## Optimization in Chemical Engineering Prof. Debasis Sarkar Department of Chemical Engineering Indian Institute of Technology, Kharagpur

# Lecture – 35 Unconstrained Multivariable Optimization: Gradient Based Methods (Contd.)

Welcome to lecture 35. So, this is the last lecture or week 7 and in this week we have been talking about gradient based methods for optimization of unconstrained multivariable functions. So, in today's lecture we will briefly talk about Quasi-Newton method and Trust Region method and then we will introduce 2 MATLAB functions from MATLABS optimization toolbox for solutions of unconstrained optimization problems.

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Quasi-Newton Method
The basic iterative process used in the Newton's method is given by
$x^{k+1} - x^k = \Delta x^k = -\left[H(x^k)\right]^{-1} \nabla f(x^k)$
where the Hessian matrix [H] is composed of the second partial derivatives of the function $f$ and varies with the current estimate for a general nonlinear objective function $f$ . Note that for a quadratic function, [H] is a constant matrix.
The basic idea behind the Quasi-Newton or variable metric methods is to approximate either [H] or [H] <sup>-1</sup> by another matrix, using only the first partial derivatives of the objective function <i>f</i> .

So, let us first briefly talk about Quasi-Newton method. The basic iterative process used in the Newton's method is given by x k plus 1 minus x k equal to minus hessian inverse into gradient of f, both evaluated at current point x k. We know that the hessian matrix is composed of the second partial derivatives of the function f and the hessian matrix in general with vary with the current estimate for a general non-linear objective function.

Note that for a quadratic function, the hessian is the constant matrix. But for a general non-linear objective function, the hessian matrix will vary with the current estimate of the optimal point. The basic idea behind the Quasi-Newton method or variable metric

methods is to approximate either the matrix H or H inverse that is a hessian or hessian inverse by another matrix using only the first partial derivatives of the objective function.

So, instead of using second partial derivatives of objective function f, we want to replace the hessian matrix or its inverse by another matrix using only first partial derivatives of the objective function f.

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J	Quasi-Newton Method
	If [H] <sup>-1</sup> is approximated by[B], we can write $x^{k+1} - x^k = \Delta x^k = -\left[H(x^k)\right]^{-1} \nabla f(x^k)$ as:
	$x^{k+1} - x^k = \Delta x^k = -\alpha^k \left[ B^k \right] \nabla f(x^k)^{*}$
	Thus the search direction $s^k$ is: $s^k = -[B^k]\nabla f(x^k)$
	Note that Steepest Descent method is a special case of above equation with [B] = [I].
	<u>Two popular methods:</u> ➢Davidon-Fletcher-Powell (DFP) method ➢Broyden-Fletcher-Goldfarb-Shanno (BFGS) method
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If the inverse of hessian matrix is approximated by a matrix B, we can write as x k plus 1 minus x k equal to alpha k into B k into gradient f at x k. The search direction then is minus B k to gradient of f at x k. Now compare this with the Steepest Descent method if B matrix is equal to identity matrix the search direction is minus gradient of f at x k, which is the search direction for Steepest Descent method.

So, Steepest Descent maker method becomes a special case of this equation with matrix B equal to identity matrix. There are 2 popular methods Davidon-Fletcher-Powell or DFP method and Broyden-Fletcher-Goldfarb and Shanno or BFGS method.

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,	Quasi Newton Method
	These methods approximate the <u>Hessian matrix</u> using only the first partial derivatives of $f(\mathbf{x})$ . Define: $\Delta \mathbf{g}^{k} = \nabla f(\mathbf{x}^{k+1}) - \nabla f(\mathbf{x}^{k})$ $\hat{\mathbf{H}}(\mathbf{x}^{k}) = \hat{\mathbf{H}}^{k}  (\text{approximation of } \mathbf{H}(\mathbf{x}^{k}))$ $\Delta \hat{\mathbf{H}}^{k} = \hat{\mathbf{H}}^{k+1} - \hat{\mathbf{H}}^{k}$
	Basically, the methods update an estimate of the Hessian matrix, or it's inverse. Two particular updating mechanisms are:
	<ul> <li>Davidon-Fletcher-Powell (DFP) method</li> <li>Broyden-Fletcher-Goldfarb-Shanno (BFGS) method</li> </ul>
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These 2 methods update an estimate of the hessian matrix or its inverse. Let us introduce this definitions.

