

Newton's Method

This Hypercard stack was prepared by:
 Dennis L. Bricker,
 Dept. of Industrial Engineering,
 University of Iowa,
 Iowa City, Iowa 52242
 e-mail: dbricker@icaen.uiowa.edu

Reference: Section 3.5 of Linear &
 Nonlinear Programming, by A. Sofer
 and S. Nash

author

Newton's Method

- ☞ Solving Nonlinear Equations
- ☞ Optimizing a Nonlinear Function



Solving Nonlinear Equations

- ☞ Single equation with single variable
 $g(x) = 0$
- ☞ System of n equations in n variables
 $g_i(x_1, x_2, \dots, x_n) = 0 \quad \forall i=1,2, \dots, n$



Let x_0 be an initial "guess" at the solution of

$$g(x) = 0$$

If $g(x_0) \neq 0$, then we wish to find a correction δ so that

$$g(x_0 + \delta) \approx 0$$

Then $x_1 = x_0 + \delta$ becomes our improved approximation, and we repeat the procedure until $g(x_k)$ is "sufficiently close" to zero.



Suppose that x_k is a "guess" or approximation to the solution of $g(x) = 0$ at iteration k.

$$g(x_k + \delta) = g(x_k) + g'(x_k)\delta + \underbrace{\frac{g''(x_k + \alpha\delta)}{2} \delta^2}_{\text{assumed negligible}} \approx 0$$

Solve the equation

$$g(x_k + \delta) = g(x_k) + g'(x_k)\delta = 0$$

for the δ which will give (hopefully) an improved approximate solution.



Solving a Nonlinear Equation $g(x) = 0$

...when an analytic solution doesn't exist.
 For example, $2x - \sin x = 0.5$,
 $x^2 + x \log x = 1$,
 $x^4 - 2x + 5 = 0$, etc.

The Newton-Raphson method is an iterative, successive-approximation method for numerically solving such equations.



Solving a Nonlinear Equation $g(x) = 0$

For some $z \in [x^*, x]$,

$$g(x) = g(x^*) + g'(x^*)(x - x^*) + \frac{g''(z)}{2} (x - x^*)^2$$

Equivalently,

$\exists \alpha \in [0,1]$ such that

$$g(x + \delta) = g(x) + g'(x)\delta + \frac{g''(x + \alpha\delta)}{2} \delta^2$$

Taylor's Formula



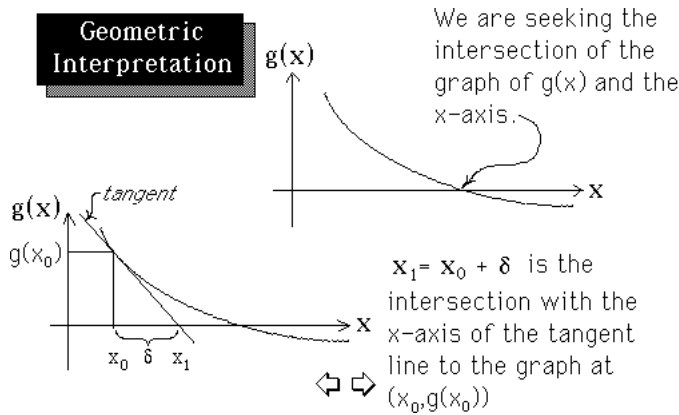
$$g(x_k) + g'(x_k)\delta = 0 \Rightarrow \delta = -\frac{g(x_k)}{g'(x_k)}$$

The new (improved?) approximation is then

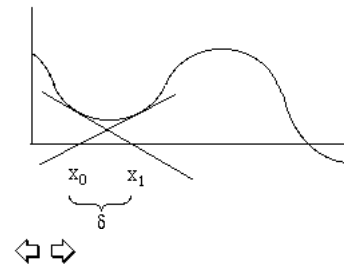
$$x_{k+1} = x_k + \delta = x_k - \frac{g(x_k)}{g'(x_k)}$$



