# Introduction to Kalman Filter in the context of Data Assimilation

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# Outline


1. Introduction
2. Best Linear Unbiased Estimate (BLUE)
3. Optimum Interpolation (OI)
4. Kalman Filter (KF)
5. Extended Kalman Filter (EKF)
6. Stochastic Ensemble Kalman Filter (EnKF)
7. Deterministic Ensemble Kalman Filter (EnSRF)

# Notations

$\mathcal{X}_b$ = Background state vector
$\mathcal{B}$ = Background error covariance matrix
$\mathcal{X}_a$ = Analysis state vector or Estimated state vector
$\mathcal{A}$ = Analysis error covariance matrix
$\mathcal{Y}_o$ = Observation vector
$\mathcal{R}$ = **Observation error** covariance matrix
$\mathcal{H}$ = **Observation operator** or transformation model (linear version, $\mathbf{H} = d\mathcal{H}/d\mathcal{X}$ @ $t$)
$\mathcal{M}$ = **Transition model** for time integration ( linear version, $\mathbf{M} = d\mathcal{M}/d\mathcal{X}$ @ $t$ )
$Q$ = **Model error** covariance matrix
$\mathcal{Y}_d$ = Innovation or observation increment $[\mathcal{Y}_o - \mathcal{H}\mathcal{X}_b]$
$\mathcal{D}$ = Innovation covariance $[\mathcal{H}\mathcal{B}\mathcal{H}^T + \mathcal{R}]$

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# **Details of the Notations:** (Basic concepts)

Time Integration model ($\mathcal{M}_{n\text{x}n}$):

$$X_{(t)} = MX_{(t-1)}$$

Observation Operator ($\mathcal{H}_{p\text{x}n}$):

$$Y = HX$$

Error covariance matrix:

$$A_{n\text{x}n} = \sum (X_a - X)(X_a - X)^T$$

$$B_{n\text{x}n} = \sum (X_b - X)(X_b - X)^T$$

$$R_{p\text{x}p} = \sum (Y_o - HX)(Y_o - HX)^T$$

$$Q_{n\text{x}n} = B - MAM^T$$

The model error is that **component of the forecast error** (background error) which arise due to **uncertainties in the model**. This **excludes the error in the initial state** propagated through time integration forward and/or backward.

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# Closed ( not isolated ) System

**Temperature inside the iron dome.**

But the variations in the interior temperature depends on the variation in the dome temperature.

Variations in the dome temperature depends on the environmental conditions.

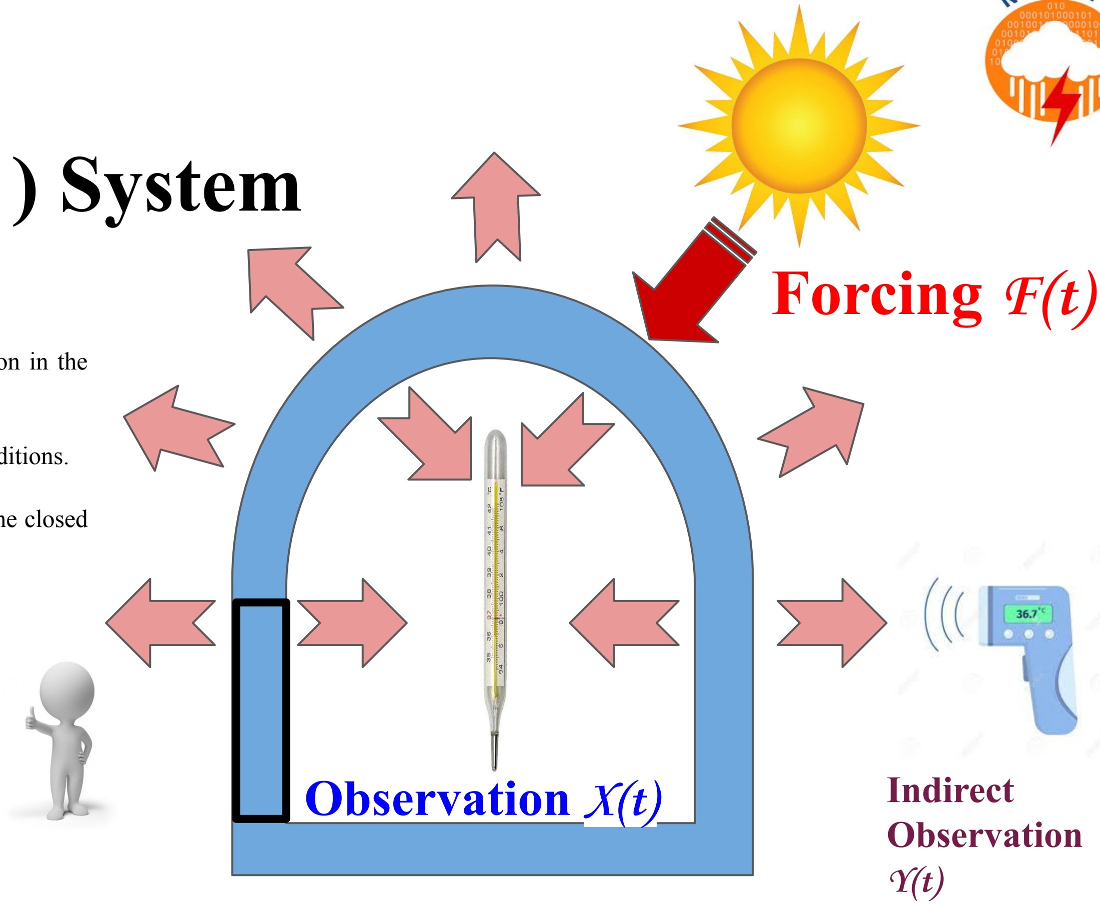
Every moment when we open the door of the iron dome we disturb the closed system and thereby introduce some error in the observation.

**Hence we need some sort of model**

$$\mathcal{X}(t) = \mathcal{M}\,[\,\mathcal{X}(t-1),\ \mathcal{F}(t)\,] + noise$$

**We can also use indirect observation.**

$$\mathcal{Y}(t) = \mathcal{H}\,[\,\mathcal{X}(t),\ \mathcal{L}(t)\,] + noise$$

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# Data Assimilation:

- **Numerical weather prediction (NWP) is an initial-value problem** for which initial data are not available in sufficient quantity and with Sufficient accuracy
- Estimation of a **realistic initial state** for a model forecast.
- Data assimilation is a method which determine the state of a system ( atmosphere or ocean or land ) as accurate as possible using **all the available information**.
- Data assimilation is a **statistical combination** of observation and short range forecast.
- Data assimilation is a **model integration nudged by innovation** (observation increment) **using proper weight** in such a way that it remains close to the reality of the system.

$$X_a = X_b + W Y_d$$

Eq (15)
in a later slide

Reference: Ghil (1981), Talagrand (1997), Kalnay (2003)

