

Lecture 6

First and Second order unconstrained optimization

The Steepest Descent Method

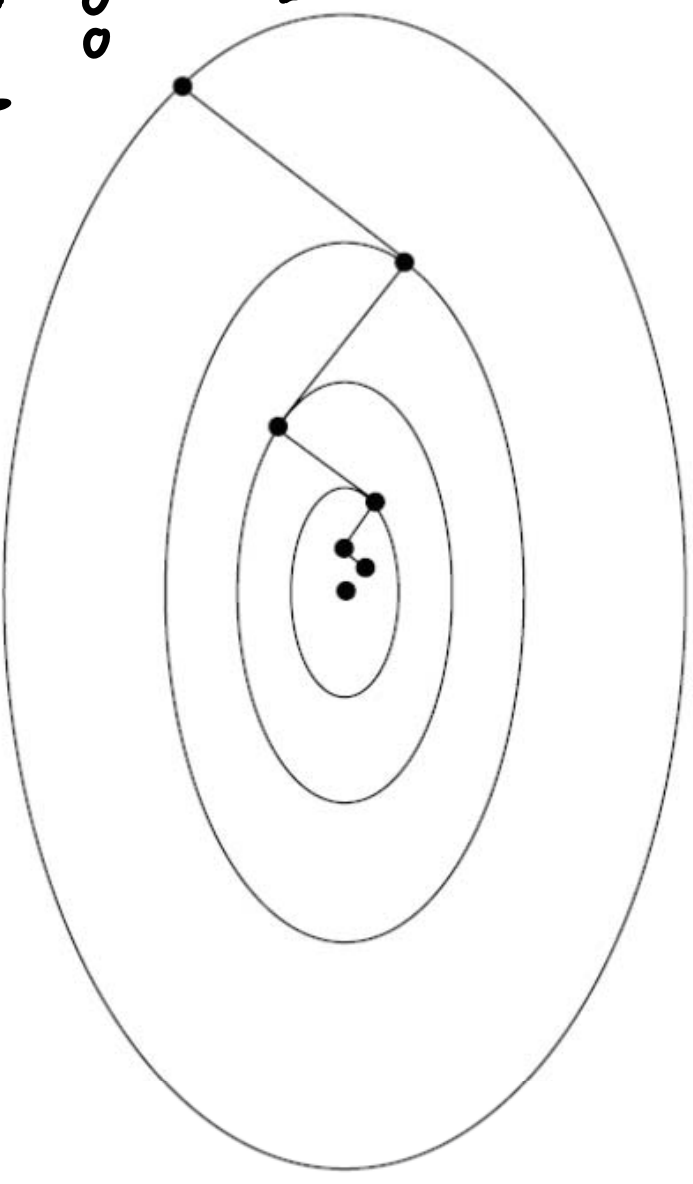
* The direction of ∇f at any point in the parameter space gives the direction of maximum function ascent $\Rightarrow -\nabla f$ is direction of steepest function descent.

* At the k th time step x_k , the new point x_{k+1} is given by $x_{k+1} = x_k + \gamma_k^* (-\nabla f)$.
 γ_k^* is obtained through line search
 $\gamma_k^* = \arg \min_{\gamma} f(x_k - \gamma \nabla f)$

Illustration

* Fast reduction
in objective
function far
from the solution

* Convergence is too
slow near solution!



Example

Use the method of steepest descent to find the minimizer of

$$f(x_1, x_2, x_3) = (x_1 - 4)^4 + (x_2 - 3)^2 + 4(x_3 + 5)^4.$$

Start from the point $x^{(0)} = [4, 2, -1]^T$ and

Carry out only 2 iterations.