Geometric Interpretation



Possible "Pathologies" of Newton's Method



Rate of Convergence

Define the error at iteration k by $\epsilon_k = x_* - x_k$
 Taylor's formula implies that, for some $z \in [x_k, x_*]$,

$$0 = g(x_*) = g(x_k + \epsilon_k) = g(x_k) + g'(x_k) \epsilon_k + \frac{1}{2} g''(z) \epsilon_k^2$$

$$-\epsilon_k - \frac{g(x_k)}{g'(x_k)} = \frac{1}{2} \frac{g''(z)}{g'(x_k)} \epsilon_k^2$$

$$-x_* + x_k - \frac{g(x_k)}{g'(x_k)} = \frac{1}{2} \frac{g''(z)}{g'(x_k)} (x_* - x_k)^2$$



$$-x_* + x_k - \frac{g(x_k)}{g'(x_k)} = \frac{1}{2} \frac{g''(z)}{g'(x_k)} (x_* - x_k)^2$$

$$\Rightarrow -x_* + x_{k+1} = \frac{1}{2} \frac{g''(z)}{g'(x_k)} (x_* - x_k)^2$$

$$\lim_{k \rightarrow \infty} \epsilon_k = 0 \Rightarrow x_{k+1} - x_* \approx \frac{1}{2} \frac{g''(z)}{g'(x_k)} (x_* - x_k)^2$$

That is, the error is approximately squared at each iteration

\Rightarrow The convergence is *quadratic* with $C = \left| \frac{1}{2} \frac{g''(z)}{g'(x_k)} \right|$



```

VV+X ROOT C,I;PIO;MAXAIT
[1] R
[2] R Newton-Raphson method applied to finding a real
[3] R root of a polynomial with coefficients C
[4] R Appeared in APL Quote Quad, June '83, pp.19-20
[5] R Author: Yuji Ijiri
[6] R
[7] I=1 O PIO=0 O MAXAIT=50
[8] Next:X+(Y+X)-X1C*X=X1C*PI,C
[9] ->Next IF (Y#X)^(MAXAIT=1+1)
V
    
```



$$3X^3 + 2X^2 + X + 1 = 0$$

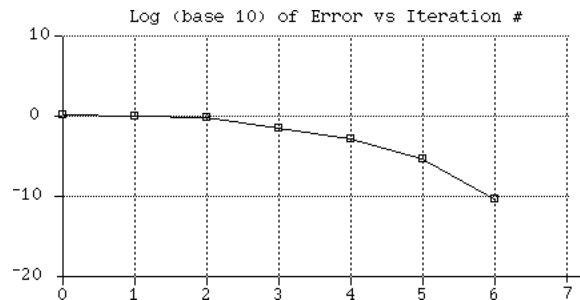
t	X_t	$G(X_t)$
0	1.0000000000000000	7.0000000000000000
1	0.5000000000000000	2.3750000000000000
2	0.047619047619048	1.052478134110787
3	-0.821562332798288	-0.135209637777137
4	-0.785872207198749	-0.006734489690139
5	-0.78390098449740	-0.000019706383372
6	-0.78389429373122	-0.00000000170329
7	-0.783894293686949	0.0000000000000000

t	X_t	$G(X_t)$
0	-1.0000000000000000	-1.0000000000000000
0	-0.8333333333333333	-0.1805555555555555
1	-0.787234042553192	-0.011394392379338
2	-0.783910803476619	-0.000056049392973
3	-0.783894294092810	-0.000000001377830
4	-0.783894293686949	0.0000000000000000

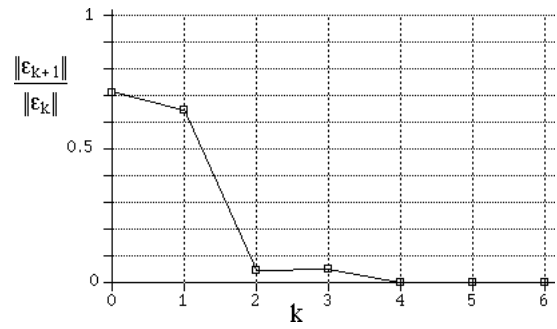


$$G(X) = 3X^3 + 2X^2 + X + 1 = 0$$

t	X_t	$G(X_t)$	ϵ_t
0	1.0000000000000000	7.0000000000000000	-1.783894293686949
1	0.5000000000000000	2.3750000000000000	-1.283894293686949
2	0.047619047619048	1.052478134110787	-0.831513341305997
3	-0.821562332798288	-0.135209637777137	0.037668039111338
4	-0.785872207198749	-0.006734489690139	0.001977913511799
5	-0.78390098449740	-0.000019706383372	0.000005804762791
6	-0.78389429373122	-0.00000000170329	0.000000000050173
7	-0.783894293686949	0.0000000000000000	0.0000000000000000