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# Methods to determine the weight for innovation:

$$X_a = X_b + WY_d$$ Eq (15)

1. **Empirical weight:** Multiple iteration using empirical weight until the convergence is achieved.
   eg:- Successive Correction Method (SCM): Berglhorsson and Doos (1955), Cressman (1959), Barnes (1964)
2. **Least Square Method:** Analysis error minimisation at each grid point.
   eg:- Optimum Interpolation (OI): Gandin 1963
3. **Cost function minimisation:** Variational Assimilation use minimization of cost function simultaneously for the entire domain.
   eg:- 3D-Var: Sasaki (1970)
   4D-Var: Boutlier and Rabier 1997
4. **Analysis error covariance minimization :**
   eg:- **Kalman Filter Family**

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# Bayes Filter

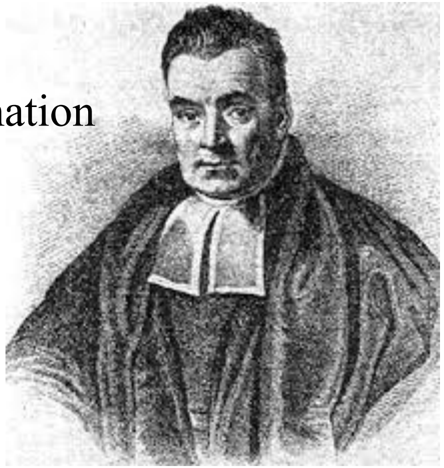
Bayes Filter is a framework for **recursive state estimation** proposed by **Thomas Bayes**

**Background (First guess): "**The **degree of belief** may be based on prior knowledge about the event, such as the **results of previous experiments** (objective evidence), or on **personal beliefs** (subjective hypothesis) about the event. **"**

**Bayesian Approach ( Recursive approach )**

(1) Construct the **background** of the state based on all available information
(2) Estimation of **background statistics** (eg: mean, variance, etc)
(3) Use new measurements for the **recursive updation** of estimate.
    (1) Batch Processing
    (2) Sequential Processing

The updated (corrected) estimate is what we call as **"analysis"**



**Thomas Bayes (1701-1761)**

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# Bayes Filter Classification

1) **Model (Transition and observation models)** based classification

Linear : $\mathcal{X}(t) = (\mathbf{M1})\, \mathcal{X}(t-1) + (\mathbf{M2})\, \mathcal{F}(t) + \textit{noise}$

$\mathcal{Y}(t) = (\mathbf{H1})\, \mathcal{X}(t) + (\mathbf{H2})\, \mathcal{L}(t) + \textit{noise}$

Non-linear : $\mathcal{X}(t) = \mathcal{M}\,[\,\mathcal{X}(t-1), \mathcal{F}(t)\,] + \textit{noise}$

$\mathcal{Y}(t) = \mathcal{H}\,[\,\mathcal{X}(t), \mathcal{L}(t)\,] + \textit{noise}$

2) Classification based on the **nature of Noise**

Gaussian

Non-Gaussian

3) **Sampling method** based classification

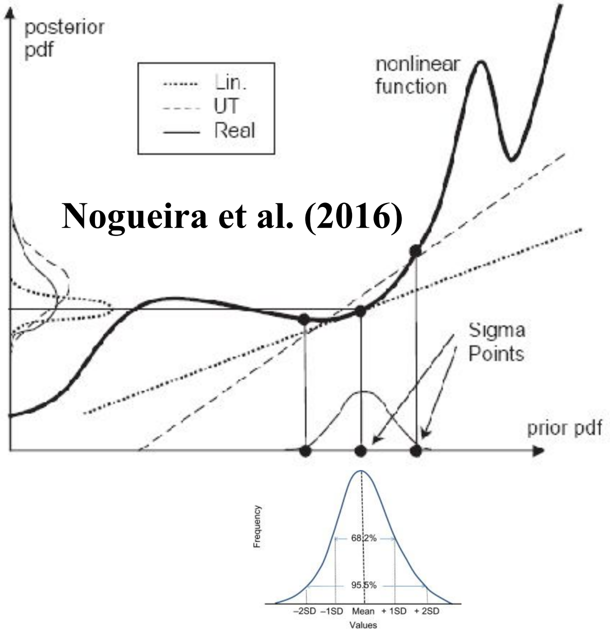
Parametric (eg: Particle filter)

Non-Parametric (eg: Monte Carlo methods)

4) **Observation processing** based classification

Batch Processing : (eg: variational DA)

Sequential Processing (eg: Kalman filter family)




**Subsets of Bayes Filter :** Kalman Filter, Particle Filter, discrete filter etc

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# Best Linear Unbiased Estimate (BLUE)

Consider the estimate ($x_a$) from the available **"independent"** information ($x_o$) and ($x_b$) using the linear function as follows.

$$x_a = w_o x_o + w_b x_b$$

Eq (1)

The estimate become unbiased if the mean

$$E(x_o) = E(x_b) = E(x_a) = E(x_t) = m$$

Eq (2)

where ($x_t$) is the unknown truth.

In other words "**mean noise is zero**" for an unbiased system.

$$E(e_o) = E(e_b) = E(e_a) = 0$$

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# Best Linear Unbiased Estimate (BLUE)

$$x_a = w_o x_o + w_b x_b$$ Eq (1)

$$E(x_a) = w_o E(x_o) + w_b E(x_b)$$

$$w_o + w_b = 1$$

$$w_b = 1 - w_o$$

$$x_a = w_o x_o + (1 - w_o) x_b$$

$$x_a = x_b + w_o (x_o - x_b)$$

Now there is only one weight $\mathbf{W} = w_1$

$$x_a = x_b + \mathbf{W} \ (x_o - x_b)$$ Eq (3)

Consider the model background ($x_b$) at a particular grid point get projected using observation operator $\mathcal{H}(x_b)$ to a nearby location and a related observable parameter and ($y_o$) be the corresponding observation at the location.

$$x_a = x_b + W[y_o - \mathcal{H}(x_b)]$$

Eq (12)
on coming slides

But still we need to get an appropriate weight $W$

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# Innovation ($X_d$)

$$x_a = x_b + \mathbf{W} \; (x_o - x_b)$$ Eq (3)

Innovation term is visible in the above equation (3)

$$X_d = X_o - X_b$$ Eq (4)

$$X_a = X_b + \mathbf{W} X_d$$ Eq (5)

Innovation (Observation Increment) is an unbiased (zero mean noise) extract of the observed information which is useful to correct the background estimate (first guess) in a data assimilation system.

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# Best Linear Unbiased Estimate (BLUE)

$$x_a = w_o x_o + w_b x_b$$ Eq (1)

$$Var(X_a) = Var[w_o x_o + w_b x_b]$$

$$Var(X_a) = E[[w_o x_o + w_b x_b] - [w_o E(x_o) + w_b E(x_b)]]^2$$

$$Var(X_a) = E[w_o[x_o - E(x_o)] + w_b[x_b - E(x_b)]]^2$$

$$Var(x_a) = w_o^2 Var(x_o) + w_b^2 Var(x_b)$$ $(a+b)^2$ expansion

Eq (6)

Informations $(x_o)$ and $(x_b)$ are **"independent"**, which makes **the cross covariance term zero**.

