Scientific Computing: An Introductory Survey

Chapter 5 – Nonlinear Equations

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Outline

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
- So problem is known as *root finding* or *zero finding*

Nonlinear Equations

Two important cases

- Single nonlinear equation in one unknown, where

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

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

- System of n *coupled* nonlinear equations in n unknowns, where

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

  Solution is vector $\boldsymbol{x}$ for which all components of $\boldsymbol{f}$ are zero *simultaneously*, $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{0}$

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 $\boldsymbol{x} = \begin{bmatrix} 0.5 & 0.5 \end{bmatrix}^T$ is solution vector

Existence and Uniqueness

- Existence and uniqueness of solutions are 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 is continuous and $\text{sign}(f(a)) \neq \text{sign}(f(b))$, then Intermediate Value Theorem implies there is $x^* \in [a, b]$ such that $f(x^*) = 0$
- There is no simple analog for n dimensions

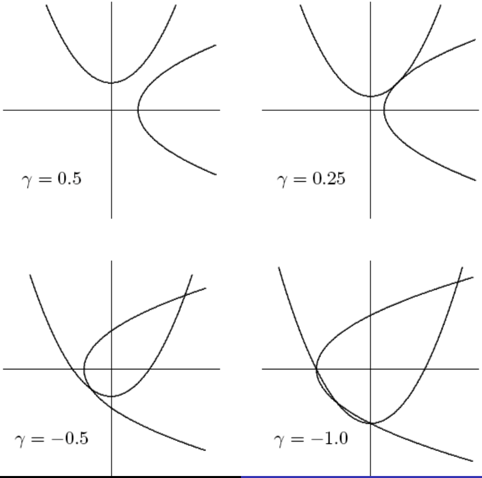
Examples: One Dimension

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

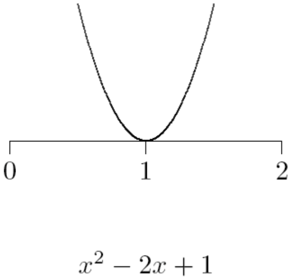
Example: Systems in Two Dimensions

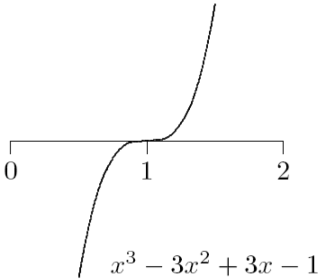
$$\begin{aligned} x_1^2 - x_2 + \gamma &= 0 \\ -x_1 + x_2^2 + \gamma &= 0 \end{aligned}$$



Multiplicity

- If $f(x^*) = f'(x^*) = f''(x^*) = \cdots = f^{(m-1)}(x^*) = 0$ but $f^{(m)}(x^*) \neq 0$ (i.e., mth derivative is lowest derivative of f that does not vanish at x^*), then root x^* has *multiplicity* m



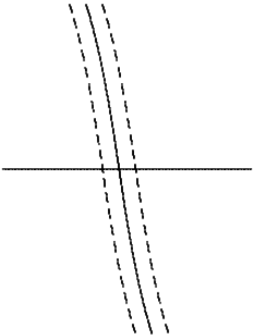


- If $m = 1$ ($f(x^*) = 0$ and $f'(x^*) \neq 0$), then x^* is *simple* root

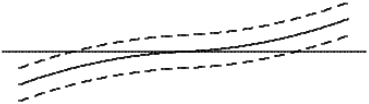
Sensitivity and Conditioning

- Conditioning of root finding problem is 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 is ill-conditioned if tangent line is nearly horizontal
- In particular, multiple root ($m > 1$) is 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 is ill-conditioned if Jacobian matrix is nearly singular

Sensitivity and Conditioning



well-conditioned



ill-conditioned

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 are not necessarily "small" simultaneously
- Small residual implies accurate solution only if problem is 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 some finite nonzero constant C

Convergence Rate, continued

Some particular cases of interest

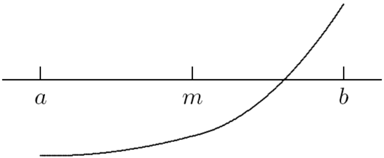
- $r = 1$: *linear* $\quad (C < 1)$
- $r > 1$: *superlinear*
- $r = 2$: *quadratic*

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 $\text{sign}(f(a)) = \text{sign}(f(m))$ **then**
    $a = m$
  else
    $b = m$
  end
end



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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

Bisection Method, continued

- Bisection method makes no use of magnitudes of function values, only their signs
- Bisection is certain to converge, but does so slowly
- At each iteration, length of interval containing solution reduced by half, convergence rate is *linear*, with $r = 1$ and $C = 0.5$
- One bit of accuracy is 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 *fixed-point iteration* scheme of form

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

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

- Also called *functional iteration*, since function g is applied repeatedly to initial starting value x_0
- For given equation $f(x) = 0$, there may be many equivalent fixed-point problems $x = g(x)$ with different choices for g

