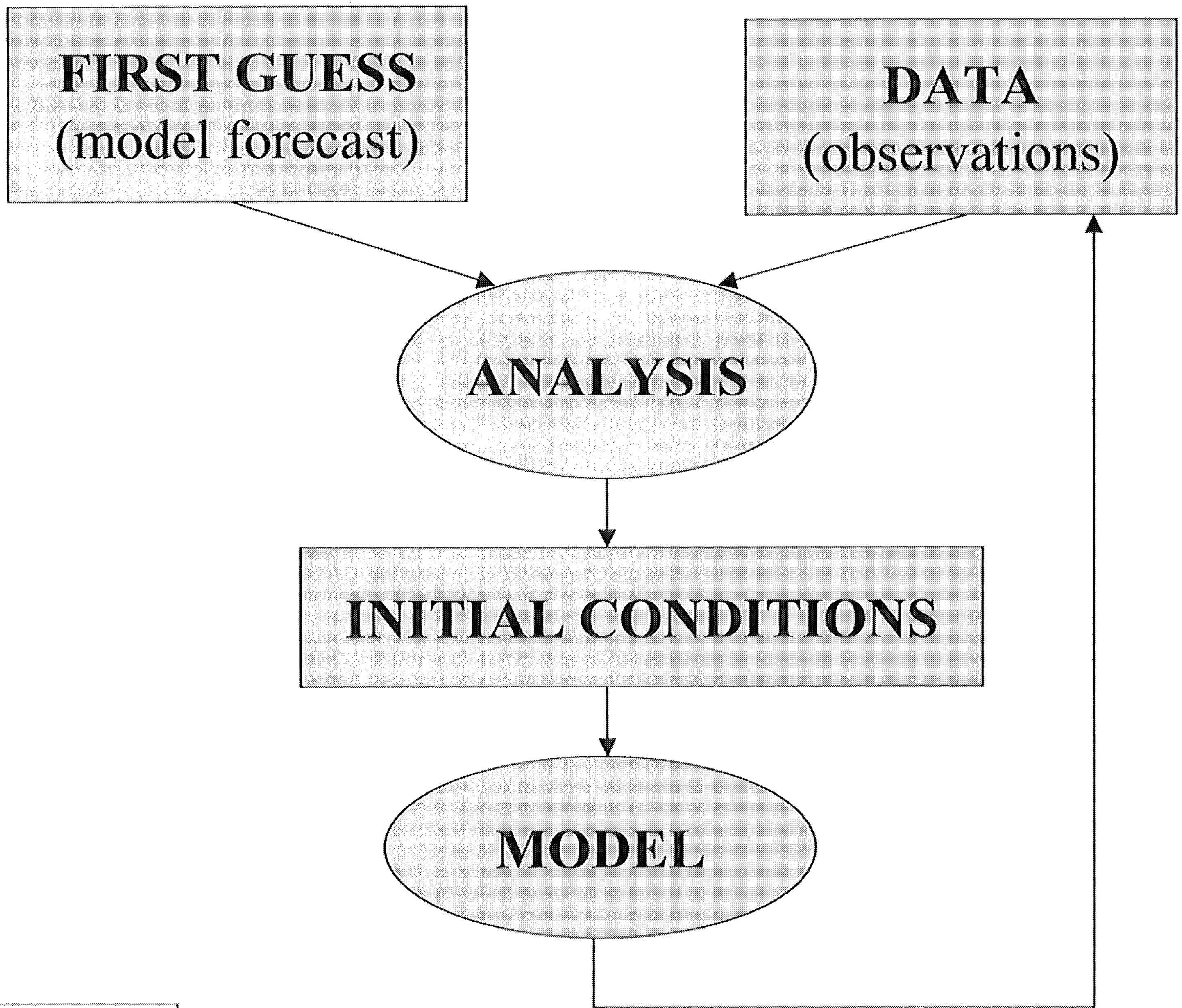
Flow-diagram of Data Assimilation Cycle



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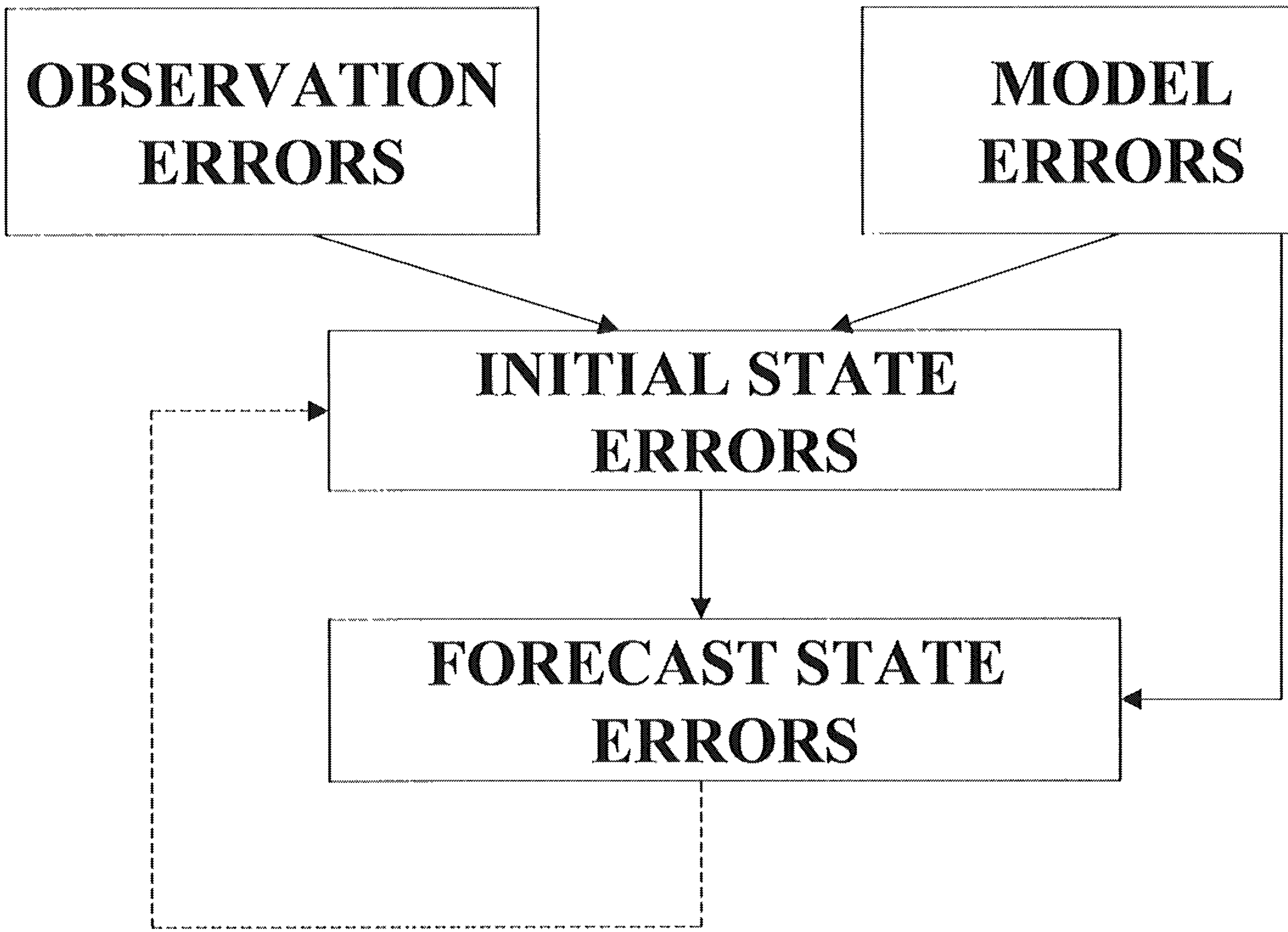
Flow-diagram of Analysis-Forecast Errors