**Answer to exercise 1 on the lecture note:**

$$2 w_o w_b [x_o - E(x_o)][x_b - E(x_b)] = 0$$

# Best Linear Unbiased Estimate (BLUE)

$$w_b = 1 - w_o$$

$$w_b^2 = (1 - w_o)^2$$

$$w_b^2 = 1 + w_o^2 - 2\,w_o$$

$$w_b^2 = 1 + W^2 - 2\,W$$

$$Var(x_a) = w_o^2\, Var(x_o) + w_b^2\, Var(x_b)$$ Eq (6)

We can rewrite Eq (6) as follows

$$Var(x_a) = Var(x_b) + W^2\,[Var(x_o) + Var(x_b)] - 2W\, Var(x_b)$$

Eq (6.1)

The derivative of Eq (6) on $W$ gives :-

$$0 + 2W\,[Var(x_o) + Var(x_b)] - 2Var(x_b) = 0$$

$$W = Var(x_b) / [Var(x_o) + Var(x_b)]$$ Eq (7)

$$1 - W = Var(x_o) / [Var(x_o) + Var(x_b)]$$ Eq (8)

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# Best Linear Unbiased Estimate (BLUE)

$$\mathbf{W} = Var(x_b) / [Var(x_o) + Var(x_b)]$$ Eq (7)

$$1\text{-}\mathbf{W} = Var(x_o) / [Var(x_o) + Var(x_b)]$$ Eq (8)

$$Var(x_a) = w_o^2\, Var(x_o) + w_b^2\, Var(x_b)$$ Eq (6)

$$Var(x_a) = \mathbf{W}^2 Var(x_o) + (1 - \mathbf{W})^2 Var(x_b)$$

$$Var(x_a) = [Var(x_b)]^2 Var(x_o) / [Var(x_o) + Var(x_b)]^2 + [Var(x_o)]^2\, Var(x_b) / [Var(x_o) + Var(x_b)]^2$$

$$Var(x_a) = Var(x_o)\, Var(x_b) / [Var(x_o) + Var(x_b)]$$

$$[Var(x_a)]^{-1} = [Var(x_o)]^{-1} + [Var(x_b)]^{-1}$$

Analysis error covariance $\mathbf{A_C} = Var(x_a)$

Background error covariance $\mathbf{B_C} = Var(x_b)$

Observation error covariance $\mathbf{R_C} = Var(x_o)$

$$\mathbf{W} = \mathbf{B_C}\,[\mathbf{R_C} + \mathbf{B_C}]^{-1}$$

$$[1\text{-}\mathbf{W}] = \mathbf{R_C}\,[\mathbf{R_C} + \mathbf{B_C}]^{-1}$$

$$\mathbf{A_C} = \mathbf{R_C}\,\mathbf{B_C}\,[\mathbf{R_C} + \mathbf{B_C}]^{-1}$$

$$\mathbf{A_C} = [1\text{-}\mathbf{W}]\,\mathbf{B_C}$$ Eq (9)

$$\mathbf{A_C} = \mathbf{R_C}\,\mathbf{W}$$ Eq (10)

Since $\mathbf{W} < \mathbf{I}$ : $\mathbf{A_C} < \mathbf{B_C}$ and $\mathbf{A_C} < \mathbf{R_C}$

$$[\mathbf{A_C}]^{-1} = [\mathbf{R_C}]^{-1} + [\mathbf{B_C}]^{-1}$$ Eq (11)

**Uncertainty (variance) in the estimate** is less than the minimum among the uncertainties (variances) of each of the available information.
**Precision of the analysis** is the sum of precisions of the individual informations.

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# Best Linear Unbiased Estimate (BLUE)

$$x_a = x_b + \mathbf{W}\ (x_o - x_b)$$

Eq (3)

Eq (3) is already linear and unbiased from the previous slides. Optimal weight is the fraction of background error variance to the total error variance.

$$\mathbf{W} = Var\,(x_b) / \ [Var(x_o) + Var\,(x_b)\,]$$

Eq (7)

The larger the background error variance the larger the correction on the first guess.

**Gauss-Markov Theorem:** Least square estimate have the minimum uncertainty among all kind of **linear unbiased** estimate.

Reference: **Theil 1971**

**Rao–Blackwell theorem :** If the **noise** associated with all the available information is gaussian, then the least square estimate is the best among all estimates (including non-linear estimates).

Reference: **Lehmann and Scheffé 1950**

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# Basic Optimality of the Estimators

1. Least sum of squared errors

   Least square estimation.

2. Minimum variance estimates

   Analysis error covariance minimisation.

3. Maximum likelihood estimates

   Maximum probability of a state vector

Reference: Lewis et al (2006) book.

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# Transformation Model or Observation Operator ($\mathcal{H}$)

Usage of observation operator ($\mathcal{H}_{\mathcal{P}x\mathcal{N}}$).

- Transformation of state variable ($\mathcal{X}_{\mathcal{N}x1}$) into observation variable ($\mathcal{Y}_{\mathcal{P}x1}$)
- Horizontal interpolation
- Vertical interpolation
- Temporal interpolation

$$(\mathcal{Y})_{\mathcal{P}x1} = (\mathcal{H})_{\mathcal{P}x\mathcal{N}}(\mathcal{X})_{\mathcal{N}x1}$$

Innovation in observation space $\mathcal{Y}_{do}$ is defined as

$$\mathcal{Y}_{do} = \mathcal{Y}_{o} - \mathcal{H}\mathcal{X}_{b}$$

Presence of observation operator along with Optimum Estimation (BLUE) algorithm enables an **Optimum Interpolation (OI)**. **Details on slide entitled** **Filtering Properties of Optimal Interpolation**

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# Innovation on the observation space ($\mathcal{Y}_d$)

$$\mathcal{X}_d = \mathcal{X}_o - \mathcal{X}_b$$

Eq (4)

Equation (4) describe the innovation in the state space. Now we can use the observation operator to define innovation in observation space.

$$\mathcal{H}\mathcal{X}_d = \mathcal{H}[\mathcal{X}_o - \mathcal{X}_b]$$

$$\mathcal{Y}_d = [\mathcal{Y}_o - \mathcal{H}\mathcal{X}_b]$$

Eq (12)

$$\mathcal{X}_a = \mathcal{X}_b + \mathbf{W}\mathcal{X}_d$$

Eq (5)

Now we require a slight modification in the weight

$$\mathcal{W} = \mathbf{W}\mathcal{H}^T$$

$$\mathcal{X}_a = \mathcal{X}_b + \mathcal{W}\mathcal{Y}_d$$

Eq (13)

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# Optimal Interpolation (OI) :

$$x_a = x_b + \mathbf{W}\ (x_o - x_b)$$ Eq (3)

Consider the model background ($x_b$) at a particular grid point get projected to a nearby location using the observation operator $\mathcal{H}(x_b)$ and ($y_o$) be an observation at the location.

