

Numerical Optimization
Prof. Shirish K. Shevade
Department of Computer Science and Automation
Indian Institute of Science, Bangalore

Lecture - 15
Trust Region and Quasi-Newton Methods

Hello, welcome back to this series of lectures on numerical optimization. In the last class we started looking at convergence of Newton method, the order two convergence of Newton method. So, let us continue with that proof.

(Refer Slide Time: 00:39)

$|x^{k+1} - x^*| = \frac{1}{2} \frac{|g''(\bar{x}^k)|}{|g'(\bar{x}^k)|} |x^k - x^*|^2$

Suppose there exist α_1 and α_2 such that

$|g''(\bar{x}^k)| < \alpha_1 \forall \bar{x}^k \in LS(x^*, x^k)$ and
 $|g'(\bar{x}^k)| > \alpha_2$ for x^k sufficiently close to x^* ,

then

$|x^{k+1} - x^*| \leq \frac{\alpha_1}{2\alpha_2} |x^k - x^*|^2$ (order two convergence if $x^k \rightarrow x^*$)

Note that

$|x^{k+1} - x^*| \leq \underbrace{\frac{\alpha_1}{2\alpha_2}}_{\text{required to be } < 1} |x^k - x^*|$

So, in the last class we showed that if the distance between x_{k+1} and x^* is equal to half of mod of $\frac{\alpha_1}{2\alpha_2} |x_k - x^*|^2$. And suppose, if you are able to get some α_1 and α_2 which both are positive such that the numerator here is less than α_1 for all \bar{x}^k and then denominator here is greater than α_2 for all x^k , sufficiently close to x^* . Then we can write that mod of $x_{k+1} - x^*$ is less than or equal to $\frac{\alpha_1}{2\alpha_2} |x_k - x^*|^2$. Now, if the sequence x_k converges to x^* , then we can clearly see that this is order two convergence.

Now, let us see how to show that x_k does converge to x^* . Now, if you look at $x_{k+1} - x^*$ mod of $|x_{k+1} - x^*|$ and that is less than or equal to this

quantity. This quantity can be split into two parts: the one part is α_1 by $2\alpha_2$ into mod of x_k minus x^* and the other quantities x_k minus x^* . Now, in order that the distance of x_{k+1} from x^* is less than the distance of x_k from x^* what we want is this quantity to be less than 1.

(Refer Slide Time: 02:14)

If $\frac{\alpha_1}{2\alpha_2} |x^k - x^*| < 1 \forall k$, then

$$|x^{k+1} - x^*| < |x^k - x^*| \forall k$$

How to choose α_1 and α_2 ?

At x^* , $g(x^*) = 0$, and $g'(x^*) > 0$

Since $g' \in C^0$, $\exists \eta > 0 \ni g'(x) > 0 \forall x \in (x^* - \eta, x^* + \eta)$

Let

$$\alpha_1 = \max_{x \in (x^* - \eta, x^* + \eta)} |g''(x)|$$

$$\alpha_2 = \min_{x \in (x^* - \eta, x^* + \eta)} g'(x)$$

Therefore,

$$\left| \frac{1}{2} \frac{g''(x^k)}{g'(x^k)} \right| \leq \frac{\alpha_1}{2\alpha_2} = \beta, \text{ say.}$$

Preferable to choose $x^0 \in (x^* - \eta, x^* + \eta)$

So, in other words if this quantity is less than 1 then we can say that mod of x_k plus minus x^* is less than mod of x_k minus x^* . So, that means that the new point is more close to x^* than the current point x_k and if this happens for every k , then certainly we would converge to x^* . Now, the question is that how do we choose that α_1 and α_2 which we mentioned earlier. Now, at x^* we know that the gradient of the derivative of the function vanishes and then the second order derivative of the function is greater than 0.

So, since we know that f in fact we have chosen f to be thrice differentiable. So, the second derivative of the function f is certainly continuous and therefore, there exists some η which is greater than 0 such that $g''(x)$ is greater than 0 for all x in the open interval $x^* - \eta$ to $x^* + \eta$ that is because of the continuity of g'' and we know that $g''(x^*)$ is greater than 0 so at least in the neighborhood of x^* the g'' has to be greater than 0.

So therefore, if you choose α_1 to be max of mod of $g''(x)$ where x lies in the interval $x^* - \eta$ to $x^* + \eta$ and α_2 to be min of $g'(x)$ where

x is again in the same interval. Then what we have is, we have mod of half into g two dash x bar k by g dash x k less than or equal to α 1 by 2 α 2 for all x bar k in that interval and x k in the same interval.

So, let us call this quantity as β . Therefore, it important for us to choose x naught to be in the interval x star minus η to x star plus η , then we can show that this holds and since, this inequality holds then if x naught is chosen properly then we have this quantity which is less than 1 and then in which the sequence in x k plus one minus x star or the mod of that quantity is less than mod of x k minus x star for all k .

(Refer Slide Time: 04:57)

Also, we want $\beta|x^k - x^*| < 1 \forall k$. That is,

$$|x^k - x^*| < 1/\beta \forall k$$

$$\Rightarrow x^k \in (x^* - 1/\beta, x^* + 1/\beta)$$

Therefore, choose $x^0 \in (x^* - \eta, x^* + \eta) \cap (x^* - 1/\beta, x^* + 1/\beta)$

Does $\{x^k\}$ converge to x^* if x^0 is chosen using this approach?

We have

$$|x^k - x^*| \leq \beta|x^{k-1} - x^*|^2$$

$$\therefore \beta|x^k - x^*| \leq (\beta|x^0 - x^*|)^{2^k}$$

$$\therefore |x^k - x^*| \leq \frac{1}{\beta} \underbrace{(\beta|x^0 - x^*|)^{2^k}}_{< 1}$$

