

Numerical Optimization
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Lecture - 5
One Dimensional Optimization (contd)

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Unconstrained Optimization

Let $f : \mathbb{R} \rightarrow \mathbb{R}$

Unconstrained problem

$$\min_{x \in \mathbb{R}} f(x)$$

- What are *necessary and sufficient conditions* for a local minimum?
 - Necessary conditions: Conditions satisfied by every local minimum
 - Sufficient conditions: Conditions which guarantee a local minimum
- Easy to characterize a local minimum if f is *sufficiently smooth*

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So, welcome back to this series of lectures on numerical optimization. So, in the last class, we were looking at unconstrained optimization problem. We saw that for solving any general constrained optimization problem, we need to solve unconstrained optimization problem. So, this one-dimensional unconstrained optimization problem plays a very important role in solving multi dimensional constant optimization problems. So, that is why, we have to spend some time studying about how to find the solution of a one dimensional constrained optimization problem.

So, here is a problem that we are looking at where f is the function from \mathbb{R} to \mathbb{R} . We want to minimize $f(x)$, x were reserve the entire set of real numbers. In the last class, we looked at the necessary and sufficient conditions for a local minimum. So, the necessary conditions are the conditions, which are satisfied by every local minimum. The sufficient conditions are the ones which guarantee a local minimum. Now, if the function f is sufficiently smooth, then we saw that it is easy to characterize a local minimum.

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Stationary Points

Let $f : \mathbb{R} \rightarrow \mathbb{R}, f \in C^1$.
Consider the problem, $\min_{x \in \mathbb{R}} f(x)$.

Definition
 x^* is called a *stationary point* if $f'(x^*) = 0$.

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We also saw the definition of a stationary point in the last class, where we defined the stationary point for a continuously differentiable function f to be a point where the derivative of the function vanishes. So, it is this stationary point that will be interested in if a function is a differentiable.

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Necessity of an Algorithm

- Consider the problem
$$\min_{x \in \mathbb{R}} (x - 2)^2$$
- We first find the stationary points (which satisfy $f'(x) = 0$).
$$f'(x) = 0 \Rightarrow 2(x - 2) = 0 \Rightarrow x^* = 2.$$
- $f''(2) = 2 > 0 \Rightarrow x^*$ is a strict local minimum.
- Stationary points are found by solving a nonlinear equation.
$$g(x) \equiv f'(x) = 0.$$
- Finding the real roots of $g(x)$ may not be always easy.
 - Consider the problem to minimize $f(x) = x^2 + e^x$.
 - $g(x) = 2x + e^x$
 - Need an algorithm to find x which satisfies $g(x) = 0$.

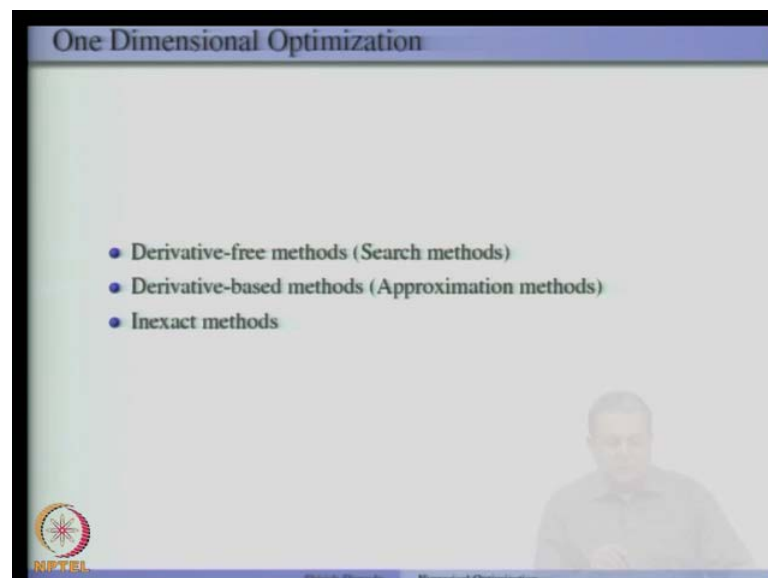
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So, if we want to find out the stationary point, we have to equate the derivative of a function to 0. So, this is the example that we saw last time that if we consider a function x minus 2 square and if you want to minimize this, so we first find out f dash x and

equate it to 0. That gives us the minimum. Then we check the second derivative and if it is greater than 0, we can say that x^* is a strict local minimum.

Now, in general, for a any non-linear function, it may not be always easy to find out a stationary point like what we have got here. For example, if we consider a function $f(x)$ is equals to $x^2 + e^x$, which is shown here. Then the derivative is $2x + e^x$. If we equate it to 0, we cannot get a closed form solution for x , so we need an algorithm to find out the x , which satisfies $g(x) = 0$. So, in today's class, we are going to look at some of those algorithms. Now, remember that we are looking at 1 dimensional optimization problem. So, there are different methods which can be used to solve this 1 dimensional optimization problem.

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So, they can be divided into different categories. So, 1 set of methods are called search free methods or search methods. So, these methods are derivative free methods. So, one looks at the function values at different places in the interval and then tries to find out, tries to reduce the interval of uncertainty and so on. The other set of methods are called approximation methods. They are based on derivative information. So, it could be either a first derivative or second derivative. Then another side of method exists, which are called inexact methods. So, in which case, we are not really worried about finding the exact solution of given 1 dimensional optimization problem?

So, this will be important when we have to solve one dimensional optimization problem many times. So, every time going towards the exact solution does not makes sense. So, one has to resort to inexact methods. So, we will study in exact methods some time later in this course, but in this class, we will study the derivative free methods and derivative based methods.

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Unimodal Functions

- Let $\phi : \mathbb{R} \rightarrow \mathbb{R}$
- Consider the problem,

$$\min_{x \in \mathbb{R}} \phi(x)$$
- Let x^* be the minimum point of $\phi(x)$ and $x^* \in [a, b]$

Definition
 The function ϕ is said to be *unimodal* on $[a, b]$ if for $a \leq x_1 < x_2 \leq b$,

$$x_2 < x^* \Rightarrow \phi(x_1) > \phi(x_2),$$

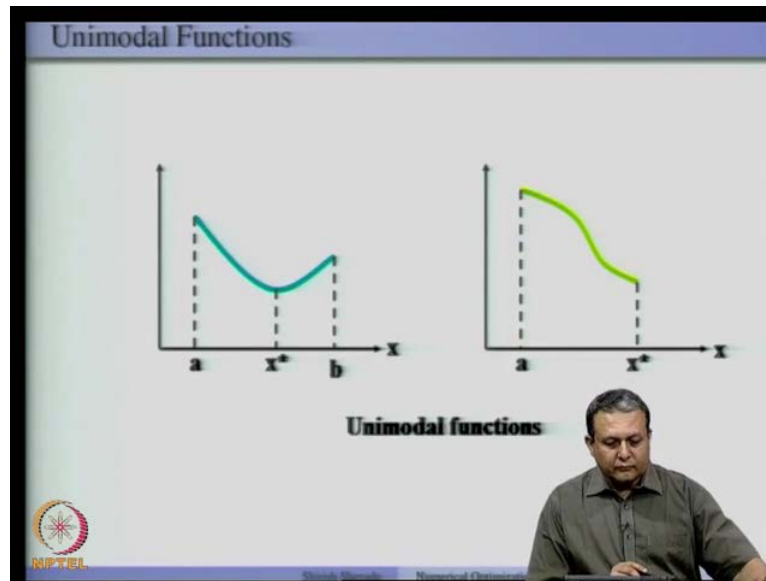
$$x_1 > x^* \Rightarrow \phi(x_2) > \phi(x_1).$$

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So, to understand these methods, we need the notion of unimodal functions. So, let ϕ be function from \mathbb{R} to \mathbb{R} . Let us consider the problem to minimize $\phi(x)$ over \mathbb{R} . Let us also assume that x^* be the minimum point of $\phi(x)$. It belongs to the closed interval a to b . Now, here is a definition of a unimodal function. The function ϕ is unimodal if if we have 2 points x_1 and x_2 in the close interval a to b , where x_1 is less than x_2 . Then x_2 less than x^* implies $\phi(x_1)$ greater than $\phi(x_2)$.

So, what it means that x_1 and x_2 both lie on the left side of x^* . In such a case, the function is strictly decreasing on the left side of x^* . If x_1 is greater than x^* , so that means that x_1 and x_2 both lie on the right side of x^* . So, on the right side of x^* , the function is strictly increasing. So, this is the definition of a unimodal function. So, let us now see how this unimodal functions look like.

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So, here are some examples of unimodal functions. So, a, b is the interval in which the minimum of the function lie. So, here b is nothing but x^* in the right panel. Now, if you look at the left panel, this is the minimum of the function in the interval a, b . so you will see that on the left side, the function is strictly decreasing. Then on the right side of x^* , the function is strictly increasing.

Similar is the case in the figure on the right side. So, on the left side of x^* , the function is strictly decreasing. Then x^* being a point of that interval, there is nothing on the right side of x^* . So, this unimodal functions function assumption will be used in most of these lectures except the last method, which is Newton method.

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Derivative-free Methods

Let $f : \mathbb{R} \rightarrow \mathbb{R}$

Unconstrained problem

$$\min_{x \in \mathbb{R}} f(x)$$

- Dichotomous search
- Fibonacci search
- Golden-section search

Require,

- Interval of uncertainty, $[a, b]$, which contains the minimum of f
- f to be unimodal in $[a, b]$.

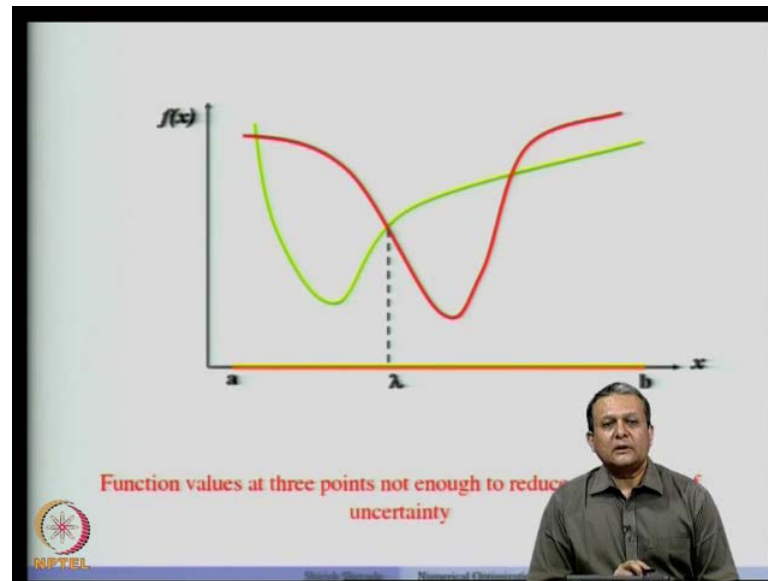
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So, with definition of unimodal functions, we will now start looking at the derivative free methods. So, as the name suggests, these methods do not use any derivative information of a function. It just tries to use the function value at different points in a given interval. So, we are again considering a unconstrained optimization problem, trying to minimize f of x , x belongs to \mathbb{R} . Here are some methods that we are going to discuss. There exist many others methods as well, but we will restrict ourselves to these 3 methods, which are quite practical methods.