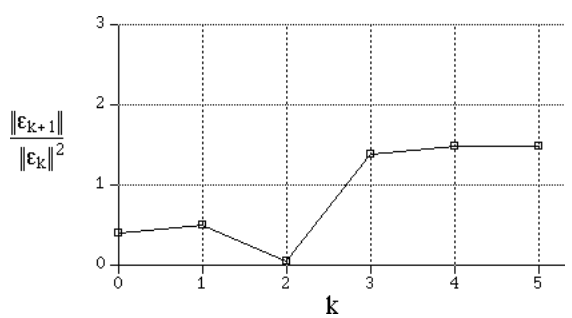


k	$\frac{\ \epsilon_{k+1} \ }{\ \epsilon_k \ }$	$\frac{\ \epsilon_{k+1} \ }{\ \epsilon_k \ ^2}$
0	7.19714334100705E-1	4.03451222781368E-1
1	6.47649378453226E-1	5.04441355988410E-1
2	4.53005829734204E-2	5.44796826738463E-2
3	5.25090649383936E-2	1.39399517939303E0
4	2.93479100899355E-3	1.48378126317763E0
5	8.64345378706824E-6	1.48902790661432E0
6	2.21278102318995E-6	4.41028491391872E4



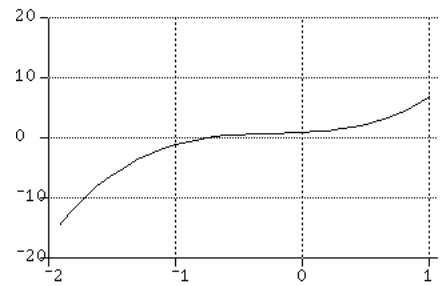
↔ ↔

↔ ↔



↔ ↔

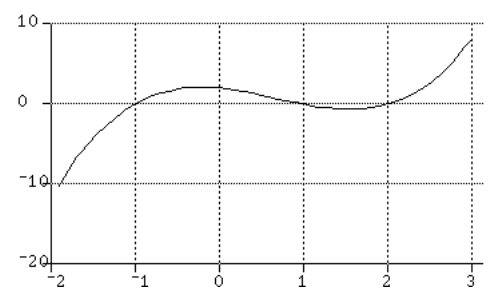
$G(X) = 3X^3 + 2X^2 + X + 1$



↔ ↔ *There appears to be only one real root!*

$G(X) = X^3 - 2X^2 - X + 2$

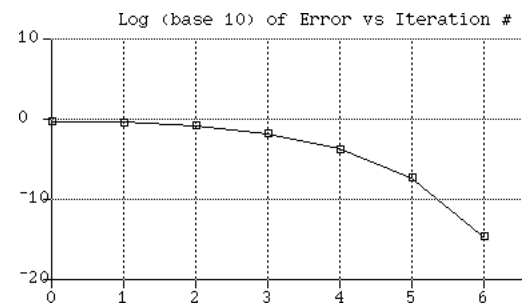
Roots are -1, 1, & 2



↔ ↔

t	X_t	$G(X_t)$	ϵ_t
0	-0.5000000000000000	1.8750000000000000	-0.5000000000000000
1	-1.571428571428571	-5.247813411078717	0.571428571428571
2	-1.158015617822692	-1.076883866081184	0.158015617822692
3	-1.017339588345219	-0.105546050034808	0.017339588345219
4	-1.000245166873965	-0.001471301792509	0.000245166873965
5	-1.000000050073447	-0.000000300440693	0.000000050073447
6	-1.000000000000002	-0.000000000000013	0.000000000000002
7	-1.000000000000000	0.000000000000000	0.000000000000000

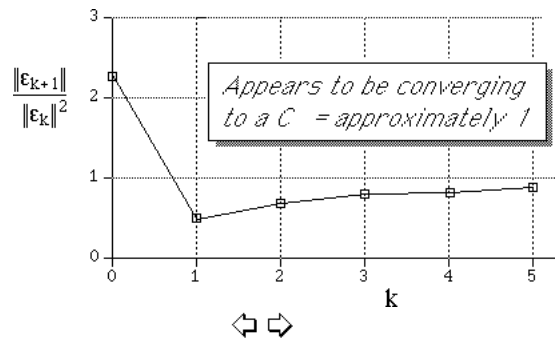
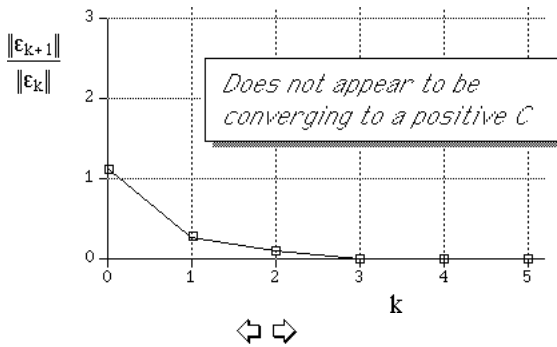
↔ ↔



