

Numerical Methods in Civil Engineering
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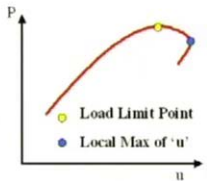
Lecture - 16
ARC Length and Gradient Based Methods

Lecture sixteen of a series numerical methods in civil engineering, we are going to talk about arc length and gradient based methods. If you recall in the last lecture, probably a last two lecture we have looked at various methods to solving non-linear equations and the method.

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Possible convergence problems

- In many structural and solid mechanics problems the load displacement curve changes slope. This occurs typically at limit points.



Legend:
● Load Limit Point
● Local Max of 'u'

- The equilibrium path following algorithm adopted so far moves from one equilibrium state to the next based on the tangent stiffness



We concentrate on first was the most well known method Newton Watson method. Then we looked at variation of the Newton Watson method modified Newton method. Finally, we looked at quasi Newton, however, it is not always possible to solve all the problems, that was in uncouncted in civil engineering application with non-linearity's using the Newton Watson method, why? Well, because load path unless it is really well be have in Newton Watson method cannot converge. We will see example of why that happens in many structural and solid mechanics problems.

The load displacement curve changes slope for instance here at plot to the load displacement curve with the red line. That is my load displacement curve and you can see that it is changing slope. It is positive up to here, positive slope goes to 0, it changes

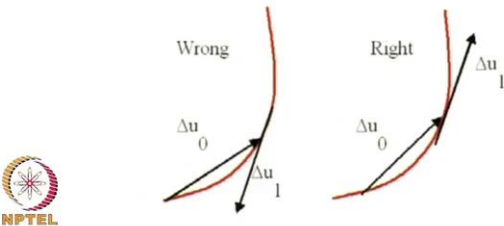
a sign right same things happen here. So, this will happen in structural mechanic application. For instance when we have a load limit point, where we will leads a maximum value of the load. This structure cannot take anymore load, that is the maximum load that it can carry. After that there is suffering load for calls I mean load decreases within increasing displacement.

So, that is a load limit point when we use Newton Watson method for solving such a problem, we encounter difficulties. This is because the equilibrium path following algorithm adopted. So, far namely the Newton Watson method moves from one equilibrium state to the next equilibrium state based on the tangent stiffness by tangent stiffness. That is evaluated at the converged equilibrium state at the previous we converge equilibrium state. We evaluate the tangent stiffness, then mass along that direction in n dimensional space.

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Possible convergence problems

- If the slope undergoes large changes along the equilibrium path, it is necessary that (a) the orientation of the path be correct (b) step sizes along the path be controlled
- Once a limit point has been exceeded, there may be a need to change the direction of the load incrementation

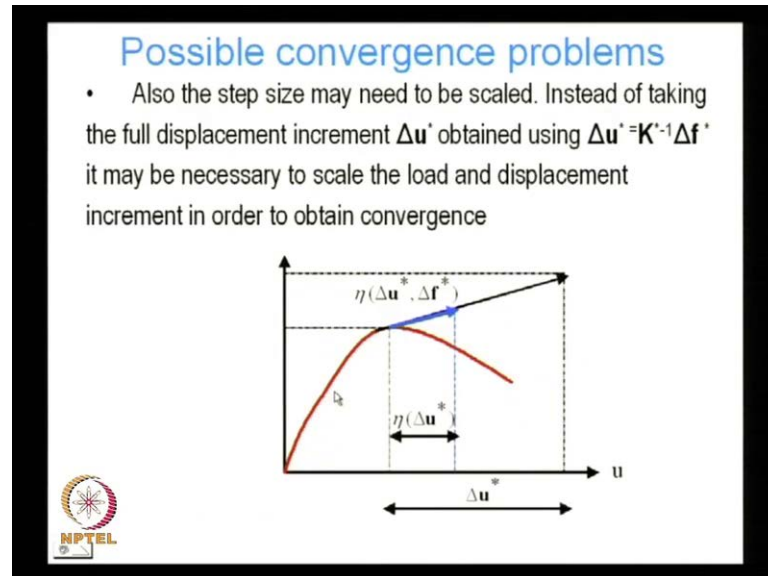


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If the slope undergoes large changes along the equilibrium path, it is necessary that a the orientation of the path be correct and b step size is along the path be controlled. For instances if we have a situation like this, where obviously, have a limit point. We are moving along this direction along the load displacement curve. We took this initial increment Δu_0 and we are evaluating the tangent here. You can see if that is the tangent point here in this direction, then the next displacement increment will point will

ask me to travel in this direction in load displacement space, which is totally wrong. It should actually be traveling in this direction.

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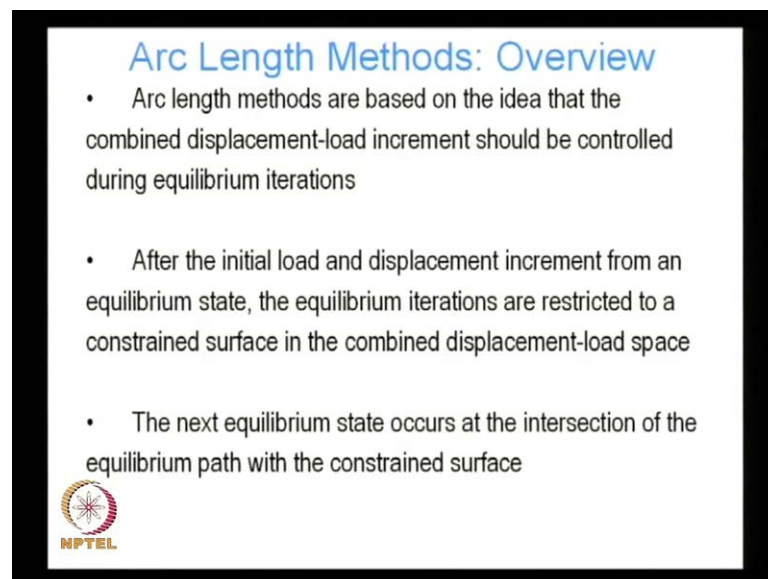
This may be necessities to check the orientation also the step size may need to be scaled. For instance we have softening behavior softening meaning that the in even though the displacement increases the load actually decreases. In a situation like this, again if you reach here. If you reach a limit point here, if you reach a limit point here like this. Then if we calculate the tangent here that is pointing in this direction. So, how do I calculate my incremental displacement?

I invert my tangent stiffness multiply it take the product invert of the tangent stiffness with my load increment and that gives me my incremental displacement. So, this is my load increment from here to here this is my load increment, this is my slope, this is my tangent stiffness. So, this tells me if I divide load to the increment by the tangent stiffness less think of 1 d. So, stock of division, if you think of that then that tells me that I must move from here to here on the displacement access, but once it moves here, you can see that the structure cannot responds, because the load displacement curve is like this. So, it cannot calculated internal an internal force to equilibrate the applied load. Then the problem diverges it cannot converge.

