Lecture Notes to Accompany

Scientific Computing

An Introductory Survey

Second Edition

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Chapter 5

Nonlinear Equations

Nonlinear Equations

Given function f, we seek value x for which

$$f(x) = 0$$

Solution x is *root* of equation, or *zero* of function f

Problem known as *root finding* or *zero finding*

Two important cases:

1. Single nonlinear equation in one unknown,

$$f\colon \mathbb{R} \to \mathbb{R}$$

Solution is scalar x for which $f(x) = 0$

2. System of n coupled nonlinear equations in n unknowns,

$$\boldsymbol{f}\colon \mathbb{R}^n \to \mathbb{R}^n$$

Solution is vector $\boldsymbol{x}$ for which all components of $\boldsymbol{f}$ are zero *simultaneously*

Examples: Nonlinear Equations

Example of nonlinear equation in one dimension:

$$x^2 - 4\sin(x) = 0,$$

for which $x = 1.9$ is one approximate solution

Example of system of nonlinear equations in two dimensions:

$$\begin{aligned} x_1^2 - x_2 + 0.25 &= 0, \\ -x_1 + x_2^2 + 0.25 &= 0, \end{aligned}$$

for which $\boldsymbol{x} = [\,0.5 \quad 0.5\,]^T$ is solution vector

Existence and Uniqueness

Existence and uniqueness of solutions more complicated for nonlinear equations than for linear equations

For function $f\colon \mathbb{R} \to \mathbb{R}$, *bracket* is interval $[a, b]$ for which sign of f differs at endpoints

If f continuous and $\text{sign}(f(a)) \neq \text{sign}(f(b))$, then Intermediate Value Theorem implies there is $x^* \in [a, b]$ such that $f(x^*) = 0$

No simple analog for n dimensions

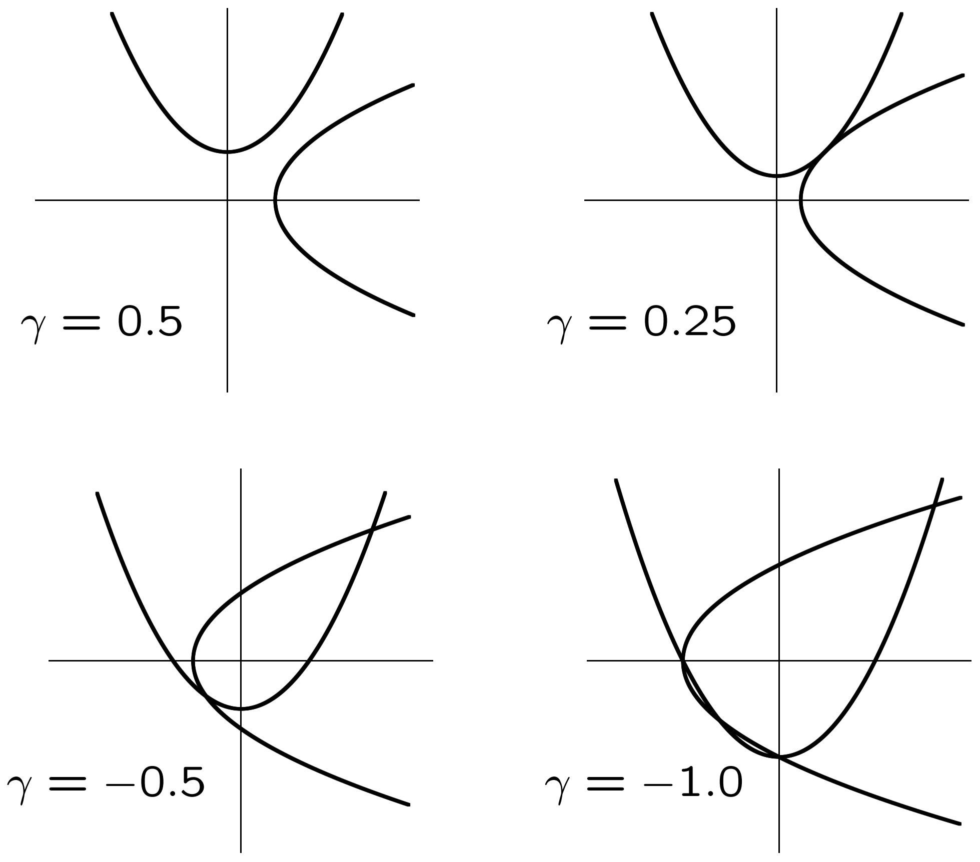
Examples

Nonlinear equations can have any number of solutions:

- $\exp(x) + 1 = 0$ has no solution
- $\exp(-x) - x = 0$ has one solution
- $x^2 - 4\sin(x) = 0$ has two solutions
- $x^3 + 6x^2 + 11x - 6 = 0$ has three solutions
- $\sin(x) = 0$ has infinitely many solutions

Example

$$\begin{aligned} x_1^2 - x_2 + \gamma &= 0 \\ -x_1 + x_2^2 + \gamma &= 0 \end{aligned}$$

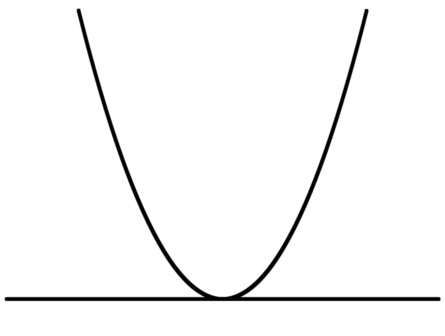


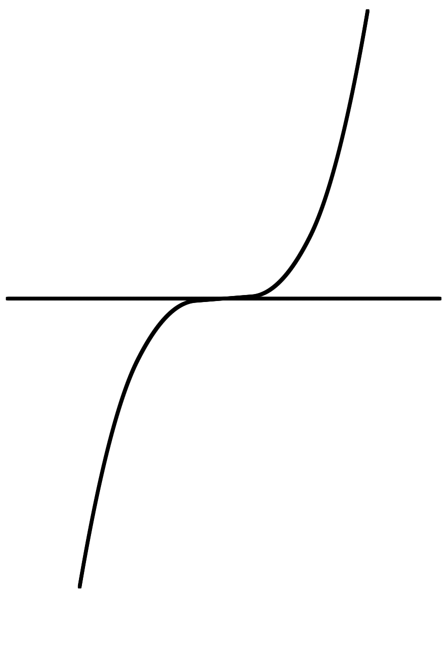
Multiple Root

Nonlinear equation may have *multiple* root, where both function *and* derivative are zero, i.e., $f(x) = 0$ and $f'(x) = 0$