↔ ↔

k	$\frac{\ \epsilon_{k+1} \ }{\ \epsilon_k \ }$	$\frac{\ \epsilon_{k+1} \ }{\ \epsilon_k \ ^2}$
0	1.14285714285714E0	2.28571428571429E0
1	2.76527331189711E-1	4.83922829581994E-1
2	1.09733383219595E-1	6.94446439735635E-1
3	1.413914039274E-2	8.15425378690662E-1
4	2.04242302038894E-4	8.33074626826414E-1
5	4.43437828748177E-8	8.85574806157926E-1

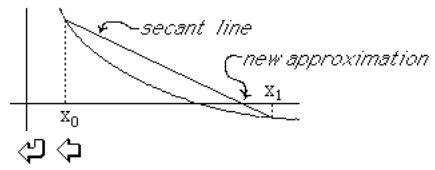
↔ ↔



Secant Method

Often the derivative $g'(x)$ is difficult to compute, making the Newton-Raphson method undesirable. The secant method avoids the use of derivatives by finding the intersection with the x -axis not of the tangent line, but a secant line.

Two initial "guesses" are required.



System of n equations in n variables

Consider the system of nonlinear equations

$$\begin{cases} g_1(x_1, x_2, \dots, x_n) = 0 \\ g_2(x_1, x_2, \dots, x_n) = 0 \\ \vdots \\ g_n(x_1, x_2, \dots, x_n) = 0 \end{cases}$$

Dropping the quadratic terms from Taylor's Formula:

$$g_i(x^t + \Delta^t) \approx g_i(x^t) + \nabla g_i(x^t) \Delta^t \quad \forall i=1,2,\dots,n$$

If we choose the step Δ^t so that $g_i(x^t + \Delta^t) \approx 0$ we get the system of *linear* equations

$$\nabla g_i(x^t) \Delta^t = -g_i(x^t) \quad \forall i=1,2,\dots,n$$

which we must solve for Δ^t

Let $J(x_1, x_2, \dots, x_n)$ be the *Jacobian* of this system, evaluated at x , i.e., the $n \times n$ matrix with row i equal to $\nabla g_i(x_1, x_2, \dots, x_n)$, the gradient of the i^{th} constraint function.

The coefficient matrix of this linear system is the *Jacobian Matrix*

$$J(x^t) \equiv \begin{bmatrix} \frac{\partial g_1(x^t)}{\partial x_1} & \frac{\partial g_1(x^t)}{\partial x_2} & \dots & \frac{\partial g_1(x^t)}{\partial x_n} \\ \frac{\partial g_2(x^t)}{\partial x_1} & \frac{\partial g_2(x^t)}{\partial x_2} & \dots & \frac{\partial g_2(x^t)}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial g_n(x^t)}{\partial x_1} & \frac{\partial g_n(x^t)}{\partial x_2} & \dots & \frac{\partial g_n(x^t)}{\partial x_n} \end{bmatrix}$$

The *Newton-Raphson Method* for solving

$$\begin{cases} g_1(x_1, x_2, \dots, x_n) = 0 \\ g_2(x_1, x_2, \dots, x_n) = 0 \\ \vdots \\ g_n(x_1, x_2, \dots, x_n) = 0 \end{cases}$$

Let x^t be the approximation to the solution at iteration $\#t$.

Then the next approximation is $x^{t+1} = x^t + \Delta^t$ where $\Delta^t = -[J(x^t)]^{-1}g(x^t)$