$$\text{Solution: } \nabla f(x) = [4(x_1 - 4) \quad 2(x_2 - 3) \quad 16(x_3 + 5)^3]^T$$

$$\nabla f(x^{(0)}) = [0 \quad -2 \quad 1024]^T$$

Example (Cont'd)

$$\underline{x}_0 = \text{arg min}_{\underline{x} > 0} f(\underline{x}^{(0)}) \rightarrow \nabla f(\underline{x}^{(0)})$$

$$f(\underline{x}) = f(\underline{x}^{(0)}) - \lambda \nabla f(\underline{x}^{(0)})$$

$$f(\underline{x}) = 0^4 + (2+2\lambda-3)^2 + 4(-1-1024\lambda+5)^4$$

Using the secant method, we obtain

$$\underline{x}_0 = 3.967 \times 10^{-3} \rightarrow \underline{x}^{(1)} = [4.000 \quad 2.668 \quad -5.062]^T$$

$$\nabla f(\underline{x}^{(1)}) = [0 \quad -1.984 \quad -0.063875]^T$$

$$\underline{x}_1 = \text{arg min}_{\underline{x} > 0} f(\underline{x}^{(1)}) \rightarrow \nabla f(\underline{x}^{(1)})$$

Example (Cont'd)

$$f(x) = (2.088x + 1.984x - 3)^2 + 4(-5.062x + 0.003875x + 5)^4$$

Using a Secant method, we obtain $x_1^* = 0.500$

$$x^{(2)} = x^{(1)} - x_1^* \Delta f(x^{(1)}) = [4.000 \quad 3.000 \quad -5.066]^T$$

$$\Delta f(x^{(2)}) = [0.000 \quad 0.000 \quad -0.003525]^T$$

MATLAB CODE

```
%This program carries out the steepest descent direction
NumberOfParameters=3; %This is n for this problem
OldPoint=[3 -3 5] %This is the starting point
OldValue=getObjective(OldPoint) %Get the objective function at the old point
Tolerance=0.001; %terminating tolerance for line search
Epsilon=0.001; %exploration step
LambdaMax=4.0; %maximum value of lambda for line search
StepNorm=1000; %initialize stepNorm
MinimumDistance=1.0e-4; %this is the terminating distance
while(StepNorm>MinimumDistance) %repeat until maximum number of iteration is achieved
    Gradient=getGradient('getObjective',OldPoint, Epsilon); %get the gradient at the old point
    NormalizedNegativeGradient=-1.0*Gradient/norm(Gradient); %normalize the gradient
    LambdaOptimal = GoldenSection('getObjective',Tolerance,OldPoint,
        NormalizedNegativeGradient,LambdaMax); %get the optimal value
    NewPoint=OldPoint+LambdaOptimal*NormalizedNegativeGradient; %Get new point
    NewValue=feval('getObjective',NewPoint); %Get the New Value
    StepNorm=norm(NewPoint-OldPoint); %get the norm of the step
    OldPoint=NewPoint %update the current point
    OldValue=NewValue %update the current value
end
```

Code Output

Minimize the objective function

$$f(x_1, x_2, x_3) = (x_1 - 1)^2 + (x_2 - 5)^2 + (x_3 - 4)^2$$

OldPoint=[3 -3 5] OldValue =69

OldPoint =[2.0368 0.8517 4.5183] OldValue = 18.5518

OldPoint = [1.0735 4.7034 4.0365] OldValue = 0.0947

OldPoint =[0.9994 5.0000 3.9994] OldValue = 6.9495e-007

Why only
3 iterations?

What Are Conjugate Directions?