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<b>**</b> **********	Page: 5 / 20
Quasi Newton Method	
Two Updating Mechanisms: (Ref: Edgar and Himmelblau)	
Davidon-Fletcher-Powell (DFP) Method:	
$[\Delta \hat{\mathbf{H}}^{k}]^{-1} = \frac{\Delta \mathbf{x}^{k} (\Delta \mathbf{x}^{k})^{T}}{(\Delta \mathbf{x}^{k})^{T} \Delta \mathbf{g}^{k}} - \frac{[\hat{\mathbf{H}}^{k}]^{-1} \Delta \mathbf{g}^{k} (\Delta \mathbf{g}^{k})^{T} [\hat{\mathbf{H}}^{k}]^{-T}}{(\Delta \mathbf{g}^{k})^{T} [\hat{\mathbf{H}}^{k}]^{-1} \Delta \mathbf{g}^{k}}$	NOTE: In both DFP and BFGS methods, the Hessian matrix method updates
Broyden-Fletcher-Goldfarb-Shanno (BFGS) Method:	remain positive
$\Delta \hat{\mathbf{H}}^{k} = \frac{\Delta \mathbf{g}^{k} (\Delta \mathbf{g}^{k})^{T}}{(\Delta \mathbf{g}^{k})^{T} \Delta \mathbf{x}^{k}} - \frac{\hat{\mathbf{H}}^{k} \Delta \mathbf{x}^{k} (\Delta \mathbf{x}^{k})^{T} \hat{\mathbf{H}}^{k}}{(\Delta \mathbf{x}^{k})^{T} \hat{\mathbf{H}}^{k} \Delta \mathbf{x}^{k}}$	definite. have this property.

With these definitions in mind, the DFP method or the BFGS methods updates the hessian or hessian inverse as shown by this expression. It may be noted that both DFP and BFGS methods keep the hessian matrix positive definite.

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Now, let us briefly define what do you mean by trust region method. We have seen that all gradient based methods use the general scheme x at k plus 1 iteration equal to x at k th iteration plus some stamp step length parameter alpha k into search direction at k. So, in case of gradient based method, we choose a search direction s k that will produce descent. Then perform a line search along this direction Sk.

So, here the emphasis is on finding the descent direction. The trust region methods use a slightly different strategy. In case of trust region methods, we form a trustworthy or safe approximation of the objective function f in a trust region, which is basically the neighborhood of the current estimate in which the current approximation of fx produces descent. So, once we have the trustworthy or safe approximation of the function fx, we find the minimum of this approximate function.

So, here the emphasis is on finding a trustworthy approximation 2 fx. So, emphasis shifts from finding the descent direction to finding a trustworthy or safe approximation to function fx.

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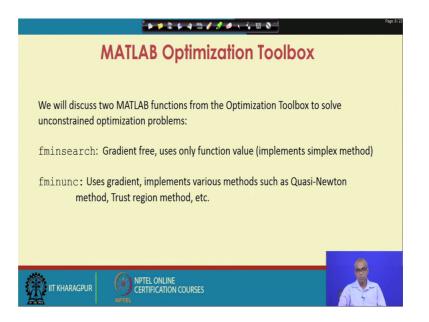
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Trust Region Method
Newton or Quasi Newton Method: $\min m(x^k + s) = f(x^k) + \nabla f(x^k)s + \frac{1}{2}s^T H^k s$
<b>Trust Region Method:</b> The model $m(x^{k+s})$ is an approximation of $f(x^{k+s})$ : $m(x^{k+s}) = f(x^{k+s})$ Alternate problem formulation may be:
$\min m(x^k + s) = f(x^k) + \nabla f(x^k)s + \frac{1}{2}s^T H^k s$
subject to $\ s\  \le \delta_k$
Here $\delta_k$ is the trust region of the model $m(x)$ , i.e. the region where we trust the model is valid.
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So, in case of Newton or Quasi-Newton methods, we solve a problem like this m of x k plus S equal to f at x x k plus gradient of f at x x k into s plus half S transpose H k s. So, basically compare it with trust series expansion and written only second order terms.

