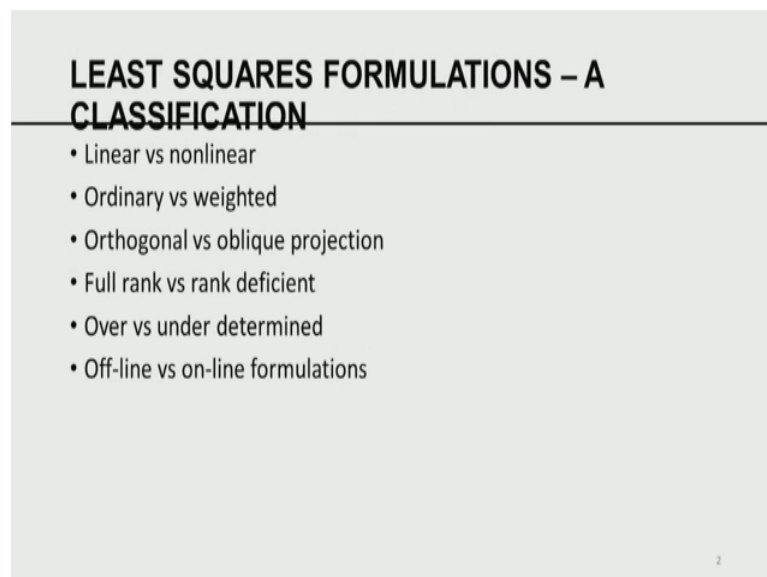


Dynamic Data Assimilation
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Lecture - 15
Interlude and a Way Forward

Now that we have seen various formulations of the static inverse problems, we would like to be able to develop numerical algorithms to solve some of the problems that we have already formulated. For example, the linear least square problem the solution process is reduced to one of solving a linear system of equation where the matrix of the linear system is symmetric and positive definite. So, it behooves us to ask a question how do I do that step especially when systems of large. So, this calls for actual numerical algorithms that we can use to get the ultimate step of being able to compute the solutions. And to see the bridge from problem formulation to actual numerical algorithms to solve the problem in this module which we call as an interlude, we are going to talk about an assessment of what we have done and the way forward.

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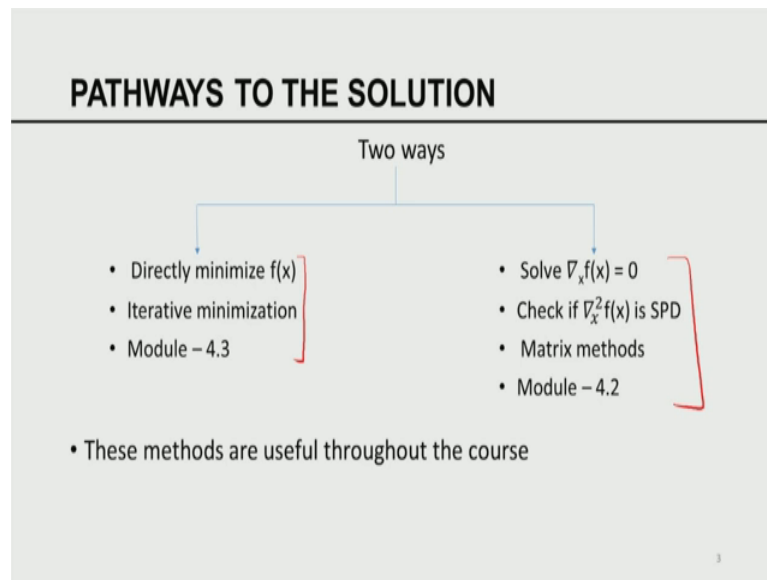
LEAST SQUARES FORMULATIONS – A CLASSIFICATION

- Linear vs nonlinear
- Ordinary vs weighted
- Orthogonal vs oblique projection
- Full rank vs rank deficient
- Over vs under determined
- Off-line vs on-line formulations

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So, the least square formulations can be classified in many ways linear, non-linear, ordinary or weighted, orthogonal or oblique projection, full rank versus rank deficient, over-determined or under determined, off-line versus on-line formulation. These are the examples of formulations of the least square problem we have covered thus far.