So, one method is the dichotomous search method. The other one is Fibonacci search method. Then the limiting Fibonacci search method is called golden section search method. Now, all these methods require given interval of uncertainty a, b which contains the minimum of f . We also assume that f is unimodal in the closed interval a, b . So, the idea is that we start with some interval of uncertainty a, b and try to reduce the length of that interval has the iterations progress.

Finally, we reach close to the solution. This interval of uncertainty is also called bracket. So, we have to ensure that the minimum of the function f always lies in the bracket and then keeps on reducing the bracket such that the minimum gets always gets trapped in the bracket. Finally, we reach the actual minimum of f . The important assumption that we are using here is that f is unimodal in the close interval a, b .

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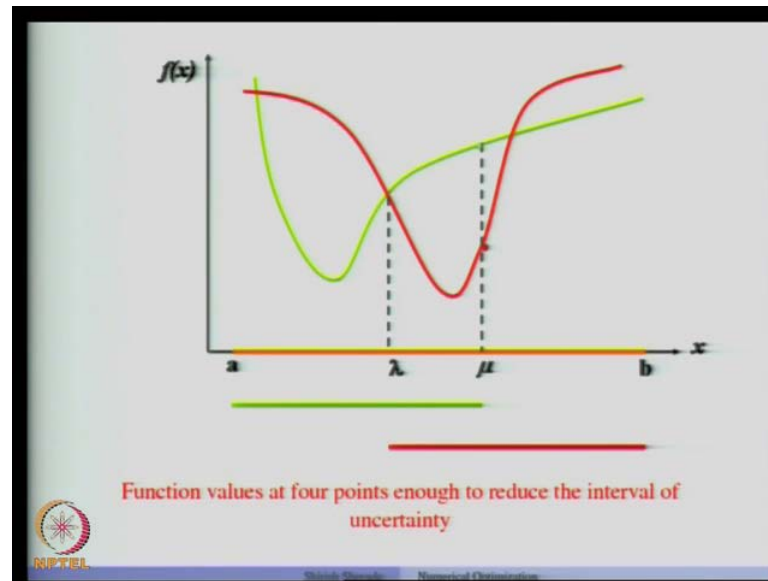


So, now, here are 2 functions. One is shown with the green line and the other one is shown with the red line. Now, a, b is the interval of uncertainty, which is given to us. So, that means that the interval a, b contains the minimum of each of these functions. Now, note also that each of these functions is unimodal. Now, suppose I know the function values at a and b . So, I know $f(a)$ and $f(b)$. Then I choose some point λ somewhere in this interval and find out the function value $f(\lambda)$.

Now, I have 3 pieces of information, $f(a)$, $f(\lambda)$ and $f(b)$ for the green line function and the red line function. Now, let us concentrate on the green line function. Now, you can see that the function has a minimum at this point and that lies in the interval a to λ . If you look at the red line function, that has the minimum at this point. That lies in the interval λ to b .

So, if I evaluate a function at a particular point, I really cannot say anything about which part of the interval does a minimum lie. It could lie either in a to λ or it could lie in λ to b also. So, function values at 3 points are not enough to reduce the interval of uncertainty. Remember that we always have to reduce the interval of uncertainty in every iteration. So, knowledge of function values at 3 points is not going to be enough.

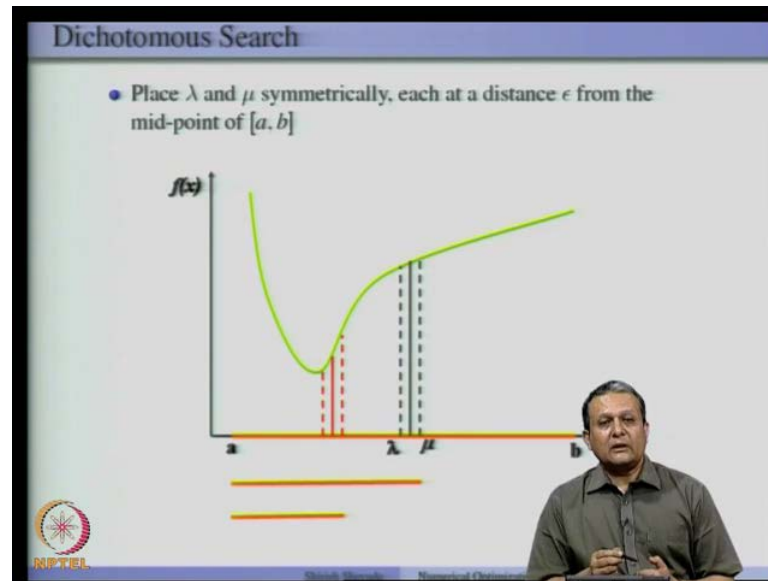
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So, we would require function value at one more point. So, again we consider the same set of functions. Now, suppose I have the knowledge of the function values at λ and μ . λ and μ both lie in the closed interval a and b . Now, let us look at the green function. Now, f of λ is less than f of μ . So, on the right, the function is strictly increasing on the right side of λ . Now, because of the unimodularity, there may not exist any minimum on the right side of μ as far as this green function is concerned. So, what we can conclude is that the minimum of this function would be bracketed in the interval a to μ .

On the other hand, if you look at the red function, red colored function, you will see that the minimum is bracketed in the interval λ to b . So, for the green color function, the minimum would lie in the interval a to μ . So, that means that we have reduced the original interval a, b to the interval a, μ , which is half size lesser than a, b . Similarly, for the red function, we have reduced the interval from a, b to λ, b . So, by having knowledge of function values at 4 points, we are able to reduce the interval of uncertainty. So, this is the very important fact that we will use for studying different derivative free methods.

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So, one of the simplest methods that is based on the derivative free approach is called the dichotomous search method. So, the idea here is very simple that given a interval a, b plus λ and μ symmetrically, each at a distance ϵ from the midpoint of a, b . So, we start with the interval a, b . This is the midpoint of that interval. Then λ and μ are plus symmetrically are at a distance of ϵ around this midpoint. Then we evaluate the function values at λ and μ . So, this functions value function values are given here.

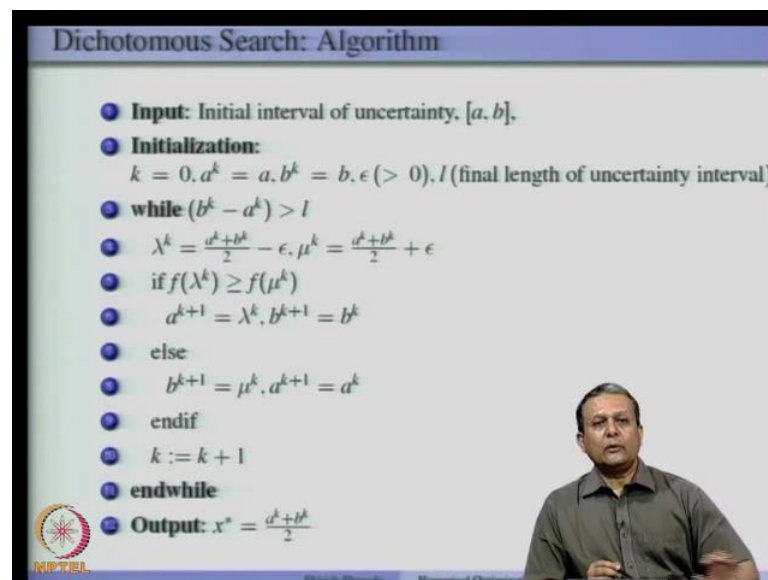
Now, you will see that $f(\lambda)$ is less than $f(\mu)$. So, this means that the function is strictly increasing on the right side of λ . So, that means that the root of this function, the minimum of this function should lie in the interval a to μ . So, the μ interval, which is shown here is the new interval of uncertainty or the new bracket. Now, you will see that this new bracket is about half the length of the original intervals length. So, that is we had this original interval a, b . We reduced it by almost a half quantity to form a new interval.

Now, now if you restrict ourselves to the interval a to μ , then again we have to do the same procedure. We will find out a midpoint of this, which is shown by the middle line. Then λ and μ are placed around it at the distance of ϵ . Then the functional values are evaluated. You will see that $f(\lambda)$ is less than $f(\mu)$. So, again we conclude

that the interval of uncertainty is on the left side of this midpoint. In fact, this f of μ and the new interval of uncertainty are shown here.

So, you will see that every time we are trying to reduce the interval of uncertainty by half. Using this procedure, one can find the minimum to a reasonable accuracy. Now, one important point to note is that in every iteration, we do 2 function evaluations. So, one is $f(\lambda)$ and the other one is $f(\mu)$. Similar thing is done here. It is a every iteration of dichotomous search requires 2 function evaluations and sometimes this number of function evaluations met are not to be expensive. So, one has to be careful about using the dichotomous search anyway.

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Dichotomous Search: Algorithm

- **Input:** Initial interval of uncertainty, $[a, b]$.
- **Initialization:**
 $k = 0, a^k = a, b^k = b, \epsilon (> 0), l$ (final length of uncertainty interval)
- **while** $(b^k - a^k) > l$
 - $\lambda^k = \frac{a^k + b^k}{2} - \epsilon, \mu^k = \frac{a^k + b^k}{2} + \epsilon$
 - **if** $f(\lambda^k) \geq f(\mu^k)$
 - $a^{k+1} = \lambda^k, b^{k+1} = b^k$
 - **else**
 - $b^{k+1} = \mu^k, a^{k+1} = a^k$
 - **endif**
 - $k := k + 1$
- **endwhile**
- **Output:** $x^* = \frac{a^k + b^k}{2}$

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It is a very simple method and very easy to implement. So, it is a simple algorithm, which implements dichotomous search method. So, we are given initial interval of uncertainty a, b and start with the initial iteration a is equal 0. The first point 0 is said to a and b 0 is said to b ϵ is some quantity, which is given, which is greater than 0. What is given to us is the final length of uncertainty interval.

So, we have to iterate till the final interval as this length. So, as long as the the interval length is greater than all greater than l , we compute λ^k and μ^k . They are computed using the midpoint of a^k and b^k minus ϵ and point of a^k and b^k plus ϵ . Now, if λ^k is greater than f of μ^k , then what we have to do is that the function is strictly decreasing on the left side of λ^k .

So, λ_k becomes a_{k+1} and b_k will remain as b_{k+1} . Otherwise, b_{k+1} will be μ_k that means that function is the $f(\lambda_k)$ is strictly less than $f(\mu_k)$. That means function is strictly increasing on the right side of λ_k . So, the right end of the bracket is μ_k . Then the left end remains as a_k . Then we increase the iteration counter and go to the next iteration.