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GENERAL PRINCIPLES

- **General Causality Principle:**
  THE PROBABILITY LAW OF THE PROCESS IN FUTURE (ONCE IT IS IN A GIVEN STATE) *DOES NOT* DEPEND ON HOW THE PROCESS ARRIVED AT THE GIVEN STATE

  - Deterministic Ordinary Differential Equations:

$$\frac{dx(t)}{dt} = f(x(t))$$

The rate of change of $\boldsymbol{x}$ depends *only* on $\boldsymbol{x}$ at t (now), *not* on $\boldsymbol{x}(\tau)$, $\tau < t$

- **Markov Process:**
  - Stochastic analog of ODE

$$\Pr\{x_{t_n}(\omega) \le \lambda \mid x_{t_1}, \ldots, x_{t_{n-1}}\} = \Pr\{x_{t_n}(\omega) \le \lambda \mid x_{t_{n-1}}\}$$

The future can be predicted from a knowledge of the present

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GENERAL PRINCIPLES

- **Stochastic differential equation:**

  $\boldsymbol{x}_t$ – n-dimensional vector state at time t

  $\boldsymbol{w}_t$ – random disturbance at time t

$$\frac{dx_t}{dt} = f(x_t, w_t, t)$$

- **This equation represents a stochastic dynamical system**
- **Probability law of w_t process assumed specified**

- **Stochastic differential equation with an additive white Gaussian forcing:**

$$\frac{dx_t}{dt} = f(x_t, t) + g(x_t, t)w_t$$

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GENERAL PRINCIPLES

- **Kolmogorov's (Fokker-Planck) equation:**

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial[p(x,t)f(x,t)]}{\partial x} + \frac{1}{2}\frac{\partial^2[p(x,t)g^2(x,t)]}{\partial x^2}$$

p – **probability density**

f – **dynamical model**

g – **stochastic forcing**

Diffusion Process:

Markov process whose transition probability density satisfies Kolmogorov's equation

Ensemble Forecasting: Estimate of the *forecast* probability density

Data Assimilation: Estimate of the *initial* probability density

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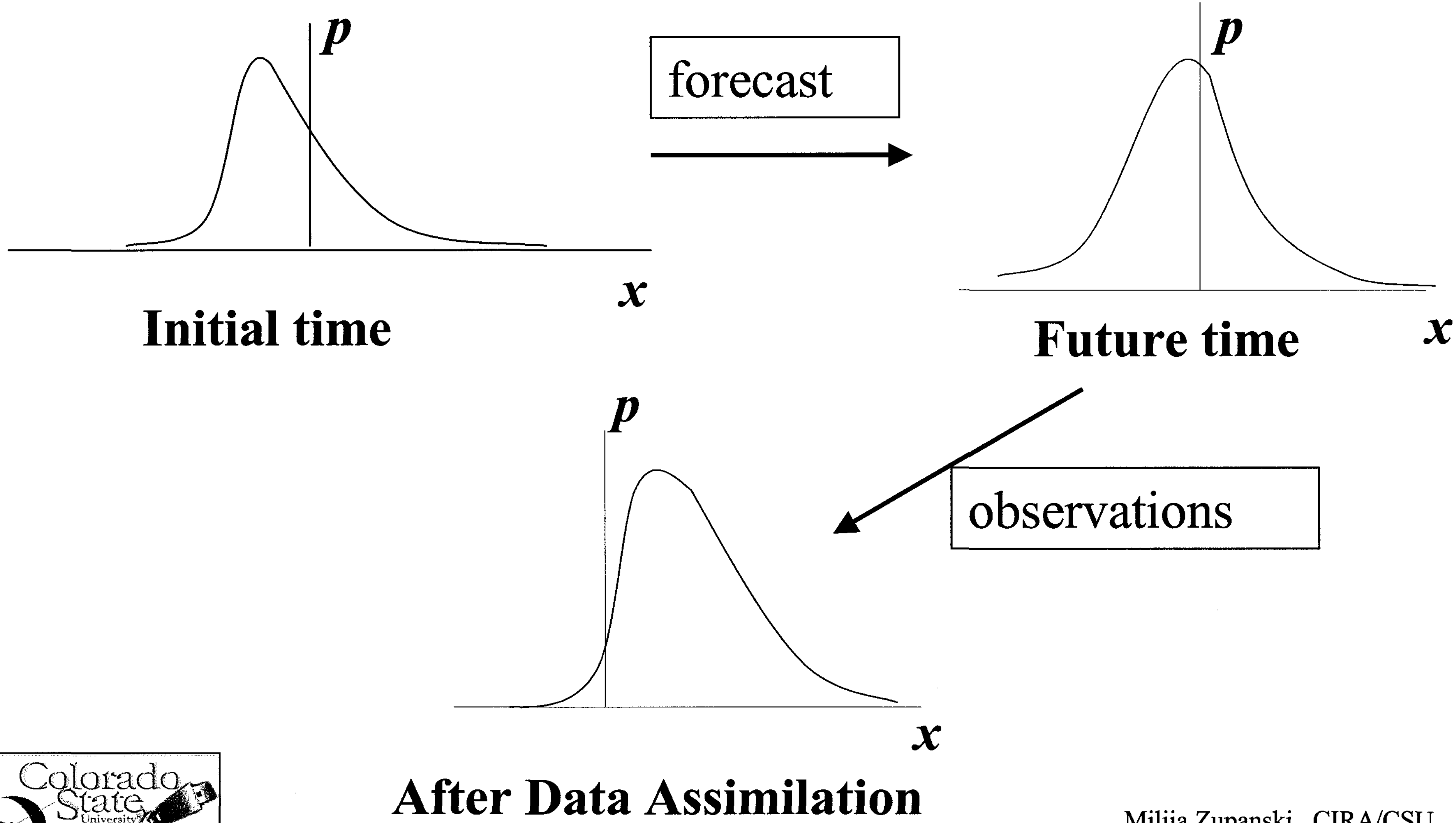
PROBABILITY DISTRIBUTION



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KALMAN FILTER

Discrete stochastic-dynamic model

$$x_k = M(x_{k-1}) + G(x_{k-1})w_{k-1}$$

w_{k-1} – **model error (stochastic forcing)**
M – **non-linear dynamic (NWP) model**
G – **model (matrix) reflecting the state dependence of model error**

Discrete stochastic observation model

$$y_k = K(x_k) + \varepsilon_{k-1}$$

ε_{k-1} – **measurement error**
K – **non-linear observation operator** (transformation from model to observations)

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KALMAN FILTER

Estimation error: $\delta_k = x_k^{true} - x_k^{est}$

Minimum variance estimate: Minimize the qudaratic *loss* function

$$L(\delta_k) = \delta_k^T \mathbf{S} \delta_k$$

$\mathbf{S}$ – positive-definite symmetric matrix

(Linear) Kalman Filter for Gaussian statistics:

$$\varepsilon_k \to N(0, \mathbf{R}) \qquad w_k \to N(0, \mathbf{Q})$$

Forecast and Analysis steps

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KALMAN FILTER EQUATIONS

Forecast step:

$$x_k = M(x_{k-1})$$

$$\boldsymbol{P}_k^f = \boldsymbol{M}(\boldsymbol{x}_{k-1})\boldsymbol{P}_{k-1}^a\boldsymbol{M}^T(\boldsymbol{x}_{k-1}) + \boldsymbol{G}(\boldsymbol{x}_{k-1})\boldsymbol{Q}_{k-1}\boldsymbol{G}^T(\boldsymbol{x}_{k-1})$$