Examples:

$x^2 - 2x + 1 = 0$ and $x^3 - 3x^2 + 3x - 1 = 0$





Sensitivity and Conditioning

Conditioning of root finding problem opposite to that for evaluating function

Absolute condition number of root finding problem for root x^* of $f\colon \mathbb{R} \to \mathbb{R}$ is $1/|f'(x^*)|$

Root ill-conditioned if tangent line nearly horizontal

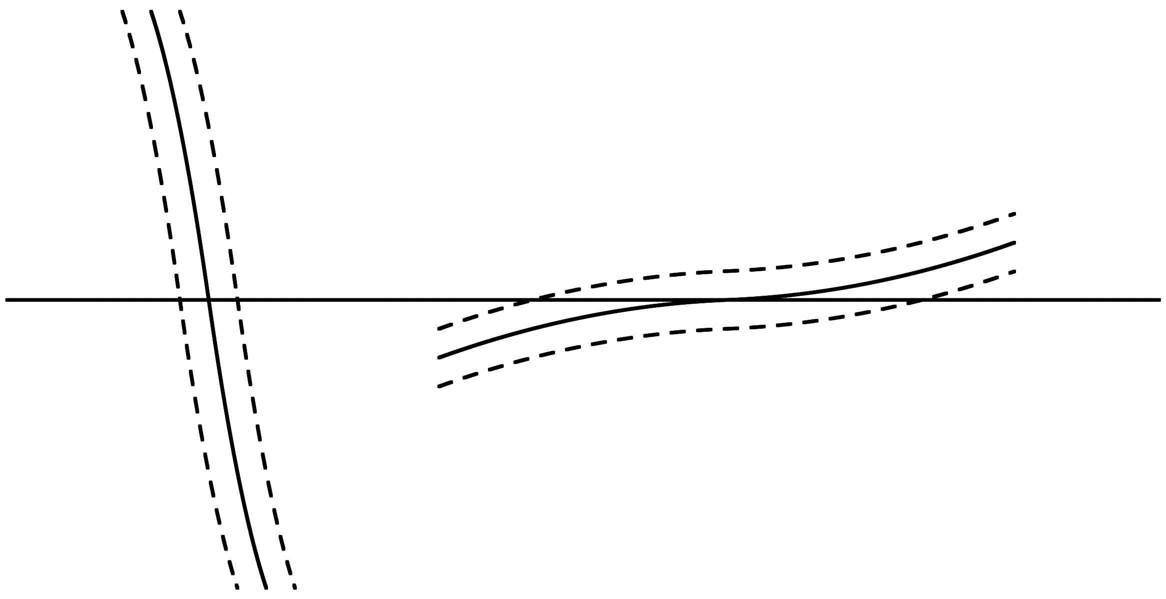
In particular, multiple root ill-conditioned

Absolute condition number of root finding problem for root $\boldsymbol{x}^*$ of $\boldsymbol{f}\colon \mathbb{R}^n \to \mathbb{R}^n$ is $\|\boldsymbol{J}_f^{-1}(\boldsymbol{x}^*)\|$, where $\boldsymbol{J}_f$ is *Jacobian* matrix of $\boldsymbol{f}$,

$$\{\boldsymbol{J}_f(\boldsymbol{x})\}_{ij} = \partial f_i(\boldsymbol{x})/\partial x_j$$

Root ill-conditioned if Jacobian matrix nearly singular

Sensitivity and Conditioning



Sensitivity and Conditioning

What do we mean by approximate solution $\hat{\boldsymbol{x}}$ to nonlinear system,

$$\|\boldsymbol{f}(\hat{\boldsymbol{x}})\| \approx 0 \qquad \text{or} \qquad \|\hat{\boldsymbol{x}} - \boldsymbol{x}^*\| \approx 0?$$

First corresponds to "small residual," second measures closeness to (usually unknown) true solution $\boldsymbol{x}^*$

Solution criteria not necessarily "small" simultaneously

Small residual implies accurate solution only if problem well-conditioned

Convergence Rate

For general iterative methods, define error at iteration k by

$$\boldsymbol{e}_k = \boldsymbol{x}_k - \boldsymbol{x}^*,$$

where $\boldsymbol{x}_k$ is approximate solution and $\boldsymbol{x}^*$ is true solution

For methods that maintain interval known to contain solution, rather than specific approximate value for solution, take error to be length of interval containing solution

Sequence converges with rate r if

$$\lim_{k\to\infty} \frac{\|\boldsymbol{e}_{k+1}\|}{\|\boldsymbol{e}_k\|^r} = C$$

for finite nonzero constant C

Convergence Rate, continued

Some particular cases of interest

$r = 1$: *linear* $(C < 1)$

$r > 1$: *superlinear*

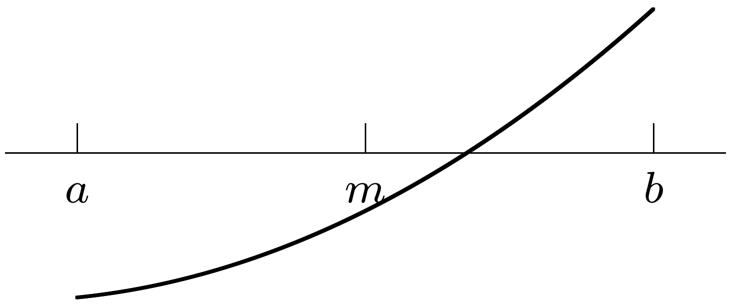
$r = 2$: *quadratic*

Convergence rate	Digits gained per iteration
linear	constant
superlinear	increasing
quadratic	double

Interval Bisection Method

Bisection method begins with initial bracket and repeatedly halves its length until solution has been isolated as accurately as desired

```
while $((b - a) > tol)$ do
    $m = a + (b - a)/2$
    if sign$(f(a))$ = sign$(f(m))$ then
        $a = m$
    else
        $b = m$
    end
end
```