Therefore,

$$\lim_{k \rightarrow \infty} |x^k - x^*| = 0$$

Not a practical approach to choose x^0

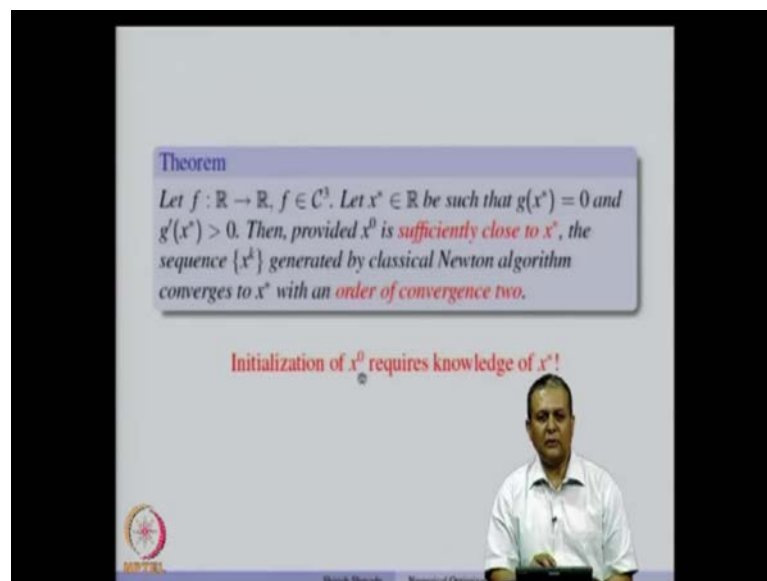
Now, we also want the α 1 by 2 α 2 into x k minus x star to be less than 1 . So, which means that the x k minus x star should be less than 1 over β for all k or in other words x k should belong to the interval x star minus 1 by β to the x star plus 1 by β . Therefore, we have to choose x naught such that, the x naught is in the intersection of x star minus η to x star plus η and x star minus 1 by β to x star plus 1 by β . And now, if we choose x naught like this, the question is that does x k converts to x star or not? Now, let us look at this expression that we had mod of x k minus x star is less than or equal to β into x k x k minus 1 minus x star square.

Now, the same quantity can be written. So, x k minus 1 x star can be written in terms of x k 2 minus x star and so on and so for. So, finally x 1 minus x star can be written as less than or equal to β into x 0 minus x star square. So, if we combine all those expressions

and write $x_k - x^*$ in terms of $x_0 - x^*$, then this is what we will get. So, we are multiplied throughout by β and we get this quantity.

Now, this $x_k - x^*$ square is less than or equal to $1/\beta$ into this quantity and this quantity since, we have seen that $\beta(x_k - x^*)$ is less than 1 for all k . So, we also know that $\beta(x_0 - x^*)$ is also less than 1. So, this quantity is less than 1. Therefore, $x_k - x^*$ is less than or equal to $1/\beta$ into very small quantity as k increases and that quantity will go to 0 as k increases. Therefore, limiters k tends to infinity $x_k - x^*$ becomes 0. But, you will notice that this is not a practical approach to choose x_0 . For example, to choose x_0 we need the knowledge of x^* . But, nevertheless this proof shows that if we start Newton method from some point x_0 which is sufficiently close to x^* , then it converges to x^* with order of convergence 2.

(Refer Slide Time: 07:54)



So, we have a theorem let f be a real valued function and in thrice continuously differentiable. The thrice continues differentiability is needed because we wanted the derivative to be Lipschitz continuous. So, that is why we need this and let x^* belong to \mathbb{R} be such that $g(x^*) = 0$, the gradient vanishes and then the second derivative is greater than 0 then provided x_0 is sufficiently close to x^* , a sequence generated by classical Newton algorithm that converges to x^* with order of convergence 2.

So, this result can be extended to a general case where you have a function f from \mathbb{R}^n into \mathbb{R} . But, the important part is that the Newton method when it starts with the point which is sufficiently close to x^* , it does converge to x^* with order of convergence two. But, the problem is that the initialization of x_0 requires the knowledge of x^* and our aim is to minimize $f(x)$ to get x^* . So, this knowledge of x^* is not there. And therefore, we cannot initialize x_0 properly so that, we can get global convergence of Newton method. In other words, the Newton method does depend a lot on x_0 a classical Newton method does depend a lot on x_0 and as this theorem says the x_0 requires knowledge of x^* which is not available. But, however the important fact is that if you start sufficiently close to x^* we do get order two convergence. Now, let us look at some modifications of Newton method which are globally convergent. So, in other words they do not require the knowledge of x^* to get the initial point x_0 . One can start from any point and converge to the local minimum.

(Refer Slide Time: 10:27)

Modified Newton Method

Modifications:

- Given x^k and $d_N^k = -(H^k)^{-1}g^k$,
Fix some constant $\delta > 0$.
Find the smallest $\zeta_k \geq 0$ such that the smallest eigenvalue of the matrix $(H^k + \zeta_k I)$ is greater than δ .
Therefore, $d^k = -(H^k + \zeta_k I)^{-1}g^k$ is a descent direction.
- Given x^k and $d^k = -(H^k + \zeta_k I)^{-1}g^k$, use line search techniques to determine α^k and x^{k+1}

$$x^{k+1} = x^k + \alpha^k d^k$$

So, those methods are called modified Newton methods. So, we will see couple of those methods in this course and let us look at the places where modifications for the Newton method are required. Now, given x^k and direction Newton direction at the point x^k which is nothing but negative of the hessian inverse into g^k . Now, there are two possibilities, one is that the hessian matrix is not invertible or is close to singular. So in that case this direction really does not make much sense. Secondly, the hessian matrix is suppose negative definite so in that case this direction is not a descent direction. So, if

either hessian matrix is negative definite or hessian matrix is close to singular. Now, how do we modify Newton method so that this expression is positive? The quantity in the parentheses is a positive definite matrix. Now, suppose if you fix some constant δ which is greater than 0 and find the smallest ζ_k which is greater than equal to 0 such that the smallest Eigen value of the matrix $H_k + \zeta_k I$ is greater than δ .

Now, by ensuring that the smallest Eigen value of this matrix is greater than δ which is a positive constant, we are ensuring that $H_k + \zeta_k I$ is a certainly a positive definite matrix. So, once we find the ζ_k for a given H_k then we can choose a direction to be minus of the new direction can be chosen as minus of $(H_k + \zeta_k I)^{-1} g_k$ and that is going to be a descent direction because $H_k + \zeta_k I$ is a positive definite matrix. So, this is one modification that one can use.

Now, secondly if you recall that the classical Newton method does not use line search or in other words, it uses α_k to be 1. Now, instead of that we can if you are given x_k and d_k which is nothing but minus $(H_k + \zeta_k I)^{-1} g_k$ what we can do is that we can use line search techniques to determine α_k and then x_{k+1} is determine as x_{k+1} is equal to $x_k + \alpha_k d_k$.

So, the two problems which are associated with classical Newton algorithm one was that the hessian is the hessian matrix at x_k is not necessarily positive definite so that, problem is taken care of by ensuring that we add some $\zeta_k I$ matrix or a constant times identity matrix to H_k . So, that the smallest Eigen value of this matrix is greater than δ where δ is positive constant. So, once you ensure that and chose this direction as our new direction for search then we certainly get a descent direction. Now, after having obtain a descent direction the next step is to get α_k using line search and update x_k to get x_{k+1} .

Now, if we ensure that this line search techniques satisfy Armijo-Goldstein or in Armijo-Wolfe condition. Then we have all the necessary criteria for global convergence of an optimization algorithm that every time the direction chosen is a descent direction. The function value decreases and there is sufficient decrease in the objective function then certainly the method is going to converge. Now, the question is that how do we get this ζ_k ? Sometimes, very simple techniques are used. Suppose we start with some reasonable value of ζ_k and do the Cholesky factorization of $H_k + \zeta_k I$.

