

Dynamic Data Assimilation
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Lecture – 22
Forward sensitivity method

In this module 5, we have been developing methods for assimilating data into deterministic dynamic models. The models are deterministic and we assume the models are perfect. The observations are noisy we are given a finite set of observations we would like to be able to assimilate this observation into the model to be able to determine the initial condition. In this context we developed the 4-D Var method, it is also called first order adjoint method. We developed the details of 4-D Var adjoint methods in the last lecture. We demonstrated the power of these methods using linear models, linear observation, non-linear models, non-linear observation.

In today's talk we are going to be talking about another related approach to assimilating data to assimilating noisy data into deterministic model which we assumed to be perfect. This method has is called the forward sensitivity method it was developed by us around 2010 and it can be shown that this method is in some sense dual of the 4-D Var and we would like to be able to present the details of the forward sensitivity method to correct forecast errors using data.

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FORWARD SENSITIVITY METHOD

- DA is viewed as forecast error correction using the forward sensitivities
- Correction to the control – I.C, B.C and parameters is expressed as the solution of a weighted linear least square problem using forward sensitivity
- No adjoint is needed but matrix recurrences for forward sensitivities need to be solved.

Data assimilation can be viewed as forecast error correction using forward sensitivities that is the view we are going to be taking in this class.

The correction to the control, please remember the solution to a dynamic model depends on the initial condition the boundary condition and parameters. So, initial condition boundary condition and parameters because changing them changes a solution it is customary to call them the control. So, we are assuming that the model is perfect. So, if you start the forecast model with the wrong control namely wrong initial condition or wrong boundary conditions or wrong parameters that would the error in the control will lead to errors in the forecast. We would like to be able to correct the errors in the control by using observations and we would like to be able to formulate this as again a linear a weighted linear least square problem using forward sensitivity.

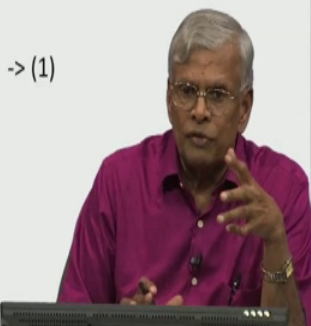
In this method we do not need any adjoint with, but we need matrix recurrences that compute the forward sensitivities of the solution with respect to the initial condition boundary conditions and parameters. So, adjoint is not needed; that means, the backward integration is not needed everything is forward, but we need to be able to solve a system of system that describes the evolution of the forward sensitivities.

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NONLINEAR MODEL – PERFECT MODEL

- State $x \in \mathbb{R}^n$, Parameters, $\alpha \in \mathbb{R}^p$
- Model map, $M: \mathbb{R}^n \times \mathbb{R}^p \rightarrow \mathbb{R}^n$
- $M(x, \alpha) = (M_1(x, \alpha), M_2(x, \alpha), \dots, M_n(x, \alpha))^T$
- Deterministic dynamics:

$$x_{k+1} = M(x_k, \alpha), x_0 = \text{I.C} \rightarrow (1)$$
- Control $c = (x_0^T, \alpha^T)^T \in \mathbb{R}^{n+p}$
- Solution: $x_k = x_k(x_0, \alpha) = x_k(c) \rightarrow (2)$



So, we are going to start with a non-linear model the assume model is perfect. Linear case will be a special case of this let x be a state, let x be state alpha be a parameter. One difference between this lecture and the previous lecture is that in the previous lecture we

assumed the model is perfect, the parameters define the model because the model is perfect we assume that there is no error in parameters, the only forecast error in the previous talk was essentially due to errors in the initial condition. One way we can think of this as a slight generalization, even though the model is perfect we have not set the values of the parameters when trying to generate forecast to the right value therefore, we assume that that could be errors in the initial condition boundary condition and our parameters.

M is the model map which is the vector valued function, M depends on two vectors one is the state vector x another is the parameter vector alpha alpha is the vector of size p, p is an integer much like N is an integer. So, M of alpha is given by M 1 of alpha, M 1 of x of alpha M 2 of x of alpha M n of x of alpha.

The deterministic dynamical equation is given in the form of a discrete time dynamics x_{k+1} is equal to M of x_k and alpha, x_{naught} is the initial condition, alpha is the parameter. I am going to assume the initial value the control c to be x_{naught} and alpha we try to generate the solution using one it can be readily seen that the solution at time k is the function of the initial condition as well as the function of the parameter. Therefore, to indicate this dependence of solution under control we call the solution x_k as x_k of c when there is no confusion we will simply say x_k .

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OBSERVATIONS

- Observations: $Z \in \mathbb{R}^m$
- Forward operator, $h: \mathbb{R}^n \rightarrow \mathbb{R}^m$
- $Z_k = h(x_k^*) + V_k \rightarrow (3)$
- x_k^* - true state of the system
- Let $c^* = ((x_0^*)^T, (\alpha^*)^T)^T$ be the unknown optimal control when $x_k^* = x_k(c^*)$
- $V_k \sim \mathcal{N}(0, R_k)$ is white Gaussian noise

Observations are given, observations are m vectors sorry I am sorry there is there is a typo this must be m vector observations belong to Z observations are m vectors they are denoted by Z and belong to \mathbb{R}^m ; h is the standard forward operator the observation at time k is given by h of x_k^* plus V_k , V_k is the true state of the system; c^* is the unknown optimal control that will lead to the true state of the system; V_k is the white Gaussian noise.

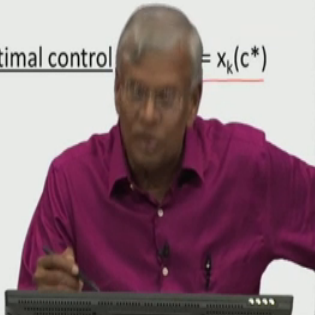
Here I would like to differentiate between two types of state one is the true state which is not known to us the mother nature does not reveal all her secrets. So, x_k^* is the true state of nature; x_k is the state predicted by the model the state predicted by the model will be equal to the true state only when the model control or set to x_0^* and α^* which corresponds to the true state of mother nature, but we do not know what x_0^* and α^* are.

But mother so, but we only know indirectly through observation what the mother nature has selected what is the value of the initial condition that corresponds to the true state which is x_0^* and α^* .

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OBSERVATIONS

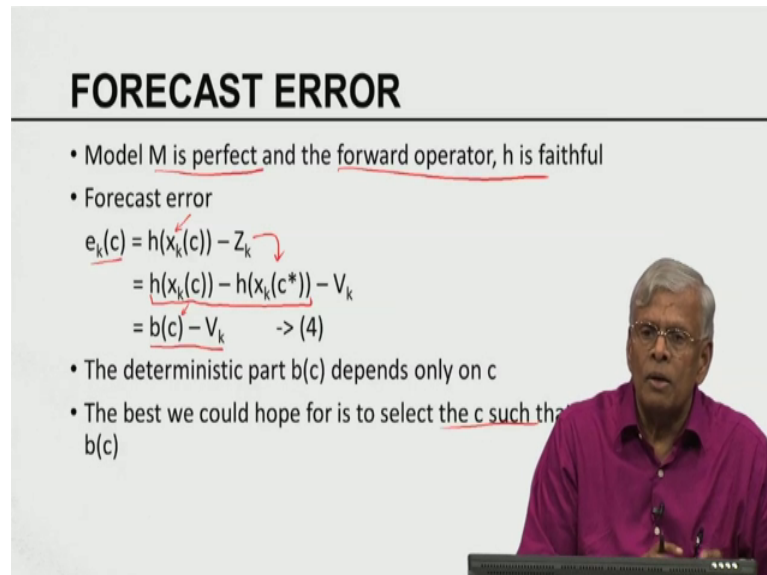
- Observations: $Z \in \mathbb{R}^{n \times m}$
- Forward operator, $h: \mathbb{R}^n \rightarrow \mathbb{R}^m$
- $Z_k = h(x_k^*) + V_k \rightarrow (3)$
- x_k^* - true state of the system
- Let $c^* = ((x_0^*)^T, (\alpha^*)^T)^T$ be the unknown optimal control $= x_k(c^*)$
- $V_k \sim N(0, R_k)$ is white Gaussian noise



So, we have we have picked x_0 and α mother nature has picked x_0^* and α^* , if x_0 is not equal to x_0^* or α is not equal to α^* the solution generated out of this will have errors that corresponds to forecast errors once you know the forecast errors our job is to be able to use these forecast errors to be able to

control to be able to alter the control x naught and α such that x naught moves closer to x star of x naught star and α moves closer to α that is the basic idea.