Inverse of the Jacobian matrix

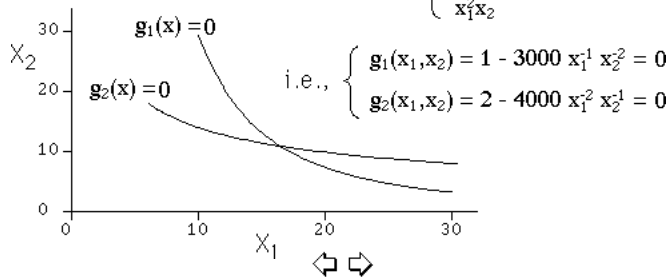
```

VY=NEWTONRAPHSON X;V;J;DY
[11] R
[12] R          SOLVE THE NONLINEAR SYSTEM OF EQUATIONS
[13] R          G(X) = 0
[14] R          WHERE G IS A VECTOR-VALUED FUNCTION
[15] R          (G AND JACOBIAN MUST BE USER-DEFINED,
[16] R          AS WELL AS TOL AND MAXITER)
[17] R
[18] R
[19] R
[20] R          DTCNL,'Tolerance (on f/|G(X)|) = ',*TOL
[21] R          start_timer 0 ITER=1 0 Y<X 0 DTCNL
[22] R          XΔPATH←((ρX),1)ρX
[23] R          NEXT:V←G Y
[24] R          →STOP IF TOL≥f/|V
[25] R          J←JACOBIAN Y
[26] R          DY←-VBJ
[27] R          →bypass IF ~detail 0 NRAOUTPUT
[28] R          bypass:XΔPATH←XΔPATH,Y←Y+DY
[29] R          →NEXT IF MAXITER≥ITER-ITER+1
[30] R          'Warning... Newton-Raphson algorithm did not converge.'
[31] R          →0
[32] R          STOP:DTCNL,'*** Converged ***'
[33] R          '(Max. Abs. Value ≤ tolerance, ',(*TOL),')'
    
```

APL code

EXAMPLE

Solve:
$$\begin{cases} \frac{3000}{x_1 x_2^2} = 1 \\ \frac{4000}{x_1^2 x_2} = 2 \end{cases}$$



```

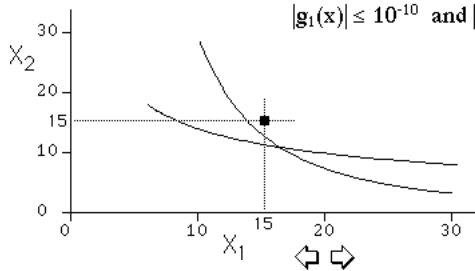
vZ←G X
[1] R
[2] R EXAMPLE EQUATIONS FOR NEWTON-RAPHSON ALGORITHM
[3] R
[4] Z←(1-3000×X×.*-2 -1) R Left side of first equation
[5] Z←Z,2-4000×X×.*-1 -2 R Left side of 2nd equation
[6] R is appended | Y
▽
▽A ← JACOBIAN X
[1] R
[2] R JACOBIAN MATRIX FOR SAMPLE SYSTEM OF EQUATIONS
[3] R TO BE SOLVED BY NEWTON-RAPHSON ALGORITHM
[4] R
[5] A←2 2ρ0
[6] A[1;1]←6000×X×.*-3 -1
[7] A[2;2]←8000×X×.*-1 -3
[8] A[1;2]←-3000×X×.*-2 -2
[9] A[2;1]←-4000×X×.*-2 -2
▽
    
```

APL code

We will start at $x = (x_1, x_2) = (15, 15)$

and terminate when

$|g_1(x)| \leq 10^{-10}$ and $|g_2(x)| \leq 10^{-10}$



Tolerance (on $|G(X)|$) = 0.0000000001

Iteration 1

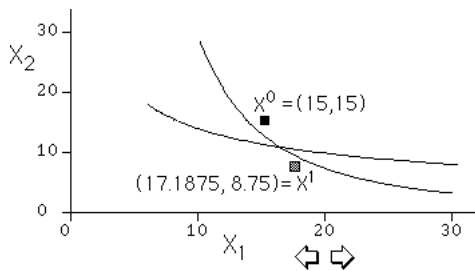
X = 15 15
 Function Values G(X) = 0.111111 0.814815
 Jacobian Matrix:
$$\begin{bmatrix} 0.118519 & 0.0592593 \\ 0.0790123 & 0.158025 \end{bmatrix}$$

 (Determinant = 0.0140466)
 Step is 2.1875 -6.25
 with length 6.62176

Iteration 2

X = 17.1875 8.75
 Function Values G(X) = -0.160614 -1.0397
 Jacobian Matrix:
$$\begin{bmatrix} 0.135053 & 0.132642 \\ 0.176855 & 0.694789 \end{bmatrix}$$

 (Determinant = 0.0703752)
 Step is -0.373925 1.59161
 with length 1.63494



Iteration 3

X = 16.8136 10.3416
 Function Values G(X) = -0.026155 -0.224455
 Jacobian Matrix:
$$\begin{bmatrix} 0.122063 & 0.0992258 \\ 0.132301 & 0.430195 \end{bmatrix}$$