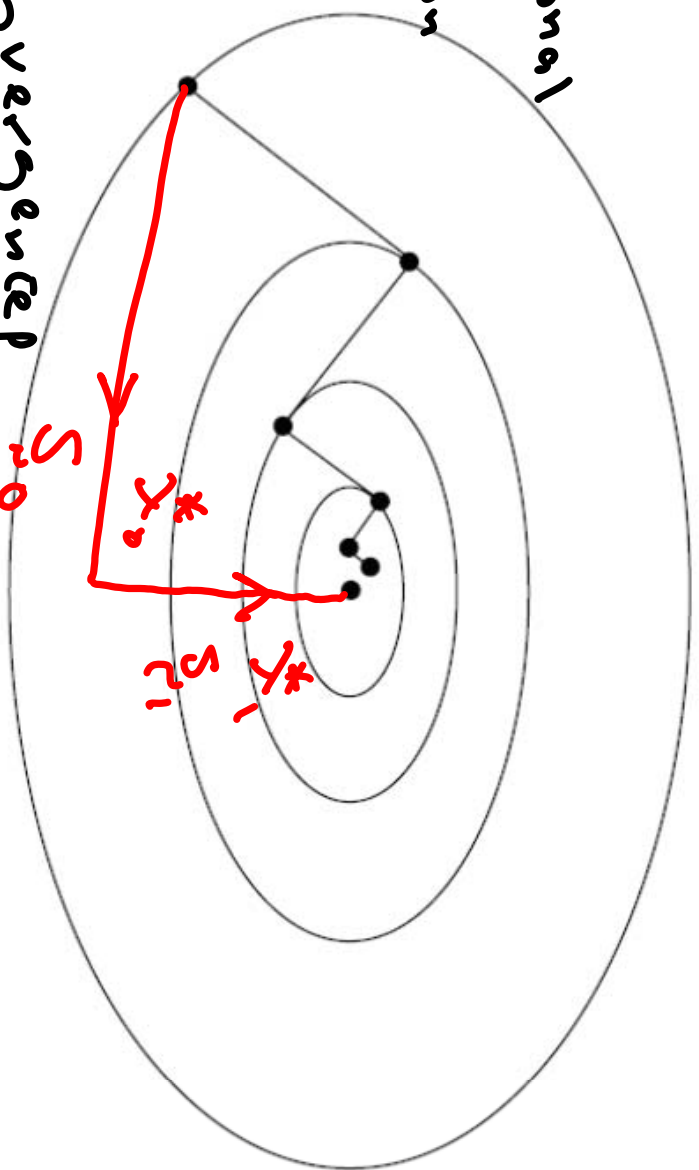
* A general quadratic function of n variables is given by $f(x) = \frac{1}{2} x^T H x + b^T x + c$
 $H \in \mathbb{R}^{n \times n}$, $b \in \mathbb{R}^n$, $c \in \mathbb{R}$.

- * Two directions s_i and s_j are H -conjugate if they satisfy $s_i^T H s_j = 0$, $i \neq j$
- * Orthogonal directions are conjugate relative to the identity matrix.

Optimization Using Conjugate Directions

The minimizer of an n -dimensional quadratic function is obtained in at most n iterations.

⇒ quadratic convergence



Derivative Free Conjugate Directions

Parallel Subspace Property:

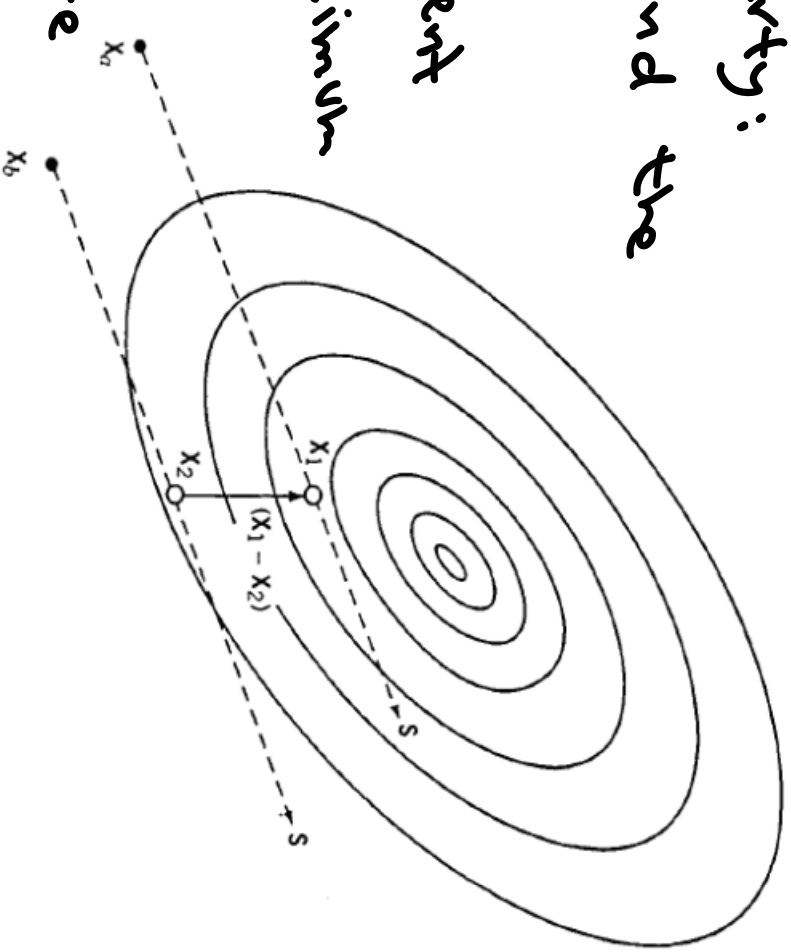
* Starting from x_a , find the minimum x_1 along S_1