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FORECAST ERROR

- Model M is perfect and the forward operator, h is faithful
- Forecast error

$$\begin{aligned}
 e_k(c) &= h(x_k(c)) - Z_k \\
 &= h(x_k(c)) - h(x_k(c^*)) - V_k \\
 &= b(c) - V_k \quad \rightarrow (4)
 \end{aligned}$$
- The deterministic part $b(c)$ depends only on c
- The best we could hope for is to select the c such that $b(c)$

So, where it is useful to think about a classification of forecast errors which we have alluded to in module one itself, but it is worth repeating some of the principles of classifications of forecast errors for our purpose.

The model is perfect, we are assuming that the model is perfect we are assuming the forward operator h is very faithful; that means, I have the physics has been the physics that if that is part of h is very good; that means, the relation between the model state in the observation is pretty accurate. In that case the forecast error e_k of c is depended on the actual forecast generated by the model. So, h of x_k of c is the model counterpart of the observation Z_k is the actual observation, but Z_k is equal to h of x_k c star minus V_k . So, if I substitute for Z_k here this I can rewrite it at b of c minus V_k where b of c is equal to the difference between the model predicted observation and the true observation if there is no noise. So, this becomes b . So, the determine, b c is called the deterministic part of the forecast error which depends money and see the control. V_k is the random part of it we cannot control the random part random part is part of the deal we have to contend with this.

So, the only way we can hope to be able to correct a forecast error is to be able to correct the deterministic part of the forecast error. So, the best way we, the best we could hope

for is to select a control c such that it annihilates $b c$, it reduces $b c$ to 0. If you can reduce this deterministic part to 0 then whatever is left is simply random errors which is beyond our control which is totally uncontrollable. So, this is what is called forecast error correction and this is the aspect of the forecast error that we are concerned with, the model is perfect, the forward operator is perfect the forecast error if any arises because of the errors in control. So, I would like to be able to move the chosen control towards the unknown using the forecast errors in a feedback loop to be able to control, to be able to correct the deterministic part and annihilate it.

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STATEMENT OF PROBLEM

- Let $c = (\underline{x}_0^T, \alpha^T)^T$ with \underline{x}_0 and α be arbitrary I.C and parameter values respectively
- Define a functional

$$J(c) = \frac{1}{2} \sum_{k=1}^n \langle \underline{e}_k(c), R_k^{-1} \underline{e}_k(c) \rangle$$

$$= \frac{1}{2} \sum_{k=1}^n \langle (\underline{Z}_k - h(\underline{x}_k))^T R_k^{-1} (\underline{Z}_k - h(\underline{x}_k)) \rangle \rightarrow (5)$$
- Find δc such that $J(c + \delta c)$ has no deterministic component and is purely the weighted sum of terms of the form $V_k^T R_k^{-1} V_k$.

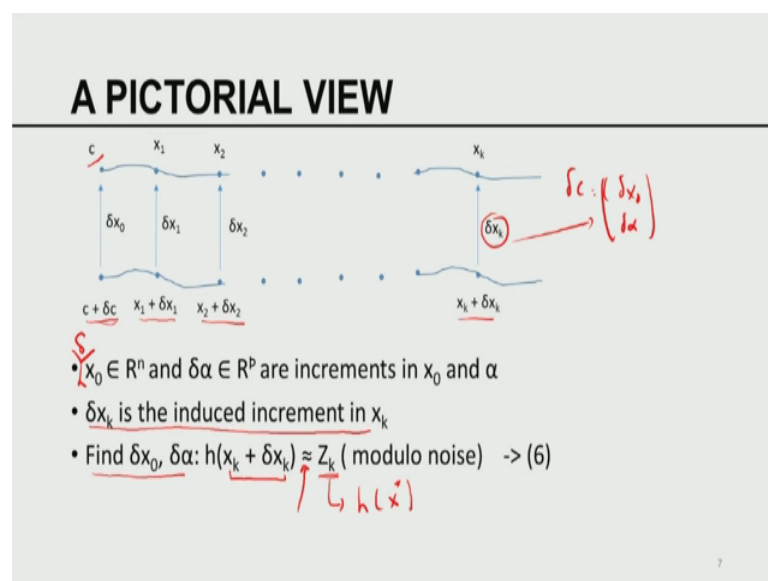
So, with that as a basis and now I am going to state the problem formally. Let c be the chosen control let c be the chosen control where \underline{x} naught and c are arbitrary. But arbitrary to the extent that general engineers and scientists know they may not know the exact value, but they do know the region where the exact value lies. So, \underline{x} naught and see while it is not equal to the true state, but they may not be too far from the true state as well, they are arbitrary.

Now, I am going to define a functional again look back in all of the developments in inverse problem there is always a cost functional which is very basic to the solution of the inverse problem the cost functional is essentially is denoted by $J(c)$ it is simply the weighted sum of squared errors, $\underline{e}_k(c)$ we have seen in the previous slide it were given by the equation 4, is the forecast error this must be R_k sorry, this must be R_k . So, this is the

weighted sum of squared of weighted sum of square of forecast errors, if I substitute for e_k from the previous slide I get this expression this is the forecast error this is the forecast error transpose and this is a very familiar equation 5 that describes the cost function, is a familiar formula that we have used repeatedly in almost all of our treatment. The reason why this relation occurs again and again because our approach is rooted in least squares the common theme of our course is least squares approach two solving inverse problem, solving data assimilation problem. So, this is the least square cost functional.

So, what is our goal? Our goal is to be able to find a perturbation δc such that if I change c to c plus δc , J of c plus δc has no deterministic component and is purely weighted sum of terms of the kind which are induced by the errors; that means, I would like to be able to add δc to the control, δc consists of δx_0 for the initial condition δc and $\delta \alpha$ for the parameter. So, how do I add corrections to the initial conditions and the parameters, so as to annihilate the deterministic part of the forecast error leaving behind only the weighted sum of squared errors of Gaussian random variables? So, please remember V_k is Gaussian, V_k transpose R_k inverse V_k it is the weighted sum of square is a normalized sum of squares of Gaussian random variables.

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Pictorially, we are going to start from c this is the forecast x_k is the forecast resulting from c . I would like to be able to change your c to c plus α ; c plus δc consists of δx naught and $\delta \alpha$. So, this is the change in the initial condition δc . So, this is the new control from the new control I can get a new state which is x_1 plus δx_1 δx_1 is the change in the state at time 1 δx_2 δx_2 is the change in the state at time 2 δx_k is the change in the state at time k all the δx_k is induced by two changes, one δx naught the initial condition, two $\delta \alpha$ and the parameters.

I must say this is δ . So, δx naught belong to \mathbb{R}^n $\delta \alpha$ belongs to \mathbb{R}^p these are increments in x naught and α . δx_k is the induced increment in x_k at time k . So, what is our goal? Our goal is to be able to find δx naught $\delta \alpha$ such that when I use this new state x_k plus δx_k which is the perturbed stage and applied to the function h it will give the observation model of the noise; that means, it will match the deterministic part of the noise what is the deterministic part of the noise this is h of x star h of x star that is that is essentially the deal here. That means, my model predicted observation will match the actual observation model of the noise that is the equation 6 and that is the goal with which we are going to be, that is the goal we are going to be working towards and this equality is to be interpreted in the least square sense, in the least square sense.