Analysis step:

$$\boldsymbol{x}^a = \boldsymbol{x}^b + \boldsymbol{P}^f\boldsymbol{K}^T(\boldsymbol{K}\boldsymbol{P}^f\boldsymbol{K}^T + \boldsymbol{R})^{-1}(\boldsymbol{y} - K(\boldsymbol{x}^b))$$

$$\boldsymbol{P}^a = [\boldsymbol{I} - \boldsymbol{P}^f\boldsymbol{K}^T(\boldsymbol{K}\boldsymbol{P}^f\boldsymbol{K}^T + \boldsymbol{R})^{-1}\boldsymbol{K}]\boldsymbol{P}^f$$

P^f: **Forecast error covariance**

P^a: **Analysis error covariance**

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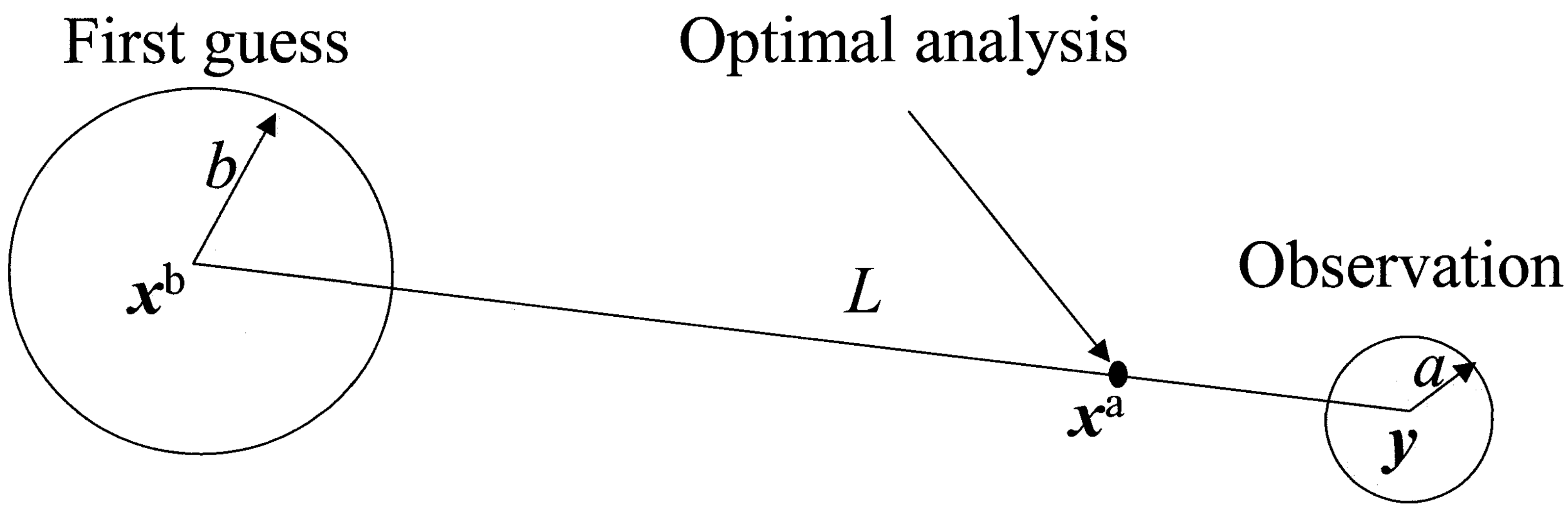
Example #1: KF analysis step



Forecast error

$$\boldsymbol{b} = (\boldsymbol{P}^f)^{\frac{1}{2}}$$

Observation error

$$\boldsymbol{a} = \boldsymbol{R}^{\frac{1}{2}}$$

Observation operator

$$\boldsymbol{K} = \boldsymbol{I}$$

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Example #1: KF analysis step

Optimal analysis

$$x^a = \frac{a^2}{a^2+b^2} x^b + \frac{b^2}{a^2+b^2} y \qquad x^a - x^b = \frac{b^2}{a^2+b^2} L$$

- Weighted sum of the first guess and observation
- Analysis adjustment proportional to the (squared) error of the first guess

1) Large *forecast* error: b>>a => $x^a = y$

2) Large *observation* error: b<<a => $x^a = x^b$

Analysis error $$(P^a)^{\frac{1}{2}} = \frac{ab}{\sqrt{a^2+b^2}}$$

1) At least one error small: $a \to 0$ or $b \to 0$ => $(P^a)^{\frac{1}{2}} \to 0$

2) One error large: $b \to \infty$ => $(P^a)^{\frac{1}{2}} \to a$

$a \to \infty$ => $(P^a)^{\frac{1}{2}} \to b$

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KALMAN FILTER

OBSERVABILITY

$$I(k,1) = \sum_{n=1}^{k} \boldsymbol{M}_{n,k}{}^{T} \boldsymbol{K}_n^T \boldsymbol{R}_n^{-1} \boldsymbol{K}_n \boldsymbol{M}_{n,k} > 0$$

- **Information matrix from observations only (*no prior*)**
- **Defined with respect to all observations ($t_1, \ldots, t_k$), or in the interval ($t_m, \ldots, t_k$)**
- k, m, n – **discrete time indexes**

$$(\boldsymbol{P}_k^a)^{-1} = \boldsymbol{M}_{0,k}^T \boldsymbol{P}_0^{-1} \boldsymbol{M}_{0,k} + \boldsymbol{I}(k,0)$$

CONTROLLABILITY

$$C(k,0) = \sum_{n=0}^{k-1} \boldsymbol{M}_{k,n+1} \boldsymbol{G}_n \boldsymbol{Q}_{n+1} \boldsymbol{G}_n^T \boldsymbol{M}_{k,n+1}{}^{T} > 0$$

- **Effect of the stochastic forcing**
- **Defined with respect to all forcing ($t_1, \ldots, t_{k-1}$), or in the interval ($t_m, \ldots, t_{k-1}$)**
- k, m, n – **discrete time indexes**

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PROBABILISTIC VIEW

Inverse analysis problem:

Find optimal analysis (z) for given observations (y) and prior information

$$y = K(z)$$

Bayes formula:

$$\Pr(A \mid B) \propto \Pr(B \mid A)\Pr(A)$$

Posterior probability of an event ***A*** occurring, given the event ***B*** has occurred, is proportional to the ***prior*** probability of ***A*** multiplied by the probability of ***B*** occurring, knowing that ***A*** has occurred

Application to the analysis problem: Maximize posterior probability

Event A: $z = z_{true}$ **Event B:** $y = y_{obs}$

$$\Pr(z = z_{true} \mid y = y_{obs}) \propto \Pr(y = y_{obs} \mid z = z_{true})\Pr(z = z_{true})$$

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VARIATIONAL PRINCIPLES

close*, *orthogonal* – imply a *measure* and a *geometry

NORM:

- **Metric (measure) of a vector space**
- $D(x,y) = \| x - y \|$

HILBERT SPACE:

- **Generalization of the Euclidian space**
- **Metric (norm) defined by inner product**
- **Orthogonality defined in terms of inner product**

BANACH SPACE:

- **Generalization of the Hilbert space**
- **Metric defined independently of inner product**