 (Determinant = 0.0393831)
 Step is -0.279815 0.607805
 with length 0.669121

Iteration 4

X = 16.5338 10.9494
 Function Values G(X) = -0.00227541 -0.0179319
 Jacobian Matrix:
$$\begin{bmatrix} 0.12124 & 0.0915369 \\ 0.122049 & 0.368592 \end{bmatrix}$$

 (Determinant = 0.033516)
 Step is -0.0239508 0.0565805
 with length 0.061441



Iteration 5

X = 16.5098 11.006
 Function Values G(X) = $-0.000017987 \ -0.000134764$
 Jacobian Matrix:

$$\begin{matrix} 0.121142 & 0.0908612 \\ 0.121148 & 0.363463 \end{matrix}$$

 (Determinant = 0.033023)
 Step is $-0.000172825 \ 0.000428384$
 with length 0.000461932

Iteration 6

X = 16.5096 11.0064
 Function Values G(X) = $-1.02881E-9 \ -7.67939E-9$
 Jacobian Matrix:

$$\begin{matrix} 0.121141 & 0.090856 \\ 0.121141 & 0.363424 \end{matrix}$$

 (Determinant = 0.0330193)
 Step is $-9.80709E-9 \ 2.43997E-8$
 with length 2.62968E-8



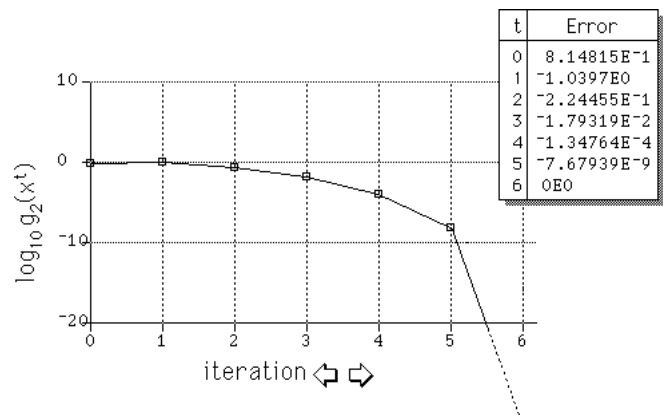
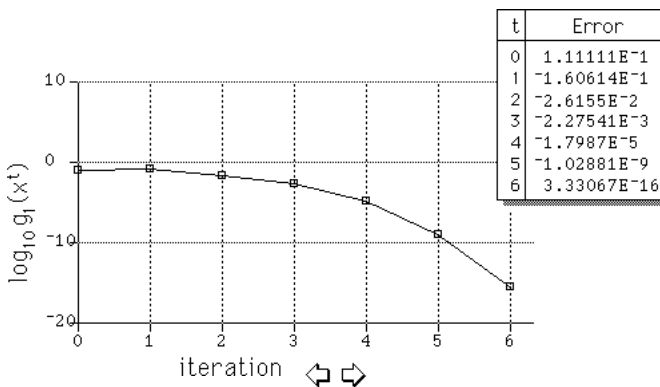
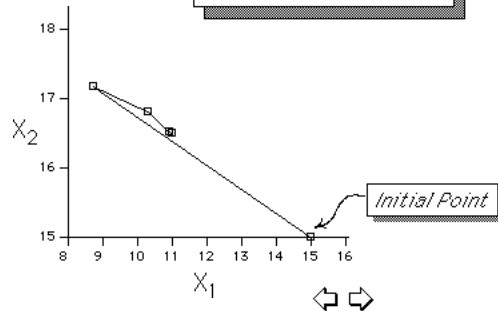
*** Converged ***
 (Max. Abs. Value \leq tolerance, 0.0000000001)

Final Solution

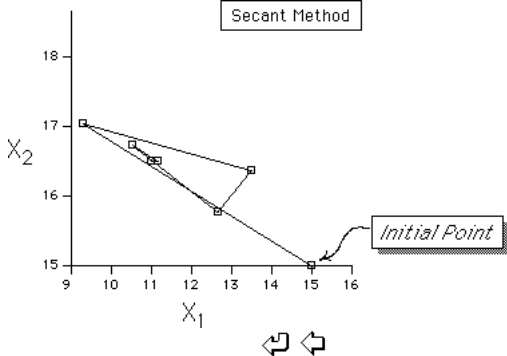
X = 16.5096 11.0064
 G(X) = 3.33067E-16 0
 CPU time: 11.95 sec.
 # of iterations = 7



Path Followed by the Algorithm



Secant Method



Optimizing a Nonlinear Function

- Function of a single variable
Minimize $f(x)$
- Function of several variables
Minimize $f(x_1, x_2, \dots, x_n)$



Function of a single variable
Minimize f(x)



This necessary condition for optimality yields a system of (in general) n *nonlinear* equations in n variables.