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STRUCTURE OF FORECAST ERROR

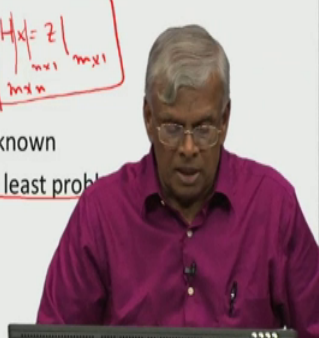
- First-order Taylor expansion:

$$Z_k = h(x_k + \delta x_k)$$

$$= h(x_k) + D_{x_k}(h) \delta x_k$$
- Using (4):

$$D_{x_k}(h) \delta x_k = -e_k(c) \quad \rightarrow (7)$$
- Jacobian, $D_x(h) \in \mathbb{R}^{m \times n}$ and $e_k(c) \in \mathbb{R}^m$ are known
- $\delta x_k \in \mathbb{R}^n$ is obtained by solving the linear least problem weighted by R_k^{-1}

$Hx = z$
 $n \times 1 \quad m \times 1$
 $m \times n$



So, I again we would like to be able to understand the structure of the forecast errors to that end. So, what is that where are we now? We have already assumed I have perturbed the control perturbed control leads to perturb state the perturb state is given by x_k plus Δx_k . So, Z_k must be equal to, we would like to be able to find Δx_k we would like to be able to force Δx_k such that Z_k is equal to h of x_k plus Δx_k . I can express this in the first order Taylor series living leading to this expression which is h of x_k plus the Jacobian of h at x_k times Δx_k .

If I using 4 let us say let us go to for a moment now. So, in 4 I have e_k of c is equal to h of x_k c minus h of x_k star c minus V_k . So, if I brought that in here, if I brought that in here this part sorry this part which is the increment is given by this equation this is equal to Z minus h of x_k Z minus h of x_k is essentially minus e_k c start up going to equation 4. You can readily see I would like to show it to you once again, equation 4, that is equation 4. So, Z_k equation 4 tells you e_k is equal to h of x_k c minus Z_k therefore, Z_k minus h of Z is minus e_k . So, that is the relation that we have here.

The Jacobian as you know is a matrix of size m by n , e_k c is a matrix of is a vector of size m . So, you can think of this like H of x is equal to Z where H is a m by n matrix, x is n by 1 and this is m by 1 that we saw in our lectures on static problems. So, you can see Δx_k , x is related replaced by Δx_k h is replaced by the Jacobian of H , and Z is replaced by minus e_k z . So, once you make this correspondence between the static problem and this problem our job is to be able to find Δx_k such that it satisfies this equation. This equation represents an equation of the linear least square type that we have discussed in earlier modules we also know the e_k is a random vector it is a its covariance is R_k . So, I can determine x_k by solving 7 as a weighted linear least square problem, as a weighted linear least square problem. So, let us summarize what we have done.

You run the model forward from an error irenaeus control. I would like to be able to compute or characterized the increment in the state Δx_k at time k . So, what is the increment we would need at time k which is Δx_k such that it will annihilate the forecast error, such a increment at time k is obtained by solving this linear least square problem as a weighted least square problem because we already know that e_k is a random vector whose covariance is a_k inverse. So, this is how.

Now, once I characterize this solution of this linearly square problem we already know Δx_k is related to Δx_0 and $\Delta \alpha$ using forward sensitivities. I am going to now relate Δx_k to Δx_0 and $\Delta \alpha$, so that is the next step in our analysis.

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FORWARD SENSITIVITY OF x_k W.R.T

I.C x_0

- Recall $x_k = x_k(x_0, \alpha)$ is a smooth function
- Let $x_{k,i}$ be the i th component of $x_k \in \mathbb{R}^n$
- Define

$$[U_k]_{ij} = \frac{\partial x_{k,i}}{\partial x_{0,j}}, 1 \leq i, j \leq n$$

= Forward sensitivity of $x_{k,i}$ w.r.to $x_{0,j}$
- $U_k = D_{x_0}(x_k) \in \mathbb{R}^{n \times n}$ = Jacobian of x_k w.r.to x_0
 = Forward sensitivity matrix of x_k with respect to x_0

$\dot{x} = f(t, x, \alpha)$
 $x(t) = x(t, x_0, \alpha)$
 ↑ ↑ ↑
 smooth

So, recall x_k which is the solution at time k is a continuous or a smooth function of x_0 and α . So, x_k depends on x_0 and α smoothly, smoothly means what x_k is differentiable with respect to x_0 and α . Those of you who have taken differential equations you know that under smooth. So, if I have a differential equation $\dot{x} = f(x, \alpha)$ if x is smooth, smooth in the sense that f has is not only continuous, but possesses continuous derivative with respect to x and α of several orders the solution x of t of x_0 and α this solution is smooth is also smooth it you can you can compute the derivative with respect to t you can compute the derivative respect to x_0 you can compute the derivative with respect to α .

That means if f is smooth in a differential equation $\dot{x} = f(x, \alpha)$ if x_0 is the initial condition the solution at any time t is equal to x of t when what we say as x of t is in fact, x of t of x_0 and α in differential equation theory one can show if f is smooth x is also smooth with respect to x_0 and α . In the case of discrete time dynamics a similar conclusion also follows if my model map m is smooth the model solution is also smooth with respect to the initial condition and α . This

smoothness essentially allows us to be able to compute the derivative of x_k with respect to x_0 the derivative of x_k with respect to α .

Now, let us denote the i th component of x_k , $x_{k,i}$. I am now going to compute the first order derivative of $x_{k,i}$ with respect to x_0 . So, this is the j th component of the initial condition this is the i th component of the solution at time k I am going to denote this as $U_{k,ij}$, U_k is a matrix i, j , i refers to the component at time k j refers the component at time 0 this derivative is called the forward sensitivity of x_k of x_0 of i with respect to x_0 of j . So, as you vary i and j in the interval 1 to n you get a matrix that matrix is called U_k . So, U_k can be thought of is simply as a Jacobian of x_k with respect to x_0 this Jacobian matrix is called the forward sensitivity matrix of x_k with respect to x_0 .

So, this is where the forward sensitivity of the solution with respect to x_0 comes in. So, what does this say? If you make a small change the initial condition at time 0 what will be the effect of that small change initial condition on the solution at time k that is what this matrix of forward sensitive captures.

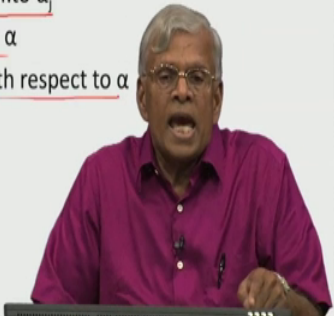
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FORWARD SENSITIVITY OF x_k W.R.TO α

- Define

$$[V_k]_{ij} = \frac{\partial x_{k,i}}{\partial \alpha_j},$$

= Forward sensitivity of $x_{k,i}$ w.r.to α_j
- $V_k = D_\alpha(x_k) \in \mathbb{R}^{n \times p}$ = Jacobian of x_k w.r.to α
 = Forward sensitivity matrix of x_k with respect to α



Likewise, I can define the forward sensitivity with respect to α . So, $V_{k,ij}$ is again the $x_{k,i}$ is the i th component of the solution at time k α_j is the j th component of the control vector. The partial derivative is the ij th element of a matrix V_k , so that is called the forward sensitivity of $x_{k,i}$ with respect to α_j . So, you can again think of V_k as a

Jacobian of x_k with respect to α this is called the forward sensitivity matrix of x_k with respect to α .

So, V_k , the matrix V_k , the matrix V_k is a n by p matrix it represents the forward sensitive to the solution at time k with respect to the p parameters is called parameter sensitivity. U_k on the other hand is the forward sensitivity solution with respect to the initial conditions. Both these sensitivities essentially tells you how a small change in the parameter value how your small change the initial condition would be amplified at time k . So, you can think of the sensitivity as a kind of an amplification factor that helps to amplify the initial error.

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RELATION BETWEEN U_k , V_k AND δx_k

- Recall $x_k = x_k(x_0, \alpha)$
- From first principles:

$$\delta x_k = \left[\frac{\partial x_k}{\partial x_0} \right] \delta x_0 + \left[\frac{\partial x_k}{\partial \alpha} \right] \delta \alpha$$

$$= U_k \delta x_0 + V_k \delta \alpha \quad \rightarrow (8)$$
- Induced increment δx_k is related to δx_0 via U_k and $\delta \alpha$ via V_k

So, having defined the concept of forward sensitivities, now I would like to use U_k and V_k to be able to characterize x_k . Please remember why are we interested in that we have already said the way to correct the forecast error is to determine δx_k as a solution of a linear least square weighted version of the problem, so that is set aside. Now we have to relate δx_k to δx_0 and $\delta \alpha$ this is where the role of U_k and V_k comes into being.