So, this procedure is repeated. Finally, what we get is the interval of uncertainty $a_k b_k$, which of the until less than or equal to r less than or equal to 1. Once we get that, the algorithm will come out. Finally, the x^* , the minimum of the function will be that midpoint of the final interval of uncertainty. So, it is a very simple algorithm, but requires 2 function evaluations, the $f(\lambda_k)$ and $f(\mu_k)$ at every iteration. That may turn out to be expensive in some cases.

So, if you look at this algorithm, every time the length of the interval is reduced by half, so after k iterations, the length will be $1/2^k$ into $b_0 - a_0$ or $b - a$, which is the original interval of uncertainty. So, by controlling k , one can reach any desired accuracy of the final length of uncertainty interval.

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Dichotomous Search: An Example

Consider, $\min_x (1/4)x^4 - (5/3)x^3 - 6x^2 + 19x - 7$

k	a^k	b^k	$b^k - a^k$
0	-4	0	4
1	-4	-1.98	2.02
2	-3.0001	-1.98	1.0201
3	-3.0001	-2.4849	.5152
⋮	⋮	⋮	⋮
10	-2.5669	-2.5626	.0043
⋮	⋮	⋮	⋮
20	-2.5652	-2.5652	4.65e-6
⋮	⋮	⋮	⋮
23	-2.5652	-2.5652	5.99e-7

$x^* = -2.5652, f(x^*) = -56.262$

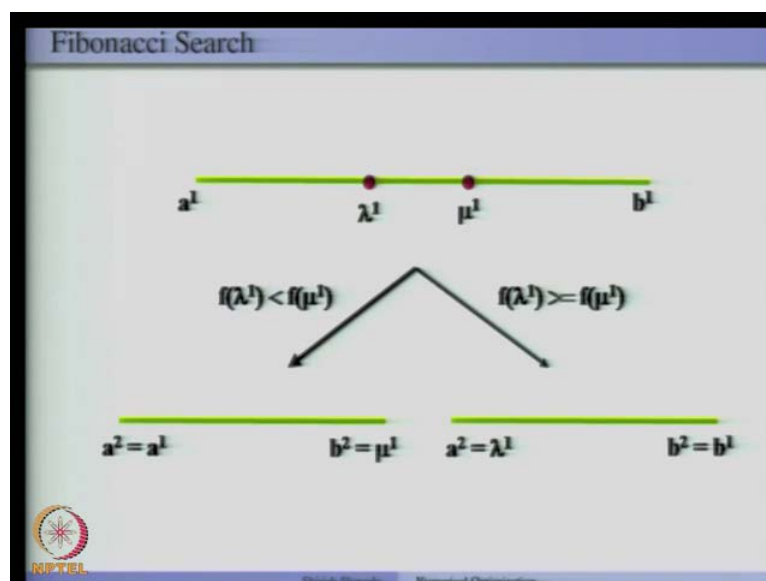
Now, here is a simple example. We have considered the function, to minimize the function, which is to be minimized is given here. Here are the iterations of dichotomous search. So, they start with the interval uncertainty to be minus 4 and 0. So, the difference

between b_k and a_k is 4. As the iterations progress, this difference between b_k and a_k comes down as you see here.

So, you will see that initially the difference was 4; and thereafter 10 iterations, it is about 0.0043. If you go down further, this difference comes down further. Suppose, if you want the final interval of uncertainty to be less than 10^{-6} , then we would end up in something in a solution like this. So, you will see that the a_k and b_k are almost close to each other with a very small value.

So, it is a very small difference between them and x^* . The minimum of the function turns out to be minus 2.5652 in this case. The corresponding value of f of x^* is given here. So, you will see that there is a significant reduction in the interval of uncertainty at every time. So, $\frac{1}{2}$ to the power k that is the reduction of the ratio of the final length of the k th interval divided by the length of the first interval that will be $\frac{1}{2}$ to the power k .

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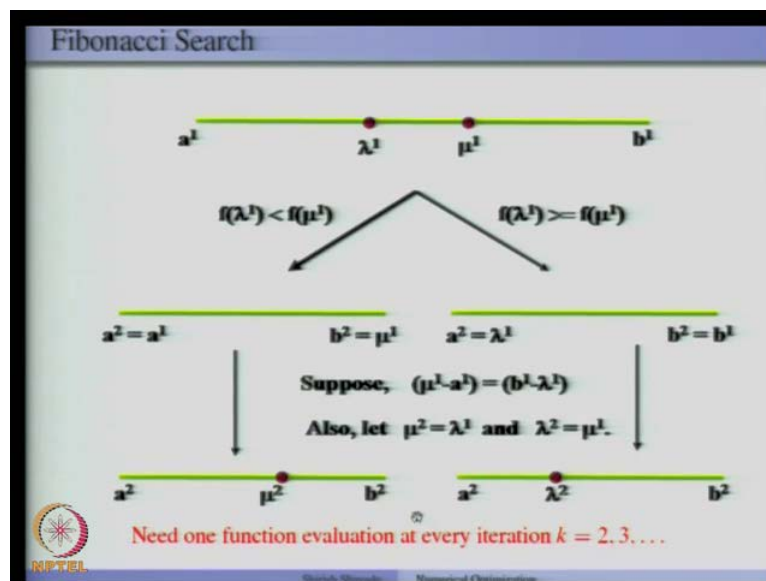


Now, in the previous method that we studied, we saw that we always needed 2 function evaluations per iteration and that 2 turned out to be expensive. So, can we better look at another case? Let us first look at a simple case. Now, a^1, b^1 is an interval of uncertainty, which is given. Suppose that we have placed λ^1 and μ^1 at 2 different places in this interval. Now, we know that the function is unimodal.

So, $f(\lambda_1)$ is less than $f(\mu_1)$. So, that means that the function is increasing on the right side of λ_1 . So, the bracket has to be a_1 to μ_1 . Similarly, if $f(\lambda_1)$ is greater than or equal to $f(\mu_1)$, then the bracket has to be λ_1 to b_1 . So, this is what is indicated here. Now, you will see that this n point of this interval is same as μ_1 . The n point of this interval in the other case is same as λ_1 . Now, we also have, if you consider this case, we also have knowledge of 1 point λ_1 in this interval. Now, can we use that to some of its some method?

Similarly, if you look at the other interval, so whose left end point is λ_1 . Now, we know the value of $f(\mu_1)$ here where μ_1 lies in this interval. Now, 1 function evaluation is already done. So, we just have to add 1 extra point, which could be on the left of this λ_1 and could be on the right side of this μ_1 . So, that would reduce the number of function evaluations. So, let us see how to do that.

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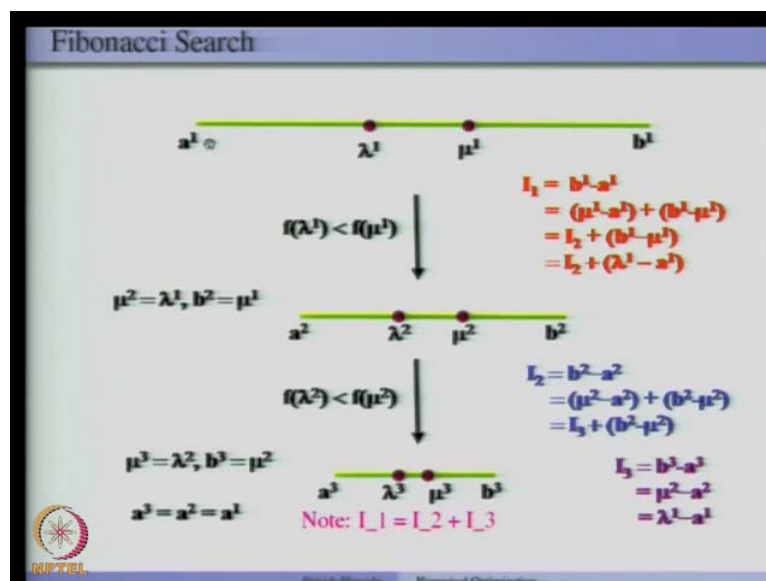
So, see the same case. Now, let us assure 2 things; 1 is that $\mu_1 - a_1$ is same as $b_1 - \lambda_1$. So, that means that λ_1 and μ_1 are always symmetrically placed. So, when we go to k th iteration, we will have λ_k and μ_k . They are symmetrically placed so that the assumption that we make, so whenever we get those 2 points, they are always the symmetrically placed in the interval. Now, let us also assume that μ_2 is equal to λ_1 .

So, if we look at this interval, this branch, we are concentrating on the interval a_1 to μ_1 . Now, this μ_1 becomes a new end point of the next iteration b_2 and a_2 is the nothing but a_1 , which is the left end point of the bracket of further k th iteration. Now, let us consider this branch. Let us assume that μ_2 is λ_1 . So, this λ_1 is basically used here. That we will, we are going to call it as μ_2 . Then what we have to do is we just have to find out λ_2 here using some method. So, that means that from the first iteration to the second iteration, we will just need 1 function evaluation as compared to 2 function evaluations used by the dichotomous search.

Similarly, it is the case if you look at the right branch where $f(\lambda_1)$ is greater than or equal to $f(\mu_1)$. Now, the left bracket of this is obtained using λ_1 . So, a_2 is set to λ_1 . The right bracket remains as b_1 . So, b_2 is b_1 . Now, what we do is that this μ_1 , which was earlier available, we will call it has λ_2 . Now, the function value at λ_2 is known because the function value of μ_1 is known.

Now, our aim is just to get μ_2 . So, that means that it will require 1 function evaluation from the second iteration onwards. So, in the first iteration, we will need both λ_1 and μ_1 ; the 2 function evaluations, but from the second iteration onwards, we will need only 1 function evaluation. If we cleverly choose our λ_2 or μ_2 depending upon the case, that is what we will see now how to do that.

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Now, we started with λ_1 μ_1 . Let us assume that f of λ_1 is less than f of μ_1 . Now, f of λ_1 less than f of μ_1 means that our new bracket will be a_1 to μ_1 . So, b_2 , which is the right end of the bracket, is μ_1 and a_2 is same as a_1 . Then λ_1 became μ_2 . Suppose that we have a way to find out a λ_2 . So, then the function evaluation of f of λ_2 is done. Now, suppose f of λ_2 also is less than f of μ_2 . So, in that case, this μ_2 will become the right bracket, which is nothing but b_3 a_2 remains as a_3 . Then this λ_2 becomes μ_3 . Then we find λ_3 . So, this is how the iterations would progress.

So, you will see that the difference between λ_k and μ_k comes down as the iterations progress. Finally, there would be situation where λ_k and μ_k would merge. So, our aim is to get this required λ s and μ s appropriately. So, we will see how to do that. Now, this is the little bit of abuse of notations here in the sense that sometimes we will call I_1 as the interval. In this case, I have used I_1 as a length of the interval. So, depending upon the context, we will know what I_1 or I_2 mean, either they could mean interval or a length of the interval.