Now, if that Cholesky factorization fails because $H_k + \zeta_k I$ is not positive definite, what one can do is that increase ζ_k or may be double the value of ζ_k and try the Cholesky factorization again. So, while the Cholesky factorization of $H_k + \zeta_k I$ is not successful, keep increasing the value of ζ_k till that becomes successful. Now, remember that this ζ_k has a very important role to play here. Now, if ζ_k is very large quantity. Then that dominates this expression $H_k + \zeta_k I$ and the method behaves like a steepest descent method. So, the order two convergence of Newton method is lost. But, if ζ_k is small then H_k will be a dominant thing.

So, typically when the quadratic approximation of the function is good, the ζ_k value will be typically small and the most dominant term here between the two is H_k and therefore, this direction will be close to the Newton direction and if ζ_k is very large then the direction becomes close to steepest descent direction. So, whenever the approximation of the quadratic approximation of a given function is good, you will see that ζ_k becomes a small quantity and therefore, we have the direction which is close to Newton direction and the convergence will be very fast and that typically happens near the solution. So, initially wherever the initial point x_0 this method because of this the extra addition of this extra term to the hessian matrix. Make sure that the steps are taken in appropriate way so that, the convergence is achieved. So, one can show that this method is globally convergent.

(Refer Slide Time: 17:29)

Modified Newton Algorithm

- (1) Initialize x^0 , ϵ and δ , set $k := 0$.
- (2) **while** $\|g^k\| > \epsilon$
 - (a) Find the smallest $\zeta_k \geq 0$ such that the smallest eigenvalue of $H^k + \zeta_k I$ is greater than δ
 - (b) Set $d^k = -(H^k + \zeta_k I)^{-1} g^k$
 - (c) Find $\alpha^k (> 0)$ along d^k such that
 - (i) $f(x^k + \alpha^k d^k) < f(x^k)$
 - (ii) α^k satisfies Armijo-Wolfe (or Armijo-Goldstein) conditions
 - (d) $x^{k+1} = x^k + \alpha^k d^k$
 - (e) $k := k + 1$

endwhile

Output : $x^k = x^k$, a stationary point of $f(x)$.

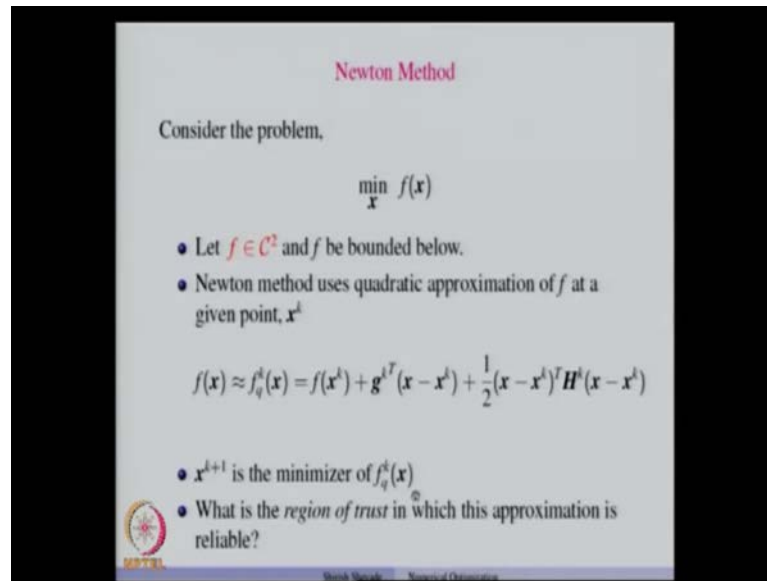
- Modified Newton algorithm has global convergence properties and has order of convergence equal to two

Now, let us look at the algorithm. So, as I mentioned that apart from the initialization of x_{naught} and ϵ what we need is parameter δ and that parameter δ is typically given by the domain expert or it requires the domain knowledge to set that parameter, the iteration counter is set to 0. So, while the norm of the gradient is at the current point x_k is greater than ϵ , you find the smallest ζ_k such that the smallest Eigen value of x_k plus ζ_k is greater than δ . Now, once we do that then the direction that it chosen is $-\zeta_k^{-1} g_k$ and this direction is certainly in descent direction because H_k plus ζ_k is a positive definite matrix. Then we use the line search so that, the function value decreases along the direction d_k and α_k satisfies the Armijo-Wolfe or Armijo-Goldstein conditions.

So, compare now this with the classical Newton algorithm that we have seen. So, this step was not there in the classical Newton algorithm. Here, in the classical Newton algorithm use d_k is equal to $-H_k^{-1} g_k$, then this the step length determination procedure was not there in the classical Newton algorithm because we chose α_k to be 1 in the classical Newton algorithm and the rest of the steps are similar to the ones that we had earlier that x_{k+1} is nothing but x_k plus $\alpha_k d_k$ and then k is equal to $k+1$ that is the iteration counter is increased and the whole procedure is repeated till norm of the gradient current point x_k is less than or equal to ϵ and then we stop and we get a stationery point x_k . So, we will not prove result related to this modified Newton algorithm. But, this modified Newton algorithm it does have global convergence properties and has order of convergence equal to 2.

So, the important thing that one should keep in mind is that the initial point x_{naught} , there are no restrictions on initial point x_{naught} . So, unlike classical Newton algorithm where, which is very sensitive to x_{naught} . This modified Newton algorithm is not sensitive to x_{naught} . Now, we will look at some other modification of Newton method also.

(Refer Slide Time: 20:25)



Newton Method

Consider the problem,

$$\min_x f(x)$$

- Let $f \in \mathcal{C}^2$ and f be bounded below.
- Newton method uses quadratic approximation of f at a given point, x^k

$$f(x) \approx f_q^k(x) = f(x^k) + g^{kT}(x - x^k) + \frac{1}{2}(x - x^k)^T H^k (x - x^k)$$

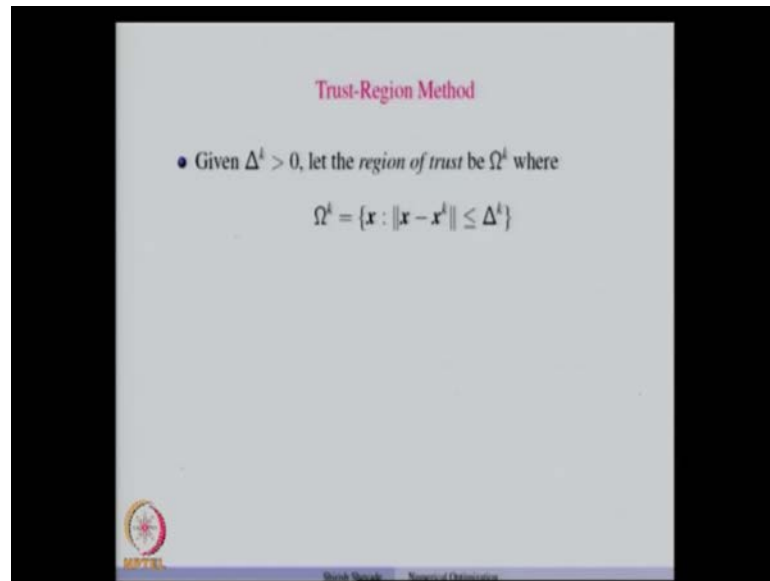
- x^{k+1} is the minimizer of $f_q^k(x)$
- What is the *region of trust* in which this approximation is reliable?