So, let x_k be the, let x_k be the model solution at time k from first principles. The variation, from this equation we can derive this. So, x_k is a function of x_0 and α therefore, the first variation of δx_k induced by δx_0 and $\delta \alpha$ is essentially given by the product of δx_k the product of the forward sensitivity of x_k

x_k with respect to x_0 times Δx_0 plus the product of the forward sensitive x_k with respect to α times $\Delta \alpha$ is a very basic principle that comes from Taylor series expansion, first variation and the notion of differentials in calculus. Now we have already seen that this matrix is V_k this matrix is U_k and this V_k . So, this matrix is a n by n matrix this matrix is a n by p matrix therefore, the induced increment is related to Δx_0 via U_k and $\Delta \alpha$ via V_k .

Please understand I need to be able to control, I need to be able to change the control changing the control means it will change the solution. So, everything must be related to time 0. So, this is how we relate the change in the state at time k to the change in the state at time 0 and change in the parameter at time 0.

So, now we have achieved one of the things that we need to be able relate Δx_k and $\Delta \alpha$. But to understand, but to use 8 to characterize Δx_k now we need to be able to characterize what is U_k and what is V_k . U_k please remember how the solution at time k varies with respect to initial condition, V_k is how the solution at time k varies with respect to the parameters these are called forward sensitivities.

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DYNAMICS OF EVOLUTION OF U_k

- Consider the i^{th} component of the model dynamics in (1) given by

$$x_{k+1,i} = M_i(x_k, \alpha) \rightarrow (9)$$
- Differentiating both sides w.r.to $x_{0,j}$:

$$\frac{\partial x_{k+1,i}}{\partial x_{0,j}} = \sum_{q=1}^n \frac{\partial M_i}{\partial x_{k,q}} \frac{\partial x_{k,q}}{\partial x_{0,j}}$$

$$= \left[\frac{\partial M_i}{\partial x_{k,1}}, \frac{\partial M_i}{\partial x_{k,2}}, \frac{\partial M_i}{\partial x_{k,3}}, \dots, \frac{\partial M_i}{\partial x_{k,n}} \right] \begin{bmatrix} \frac{\partial x_{k,1}}{\partial x_{0,j}} \\ \frac{\partial x_{k,2}}{\partial x_{0,j}} \\ \frac{\partial x_{k,3}}{\partial x_{0,j}} \\ \vdots \\ \frac{\partial x_{k,n}}{\partial x_{0,j}} \end{bmatrix}$$

$$= [\text{ith row of } D_{x_k}(M)] [\text{jth column of } U_k]$$

$x_{k+1} = M(x_k, \alpha) \rightarrow (1)$

So, we need to be able to explain are we need to be able to find out a way to characterize the evolution of U_k and V_k please recall these are matrices. So, we have going to collectively talk about the evolution of all these of these two matrices in time. So, the dynamics of evolutionary U_k is our next topic consider, the i^{th} component of the model

dynamics in one. So, please remember the model dynamics is given by x_{k+1} is equal to M of x_k of α . So, if I consider the i th component on the left hand side I should be able to consider the i th component on the right hand side and that is what equation nine is all about consider the i th component of the equation the model equation in one. So, this is the equation in one which I have written for us to be able to recall.

Now, I would like to be able to differentiate both sides with respect to the j th component to the initial condition. So, the differential coefficient of the i th component at time $k+1$ with respect to the j th component time 0 that the left hand side, now I can use the chain rule α depend does not depend on x_{naught} x_k depends on x_{naught} M_i depends on x_k and x_k depends on x_{naught} . So, I have to use the chain rule in standard calculus. So, the left hand side is equal to partial of M_i with respect to partial of the q th component of x_k and the partial of q th component of x_k 2 the partial of j th component of x_{naught} so the product of these two partial derivatives.

Now, q is an arbitrary 1, q can take the value 1 2 3 all the way up to n . So, I have to sum it up over q . So, this is the fundamental relation that relates the dynamics of evolution of the forward sensitivity. Please recall this is the forward sensitivity the i th component with respect to the j th component time $k+1$, time $k+1$ and this is the sensitive of the q th component with respect to the j th component. I can rewrite this in the form of a inner product that is the row, that is the column you can convince yourself very easily. This is the i th row of $D_{k,m}$, this is $D_{k,m}$ and this is the j th column of U_k that is being, that is a fundamental interest right now, that is a fundamental interest right now.

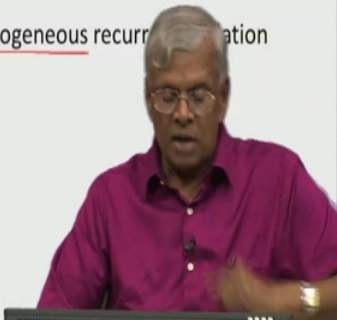
So, let us go back now. So, one sensitivity component is given by the product of the i th row and the j th column.

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DYNAMICS OF EVOLUTION OF U_k

- Collecting all the n^2 sensitivity relations:

$$U_{k+1} = D_k(M)U_k \quad \rightarrow (10)$$
- $U_0 = \left[\frac{\partial x_0}{\partial x_0} \right] = I, D_k(M) = D_{x_k}(M)$
- (10) is a linear, non-autonomous, homogeneous recurrence relation
- $U_k = D_{x_0}(x_k)$ – Jacobian of x_k w.r.to x



If I want to consider all the sensitivity matrices simultaneously there are n square such sensitivity relations the set of all n square such sensitivity relations is captured in the form of a matrix dynamics. So, U_{k+1} is a sensitivity at time $k+1$, U_k is a sensitivity time k , U_{k+1} is the matrix U_k is a matrix, $D_k(M)$ is the $D_k(M)$ is the sensitivity, I am sorry it is the model Jacobian with respect to x_k . So, here I am using a simplified notation I want you to remember that instead of writing d of x_k of M we are simply write $D_k(M)$, $D_k(M)$. So, $D_k(M)$ is the model Jacobian. So, this is a dynamical equation in discrete time.

I need an initial condition U_0 is given by partial of x_0 with respect to x_0 that is an identity matrix. And I have already talked about the change in slight change in notation for the better. Now please remember (10) is a linear equation (10) is a non autonomous equation, it changes along the trajectory it is a homogeneous recurrence relation, it is a homogeneous recurrence relation. Please recall U_k is the sensitivity of x_k with respect to x_0 therefore, equation (10) tells you how the forward sensitivity of the solution with respect to the initial condition evolves starting from the initial value of i . So, I have to compute all these along the trajectory you may recall in the context of in the context of non-linear version of the 4-D Var we talked about the tangent linear system you can think, I am going to challenge the reader to be able to compare this with the tangent linear system and verify this is very similar to the tangent

linear system that we talked about in the context of 4-D Var in the context of 4-D Var. So, 10 is a forward dynamics, it is called the forward sensitivity.

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EXPRESSION FOR U_k

- Iterating (10): Since $V_0 = I$

$$U_k V_k = D_{k-1}(M) D_{k-2}(M) \dots D_1(M) D_0(M)$$

$$= \prod_{i=0}^{k-1} D_i(M) = D_{k-1:0}(M) \rightarrow (11)$$
- \prod denotes the reverse product (from k-1 to 0) of the Jacobians of M along the trajectory
- U_k contains information on the behavior of the trajectories

Now, I can iterate 10 starting from I therefore, V_k I can iterate sorry I can iterate 10 sorry this is U_k , I can iterate 10 and so U_k is the is the given by the product of the Jacobian along the path this can be written as the product succinctly like this which can again using the notation that we have already used is the product of the Jacobian along the trajectory. \prod denotes the reverse product from k minus one to 0 of the Jacobian of V m along the trajectory please realize this must be sorry we will correct that this must be U. Therefore U, contains information about the behavior of the trajectories.

In what way does this contain the information with the trajectory? If I perturb the initial condition by a small amount how sensitive the solution is going to be at a future time that is why it is called forward sensitivity. So, we not only derived the forward sensitivity equation 10, but also have solved for the forwards m, found an expression for the forward sensitivity it is simply the product of the Jacobian of the model map along the trajectory.