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Now, the pathways to the solution we have to convert that formulate mathematical formulation to actual numerical computation leading to the numerical methods for solving the problem. There are two ways to approach this. One is to directly minimize f of x , this leads to the so called iterative minimization algorithms we are going to talk about these iterative minimization algorithms as a part of the module 4.3 coming attractions. An alternate way would be we want to be able to minimize the f of x we compute the gradient of f of x , we compute the hessian of f of x , we solve the equation f of x is equal to 0, and verify at the solution this system is symmetric and positive definite. That leads to solving linear systems of equations these linear systems of equation solution process leads to a variety of matrix methods, and these are covered in module 4.2.

So, in this module 4.1, we provide a global view of what we have done and where we need to go and the two pathways, the two pathways to achieving the goal. In addition to achieving the goal of solving the static inverse problem, the methods that we are going to be looking at in this module are useful throughout the course whether it is the 3-D var problem or a 4 D var problem. So, these methods are the workhorse, the iterative methods and matrix methods are the workhorse that underlie computation of solutions of inverse problems or data assimilation problems in particular.

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PATHWAYS TO SOLUTION – LINEAR CASE

- Off-line, ordinary linear, full rank formulation: Module – 3.1
 $(H^T H)x = H^T Z$, $(H^T H) - \text{SPD}$, $m > n$
 $(HH^T)y = Z$ and $x = H^T y$, $(HH^T) - \text{SPD}$, $m < n$
- Off-line, weighted, linear full rank formulation: Module – 3.1
 $(H^T W H)x = H^T W Z$, $(H^T W H) - \text{SPD}$, $m > n$
 $(H W H^T)y = Z$ and $x = W H^T y$, $(H W H^T) - \text{SPD}$, $m < n$
- $W - \text{SPD}$

So, in the linear case off-line ordinary linear, full rank formulation in module 3.1 we were called upon to solve. This system H transpose H is equal to H transpose Z ; in here H transpose H is a symmetric positive definite matrix, m is greater than n that is the over determine case. In the under determine case, when m is less than n , HH transpose y is equal to Z , you solve for y ; and then the least square solution is obtained by the H transpose y . Here again HH transpose these two matrices are the gramian matrices which we know; the gramian is full rank, when H is of full rank; the gramian is symmetric it is positive definite. So, in these two cases, we are called upon to solve linear systems with symmetric positive definite matrices HH transpose H transpose H .

In the off-line weighted linear full rank formulation as we saw in module three point one we are called upon to solve a system with this matrix and the right hand side. Here H transpose $W H$ is a symmetric positive definite matrix. In the underdetermined case, again we are going to have to solve this problem and compute the weighted solution like this. Again in these cases we are called to solve a linear system of the kind $A x$ is equal to b , where A is symmetric and positive definite.

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PATHWAYS TO SOLUTION – LINEAR CASE

- Off-line, ordinary linear, rank-deficient formulation: Module – 3.2

$$(H^T H + \alpha I)x = H^T Z, \quad (H^T H + \alpha I) - \text{SPD}, \alpha > 0, \quad m > n$$

$$(H H^T + \alpha I)y = Z \text{ and } x = H^T y, \quad (H H^T + \alpha I) - \text{SPD}, \alpha > 0, \quad m < n$$

- On-line, ordinary linear, full rank case: Module – 10

$$X^*(m+1) = X^*(m) + K_{m+1} h_{m+1} [z_{m+1} - h_{m+1}^T X^*(m)]$$

$$K_m^{-1} = H^T H$$

$$K_{m+1}^{-1} = K_m^{-1} + h_{m+1} h_{m+1}^T$$

- K_{m+1} is obtained by Sherman-Morrison-Woodbury formula

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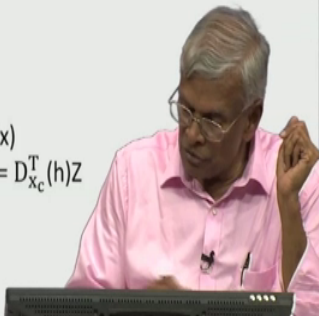
In the off-line ordinary linear rank deficient formulation, we are trying to provide a summary of everything we have done. We are called upon to solve $H^T H + \alpha I$ x is equal to $H^T Z$, this is a symmetric positive definite matrix. This kind of formulation arose for the rank deficient or the ill conditioned problem, these methods arose out of the use of regularization. This is for the overdetermined case; for the underdetermined case, again we solve a linear system of this type.