In case of trust region method, the model this m x k plus s is basically an approximation of f at x k plus s. So, an alternate problem formulation may be we minimize m at x k plus s which is given as f of x k plus gradient of f x k plus into s plus half s transpose H s a subject to s confined in a small region. So, norm of s is less or equal to a parameter delta. So, delta k is the trust region of the model m that is the region where the trust where the model is trusted to be valid.

So, basically in case of Newton or Quasi-Newton method the focus is on finding the descent direction, the descent direction s, in case of trust region method we want to find out the approximation of the function in a trust region and minimize the function in the trust region.

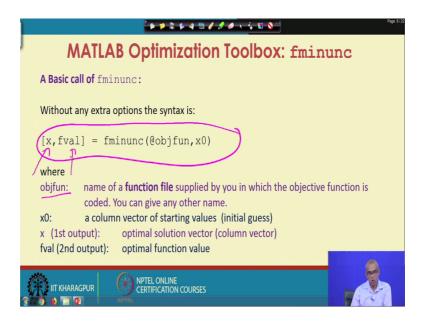
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Now, we will discuss 2 MATLAB functions from the MATLAB optimization toolbox to solve unconstrained optimization problems. In particular we will discuss fminsearch and fminunc. In fminsearch is the gradient free method whereas, fmin unconstrained fminunc uses gradient, fminsearch being a gradient free method uses only function value method, function value of the objective function.

It is a direct search method, it implements simplex method whereas, fminunc uses gradient. So, you have to supply the gradient of the objective function and if we do not supply, it may use numerical computation of the gradient. fminunc you implements various algorithms such as Quasi-Newton method trust region method etcetera.

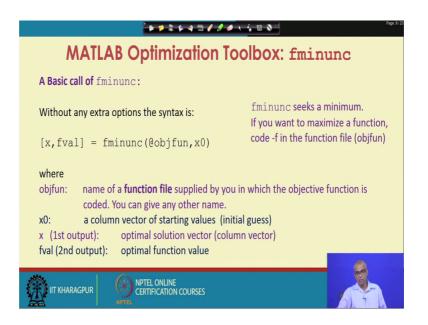
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So, let us first talk about fminunc, fminunc. A basic call is x comma fval is the function name fminunc at objfun objective function, x0 here objfun is the name of a function file supplied by you in which the objective function is coded in MATLAB language.

It is not necessary that you have to give only this name you are free to supply any other valid name.  $x \ 0$  is the column vector of starting values; that means, initial guess, the first output x presents the optimal solution vector. Again it is a column vector and the second output fval presents the optimal function value that is the function value at optimally determined point x.

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By default fminunc seeks a minimum, if you want to maximize a function you simply code minus f in the function file objfun.

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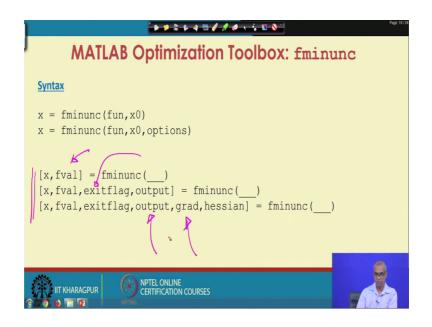
]	MATLAB Optimization Toolbox: fminunc
	<pre>Syntax x = fminunc(fun,x0) x = fminunc(fun,x0,options) [x,fval] = fminunc() [x,fval,exitflag,output] = fminunc() [x,fval,exitflag,output,grad,hessian] = fminunc()</pre>
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So, these presents some more details about the syntax or how you call the MATLAB function, fminunc note x equal to the function file name, the built in function file name the solver fmin unconstrained fminunc it takes 2 arguments the name of the function file in which you have written, the function that you are going to minimize and the initial

guess. Note this if I supply this if I write this, I have no way of telling MATLAB that I am supplying the gradient which needs to be used.