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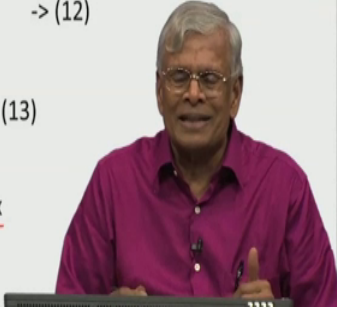
DYNAMICS OF EVOLUTION OF V_k

- Consider (9):

$$x_{k+1,i} = M_i(x_k, \alpha)$$
- Differentiate both sides w.r.to α_j :

$$\frac{\partial x_{k+1,i}}{\partial \alpha_j} = \sum_{q=1}^n \frac{\partial M_i}{\partial x_{k,q}} \cdot \frac{\partial x_{k,q}}{\partial \alpha_j} + \frac{\partial M_i}{\partial \alpha_j} \quad \rightarrow (12)$$
- Expressing the np relations together:

$$V_{k+1} = D_k(M)V_k + D_\alpha(M) \quad \rightarrow (13)$$
- $D_\alpha(M) \in \mathbb{R}^{n \times p}$, Jacobian of M w.r.to α
- Clearly, $V_0 = \left[\frac{\partial x_0}{\partial \alpha} \right] = 0 \in \mathbb{R}^{n \times p}$, zero matrix



Now, we are going to concentrate on deriving a similar dynamics for V_k . Please remember V_k is the sensitivity the solution with respect to the parameters. Again I am going to consider the i th component of the model equation that was also the starting point previously. Earlier we found the derivative of this with respect to the j th component of the initial condition here we are going to differentiate this with the j th component of α .

Therefore the left hand side is simply the derivative of this scalar with respect to α , the right hand side it is slightly different from the previous derivation x_k depends on α . So, so M_i depends on α in two ways M_i depends on α directly M_i also depends on α indirectly through x_k . So, one is the direct term another is to be obtained by chain rule. This is the term that comes from the chain rule to accommodate to accommodate the implicit dependence, this is the explicit dependence. So, the sensitivity of x_{k+1} the i th component of it with respect to the j th component of α is essentially the sum of two terms, the first one is an implicit dependence second one is an explicit dependence.

Again expressing, there i varies from 1 to n , j varies from 1 to p . So, there are $n \times p$ such relations by collecting all these $n \times p$ such relations and arranging them in the form of a matrix we get a matrix recurrence. This is the model Jacobian, this is the model Jacobian

with respect to parameter with respect to the parameter. So, this is the, $D M \alpha$ is the Jacobian of M with respect to α .

Now, what is the initial condition from this? Initial condition is dealt is the partial of x naught with respect to α . The state or the initial term is x naught α is the initial settings of the parameters the initial condition has no bearing on the parameter value and the parameters has no bearings on the initial condition therefore, the initial condition is identically 0, it is a 0 matrix. So, this is the starting initial condition. So, 13 is a recurrence relation that starts from a 0 matrix whereas, in the previous one started from identity as the initial condition.

So, we have derived recurrence relation for the evolution of both the forward sensitivity with respect to initial condition and parameters.

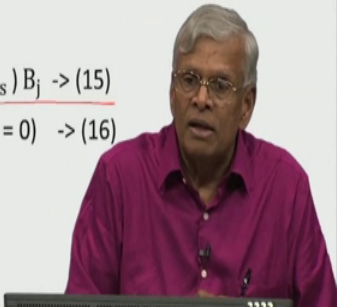
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EXPRESSION FOR V_k

- Equation (13) is a linear, non-autonomous, non-homogenous recurrence relation
- Setting $A_k = D_k(M)$ and $B_k = D_\alpha(M(x_k, \alpha))$
- $V_{k+1} = A_k V_k + B_k \quad \rightarrow (14)$
- Solving:

$$V_k = \left(\prod_{j=0}^k A_j \right) V_0 + \sum_{j=0}^{k-1} \left(\prod_{s=j+1}^k A_s \right) B_j \quad \rightarrow (15)$$

$$= \sum_{j=0}^{k-1} \left(\prod_{s=j+1}^k A_s \right) B_j \quad (\text{since } V_0 = 0) \quad \rightarrow (16)$$



Equation 13 is a sin is again a linear non autonomous non homogenous recurrence relation. The previous one was linear non autonomous it is homogeneous, now I have a forcing term $D M$ of α is the forcing term. We are now going to simplify the solution of this. We are going to change notation let A_k be $D_k M$, let B_k be that in this case the previous relation 13 can be rewritten as 14 V_k plus 1. So, V_k plus 1 is equal to A_k times V_k plus B_k .

I can substitute back that is a very good interesting exercise I am going to ask you to do this as an exercise by solving 14 one can verify that the solution V_k is expressed as 15 where V_{naught} is the initial condition, but please recall V_{naught} is a 0 matrix therefore, the first term vanishes, the second term is the solution therefore, V_k is given by this sums of products of matrices as and bs. As or the model Jacobian with respect to with respect to the state bs are model Jacobian with respect to this is with respect to the state this is with respect to the alpha. So, it is the products of Jacobians model, Jacobians both respect to the state and the parameter the sum that off is a complicated expression much more complicated than the U_k , but however, we have an explicit expression for the sensitivity of the solution with respect to the parameters.

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DEPENDENCE OF FORECAST ERROR ON δx_0 AND $\delta \alpha$

- Recall from (7):

$$D_{x_k}(h)\delta x_k = -e_k(c) \quad \rightarrow (7)$$
- Also from (8):

$$\delta x_k = U_k \delta x_0 + V_k \delta \alpha \quad \rightarrow (8)$$
- Substituting (8) in (7):

$$[D_{x_k}(h)U_k, D_{x_k}(h)V_k] \begin{bmatrix} \delta x_0 \\ \delta \alpha \end{bmatrix} = -e_k(c) \quad \rightarrow (17)$$

$x_k = x(t, x_0, \alpha)$
 $\delta x_k = \left(\frac{\partial x}{\partial x_0} \right) \delta x_0 + \left(\frac{\partial x}{\partial \alpha} \right) \delta \alpha$
 $= U_k \delta x_0 + V_k \delta \alpha$

I think we have we are almost there to state the final version of the problem. So, please recall from 7 we know the delta x_k that will help to inoculate the deterministic part of the error is given by 7, I have quoted the 7 back again here.

From 8 we know, now let us let us talk about the change. So, x_k is equal to x of k of x_{naught} and α therefore, delta x_k from basic differential equation our basic theory of differentials is that delta x by delta x_{naught} times delta x_{naught} plus delta x by delta α times delta α . So, this is the matrix, this is the matrix and this matrix is U of k of delta x_{naught} plus this is V of k plus delta α and that is what equation 8 is all

about. Therefore, we are able to express the x_k in terms of δx and $\delta \alpha$.

Now, I can substitute this δx_k from here to the equation 7. If I substituted this and simplify a little bit I get $D_{x_k}(h) U_k$ come on $D_{x_k}(h) V_k$ times δx_k must be equal to $-e_k$ minus e_k of c that is equation 17. Now let us look at the left hand side, I know the Jacobian of h I know the forward sensitivity because I have already solved the recurrence relation again these two are the same. So, I know this, this is again computed from solving the forward sensitivity e_k is known.

So, now, we can see the left hand side is a matrix that is the vector that is the vector we know this, we know this, we do not know this part, we can essentially see I got a classical linear least square problem. Why this is linear? The unknowns are or the unknowns what are the unknowns δx_k $\delta \alpha$ they occur to their first degree. Therefore, we have converted the forecast correction problem to one of being able to compute the increments in the initial condition δx and $\delta \alpha$ and these increments are going to be decided by the solution of this linear least square problem and we will formulate it as a weighted linearly square problem because in the right hand side is stochastic and I know its variances r_k .

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FORECAST ERROR CORRECTION AS INVERSE PROBLEM

- Define:

$$H_k^{(1)} = D_{x_k}(h) U_k \in \mathbb{R}^{m \times n}$$

$$H_k^{(2)} = D_{x_k}(h) V_k \in \mathbb{R}^{m \times p}$$

$$H_k = [H_k^{(1)}, H_k^{(2)}] \in \mathbb{R}^{m \times (n+p)} \rightarrow (18)$$
- Combining with (17):

$$H_k \delta c = -e_k(\alpha) \quad \delta c \rightarrow (19)$$
- By solving this linear weighted least squares problem with R_k^{-1} as the weight using the methods in Module 6, obtain corrections δc to c .