So, if you have a situation like that one solution is to scale the displacement increment may when the load increment. So, I have got my initial displacement increment and load


increment. Suppose, Δu^* and Δu^* . So, I say no take I cannot take the load that because load displacement. So, let be scale it by factor 8. If I do that I probably end up some points here, where there is a load response, where there is valid response for this structure, where there is internal force is not undefined. So, I have chance of reaching equilibrium. So, that is the simplest possible thing that we can do the control the load steps and the displacement step. So, up till now Newton Watson we have, so we controlling the load steps and the displacement steps.

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Arc Length Methods: Overview

- Arc length methods are based on the idea that the combined displacement-load increment should be controlled during equilibrium iterations
- After the initial load and displacement increment from an equilibrium state, the equilibrium iterations are restricted to a constrained surface in the combined displacement-load space
- The next equilibrium state occurs at the intersection of the equilibrium path with the constrained surface

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So, that brings us to say new concept, which is known as the arc length type. Let us look at what this are arc length methods are based on the idea that the combined displacement. Load increment should be controlled during equilibrium iteration. So, not just the load not even in displacement, not a load given problem we controlled the load. When displacement ravine problem, we controlled the displacement, but this is in this case we are controlling both the load and.

The displacement we are saying that neither the displacement increment not the load increment should exceed certain cart of value, during the equilibrium hydrations. There is will help the problem to converge this help my non-linear iteration to convert. So, based on the idea that the combine load displacement is increment should be control. So, how this is that don? Well, we take an initial load and displacement increment from equilibrium step. Suppose, I have any equilibrium steps with this displacement is 0 and

force f_0 I calculated incremental force Δf applying incremental force Δf . Then I calculated incremental displacement Δu_0 using 0 my tangent stiffness $\Delta u_0 f_0$. So, that gives me the first step in my iteration, but following that the equilibrium iteration are restricted to a constraint surface in the combine load displacement space. So, let me show picture and this probably help you to understand this.

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Arc Length Methods: Overview

- In the first iteration of an increment, the displacement is determined from a load increment by the usual linearized stiffness matrix: $\mathbf{K}\Delta\mathbf{u}_1 = \Delta\mathbf{f}_1$
- This is followed by simultaneous combined displacement and load sub-increments $(\delta\mathbf{u}_i, \delta\mathbf{f}_i)$ after which the increments are updated as: $\Delta\mathbf{u}_i = \Delta\mathbf{u}_{i-1} + \delta\mathbf{u}_i$ $\Delta\mathbf{f}_i = \Delta\mathbf{f}_{i-1} + \delta\mathbf{f}_i$

So, this is my equilibrated step $u_0 f_0$, from here I have taken initial increment $\Delta u_1 \Delta f_1$, how did I calculate this I talk my Δf_1 , which was my force increment? I took my tangent stiffness here, I inverted my tangent stiffness took the product with Δf_1 and got my Δu_1 , but this is obviously, does not equilibrated state. So, I have what will be an equilibrium state upon that must lie on my red color. Where, my internal force going to be my external force. So, what do I do?

Well, I say that I take a step here to here, this is my trial step. This is like my predictor, this is what I predicted to be this concept are common to lots of numerical method, but basically the idea I take initial predictor. Then I take corrector, I corrected to reach the red line, which is my desire solution, but I do not do my correctors are constraints, why are the constrained. Well, it says that the correctors that I must take the move from this point to this point to this point my equilibrated solution. My equilibrated solution must move along this curve, this is my constraint curve. So, I can only move from here to hereby travelling along this arc.

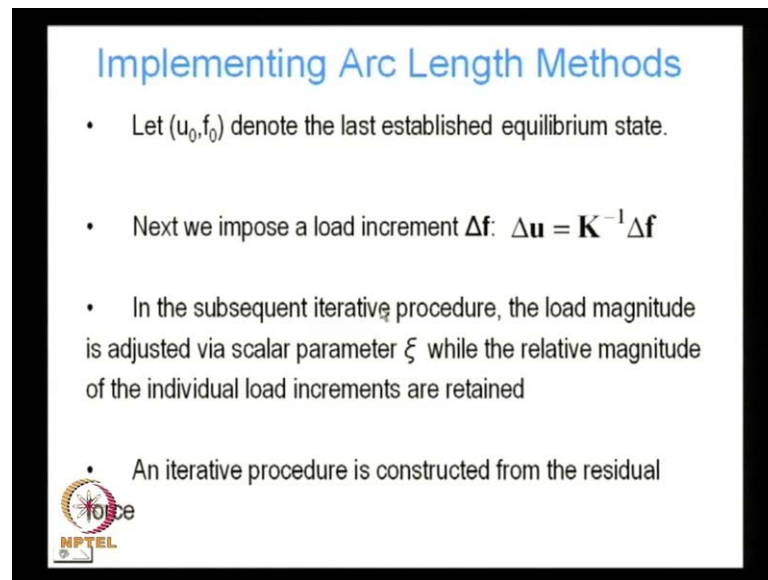
So, that is why it is known as arc length methods. So, I'm moving from here to here, I'm traveling along that curve. This curve is a surface in the load displacement space, this is just a 2D idealization. So, basically a hyperplane or some surface in a multi-dimensional surface. I have to move along that surface from my initial predictor solution to my equilibrated solution. So, after the initial load and displacement increment from an equilibrium state, the equilibrium iterations are restricted to a constrained surface in the combined load and load displacement space. The next equilibrium state occurs at the intersection of the equilibrium path with the constrained surface.

It occurs at the intersection of the equilibrium path with the constrained surface. So, this is my equilibrium path, this is my constrained surface, this is my new equilibrated state in the first iteration of an increment. The displacement is determined from a load increment by the usual linearized stiffness matrix. That's how I determine my Δu from here? I know Δf , I know the tangent, I can calculate Δu .

This is followed by simultaneous combined displacement and load sub-incremental following that initial increment following that initial increment. When my load is fixed, Δf is fixed. I calculate my displacement increment now in the subsequent iteration, I can change both my load and my displacement. You can see obviously, that if I have to travel from here to here, I have to change both the load and displacement.


So, I have to change both my load and displacement in order to reach this point on the intersection point. So, this is followed by simultaneous combined displacement and load sub-increment Δu_i and Δf_i , where these are the i th iteration compared. I keep on iterating after each iteration, I update my incremental displacement. My incremental load until I finally reach my convergence state. So, $\Delta u_i = \Delta u_{i-1} + \Delta u_i$ and $\Delta f_i = \Delta f_{i-1} + \Delta f_i$. So, I am going from here to here and little iteration steps, which are denoted by i iteration.