© 2013 MIT. All rights reserved. Newton Optimization

Let us recall that we are trying to minimize this problem. Minimize f of x and in Newton method, we consider f to be twice continuously differentiable and bounded below. So, we continue to use this assumption that f is bounded below. Now, the Newton method you just quadratic approximation of a given function f at a given point and x^{k+1} is the minimizer of this quadratic approximation. So, the quadratic approximation uses the first order derivative and second order derivative information and so, this quadratic approximation is used at a current point x^k and x^{k+1} is found as the minimizer of this quantity. Now, the question that one would like to ask is that how good is this quadratic approximation at a given point?

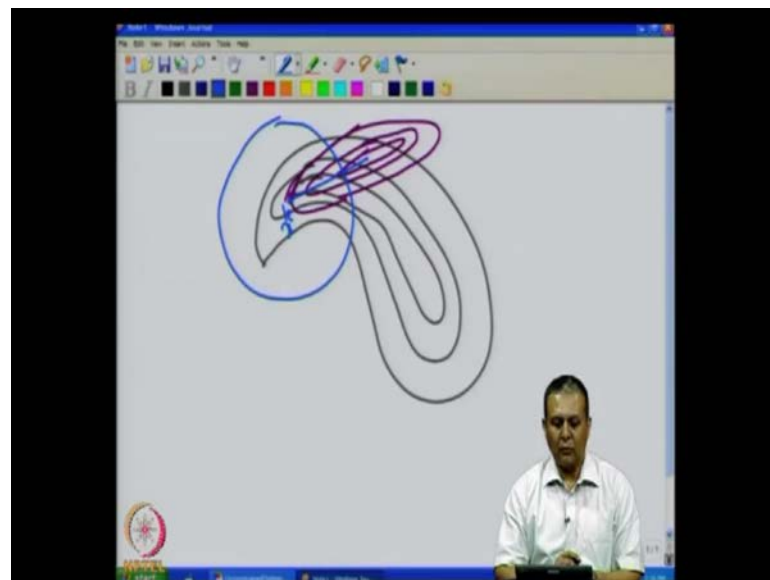
Here, in other words what is the region of trust in which this approximation is reliable. Now, if the quadratic approximation is reliable, then we certainly would like to minimize this quantity and go to the next step x^{k+1} . But, if the region of trust is not reliable or the quadratic approximation is not reliable in the region then we would like to reduce the region of trust or reduce a region in which we can approximate f by a quadratic function. So, such methods which use the region of trust of the quadratic approximation are called trust region methods.

(Refer Slide Time: 22:31)



Now, suppose Δ^k is a positive quantity which is given to us then one can define the region of trust to be Ω^k and Ω^k is defined as set of all points around x^k which are at a distance at the most Δ^k from x^k . So, this norm is typically a Euclidean norm.

(Refer Slide Time: 23:16)



Now, let us look at an example suppose that we have the function contours like this. And suppose this is our current point and suppose the quadratic approximation of the function like this. Now, if one wants to go to the minimum we simply take a step like this and that may not reduce the objective function or you (()) it reduces, if we do the line search the

reduction in the objective function will be typically small. So, instead what one can do is that in such cases remember that the minimum like somewhere in this direction. So, in such cases what one can do is that, one can construct a region of trust around x_k . So, this is x_k we can construct a region of trust around x_k and then minimize the quadratic approximation that we have got in this region of trust and then go to the new point.

Now, if it so happens that the region of trust is good then if we go to the new point and if we find that the approximation is really good, then we can expand this region of trust. On the other hand, if we realize that when we move from x_k to x_{k+1} that function value has actually increased which we do not want, then one can shrink the region of trust.

So, depending upon how good is the above quadratic approximation of the function at a given point, we can decide whether to expand this region of trust or reduce this region of trust. So, by adopting the size of this region of trust one can move to a new point and that will ensure that we are not going in a direction which is away from the local minimum. So, let us see how to do that.

(Refer Slide Time: 25:58)

Trust-Region Method

- Given $\Delta^k > 0$, let the *region of trust* be Ω^k where

$$\Omega^k = \{x : \|x - x^k\| \leq \Delta^k\}$$
- Solve the following constrained problem to get x^{k+1} :

$$\begin{aligned} \min & f_q^k(x) \\ \text{s.t.} & x \in \Omega^k \end{aligned}$$
- How to determine Ω^{k+1} (or Δ^{k+1})? Can use the *actual* and *predicted* reduction in f

So, Ω_k is the region of trust that we have define based on the value of Δ_k . Now, instead of directly minimizing the quadratic approximation of the function which is $f_q(x)$, what we do is that we minimize the quadratic approximation subject to the constrained that x belongs to Ω_k .

Now, remember that this $f_q(x)$ is a quadratic approximation. So, the subscript q stands for the quadratic approximation and k star stands for the k -th iteration so that means that the quadratic approximation is defined at the point x_k and or it is defined around point x_k .

So, this is a slight change in notation here that, I have now used this quadratic. This constraint approximation problem is easy to solve. But, now the question is that once we find x_{k+1} which is solution of this problem, then how do we determine the new region of trust which is ω_{k+1} or how do you determine Δ_{k+1} because once you determine Δ_{k+1} that can easily determine what is ω_{k+1} .

So, in other words what we are interested in is finding out that how this Δ_{k+1} is obtained? If we have knowledge of x_{k+1} which is a constrained minimizer of this optimization problem now, one can use the ratio of the actual reduction in f to the predicted reduction in f to find out Δ_{k+1} . And we will see how to do that.