Example: Bisection Method

$$f(x) = x^2 - 4\sin(x) = 0$$

a	$f(a)$	b	$f(b)$
1.000000	-2.365884	3.000000	8.435520
1.000000	-2.365884	2.000000	0.362810
1.500000	-1.739980	2.000000	0.362810
1.750000	-0.873444	2.000000	0.362810
1.875000	-0.300718	2.000000	0.362810
1.875000	-0.300718	1.937500	0.019849
1.906250	-0.143255	1.937500	0.019849
1.921875	-0.062406	1.937500	0.019849
1.929688	-0.021454	1.937500	0.019849
1.933594	-0.000846	1.937500	0.019849
1.933594	-0.000846	1.935547	0.009491
1.933594	-0.000846	1.934570	0.004320
1.933594	-0.000846	1.934082	0.001736
1.933594	-0.000846	1.933838	0.000445
1.933716	-0.000201	1.933838	0.000445

Bisection Method, continued

Bisection method makes no use of magnitudes of function values, only their signs

Bisection certain to converge, but does so slowly

At each iteration, length of interval containing solution reduced by half, so method linearly convergent, with $r = 1$ and $C = 0.5$

One bit of accuracy gained in approximate solution for each iteration of bisection

Given starting interval $[a, b]$, length of interval after k iterations is $(b-a)/2^k$, so achieving error tolerance of tol requires

$$\left\lceil \log_2\left(\frac{b-a}{tol}\right)\right\rceil$$

iterations, regardless of function f involved

Fixed-Point Problems

Fixed point of given function $g\colon \mathbb{R} \to \mathbb{R}$ is value x such that

$$x = g(x)$$

Many iterative methods for solving nonlinear equations use iteration scheme of form

$$x_{k+1} = g(x_k),$$

where g is function whose fixed points are solutions for $f(x) = 0$

Scheme called *fixed-point iteration* or *functional iteration*, since function g applied repeatedly to initial starting value x_0

For given equation $f(x) = 0$, may be many equivalent fixed-point problems $x = g(x)$ with different choices for g