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Implementing Arc Length Methods

- Let (u_0, f_0) denote the last established equilibrium state.
- Next we impose a load increment Δf : $\Delta u = \mathbf{K}^{-1} \Delta f$
- In the subsequent iterative procedure, the load magnitude is adjusted via scalar parameter ξ while the relative magnitude of the individual load increments are retained
- An iterative procedure is constructed from the residual



So, let us use f_0, u_0 to denote the last established equilibrium state. From this going to somewhat more detail, we impose a load increment Δf . We calculate the displacement increment Δu is equal to $\mathbf{K}^{-1} \Delta f$ in the subsequent iterative procedure. The load magnitude is adjusted via scalar parameters ξ , where the relative magnitude of the individual load increments are retained, what does it mean? Well, I know my load increment Δf , this is what I am controlling. It is a load control problem and prescribing Δf I want I am increasing load by Δf , but that Δf is vector is got many, many components.


So, how am I going to scale that Δf to bring it to my converge state well the way I am going to scale is it. I am going to change the magnitude and I am just going to keep all the components the directions the same. I am going to keep the direction of the load vector this the same and I am just going to scale its magnitude. So, this factor is ξ this parameters ξ its scale magnitude of the load vector, but it keeps the leaves the direction unchanged the direction of the load vector and changed. So, the each load ratio between the load components remains the same its only the magnitude that is change.

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Implementing Arc Length Methods

$$\begin{aligned} \mathbf{r} &= \mathbf{f} - \mathbf{g}(\mathbf{u}) = \mathbf{f}_0 + \xi \Delta \mathbf{f} - \mathbf{g}(\mathbf{u}_0 + \delta \mathbf{u}) \\ &= \xi \Delta \mathbf{f} - \Delta \mathbf{g} \quad [\text{Using } \mathbf{f}_0 = \mathbf{g}(\mathbf{u}_0)] \quad (*) \end{aligned}$$

- In addition we have a constraint equation relating the current displacement increment $\delta \mathbf{u}$ to the current load increment $\xi \Delta \mathbf{f}$, which can in general be a nonlinear equation:
$$c(\delta \mathbf{u}, \xi \Delta \mathbf{f}) = 0$$
- The combined equilibrium and constraint equations are then solved using a Newton Raphson procedure



So, an iterative procedure construct from the residual force like this. So, basically we say that residual is equal to \mathbf{f} minus $\mathbf{g}(\mathbf{u})$, which you have seen maintained before. This apply load, this is my response internal force. This I am going to write as \mathbf{f}_0 plus ξ times $\Delta \mathbf{f}$. \mathbf{f}_0 was my last equilibrated load right $\Delta \mathbf{f}$ is my initial increment and ξ is my scalar parameter, which I am going to scale load that load increment.

So, \mathbf{f}_0 plus $\xi \Delta \mathbf{f}$ must be equal to sorry \mathbf{f}_0 plus $\xi \Delta \mathbf{f}$ minus my internal force by response, which is the function of the initial displacement \mathbf{u}_0 , plus my increment $\delta \mathbf{u}$ is going to whatever the differences that is going to be my residual. That is going to be my residual. I am going to represent write this as $\xi \Delta \mathbf{f}$ minus $\Delta \mathbf{g}$, because I am going to write minus $\mathbf{g}(\mathbf{u}_0 + \delta \mathbf{u})$ as $\mathbf{g}(\mathbf{u}_0) + \Delta \mathbf{g}$.

So, I am just representing $\mathbf{g}(\mathbf{u}_0 + \delta \mathbf{u})$ as $\mathbf{g}(\mathbf{u}_0)$, the internal force at displacement \mathbf{u}_0 plus the increment in the internal force $\Delta \mathbf{g}$. So, say this $\mathbf{g}(\mathbf{u}_0)$ must be equal \mathbf{f}_0 , because the 0 is an equilibrate state right \mathbf{f}_0 must be equal to $\mathbf{g}(\mathbf{u}_0)$. So, \mathbf{f}_0 cancel with $\mathbf{g}(\mathbf{u}_0)$ and a $\xi \Delta \mathbf{f}$ minus $\Delta \mathbf{g}$. So, that is going to be my residual in addition we have constraint equation, which relates the current displacement increment $\delta \mathbf{u}$ to the current load increment $\xi \Delta \mathbf{f}$. So, my current displacement increment is $\delta \mathbf{u}$, it is this is thing. My current load increment is $\xi \Delta \mathbf{f}$ of the $\Delta \mathbf{f}$ and I am saying that this $\delta \mathbf{u}$ and this $\xi \Delta \mathbf{f}$ displacement increment and cannot be arbiter they must lie on the constraint surface.

That is must satisfy this constraint equations, this constraint equation is function of delta u and x I delta f. So, these increment my satisfy that equation. So, now, we have two equations, we have couples system. We have equation there, which is my residual, which is my usual residual equation. Then I have this constrained equations, which also involves delta u and x I delta. These two equations are coupled, because both involve delta u and delta f. So, now, I have to solve a coupled system a coupled system the combine equilibrium and constrained equation are then solved using a Newton Watson procedure. How do we do that? Well, let see.

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Implementing Arc Length Methods

$$\mathbf{r} + \delta \mathbf{r} = 0 \qquad \mathbf{c} + \delta \mathbf{c} = 0$$

$$-\frac{\partial \mathbf{r}}{\partial \mathbf{u}} \delta \mathbf{u} - \frac{\partial \mathbf{r}}{\partial \xi} \delta \xi = \mathbf{r} \qquad -\frac{\partial \mathbf{c}}{\partial \mathbf{u}} \delta \mathbf{u} - \frac{\partial \mathbf{c}}{\partial \xi} \delta \xi = 0$$

Recalling that $\frac{\partial \mathbf{r}}{\partial \mathbf{u}} = -\mathbf{K}$ and from (*) $\frac{\partial \mathbf{r}}{\partial \xi} = \Delta \mathbf{f}$

and denoting $\frac{\partial \mathbf{c}}{\partial \mathbf{u}} = \mathbf{c}_u^T$ and $\frac{\partial \mathbf{c}}{\partial \xi} = c_\xi$, we get :

$$\begin{bmatrix} \mathbf{K} & -\Delta \mathbf{f} \\ -\mathbf{c}_u^T & -c_\xi \end{bmatrix} \begin{bmatrix} \delta \mathbf{u} \\ \delta \xi \end{bmatrix} = \begin{Bmatrix} \mathbf{r} \\ c \end{Bmatrix}$$


Again Newton Watson means linearization linearization above the last converge state. So, again we writer plus delta r equal to 0, we assume that at my new after I calculate my new update my exceeds it intersects the x exceeds. So, the Coordinate is 0 linearization, so, r plus delta r is equal to 0 c plus delta c is equal to 0 linearised that del r I write as del r del u, where is del u my plus del x i. This must be equal to plus are must be equal to 0. So, the minus of this must be equal to r.

Basically, delta r is equal to just by linearization is equal to del r del u del i del x i. So, r plus this is equal to 0 this must be equal to r. Similarly, I do the same thing here again my linearized del c del u del c del r x I and c is a function both u and x i. So, I can when I linear get this and this is equal to 0 right we call del r del u is equal to minus k, del r del u is equal to minus k.