* Starting from a different point x_b , find the minimum

x_2 along S_2

$\Rightarrow (x_1 - x_2)$ is Conjugate

to S_1 !



Proof: Assume $f(x) = \frac{1}{2} x^T H x + b^T x + c$

$$\Rightarrow \nabla f(x) = Hx + b$$

$$\nabla f(x_1) = Hx_1 + b, \quad \nabla f(x_2) = Hx_2 + b$$

$$\nabla f(x_1) - \nabla f(x_2) = H(x_1 - x_2) \quad \leftarrow \textcircled{1}$$

Because x_1 and x_2 are minimizers in the

direction of s_1 , we have $s_1^T \nabla f(x_1) = s_1^T \nabla f(x_2) = 0$

$$s_1^T Hx_1 + s_1^T b = 0, \quad s_1^T Hx_2 + s_1^T b = 0$$

$$\Rightarrow s_1^T H(x_1 - x_2) = 0 \Rightarrow (x_1 - x_2) \text{ is conjugate}$$

to s_1 !

A Method For Conjugate Directions

For $n=3$

- * Initialize all 3 directions to $e_i, i=1,2,3$
- * Starting from x_0 find minimum along e_3 to get x_1
- * From x_1 , sequentially minimize along e_1, e_2, e_3 to get z_1
- * $p_{1,1} = (z_1 - x_1)$ is conjugate to e_3 (why?)
- * Search from z_1 along $p_{1,1}$ to get x_2 .
- * Repeat next star using $e_2, e_3, p_{1,1}$

Illustration

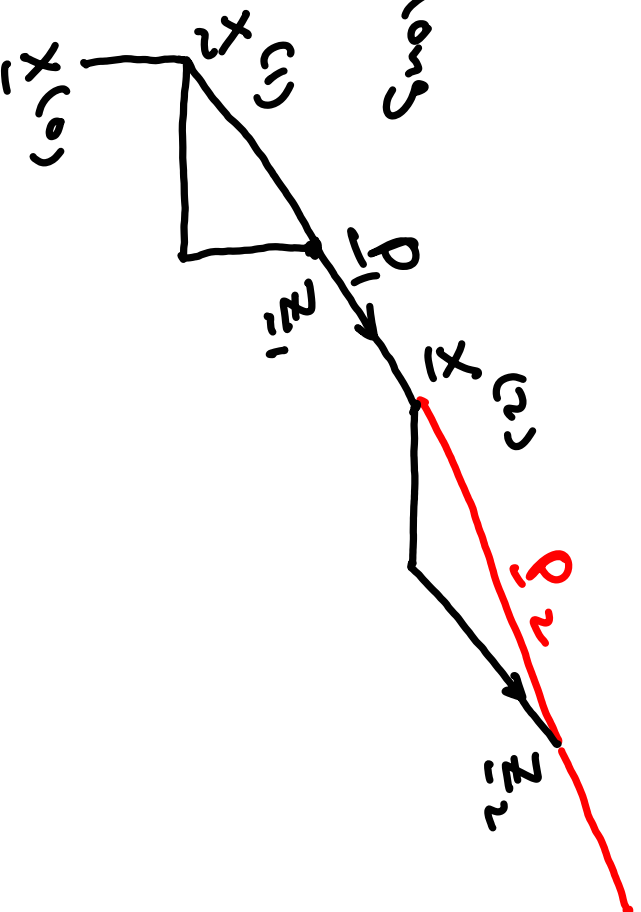
* from x_0 minimize along

e_2 to get x_1

* from x_1 , minimize

along both e_1 and e_2

to get x_2



* $P_1 = Z_1 - x_1$ is conjugate to e_2 . Search along

P_1 to get x_2 . Repeat using e_1 and P_1

The Algorithm

Initialization: Set x_0 . Set $p_i = e_i, i=1, 2, \dots, n$.