Now, if you look at the the interval length at the first iteration, so the interval length is b_1 minus a_1 . Now, b_1 minus a_1 is same as μ_1 minus a_1 plus b_1 minus μ_1 . So, μ_1 minus a_1 assume that f of λ_1 is length than f of μ_1 . So, that means that a_1 to μ_1 is the interval length at the second iteration. So, μ_1 minus a_1 is I_2 and that is added to b_1 minus μ_1 .

Now, remember that we have placed λ_1 and μ_1 symmetrically. So, what it means is that b_1 minus μ_1 is same as μ_1 minus a_1 . So, I can write b_1 minus a_1 as λ_1 minus a_1 . Now, now, let us go to second step. Suppose we find out λ_2 because we already have got μ_2 that is equal to λ_1 . Now, suppose that we have found μ_2 and f of λ_2 is less than f of μ_2 . Then we find out that we are interested in the interval a_2 to μ_2 . Now, b_3 is nothing but μ_2 and μ_3 is nothing but λ_2 . We find λ_3 . So, you will see that the interval length I_2 is nothing but b_2 minus a_2 . One can calculate to be I_3 plus b_2 minus μ_2 ; so I_3 plus b_2 minus μ_2 .

Now, if you look at I_3 , how is I_3 derived? I_3 is derived from b_3 a_3 to b_3 interval. So, the length of interval I_3 is b_3 minus I_3 and b_3 minus I_3 a_3 is same as μ_2 minus a_2 .

So, $b_3 - a_3$ is same as $\mu_2 - a_2$ because we have got this interval based on this condition and $\mu_2 - a_2$ because of the symmetry is same as $\lambda_1 - a_1$. So, what we can see is that I_1 can be written as $I_2 + I_3$.

So, this is the very important observation that we have made here that the length of the interval, the first interval is the sum of the lengths of second interval and the interval obtained at the third iteration. So, you will see that this is I_1 . Then I_2 is nothing but a $\frac{1}{2} \mu_1$. Since, λ_1 and μ_1 are symmetrically placed, so a_1 to μ_1 is same as λ_1 to b_1 . This a_1 to λ_1 is same as a_3 to b_3 . So, you will see that I_3 is same as I_1 is same as $I_3 + I_2$. So, this is the very important observation that we are going to use.

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Fibonacci Search

We have $I_1 = I_2 + I_3$.
Generalizing further, we get

$$\begin{aligned} I_1 &= I_2 + I_3 \\ I_2 &= I_3 + I_4 \\ &\vdots \\ I_n &= I_{n+1} + I_{n+2} \end{aligned}$$

Assumption: The interval for iteration $n + 2$ vanishes ($I_{n+2} = 0$).

Now, we have this I_1 is equal to $I_2 + I_3$. Now, if you generalize further, so what we get is I_2 is equal to $I_3 + I_4$ and so on. Then we get I_n is equal to $I_{n+1} + I_{n+2}$. So, now, we have n equations. Now, out of these n equations, I_1 is a given interval of uncertainty that before we started using our approach. So, I_1 is known. Now, there are n equations and $n - 1$ variables. So, there exists infinite number of solutions assuming that they are consistent. Now, suppose we make 1 assumption that I_{n+2} is 0. So, that means that after $n + 2$ iterations, the length of the interval is going to vanish.

So, let us make this assumption that after $n+2$ iterations, I_{n+2} will be equal to 0. So, that means that we are now left with n variables, which are I_2 to I_{n+1} and n unknowns. So, we can find out, we can generate a sequence of intervals I_2 to I_{n+1} with I_1 given and $I_{n+2} = 0$. So, let us see how to do that.

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$$I_{n+1} = I_n - I_{n+2} = 1I_n$$

$$I_n = I_{n+1} + I_{n+2} = 1I_n$$

$$I_{n-1} = I_n + I_{n+1} = 2I_n$$

$$I_{n-2} = I_{n-1} + I_n = 3I_n$$

$$I_{n-3} = I_{n-2} + I_{n-1} = 5I_n$$

$$I_{n-4} = I_{n-3} + I_{n-2} = 8I_n$$

$$\vdots$$

$$I_1 = I_2 + I_3 = ?I_n$$

Fibonacci Sequence : {1, 1, 2, 3, 5, 8, 13, 21, 34, 55, ...}

$$F_k = F_{k-1} + F_{k-2}, k = 2, 3, \dots$$

$$F_0 = 1, F_1 = 1.$$

So, let us look I_{n+1} . Now, if you look at I_{n+1} , I_{n+1} is nothing but I_n minus I_{n+2} . So, I_n minus I_{n+2} is nothing but I_{n+1} . We know that I_{n+2} is going to be 0. So, that is nothing but I_n . So, I_{n+1} is equal to 1 into I_n . Now, if we go further, let us write write down I_n . So, I_n is nothing but I_{n+1} plus I_{n+2} . Now, I_{n+2} is 0 and I_{n+1} that we have already seen. That is I_n . So, I_n is nothing but I_{n+1} that is nothing but 1 I_n .

Now, we go 1 step further. So, let us look at I_{n-1} . So, I_{n-1} is I_n plus I_{n+1} . Now, you will see that I_{n+1} is 1 into I_n , I_n is 1 into I_n . so I_{n-1} will be 1 I_n plus 1 I_n that is nothing but 2 I_n . So, what we have done is that we have started with I_{n+1} and I_n . Then we can now find out I_{n-1} . So, what it means is that at the $n-1$ th iteration, the interval is the interval length is 2 into I_n , if you go further, so you will see that I_{n-2} is nothing but 3 into I_n . So, the interval length at I_{n-2} is 3 into I_n . How is this 3 derived? This 3 is derived from I_n and I_{n-1} . So, it means that we have derived it from this 2.

So, we take a sum of the previous 2 entries. Then we get 3. So, if you proceed further, so you will see that the length of every interval is obtained using the previous 2. If you go from I_{n+1} down to I_1 , so I_1 is nothing but I_2 plus I_3 . Then what should be the length here? So, that is the question that we would like to ask. Now, if you look at this sequence 1, 1, 2, 3, so let us assume that this 2 are given to us 1 and 1. Then we sum the previous 2 to get this quantity. Then similarly, from the previous 2 to get this, then 5 plus 3 will give us 8 and so on. So, that is how the lengths are obtained.

Now, this sequence that we have given here in the red color is called the Fibonacci sequence. The recursive relation for this Fibonacci sequence is F_k is equal to F_{k-1} plus F_{k-2} . So, that means from k equal 2 onwards, you obtain this sequence by finding the sum of the previous 2 elements in the sequence. Then of course, we will assume that the first member of this sequence is 1 and the second member is 1. So, these 2 are 1. So, once they are given, we can start calculating F_2 onwards. So, this is called the Fibonacci sequence. Then if we assume that I_{n+2} is 0, then we can get the lengths of all the intervals based on the element of which element of the sequence we are talking about.

(Refer Slide Time: 35:11)

Fibonacci Search

$$\begin{aligned}
 I_{n+1} &= I_n - I_{n+2} = 1I_n && \equiv F_0 I_n \\
 I_n &= I_{n+1} + I_{n+2} = 1I_n && \equiv F_1 I_n \\
 I_{n-1} &= I_n + I_{n+1} = 2I_n && \equiv F_2 I_n \\
 I_{n-2} &= I_{n-1} + I_n = 3I_n && \equiv F_3 I_n \\
 I_{n-3} &= I_{n-2} + I_{n-1} = 5I_n && \equiv F_4 I_n \\
 I_{n-4} &= I_{n-3} + I_{n-2} = 8I_n && \equiv F_5 I_n \\
 &\vdots && \vdots \\
 I_k &= I_{k+1} + I_{k+2} = F_{n-k+1} I_n \\
 &\vdots && \vdots \\
 I_1 &= I_2 + I_3 = F_n I_n
 \end{aligned}$$

Note: After n iterations,

$$I_n = \frac{I_1}{F_n}$$

So, we will see how to do that. So, I_n we saw that I_{n+1} is nothing but $1 I_n$. That is the first element of the Fibonacci sequence. So, $F_0 I_n$ is also $1 I_n$ that is nothing but $F_1 I_n$ and so on. So, we can based on the value of n , we can decide which sequence,

which element of the sequence of Fibonacci sequence are talking about. So, if we go further at the at the k th iteration, we are talking about F_{n-k+1} .

Therefore, at I_1 , it will be $F_n I_n$. Now, this is the very important relation. I_1 is nothing but $F_n I_n$, which means that after any iterations, the length of the original interval I_1 . So, the ratio of I_n , the length of the interval after any iterations and the length of the interval at the original iteration is 1 over F_n . In other words, I_n is nothing but I_1 by F_n . So, this is the important relation that we would like to use. So, if we generate the sequence like this, then how is it going to be useful in generating our λ and μ ? That is what we will see now.

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Fibonacci Search

- After n iterations,

$$I_n = \frac{I_1}{F_n}$$

For example, after 10 iterations, $I_n = \frac{I_1}{89}$

- n should be known beforehand

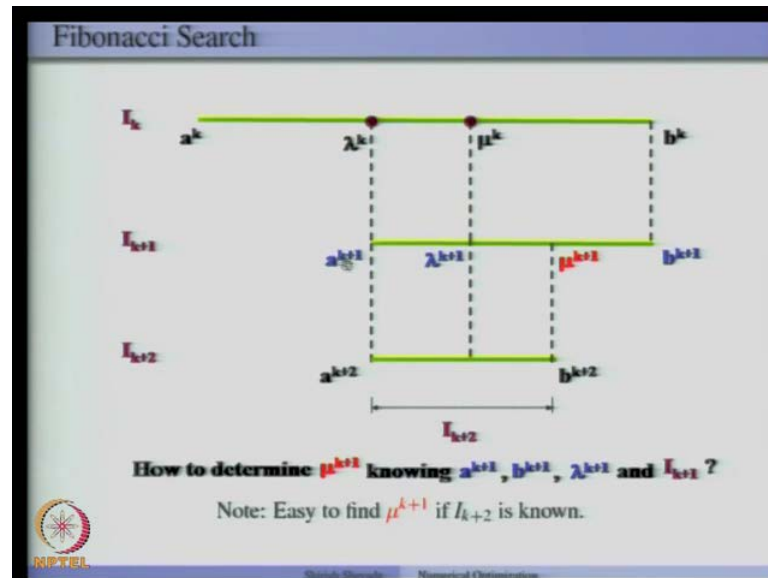
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Now, a quick comment about the number of iterations needed by this Fibonacci search method is that after n iterations, the length of the interval comes to I_1 by F_n . Now, F_n if we consider 10 iterations, so F_n is F_{10} . F_{10} is 89. So, I_n becomes I_1 by 89. Now, after 10 iterations, the number of function evaluations will be 2 for the first iteration. This is because initially, we do not have any idea. Suppose if you cleverly choose λ and μ , then for the remaining 9 iterations, we will require 9 function evaluations.