So, $\frac{\partial r}{\partial u}$ is minus k , because x my tangent stiffness and $\frac{\partial r}{\partial x}$ I is equal to Δf vice that. Let's go back and take a look see here we have an expression for all. If I take the partial of r with respect to x_i I get Δf . So, $\frac{\partial r}{\partial x_i}$ is equal to Δf . Then if I denote $\frac{\partial c}{\partial u}$ by c_u transpose and $\frac{\partial c}{\partial x_i}$ by c_{x_i} . I get a coupled system like this.

So, now, I have k which is this term $k \Delta u$ $k \Delta u \frac{\partial r}{\partial x_i}$, which is equal to Δf $\Delta f \frac{\partial r}{\partial x_i}$. That is equal to r and here I have $\frac{\partial c}{\partial u}$ which I denoted by c_u transpose c_u transpose. Here, I have $\frac{\partial c}{\partial x_i}$ which is c_{x_i} . So, this c_u transpose Δu $c_{x_i} \Delta x_i$ equal to c . There is a type of here I am sorry this should be c that is that that has to hold. So, let us look at the first equation $k \Delta u$ minus $\Delta f \frac{\partial r}{\partial x_i}$ is equal to r .

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Implementing Arc Length Methods


Considering the first term:

$$\delta \mathbf{u} = \mathbf{K}^{-1} \mathbf{r} + \delta \xi \mathbf{K}^{-1} \Delta \mathbf{f} \quad (**)$$

Denoting $\mathbf{K}^{-1} \mathbf{r} = \delta \mathbf{u}_r$, $\mathbf{K}^{-1} \Delta \mathbf{f} = \Delta \mathbf{u}_f$

we get: $\delta \mathbf{u} = \delta \mathbf{u}_r + \delta \xi \Delta \mathbf{u}_f \quad (*)$

- The first term is the displacement sub-increment $\delta \mathbf{u}_r$, generated by the residual force \mathbf{r} corresponding to that used by the Newton Raphson method.
- The second term represents the displacement increment following from the adjustment of the load increment



So, this from this equations I can write Δu I can write Δu Δu is equal to $\mathbf{K}^{-1} \mathbf{r}$ plus $\Delta x_i \mathbf{K}^{-1} \Delta f$ just by taking $\Delta f \Delta f \Delta x_i$ to the right hand side. Then inverting \mathbf{K} right I can get an expression for Δu is the typical conversation type of operation. So, I get an expression for Δu , which is $\mathbf{K}^{-1} \mathbf{r}$ plus $\Delta x_i \mathbf{K}^{-1} \Delta f$. Then I denote $\mathbf{K}^{-1} \mathbf{r}$ as Δu_r and $\mathbf{K}^{-1} \Delta f$ as Δu_f . Then I get again Δu is equal to Δu_r plus $\Delta x_i \Delta u_f$, the first term the first term is the usual update. The first term is the usual update why is the usual update? First

term is the usual update, why is the usual update? Well, just calculated by taking k inverse r like we did for normal Newton Watson that the usual.

This is the contribution this is the coupling term contribution, because there is that coupling term. That is why I get this additional correction. The first term is the displacement sub increment delta u r generated by the residual force r corresponding to that used by the Newton Watson method. The second term represents the displacement increment following from the adjustment of the load increment, if there was no adjustment of the load increment. Then delta x i would be 0 and this term would vanish, but since there is delta x i not equal to 0 I have this additional contribution, delta u is equal to delta u r plus delta x i delta u f. Then, what do I do? Well, after evaluate I that. So, this is typical type of solution that we are talking about is very common its known as condensation type solution.


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Implementing Arc Length Methods

Using (*) in the second equation:
$$\delta \xi = - \frac{c_{\mathbf{u}}^T \delta \mathbf{u}_r + c}{c_{\mathbf{u}}^T \Delta \mathbf{u}_f + c_{\xi}}$$

Once $\delta \xi$ has been calculated as above, $\delta \mathbf{u}$ can be calculated from (**). For a non-linear constraint c , $\frac{\partial c}{\partial \mathbf{u}}$ and $\frac{\partial c}{\partial \xi}$ are not constant. Hence the above system has to be solved iteratively.

However for linear constraints (hyperplane constraints) or quadratic constraints (hypersphere constraints) allow closed form solution of the constraint equations



So, in the first equation what we did we obtained delta u. We solve that equation to get delta u in terms of in terms of delta x i. Then once we obtained we wrote delta u like that we are going to substitute that in the second equation minus c u transpose delta u. So, we are going to replace that delta u in terms of x I, there is always delta x i here. So, that will give me equation purely in terms of delta x I. Then I am going to solve that equation to get my delta x i. So, using star in the second equation I solve for delta x i like this. Once I have calculate delta x I, I again substitute that in this equation I get my delta u.


So, once delta has been calculated as above delta u can be calculated by my previous equation, which was this one thing one most note that this equation to solve this equation is not that simple, because why is not simple? Well, because all in this in case if I have non-linear constraint, if my c is non-linear function if my c is a non-linear functions of delta u and x i delta f. When I just cannot just cannot solve directly, I have to iterate because, every time I change I change this solution these const. These things are going to change this c u transpose. That is going to change, because that depends on the delta u and delta x I. So, that is going to change, so, I have to solve this equation iteratively.

So, this system has to be solve iteratively again iteratively means we assume some value of delta x i solve for until it converges iterative converges, for linear constraints. For instance I have hyper plane constraints for a quadratic constraints. I can get close form solution that is I do not have to iterate I can just solve this equation is close form. Because, these things are no longer they are no longer function of delta u and x i delta x I, they become constant. That case I can solve that for del x i directly, once I solve delta x i I can substitute it in my previous equation solve for delta u.

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Gradient based iterative Methods

- Up till now the methods considered for obtaining the solution update involve solving at each iteration the system $\mathbf{K}^{(i)} \Delta \mathbf{u}_n^{(i)} = \Delta \mathbf{f}$ for the Newton Raphson method and the constrained system for arc length methods
- If $\mathbf{K}^{(i)}$ is a full matrix, then direct solution of this system by Gauss elimination or its variants is most economical
- However if $\mathbf{K}^{(i)}$ is sparse, then as seen before, it may be more efficient computationally to consider iterative methods



So, that was very brief introduction to arc length method arc length method are extremely important. Probably, the only the technique that can be used solving the wide range of problems wide range of problems, problems with limit point problem bifurcation tabbed solution stability things like that. Suppose, in a typical civil

engineering application if you have sparse link sparse link when a structure sparselets. These in stability obviously, at that point the load displacement curves changes slope. If you have interesting not only at knowing at what load structure sparselets, but you also interested in knowing the post sparse link behavior.