Example: Fixed-Point Problems

If

$$f(x) = x^2 - x - 2,$$

then fixed points of each of functions

$$g(x) = x^2 - 2$$

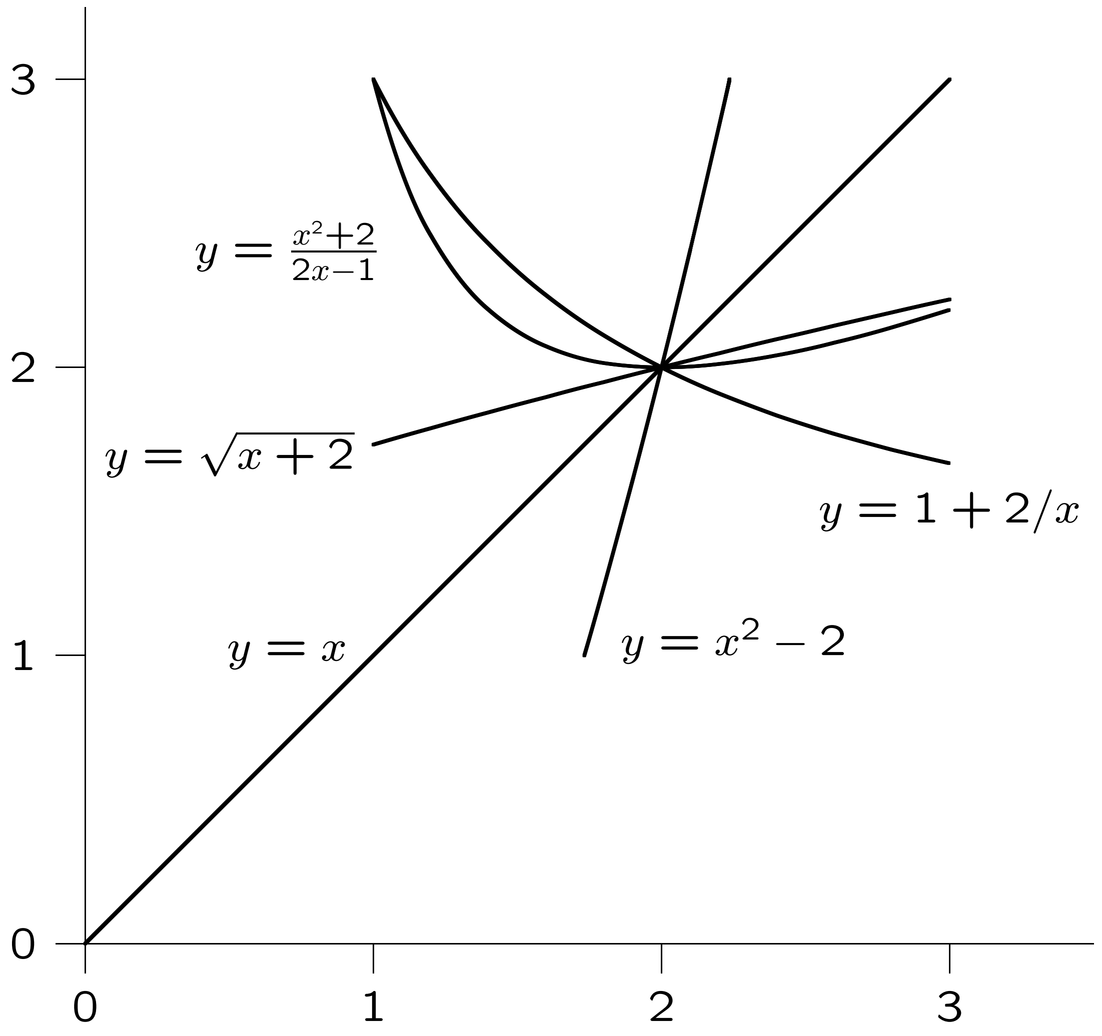
$$g(x) = \sqrt{x + 2}$$

$$g(x) = 1 + 2/x$$

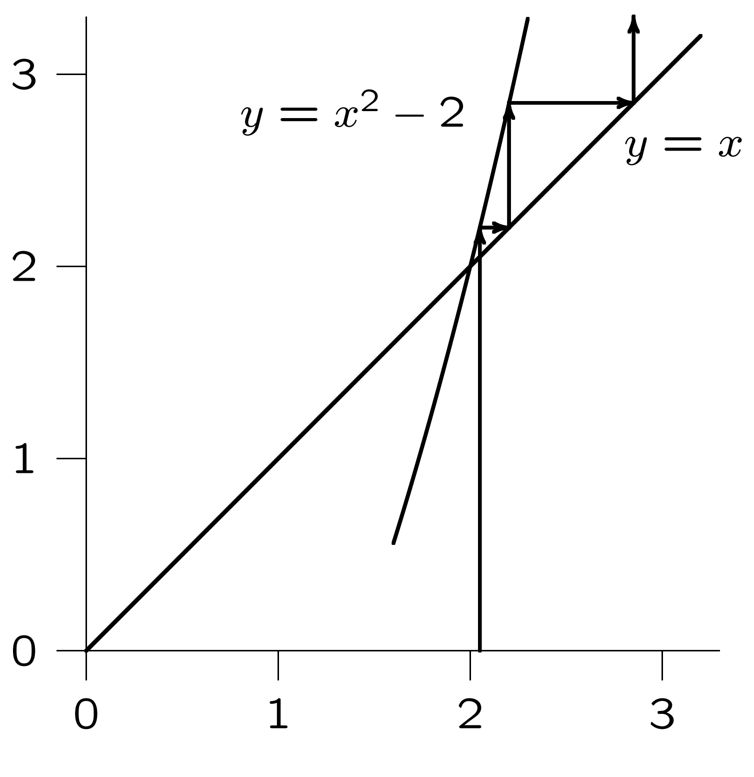
$$g(x) = \frac{x^2 + 2}{2x - 1}$$

are solutions to equation $f(x) = 0$

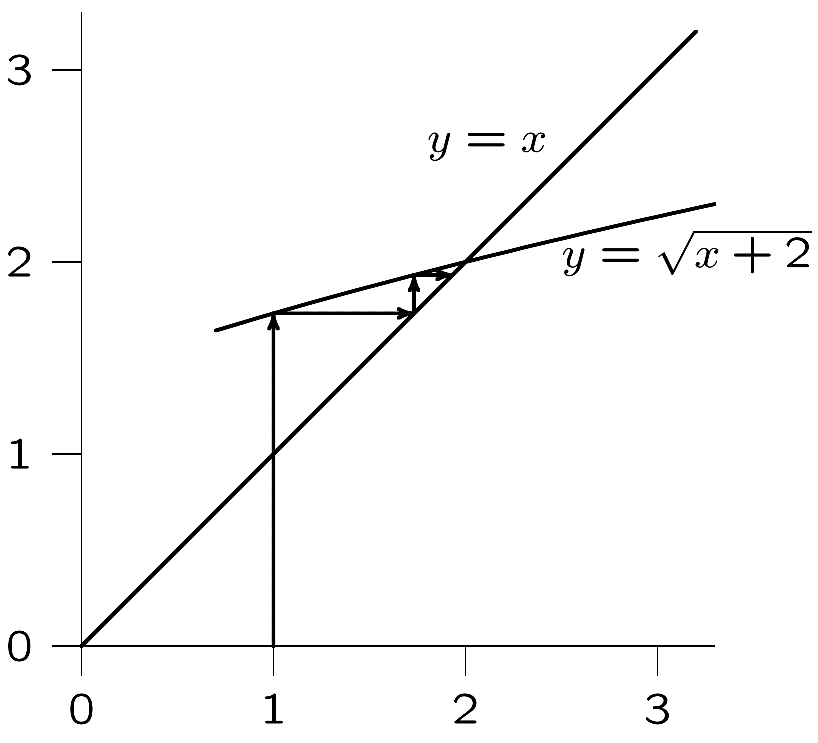
Example: Fixed-Point Problems



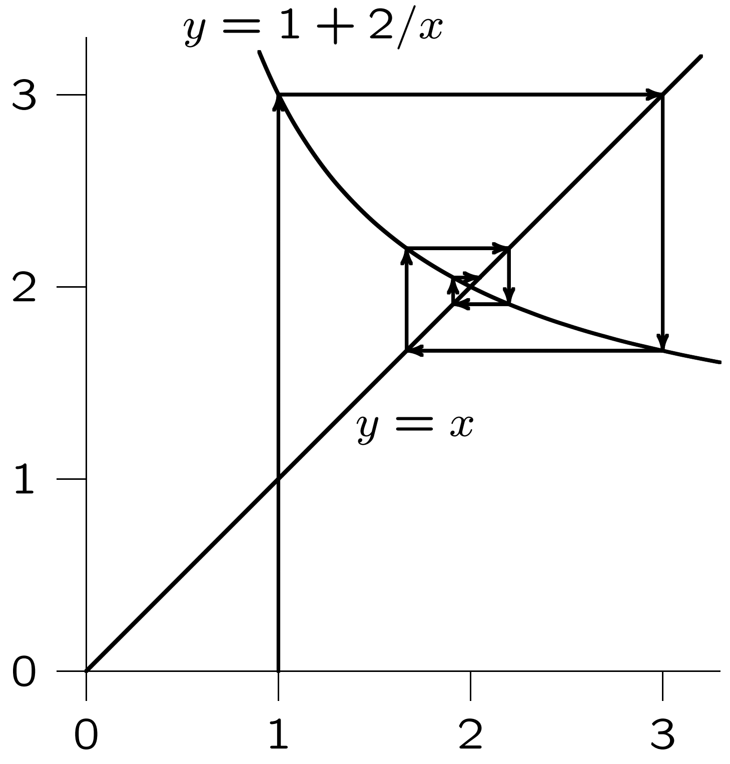
Example: Fixed-Point Iteration



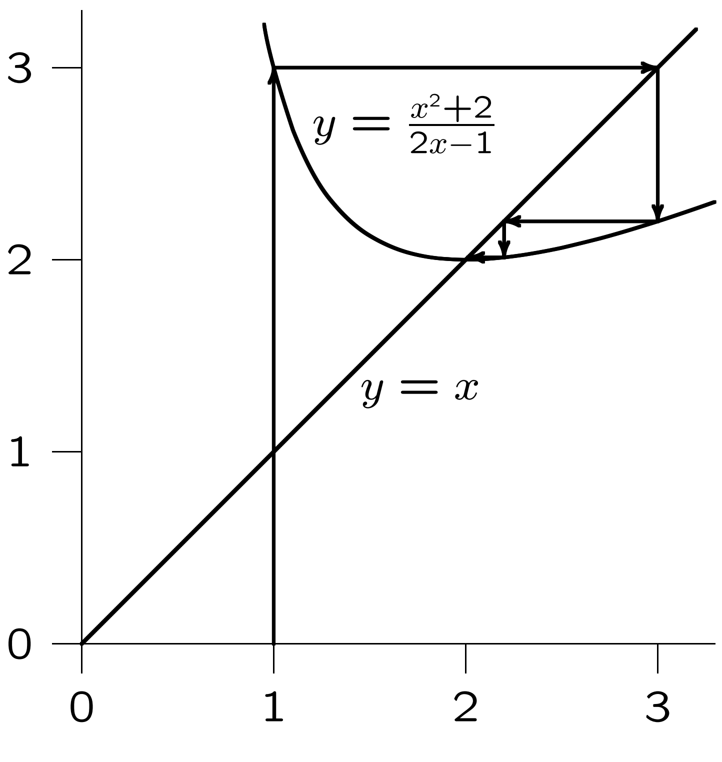
Example: Fixed-Point Iteration



Example: Fixed-Point Iteration



Example: Fixed-Point Iteration



Convergence of Fixed-Point Iteration

If $x^* = g(x^*)$ and $|g'(x^*)| < 1$, then there is interval containing x^* such that iteration

$$x_{k+1} = g(x_k)$$

converges to x^* if started within that interval

If $|g'(x^*)| > 1$, then iterative scheme diverges

Asymptotic convergence rate of fixed-point iteration usually linear, with constant $C = |g'(x^*)|$

But if $g'(x^*) = 0$, then convergence rate at least quadratic

Newton's Method

Truncated Taylor series

$$f(x+h) \approx f(x) + f'(x)h$$

is linear function of h approximating f near x

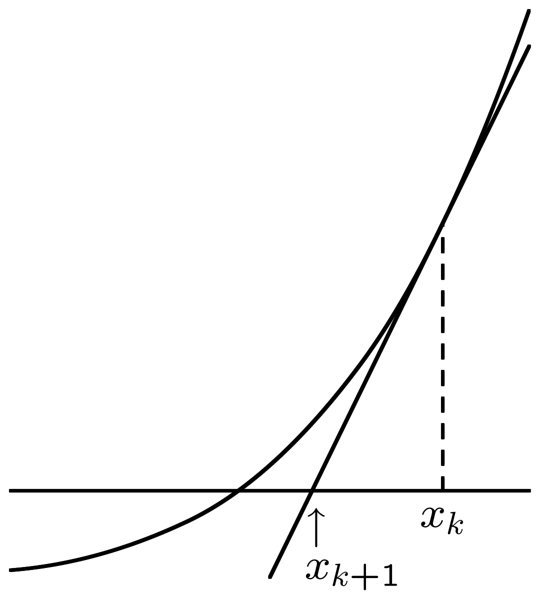
Replace nonlinear function f by this linear function, whose zero is $h = -f(x)/f'(x)$

Zeros of original function and linear approximation not identical, so repeat process, giving *Newton's method*

$$x_{k+1} = x_k - f(x_k)/f'(x_k)$$

Newton's Method, continued

Newton's method approximates nonlinear function f near x_k by tangent line at $f(x_k)$