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So, to further simplify the notation, the forecast error correction as an inverse problem, I have already alluded to this and that is what we are going to be emphasizing again. So, I

am going to define H_k of 1 as the product of these two matrices, H_k of 2 as the product of these two matrices. I am going to define a new matrix which is H_k which is the two matrices put together side by side. So, this matrix H_k is a m by n plus p matrix. So, combining this with 17 via please recall δx naught and $\delta \alpha$ is the vector have δc this is a size n , this is a size p . So, the whole thing belongs to \mathbb{R}^{n+p} , therefore, by solving this linear least weighted least square problem with R_k inverse as the weight using the methods that we have already discussed, using the methods I do not think the module 6 is correct I will correct that.

Obtain the corrections to correction δt to c and I can then compute δc by the solution that is the whole idea of the forward sensitivity method. Now you can see how the forward sensitivity method gets into the matrix H_k on the left hand side of 19.

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FORWARD SENSITIVITY METHOD – (FSM)

- Start with the initial value of control c and compute the model trajectory $\{x_0, x_1, x_2 \dots x_k\}$
- Let Z_k be the observation at time k , given ✓
- Compute $e_k(c) = h(x_k) - Z_k$
- Compute U_k, V_k
- Assemble $H_k = [H_k^{(1)}, H_k^{(2)}]$
- Solve $H_k \delta c = -e_k(c)$ \rightarrow (20) as a weighted linear least squares using the weight R_k^{-1}
- Set $c^{new} \leftarrow c + \delta c$ and repeat until convergence

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So, I am going to talk about an algorithm which is called the forward sensitivity method FSM is an acronym. Start with the initial value of the control c start with the initial value of the control c , compute the model trajectory x naught through x_k let Z_k be the observation at time k that is given to you that is that is Z_k is given to you compute the error which is h of x_k . So, you know h you know x_k . So, you know h of x_k , h of x_k minus Z is the error.

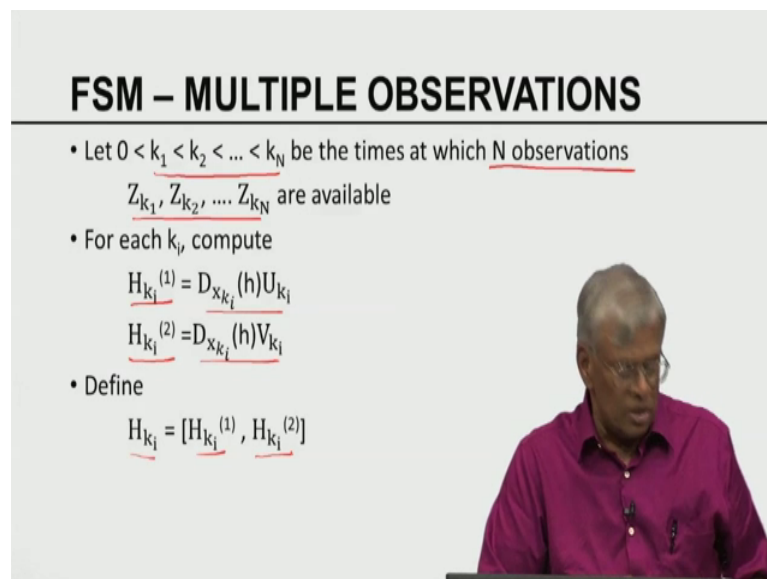
Compute $U_k V_k$ by solving the forward sensitivity dynamics the matrix recurrence relation assemble the matrix H_k 1, H_k 2 that gives you the matrix H . Then solve the

resulting least square problem as a weighted linear least square problem with the weight R_k inverse.

Once you compute Δc you can add Δt to c I get a new control. Since we have used the first order method well the new control will be better than the old control in the annihilating error you can expect the error will not be annihilated in its entirety because we have used only first order recurrence of first order Taylor series expansion in our theory. Therefore, what is a way to further reduce the forecast error you repeat the whole procedure again starting with c_{nu} and do whatever you did with c . So, if you iterate this several times each time you are going to keep adding increments to the control that continuously keep moving the forecast error towards purely random part it annihilates continuously the deterministic part that is the idea, that is the idea.

So, in all these discussions we essentially said if I had only one observation how I can use one observation to be able to compute the control.

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FSM – MULTIPLE OBSERVATIONS

- Let $0 < k_1 < k_2 < \dots < k_N$ be the times at which N observations
 $Z_{k_1}, Z_{k_2}, \dots, Z_{k_N}$ are available
- For each k_i , compute

$$\underline{H_{k_i}^{(1)}} = \underline{D_{x_{k_i}}(h)U_{k_i}}$$

$$\underline{H_{k_i}^{(2)}} = \underline{D_{x_{k_i}}(h)V_{k_i}}$$
- Define

$$\underline{H_{k_i}} = [\underline{H_{k_i}^{(1)}}, \underline{H_{k_i}^{(2)}}]$$

In principle you may have multiple observations. So, I am going to provide a quick extension of this let there be N times, let there be N observations the observation that these N times be given by $Z_{k_1}, Z_{k_2}, Z_{k_N}$. For each k I now I simply need to repeat what I did for one observation to each of these observations and then collide them all together that is all the idea there is nothing more because each observation is going to give me give me information about the increment. So, I have to repeat as many times as I

had. So, I need to be able to compute H_{k+1} , earlier I had H_k here I have H_{k+1} , H_{k+2} which is given by this which is given by this U_k , V_k are the sensitivities of the solution at time k , x_{k+1} , x_{k+2} are the Jacobian the forward operator at time k I therefore, H_k is the concatenation of these two matrices side by side.

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FSM – MULTIPLE OBSERVATIONS

- Define

$$H = \begin{bmatrix} H_{k_1} \\ H_{k_2} \\ \vdots \\ H_{k_N} \end{bmatrix} \in \mathbb{R}^{Nm \times (n+p)} \quad e = \begin{bmatrix} e_{k_1} \\ e_{k_2} \\ \vdots \\ e_{k_N} \end{bmatrix} \in \mathbb{R}^{Nm}$$
- Solve the linear weighted least square problem

$$H\delta c = e \quad \rightarrow (21)$$
 with weight matrix, R^{-1} where

$$R = \text{Diag}(R_{k_1}, R_{k_2}, \dots, R_{k_N}) \in \mathbb{R}^{Nm \times Nm}$$
 using the iterative framework defined in slide 19

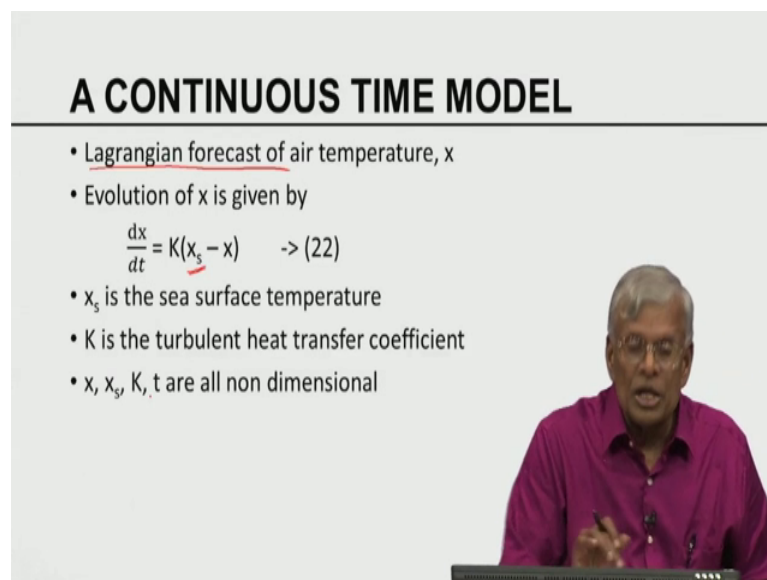
Now, for each time k , I have this matrix, now I have N such times now I have to prepare another gigantic matrix. So, create a newer metric h where I stack H_{k_1} , H_{k_2} , H_{k_N} , this matrix is of size or Nm cross n by p likewise I also stack all the errors forecast errors at time k_1 , k_2 k_N and that is going to be giving you a large vector of size Nm . So, if you pull them altogether I have now a new linear least square problem please remember δc has not changed only the matrix h has changed only the vector e has changed, in this case I have I think it should be minus e minus e .