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VARIATIONAL PRINCIPLES

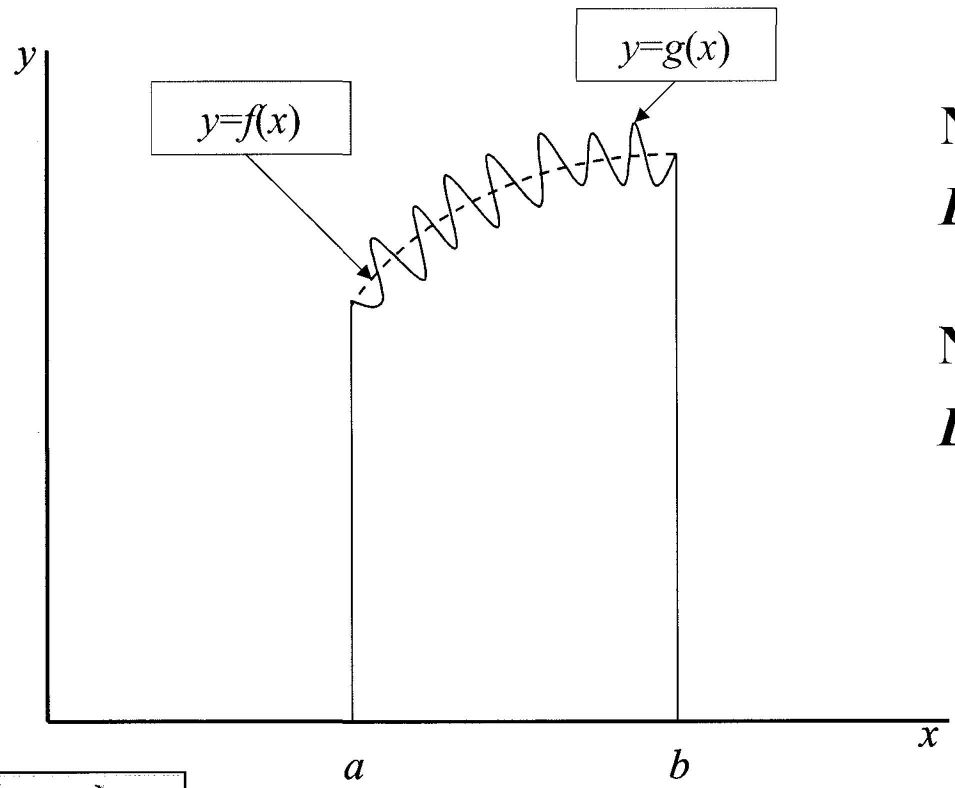
Example #2: Norm definition and distance

Norm 1

$$C[a,b]: \| f \| = \max | f(x) |$$

Norm 2

$$C_1[a,b]: \| f \| = \max | f(x) | + \max \left| \frac{df(x)}{dx} \right|$$



Norm 1: *f*(*x*) and *g*(*x*) are *close*

D(f,g)=||f-g|| is small

Norm 2: *f*(*x*) and *g*(*x*) are *far away*

D(f,g)=||f-g|| is large

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VARIATIONAL PRINCIPLES

Maximum (minimum) of the functional (cost function): max (min) $J(x)$

$$J(x+\delta x)-J(x)=\delta J\{x;\delta x\}+\frac{1}{2!}\delta^2 J\{x;\delta x\}+\frac{1}{3!}\delta^3 J\{x;\delta x\}+\ldots$$

FIRST VARIATION:

- **Main linear contribution to the non-linear perturbation of the cost function**
- **First variation equivalent to *linearization***

$$\delta J(x;\delta x)=\frac{\partial J(x)}{\partial x}\delta x$$

CONDITIONS FOR EXTREMUM:

1) First variation is zero: $\delta J(x;\delta x)=0$

Minimum:

2) Second variation positive: $\delta^2 J(x;\delta x)>0$ for arbitrary δx

Maximum:

3) Second variation negative: $\delta^2 J(x;\delta x)<0$ for arbitrary δx

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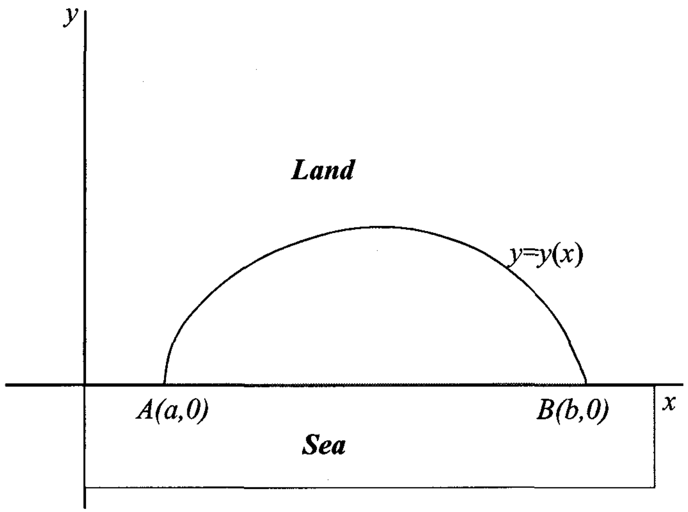
Example #3: The legend of Carthage

Queen Dido escaped from Greece to northern Africa. She was promised by the natives the land she can surround by the ox's skin. Dido had the skin cut in tiny stripes, connected all into one long rope. The ancient Carthage was founded on the land surrounded by the rope.

"First" variational problem: Given the length of the rope, what is the largest area that can be surrounded ?



Maximize the area $S = \int_a^b y(x)dx$

Length of the rope $L = \int_a^b \sqrt{1+(dy/dx)^2}\,dx$

Constraints $y(a)=0 \qquad y(b)=0$

ANSWER: ***Circle*** $(x-C_1)^2 + (y-C_2)^2 = \lambda^2$

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CONTROL THEORY (OPTIMIZATION)

Constrained optimization problem:

$$\begin{aligned} &\textit{minimize} && J(\boldsymbol{x}) \\ &\textit{subject to} && c_i(x) = 0, \quad i = 1,2,\ldots,m_1 \\ &&& c_i(x) \geq 0, \quad i = m_1+1,\ldots,m \end{aligned}$$

Unconstrained optimization:

$$\textit{minimize} \qquad J(\boldsymbol{x})$$

In practice, constrained optimization can be defined in terms of unconstrained minimization: constraints embedded in $J(x)$ definition

Unconstrained minimization algorithms:

- **Conjugate gradient**
- **Quasi-Newton**

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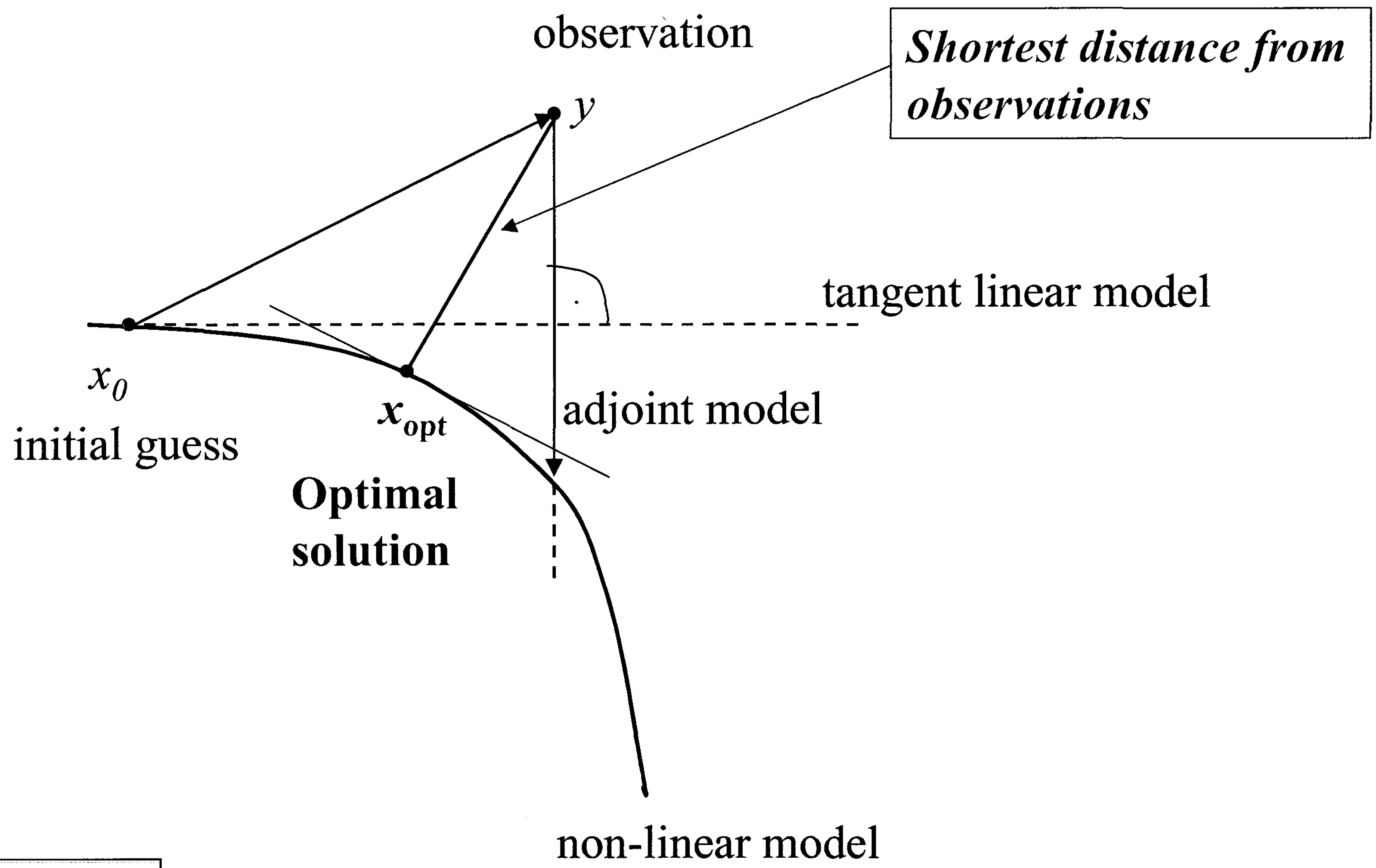
CONTROL THEORY (OPTIMIZATION)

Constrained optimization:



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COST FUNCTION

GAUSSIAN PROBABILITY DISTRIBUTION

$$\Pr(\boldsymbol{x}) \propto \exp[-\frac{1}{2}(\boldsymbol{x} - E(\boldsymbol{x}))^T \boldsymbol{P}_x^{-1}(\boldsymbol{x} - E(\boldsymbol{x}))]$$

P_x – covariance (2nd moment)

$E(x)$ – mean value, mathematical expectation (1st moment)

Maximum likelihood:

Find x for which $\Pr(x)$ is maximum => max [$\Pr(x)$]

Cost Function: $J(x) = -ln[\Pr(x)]$

Maximum likelihood: Find x for which $J(x)$ is minimum => min [$J(x)$]

$$J(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x} - E(\boldsymbol{x}))^T \boldsymbol{P}_x^{-1}(\boldsymbol{x} - E(\boldsymbol{x}))$$

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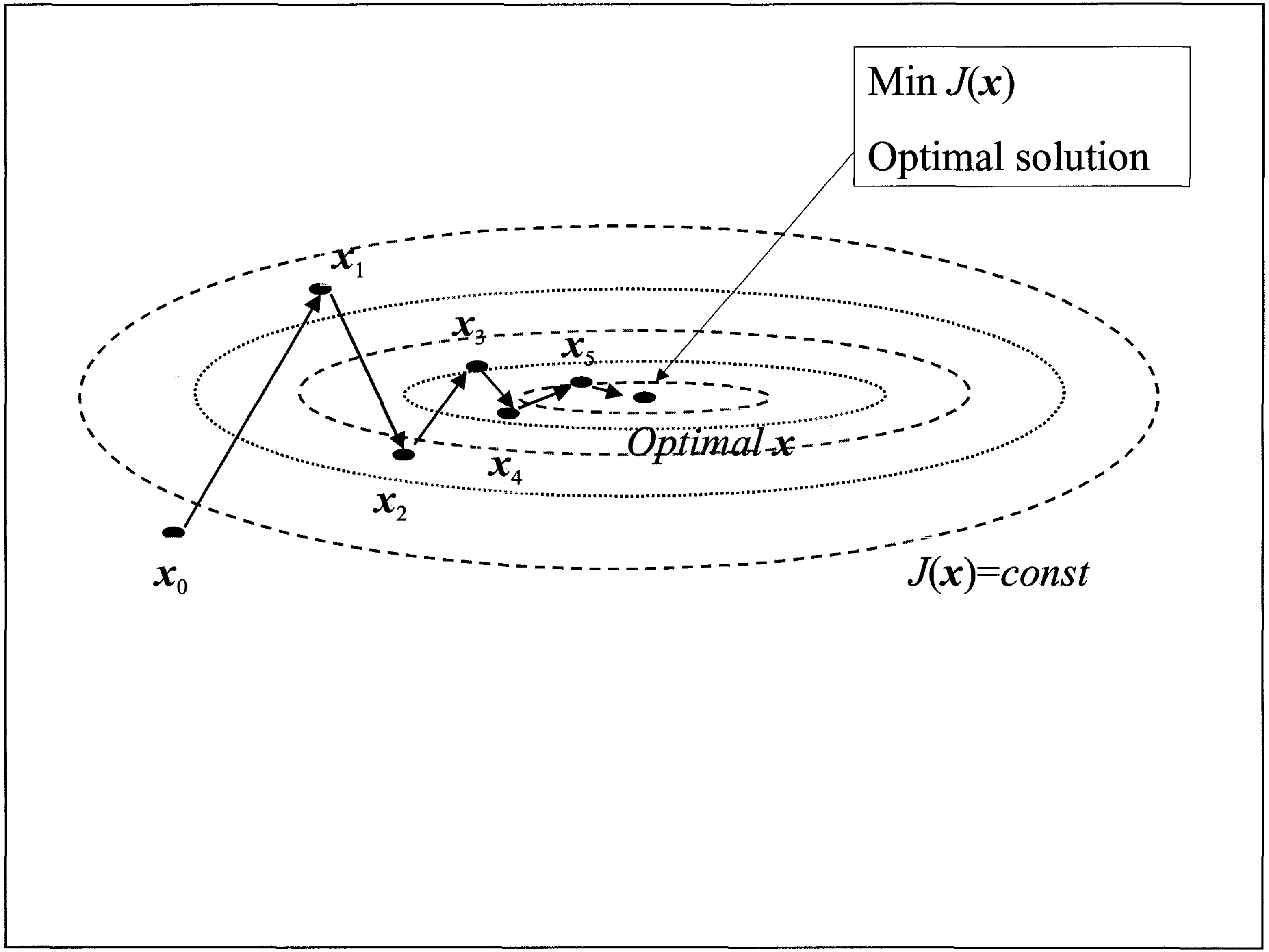
ITERATIVE MINIMIZATION