So, for that you have to add one more argument options and through options you can tell MATLAB or this solver fminunc that you are supplying the gradient of the objective function which can be used for minimization and then this gradient can be written in the same function file where your coding the objective function that you are minimizing.

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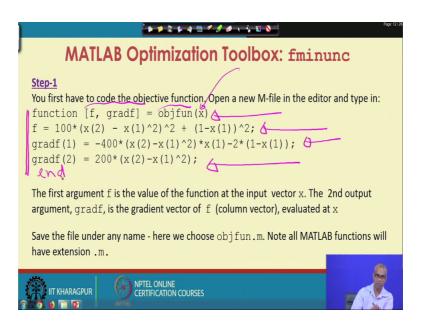


Now, here are more details about the syntax if we look at the left hand part see these are the values that are returned by fminunc. So, x is the optimal function value, fval is the function value at optimum x. So, x is the optimal solution and fval is the function value at the optimal solution. Exit flag is a parameter which tells you about whether the optimization was successful how it existed, similarly output is a structure where you have more information's like number of functions value, number of function calls, number of iterations so on and so forth. You can ask the solver to return information on gradient and hessian as well. (Refer Slide Time: 17:39)

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,	MATLAB Optimization Toolbox: fminunc
	Example: The Rosenbrock Function
	$f(x_1, x_2) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$
	Gradient:
	$\nabla f(x_1, x_2) = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}\right]^T$
	$= \left[-400(x_2 - x_1^2)x_1 - 2(1 - x_1), 200(x_2 - x_1^2)\right]^T$
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So, now let us take an example, let us consider the Rosenbrock function which is the 2 dimensional function 100 into x 2 minus x 1 square whole square plus 1 minus x 1 whole square. So, if we look at this function the minimum value is; obviously, x 1 equal to 1, x 2 equal to 1 and the function value becomes 0. So, the optimal solution for this Rosenbrock function is x 1 equal to 1, x 2 equal to 1 and at this optimal point the function value is 0. So, take the gradient, so we have evaluated the gradient.

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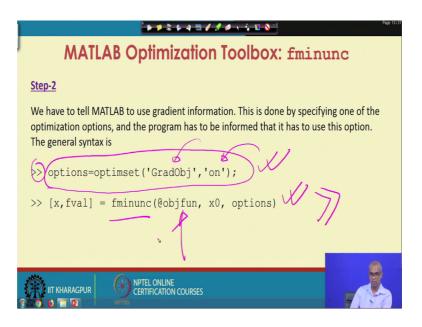


So, in the first step you have to code the objective function. So, open a new M-file in the editor and you have to tie these lines. First line is the definition of the function file this is how we write the function file function then f grad f these are the 2 values that will be returned by the function objfun and x is the input argument to the objfun function.

So, here the Rosenbrock function is coded note that it is 2 dimensional function  $x \ 1$  and  $x \ 2$ . So, the vector x has 2 component x of 1 and x of 2 x of 1 equal to  $x \ 1 x$  of 2 equal to  $x \ 2$ . So, we write the Rosenbrock we code the Rosenbrock function then the 2 components del f del  $x \ 1$  and del f del  $x \ 2$  are coded as grad f 1 and grad f 2. So, that is all if you want you can write n here.

So, the first argument f is the value of the function at the input vector x, the second output argument grad f is the gradient vector of f which is again column vector evaluated at x. Now you save the file under any name here we choose objfun dot m all MATLAB functions will have extension dot m.