Compute x_1 as the minimizer of f along the

line $x_0 + \lambda p_n$

Repeat

Set $z_{n+1} = x_k$

Get $z_{n+1} = z_1 + \lambda_1^* p_1 + \lambda_2^* p_2 + \dots + \lambda_n^* p_n$

Set $p_j = p_{j+1}$ for $j=1, 2, \dots, n-1$. Set $p_n = z_{n+1} - z_1$.

Get $x_{k+1} = z_{n+1} + \lambda^* p_n$.

$k = k+1$

end

MATLAB CODE

```
up=Directions(:,NumberOfParameters); %get the vector ei
um=-1.0*up; %get the vector -ei
fp=feval('getObjective',OldPoint+Epsilon*up); %get +ve value
if(fp<OldValue) u=up; else u=um; end
LambdaOptimal = Goldensection
('getObjective',Tolerance,OldPoint,u,LambdaMax);
NewPoint=OldPoint+LambdaOptimal*u; %get new point
NewValue=getObjective(NewPoint);
OldPoint=NewPoint;
OldValue=NewValue;
while(StepNorm>1.0e-4) %repeat
    YOld=OldPoint; %start exploring
    YOldValue=OldValue; %store also the old value
    for i=1:NumberOfParameters %repeat for all coordinates
        up=Directions(:,i); %get the vector ei
        um=-1.0*up; %get the vector -ei
        fp=feval('getObjective',YOld+Epsilon*up); %get value
        if(fp<OldValue) u=up; else u=um; end
        LambdaOptimal = Goldensection
        ('getObjective',Tolerance,YOld,u,LambdaMax); %get optimal
        YNew=YOld+LambdaOptimal*u; %get new exploration point
        YNewValue=feval('getObjective',YNew); %get new value
        YOld=YNew;
        YOldValue=YNewValue;
    end
end

ConjugatedDirection=YOld-OldPoint; %determine new
direction
LambdaOptimal = Goldensection
('getObjective',Tolerance,YOld,ConjugatedDirection,Lambda
Max);
NewPoint=YOld+LambdaOptimal*ConjugatedDirection; %Get
new point
NewValue=feval('getObjective',NewPoint); %Get the
New Value
StepNorm=norm(NewPoint-OldPoint); %get the norm of
the step
for j=1:(NumberOfParameters-1)
    Directions(:,j)=Directions(:,(j+1));
end
Directions(:,NumberOfParameters)=ConjugatedDirection;
%store the new conjugate direction
OldPoint=NewPoint %update the current point
OldValue=NewValue %update the current value
pause
end
OldPoint
OldValue
```


Example 1

Utilize the Conjugate Directions method to minimize the function

$$f(x) = 4(x_1 - 1)^2 + 3(x_2 - 5)^2 + (x_3 - 4)^2 \quad \text{starting}$$

$$\text{from } \underline{x}^{(0)} = \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}^T.$$

OldPoint = [0 0 0]^T OldValue = 95

OldPoint = [1.0001 5.0003 4.0001]^T OldValue = 2.1657e-007

Solution is
obtained in one
iteration!

Example 2

Find the minimum of the function

$$f(x_1, x_2, x_3) = 1.5x_1^2 + 2x_2^2 + 1.5x_3^2 + x_1x_3 + 2x_2x_3 - 3x_1 - x_3$$

Starting from the point $x^{(0)} = [0 \ 0 \ 0]^T$:

OldPoint = [0 0 0] OldValue = 0

OldPoint = [0.8889 0.0000 0.3333] OldValue = -1.3518

OldPoint = [0.8889 -0.1667 0.3333] OldValue = -1.4074

OldPoint = [0.9583 -0.1667 0.1250] OldValue = -1.4653

OldPoint = [1.0000 0.0000 -0.0000] OldValue = -1.5000

Analytical Solution

$$\nabla f(x) = \begin{bmatrix} 3x_1 + x_3 - 3 \\ 4x_2 + 2x_3 \\ x_1 + 2x_2 + 2x_3 - 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Solving these 3 eqns, we get

$$\bar{x}^* = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad f(\bar{x}^*) = -1.5 \quad \checkmark$$

Conjugate Gradient Methods

* These methods exploit the gradient at each point to construct the conjugate direction at the current step.