You want to know the deformation patterns after the structures as sparselets. In that case Newton Watson is simply going to fail, it cannot work is never going to converge in that case we are using arc length method as a most you cannot get anywhere. If cannot get any reasonable sparkling solution without using in arc length method several arc length methods are used, when risks method r i k s the risks method is a common arc length method. That is suppose to one of the most arc length method in used. So, that was a very brief introduction to arc length method.

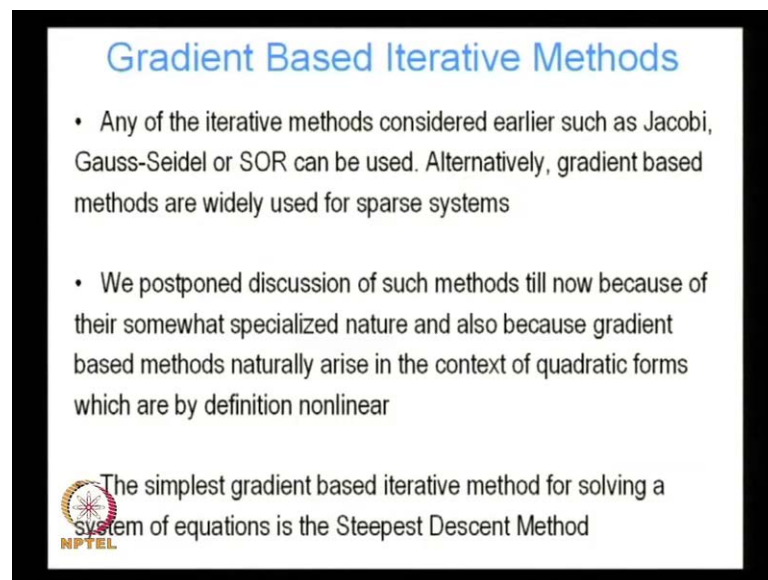
Now, want to switch to what I known as gradient based iterative methods look at the methods we have use so far for solving non-linear equation. All of them are direct methods all of them involve inverting a matrix, finding update doing that over and over and over again, until we will get the equilibrium solution. So, that involves direct solution involves matrix inversion. Instead of that we can use iterative methods iterative methods for solving this system, up till now the methods we are considered for obtaining the solution. Update involve solving at each iteration the system $k_i \Delta u_n$ is equal to Δf for the Newton Watson method, the constrained system for arc length methods. If I use the Newton Watson method Newton Watson I solves this system I had arc length method. I solve the coupled system the constrained system if k_i is a full metrics.

Then the direct solution of this system by gauss elimination or its variants is probably the most economical. If my stiffness, if my coefficient metrics is a full metrics, then probably gauss elimination or in variants of those. Those are probably the most are the most economical method, but in case those tangents stiffness are not full matrices. Let as they are pass matrices we looked at when we looked a Gauss elimination. We saw that one major problem with gauss elimination was that during this pivoting during the pivoting process, which is of course, essential for gauss elimination. In most problem during the preventing problem process, it converts a pass matrix into a populated matrix.

As soon as that is losses all the benefits possess it increases the number of computation. It increases the number of it increase the computation time becomes uneconomic. We

also saw that iterative methods are probably the preferred methods for problem, where you have sparse matrices that was for linear systems, non-linear case. Also, the same holds if k_i is sparse then it may be more efficient to computationally more efficient computationally to consider iterative methods to consider iterative method.

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The slide is titled "Gradient Based Iterative Methods" in blue text. It contains two bullet points: "Any of the iterative methods considered earlier such as Jacobi, Gauss-Seidel or SOR can be used. Alternatively, gradient based methods are widely used for sparse systems" and "We postponed discussion of such methods till now because of their somewhat specialized nature and also because gradient based methods naturally arise in the context of quadratic forms which are by definition nonlinear". At the bottom left is the NPTEL logo, and at the bottom right is the text "The simplest gradient based iterative method for solving a system of equations is the Steepest Descent Method".


Any of the iterative method we consider earlier such as the several, as which are gusseded method or successive over elation method can be used alternatively. We are now going to propose something, which we did not talk about before gradient based method till now. Because, of somewhat specialize nature and also because gradient based method naturally arise in the context of quadratic forms, which are by definition non-linear.

So, gradients method are typically arise in solving, what as known as quadratic form in finding minimum for quadratic form. For instant, that why we did not talk about gradients method, when we talk earlier about pure linear system, but this are very important methods first solving non-linear problems. One of the most important, one of the most probably the most simplest gradient based iterative method is the method of steepest decent, which we are going to talk about in some detail.

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Quadratic form

- The Steepest Descent Method can be used to find the minimum of a quadratic form which is a scalar, quadratic function of a n-dimensional vector \mathbf{x} :
$$f(\mathbf{x}) = \frac{1}{2} \mathbf{x}^T \mathbf{A} \mathbf{x} - \mathbf{b}^T \mathbf{x} + c$$
where \mathbf{A} is a matrix, \mathbf{b} a vector and c a scalar constant
- If we plot the function $f(\mathbf{x})$ in n-dimensional space for various values of d_i , where $d_i = f(\mathbf{x})$, we find each value of d_i corresponds to an ellipsoidal curve in n-dimensional space



The steepest descent method can be used to find the minimum of a quadratic form, what is a quadratic form? It is basically just generalization of a simple quadratic equation in one variable. That way you are occurs into 2 a square plus b x equal to c. That is your typical polynomial, quadratic polynomial of order two quadratic general form $A x^2 + b x + c$ quadratic form is just a generalization of that to multi dimensional vectors. Your multi dimensional space, how is that quadratic form instant of $A x^2$.

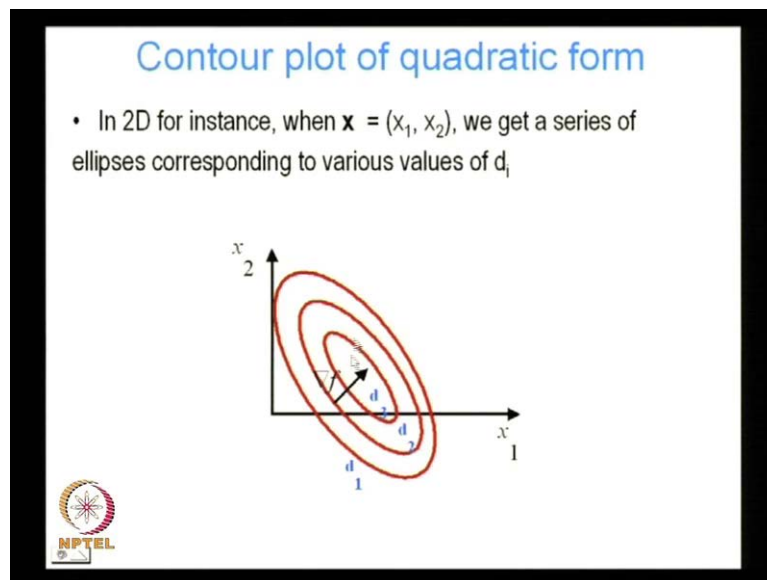
I have this vector \mathbf{x} with all this components one through n $\mathbf{x}^T \mathbf{A} \mathbf{x}$, where \mathbf{A} is the matrix right \mathbf{A} is the matrix \mathbf{A} signs n by n . When \mathbf{A} is the vector of size n $\mathbf{x}^T \mathbf{e} - \mathbf{b}^T \mathbf{x}$ this is the quadratic term. This is my linear term we transpose \mathbf{x} , this is the scalar. So, this is the just generalization of quadratic equation. Suppose, we want to find the minimum of the quadratic form minimum of the quadratic, what is the value of \mathbf{x} which makes f minimum? What is the value of \mathbf{x} , which makes the quadratic form a minimum.