Newton's Method is simply the application of the Newton-Raphson method to solving this system of equations.



Necessary Condition for Optimality:
 If X^* is optimal, then $\nabla f(X^*) = 0$, i.e., $\frac{\partial f(X^*)}{\partial x_i} = 0$ for each $i=1,2,\dots,n$

Consider the problem of minimizing a function of several variables:

Minimize $f(x_1, x_2, \dots, x_n)$

Suppose that f is differentiable, i.e., the gradient

$$\nabla f(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix} \text{ is defined.}$$



Necessary Condition for Optimality:
 If X^* is optimal, then $\nabla f(X^*) = 0$, i.e., $\frac{\partial f(X^*)}{\partial x_i} = 0$ for each $i=1,2,\dots,n$

Applying the Newton-Raphson method to the solution of the equations $\nabla f(X^*) = 0$,

$$\text{i.e., } \begin{cases} g_1(x_1, x_2, \dots, x_n) = \frac{\partial f}{\partial x_1} = 0 \\ g_2(x_1, x_2, \dots, x_n) = \frac{\partial f}{\partial x_2} = 0 \\ \vdots \\ g_n(x_1, x_2, \dots, x_n) = \frac{\partial f}{\partial x_n} = 0 \end{cases}$$

we find that the Jacobian matrix of this system is the **Hessian** matrix of the function f , i.e., $\nabla^2 f(x)$



Hessian Matrix

$$\nabla^2 f(x^t) \equiv \begin{bmatrix} \frac{\partial^2 f(x^t)}{\partial x_1^2} & \frac{\partial^2 f(x^t)}{\partial x_1 \partial x_2} & \dots & \frac{\partial^2 f(x^t)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x^t)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x^t)}{\partial x_2^2} & \dots & \frac{\partial^2 f(x^t)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x^t)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x^t)}{\partial x_n \partial x_2} & \dots & \frac{\partial^2 f(x^t)}{\partial x_n^2} \end{bmatrix}$$



Newton's Method

Let x^t be the approximation to the solution at iteration t .

Then the approximation at iteration $t+1$ is given by

$$x^{t+1} = x^t + \Delta^t, \text{ where } \Delta^t \text{ is the solution of the (linear) equation}$$

$$\nabla^2 f(x^t) \Delta^t = -\nabla f(x^t)$$

$$\text{i.e., } \Delta^t = -[\nabla^2 f(x^t)]^{-1} \nabla f(x^t)$$



Comments

- If $f(x)$ is a quadratic function, Newton's method converges to a stationary point in a single iteration.
- Newton's method does not discriminate among minimizers, maximizers, and saddle points
- If the Hessian matrix at an iteration is positive definite, then the direction δ^t is a direction of descent, i.e., $f(x^t + \epsilon \delta^t) < f(x^t)$ for some $\epsilon > 0$, even though it might be that $f(x^t + \Delta^t) \geq f(x^t)$.
- It is more efficient and more numerically stable to solve the system of equations $\nabla^2 f(x^t) \Delta^t = -\nabla f(x^t)$

by means other than inverting the Hessian matrix.



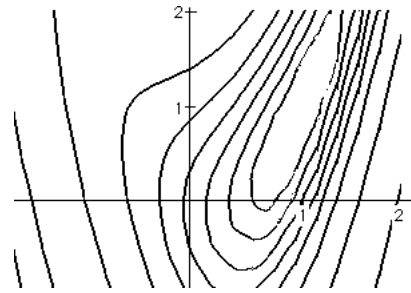
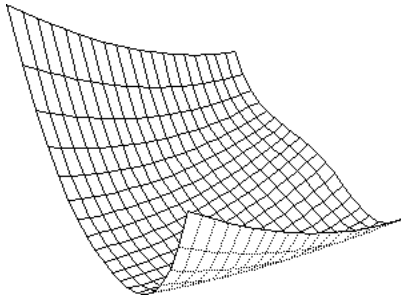
Example