So, in all, we will require 2 plus 9 that is 11 function evaluations. In 11 function evaluations, we were able to reduce the length of the interval by about 1 percent. So, 1 by 89 is almost close to 1 by 100. So, the length of the interval after n iterations is almost

close to 1 percent of the original length of interval. Now, the only disadvantage here is that we should know n beforehand. Only then we can calculate what is what is going to be the final interval length.

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Now, let us see how to get λ^k and μ^k from the previous iterations. So, at the k th iteration, we have a^k and b^k . Then λ^k and μ^k are given here which are known. Now, let us assume that in the next interval, in the next iteration we are talking about the interval λ^k to b^k . So, that means b^{k+1} is b^k and a^{k+1} is λ^k . Then λ^{k+1} is nothing but μ^k as we saw earlier.

Our aim is to get μ^{k+1} . Now, we know that they are to be symmetrically placed right. Then suppose we know μ^{k+1} right and it turns out that in the next iteration that $k+2$. The iteration we have to only worry about is the interval a^{k+1} to μ^{k+1} . So, by the things that we have studied so far, we know that this μ^{k+1} will be the right end point of the bracket at I_{k+2} . So, if I can get the interval length at the $k+2$ iteration, then I can, what I can do is that I can add that interval length to get μ^{k+1} . Since, they are symmetrically placed; $\mu^{k+1} - a^{k+1}$ will be same as $b^{k+1} - \lambda^{k+1}$.

So, if we know a^{k+1} , if we know b^{k+1} , if we know λ^{k+1} , I_{k+2} and I_{k+1} , I_{k+2} , how do we get μ^{k+1} ? So, that is the question that we would like to answer. So, it turns out that if I know I_{k+2} , μ^{k+1} is easily

available. So, what I have to do is that I just have to add this interval length to a k plus 1 to get mu k plus 1.

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Fibonacci Search

Recall, $I_k = F_{n-k+1}I_n$.

Therefore, $I_{k+2} = F_{n-k-1}I_n$.

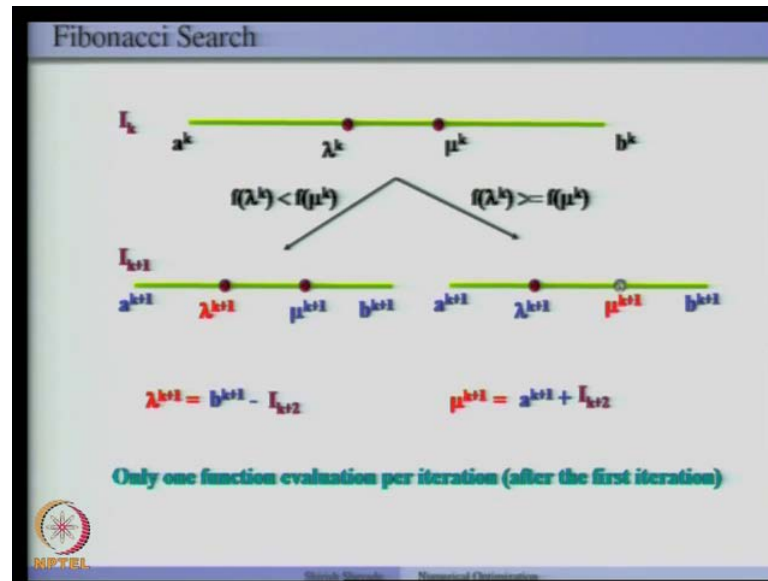
and $I_{k+1} = F_{n-k}I_n$.

This gives, $I_{k+2} = \frac{F_{n-k-1}}{F_{n-k}}I_{k+1}$.

Now, here is a procedure to do that. So, let us recall that I_k was found to be $F_{n-k+1}I_n$. Therefore, I_{k+2} also can be written as $F_{n-k-1}I_n$. Now, I_{k+1} also is written as $F_{n-k}I_n$. Therefore, if you take using if you use these 2 equalities, then one can write I_{k+2} as the ratio of F_{n-k-1} and F_{n-k} into I_{k+1} .

So, if I know I_{k+1} , if I know n and k , then I can derive I_{k+2} . All this was possible because of this relation. This relation was possible because of the way we generated the sequence. So, we assume that given I_n given I_1 and given that I_{n+2} equal to 0. We were able to generate a Fibonacci sequence and from which we derived this expression for I_k . This is because of which we are able to get I_{k+2} with the knowledge of the length of the interval at $k+1$ th iteration. This ratio is easy to find.

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So, here is a procedure. So, we have the interval I_k , which is a^k to b^k . λ^k and μ^k are given. The function values at these 2 λ^k and μ^k are evaluated. $f(\lambda^k)$ suppose is less than $f(\mu^k)$, then we know that b^{k+1} is nothing but μ^k . μ^{k+1} nothing but λ^k . a^{k+1} is nothing but a^k . λ^{k+1} is evaluated using $b^{k+1} - I_{k+2}$. Similarly, in the other case, when $f(\lambda^k)$ is greater than or equal to $f(\mu^k)$, so in this case, these quantities are known. Only this quantity which is shown in a red is unknown and that is evaluated by adding I_{k+2} to a^{k+1} . So, that is what is shown here that μ^{k+1} is equal to $a^{k+1} + I_{k+2}$.


So, that important point to note is that after the first iteration, what we need to evaluate is only either λ^{k+1} or μ^{k+1} , the function and then the function value at that. So, only 1 function evaluation per iteration is needed after the first iteration. Also, it is easy to calculate these values if we know I_{k+2} . So, with that, the algorithm becomes very simple. So, the idea is that we start with some initial interval a^1 b^1 and then keep on reducing the interval of uncertainty. Then at final point, if we look at the previous expressions, we see this.

(Refer Slide Time: 43:13)

Fibonacci Search

$$\begin{aligned}
 I_{n+1} &= I_n - I_{n+2} = 1I_n && \equiv F_0 I_n \\
 I_n &= I_{n+1} + I_{n+2} = 1I_n && \equiv F_1 I_n \\
 I_{n-1} &= I_n + I_{n+1} = 2I_n && \equiv F_2 I_n \\
 I_{n-2} &= I_{n-1} + I_n = 3I_n && \equiv F_3 I_n \\
 I_{n-3} &= I_{n-2} + I_{n-1} = 5I_n && \equiv F_4 I_n \\
 I_{n-4} &= I_{n-3} + I_{n-2} = 8I_n && \equiv F_5 I_n \\
 &\vdots && \vdots \\
 I_k &= I_{k+1} + I_{k+2} = F_{n-k+1} I_n \\
 &\vdots && \vdots \\
 I_1 &= I_2 + I_3 = F_n I_n
 \end{aligned}$$

Note: After n iterations,

$$I_n = \frac{I_1}{F_n}$$




So, you will see that I_{n-1} is nothing but $2 I_n$. Then after this interval of uncertainty becomes half of the previous interval of uncertainty, so at that point, the λ and μ merge into each other. So, after $n-1$ iterations, we will have $\lambda_{n-1} = \mu_{n-1}$. Then one just has to look at either the left interval that is $a_{n-1} = a - \frac{1}{2} \lambda_{n-1}$ or $\lambda_{n-1} = b - \lambda_{n-1}$. Then do an iteration of dichotomous search to find out what is the minimum point. So, if you use this algorithm, the algorithm is easy to write. So, let us consider the same example that we saw earlier.

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The Fibonacci Search

- Consider, $\min_x (1/4)x^4 - (5/3)x^3 - 6x^2 + 19x - 7$
- Initial interval of uncertainty : $[-4, 0]$
- Required length of interval of uncertainty: 0.2
- Set n such that $F_n > \frac{4}{0.2} = 20, n = 7$

k	a^k	b^k	$b^k - a^k$
0	-4	0	4
1	-4	-1.52	2.48
2	-3.05	-1.52	1.53
3	-3.05	-2.11	0.94
4	-2.70	-2.11	0.59
5	-2.70	-2.34	0.36
6	-2.70	-2.47	0.23
7	-2.61	-2.47	0.14

We are trying to minimize this function. The interval of uncertainty is the close interval minus 4 to 0. Suppose that the required length of interval of uncertainty is 0.2, then if you set n to b say one that is based on F n, then this is the set of iterations, which are given here for Fibonacci search method. So, you will see that the length of the uncertainty interval, which was 4 initially after 7 iterations, it came to 0.14. Then one has to use the appropriate method, 1 iteration of dichotomous search after n minus 1 iterations. That will give us the final minimum of the function at 2 certain accuracy.

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Golden Section Search

- Fibonacci Search requires the number of iterations as input
- Golden section search : Ratio of two adjacent intervals is constant

$$\frac{I_k}{I_{k+1}} = \frac{I_{k+1}}{I_{k+2}} = \frac{I_{k+2}}{I_{k+3}} = \dots = r$$

Therefore,

$$\frac{I_k}{I_{k+2}} = r^2$$

and

$$\frac{I_k}{I_{k+3}} = r^3$$

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Now, as I said earlier that Fibonacci search requires n as the input. We have to fix n beforehand. Only then we can use Fibonacci search. Now, there is another method, which is called golden section search method, which is a limiting case of a Fibonacci search. So, here we assume that the ratio of 2 adjacent intervals is constant. So, that is I k by I k plus 1 is same as I k plus 1 by I k plus 2 and I k plus 2 by I k plus 3 and so on. This should be I k plus 2. Therefore, if take I k by I k plus 2, so that will be r square. Then I k by I k plus 3 is equal to r to the power 3 and so on.

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Golden Section Search

Suppose, $I_k = I_{k+1} + I_{k+2}$. That is,

$$\frac{I_k}{I_{k+2}} = \frac{I_{k+1}}{I_{k+2}} + 1$$

This gives

$$r^2 = r + 1 \Rightarrow r = \frac{1 + \sqrt{5}}{2} = 1.618034 \quad (\text{negative } r \text{ is irrelevant})$$

Golden Ratio = 1.618034

So, if we suppose continue to use the same relationship that we had for the Fibonacci search that is I_k is equal to I_{k+1} plus I_{k+2} or in other words, I_k by I_{k+2} is same as I_{k+1} by I_{k+2} plus 1. So, now, I_k by I_{k+2} is r square. I_{k+1} by I_{k+2} is r . so we can write r square is equal to r plus 1. If we consider the positive root of this polynomial, then we get r equal to 1 plus root 5 by 2 . This is nothing but 1.618034 . We are neglecting the negative root of r because we do not want the negative ratios. So, this ratio is called the golden ratio. Hence, the name of the method has the golden section search.