So, that is the typical problem, which is use in order to propose this gradient methods. Later, we will see that gradient base method are not restricted to quadratics form quadratic form are a special class of non-linear equation. There were the probably simplest type of non-linear equation. So, we propose this gradient based method, we discussed their properties in the context of quadratic form. Because, it is easy to understand, but we should always keep in mind that my real problem is problem is never

going to be quadratic form. So, I must I should able to extent extent this methods this gradients base methods to non-linear general non-linear problems, which are not quadratics cubic quadratics anything that should work too.

So, if we plot the function f of x in dimensional space for various now I am concentrating on the quadratic form the simplest non-linear problem. So, we looking at steepest descent method, we are looking at gradients based methods in the context of simplest possible non-linear problem, which is a quadratic form. We say if we plot this quadratic form in and dimensional space for various values of constant d , where d is equal to f of x . Then we find each value of d is correspond to ellipse sidle curve in dimensional space.

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If I plot if I consider this two variables an if I have a quadratic form then I plot this quadratic form. Basically, I plot f of x equal to d_1 f of x equal to d_2 f of x equal to d_3 I plot for this various values of f of x . For each value of f of x my quadratic form is an ellipses. Since, it is 2 D it in ellipse in multi dimensional space ellipse is an in that dimension and dimensional space. It is an dimensional ellipse sides in two dimensional space, it becomes a ellipse. So, 2 D for instant when x is equal to $x_1 x_2$ that is x has got only two components. Ee get c of ellipses corresponding to various values of d_i .

So, each of this ellipse is correspond to particular value of the quadratic along this ellipse f of x is constant. It is equal to d_1 along this ellipse second ellipse and f of x is constant

two and its equal to d 2. Similarly, here f of x is constant equal to d 3 and problem that I am posing is that, how am I going to calculate the value of x which minimize. However, I am going to calculate the value is x 1 and x 2. This the function and f of x is you this, you can think of like this is are ellipses, this are like contours.

So, I am going to try to go to the contour with the smallest value. That is going to minimize my function f of x. So, starting from some location, how I am going to reach the contour with the smallest value, starting at the certain location and I am going to go there.

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The gradient vector

If we evaluate the gradient of the quadratic form, we get :

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f(\mathbf{x})}{\partial x_1} \\ \vdots \\ \frac{\partial f(\mathbf{x})}{\partial x_n} \end{bmatrix} = \frac{1}{2} \mathbf{A}^T \mathbf{x} + \frac{1}{2} \mathbf{A} \mathbf{x} - \mathbf{b}$$

If \mathbf{A} is symmetric, this equation becomes : $\nabla f(\mathbf{x}) = \mathbf{A} \mathbf{x} - \mathbf{b}$

Geometrically, the negative of the gradient is a vector field that for a given location \mathbf{x} in the n-dimensional space, points in the direction of the greatest decrease (steepest descent) in $f(\mathbf{x})$



We will see that one way to get is use the gradients, what is the gradient the gradient of the quadratic, which is just this right gradient of f and x in multi dimension is del of x del f x 1 del f x 2 del f x n 3 n. It is a vector and dimensional vector each component is given by that it just here later calculus. So, if I take since I had f of x like this, if I calculate grade of x. If I calculate grade of x i get half a transpose x plus half A x minus b, I get that right. If a is symmetric, what does a symmetric means. We talking about this many times before it means a is equal to half a plus a transpose. There is no excuse symmetric part. So, a is always going to be always equal to half a plus a transpose.

So, in that case I can bring out x and write this as grade of f x effect is equal to A x minus b. Just I am writing this, I am taking advantage of the symmetry in a geometrically the negative of the gradient is a vector that for a given location x points to the direction

of steepest descent. It points to the directions whether function decreases by the maximum amount. So, at any point lets go back to this picture again. So, I start from here suppose this is my starting point. I calculate my gradient will always point in the direction in which f decreases by the maximum amount. That in this case this point in this direction, because, f is going to decrease `by the maximum amount, if travel in this direction and $x_1 \times x_2$ space.

So, the gradient to the negative of the gradient is point to the direction of steepest descent. It point to directions of steepest descent is a vector field for a given location x in dimensional space points to the direction of the greatest decrease. That means, the steepest descent. So, I am going downhill, it gradient if I going down the hill the gradient is pointing in the direction in which if you go you lose the max I multitude, you lose the maximum height.

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Local Minima

- Hence when $f(\mathbf{x})$ has a minimum, $\nabla f(\mathbf{x}) = 0$. If A is symmetric and positive definite, since $\nabla f(\mathbf{x}) = A\mathbf{x} - \mathbf{b}$ the minimum occurs when \mathbf{x} satisfies $A\mathbf{x} = \mathbf{b}$
- Non linear functions in general possess a large number of local minima. This can be seen by considering a 1D nonlinear function $g(x)$ shown in the figure:

So, the gradient is the direction of steepest descent hence when f of has a minimum greater gradient of f of x must be equal to 0. That well the gradient points in the direction of steepest descent, but when f of x r i chest the minimum is there direction of steepest descent. Anywhere you go the function is going to increase, because that is the minimum. So, the direction of steepest descent has got to be 0 at that point at that minimum direction of stiffness descent as this is the gradient. That means, the gradients

got to be 0 at that point. If A is symmetric and positive definite since gradient of effect is equal to $Ax - b$. So, that means, at the minimum gradient of $f(x)$ must equal to be 0.

So, $Ax - b = 0$, so in order to find the value of x which minimizes the function I have to solve $Ax - b = 0$. The minimum occurs when x satisfied $Ax = b$. After now we are talking about quadratics forms quadratic function quadratic forms and nice well behaved function. We will show later they have, what is known as global minimum.


So, one point, which is the minimum its well behave function with minimum at the point, but in general not linear function do not posses global minimum, they poses local many local minimum. This can be consider by seeing by considering 1 D non-linear function of x right $g(x)$. If I plot that non-linear function $g(x)$ I have a function like this. Suppose, we can see it has got multiple local minimum 1 2 3 4 all of these are tropes. So, these are local minimum.