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Now in the step two we have to tell MATLAB that the solver fminunc has to use the gradient information. This is done by specifying one of the optimization options and the program has to be informed that it has to use this option.

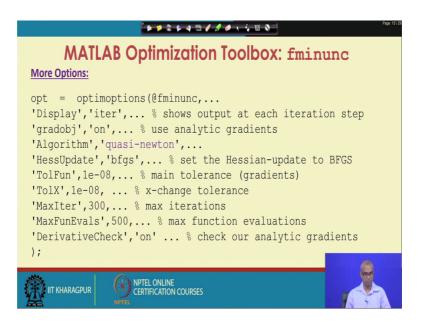
So, the general syntax is options equal to optimset gradobj on; that means, we are supplying gradient and a solver has to use the supplied gradient information. This means

that this symbol represents the comment line. So, you can type it in comment line or you can create another m file give it some other name and write this statement and then call the solver fminunc to solve the problem to minimize the function written in objfun.

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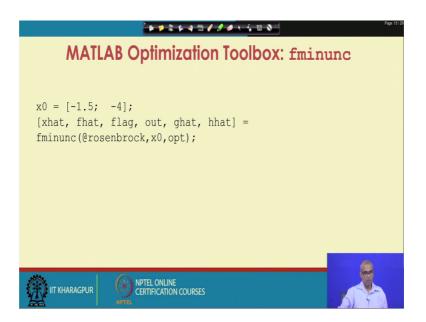
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MATLAB Optimization Toolbox: fminunc
<u>Step-2</u>
We have to tell MATLAB to use gradient information. This is done by specifying one of the optimization options, and the program has to be informed that it has to use this option. The general syntax is >> options=optimset('GradObj','on');
>> [x,fval] = fminunc(@objfun, x0, options)
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So, we are already familiar with the basic sequence basic syntax which is x, fval equal to the solver name, then arguments say our first argument is at then name of the objective name of the function where name of the function file where you have written the objective function as well as gradient. Second argument is the vector having initial guess and third is the options where you have given the option of using gradient information. (Refer Slide Time: 23:28)



Now, so there are many other options that we can use. These options are shown here you can define these options as. So, you define as opt equal to optim options within bracket at fminunc; that means, the name of the solver and then all the options display iter; that means, it will show output at each iteration step grad obj on; that means, it will use analytic gradients. So, analytic gradients will be supplied by you in the function file.

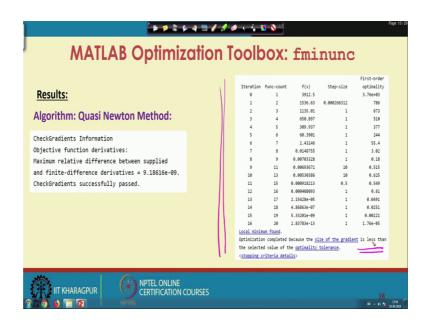
Here we have named that as obj fun algorithm Quasi-Newton. So, I am asking the solver to use quasi Newton method to minimize the function the Rosenbrocks function using Quasi-Newton method HessUpdate means hessian update means hessian update use BFGS method. We talked about BFGS method cross region method TolFun is the tolerance main tolerance for gradients TolX, x change tolerance x is the solution vector MaxIter, 300 means maximum number of iterations is not more than 300, MaxFunEvals maximum number of function evaluations. DerivativeCheck on: So, it will check our analytic gradients. So, different options now are available and you can use all these options or some of these options. (Refer Slide Time: 25:24)



Now, let us solve the Rosenbrock problem with let us say this Quasi-Newton algorithm. So, we are supplying all these options and solving the problem using Quasi-Newton algorithm. So, I supply x 0 equal to minus 1.5 and minus 4 as initial guess, then use the syntax as shown to solve the problem.

So, I have given the name as now say Rosenbrock the objfun. Now I am renaming at as Rosenbrock. You can also give it any other name you want.