Eq (12)

$$Y_d = [Y_o - \mathcal{H}X_b]$$

$$X_a = X_b + WY_d$$ Eq (13)

Weight $W$ *is given by*

$$W = Var(x_b) / [Var(x_o) + Var(x_b)]$$

Eq (7)

Consider $Y_{Px1}$ where 'P' is total number of observation, that is the product of number of observation parameters with number of observation locations.

Consider $X_{Nx1}$ where 'N' is total number of background information, that is the product of the number of model variables with number of model grid points.

The observation operator $\mathcal{H}_{PxN}$ is a transformation matrix, in such a way that $(\mathcal{H}X)_{Px1}$ have the same dimension as that of $Y_{Px1}$ and the difference

$$Y_d = (\mathcal{H})_{PxN}(X_d)_{Nx1} = [(Y_o)_{Px1} - (\mathcal{H})_{PxN}(X)_{Nx1}]$$ Eq (12)

provide the innovation according to the dimension.

$$(X_a)_{Nx1} = (X_b)_{Nx1} + W_{NxP}(Y_d)_{Px1}$$

Here is the vector form of Eq(13)

Eq (13)

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# Optimal Interpolation (OI)

$x_a = x_b + W\,(x_o - x_b)$ Eq (3)

Consider the model background ($x_b$) at a particular grid point get projected to a nearby location using the observation operator $H\,(\,x_b\,)$ and ($y_o$) be an observation at the location.

Eq (12)

$$Y_d = [Y_o - HX_b]$$

$$X_a = X_b + WY_d$$

Eq (13)

Weight $W$ *is given by*

$$W = Var\,(x_b) / \,[Var(x_o) + Var\,(x_b)\,]$$

Eq (7)

$(X_a)_{Nx1} = (X_b)_{Nx1} + W_{NxP}\,(Y_d)_{Px1}$ Eq (13)

Here is the vector form of Eq(13)

Now we need to get the weight function in the vector form.

Consider the background error covariance $B_{NxN}$ and observation error covariance $R_{PxP}$ along with the observation operator $H_{PxN}$ and its transpose $H^T{}_{NxP}$

Observation error covariance in state space is $H^T{}_{NxP} R_{PxP} H_{PxN}$

Background error covariance in observation space is $H_{PxN} B_{NxN} H^T{}_{NxP}$

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# Optimal Interpolation (OI)

$$x_a = x_b + W\,(x_o - x_b)$$ Eq (3)

Consider the model background ($x_b$) at a particular grid point get projected to a nearby location using the observation operator $H(x_b)$ and ($y_o$) be an observation at the location.

$$Y_d = [Y_o - HX_b]$$ Eq (12)

$$X_a = X_b + WY_d$$ Eq (13)

Weight $W$ *is given by*

$$W = Var(x_b) / [Var(x_o) + Var(x_b)]$$ Eq (7)

$$(X_a)_{N\mathrm{x}1} = (X_b)_{N\mathrm{x}1} + W_{N\mathrm{x}P}\,(Y_d)_{P\mathrm{x}1}$$ Eq (13)

Here is the vector form of Eq(13)

Now we need to get the weight function in the vector form.

Consider the background error covariance $B_{N\mathrm{x}N}$ and observation error covariance $R_{P\mathrm{x}P}$ along with the observation operator $H_{P\mathrm{x}N}$ and its transpose $H^T_{N\mathrm{x}P}$

$$W_{N\mathrm{x}P} = B_{N\mathrm{x}N} H^T_{N\mathrm{x}P} [R_{P\mathrm{x}P} + H_{P\mathrm{x}N} B_{N\mathrm{x}N} H^T_{N\mathrm{x}P}]^{-1}$$ Eq (14)

Here is the vector form of Eq(7)

We can write a combined equation as below

$$X_a = X_b + WY_d$$

$$X_a = X_b + B H^T [R + H B H^T]^{-1} [Y_o - H X]$$ Eq (15)

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# Optimal Interpolation (OI)

$$x_a = x_b + W\,(x_o - x_b) \qquad \text{Eq (3)}$$

$$W = Var\,(x_b) \,/\, [Var(x_o) + Var\,(x_b)\,] \qquad \text{Eq (7)}$$

$$Var\,(x_a) = Var(x_o)\,Var\,(x_b) \,/\, [Var(x_o) + Var\,(x_b)\,]$$

Notation form:

$$A_C = R_C\,B_C\,[\,R_C + B_C\,]^{-1}$$

Eq (9)

$$A_C = [\,1-W]\,B_C$$

$$[A_C]^{-1} = [R_C]^{-1} + [B_C]^{-1} \qquad \text{Eq (10)}$$

Eq (11)

$$(X_a) = (X_b) + W\,(\,Y_o - HX_b\,) \qquad \text{Eq (13)}$$

$$A = E[e_a e_a^T] = E\,[e_b + W^T(e_o - He_b)][e_b + W^T(e_o - He_b)]^T$$

$$A = E\,[e_b e_b^T + e_b\,(e_o - He_b)^T W^T + W\,(e_o - He_b)e_b^T + W\,(e_o - He_b)(e_o - He_b)^T W^T]$$

$$A = B - BH^T W^T + WHB + WRW^T + WHBH^T W^T$$

$$A = B - BH^T[B H^T [R + H B H^T]^{-1}]^T + [B H^T [R + H B H^T]^{-1}]HB + [B H^T [R + H B H^T]^{-1}]R[B H^T [R + H B H^T]^{-1}]^T + [B H^T [R + H B H^T]^{-1}]HBH^T[B H^T [R + H B H^T]^{-1}]^T$$

$$A_{NxN} = [\,I_{NxN} - W_{NxP}H_{PxN}]B_{NxN} \qquad \text{Eq (16)}$$

Here is the matrix form of Eq(10)

$$[A]^{-1} = H^T[R]^{-1}H + [B]^{-1}$$

Here is the matrix form of Eq(11)

$$A = [H^T[R]^{-1}H + [B]^{-1}]^{-1} \qquad \text{Eq (17)}$$

The cross-covariance terms in the expansion are eliminated by considering the independence of information. That is the observation and background are not correlated to each other.