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Local vs Global Minimum

- Points 1, 2, 3 and 4 are all local minima of $g(x)$ and $\nabla g(x) = 0$ at all these locations
- However, 2 is a global minimum since $|g(x_2)| < |g(x)| \forall x \neq x_2$
- Ordinarily for a n-dimensional nonlinear equation there is no numerical method that will assuredly converge to a global minimum

Convergence to a particular local minimum can be assured so long as the starting point is "close" to that local minimum



So, points 1 2 3 and 4 are all local minimum of $g(x)$ and grad of $g(x)$ is equal to 0 at all this locations. However, two is a global minimum ways two global minimum while you can see two has the lowest value of the function, two has the lowest value of the function. Since, $g(x)$ of 2 is less than or equal to $g(x)$ for all value of x not equal to x_2 , ordinarily for n dimensional non-linear equation. There is no algorithm, which can guarantee that you are going to reach a global minimum. There is no numerical method

that will surely convert to a global minimum convergent, can at most be pressured to a local minimum. So, long as the starting point is close to that local minimum.

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Local vs Global Minimum

- "Close" to the minimum means that the starting point is within the neighborhood where the convergence requirements of the algorithm are satisfied (recall convergence requirements of Newton Raphson for instance)
- The particular local minimum the iteration converges to depends on the initial value of the iterate
- For example if we start from **a** in the figure we will converge to local minimum **1** while if we start from **b** we will converge to **2**

Which is a global minimum

So, what does close means close to the minimum means, that the starting point is within the neighborhood. When the convergent where the convergent requirement of the algorithm satisfied. We call our convergent requirement of the Newton Watson method. He said that in Newton method is assure to converge only within a certain neighborhood of the root and in that neighborhood the function. The derivative of the function had to satisfied special and characteristics fashion special properties. So, we are assure to converge to global minimum only, when we are within that neighborhood within that neighborhood.


The particle local minimum that iteration convergent to depends on the starting values of my iterate. For instance if we start from a in the figure if I start from a. So, this is my starting point and I am going to converge this local minimum local minimum 1. If d is my starting point and I am not going to converge to 1, I am going to converge two. So, the result I get from my solving my system of equations is going to be dependent on my starting. Guess on where I start from, that is why it is very hard to get a global minimum to reach the global minimum for a general non-linear equation, which does not have a which is not a quadratic form. This start means in the figures we will converge local

minimum one, while we start from \mathbf{b} we will converge to $\mathbf{2}$, which return out is the global minimum, but we never know where start from.

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Global Minimum for Quadratic forms

- Non linear functions which are quadratic forms are exceptions to this general rule
- This is because quadratic forms with a positive definite coefficient matrix \mathbf{A} have the property that the minimum \mathbf{x} obtained by solving $\mathbf{Ax} = \mathbf{b}$ is not only a local minimum of the function but also a global minimum



So, non-linear function which are quadratics forms are acceptance to this general root. They will always converge to the global minimum this is because quadratics forms with the positive definite coefficient matrix \mathbf{a} have the property. That minimum \mathbf{x} obtain by solving \mathbf{x} equal to \mathbf{b} is not only a local minimum of the function, but it also a global minimum of the function.

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Global Minimum for Quadratic forms

- To show this let us evaluate $f(\mathbf{x})$ at some arbitrary point \mathbf{p} which is not a minimum of $f(\mathbf{x})$:

$$f(\mathbf{p}) = \frac{1}{2} \mathbf{p}^T \mathbf{A} \mathbf{p} - \mathbf{b}^T \mathbf{p} + c$$

Also let the minimum be given by $\mathbf{x} = \mathbf{A}^{-1} \mathbf{b}$. Denoting $\mathbf{p} = \mathbf{x} + \mathbf{e}$ where \mathbf{e} is an "error" term, we get:

$$f(\mathbf{p}) = \frac{1}{2} (\mathbf{x} + \mathbf{e})^T \mathbf{A} (\mathbf{x} + \mathbf{e}) - \mathbf{b}^T (\mathbf{x} + \mathbf{e}) + c$$

$$= \frac{1}{2} \mathbf{x}^T \mathbf{A} \mathbf{x} + \frac{1}{2} \mathbf{e}^T \mathbf{A} \mathbf{e} + \frac{1}{2} \mathbf{x}^T \mathbf{A} \mathbf{e} + \frac{1}{2} \mathbf{e}^T \mathbf{A} \mathbf{x} - \mathbf{b}^T \mathbf{x} - \mathbf{b}^T \mathbf{e} + c$$


Let show that to show that, let us evaluate effects at some arbitrary point p , which is not minimum f of x . Suppose, evaluate the quadratic form at some location p , which is not at my root. It is not at my minimum at p the quadratic form assume this function value. Let us suppose the minimum is given by x , which x is equal to a inverse b . So, we denote p is equal to x plus e , where e is error term. Because, p is not equal to x is my 2 minimum sides and p is not equal to x , I did not the difference by e vector e .

So, I can write p is equal to x plus e . So, that is true in this equation I can replace p by x plus e . If I do that I get half x plus e transpose A x plus e minus b transpose x plus e plus c , expand this out half transpose x half e transpose A e plus half x transpose A e plus half e transpose A x right plus half e transpose x . That last term minus b transpose minus x b transpose e plus c , but half x transpose A e is equal to half e transpose x , if there is symmetry in A if A is symmetric.

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Global Minimum for Quadratic forms

But $\frac{1}{2}x^T A e = \frac{1}{2}e^T A x$ by symmetry of A

$$\begin{aligned} \therefore f(p) &= \frac{1}{2}x^T A x + \frac{1}{2}e^T A e + \frac{1}{2}x^T A e + \frac{1}{2}e^T A x - b^T x - b^T e + c \\ &= \frac{1}{2}x^T A x - b^T x + c + \frac{1}{2}e^T A e + e^T A x - b^T e \\ &= \frac{1}{2}x^T A x - b^T x + c + \frac{1}{2}e^T A e + e^T b - b^T e \\ &= f(x) + \frac{1}{2}e^T A e \end{aligned}$$

Since A is positive definite, $\frac{1}{2}e^T A e > 0 \forall e \neq 0$

Hence x is a global minimum of f



Then x transpose A e got to be equal to e transpose x . It should be obvious, it is a symmetric metric that does not made. If I post multiply of free multiply with e and x right if I do that. Then I have f p is equal to half x transpose A x plus that half e transpose A e plus half x transpose A e plus half e transpose A x . It was basically just a previous equation we written, that is we convenience, then I can replace. So, half extra transpose A x and then bring minus b transpose x plus c I collect those term. Then I have half e transpose A

e, since these two terms are equal I can replace I can sum them together, replace them with e transpose x.