* The new iteration is obtained by carrying out a line search along the current conjugate direction.

Fletcher-Reeves Method

* Start with an initial point x_1 . The first conjugate direction is $S_1 = -\nabla f(x_1)$

* At the k th iteration, the new solution is obtained through a line search $x_{k+1} = x_k + \alpha_k^* S_k$.

* The new conjugate direction S_{k+1} is given by

$$S_{k+1} = -\nabla f(x_{k+1}) + \frac{\|\nabla f(x_{k+1})\|^2}{\|\nabla f(x_k)\|^2} S_k$$

* Set $n = k+1$ and repeat!

MATLAB CODE

```
NumberOfParameters=3; %This is n for this problem
OldPoint=[3 -7 0] %This is the starting point
OldValue=getObjective(OldPoint) %Get the objective function at the old point
Epsilon=1.0e-3; %this is the perturbation
LambdaMax=5; %maximum lambda for line search
Tolerance=1.0e-4; %termination condition for line search
Gradient=getGradient('getObjective', OldPoint, Epsilon); %get the gradient at the first point
NormGradientOld=norm(Gradient); %get the norm of the gradient at the current point
ConjugatedDirection=-1.0*Gradient; %initialize the first direction
IterationCounter=0;
while(IterationCounter<NumberOfParameters) %do only n iterations
    LambdaOptimal = GoldenSection('getObjective',Tolerance,OldPoint,ConjugatedDirection,LambdaMax);%do line search
    NewPoint=OldPoint+LambdaOptimal*ConjugatedDirection; %get new point
    NewValue=feval('getObjective',NewPoint); %get new objective function value
    NewGradient=getGradient('getObjective', NewPoint, Epsilon); %get new gradient
    NormGradientNew=norm(NewGradient); %get norm of the new gradient
    %now we determine the new conjugate direction
    NewConjugatedDirection=-1.0*NewGradient+((NormGradientNew*NormGradientNew)/(NormGradientOld*NormGradientOld))
    *ConjugatedDirection;
    %now we make the new point the current point
    OldPoint=NewPoint
    OldValue=NewValue
    Gradient=NewGradient;
    NormGradientOld=NormGradientNew;
    ConjugatedDirection=NewConjugatedDirection;
    IterationCounter=IterationCounter+1;
end
```

Code Output

Utilize the Fletcher-Reeves method to minimize the function

$$f(x) = 4(x_1 - 1)^2 + 3(x_2 - 5)^2 + (x_3 - 4)^2 \quad \text{Starting from } \underline{x}^{(0)} = [3 \quad -7 \quad 0]^T.$$

OldPoint = [3 -7 0] OldValue = 464

OldPoint = [0.3529 4.9085 1.3231] OldValue = 8.8661

OldPoint = [1.3885 5.1720 2.4461] OldValue = 3.1071

OldPoint = [0.9996 4.9990 3.9992] OldValue = 4.6080e-006

Newton's Method

* This method exploits the 2nd order information of the function under consideration

$$\nabla_1 f(x_k) = \nabla_1^2 f(x_k) * H_2^{-1}(x_k - x_{k-1})$$

by setting $\nabla_1 f(x_k) = 0$, we obtain

$$H_2 \Delta x_k = -\nabla_1 f(x_k) \Rightarrow x_{k+1} = x_k - H_2^{-1} \nabla_1 f(x_k)$$

* The method may diverge if the starting point is far!

Newton's Method (cont'd)

* For a quadratic function, this method converges in only ONE iteration.