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Golden Section Search

- Every iteration is independent of n

$$\frac{I_k}{I_{k+1}} = \frac{I_{k+1}}{I_{k+2}} = \frac{I_{k+2}}{I_{k+3}} = \dots = r$$

- Lengths of generated intervals,
 $\{I_1, I_1/r, I_1/r^2, \dots\}$

- After n function evaluations, $I_n^{GS} = I_1 / r^{n-1}$

Now, one important point to note for golden section search is that every iteration is independent of n that we saw earlier. Again, this should be I_k plus 2 by I_k plus 3. Now, if you look at the lengths of the intervals, which are generated after every iteration, so we start with I_1 . Then the length of the next interval is I_1 by r and then I_1 by r square and so on. So, after n function evaluations, assuming that we use the same technique as we used earlier, we will see that for the golden section search, the length of the interval after n iterations is I_1 by r to the power n minus 1. Now, how does it compare with Fibonacci search?

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Golden Section Search

- For Golden Section search, $I_n^{GS} = I_1 / r^{n-1}$
- For Fibonacci search, $I_n^F = I_1 / F_n$
- When n is large,

$$F_n \cong \frac{r^{n+1}}{\sqrt{5}}$$

Therefore, $I_n^F \cong \frac{\sqrt{5}}{r^{n+1}} I_1$

- $$\frac{I_n^G}{I_n^F} = \frac{r^2}{\sqrt{5}} \approx 1.17$$
- If the number of iterations is same, I_n^{GS} is larger by about 17%

Now, if you look at the Fibonacci search, the length of the interval after n iterations is I_1 by F_n and for the golden sections search, we saw that it is I_1 by r to the power n minus 1. So, how do they compare? Now, one uses a relationship, which holds when n is very large. So, the relationship is that F_n is approximately equal to r to the power n plus 1 by root 5. Therefore, one can write I_n^F as this.

Then, the ratio of this 2 turns out to be r^2 by root 5, which is 1.17. So, what it tells is that when n is large, when this relationship holds after n evaluations, the length of the interval given by the golden section search is about 17 percent higher than the length given by the Fibonacci search. But, one advantage of golden section search is that it does not require knowledge of n beforehand, while Fibonacci search needed the knowledge of n beforehand. So, golden section search is typically used in practice because one need

not know the value of n . One can reach the desired interval, one can reach the desired length of the interval of uncertainty has the iterations progress.

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The slide is titled "Derivative-based Methods" and contains the following text:

Let $f : \mathbb{R} \rightarrow \mathbb{R}$

Unconstrained problem

$$\min_{x \in \mathbb{R}} f(x)$$

- Bisection method
 - Assumes $f \in \mathcal{C}^1$.
 - Interval of uncertainty, $[a, b]$, which contains the minimum of f needs to be provided.
 - Assumes that f is *unimodal* in $[a, b]$.
- Newton method
 - Assumes $f \in \mathcal{C}^2$.
 - Based on using the quadratic approximation

The slide also features the NPTEL logo in the bottom left corner and a small inset image of a man in the bottom right corner.

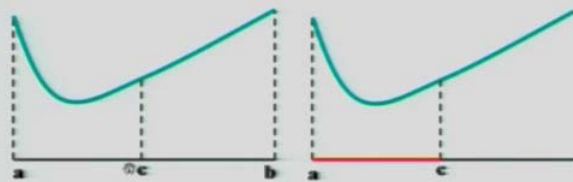
Now, let us look at some derivative based methods. Remember that we are trying to solve this unconstrained optimization problem. We are going to see a couple of methods. One of them is bisection method. These methods are derivative based. We assume that f is continuously differentiable for this bisection method. We also assume that the function f is unimodal. There is another method called Newton method, for which the function is assumed to be continuously twice differentiable. Then this is based on the quadratic approximation of the function at every iteration.

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Bisection Method

Assumption:

- $f \in C^1$
- f is unimodal in the initial interval of uncertainty, $[a, b]$.



Idea: Compute $f'(c)$ where c is the midpoint of $[a, b]$

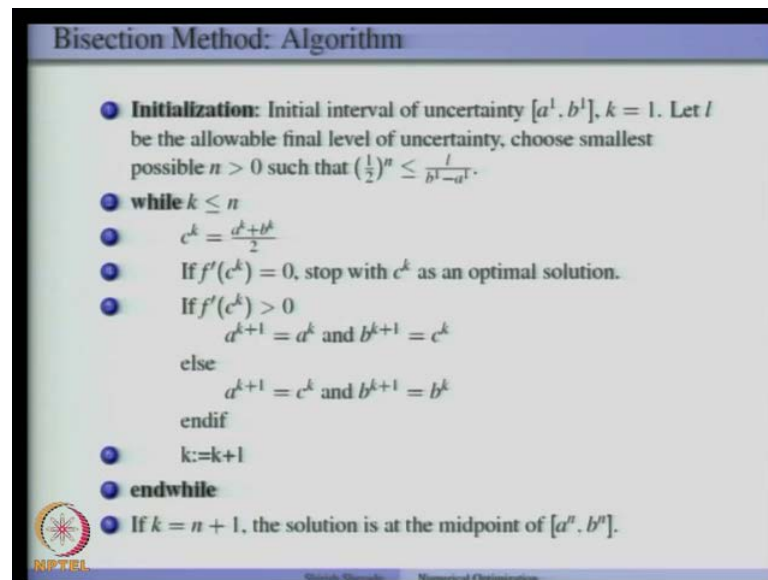
- If $f'(c) = 0$, then c is a minimum point.
- $f'(c) > 0 \Rightarrow [a, c]$ is the new interval of uncertainty
- $f'(c) < 0 \Rightarrow [c, b]$ is the new interval of uncertainty

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Now, let us see how the bisection method works. So, this is basically a variant of the dichotomous search that we studied. So, if you can recall that in the dichotomous search, we find the midpoint of the interval and then look at the function values at those 2 points, which are at a distance of epsilon from the midpoint. Now, instead of doing that, we find the midpoint and at this midpoint, we find out how what is the sign of the derivative? Now, if the sign of the derivative is positive as in this case, so that means that the function is going to increase further. Remember that we are using the assumption that the function is unimodal. So, next time we have to worry only about the interval a, c . So, the length of the interval gets reduced by half every time.

So, we compute $f'(c)$ where c is the midpoint of a, b . Then if $f'(c) = 0$, then we stop. If it is not 0, if it is greater than 0 that means we only concentrate on the left side interval a, c . $f'(c) < 0$ means we concentrate on the right side interval c, b . so every time the interval is reduced by half, so this is just a variant of the dichotomous search. So, instead of using 2 function evaluations around the midpoint, we use the derivative of the function at the midpoint.

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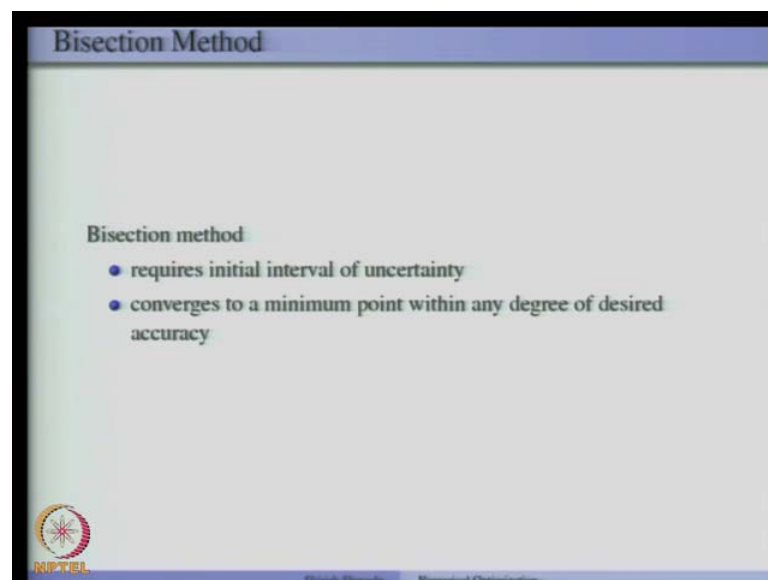
Bisection Method: Algorithm

- **Initialization:** Initial interval of uncertainty $[a^1, b^1]$, $k = 1$. Let l be the allowable final level of uncertainty, choose smallest possible $n > 0$ such that $(\frac{1}{2})^n \leq \frac{l}{b^1 - a^1}$.
- **while** $k \leq n$
- $c^k = \frac{a^k + b^k}{2}$
- If $f'(c^k) = 0$, stop with c^k as an optimal solution.
- If $f'(c^k) > 0$
 $a^{k+1} = a^k$ and $b^{k+1} = c^k$
else
 $a^{k+1} = c^k$ and $b^{k+1} = b^k$
endif
- $k := k + 1$
- **endwhile**
- If $k = n + 1$, the solution is at the midpoint of $[a^n, b^n]$.

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So, the algorithm is a very simple. So, it is easy to understand this algorithm. So, I will not spend much time on this.

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Bisection Method

Bisection method

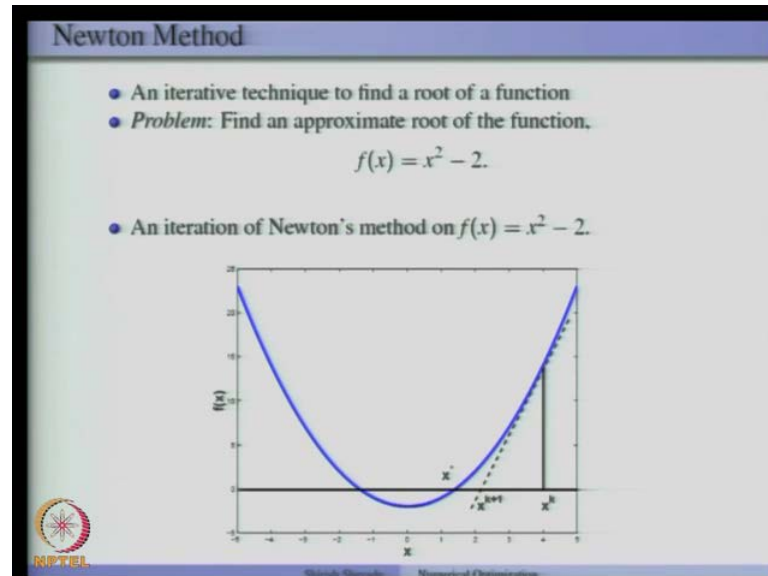
- requires initial interval of uncertainty
- converges to a minimum point within any degree of desired accuracy

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So, let us go to the some of the properties of the bisection method. So, it requires initial interval of uncertainty. It converges to a minimum point within any degree of desired accuracy. So, like the dichotomous search case, every time the interval length gets reduced by half in the dichotomous search case. It was almost close to half. Where?

Here, it is every time; it is half of the previous length. So, based on the desired degree of accuracy, one can reach the minimum point. Now, let us look at Newton method.

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This is the iterative technique to find a root of a function. You might have studied it in earlier classes. Let us look at some simple problem, where we want to find an approximate root of the function. So, root of a function is a point where the function crosses the x axis. Now, there could be multiple points or multiple roots or a function. But, suppose that we are interested in finding one particular root. So, you might have used this method earlier. So, suppose, we start with a point which is x_k , at x_k , we draw a tangent to the function and where this tangent hits the x axis, that point will be our new point x_{k+1} .