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ITERATIVE MINIMIZATION OF THE COST FUNCTION

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k \qquad (k = 0,1,2,\ldots)$$

x – **Control variable**

x_0 – **Initial guess**

d – **Descent direction**

α – **Step-length**

$$\boldsymbol{g} = \frac{\partial J(\boldsymbol{x})}{\partial \boldsymbol{x}}$$ - ***Gradient*** **(adjoint, finite difference)**

$$\boldsymbol{H} = \frac{\partial^2 J(\boldsymbol{x})}{\partial \boldsymbol{x}^2}$$ - ***Hessian matrix***

$$\boldsymbol{d} = -\boldsymbol{H}^{-1}\boldsymbol{g}$$

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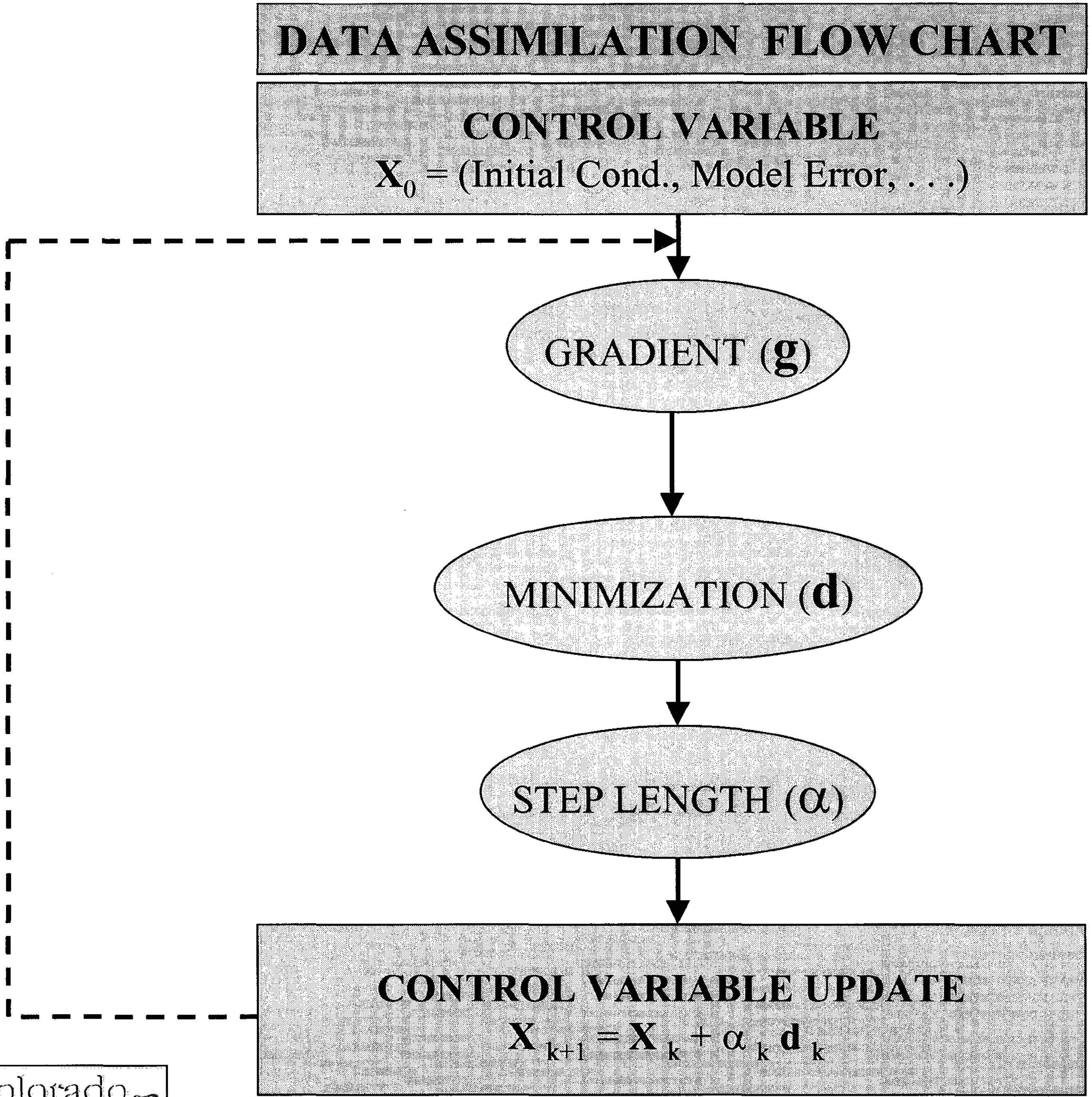

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3DVAR COST FUNCTION

FOR GAUSSIAN ERROR STATISTICS (with *zero* mean):

$$\Pr(z = z_{true}) \propto \exp[-\frac{1}{2}(z - z_b)^T (P^f)^{-1}(z - z_b)]$$

$$\Pr(y = y_{obs} \mid z = z_{true}) \propto \exp[-\frac{1}{2}(y_{obs} - K(z))^T R^{-1}(y_{obs} - K(z))]$$

P_f – **forecast (background) error covariance**

R – **observation error covariance** (measurement + observation transformation)

Minimize cost function:

$$J(z) = \frac{1}{2}(z - z_b)^T (P^f)^{-1}(z - z_b) + \frac{1}{2}[y_{obs} - K(z)]^T R^{-1}[y_{obs} - K(z)]$$

Gradient

$$\frac{\partial J}{\partial z} = (P^f)^{-1}(z - z_b) + K^T R^{-1}[K(z) - y_{obs}]$$

Hessian matrix

$$\frac{\partial^2 J}{\partial z^2} = (P^f)^{-1} + K^T R^{-1} K$$

K^T – *adjoint* of observation operator

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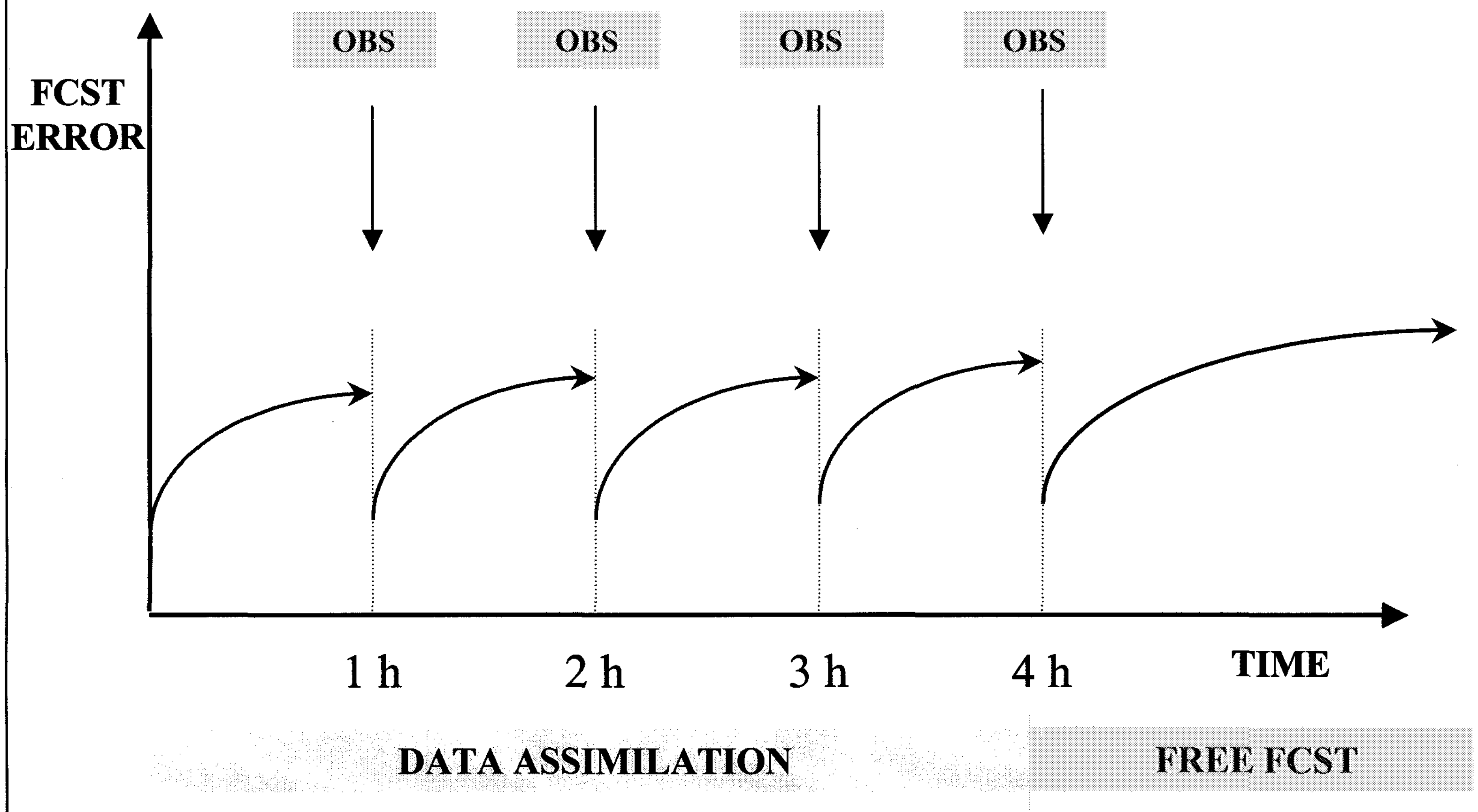
SEQUENTIAL DATA ASSIMILATION (3DVAR, EnKF)