* This method may converge to a local maximum, a local minimum, or a saddle point

* Notice that we move along the direction

$$S_2 = -H_2^{-1} \nabla f(x_2) \text{ a distance of } \lambda=1.$$

* For non quadratic function, we do a line search

Example Use Newton's method to minimize the function

$$F(x) = (x_1 + 10x_2)^2 + 5(x_3 - x_4)^2 + (x_2 - 2x_3)^4 + 10(x_1 - x_4)^4$$

Starting from the point $x^{(0)} = [3 \quad -1.0 \quad 0 \quad 1]^T$

Solution: $\nabla F(x) =$

$$\begin{bmatrix} 2(x_1 + 10x_2) + 40(x_1 - x_4)^3 \\ 20(x_1 + 10x_2) + 4(x_2 - 2x_3)^3 \\ 10(x_3 - x_4) - 4(x_2 - 2x_3) \\ -10(x_3 - x_4) - 40(x_1 - x_4)^3 \end{bmatrix}$$

Example (Cont'd)

$$H = \begin{bmatrix} 2 + 120(x_1 - x_4)^3 & 20 & 0 & -120(x_1 - x_4)^2 \\ 20 & 200 + 12(x_2 - 2x_3)^2 & -24(x_2 - 2x_3)^2 & 0 \\ 0 & -24(x_2 - 2x_3)^2 & 10 + 48(x_2 - 2x_3)^2 & -10 \\ -120(x_1 - x_4)^2 & 0 & -10 & 10 + 120(x_1 - x_4)^2 \end{bmatrix}$$

First iteration

$$f(x^{(0)}) = 215$$

$$\nabla f(x^{(0)}) = \begin{bmatrix} 306 \\ -144 \\ -2 \\ -310 \end{bmatrix}$$

Example (Cont'd)

$$\bar{H}(\bar{x}^{(9)}) =$$

$$\begin{bmatrix} 482 & 20 & 0 & -480 \\ 20 & 212 & -24 & 0 \\ 0 & -24 & 58 & -10 \\ -480 & 0 & -10 & 480 \end{bmatrix}$$

$$(\bar{H}(\bar{x}^{(9)}))^{-1} =$$

$$\begin{bmatrix} 0.1126 & -0.0089 & 0.0154 & 0.1106 \\ -0.0089 & 0.0057 & 0.0008 & -0.0087 \\ 0.0154 & 0.0008 & 0.0203 & 0.0155 \\ 0.1106 & -0.0087 & 0.0155 & 0.1107 \end{bmatrix}$$

Example (Cont'd)

$$\Delta \bar{x}^{(0)} = -\bar{H}^{(0)^{-1}} \nabla f(\bar{x}^{(0)}) = -1*$$

$$\begin{bmatrix} 1.4127 \\ -0.8413 \\ -0.2540 \\ 0.7460 \end{bmatrix}$$

$$\bar{x}^{(1)} = \bar{x}^{(0)} + \Delta \bar{x}^{(0)} = \begin{bmatrix} 3 \\ -1.0 \\ 0 \\ 1.0 \end{bmatrix} -$$

$$\begin{bmatrix} 1.4127 \\ -0.8413 \\ -0.2540 \\ 0.7460 \end{bmatrix} =$$

$$\begin{bmatrix} 1.5873 \\ -0.1587 \\ 0.2540 \\ 0.2540 \end{bmatrix}$$

$$f(\bar{x}^{(1)}) = 31.8$$

Example (Cont'd)

Second iteration

$$\nabla f(x^{(2)}) = \begin{bmatrix} 94.81 \\ -1.179 \\ 2.371 \\ -94.81 \end{bmatrix}$$

$$H^{(2)} = \begin{bmatrix} 215.3 & 20 & 0 & -213.3 \\ 20 & 205.3 & -10.67 & 0 \\ 0 & -10.67 & 31.34 & -10 \\ -213.3 & 0 & -10 & 222.3 \end{bmatrix}$$

$$H^{(2)} \nabla f(x^{(2)}) = \begin{bmatrix} 6.5291 \\ -0.0529 \\ 0.0846 \\ 0.0846 \end{bmatrix}$$

$$\begin{aligned} \bar{x}^{(2)} &= x^{(1)} + \Delta \bar{x}^{(2)} \\ f(\bar{x}^{(2)}) &= 6.28 \end{aligned}$$

$$\begin{bmatrix} 1.5873 \\ -0.1587 \\ 0.2540 \\ 0.2540 \end{bmatrix}$$

$$\begin{bmatrix} 0.5291 \\ -0.0529 \\ 0.0846 \\ 0.0846 \end{bmatrix}$$

$$\begin{bmatrix} 1.0582 \\ -0.1058 \\ 0.1694 \\ 0.1694 \end{bmatrix}$$

MAIN ISSUES WITH Newton's Method

- * The direction $S_{n+1} = -H_n^{-1} \nabla f$ may not be a descent direction if the Hessian is not positive definite.
- * The Hessian matrix of a non quadratic function is not definite near local minima.
- * Starting from a far point, the method may diverge.