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# Basic characteristics of Optimum Interpolation

- The analysis is obtained by adding optimal weighted innovation to the background

$$(X_a) = (X_b) + W\,(Y_o - HX_b) \qquad \text{Eq (13)}$$

- Optimal weight is the fraction of background error covariance to the total error covariance

$$W = B H^T [R + H B H^T]^{-1} \qquad \text{Eq (14)}$$

- Error variance of the background reduced by a factor ( $1 - WH$ ) gives the error variance of the analysis

$$A = [\,I - WH]B \qquad \text{Eq (16)}$$

- The precision of the analysis is the sum of the precisions of both the background and the observation (in state space).

$$[A]^{-1} = H^T[R]^{-1} H + [B]^{-1} \qquad \text{Eq (17)}$$

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# Filtering Properties of Optimal Interpolation

**Eliminate the interpolation aspects** of the analysis by assuming

**Observation Operator ($\mathcal{H}$)** to be Identity Matrix ($I$)

$$(Y_o) = (X_o)$$

$$X_a - X_b = B H^T [R + H B H^T]^{-1} [Y_o - H X_b] \qquad \text{Eq (15)}$$

$$X_a - X_b = B[R + B]^{-1} [X_o - X_b]$$

$$X_a - X_b = B A^{-1} [X_o - X_b] \qquad \text{Eq (17)}$$

$$X_{da} = B A^{-1} X_{do}$$

Increment of analysis in state space ($X_{Nx1}$)

$$X_{da} = X_a - X_b$$

Increment of observation in state space ($X_{Nx1}$)

$$X_{do} = X_o - X_b$$

Reference: Daley (1991)

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# Transition model ($\mathcal{M}$)

The mathematical representation of the physical process which drives the time evolution of the state vector.

$$X(t) = \mathcal{M}[X(t-1)] \quad \text{Eq (18)}$$

One of the primary essential for the data assimilation system is a well defined time forwarding model (transition model).

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# <u>**Markovian assumption:**</u> **(sequential processing)**

Probability of $\mathcal{X}$ intersection $\mathcal{Y}$ defined by **markovian chain rule** as

$$\mathcal{P}[\mathcal{X} \cap \mathcal{Y}] = \mathcal{P}[\mathcal{Y}|\mathcal{X}] \,.\, \mathcal{P}[\mathcal{X}]$$

$$\mathcal{P}[\mathcal{X} \,|\, \mathcal{Y}]\mathcal{P}[\mathcal{Y}] = \mathcal{P}[\mathcal{Y} \,|\, \mathcal{X}]\, \mathcal{P}[\mathcal{X}]$$

(based on commutative property of intersection)

<u>**Assumptions:**</u>

(1) The <u>**conditional independence of observation**</u> given the state

$$\mathcal{Y}(t) = \mathcal{H}[\mathcal{X}(t), l(t)] \quad \text{or} \quad \mathcal{P}[\mathcal{Y}(t) \,|\, \mathcal{X}(t)]$$

where $l_t$ is known observation control info (eg: perturbation, location, bias).

(2) Markovian process: well defined time evolution (predictability)

$$\mathcal{X}(t) = \mathcal{M}[\mathcal{X}(t-1), f(t)] \quad \text{or} \quad \mathcal{P}[\mathcal{X}(t) \,|\, \mathcal{X}(t-1)]$$

where $f_t$ is known state control info (eg: perturbation, forcing, bias).

(3) Initial state is known.

$$\mathcal{P}[\mathcal{X}(0) \,|\, \mathcal{Y}(0)] = \mathcal{P}[\mathcal{X}(0)]$$

(4) Continuous Observations are available

$$\mathcal{Y} = [\mathcal{Y}]_0^t$$

from initial time (t=0) to present ( t=t )

**Andrey Andreyevich Markov (1856 - 1922)**

# Markovian Chain of Bayesian Estimation Cycle

**Prediction step** ( a-priori ) : generate the **background (first guess)** using the time transition model**.**

$$x(t) = \mathcal{M}[x(t-1), f(t)]$$
$$\mathcal{P}[X(t) \mid X(t-1)]$$

**Correction step** ( a-posteriori ) : generate the **analysis** using the observation model**.**

$$y(t) = \mathcal{H}[x(t), l(t)]$$
$$\mathcal{P}[Y(t) \mid X(t)]$$

$$\mathcal{P}[X \cap Y] = \mathcal{P}[Y|X] \,.\, \mathcal{P}[X]$$

$$\mathcal{P}[X(t) \mid Y(t)]\mathcal{P}[Y(t)] = \mathcal{P}[Y(t) \mid X(t)]\, \mathcal{P}[X(t)]$$

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# Optimum Interpolation Algorithm

Minimum communication between estimator and transition model ($\mathcal{M}$)

1) Optimum Interpolation [ $(X_a)_{t-1}, \mathcal{A}_{t-1}, Y_t$ ]
2) Background state $X_b = \mathcal{M}(X_a)_{(t-1)}$ Eq (18)
3) Bg err covariance $\mathcal{B} = a\mathcal{A}$
4) Optimum Weight $\mathcal{W} = \mathcal{B}\mathcal{H}^T[\mathcal{H}\mathcal{B}\mathcal{H}^T + \mathcal{R}]$ Eq (14)
5) Innovation $Y_d = [Y_o - \mathcal{H}(X_b)]$ Eq (12)
6) Corrected state $(X_a) = (X_b) + \mathcal{W} Y_d$ Eq (15)
7) Analysis covariance $\mathcal{A} = (I - \mathcal{W}\mathcal{H})\mathcal{B}$ Eq (16)
8) Return [ $(X_a), \mathcal{A}$ ]

Outline>>

# Kalman Filter

A state-space approach of optimal estimation algorithm based on Bayesian Filter for linear systems with Gaussian noise distribution is known as Kalman Filter.

formulated by Kalman (1960)

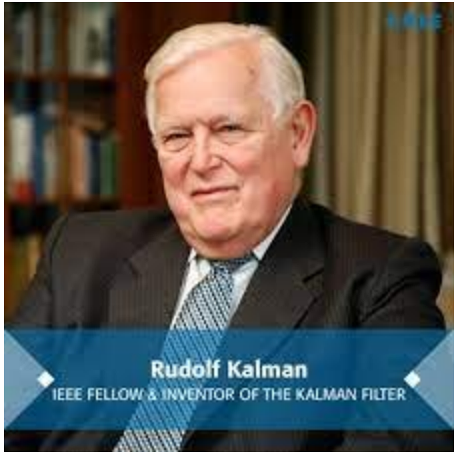
further improved by Kalman and Bucy (1961)

Conditions for applicability of Kalman Filter:

1) Transition model and observation model are **linear** (or linearized or tangent-linear )
2) Noise have **Zero mean Gaussian Distribution**

Use:

1) Estimation of variables where direct measurement is difficult.
2) Combining of multiple observations (signal+noise) to get best estimate.