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So, this is the solution you get. So, this is a snapshot of the run of the algorithm result of the run of the algorithm. So, it first takes the gradient information's because derivative check option was on and these are the iterations wise results. So, after 16th iteration optimization is complete. The persistent iteration the size of the gradient becomes very small.

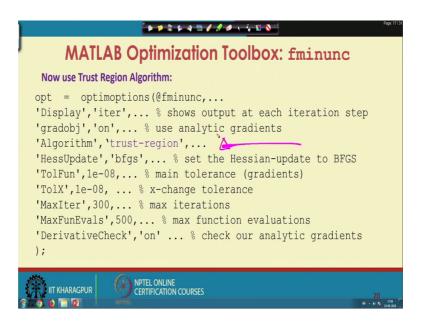
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MA	TLAB Optimization Toolbox: fminu	nc
Results:	xhat = 1.0000 1.0000 fhat =	
	2.8378e-13 flag = 1 out =	
	<pre>struct with fields: iterations: 16 funcCount: 20 stepsize: 1.0617e-04 losselatt: 1</pre>	
	<pre>lssteplength: 1 firstorderopt: 1.2588-05 algorithm: 'quasi-newton' message: 'Local minimum found.""Optimization completed because the size of the gradient is less than"the selected value of the optimality tolerance.""Stopping</pre>	
	criteria details:440ptimization completed: The first-order optimality measure,	
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So, now, look at the solution that you have got 1 1 and we know that x 1 equal to 1 and x 2 equal to 1 is the solution and the function value is 0. So, we get that as 2.83 minus 10 to the power 13. So, very close very small value can be considered as 0.

So, these are the some information's, which is obtained with the structure name out, iterations equal to 16 function count 20 steps size as 1.0617 into 10 to the minus 4 first step length was 1 so on and so forth algorithm uses Quasi-Newton. So, all these details can be obtained.

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Let us now solve the same problem using Trust Region method. So, you just change the option here algorithm, it was Quasi-Newton method. Now I change the algorithm to Trust Region. So, now, I am telling the solver that the algorithm that needs to be use is trust region everything else remains unchanged. So, this is the result.

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		Norm of	First-order		must marked all a differences
Iteration	f(x)	step	cotinality	CG-iterations	Trust Region Algorithm:
0	3912.5		3.76e+03		
1	6.24001	6.24491	5	1	and the second
2	6.24001	7.88371	5	1	fminunc stopped because the final change in function value relative to
3	6.24001	1.97093	5	0	its initial value is less than the selected value of the function tolerance.
4	5.50743	0.492732	14.3	0	
5	5.41817	0.985464	51.8	1	< <u>stopping criteria details</u> >
6	3.65108	0.0864031	6.09	1	xhat =
7	3.19595	0.246366	6.28	1	1.0000
8	2.76465	0.492732	17.1	1	1.0000
9	2.00507	0.109746	4.57	1	1.0000
10	2.00507	0.578825	4.57	1	
11	1.71896	0.123183	3.33	0	
12	1.37804	0.246366	8.39	1	fhat =
13	0.978233	0.118359	2.73	1	1.5226e-19
14	0.978233	0.264033	2.73	1	flag =
15	0.848752	0.0615915	1.67	0	3
16	0.663295	0.123183 0.212605	3.18	1	out +
18	0.288515	0.118991	1.07	1	struct with fields:
19	0.232956	0.246366	7.67	1	iterations: 27
20	0.0959621	0.104984	0.451	1	funcCount: 28
21	0.0718443	0.246366	6.71	1	stepsize: 1.3917e-05
22	0.0179744	0.0804931	0.201	1	
23	0.015862	0.223585	4.8	1	cgiterations: 23
24	0.000254066	0.0257771	0.0155	1	firstonderopt: 1.5332e-08
25	6.25444e-06	0.0349246	0.0995	1	algorithm: 'trust-region'
26	3.86852e-11	0.000513953	6.24e-05	1	message: 'Local minimum possible.44fminunc stopped because the final
27	1.52262e-19	1.39171e-05	1.53e-08	1	change in function value relative to wits initial value is less than the selected
	m possible.				