Now, at x_{k+1} , we follow the same procedure that we draw a tangent to a function at x at this point and then again, do this. Finally, we will reach the point x^* . Now, this function has another root, which is here. So, if we suppose start from a point here, we may end up in this root. So, depending upon the initial point, your root, your functions, the the root obtained using Newton's method would change.

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Newton Method

- Consider the problem to minimize $f(x)$, $x \in \mathbb{R}$
- Assumption: $f \in \mathcal{C}^2$.
- Idea:
 - At any iteration k , construct a quadratic model $q(x)$ which agrees with f at x^k up to second derivative.

$$q(x) = f(x^k) + f'(x^k)(x - x^k) + \frac{1}{2}f''(x^k)(x - x^k)^2$$

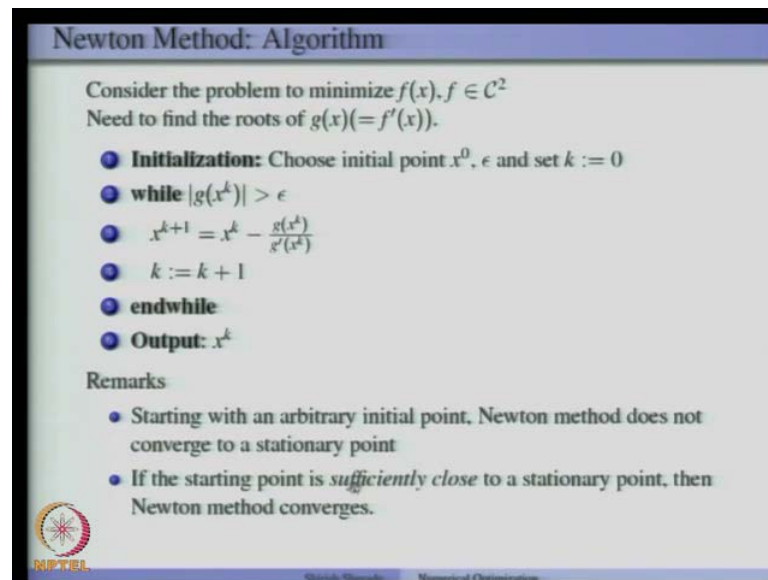
- Estimate x^{k+1} by minimizing $q(x)$.
- $q'(x^{k+1}) = 0 \Rightarrow f'(x^k) + f''(x^k)(x^{k+1} - x^k) = 0$
- $x^{k+1} = x^k - \frac{f'(x^k)}{f''(x^k)}$
- Repeat this process at x^{k+1} .

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Now, how do we use this method to find the minimum of a function? So, let us assume that the function is twice continuously differentiable. Then the idea of the Newton method is very simple. So, at every iteration k , you approximate a function b by a quadratic function. So, $q(x)$ is the quadratic approximation of f at x^k . So, that is obtained using the approximate using the Taylor series. But, Taylor series is up to second order. Remember that this is not the truncate at Taylor series. We are using $f''(x^k)$, so this is a quadratic approximation of the function.

So, we estimate the new point of the iteration by minimum, finding the minimum of quadratic. Minimum of quadratic is easy to find. We just take the derivative and equate to 0. That will give us the minimum. So, here is a derivative $q'(x^{k+1})$ is nothing but that is equated to 0. That gives us $x^{k+1} = x^k - \frac{f'(x^k)}{f''(x^k)}$. Now, the same procedure is again repeated that you go to a new point, again find the quadratic approximation of the function and go to the minimum of that quadratic approximation and repeat. So, this is the Newton method for finding the minimum of a function.

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The slide is titled "Newton Method: Algorithm" and contains the following text:

Consider the problem to minimize $f(x)$, $f \in C^2$
Need to find the roots of $g(x)(=f'(x))$.

- **Initialization:** Choose initial point x^0 , ϵ and set $k := 0$
- **while** $|g(x^k)| > \epsilon$
- $x^{k+1} = x^k - \frac{g(x^k)}{g'(x^k)}$
- $k := k + 1$
- **endwhile**
- **Output:** x^k

Remarks

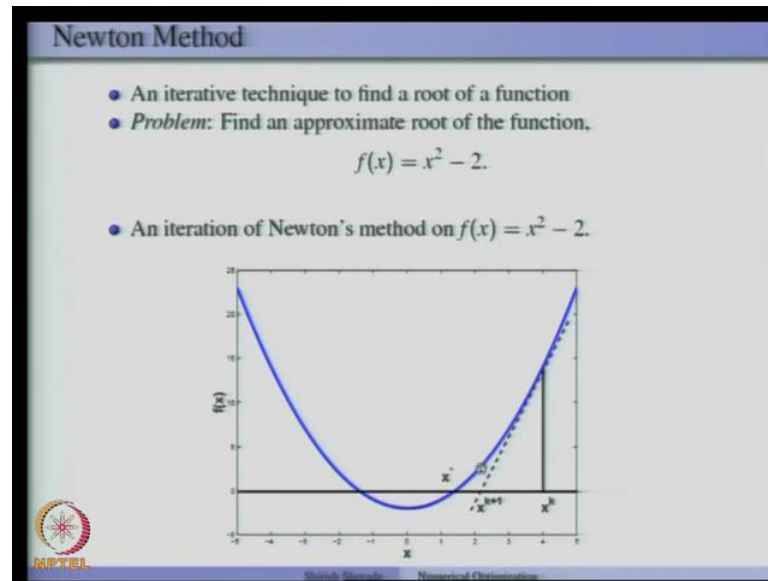
- Starting with an arbitrary initial point, Newton method does not converge to a stationary point
- If the starting point is *sufficiently close* to a stationary point, then Newton method converges.

MPTEL logo is visible in the bottom left corner.

So, it is very simple that we start with some initial point, as long as the gradient is within is greater than the desired epsilon value. So, we just iterate x_{k+1} is nothing but x_k minus g of x_k . So, remember that we are trying to find the stationary point. So, we have to look at the problem where we want to find the roots of the $g(x)$, the gradient of the function rather than the $f(x)$ we are trying to minimize. So, to get a stationary point, we want to find the root of $g(x)$. This is an algorithm to find the root of $g(x)$.

Finally, you will get x_k , the n point. Now, this entire procedure works provided the second additive of the function f is the first derivative of function g is positive. Then as you will see now that Newton method depends on the initial point. So, we are sufficiently close to the solution. Then the Newton method will converge. Now, we will see some evaluation Newton method on different functions.

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So, Newton method as all of you know, you must have used it to find the roots of a function. It is an iterative technique to find the root of a function. So, suppose if you consider a problem that we want to find an approximate root of the function $f(x) = x^2 - 2$. Then what we do is that we use Newton method to solve this problem. So, we start with some point x_k , which is shown here. At x_k , you take a tangent to the curve at x_k and where the point at which the tangent meets, that becomes your new point x_{k+1} . At x_{k+1} , again, you follow the same procedure. Again, draw a tangent to this curve. The point at which it intersects the x axis will be your x_{k+2} and so on.

So, finally, you will see that as the iterations progress, you will move to the point, which is x^* . It is one of the roots of this function. Now, if we start from a point somewhere in this region, then we may end up in getting a root. It is this. So, remember that this function has 2 roots. One is located on the positive side. One is located on the negative side.

Depending upon what our initial point is, we will end up going to the closest root. So, this is the Newton method and that can be used to minimize a function. So, when you want to minimize a function, we basically want to find out the stationary points. So, the points where $f'(x) = 0$, we are interested in finding the roots of $f'(x)$ when we want to minimize $f(x)$.

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Newton Method

- Consider the problem to minimize $f(x)$, $x \in \mathbb{R}$
- Assumption: $f \in C^2$.
- Idea:
 - At any iteration k , construct a quadratic model $q(x)$ which agrees with f at x^k up to second derivative.

$$q(x) = f(x^k) + f'(x^k)(x - x^k) + \frac{1}{2}f''(x^k)(x - x^k)^2$$

- Estimate x^{k+1} by minimizing $q(x)$.
- $q'(x^{k+1}) = 0 \Rightarrow f'(x^k) + f''(x^k)(x^{k+1} - x^k) = 0$
- $x^{k+1} = x^k - \frac{f'(x^k)}{f''(x^k)}$
- Repeat this process at x^{k+1} .

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So, let us see how to do that when we use Newton method. So, let us consider the problem to minimize f of x where x is value from the set of real numbers. Now, the important thing that we have to assume is that f belongs to C^2 . So, the second derivatives of f are continuous or f is twice continuously differentiable. Now, given that the Newton method is just a simple idea that at every iteration, it tries to construct a quadratic model of a function, which based which agrees with the function at x^k up to the second derivative.

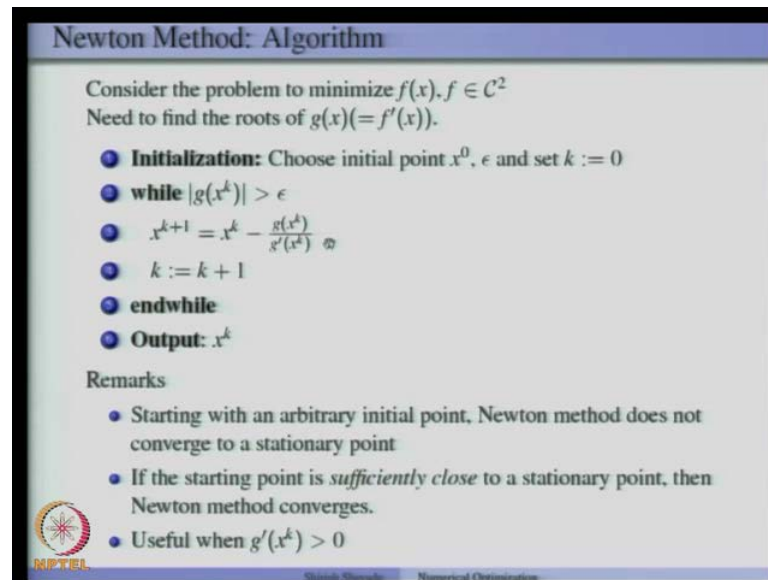
So, at x^k , if we can find out f' at x^k and f'' at x^k , then we can construct a quadratic model of the given function at x^k . Now, given this quadratic model, then the Newton method simply finds out the minimum of this quadratic function. So, to find minimum of this quadratic function, what we have to do is that we have to take the derivative of this with respect to x with respect to x equated to 0.

We estimate the new point x^{k+1} . So, $q'(x^{k+1})$ if we calculate, you will see that $q'(x^{k+1})$ is nothing but $f'(x^k) + f''(x^k)(x^{k+1} - x^k)$. Now, at x^{k+1} , this derivative of q should vanish. So, that means that $f'(x^k) + f''(x^k)(x^{k+1} - x^k) = 0$. So, from this, we can get a formula for x^{k+1} .