(Refer Slide Time: 27:50)

Trust-Region Method

Algorithm to determine Δ^{k+1} and R^k

- (1) Given Δ^k, x^k, x_{k+1}
- (2) $R^k = \frac{f(x^k) - f(x_{k+1})}{f'_q(x^k) - f'_q(x_{k+1})}$
- (3) if $R^k < 0.25$
 $\Delta^{k+1} = \|x_{k+1} - x^k\|/4$
 else if $R^k > 0.75$ and $\|x_{k+1} - x^k\| = \Delta^k$
 $\Delta^{k+1} = 2\Delta^k$
 else
 $\Delta^{k+1} = \Delta^k$
 endif

Output : Δ^{k+1}, R^k

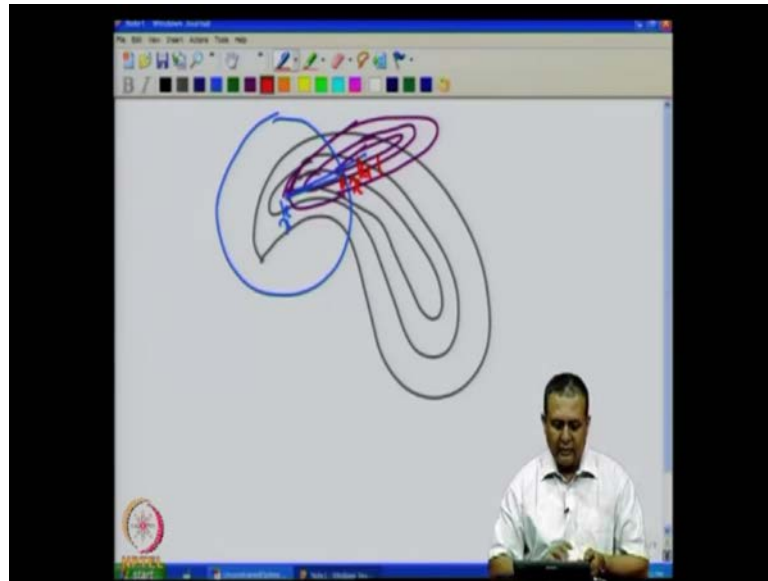
Now, here is simple algorithm to determine Δ_{k+1} and this R_k we will define it now, so given that Δ_k, x_k and x_{k+1} . So, we initially start with x_k and then solve this optimization problem to get x_{k+1} and that optimization problem used Δ_k . So, given the knowledge of x_k, Δ_k and x_{k+1} . How do we determine Δ_{k+1} that is the question that we would like to ask.

So, let us define the ratio R_k to be the function value at x_k minus function value at x_{k+1} divided by $f_q(x_k) - f_q(x_{k+1})$. So, $f_q(x_k)$ is the quadratic approximation of the function at a given x_k and $f_q(x_{k+1})$ is the function that quadratic approximation value at the point x_{k+1} . So, this the numerator denotes the actual decrease in the objective function and denominator denotes the predicted decrease in the objective function. Now, if the quadratic approximation is good, then this ratio is close to 1.

And if, the quadratic approximation at a current point x_k is bad, this ratio will be close to 0 and there could be situations where there could be a increase in the function value at x_{k+1} , so that means that this ratio could be negative. So, there are different possibilities for R_k . Now, if R_k is less than 0.25 such these numbers which are mentioned here. The algorithm is not so much sensitive to this numbers so, one can change appropriately.

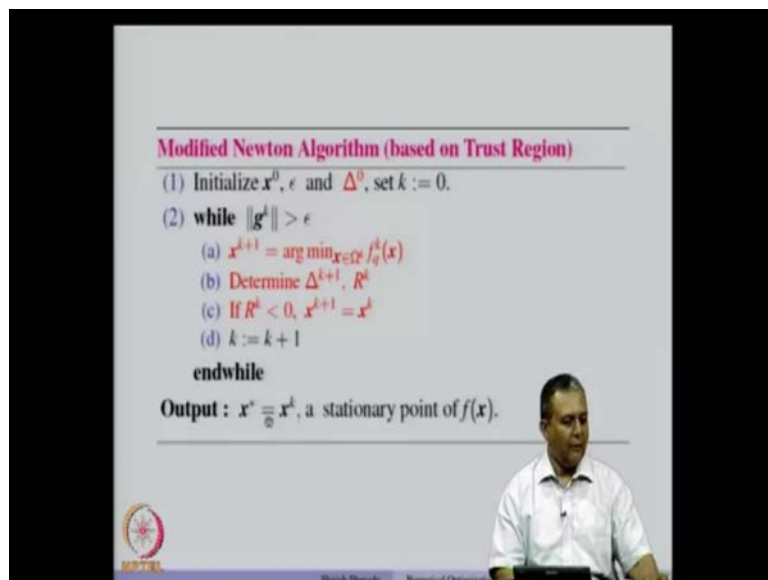
So, if the ratio is small which means that the actual decrease, by the predicted decreases is very close to or less than 0.25, then which means that the quadratic approximation is not good enough. Now, if the quadratic approximation is not good enough that means that we have to shrink the region of trust and that is done by typically setting Δ_{k+1} to be the distance between the $x_{k+1} - x_k$ by 4. So, all the numbers mentioned here are typical numbers and if one wants, one can change it based on the application. So, the Δ_{k+1} reduces and hence the region of trust also reduces for the next iteration. That is, because the current approximation is not good enough. On the other hand, if the current approximation is good and the step taken is equal to Δ_k . So, if you look at this figure.

(Refer Slide Time: 31:24)



So, if starting from x^k if we go to a point x^{k+1} and x^{k+1} lies on the boundary so, that means that the distance between x^{k+1} and x^k is nothing but Δ^k . So, in such a case what one can do is increase the region of trust to $2\Delta^k$. So, whatever was the previous region of trust or previous Δ^k that is multiplied by 2 and if none of these two things happen then you return Δ^{k+1} to be Δ^k and the algorithm returns Δ^{k+1} and r^k r^k is this ratio and Δ^{k+1} is the new Δ value for the new region of trust.

(Refer Slide Time: 32:25)

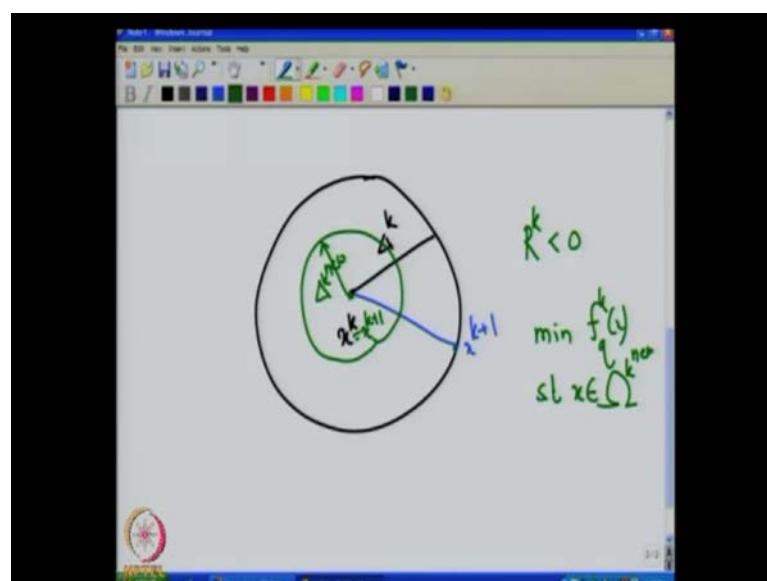


Now, how does the modified Newton algorithm which is based on trust region method look like. So, as usual we initialize x_0 and epsilon and also initialize Δ_0 . So, this is a parameter of that, we will need and the iteration count is set to 0. Now, while the norm of the gradient is greater than epsilon you find x_{k+1} to be $\arg \min_{x \in \omega_k} \| \nabla f(x) \|^2$.