Then I have this term left which is this term left, which is b transpose e i have this term, which is identical to that. I have this term half e transpose A e transpose x, but I know that x is equal to b. So, I can replace that with e transpose b. Then I have e transpose b minus b transpose e. So, those terms canceled out, it taking dot product of e dotted with b is same taken as the dot product of b dotted with the dot products commutative. So, this two cancel out and a I have left half x transpose a x minus b transpose x plus c, but what is this is my quadratic form in x. This is my f of x and I have this term remaining, which is half e transpose e, but remember we assume that a is a positive definite matrix positive definite matrix. Means that for any e, which is not identically equal to 0 e transpose a got to be greater than 0.

So, this term is always going to be positive. So, dot what is that mean that if p is not equal to x, any p not equal to x is always going to be greater than f of x. Hence, x is a global minimum of x, because this term is not 0 can never be 0. Because, a is positive definite e cannot be equal to 0 p is not equal to x. So, we are assure that a quadratic form a has a global minimum. So, all this descent methods they are going to converge a global minimum.

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Steepest Descent for Quadratic forms


- We can use the steepest descent method to find \mathbf{x} such that it minimizes a quadratic form
- At any step in the iteration we use the direction of steepest descent (the negative gradient direction) in the update formula:

$$\mathbf{x}_{i+1} = \mathbf{x}_i - \alpha \nabla f(\mathbf{x}_i)$$
 where α is the step size

Recall that for a quadratic form:

$$-\nabla f(\mathbf{x}_i) = \mathbf{r}_i = \mathbf{b} - \mathbf{A}\mathbf{x}_i = \mathbf{A}\mathbf{x} - \mathbf{A}\mathbf{x}_i = \mathbf{A}\mathbf{e}_i$$

The step size α is determined by a line search procedure adopted to minimize the value of f along $\nabla f(\mathbf{x}_i)$



So, we can use the steepest decent method to find to x seize, that its minimizes a quadratic form half, how we use this steepest descent method at any step in the iteration. We use the direction of steepest descent in the update formula. So, I say that suppose I am location at a x_i . I gone to any iteration basic ideas x_{i+1} want to go x_{i+1} plus one how am I going to get the that is the whole idea of quadratic method. Still, you have to go from x_i to x_{i+1} . Hopefully, when you go from s_i to s_{i+1} we are not going in the wrong direction. We are converging towards the solution rather than diverging. Suppose, I have x_i I am going to x_{i+1} .

So, I am going to take and I am going to take the part in which is along the steepest descent along the gradient direction at x_i . So, I x_i the steepest descent direction the direction in which the function decreases by maximum pound is given by gradient of f of x_i . So, I am going to take a part I am going to take a step in this direction. The magnitude of the step that I am going to take is given by this scalar α . So, I am going to travel in this direction, I am going to travel in this direction, but the extent I am going to travel is Gaussian by my step α . You can see that the step styles is very important. If I take a very large step suppose my minimum is somewhere here, I am somewhere here.

If I am going in this direction we might take a huge step. I will end upon this reach that I totally cross the minimum, which lies somewhere here. So, land on the opposite rigid you can think as this as a value, this as the richest mountain. So, this are two mountain peaks in dynamics. There is a value in between if I want from go from here to the bottom of the valley, but if I take a very large step. I am going to reach the opposite peak, I am going to reach point in the opposite wage. So, the extent of the step I take is very important. So, the α the value of α is very important, so how to determine α ? So, that is all it boils down to how the determine steps has, because the direction have to move. We know at gradient direction the steepest descent method.

We move along the gradient direction, how much it will move well to determine that recall the for the quadratic form gradient off of x_i is equal to r_i is equal to $b - Ax_i$. We saw that earlier, where we did see that probably did not see the that it should be obvious to view. We did see somewhere that anyways let us not worry about that right now. So, gradient of x_i is equal to $b - Ax_i$, which is equal to by definition the residual $b - Ax_i$ when x_i is equal to x then residual become 0. So, gradient of x_i

equal to 0, that we have seen before equal to $\mathbf{b} - \mathbf{A} \mathbf{x}_i$ and \mathbf{b} is equal to $\mathbf{A} \mathbf{x}$. When I reach my minimum that must be equal to $\mathbf{A} \mathbf{x}$.

So, I have $\mathbf{A} \mathbf{x} - \mathbf{A} \mathbf{x}_i$. That if I write it like this if I represent this as error vector $\mathbf{r}_i = \mathbf{x} - \mathbf{x}_i$ I can write as \mathbf{a}_i of \mathbf{e}_i this step size. So, this is this is just to calculate my gradient the direction in which I have got to move if I take \mathbf{x}_i and \mathbf{a} . I know my error, if I know my error or I know my residual in calculate my gradient or can just, but the amount, which have got to move steps size α is determine by what is known as the line search procedure. What does a line procedure do it tries to minimize the value of the function along that directions. I am at certain points and I have a certain function value.

I am moving along certain direction and I want to travel I want to only move α along the direction to that point, where I minimize the function value along that direction. So, this is the multi dimensions space I am taking line in that multi dimension space. Now, multi dimensional space I only want to move to location along that line, where I get a minimum value for my function along that line.

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Steepest Descent for Quadratic forms

α minimizes f when the directional derivative $\frac{d}{d\alpha} f(\mathbf{x}_{i+1}) = 0$

By the chain rule, $\frac{d}{d\alpha} f(\mathbf{x}_{i+1}) = \nabla f(\mathbf{x}_{i+1})^T \frac{d}{d\alpha} \mathbf{x}_{i+1} = \nabla f(\mathbf{x}_{i+1})^T \mathbf{r}_i$
 where the steepest descent update formula has been used.

Thus α should be chosen so that \mathbf{r}_i and $\nabla f(\mathbf{x}_{i+1})$ are orthogonal
 But $\nabla f(\mathbf{x}_{i+1}) = \mathbf{r}_{i+1}$
 Hence $\mathbf{r}_{i+1}^T \mathbf{r}_i = (\mathbf{b} - \mathbf{A} \mathbf{x}_{i+1})^T \mathbf{r}_i = [\mathbf{b} - \mathbf{A}(\mathbf{x}_i + \alpha \mathbf{r}_i)]^T \mathbf{r}_i = 0$.

Solving for α we get $\alpha = \frac{\mathbf{r}_i^T \mathbf{r}_i}{\mathbf{r}_i^T \mathbf{A} \mathbf{r}_i}$



So, α minimizes f where the directional derivative $\frac{d}{d\alpha} f$ of \mathbf{x}_i plus 1 is equal to 0. So, let us stop here today next class we are going to continue talking about this we are going to talk about directions derivatives. We are going to find out how to do the line search, how to find the value of α . At least we can find of value α in a we can get

a close form solution. So, alpha for quadratic forms non quadratics forms, that is no possible right the otherwise the other algorithm, which can give a proximate solution, but not exact solution for the step size alpha.

So, we will look at that then we look at converging criteria for the steepest descent methods. What are the condition, which will allow the steepest descent method to converge. This is our privately to talking about what is the probably one of the most slightly use gradient based method for solving sparse system. The conjugated gradient method, we going to talk about conjugate start talking about the conjugate gradient method, next class.

Thank you.