So, given x^k , given the first derivative of the function, the second derivative of the function at x^k , then x^{k+1} can be calculated as $x^{k+1} = x^k - \frac{f'(x^k)}{f''(x^k)}$.

$f'(x_k)$ divided by $f''(x_k)$. Of course, we have to assume that $f''(x_k)$ is non 0 in this case so that this division makes sense. Now, this procedure is repeated at $x_k + 1$. Again, we form a quadratic model at $x_k + 1$ and so on till some stopping criterion is reached.

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Newton Method: Algorithm

Consider the problem to minimize $f(x), f \in C^2$
 Need to find the roots of $g(x) (= f'(x))$.

- **Initialization:** Choose initial point x^0, ϵ and set $k := 0$
- **while** $|g(x^k)| > \epsilon$
- $x^{k+1} = x^k - \frac{g(x^k)}{g'(x^k)}$
- $k := k + 1$
- **endwhile**
- **Output:** x^k

Remarks

- Starting with an arbitrary initial point, Newton method does not converge to a stationary point
- If the starting point is *sufficiently close* to a stationary point, then Newton method converges.
- Useful when $g'(x^k) > 0$

NPTEL

So, here is the simple algorithm called Newton method. Remember that, we are trying to minimize f of x where f is f belongs to C^2 . We are interested in finding the roots of $g(x)$ and $g(x)$ is nothing but $f'(x)$. Now, the first step in the Newton method is to initialize the point x^0 . So, one can randomly choose the initial point x^0 . Then choose some epsilon, which is going to be used for deciding the stopping criteria and set the iteration number to 0.

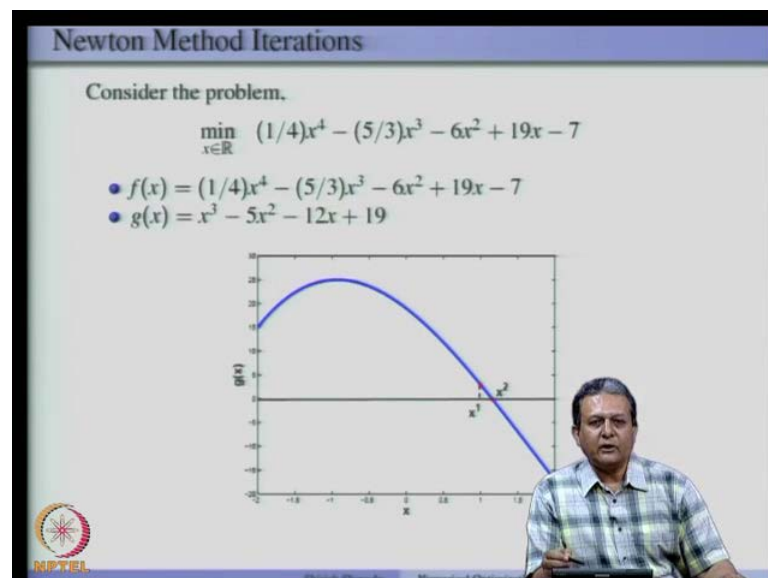
Now, while the gradient of the function at x^k , the absolute value of the gradient is greater than epsilon. So, that is why, this epsilon is used. So, one does another iteration of Newton method, where one finds x^{k+1} based on x^k and $f'(x^k)$. It is nothing but $g(x^k)$ and $f''(x^k)$. Then the iteration counter is increased and the whole process is repeated till the absolute value of the gradient at x^k is less than or equal to epsilon and the output of this algorithm. When the algorithm terminates, what we get is x^k and $f(x^k)$ is the optimal of objective function value.

Now, the algorithm looks very simple, but a lot depends on your initial point as we will see some examples now. If the initial points are far away, then this method will Newton

method will not converge. The second point that is important is that the $g'(x)$ should always be positive, only then the minimization will make sense. If $g'(x)$ turns out to be 0, then this division is not possible and $g'(x)$ turns out to be negative. Then we may not be able to solve this problem minimize f of x .

So, one has to be careful about these 2 points. Some remarks that if we start with an arbitrary initial point, the Newton method does not converge to a stationary point. So, this is the important remark. If we start sufficiently close to a stationary point, then the Newton method converges. This method is useful only when $g'(x)$ is greater than 0. That means that the the curve has a positive curvature at every point. Now, let us see how the Newton method works on different problems.

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So, let us take the same problem that we considered earlier to minimize a function, which is shown here. Its derivative $g(x)$ that is $f'(x)$ is also shown here. We are interested in finding the roots of this function $g(x)$. Now, here is the graph of that function $g(x)$. You will see that one of the roots of that function is somewhere here. Now, if I if we choose x_1 somewhere in the vicinity of that route, you will see that from x_1 we go to x_2 which is very close to the root here and then so on. So, after a few iterations, the algorithm will converge to the actual x^* . Now, for the same function, you start with a different initial point.

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Newton Method Iterations

Consider the problem.

$$\min_{x \in \mathbb{R}} (1/4)x^4 - (5/3)x^3 - 6x^2 + 19x - 7$$

- $f(x) = (1/4)x^4 - (5/3)x^3 - 6x^2 + 19x - 7$
- $g(x) = x^3 - 5x^2 - 12x + 19$

The slide features a graph of the function $g(x)$ with several points x^1, x^2, x^3, x^4 marked on the x-axis. A man in a plaid shirt is visible in the bottom right corner of the slide frame.

So, earlier we started with somewhat close to this root. Now, suppose if you start with close to this root. So, suppose our x_1 is here. One can check that from x_1 . Then next point x_2 is somewhere here; then x_3, x_4 and so on. Then finally, it converges to the root. So, the important point is that depending upon the initial point x_1 , the solution that we would get would differ.

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Newton Method Iterations

Consider the problem.

$$\min_{x \in \mathbb{R}} \log(e^x + e^{-x})$$

- $f(x) = \log(e^x + e^{-x})$
- $g(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$

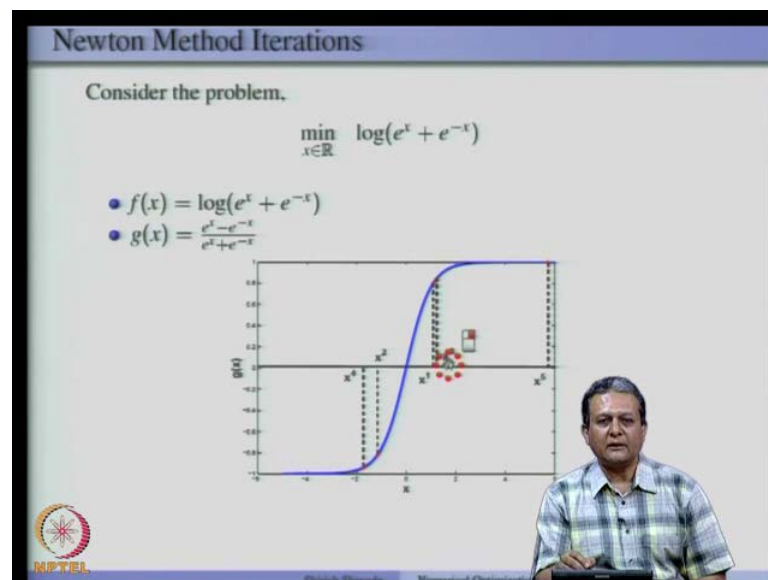
The slide features a graph of the function $g(x)$ with several points x^1, x^2, x^3 marked on the x-axis. A man in a plaid shirt is visible in the bottom right corner of the slide frame.

Now, suppose that we consider a function, which is to minimize \log of e to the power x plus x to power minus x . If you write the derivative of that, it turns out to be e to the

power x minus x to the power minus x divided by e to the power x plus e to the power minus x . So, remember that this function is twice continuously differentiable. So, we can use Newton method. Now, if we plot the graph of $g(x)$, so it would look something like this. Suppose, we start from a point x_1 , then x_2 point is somewhere here.

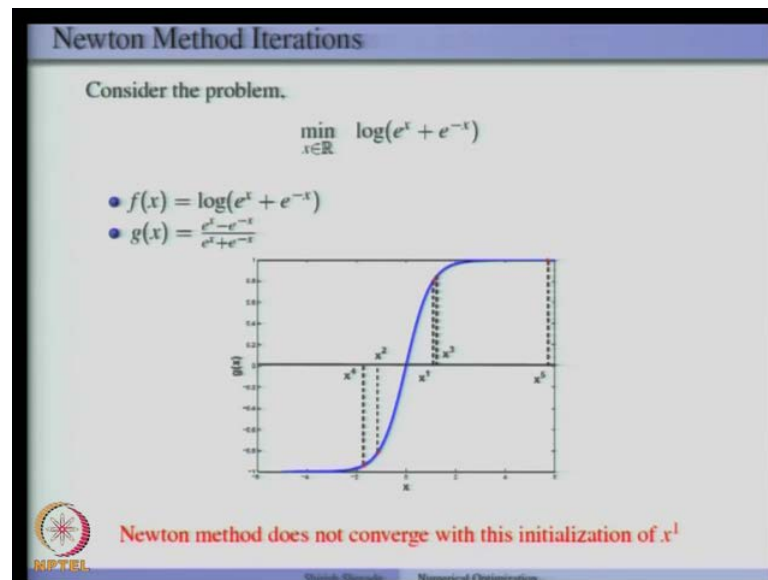
So, if you take a tangent to this curve at x_1 , it is the x axis. At x_2 , at x_2 , we again take the tangent to this curve. It cuts the x axis at x_3 and so on. So, you will see that slowly this method will converge to the point x^* where $g(x)$ becomes 0. Now, this is the only root of this function $g(x)$ and a , because as x increases, it goes further up and as x decreases, it goes down. So, it never touches the x axis at any point of time.

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Now, let us again consider the same function. But, start with a different initial point. So, our initial point is supposing somewhere here. We are talking about the same function $f(x)$ and then the same $g(x)$. Now, if our initial point x_1 is here, then take a tangent to the curve $g(x)$ at x_1 . So, it will meet the x axis at x_2 and we repeat the procedure. So, x_2 is here. Then x_3 comes on the right side of x_1 .

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x^3 becomes on the right side of x^1 . Then x^4 is again on the left side of x^2 . Now, you will see that x^2, x^5 has gone beyond much beyond x^3 . Now, the algorithm does not have any hope to converge to this point. So, you will see that at every iteration, because our initial point was such that it tended to move away from the stationary point. You will see that after x^5 , it will be difficult to again come back to this. So, this algorithm will not converge if we start with this particular x^1 . So, Newton method is very sensitive to the initial point. If we start sufficiently close to the solution only then there is a chance that it will converge.

So, with this I will end up my discussion on 1 dimensional unconstrained optimization algorithms. Later on, we will come back to multi dimensional unconstrained optimization problems, where these 1 dimensional unconstrained optimization algorithms are useful. But, before we move on to that, let us start with a new topic, which are convex sets.