So, we minimize this quadratic approximation of f at x_k subject to the constraint that x belongs to the set ω_k . Now, we have x_k , x_{k+1} and Δ_k . Now, we are in a position to use our previous algorithm to determine Δ_{k+1} so that Δ_{k+1} and R_k are determined using the previous algorithm. Now, if we realize that R_k is less than 0 that means actually there is an increase in the function value from x_k to x_{k+1} then what we do is that x_{k+1} is set equal to x_k . So, that means that the new point is same as the current point. So, we do not move to the new point. So, the change which was made here that will be undone by this statement x_{k+1} is equal to x_k . And remember that if R_k is less than point twenty five, we had shrunk the region of trust.

So, that anyway will hold here and therefore, will be seen the initial region of trust was not good. We again use thus, reduce the region of trust if R_k is less than 0 and see how to move from x_k to the new point and then the rest of the procedure is at k equal to $k+1$ the iteration counter is increased and the process is repeated till norm of g_k is less than or equal to epsilon and as output what we get is stationary point.

(Refer Slide Time: 34:57)

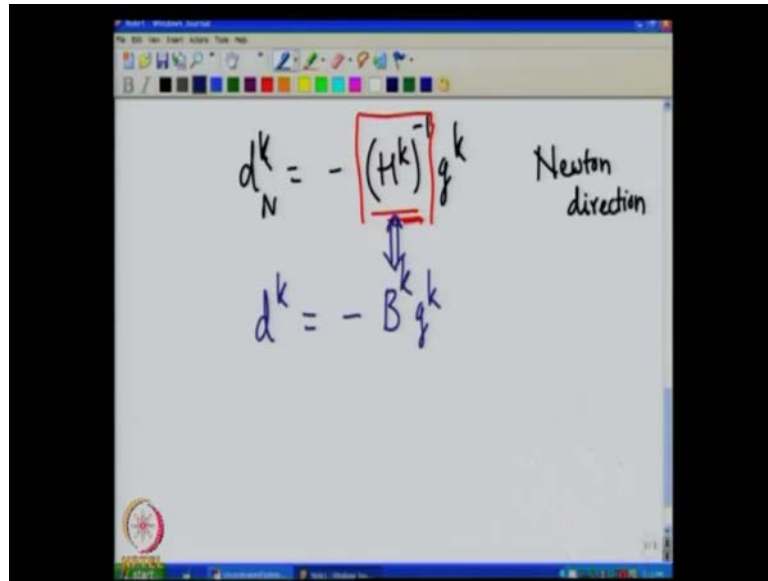


So, in other words if this is our x_k , and this is the region of trust that we have and the corresponding radius is Δ_k . Now, at this suppose the algorithm takes a step to be new point x_{k+1} and if at this point, we realize that the function value has increased so, that means that this region of trust was really not good. So, we reduce the region of trust to a new boundary. So, this is the case where R_k is less than 0.

So, the new region of trust is defined and then we against so, x_{k+1} is same as x_k plus Δ_{k+1} . So, instead of taking this step where the function value actually increased what we do is we come back to x_k reduce the region of trust and then this is our new point x_{k+1} and then we try to solve the problem minimize $f(x)$ subject to x belongs to Ω_{k+1} . So, let me call this as Δ_{k+1} and so the corresponding ω_{k+1} . So, that way we make sure that the function value does decrease at the end of every iteration. So, this method is called trust region method.

So, both these methods, the earlier method that we saw and this method they still use the Newton method ideas. But, the way the steps are taken is not like classical Newton method. So, in the previous method that we saw it was make sure that the hessian matrix are the direction, that the direction d_k that we get is a descent direction which is unlike Newton method. Where the direction is always is in the classical Newton method the direction always minus $H_k^{-1} g_k$ and which need not be a decent direction. The second approach that we saw here, the trust region based approach that makes sure that the maximum step is taken the approximation is good otherwise or in the region of trust is large, otherwise the region of trust is shrunk so that, we do not reverse it. Now, let us look at some modifications of Newton methods.

(Refer Slide Time: 38:55)


$$d_N^k = - (H^k)^{-1} g^k \quad \text{Newton direction}$$
$$d^k = - B^k g^k$$

Now, remember that in the Newton method we have the direction d^k to be minus H^k inverse g^k and this requires. So, this is Newton direction now, this requires the hessian matrix and its inverse now that is many a times computationally expensive operation, especially when the size of H^k is very large. So, a set of methods were suggested and what they do is that they approximate this hessian inverse by a matrix and then choose a direction d^k to be minus $B^k g^k$.

Now, if B^k is a positive definite matrix then we know that this is a descent direction. The direction d^k is the descent direction. Now, how good is this approximation that is the question that we would like to answer. So, in some cases it turns out that especially for quadratic functions. If this B^k matrix is obtained in such a careful way, then this B^k after certain number of iterations approximates the inverse of the hessian. That is, the typical of a quadratic function but may not least hold. But, nevertheless this approximation of Newton method or modification of Newton method is very popular because if you look at this operation. This does not require inversion of a matrix.

So, computational effort required by this method to find the direction is much less or is much less compared to the computational effort required by the Newton direction. Typically, if we want to invert n by n matrix the complexity of the operations order n^3 and that is avoided in this case, because to get the new direction d^k . We just need matrix vector multiplication and that needs order n^2 effort so the computational effort is

saved in this method. So, such methods are called quasi-Newton methods and let us now study some of those methods.

(Refer Slide Time: 42:02)

Quasi-Newton Methods

Consider the problem,

$$\min_{\mathbf{x}} f(\mathbf{x}),$$

where $f: \mathbb{R}^n \rightarrow \mathbb{R}$, $f \in C^1$.