**Rudolf E. Kalman (1930-2016)**

Outline>>

# Kalman Filter Family

- Kalman Filter(KF):
  Ghil et al 1981
- Extended Kalman Filter (EKF):
  Einicke and White (1999)
- Ensemble Kalman Filter (EnKF):
  Evensen (1994), Houtekamer and Mitchell (1998)
- Deterministic Ensemble Kalman Filter (EnSRF):
  Tippett et al. (2003)
  - Ensemble Transform Kalman Filter (ETKF):
    Bishop et al. (2001), Majumdar (2002)
  - Local Ensemble Kalman Filter (LEKF):
    Kalnay and Toth (1994), Ott et al. (2002,2004)
  - Local Ensemble Transform Kalman Filter (LETKF):
    Harlim and Hunt (2005)

# Properties of Gaussian Distribution

Product of two gaussians is a gaussian.

**Gaussians stay gaussians under linear transformation**.

Marginal and conditional distribution of a gaussian stays a gaussian.

Mean and covariance of a gaussian distribution is computable.

Matrix are invertible in a gaussian system.

Outline>>

# Error Variance Tracking in Kalman Filter

$$X_b(t) = \mathbf{M} X_a(t-1)$$

Eq (18)

Model error is defined by the expression as follows

$$X_t(t) = \mathbf{M} X_t(t-1) + e_m$$

Background error is defined as

$$e_b(t) = X_b(t) - X_t(t)$$

$$e_b(t) = \mathbf{M} X_a(t-1) - \mathbf{M} X_t(t-1) - e_m$$

**( In the case of Extended Kalman Filter, Linearized model is used. ie $\mathbf{M} = d\mathcal{M}/dX @ t$)**

$$e_b(t) = \mathbf{M}[X_a(t-1) - X_t(t-1)] - e_m$$

$$e_b(t) = \mathbf{M} e_a(t-1) - e_m$$

Mean error (bias)

$$\mathcal{E}[e_b(t)] = \mathbf{M}\mathcal{E}[e_a(t-1)] - \mathcal{E}[e_m]$$

Outline>>

# Error Variance Tracking in Kalman Filter

Background error covariance matrix $\mathcal{B}$ is defined by

$$\mathcal{B} = \mathcal{E}[e_b e_b^{\mathcal{T}}]$$

$$\mathcal{B} = \mathcal{E}[[\mathbf{M} e_a(t-1) - e_m][\mathbf{M} e_a(t-1) - e_m]^{\mathcal{T}}]$$

$$\mathcal{B} = \mathcal{E}[\mathbf{M} e_a(t-1) e_a^{\mathcal{T}}(t-1) \mathbf{M}^{\mathcal{T}} - e_m e_a^{\mathcal{T}}(t-1) \mathbf{M}^{\mathcal{T}} - \mathbf{M} e_a(t-1) e^{\mathcal{T}}_m + e_m e^{\mathcal{T}}_m]$$

As per variance of the sum theorem, for independent variables ($e_a$ and $e_m$), the cross covariance term become zero on summation.

$$\mathcal{B} = \mathbf{M}\ \mathcal{E}[e_a(t-1) e_a^{\mathcal{T}}(t-1)] \mathbf{M}^{\mathcal{T}} + \mathcal{E}[e_m e^{\mathcal{T}}_m]$$

$$\mathcal{B} = \mathbf{M}\, \mathcal{A}\, \mathbf{M}^{\mathcal{T}} + Q \qquad \text{Eq (19)}$$

Where $Q = \mathcal{E}[e_m e^{\mathcal{T}}_m]$ is the model error covariance matrix.

Outline>>

# Error Variance Tracking in Kalman Filter

**Analysis:** Optimum interpolation provide analysis state vector and analysis error variance.

$$(X_a) = (X_b) + W(Y_o - \mathbf{H} X_b) \quad \text{Eq (13)}$$

$$W = B\mathbf{H}^T[R + \mathbf{H}B\mathbf{H}^T]^{-1} \quad \text{Eq (14)}$$

$$A = [I - W\mathbf{H}]B \quad \text{Eq (16)}$$

**Prediction:** Optimum interpolation prediction stage only provide the forecast state vector.

$$x_b(t_{i+1}) = \mathbf{M}\,[x_a(t_i)] \quad \text{Eq (18)}$$

$$B = ?$$

Inability to track background error variance is the major limitation of **Optimum interpolation.**

$$B = a A$$

But the background error variance is well tracked in **Kalman Filter**

$$B = \mathbf{M}A\mathbf{M}^T + Q \quad \text{Eq (19)}$$

Outline>>

# Kalman Filter Algorithm

1) Kalman Filter $[(\mathcal{X}_a)_{t-1}, \mathcal{A}_{t-1}, \mathcal{Y}_t]$
2) Background state $(\mathcal{X}_b) = \mathbf{M}(\mathcal{X}_a)_{(t-1)}$ Eq (18)
3) Bg. Err. covariance $\mathcal{B} = \mathbf{M}\mathcal{A}\mathbf{M}^{\mathcal{T}} + \mathbf{Q}_t$ Eq (19)
4) Kalman gain $\mathcal{W} = \mathcal{B}\mathbf{H}^{\mathcal{T}}[\mathbf{H}\mathcal{B}\mathbf{H}^{\mathcal{T}} + \mathcal{R}]^{-1}$ Eq (14)
5) Innovation $\mathcal{Y}_d = [\mathcal{Y}_t - \mathbf{H}(\mathcal{X}_b)]$ Eq (12)
6) Corrected state $(\mathcal{X}_a) = (\mathcal{X}_b) + \mathcal{W}\,\mathcal{Y}_d$ Eq (15)
7) Analysis Err. covariance $\mathcal{A} = (\,I - \mathcal{W}\mathbf{H}\,)\,\mathcal{B}$ Eq (16)
8) Return $[(\mathcal{X}_a), \mathcal{A}]$

Outline>>

# Challenges in Kalman Filter for Realistic Problems

(i) Expensive background error covariance computation,

$$\mathcal{B}_{\mathcal{N}\mathrm{x}\mathcal{N}} = \mathbf{M}_{\mathcal{N}\mathrm{x}\mathcal{N}} \mathcal{A}_{\mathcal{N}\mathrm{x}\mathcal{N}} \mathbf{M}^{\mathcal{T}}_{\mathcal{N}\mathrm{x}\mathcal{N}} + Q_t$$

(ii) Inability to accommodate the nonlinearity of the real world dynamics,

(iii) poorly characterized error sources.

Unless special measures are taken, accumulation of roundoff error lose the positive definiteness of the error covariance matrix.

Outline>>

# Extended Kalman Filter (EKF)

The extended Kalman filter (EKF) is the **nonlinear version of the Kalman filter** which linearizes about an estimate of the current mean and covariance.