Minimize $f(x_1, x_2) = (x_2 - x_1^2)^2 + (1 - x_1)^2$

$$\nabla f(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 4x_1^3 - 4x_1x_2 + 2x_1 - 2 \\ 2(x_2 - x_1^2) \end{bmatrix}$$

$$\nabla^2 f(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix} = \begin{bmatrix} 12x_1^2 - 4x_2 + 2 & -4x_1 \\ -4x_1 & 2 \end{bmatrix}$$





Let's begin at the point $x^0 = (2, 1)$

$$\begin{cases} \delta_1 = -0.1428 \\ \delta_2 = 2.4286 \end{cases} \Rightarrow \begin{aligned} x_1^1 &= x_1^0 + \delta_1 = 2 - 0.1428 \\ x_2^1 &= x_2^0 + \delta_2 = 2 + 2.4286 \end{aligned}$$

Iteration 1

Iteration 2

$x = 2 \ 1$
 $F(x) = 10$
 $\nabla F(x) = 26 \ -6$
 Hessian Matrix = $\begin{bmatrix} 46 & -8 \\ -8 & 2 \end{bmatrix}$

$x = 1.857142857 \ 3.428571429$
 $F(x) = 0.7351103707$
 $\nabla F(x) = 1.865889213 \ -0.04081632653$
 Hessian Matrix = $\begin{bmatrix} 29.67346939 & -7.428571429 \\ -7.428571429 & 2 \end{bmatrix}$

We need to solve the equations $\begin{cases} 46\delta_1 - 8\delta_2 = -26 \\ -8\delta_1 + 2\delta_2 = 6 \end{cases}$

Improvement: 9.264889629

$$\Rightarrow \begin{cases} \delta_1 = -0.1428 \\ \delta_2 = 2.4286 \end{cases} \quad \leftrightarrow$$



Iteration 3

Iteration 4

$x = 1.033613445 \ 0.3901560624$
 $F(x) = 0.4610860424$
 $\nabla F(x) = 2.871216307 \ -1.356401384$
 Hessian Matrix = $\begin{bmatrix} 13.2596568 & -4.134453782 \\ -4.134453782 & 2 \end{bmatrix}$

$x = 1.019348709 \ 1.038868307$
 $F(x) = 0.0003744139315$
 $\nabla F(x) = 0.03952709666 \ -0.000406965428$
 Hessian Matrix = $\begin{bmatrix} 10.31338825 & -4.077394835 \\ -4.077394835 & 2 \end{bmatrix}$

Improvement: 0.2740243283

Improvement: 0.4607116285



Iteration 5

Iteration 5

$x = 1.000007871 \ 0.9996416742$
 $F(x) = 1.399888212E^{-7}$
 $\nabla F(x) = 0.001512025877 \ -0.0007481359977$
 Hessian Matrix = $\begin{bmatrix} 10.00162221 & -4.000031484 \\ -4.000031484 & 2 \end{bmatrix}$

$x = 1.000000006 \ 1.000000012$
 $F(x) = 3.462781953E^{-17}$
 $\nabla F(x) = 1.201587541E^{-8} \ -1.237219216E^{-10}$
 Hessian Matrix = $\begin{bmatrix} 10.00000009 & -4.000000024 \\ -4.000000024 & 2 \end{bmatrix}$

Improvement: 0.0003742739427

Improvement: 1.399888212E^{-7}



Convergence criterion satisfied:

```

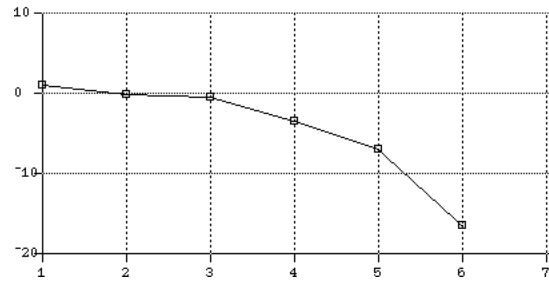
Improvement in objective
Step size
Gradient
*** CONVERGED ***

Solution found is 1.000000006 1.000000012
where F is 3.462781953E-17
and VF is 1.201587541E-8 1.237219216E-10

# iterations = 6
Elapsed CPU time: 11.85 seconds
    
```



Plot of Log ΔF by iteration



Disadvantages

- Newton's method converges to a stationary point, which may or may not be a minimizer
- Newton's method requires the computation of $\frac{1}{2} n^2$ 2nd partial derivatives (i.e., the Hessian matrix)
- Newton's method requires at each iteration the inversion of a matrix of order n (or the solution of a linear system of equations in n variables)

For these reasons, Newton's method is not of practical significance for unconstrained optimization.