I can now solve this as a weighted linear least square problem the weight matrixes R inverse. R inverse is simply a diagonal matrix, R inverse is a matrix of size $[Noise]$, cross Nm . So, each of the yeah each of the N matrices are put along the diagonal of a matrix R this R will be a collection of all the covariances of observations at each time, so is a gigantic matrix. And you can formulate this as a linearly square problem since we have solved the static linearly square problem weighted unweighted versions, in detail in previous modules we are not going to describe that part. But one can see that if you

know the linear least square static problem you can solve this dynamic problem simply an application of those concepts here.

So, what is the interesting thing here is that even though it is a dynamic data assimilation problem we convert the dynamic data assimilation problem to a static deterministic inverse problem and that is the essence of forward sensitivity method.

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A CONTINUOUS TIME MODEL

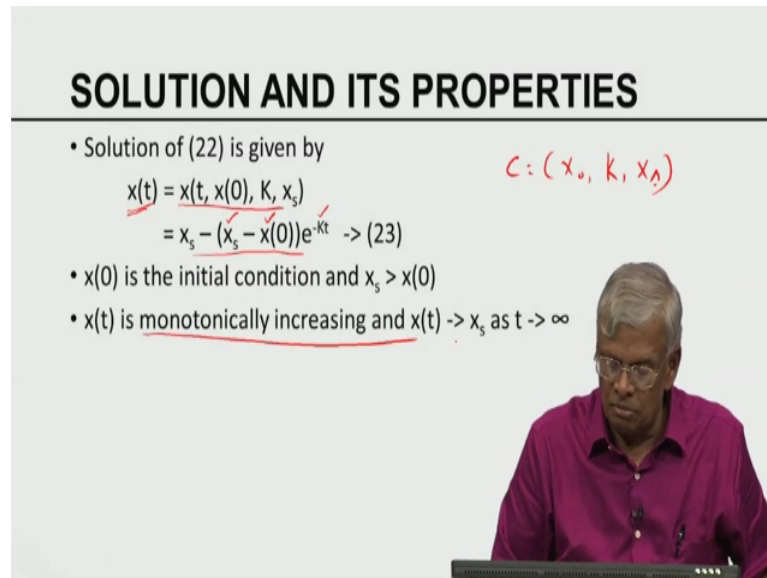
- Lagrangian forecast of air temperature, x
- Evolution of x is given by
$$\frac{dx}{dt} = K(x_s - x) \quad \rightarrow (22)$$
- x_s is the sea surface temperature
- K is the turbulent heat transfer coefficient
- x, x_s, K, t are all non dimensional

We can also talk about a continuous time versions we simply for the sake of simplicity used the discrete time version. Now I am going to present a quick example of the forward sensitivity method using a continuous time model. This is a model that describes a motion of cold air over a hot ocean. So, this is called the Lagrangian forecast in meteorological circles. The air temperature is x , x_s is the temperature of the sea surface x_s is greater than. So, in United States we have the gulf of Mexico during wintertime cold air sweeps from the north the waters of the gulf are very warm in October November, it holds lot of the heat from the summer. So, when the cold air moves over the warm gulf there is a heat transfer from the warm gulf waters to the cold air. So, the air becomes warmer and warmer.

So, I am now the equation 22 gives you the dynamics of evolution of the temperature x of the air column k . So, x_s is the sea surface temperature k is the turbulent mixing are a turbulent heat transfer coefficient and we are assuming x, k, t are all non dimensional in other words originally I had a dimensionalized version assume that I have non-

dimensionalized it we have already done that. So, this is the non dimensional version of the model equation.

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SOLUTION AND ITS PROPERTIES

- Solution of (22) is given by

$$\underline{x(t) = x(t, x(0), K, x_s)}$$

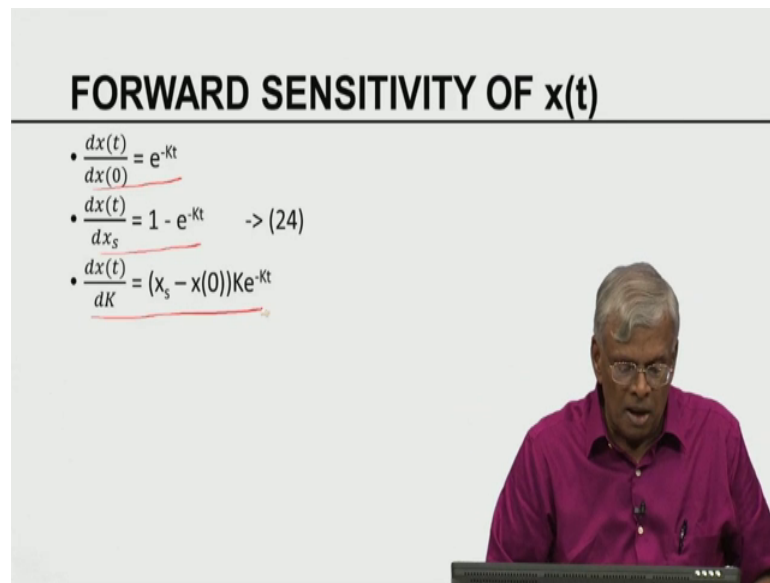
$$= x_s - (x_s - x(0))e^{-Kt} \rightarrow (23)$$
- $x(0)$ is the initial condition and $x_s > x(0)$
- $x(t)$ is monotonically increasing and $x(t) \rightarrow x_s$ as $t \rightarrow \infty$

Handwritten note in red: $C: (x_0, K, x_s)$

The solution of this model can be given explicitly because simply a first order differential equation we can readily solve from standard experience in calculus. So, this is the solution this is the form of the solution x naught is the, you can see the solution depends on x naught the solution depends on x_s which is called the boundary condition and the solution also depends on the parameter K . So, the control here c consists of x naught, K and x_s .

So, the control has three components one is the state of the system one is the initial state of the system another is the parameter, another is the sea surface temperature. The solution is monotonically increasing and x_t tends to x_s as t goes to infinity; that means, as the water are as the air moves over the water the heat transfer takes place the air temperature rises the heat transfer stops when the air temperature is equal to the sea surface temperature that is this very simple dynamics.

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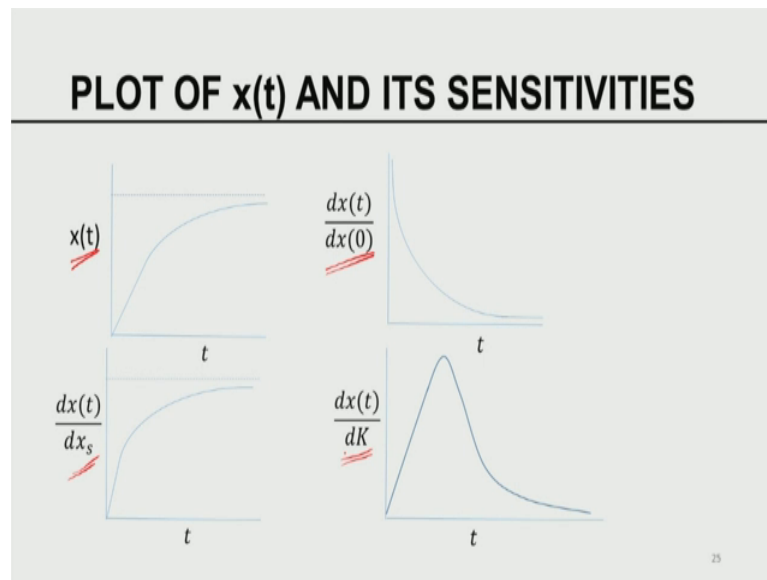
FORWARD SENSITIVITY OF $x(t)$

- $\frac{dx(t)}{dx(0)} = e^{-Kt}$
- $\frac{dx(t)}{dx_s} = 1 - e^{-Kt} \rightarrow (24)$
- $\frac{dx(t)}{dK} = (x_s - x(0))Ke^{-Kt}$

So, because the solution is known I can compute the sensitivities rather explicitly, I do not have to use the differential equation to compute the evolution of the sensitivity. So, that is the initial condition sensitivity, boundary condition sensitivity, parameter sensitivity.