Example: Newton's Method

Use Newton's method to find root of

$$f(x) = x^2 - 4\sin(x) = 0$$

Derivative is

$$f'(x) = 2x - 4\cos(x),$$

so iteration scheme is

$$x_{k+1} = x_k - \frac{x_k^2 - 4\sin(x_k)}{2x_k - 4\cos(x_k)}$$

Taking $x_0 = 3$ as starting value, we obtain

x	$f(x)$	$f'(x)$	h
3.000000	8.435520	9.959970	-0.846942
2.153058	1.294772	6.505771	-0.199019
1.954039	0.108438	5.403795	-0.020067
1.933972	0.001152	5.288919	-0.000218
1.933754	0.000000	5.287670	0.000000

Convergence of Newton's Method

Newton's method transforms nonlinear equation $f(x) = 0$ into fixed-point problem $x = g(x)$, where

$$g(x) = x - f(x)/f'(x),$$

and hence

$$g'(x) = f(x)f''(x)/(f'(x))^2$$

If x^* is simple root (i.e., $f(x^*) = 0$ and $f'(x^*) \neq 0$), then $g'(x^*) = 0$

Convergence rate of Newton's method for simple root is quadratic, $r = 2$

But must start close enough to root to converge

Newton's Method, continued

For multiple root, Newton's method linearly convergent (with constant $C = 1-(1/m)$, where m is multiplicity)

Both cases illustrated below

k	$f(x) = x^2 - 1$	$f(x) = x^2 - 2x + 1$
0	2.0	2.0
1	1.25	1.5
2	1.025	1.25
3	1.0003	1.125
4	1.00000005	1.0625
5	1.0	1.03125

Secant Method

Newton's method requires evaluation of both function and derivative at each iteration

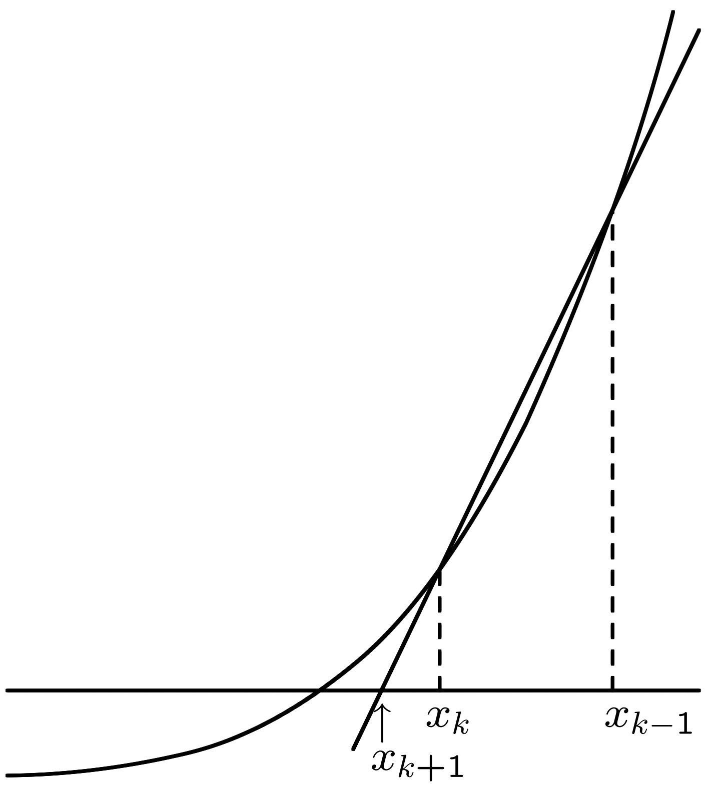
Evaluating derivative may be inconvenient or expensive, so replace it by finite difference approximation using two successive iterates,

$$x_{k+1} = x_k - f(x_k)\frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})}$$