Now after 27 iterations we obtain the minimum and minimum again is obtained as x = 1 equal to 1 x 2 equal to 1. The function value is 1.5226 into 10 to the power minus 19

which is very small. The details are available in the structure called out 27 iterations were required function count is 28 Trust Region algorithm was used.

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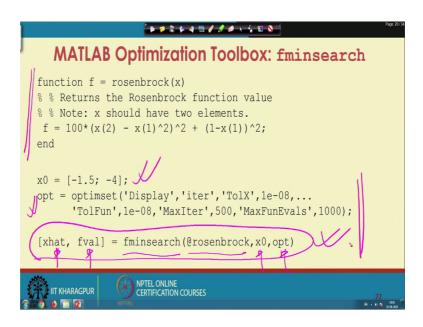
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1	MATLAB Optimization Toolbox: fminsearch
	<pre>function f = rosenbrock(x) % % Returns the Rosenbrock function value % % Note: x should have two elements. f = 100*(x(2) - x(1)^2)^2 + (1-x(1))^2; end</pre>
	<pre>x0 = [-1.5; -4]; opt = optimset('Display', 'iter', 'TolX', 1e-08, 'TolFun', 1e-08, 'MaxIter', 500, 'MaxFunEvals', 1000); [xhat, fval] = fminsearch(@rosenbrock, x0, opt)</pre>
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Now, let us look at the use of fminsearch. Once you are familiar with use of any solver you can easily understand the use of other solvers. For example, as of now we have seen how fminunc works. Now we are talking about fminsearch, fminsearch does not use gradient information. In fact, it implements simplest method to solve an unconstrained optimization problem.

But you will see that the basic syntax that will use are very similar. Again we define a function file let us call Rosenbrock where I quote the Rosenbrock function. He does not use gradient information, so, no need to supply the gradient information. Initial guess is given as x 0 vector same starting point I use minus 1.5 minus 4. Now let us say I give these options. So, opt equal to optimset display iter; that means, each iterations will be displayed.

X tolerance is 10 to the power minus 8, function tolerance 10 to the power minus 8, maximum iterations 500, maximum function evaluations 1000. So, once these are defined in the options.

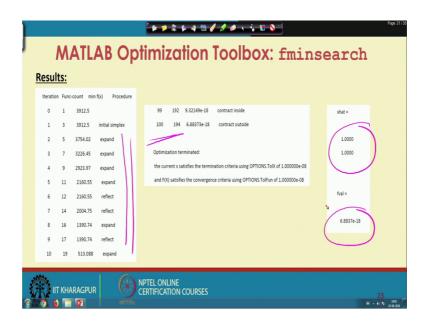
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We call fminsearch using this syntax xhat fval, xhat returns the solution optimal solution, fval is the function value at optimal solution, fminsearch is the name of the solver at rosenbrock. So, this is the function file where you have coded the function x 0 is the initial starting point, initial vector is a column vector and opt is the options that we are specified.

So, you write these statements as an M-file let us call them file as Rosenberg dot m then you either type in these in the common mode both these 3 lines or write another M-file where you write these three lines and then hit the run button and you will get this solution.

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Note, it is using simple x method, so it is talking about expansion of simplex, contraction of simplex, reflection all these things.

We have gone up to 100 iterations and the solution is again is obtained as x 1 equal to 1, x 2 equal to 1 the function value is 6.8837 into 10 to the power minus a which is extremely small can be considered as 0. So, we learn how to make use of MATLAB optimization toolbox. In fact, 2 function files 2 functions from MATLAB optimization toolbox namely fminunc and fminsearch. Both are used for solutions of unconstrained minimization problem. You can solve for maximization of problem simply by taking negative of f. With this, we stop our lecture number 35 here.