The Levenberg-Marquardt Method

* This Method addresses the drawbacks of Newton Method.

* The k th iteration step is given by

$$\Delta x_k = - (H_k^{(m)} + \mu I)^{-1} \nabla f(x_k)$$

μ is selected such that $H_k^{(m)} + \mu I$ is +ve definite.

* What are the eigenvalues of $H_k^{(m)} + \mu I$?

The Levenberg-Marquardt Method (Cont'd)

* Notice that if $\mu = 0$, $\Delta x = -\tilde{H}^{-1} \nabla f \Rightarrow$
regular Newton's step

* If μ is large enough $\mu \tilde{I} \gg \tilde{H} \Rightarrow$

$\Delta x \approx -\frac{1}{\mu} \nabla f \Rightarrow$ steepest descent direction

* Usually we start each iteration with a small μ and increase μ until a descent step is achieved.

MATLAB CODE

```
NumberOfParameters=3; %This is n for this problem
Epsilon=1.0e-3; %perturbation used in finite differences
OldPoint=[3 -7 0]'; %This is the starting point
OldValue=getObjective(OldPoint)
OldGradient=getGradient('getObjective', OldPoint, Epsilon)
OldGradientNorm=norm(OldGradient); %get the old gradient norm
OldHessian=getHessian('getObjective', OldPoint, Epsilon)
Identity=eye(NumberOfParameters); %This is the identity matrix
while (OldGradientNorm>1.0e-5)
    TrustRegionParameter=0.001; %initialize trust region parameter
    DescentFlag=0;
    while (DescentFlag==0)
        MarquardtMatrix=OldHessian+TrustRegionParameter*Identity;
        NewStep=-1.0*inv(MarquardtMatrix)*OldGradient
        NewPoint=OldPoint+NewStep %get the new trial point
        NewValue=fval('getObjective',NewPoint); %calculate new value
        if (NewValue<OldValue) %a descent step
            DescentFlag=1.0;
        else
            TrustRegionParameter=TrustRegionParameter*4;
        end
    end
end

step=NewPoint-OldPoint; %get the new step
stepNorm=norm(step); %get the step norm
NewGradient=getGradient('getObjective',
    NewPoint, Epsilon); %get new gradient
    NewHessian=getHessian('getObjective', NewPoint,
        Epsilon); %get new Hessian
        %now we swap parameters
        OldPoint=NewPoint;
        OldGradient=NewGradient;
        OldHessian=NewHessian;
        OldGradientNorm=norm(OldGradient);
    end
end
```

Example 2

Find the minimum of the function

$$f(x) = 1.5x_1^2 + 2x_2^2 + 1.5x_3^2 + x_1x_3 + 2x_2x_3 - 3x_1 - x_3$$

Starting from $x^{(0)} = [3 \ -7 \ 0]^T$.

$$\text{OldPoint} = [3 \ -7 \ 0]^T \quad \text{OldValue} = 102.5000$$

$$\text{OldGradient} = [6.0015 \ -27.9980 \ -11.9985]^T$$

$$\text{OldHessian} = \begin{bmatrix} 3.0000 & 0 & 1.0000 \\ 0 & 4.0000 & 2.0000 \\ 1.0000 & 2.0000 & 3.0000 \end{bmatrix}$$

$$\text{NewStep} = [-2.0004 \ 6.9969 \ 0.0017]^T$$

$$\text{NewPoint} = [0.9996 \ -0.0031 \ 0.0017]^T$$

$$\text{NewValue} = -1.5000$$

exact solution

$$x^* = [1.0 \ 0 \ 0]^T$$