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4DVAR COST FUNCTION

FOR GAUSSIAN ERROR STATISTICS (with *zero* mean):

$$\Pr(\boldsymbol{z} = \boldsymbol{z}_{true}) \propto \exp[-\frac{1}{2}(x - x_b)^T (\boldsymbol{P}^f)^{-1}(x - x_b) - \frac{1}{2}(r - r_b)^T \boldsymbol{Q}^{-1}(r - r_b)]$$

$$\Pr(\boldsymbol{y} = \boldsymbol{y}_{obs} \mid \boldsymbol{z} = \boldsymbol{z}_{true}) \propto \exp[-\frac{1}{2}\sum_n [K(M(\boldsymbol{x},\boldsymbol{r})) - \boldsymbol{y}]_n^T \boldsymbol{R}_n^{-1} [K(M(\boldsymbol{x},\boldsymbol{r}) - \boldsymbol{y}]_n]$$

$\boldsymbol{Q}$ – **random model error covariance**

$\boldsymbol{x}$ - **initial conditions** (in the past, beginning of assimilation)

$\boldsymbol{r}$ - **random model error** (in the past, during the assimilation)

$\boldsymbol{z}$ - **analysis** (present time)

Minimize cost function:

$$J(\boldsymbol{z}) = \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}_b)^T (\boldsymbol{P}^f)^{-1}(\boldsymbol{x} - \boldsymbol{x}_b) + \frac{1}{2}(\boldsymbol{r} - \boldsymbol{r}_b)^T \boldsymbol{Q}^{-1}(\boldsymbol{r} - \boldsymbol{r}_b) + \frac{1}{2}\sum_n [K(M(\boldsymbol{x},\boldsymbol{r})) - \boldsymbol{y}]_n^T \boldsymbol{R}_n^{-1} [K(M(\boldsymbol{x},\boldsymbol{r})) - \boldsymbol{y}]_n$$

Gradient

$$\frac{\partial J}{\partial \boldsymbol{x}} = (\boldsymbol{P}^f)^{-1}(\boldsymbol{x} - \boldsymbol{x}_b) + \sum_n \boldsymbol{M}_x^{\ T} [\boldsymbol{K}]_n^T \boldsymbol{R}_n^{-1} [K(M(\boldsymbol{x},\boldsymbol{r}) - \boldsymbol{y}]_n$$

$$\frac{\partial J}{\partial \boldsymbol{r}} = \boldsymbol{Q}^{-1}(\boldsymbol{r} - \boldsymbol{r}_b) + \sum_n \boldsymbol{M}_r^{\ T} [\boldsymbol{K}]_n^T \boldsymbol{R}_n^{-1} [K(M(\boldsymbol{x},\boldsymbol{r}) - \boldsymbol{y}]_n$$

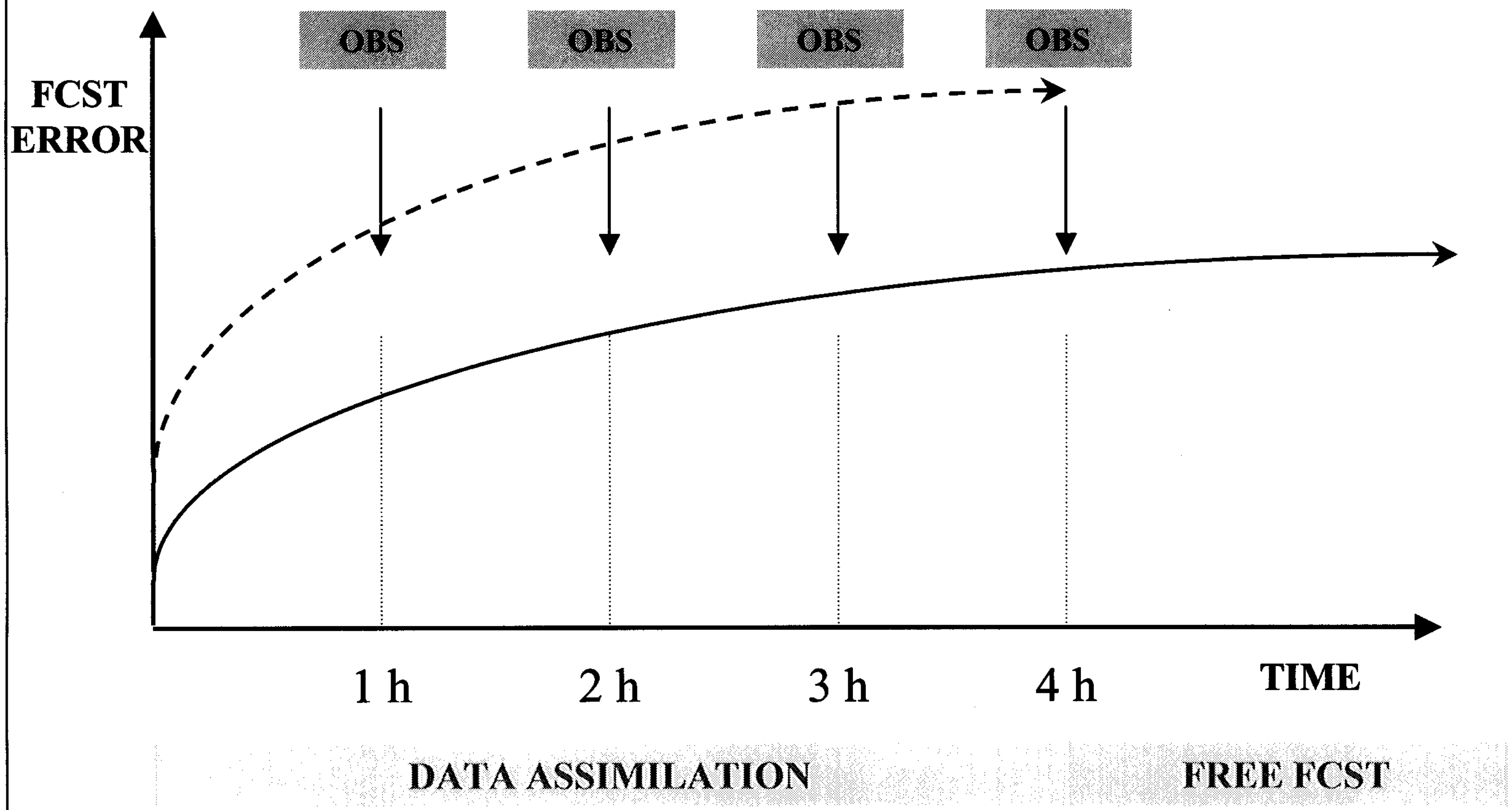
Hessian matrix

$$\frac{\partial^2 J}{\partial \boldsymbol{x}^2} = (\boldsymbol{P}^f)^{-1} + \sum_n \boldsymbol{M}_x^{\ T} [\boldsymbol{K}]_n^T \boldsymbol{R}_n^{-1} \boldsymbol{M}_x$$

$$\frac{\partial^2 J}{\partial \boldsymbol{r}^2} = \boldsymbol{Q}^{-1} + \sum_n \boldsymbol{M}_r^{\ T} [\boldsymbol{K}]_n^T \boldsymbol{R}_n^{-1} \boldsymbol{M}_r$$