Secant method normally superlinearly convergent, with $r \approx 1.618$

Secant Method, continued

Secant method approximates nonlinear function f by secant line through previous two iterates



Example: Secant Method

Use secant method to find root of

$$f(x) = x^2 - 4\sin(x) = 0$$

Taking $x_0 = 1$ and $x_1 = 3$ as starting guesses, we obtain

x	$f(x)$	h
1.000000	-2.365884	
3.000000	8.435520	-1.561930
1.438070	-1.896774	0.286735
1.724805	-0.977706	0.305029
2.029833	0.534305	-0.107789
1.922044	-0.061523	0.011130
1.933174	-0.003064	0.000583
1.933757	0.000019	-0.000004
1.933754	0.000000	0.000000

Higher-Degree Interpolation

Secant method uses linear interpolation to approximate function whose zero is sought

Higher convergence rate can be obtained by using higher-degree polynomial interpolation

Quadratic interpolation (Muller's method) has convergence rate of $r \approx 1.839$, for example

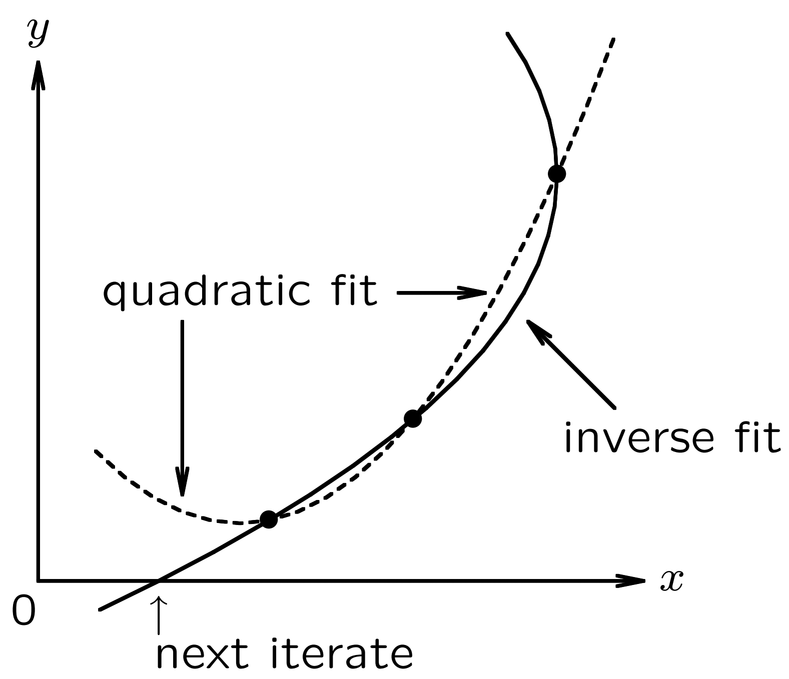
Unfortunately,

- interpolating polynomial may not have real roots
- roots may not be easy to compute
- choice of root to use as next iterate may not be obvious

Inverse Interpolation

Good alternative is *inverse interpolation*, where x_k are interpolated as function of $y_k = f(x_k)$ by polynomial $p(y)$, so next approximate solution is $p(0)$

Most commonly used for root finding is inverse quadratic interpolation



Inverse Quadratic Interpolation

Given approximate solution values a, b, c, with function values f_a, f_b, f_c, next approximate solution found by fitting quadratic polynomial to a, b, c as function of f_a, f_b, f_c, then evaluating polynomial at 0

We compute

$$u = f_b/f_c, \quad v = f_b/f_a, \quad w = f_a/f_c,$$

$$p = v(w(u-w)(c-b) - (1-u)(b-a)),$$

$$q = (w-1)(u-1)(v-1),$$

then new approximate solution is $b + p/q$

Convergence rate normally $r \approx 1.839$

Example: Inverse Quadratic Interpolation

Use inverse quadratic interpolation to find root of

$$f(x) = x^2 - 4\sin(x) = 0$$

Taking $x = 1$, 2, and 3 as starting values, we obtain

x	$f(x)$	h
1.000000	-2.365884	
2.000000	0.362810	
3.000000	8.435520	
1.886318	-0.244343	-0.113682
1.939558	0.030786	0.053240
1.933742	-0.000060	-0.005815
1.933754	0.000000	0.000011
1.933754	0.000000	0.000000

Linear Fractional Interpolation

Interpolation using rational fraction of form

$$\phi(x) = \frac{x-u}{vx-w}$$

especially useful for finding zeros of functions having horizontal or vertical asymptotes

ϕ has zero at $x = u$, vertical asymptote at $x = w/v$, and horizontal asymptote at $y = 1/v$

Given approximate solution values a, b, c, with function values f_a, f_b, f_c, next approximate solution is $c + h$, where

$$h = \frac{(a-c)(b-c)(f_a - f_b)f_c}{(a-c)(f_c - f_b)f_a - (b-c)(f_c - f_a)f_b}$$

Convergence rate normally $r \approx 1.839$, same as for quadratic interpolation (inverse or regular)

Example: Linear Fractional Interpolation

Use linear fractional interpolation to find root of

$$f(x) = x^2 - 4\sin(x) = 0$$

Taking $x = 1$, 2, and 3 as starting values, we obtain

x	$f(x)$	h
1.000000	−2.365884	
2.000000	0.362810	
3.000000	8.435520	
1.906953	−0.139647	−1.093047
1.933351	−0.002131	0.026398
1.933756	0.000013	−0.000406
1.933754	0.000000	−0.000003

Safeguarded Methods

Rapidly convergent methods for solving nonlinear equations may not converge unless started close to solution, but safe methods are slow

Hybrid methods combine features of both types of methods to achieve both speed and reliability

Use rapidly convergent method, but maintain bracket around solution

If next approximate solution given by fast method falls outside bracketing interval, perform one iteration of safe method, such as bisection