So, once I know the sensitivity I am ready to compute the matrix h , but before that I need to be able to compute the observations or have the observations. So, using the observations starting from the initial condition make the forecast compute, the errors compute the forward sensitivity, you know the error using the forward sensitivity I can compute the matrix h we got the standard linearly square problem.

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Here are the examples for this model the model solutions this is the model solution x of t , this is the model solution this is the sensitivity the model solution with respect to x naught, this is the sensitivity of the model solution with respect to the boundary condition, this is the sensitivity of the model solutions with respect to parameters.

So, you can see solution and three sensitivities are graphically given here.

(Refer Slide Time: 58:21)

DISCRETIZATION

- Consider a uniform grid with interval Δt

- Let $x_k = x(k\Delta t) = x(t)$
- (22) becomes

$$\frac{x_{k+1} - x_k}{\Delta t} = K(x_s - x_k) \rightarrow (25)$$
- Simplifying (25);

$$x_{k+1} = (1 - \beta)x_k + \beta x_s \rightarrow (26)$$
- $\beta = K\Delta t$, $0 < \beta < 1$
- Solution of (26): $x_s > x_0$, the I.C

$$x_k = x_s - (1 - \beta)^k(x_s - x_0) \rightarrow (27)$$

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I am now going to discretize the model equation using standard Euler scheme this is the standard Euler scheme. So, if I simplify this 25 I get this equation. This is again a linear

equation because we started with a linear model β is k times Δt , Δt is the time interval for time discretization. I can solve this model equation explicitly and this is the discrete version of the model solution that is given in 27 we have already given the continuous time version of the model solution earlier.

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EXERCISES

1) Let $x \in \mathbb{R}$ and $\alpha \in \mathbb{R}^p$. $f: \mathbb{R} \times \mathbb{R}^p \rightarrow \mathbb{R}$. Consider

$$\frac{dx}{dt} = f(x, \alpha) \text{ with } x(0), \text{ I.C}$$

a) Differentiate both sides w.r.to $x(0)$ and derive the dynamics of evolution $\frac{dx(t)}{dx(0)}$

b) Differentiate both sides w.r.to α and and derive the dynamics of evolution $\frac{dx(t)}{d\alpha} \in \mathbb{R}^p$

2) Verify that the solution of the recurrence

$$x_{k+1} = (1 - \beta)x_k + \beta x_s$$

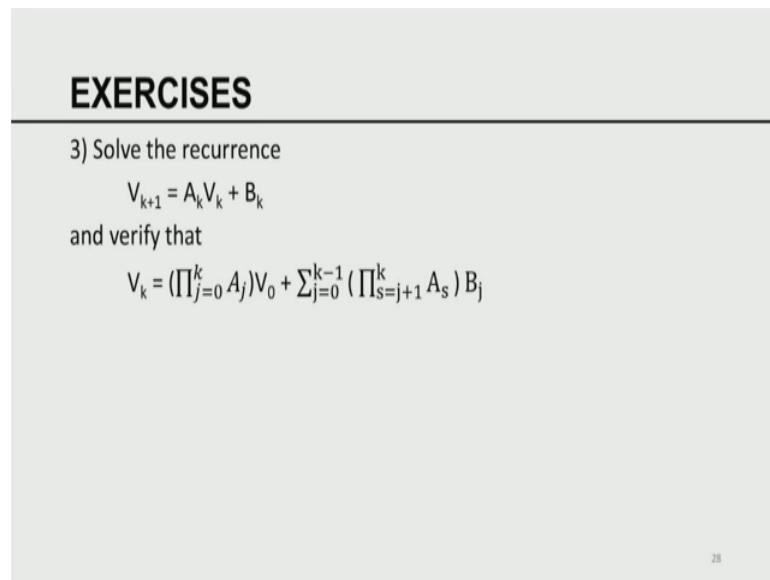
is given by

$$x_k = (1 - \beta)^k (x_0 - x_s) + x_s$$

27

So, what is that we are going to ask you to do? We are going to ask you to be able to with that is what problem two is all about, verify that the solution of the recurrence is given by this. We also want you to be able to solve the recurrence relation that are given in the previous slides when we did that.

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EXERCISES

3) Solve the recurrence

$$V_{k+1} = A_k V_k + B_k$$

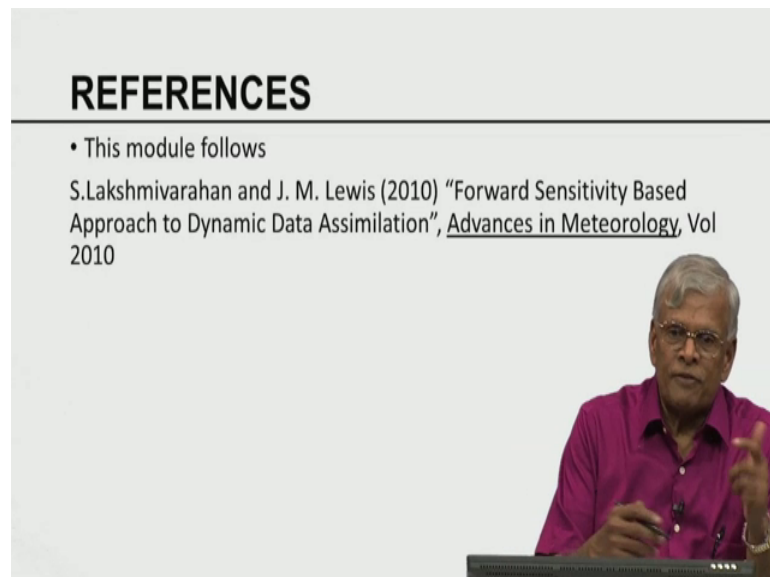
and verify that

$$V_k = (\prod_{j=0}^k A_j) V_0 + \sum_{j=0}^{k-1} (\prod_{s=j+1}^k A_s) B_j$$

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I also want you to be able to derive for the continuous time dynamics that is problem number 1. I would like you to be able to differentiate the continuum dynamics and derive the dynamics of evolution for the forward sensitivities both with respect to the parameter and the initial conditions.

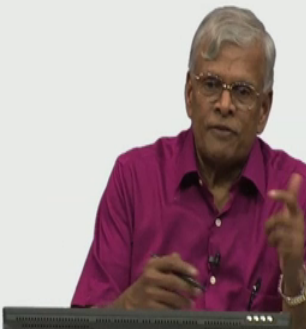
(Refer Slide Time: 59:49)



REFERENCES

- This module follows
- S.Lakshmivarahan and J. M. Lewis (2010) "Forward Sensitivity Based Approach to Dynamic Data Assimilation", Advances in Meteorology, Vol 2010

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This FSM method was developed by as it was published in a paper in 2010 entitled Forward Sensitivity Based Approach to Dynamic Data Assimilation which appeared in, Advances in Meteorology, volume in 2010. In this paper we describe both continuous

time as well as a discrete time. The example that I talked about we discuss in complete detail, we would like to refer the reader to this paper and I would also very strongly encourage you to be able to reproduce the results in this paper to make sure that you have a total and a thorough understanding of this methodology.

With this we conclude our discussion of data simulation using FSM forward sensitivity method. You can really see this is another way to do this. In our next lecture we will talk about the relation between 4-D Var and FSM. I strongly encourage you to be able to perform a data assimilation using it using the forward sensitivity. How do we do that? You assume certain values of the parameters, you generate the solution, you generate observation and in change the initial condition create erroneous forecast then use the generated observation to be able to control the erroneous forecast and that is what is called a twin experiment which we have been doing all along. Why? What is the best way to be able to benchmark your algorithm is to be able to generate data artificially using the model and if the model, if the method is capable of being able to recover the true initial condition then you have shown the proof of concept using these artificially designed observations that essentially gives you a clue that it should also work in real situations. So, that is the basic idea of the whole approach.

With this we have completed the discussion of FSM. We will in the next lecture talk about the relation between FSM and 4-D Var.

Thank you.