$\boldsymbol{M}^{T}$ – *adjoint* of NWP model

SIMULTANEOUS DATA ASSIMILATION (4DVAR, EnKS)



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ENSEMBLE DATA ASSIMILATION

- **Solving the Kolmogorov equation**
- **Sampling of probability density by non-linear ensembles**
- **Unification of ensemble forecasting and data assimilation:**
  Given the *initial* estimate of probability density (*data assimilation*), find the *forecast* probability density (*ensemble forecasting*)
- **Feedback between data assimilation and ensemble forecasting**
- **Superior parallel computing**

ENSEMBLE *KALMAN FILTER* AND *SMOOTHER*:

- **Forecast error covariance using the non-linear ensemble forecasts**
- **Solve analysis inverse problem in the subspace spanned by ensembles**
- **Error covariance localization for small ensemble size**
- **Perturbations of observations, or model state**
- **Can be embedded in variational optimization algorithm**

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ENSEMBLE DATA ASSIMILATION:
Forecast Error Covariance

- **Kalman Filter (Smoother) forecast step**

$$\boldsymbol{P}^f \approx \boldsymbol{M}\boldsymbol{P}^a\boldsymbol{M}^T = [\boldsymbol{M}(\boldsymbol{P}^a)^{1/2}][\boldsymbol{M}(\boldsymbol{P}^a)^{1/2}]^T$$

- **If the columns of P_a ½ are known (p_i) the forecast error covariance is**

$$(\boldsymbol{P}^f)^{i,j} = [M(\boldsymbol{x}+\boldsymbol{p}_i)-M(\boldsymbol{x})][M(\boldsymbol{x}+\boldsymbol{p}_j)-M(\boldsymbol{x})]^T$$

Need only the *non-linear ensemble* forecast difference

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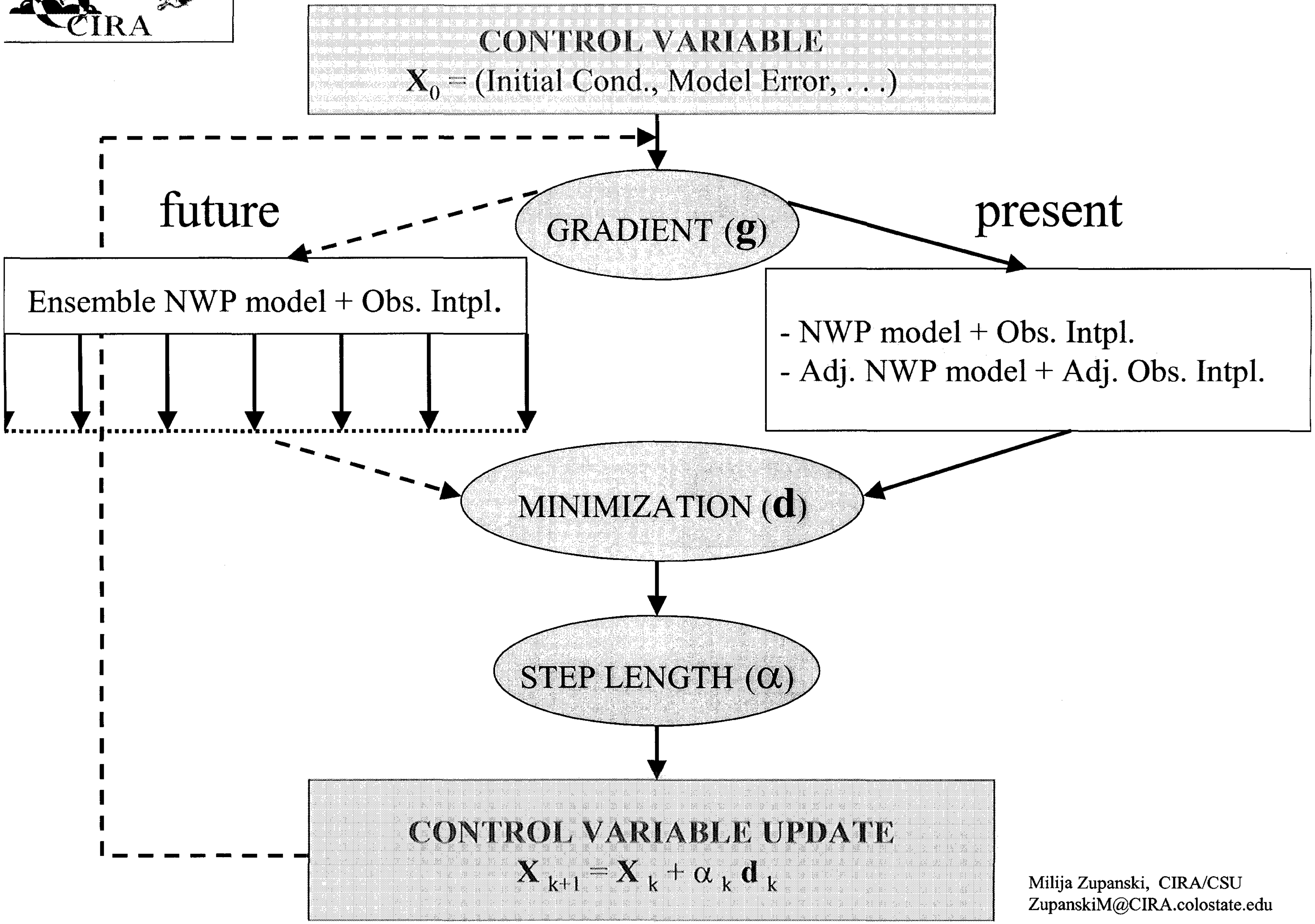
DATA ASSIMILATION FLOW CHART



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WHAT IS IN FUTURE?

- **PROBABILISTIC ESTIMATE OF ANALYSIS AND FORECAST ERRORS**
  - **Initial state probability distribution (*ensemble data assimilation*)**
  - **Forecast probability distribution (*ensemble forecasting*)**
  - ***Unified* data assimilation-forecasting system**

- **NON-GAUSSIAN ERROR STATISTICS**
  - **All current practical data assimilation methods assume Gaussian error statistics**

- **TRULY NON-LINEAR METHODS FOR DATA ASSIMILATION**
  - **Solve directly for the probability density function**

- **BEYOND THE CHAOS**
  - **All presented theory based on *deterministic* equations, with stochastic forcing**
  - **Ensemble forecasting is a set of *deterministic* model runs**
  - **The theory breaks down when chaos starts**
  - **A *non-deterministic* analog of Kolmogorov Equation**

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