Safeguarded Methods, continued

Fast method can then be tried again on smaller interval with greater chance of success

Ultimately, convergence rate of fast method should prevail

Hybrid approach seldom does worse than safe method, and usually does much better

Popular combination is bisection and inverse quadratic interpolation, for which no derivatives required

Zeros of Polynomials

For polynomial $p(x)$ of degree n, one may want to find all n of its zeros, which may be complex even if coefficients are real

Several approaches available

- Use root-finding method such as Newton's or Muller's method to find one root, deflate it out, and repeat
- Form companion matrix of polynomial and use eigenvalue routine to compute all its eigenvalues
- Use method designed specifically for finding all roots of polynomial, such as Jenkins-Traub

Systems of Nonlinear Equations

Solving systems of nonlinear equations much more difficult than scalar case because

- Wider variety of behavior possible, so determining existence and number of solutions or good starting guess much more complex
- No simple way, in general, to guarantee convergence to desired solution or to bracket solution to produce absolutely safe method
- Computational overhead increases rapidly with dimension of problem

Fixed-Point Iteration

Fixed-point problem for $\boldsymbol{g}\colon \mathbb{R}^n \to \mathbb{R}^n$ is to find vector $\boldsymbol{x}$ such that

$$\boldsymbol{x} = \boldsymbol{g}(\boldsymbol{x})$$

Corresponding fixed-point iteration is

$$\boldsymbol{x}_{k+1} = \boldsymbol{g}(\boldsymbol{x}_k),$$

given starting vector $\boldsymbol{x}_0$

If

$$\rho(\boldsymbol{G}(\boldsymbol{x}^*)) < 1,$$

where ρ is *spectral radius* and $\boldsymbol{G}(\boldsymbol{x})$ is Jacobian matrix of $\boldsymbol{g}$ evaluated at $\boldsymbol{x}$, then fixed-point iteration converges if started close enough to solution

Smaller spectral radius yields faster convergence rate

If $\boldsymbol{G}(\boldsymbol{x}^*) = \boldsymbol{O}$, then convergence rate quadratic

Newton's Method

In n dimensions Newton's method has form

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \boldsymbol{J}(\boldsymbol{x}_k)^{-1}\boldsymbol{f}(\boldsymbol{x}_k),$$

where $\boldsymbol{J}(\boldsymbol{x})$ is Jacobian matrix of $\boldsymbol{f}$,

$$\{\boldsymbol{J}(\boldsymbol{x})\}_{ij} = \frac{\partial f_i(\boldsymbol{x})}{\partial x_j}$$

In practice, do not explicitly invert $\boldsymbol{J}(\boldsymbol{x}_k)$, but instead solve linear system

$$\boldsymbol{J}(\boldsymbol{x}_k)\boldsymbol{s}_k = -\boldsymbol{f}(\boldsymbol{x}_k),$$

for *Newton step* $\boldsymbol{s}_k$, then take as next iterate

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \boldsymbol{s}_k$$

Example: Newton's Method

Use Newton's method to solve nonlinear system

$$\boldsymbol{f}(\boldsymbol{x}) = \begin{bmatrix} x_1 + 2x_2 - 2 \\ x_1^2 + 4x_2^2 - 4 \end{bmatrix} = \boldsymbol{o}$$

Jacobian matrix is $\boldsymbol{J}_f(\boldsymbol{x}) = \begin{bmatrix} 1 & 2 \\ 2x_1 & 8x_2 \end{bmatrix}$

If we take $\boldsymbol{x}_0 = [\,1 \quad 2\,]^T$, then

$$\boldsymbol{f}(\boldsymbol{x}_0) = \begin{bmatrix} 3 \\ 13 \end{bmatrix}, \quad \boldsymbol{J}_f(\boldsymbol{x}_0) = \begin{bmatrix} 1 & 2 \\ 2 & 16 \end{bmatrix}$$

Solving system

$$\begin{bmatrix} 1 & 2 \\ 2 & 16 \end{bmatrix} \boldsymbol{s}_0 = \begin{bmatrix} -3 \\ -13 \end{bmatrix}$$

gives $\boldsymbol{s}_0 = [\,-1.83 \quad -0.58\,]^T$, and hence

$$\boldsymbol{x}_1 = \boldsymbol{x}_0 + \boldsymbol{s}_0 = \begin{bmatrix} -0.83 \\ 1.42 \end{bmatrix},$$

Example Continued

$$\boldsymbol{f}(\boldsymbol{x}_1) = \begin{bmatrix} 0 \\ 4.72 \end{bmatrix}, \quad \boldsymbol{J}_f(\boldsymbol{x}_1) = \begin{bmatrix} 1 & 2 \\ -1.67 & 11.3 \end{bmatrix}$$

Solving system

$$\begin{bmatrix} 1 & 2 \\ -1.67 & 11.3 \end{bmatrix} \boldsymbol{s}_1 = \begin{bmatrix} 0 \\ -4.72 \end{bmatrix}$$

gives $\boldsymbol{s}_1 = [\,0.64 \quad -0.32\,]^T$, and hence

$$\boldsymbol{x}_2 = \boldsymbol{x}_1 + \boldsymbol{s}_1 = \begin{bmatrix} -0.19 \\ 1.10 \end{bmatrix},$$

$$\boldsymbol{f}(\boldsymbol{x}_2) = \begin{bmatrix} 0 \\ 0.83 \end{bmatrix}, \quad \boldsymbol{J}_f(\boldsymbol{x}_2) = \begin{bmatrix} 1 & 2 \\ -0.38 & 8.76 \end{bmatrix}$$

Iterations continue until convergence to solution $x^* = [\,0 \quad 1\,]^T$

Convergence of Newton's Method

Differentiating corresponding fixed-point operator

$$\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{x} - \boldsymbol{J}(\boldsymbol{x})^{-1}\boldsymbol{f}(\boldsymbol{x})$$

and evaluating at solution $\boldsymbol{x}^*$ gives $\boldsymbol{G}(\boldsymbol{x}^*) =$

$$\boldsymbol{I} - (\boldsymbol{J}(\boldsymbol{x}^*)^{-1}\boldsymbol{J}(\boldsymbol{x}^*) + \sum_{i=1}^{n} f_i(\boldsymbol{x}^*)\boldsymbol{H}_i(\boldsymbol{x}^*)) = \boldsymbol{O},$$

where $\boldsymbol{H}_i(\boldsymbol{x})$ is component matrix of derivative of $\boldsymbol{J}(\boldsymbol{x})^{-1}$