Linearized model $\mathbf{M} = dM/dX @ t$ Eq (20)

Linearized Observation Operator $\mathbf{H} = dH/dX @ t$ Eq (21)

Background error covariance is obtained by linearizing the model about the nonlinear trajectory within the cycle interval.

$$\mathcal{B} = \mathcal{M}(@t)\,\mathcal{E}\,[\,e_a(t-1)\,e_a^{\mathcal{T}}(t-1)\,]\mathcal{M}^{\mathcal{T}}(@t) + \mathcal{E}[e_m e^{\mathcal{T}}_m]$$

$$\mathcal{B} = [\mathbf{M}\mathcal{A}\mathbf{M}^{\mathcal{T}}] + Q \quad \text{Eq (22)}$$

$$\mathcal{W} = \mathcal{B}\mathbf{H}^{\mathcal{T}}[\mathbf{H}\mathcal{B}\mathbf{H}^{\mathcal{T}} + \mathcal{R}]^{-1} \quad \text{Eq (23)}$$

Reference:

Outline>>

# Extended Kalman Filter Algorithm

Nonlinear transition model $\mathcal{M}$ and Nonlinear observation operator $\mathcal{H}$ are used in EKF.

1) Kalman Filter [$(\mathcal{X}_a)_{t-1}, \mathcal{A}_{t-1}, \mathcal{Y}_t$ ]

2) Background state (non linear) $[\mathcal{X}_b] = \mathcal{M}[(\mathcal{X}_a)_{(t-1)}]$ Eq (18)

3) Linearized model $\mathbf{M} = d\mathcal{M}/d\mathcal{X}\ @\ t$ Eq (20)

4) Background Err. covariance $\mathcal{B} = [\mathbf{M}\mathcal{A}\mathbf{M}^{\mathcal{T}}] + Q$ Eq (22)

5) Linearized Obs-Operator $\mathbf{H} = d\mathcal{H}/d\mathcal{X}\ @\ t$ Eq (21)

6) Kalman gain $\mathcal{W} = \mathcal{B}\mathbf{H}^{\mathcal{T}}[\mathbf{H}\mathcal{B}\mathbf{H}^{\mathcal{T}} + \mathcal{R}]^{-1}$ Eq (23)

7) Innovation (non linear) $\mathcal{Y}_d = [\mathcal{Y}_o - \mathcal{H}(\mathcal{X}_b)]$ Eq (12)

8) Corrected state $(\mathcal{X}_a) = (\mathcal{X}_b) + \mathcal{W}\mathcal{Y}_d$ Eq (15)

9) Analysis Err. covariance $\mathcal{A} = (I - \mathcal{W}\mathbf{H})\mathcal{B}$ Eq (16)

10) Return [$(\mathcal{X}_a), \mathcal{A}$ ]

Outline>>

# Ensemble Kalman Filter (EnKF)

- State-space estimation methods.
- Low-rank representations of forecast and analysis error covariances.
- **Stochastic analysis ensemble update methods**: stochastic transformation of the forecast ensemble into an analysis ensemble.
- Tangent linear and adjoint models of the dynamics are **not required**.

Limitations

- Neglecting forecast error due to model deficiencies.
- requires an ensemble of “perturbed observations” for statistical consistency.
- “perturbed observations” may cause sampling issue.
- Computationally expensive

Reference : Evensen (1994), Houtekamer and Mitchell (1998)

Outline>>

# Ensemble Kalman Filter (EnKF)

**Observations perturbed randomly** in generating each ensemble member. All the individual members assimilate the same real observation with different set of random perturbations (to make them **realistically independent**).

$$(Y_d) = (Y_o + \epsilon - \mathcal{H}X_b) \qquad \text{Eq (24)}$$

An ensemble of Kalman Filter data assimilation cycles are carried out simultaneously.

$$[X_b(t)]_{1,2,3,\ldots K} = \mathcal{M}[X_a(t-1)]_{1,2,3,\ldots K} \qquad \text{Eq (25)}$$

Reference : Evensen (1994), Houtekamer and Mitchell (1998)

Outline>>

# Ensemble Kalman Filter (EnKF)

Flow dependent Background error covariance is determined from the ensemble of data assimilation cycles.

$$Z_b = B^{1/2} = [K-1]^{-1/2} \Sigma_{k=1}^{K} ( X_k - [K^{-1}] \Sigma_{k=1}^{K} X_k )$$

Eq (26)

$$B = Z_b Z_b^T = [1/[K-1]] \Sigma_{k=1}^{K} ( X_k - [1/K] \Sigma_{k=1}^{K} X_k )( X_k - [1/K] \Sigma_{k=1}^{K} X_k )^T$$

$$BH^T = Z_b (HZ_b)^T = [1/[K-1]] \Sigma_{k=1}^{K} ( X_k - [1/K] \Sigma_{k=1}^{K} X_k )( HX_k - [1/K] \Sigma_{k=1}^{K} HX_k )^T$$

$$HBH^T = HZ_b (HZ_b)^T = [1/[K-1]] \Sigma_{k=1}^{K} ( HX_k - [1/K] \Sigma_{k=1}^{K} HX_k )( HX_n - [1/K] \Sigma_{k=1}^{K} HX_k )^T$$

$$W = Z_b (HZ_b)^T [ HZ_b (HZ_b)^T + R ]^{-1}$$

Eq (27)

$$A = ( I - WH ) Z_b (Z_b)^T$$

Eq (28)

Reference : Evensen (1994), Houtekamer and Mitchell (1998)

Outline>>

# Ensemble Kalman Filter Algorithm

1) Ensemble Kalman Filter $[(X_a)_{t-1}, A_{t-1}, Y_t]_{k=1,2,3,...K}$
2) Background State $[X_b]_{k=1,2,3,...K} = m[(X_a)_{(t-1)}]_{k=1,2,3,...K}$ Eq (25)
3) Background Err. covariance $Z_b = [K-1]^{-1/2} \Sigma_{k=1,2,3,...K} (X_k - [K^{-1}] \Sigma_{k=1,2,3,...K} X_k)$ Eq (26)
4) Kalman gain $W = Z_b(HZ_b)^T [HZ_b(HZ_b)^T + R]^{-1}$ Eq (27)
5) Innovation $(Y_d)_{k=1,2,3,...K} = [Y_o + \epsilon_{k=1,2,3,...K} - h(X_b)]$ Eq (24)

($Y_o$ is the observation and $\epsilon_{k=1,2,3,...K}$ are the stochastic perturbations on the innovation)

6) Corrected State $(X_a)_{k=1,2,3,...K} = (X_b)_{k=1,2,3,...K} + W(Y_d)_{k=1,2,3,...K}$ Eq (15)
7) Analysis Err. covariance $A = (I - WH) Z_b (Z_b)^T$ Eq (28)
8) Return $[(X_a), A]_{k=1,2,3,...K}$

Outline>>

# Deterministic Ensemble Kalman Filter (EnSRF)

- **Deterministic EnKF** use **Matrix square roots** of error covariance and hence known as **Kalman square root filters or Ensemble square root filters**.
- **Deterministic analysis ensemble update methods:** analysis perturbations satisfy the Kalman filter analysis error covariance equation.
- Avoid sampling issues associated with the use of "perturbed observations".