- Let $f \in C^2$.
- Newton method:

$$f(\mathbf{x}) \approx f_q^k(\mathbf{x}) = f(\mathbf{x}^k) + \mathbf{g}^{kT}(\mathbf{x} - \mathbf{x}^k) + \frac{1}{2}(\mathbf{x} - \mathbf{x}^k)^T \mathbf{H}^k (\mathbf{x} - \mathbf{x}^k)$$
- Newton direction: $\mathbf{d}_N^k = -(\mathbf{H}^k)^{-1} \mathbf{g}^k$
- Given $f \in C^1$, form a quadratic model of f at \mathbf{x}^k :

$$y_k(\mathbf{x}) = f(\mathbf{x}^k) + \mathbf{g}^{kT}(\mathbf{x} - \mathbf{x}^k) + \frac{1}{2}(\mathbf{x} - \mathbf{x}^k)^T \mathbf{B}^{k-1} (\mathbf{x} - \mathbf{x}^k)$$

where \mathbf{B}^k is a symmetric positive definite matrix.

- Quasi-Newton direction: $\mathbf{d}_{QN}^k = -\mathbf{B}^k \mathbf{g}^k$

Now, consider the problem to minimize f of x , where f is function from \mathbb{R}^n to \mathbb{R} and more importantly f is a continuously differentiable function. Now, if we use Newton method we have to assume that f belongs to C^2 . And then as we saw earlier, that Newton method depends on quadratic approximation of the function at a given point x^k . So, this is the quadratic approximation which requires the first derivative and the second derivative information and the Newton direction chosen is $-\mathbf{H}^k \mathbf{g}^k$.

But, now suppose we want to work in this setup where you want to minimize $f(x)$, where f is a continuously differentiable function that means we do not want to use the second order information for this purpose now, given f which is a continuously differentiable. Suppose we form quadratic model of f at x and let us denote it by y_k . So, $y_k(x)$. So, this y_k stands for the quadratic approximation of f at x^k . So, using Taylor series, if you write f of x^k plus $\mathbf{g}^{kT}(\mathbf{x} - \mathbf{x}^k)$ plus half $(\mathbf{x} - \mathbf{x}^k)^T \mathbf{H}^k (\mathbf{x} - \mathbf{x}^k)$ now, instead of the hessian matrix because the functions are only continuously differentiable. So, the second order information is not available. So, we write some matrix \mathbf{B}^k inverse into $(\mathbf{x} - \mathbf{x}^k)^T \mathbf{B}^k (\mathbf{x} - \mathbf{x}^k)$, where \mathbf{B}^k is a symmetric and positive definite matrix.

So, make sure that this matrix \mathbf{B}^k whatever we have is a symmetric matrix. This is like hessian matrix which is also symmetric and also positive definite. Now, the hessian matrix

is not always positive definite that is what you saw earlier, when we studied Newton method and in fact, that is one of the drawbacks of Newton method that every time the hessian matrix is not positive definite. So, if we make sure this matrix B_k is positive definite then one can chose a direction d_k to be minus $B_k^{-1} g_k$ and that direction is called a quasi-Newton direction. Now, let us see how to use this quasi-Newton direction in our approach.

(Refer Slide Time: 44:38)

Quasi-Newton Methods

$$y_k(x) = f(x^k) + g^{kT}(x - x^k) + \frac{1}{2}(x - x^k)^T B^{k-1}(x - x^k)$$

- $(B^k)^{-1}$ is either H^k or its approximation
- $x^{k+1} = x^k + \alpha^k d_{QN}^k = x^k - \alpha^k B^k g^k$
- Given $x^k, x^{k+1}, g^k, g^{k+1}$ and B^k , how to update B^k to get a symmetric positive definite matrix B^{k+1} ?
- Is $B^k \approx (H^k)^{-1}$?
- Are there any conditions that B^{k+1} should satisfy?

So, the quasi-Newton methods use the quadratic model of f around x_k using the matrix B_k inverse rather than the matrix h_k . Now, as I said earlier that this B_k inverse is either h_k ideally, you would like it to be h_k or its approximation. So, the question is that if we use the direction d_k to be minus $B_k^{-1} g_k$ which is quasi-Newton direction and get x_{k+1} to be $x_k + \alpha_k d_k$ which is nothing but $x_k - \alpha_k B_k^{-1} g_k$. So, how good is the approximation of B_k^{-1} with respect to h_k ? And the second question is that once we move to the point x_{k+1} , how do we get B_{k+1} ? How to update B_k using the information $x_k, x_{k+1}, g_k, g_{k+1}$ and B_k to get a symmetric positive definite matrix B_{k+1} ? So, this is an important question that we would like to answer and whenever, we update B_k to be B_{k+1} . How good is that approximation to corresponding h_{k+1} inverse and when we do this update or there any conditions that B_{k+1} should satisfy.

(Refer Slide Time: 46:32)

Given x^{k+1} , we construct a quadratic approximation of f at x^{k+1} :

$$y_{k+1}(x) = f(x^{k+1}) + g^{k+1T}(x - x^{k+1}) + \frac{1}{2}(x - x^{k+1})^T (B^{k+1})^{-1} (x - x^{k+1})$$

Require

$$\begin{aligned} \nabla y_{k+1}(x^k) &= \nabla f(x^k) \\ \nabla y_{k+1}(x^{k+1}) &= \nabla f(x^{k+1}) = g^{k+1} \end{aligned}$$

Therefore, we require,

$$\nabla y_{k+1}(x^k) = \nabla f(x^k) = g^k = g^{k+1} + (B^{k+1})^{-1} (x^k - x^{k+1})$$

Letting $g^{k+1} - g^k = \gamma^k$ and $x^{k+1} - x^k = \delta^k$, we get

$$B^{k+1} \gamma^k = \delta^k \quad (\text{Quasi-Newton condition})$$

So, these are some of the questions that we would like to answer. So, let us take a given point x_{k+1} and construct the quadratic approximation of f at x_{k+1} and that quadratic approximation will be denoted by y_{k+1} . So, this $k+1$ stands for file that quadratic approximation is obtained around x_{k+1} . So, this function would look like $f(x_{k+1}) + g_{k+1}^T(x - x_{k+1}) + \frac{1}{2}(x - x_{k+1})^T B_{k+1}^{-1}(x - x_{k+1})$.

Now, how good is this quadratic approximation? Now, for this quadratic approximation to be good, what we want is that the gradient of this information at x_{k+1} should be the gradient of f at x_{k+1} . And gradient of this function at x_k should be equal to the gradient of the function at x_k . So, at the 2 consecutive points x_k and x_{k+1} the gradients of the actual function f and the gradient of the function y , they should match with each other. So, in other words what we want is that gradient of y_{k+1} , gradient of y_{k+1} is evaluated at x_k should be equal to gradient of x_k and gradient y_{k+1} evaluated at x_{k+1} should be equal to gradient of f of x_{k+1} .