Convergence rate of Newton's method for nonlinear systems is normally quadratic, provided Jacobian matrix $\boldsymbol{J}(\boldsymbol{x}^*)$ is nonsingular

Must be started close enough to solution to converge

Cost of Newton's Method

Cost per iteration of Newton's method for dense problem in n dimensions is substantial

- Computing Jacobian matrix costs n^2 scalar function evaluations
- Solving linear system costs $\mathcal{O}(n^3)$ operations

Secant Updating Methods

Secant updating methods reduce cost of Newton's method by

- Using function values at successive iterates to build approximate Jacobian and avoiding explicit evaluation of derivatives
- Updating factorization of approximate Jacobian rather than refactoring it each iteration

Most secant updating methods have superlinear but not quadratic convergence rate; often cost less overall than Newton's method

Broyden's Method

Broyden's method is typical secant updating method

```
$\boldsymbol{x}_0 =$ initial guess
$\boldsymbol{B}_0 =$ initial Jacobian approximation
**for** $k = 0, 1, 2, \ldots$
    Solve $\boldsymbol{B}_k \, \boldsymbol{s}_k = -\boldsymbol{f}(\boldsymbol{x}_k)$ for $\boldsymbol{s}_k$
    $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \boldsymbol{s}_k$
    $\boldsymbol{y}_k = \boldsymbol{f}(\boldsymbol{x}_{k+1}) - \boldsymbol{f}(\boldsymbol{x}_k)$
    $\boldsymbol{B}_{k+1} = \boldsymbol{B}_k + ((\boldsymbol{y}_k - \boldsymbol{B}_k \boldsymbol{s}_k)\boldsymbol{s}_k^T)/(\boldsymbol{s}_k^T \boldsymbol{s}_k)$
**end**
```

Broyden's Method, continued

Motivation for formula for $\boldsymbol{B}_{k+1}$ is to make least change to $\boldsymbol{B}_k$ subject to satisfying *secant equation*

$$\boldsymbol{B}_{k+1}(\boldsymbol{x}_{k+1} - \boldsymbol{x}_k) = \boldsymbol{f}(\boldsymbol{x}_{k+1}) - \boldsymbol{f}(\boldsymbol{x}_k)$$

In practice, factorization of $\boldsymbol{B}_k$ updated instead of updating $\boldsymbol{B}_k$ directly, so total cost per iteration is only $\mathcal{O}(n^2)$

Example: Broyden's Method

Use Broyden's method to solve nonlinear system

$$\boldsymbol{f}(\boldsymbol{x}) = \begin{bmatrix} x_1 + 2x_2 - 2 \\ x_1^2 + 4x_2^2 - 4 \end{bmatrix} = \boldsymbol{o}$$

If $\boldsymbol{x}_0 = [\,1 \quad 2\,]^T$, then $\boldsymbol{f}(\boldsymbol{x}_0) = [\,3 \quad 13\,]^T$, and we choose

$$\boldsymbol{B}_0 = \boldsymbol{J}_f(\boldsymbol{x}_0) = \begin{bmatrix} 1 & 2 \\ 2 & 16 \end{bmatrix}$$

Solving system

$$\begin{bmatrix} 1 & 2 \\ 2 & 16 \end{bmatrix} \boldsymbol{s}_0 = \begin{bmatrix} -3 \\ -13 \end{bmatrix}$$

gives $\boldsymbol{s}_0 = [\,-1.83 \quad -0.58\,]^T$, and hence

$$\boldsymbol{x}_1 = \boldsymbol{x}_0 + \boldsymbol{s}_0 = \begin{bmatrix} -0.83 \\ 1.42 \end{bmatrix},$$

Example Continued

$$\boldsymbol{f}(\boldsymbol{x}_1) = \begin{bmatrix} 0 \\ 4.72 \end{bmatrix}, \quad \boldsymbol{y}_0 = \begin{bmatrix} -3 \\ -8.28 \end{bmatrix}$$

From updating formula, we obtain

$$\boldsymbol{B}_1 = \begin{bmatrix} 1 & 2 \\ 2 & 16 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ -2.34 & -0.74 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 2 \\ -0.34 & 15.3 \end{bmatrix}$$

Solving system

$$\begin{bmatrix} 1 & 2 \\ -0.34 & 15.3 \end{bmatrix} \boldsymbol{s}_1 = \begin{bmatrix} 0 \\ -4.72 \end{bmatrix}$$

gives $\boldsymbol{s}_1 = [\,0.59 \quad -0.30\,]^T$, and hence

$$\boldsymbol{x}_2 = \boldsymbol{x}_1 + \boldsymbol{s}_1 = \begin{bmatrix} -0.24 \\ 1.120 \end{bmatrix},$$

Example Continued

$$\boldsymbol{f}(\boldsymbol{x}_2) = \begin{bmatrix} 0 \\ 1.08 \end{bmatrix}, \quad \boldsymbol{y}_1 = \begin{bmatrix} 0 \\ -3.64 \end{bmatrix}$$

From updating formula, we obtain

$$\boldsymbol{B}_2 = \begin{bmatrix} 1 & 2 \\ -0.34 & 15.3 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 1.46 & -0.73 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 2 \\ 1.12 & 14.5 \end{bmatrix}$$

Iterations continue until convergence to solution $\boldsymbol{x}^* = [\,0 \quad 1\,]^T$

Robust Newton-Like Methods

Newton's method and its variants may fail to converge when started far from solution

Safeguards can enlarge region of convergence of Newton-like methods

Simplest precaution is *damped Newton method*, in which new iterate is

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{s}_k,$$

where $\boldsymbol{s}_k$ is Newton (or Newton-like) step and α_k is scalar parameter chosen to ensure progress toward solution

Parameter α_k reduces Newton step when it is too large, but $\alpha_k = 1$ suffices near solution and still yields fast asymptotic convergence rate

Trust-Region Methods

Another approach is to maintain estimate of *trust region* where Taylor series approximation, upon which Newton's method is based, is sufficiently accurate for resulting computed step to be reliable

Adjusting size of trust region to constrain step size when necessary usually enables progress toward solution even starting far away, yet still permits rapid converge once near solution

Unlike damped Newton method, trust region method may modify direction as well as length of Newton step

More details on this approach in Chapter 6