Reference : Tippett et al. (2003)

Outline>>

# Deterministic Ensemble Kalman Filter (EnSRF)

$$\mathcal{A} = [\, I - \mathcal{W}\mathcal{H}]\mathcal{B}$$

$$\mathcal{A} = [I - [\mathcal{B}\mathcal{H}^T[\, \mathcal{H}\mathcal{B}\mathcal{H}^T + \mathcal{R}\,]^{-1}\,]\mathcal{H}]\mathcal{B}$$

$$\mathcal{A} = [I - [Z_b Z_b^{\,T}\mathcal{H}^T[\, \mathcal{H} Z_b Z_b^{\,T}\mathcal{H}^T + \mathcal{R}\,]^{-1}\,]\mathcal{H}] Z_b Z_b^{\,T}$$

$$\mathcal{A} = [I - [Z_b(\mathcal{H}Z_b)^T[(\mathcal{H}Z_b)(\mathcal{H}Z_b)^T + \mathcal{R}\,]^{-1}\,]\mathcal{H}] Z_b Z_b^{\,T}$$

$$\mathcal{A} = [Z_b - [Z_b(\mathcal{H}Z_b)^T[(\mathcal{H}Z_b)(\mathcal{H}Z_b)^T + \mathcal{R}\,]^{-1}\,]\mathcal{H}Z_b] Z_b^{\,T}$$

$$\mathcal{A} = Z_b\, [\, I - (\mathcal{H}Z_b)^T[(\mathcal{H}Z_b)(\mathcal{H}Z_b)^T + \mathcal{R}\,]^{-1}(\mathcal{H}Z_b)] Z_b^{\,T}$$

$$\mathcal{A} = Z_b\, [\, I - \mathcal{V}[\mathcal{V}^T\, \mathcal{V} + \mathcal{R}\,]^{-1}\mathcal{V}^T\, ] Z_b^{\,T}$$

$$\mathcal{A} = Z_b[\, I - \mathcal{V}[\mathcal{D}]^{-1}\mathcal{V}^T] Z_b^{\,T}$$

$$Z_a = Z_b[\, I - \mathcal{V}[\mathcal{D}]^{-1}\mathcal{V}^T]^{1/2}$$

$$Z_a = (K\text{-}1)^{-1/2} \sum [......]$$

$$Z_b = (K\text{-}1)^{-1/2} \sum [......]$$ Eq (26)

$$\mathcal{A} = Z_a Z_a^{\,T}$$ Eq (29)

$$\mathcal{B} = Z_b Z_b^{\,T}$$ Eq (30)

$$\mathcal{V} = (\mathcal{H}Z_b)^T$$ Eq (31)

$$\mathcal{D} = \mathcal{V}^T\, \mathcal{V} + \mathcal{R}$$ Eq (32)

$$X_k = [\, I - \mathcal{V}[\mathcal{D}]^{-1}\mathcal{V}^T]^{1/2}$$ Eq (33)

$$[Y_d] = [\, Y_o - \mathcal{H}\, X_b - \mathcal{H}\, X_k\, ]$$ Eq (34)

Outline>>

# Deterministic Ensemble Kalman Filter (EnSRF)

## Kalman Filter

$$\mathcal{A} = [\, I - \mathcal{W}\mathcal{H}]\mathcal{B} \qquad \text{Eq (16)}$$

$$\mathcal{W} = \mathcal{B}\mathcal{H}^T[\, \mathcal{H}\mathcal{B}\mathcal{H}^T + \mathcal{R}\,]^{-1} \qquad \text{Eq (27)}$$

$$\mathcal{B} = \mathcal{M}\mathcal{A}\mathcal{M}^T + Q \qquad \text{Eq (19)}$$

## Square Root Kalman Filter

$$\mathcal{Z}_a = \mathcal{Z}_b \mathcal{X}_k \qquad \text{Eq (35)}$$

$$\mathcal{W} = \mathcal{Z}_b \mathcal{V}[\, \mathcal{D}\,]^{-1} \qquad \text{Eq (36)}$$

$$\mathcal{Z}_b = \mathcal{M}\mathcal{Z}_a \qquad \text{Eq (37)}$$

$$\mathcal{V} = (\mathcal{H}\mathcal{Z}_b)^T \qquad \text{Eq (31)}$$

$$\mathcal{V} = [\mathcal{H}\mathcal{M}(\mathcal{Z}_a)_{t-1}]^T \qquad \text{Eq (38)}$$

The transformation operator which generate deterministic perturbation

Outline>>

# Deterministic Ensemble Kalman Filter Algorithm

| | | |
|---|---|---|
| 1) **EnSRF [** $(X_a)_D$ $(x_a)_{t-1\ k=1,2,3,\ldots K}$, $(Z_a)_{t-1}$, $Y_t$ **]** | | |
| 2) Background **(deterministic)** | $[X_b] = M\,[X_a]_{(t-1)}$ | Eq (18) |
| 3) Background covariance **matrix square root** | $Z_b = MZ_a$ | Eq (37) |
| 4) **Transformation Operator** | $V = [HZ_b]^T$ | Eq (38) |
| 5) Innovation Covariance Matrix | $D = V^T V + R$ | Eq (32) |
| 6) Kalman gain | $W = Z_b V[\,D\,]^{-1}$ | Eq (36) |
| 7) Analysis Perturbations (state perturbation) | $X_k = [\,I - V[D]^{-1}V^T]^{1/2}$ | Eq (33) |
| 8) Innovation Estimate (with deterministic pert.) | $[Y_d] = [\,Y_o - HX_b - HX_k\,]$ | Eq (34) |
| 9) Corrected State **(deterministic)** | $[X_a] = [X_b] + W[Y_d]$ | Eq (15) |
| 10) Analysis Err. covariance **matrix square root** | $Z_a = Z_b X_k$ | Eq (35) |
| 11) Return [$(X_a)_D$ $(x_a)_{k=1,2,3,\ldots K}$, $(Z_a)$] | | |

Outline>>

# Deterministic Ensemble Kalman Filter (EnSRF)

**Classifications:**

1) Ensemble Adjustment Kalman Filter (EAKF):

    Anderson (2001)

2) Ensemble Transform Kalman Filter (ETKF):

    Bishop et al. (2001), Majumdar et al. (2002)

3) Local Ensemble Kalman Filter (LEKF):

    Ott et al. (2002, 2004)

4) Local Ensemble Transform Kalman Filter (LETKF):

    Harlim and Hunt (2005)

Outline>>

# Use of Kalman Filter at NCMRWF

**Atmosphere Data Assimilation**

- Local Ensemble Transform Kalman Filter (LETKF) based system for atmosphere provide
    - **Flow dependent background error covariance matrix** for hybrid 4D-Var system.
    - **Analysis perterbations** for the Global (and Regional) Ensemble Prediction Systems

**Land Surface Data Assimilation System**

- Extended Kalman Filter (EKF) based SURFace data assimilation system updates
    - Soil Moisture, Land Surface Temperature etc

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# Thanks
# for your kind attention!

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