For the on-line ordinary linear full rank the emphasis is on-line we saw it is not module 10, I think we have to correct that a different module we will give the numbers soon. The equations were given by this. Here again K_m is continually calculated like this. Here again I am interested in computing the inverses of certain matrices K_{m+1} is obtained by the Sherman-Morrison-Woodbury formula we may remember this. So, we have covered off-line problems as well as on-line problems; and we have summarized all the equations. Solutions of these equations give rise to the least square solution of the least square problem.

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PATHWAYS TO SOLUTION – NONLINEAR CASE

- Off-line, ordinary, nonlinear case: Module – 3.4
 - Solve a set of non-linear equations:
$$\nabla_x^T f(x) = D_x^T(h)[h(x) - Z] = 0$$
- On-line, ordinary, nonlinear case:
 - Use first-order approximation to $h(x)$
$$[D_{x_c}^T(h)D_{x_c}(h)](x - x_c) = D_{x_c}^T(h)Z$$
$$x_c^{new} \leftarrow x_c + (x - x_c)$$
 - Use second-order approximation to $h(x)$
$$[D_{x_c}^T(h)D_{x_c}(h) - \sum_{i=1}^m g_i \nabla_x^2 h_i(x_c)](x - x_c) = D_{x_c}^T(h)Z$$
$$g = z - h(x_c), x_c^{new} \leftarrow x_c + (x - x_c)$$



For the off-line ordinary non-linear case, we have to solve a set of non-linear equations, we have to solve a set of non-linear equations. The non-linear equation is solved by setting the gradient equal to 0. In the on-line ordinary non-linear case, again we are going to be solving these kinds of equations. This is for the first order case. In the second order case, again we are going to be solving systems where the system matrix is given by this, the system matrix is given by that. The system matrix is a large matrix; the expression for it is large, we have to solve this system matrix. So, you can see no matter what formulation we have used.

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A WAY FORWARD – COMING ATTRactions:

- Method of normal equations
- At its core, need methods for solving
$$(H^T H)x = H^T Z \text{ or } (HH^T)y = Z$$
- These are linear systems of the form
$$Ax = b$$
with A as a symmetric positive definite (SPD) matrix
- A stand method to linear systems with SPD matrix is the Cholesky decomposition method – (Module 4.2)

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The method of normal equations at its core calls for solving linear systems of the form $Ax = b$ where A is a symmetric positive definite matrix, so that is the bottom line no matter where you start off-line, on-line, linear, non-linear, well conditioned ill conditioned. In all these cases, all these different formulations, all lead to from a mathematical perspective result in solving one simple problem $Ax = b$, where the matrix A is not any matrix is a symmetric positive definite matrix. A standard method for solving this linear system with symmetric positive matrix is called Cholesky decomposition method, we will talk about this method in module 4.2. Again we are trying to build a bridge between what had happened and what is likely to happen, and why and how what happened and what is how supposed to happen are interrelated with each other are interrelated with each other.

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ALTERNATE DECOMPOSITION (QR AND SVD) METHODS

- Instead of decomposing $(H^T H)$ or $(H H^T)$ using Cholesky method, we can directly decompose H that will simplify the form of the least squares solution
- QR - decomposition - (Module 4.2)
- (SVD) - (Module 4.2)

Most of the methods for solving linear systems they all rests on what is called decomposition techniques. So, in the Cholesky decomposition, what is that first you need to do, you need to be able to compute the matrix A .

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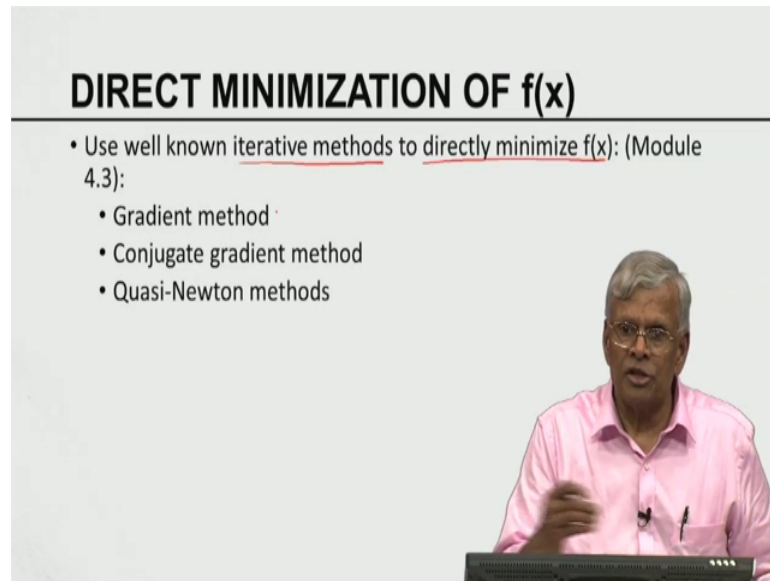
A WAY FORWARD – COMING ATTRACTIONS:

- Method of normal equations
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$A = H^T H / H H^T$

A in general is given by H transpose H or H H transpose. So, in using cholesky method for solving this we first have to multiply H with H transpose H transpose with H to obtain a and then we need to do a decomposition method, we will see some of the details in module 4.2. An alternate way it would be instead of first composing H transpose H and then decomposing using Cholesky method, so you first wind then unwind. So, instead of multiplying H with the H transpose in H transpose with the H, and then applying Cholesky for H transpose H or H H transpose, we can directly decompose H to simplify the form of the least square solution. These two method there are two methods we will indicate, these are called QR decomposition and SVD. SVD stands for singular value decomposition, QR decomposition, Cholesky decomposition these are the three popular methods which we have come to call matrix methods for solving the resulting system of $Ax = b$, where A is a symmetric positive definite matrix.

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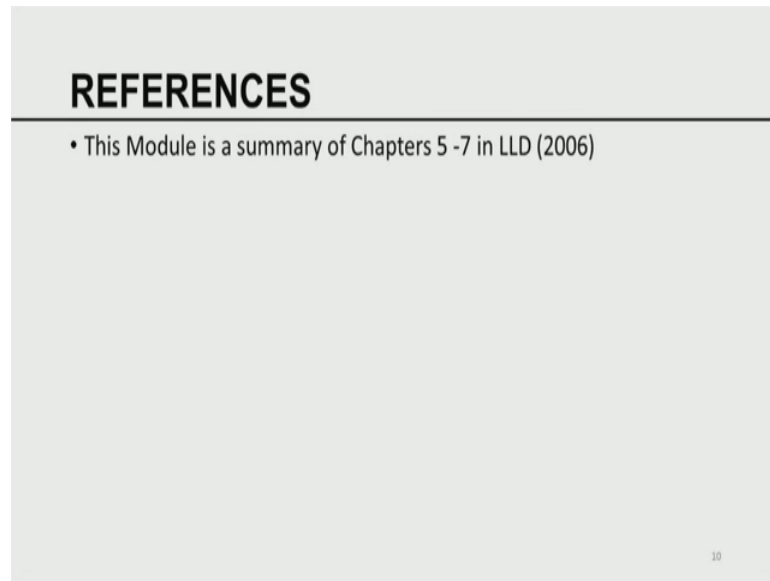


DIRECT MINIMIZATION OF $f(x)$

- Use well known iterative methods to directly minimize $f(x)$: (Module 4.3):
 - Gradient method
 - Conjugate gradient method
 - Quasi-Newton methods

Since our approach is quite mathematical since our goal is to provide all the mathematical basis instead of simply saying use QR, use SVD, use Cholesky. We are going to also fill up the blanks as to how Cholesky works, how QR works, how SVD works because if you understand some of the intricate details of these methodologies then you will be able to exploit that knowledge to be able to accelerate convergence in solving specific problems that is the goal. The alternate method would be instead of solving the gradient equal to 0 and resulting linear equation we could have directly minimized f of x , which is the square of the sum of the residuals f of x . I could directly minimize it using iterative methods, some of the well known methods for iterative minimizations are called gradient methods, conjugate gradient methods, and Quasi-Newton methods we are going to provide some overview of the workings of these methods as well these methods become integral part of the data assimilation process. In fact, anybody who is interested in trying to develop a data assimilation system have to program many of these methods one or two of these methods to be able to bring the mathematical formulations to the computational domain and that is where these methods are very useful.

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So, in summary in this module we have provided a quick overview of all the results we have done so far in all the previous modules. These are summaries of chapters five through seven in our textbook Lewis (Refer Time: 13:46) 2006. With this as a background, with this as a bridge between the previous modules and the coming attractions, now I am going to get into the nitty-gritty details of matrix methods as well as direct memorization techniques for minimizing f of x . And these two classes of methods constitute the basic workhorse of the data assimilation process. With this we conclude this module.

Thank you.