Now, you will see that the gradient of y_{k+1} is nothing but g_{k+1} which is the gradient of y_{k+1} evaluated at x_{k+1} is g_{k+1} which is same as that of f at x_{k+1} . So, this equation is all satisfied. Now what about the first equation? We want that equation also to hold or in other words, gradient of function f at x_k should be same as the gradient of y_{k+1} at x_k and so, we know that gradient of f at x_k is nothing but g_k .

\mathbf{g}^k and the this \mathbf{g}^k should be equal to the gradient of y^k plus 1. Evaluate at \mathbf{x}^k . Now, if we evaluate gradient of this function at \mathbf{x}^k , what we get is \mathbf{g}^k plus 1 transpose into plus \mathbf{B}^k plus inverse into \mathbf{x}^k minus \mathbf{x}^k plus 1.

So, we want \mathbf{B}^k plus 1 or we want this quadratic approximation to be such that, this condition is satisfied or in other words, \mathbf{B}^k plus 1 should be such that \mathbf{B}^k plus 1 equal to \mathbf{B}^k plus one γ^k is equal to γ^k , the way this is obtain is using this expression. So since, \mathbf{B}^k plus 1 is, we want is a invertible matrix. So, we can write \mathbf{g}^k plus 1 minus \mathbf{g}^k to be γ^k and \mathbf{x}^k plus 1 minus \mathbf{x}^k to be δ^k and write this quantity as \mathbf{B}^k plus 1 γ^k equal to δ^k . So, this we want \mathbf{B}^k plus 1 to satisfy this condition and this condition is called quasi-Newton condition.

(Refer Slide Time: 50:21)

• Quasi-Newton condition

$$\mathbf{B}^{k+1} \gamma^k = \delta^k$$

• \mathbf{B}^{k+1} should be positive definite

$$\gamma^{kT} \mathbf{B}^{k+1} \gamma^k = \gamma^{kT} \delta^k > 0 \quad \forall \gamma^k \neq 0$$

• From Wolfe conditions for line search,

$$\mathbf{g}^{k+1T} \mathbf{d}^k \geq c_2 \mathbf{g}^{kT} \mathbf{d}^k, \quad c_2 \in (0, 1) \Rightarrow \gamma^{kT} \delta^k > 0$$

\therefore When Wolfe condition is satisfied in a line search,
 $\exists \mathbf{B}^{k+1}$ which satisfies Quasi-Newton condition

• $\frac{n(n+1)}{2}$ variables to be found using n equations and n inequalities

Now, let us look at this quasi-Newton condition \mathbf{B}^k plus 1 γ^k equal to δ^k . Now, certainly \mathbf{B}^k plus 1, we want it to be positive definite. Now, γ^k transpose \mathbf{B}^k plus 1 γ^k is nothing. But, γ^k transpose δ^k and that is greater than 0 for all γ^k not equal to 0. If we use Wolfe conditions for line search or in other words, suppose if we take Wolfe conditions for line search. So, what we get is \mathbf{g}^k plus 1 transpose \mathbf{d}^k is greater than or equal to $c_2 \mathbf{g}^k$ transpose \mathbf{d}^k lets c_2 is a positive fraction, in such c_2 should be in the intervals c_1 to 1 but here i have intentionally mentioned to be 0 to 1. Just to indicate that it is a positive fraction and so, if you take the right hand side to the left side so that we get is \mathbf{g}^k plus 1 minus $c_2 \mathbf{g}^k$ into whole

transpose δ^k is greater than or equal to 0 or in other words, so what we get from this is that $\gamma^k \text{transpose } \delta^k$ which is greater than 0.

So, if we make sure that Wolfe conditions for line search are satisfied. Then we ensure that $\gamma^k \text{transpose } \delta^k$ is greater than 0 and $\gamma^k \text{transpose } \delta^k$ greater than 0 essentially means that the B^k plus 1 matrix should be positive-definite matrix. Therefore, when Wolfe condition is satisfied in a line search then exists of B^k plus 1 satisfies quasi-Newton condition.

Now, how to get this B^k B^k plus 1? Now, B^k plus 1 is a symmetric matrix. So, a symmetric matrix has of size n as n into m plus 1 by 2 are independent variables. So, the number of variables here is n into m plus 1 by 2 number of equality constraints here or number of equalities here are n and in addition to symmetricity, we also need positive definiteness of B^k plus 1 that is, all the principle minus of B^k plus 1 should be positive so that will result in n inequalities. So, in all we have n into n plus 1 by 2 variables n equalities and because of the positive definiteness, we want n inequalities to be satisfied. So, in other words this is a problem in m n plus 1 by 2 variable which are to be found using n equations and n inequalities. So, you will see that the number of variables is much larger than the number of equations are inequalities. So, there exist many solutions which satisfy this quasi-Newton condition. Now, let us look at some simple ways of finding B^k plus 1.

(Refer Slide Time: 53:56)

Consider a simple way to update B^k : Let $\alpha \neq 0, u \in \mathbb{R}^n, u \neq 0$

$$B^{k+1} = B^k + \alpha uu^T \quad (\text{Rank-one correction})$$

Choose α and u such that B^{k+1} satisfies *Quasi-Newton condition*

$$\begin{aligned} \therefore (B^k + \alpha uu^T) \gamma^k &= \delta^k \\ \therefore \alpha u^T \gamma^k u &= \delta^k - B^k \gamma^k \end{aligned}$$

So, let us consider simple way to update B_k and let us assume that α is scalar which is non-0 and u is n -dimensional vector which is again non-0 and let us update B_k to B_{k+1} as $B_{k+1} = B_k + \alpha u u^T$. Now, $\alpha u u^T$ is a symmetric matrix of rank 1. So, that is why this is called the rank 1 correction. So, if B_k is a symmetric matrix, then certainly B_{k+1} will be a symmetric matrix.

Now, if B_k is positive definite, is there a guarantee that B_{k+1} is also positive definite that is the question, that we would like to answer. Now, before we do that we want to find out what are possible values of α and u that could be used. So, that quasi-Newton condition is satisfied by the matrix B_{k+1} or in other words, what is that α and u such that $B_{k+1} \gamma_k = \delta_k$. So, we will choose α and u such that B_{k+1} satisfies the quasi-Newton condition or in other words, $B_{k+1} \gamma_k = \delta_k$ implies $B_k + \alpha u u^T \gamma_k = \delta_k$.

Now, how do we make sure that or how do you get this α and u from this equation. So, as you will see that there are lots of possibilities to do this and we look at a simplest possibilities, so if you expand this and then equate u to be $\delta_k - B_k \gamma_k$ then we can choose α equal to $1 / (u^T \gamma_k)$ or in other words, $\alpha u^T \gamma_k = 1$ and then that will satisfy this equality and B_k in B_{k+1} . In this case will satisfied quasi-Newton condition, now will that B_k also B_{k+1} also be positive definite and how good is this rank 1 correction. We will discuss about those things in the next class.

Thank you.