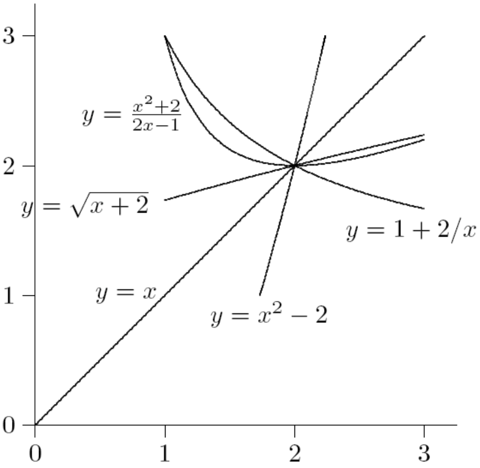
Example: Fixed-Point Problems

If $f(x) = x^2 - x - 2$, then fixed points of each of functions

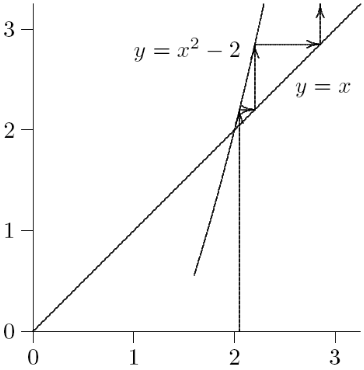
- $g(x) = x^2 - 2$
- $g(x) = \sqrt{x + 2}$
- $g(x) = 1 + 2/x$
- $g(x) = \dfrac{x^2 + 2}{2x - 1}$

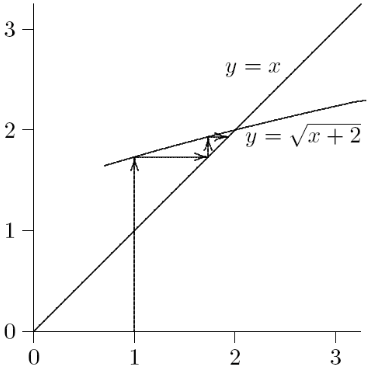
are solutions to equation $f(x) = 0$

Example: Fixed-Point Problems

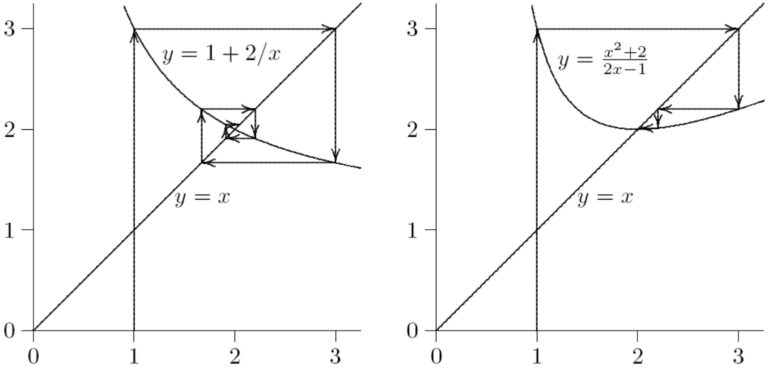


Example: Fixed-Point Iteration





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 is usually linear, with constant $C = |g'(x^*)|$
- But if $g'(x^*) = 0$, then convergence rate is at least quadratic

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Newton's Method

- Truncated Taylor series

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

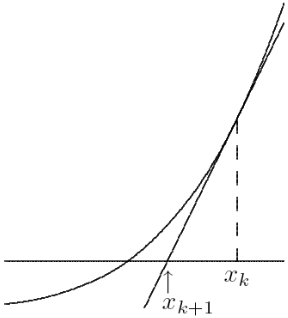
is linear function of h approximating f near x

- Replace nonlinear function f by this linear function, whose zero is $h = -f(x)/f'(x)$
- Zeros of original function and linear approximation are not identical, so repeat process, giving *Newton's method*

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

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 therefore *quadratic* ($r = 2$)
- But iterations must start close enough to root to converge

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Newton's Method, continued

For multiple root, convergence rate of Newton's method is only linear, with constant $C = 1 - (1/m)$, where m is multiplicity

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

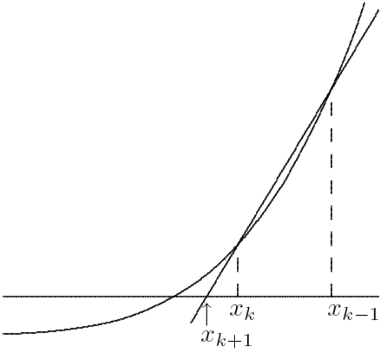
- For each iteration, Newton's method requires evaluation of both function and its derivative, which may be inconvenient or expensive
- In *secant method*, derivative is approximated by finite difference using two successive iterates, so iteration becomes

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

- Convergence rate of secant method is normally *superlinear*, with $r \approx 1.618$

Secant Method, continued

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



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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

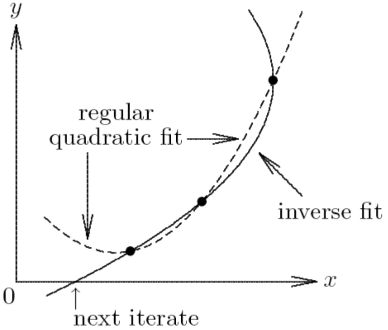
x	$f(x)$	h
1.000000	−2.365884	
3.000000	8.435520	−1.561930
1.438070	−1.896774	0.286735
1.724805	−0.977706	0.305029
2.029833	0.534305	−0.107789
1.922044	−0.061523	0.011130
1.933174	−0.003064	0.000583
1.933757	0.000019	−0.000004
1.933754	0.000000	0.000000

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
- For example, quadratic interpolation (Muller's method) has superlinear convergence rate with $r \approx 1.839$
- Unfortunately, using higher degree polynomial also has disadvantages
  - 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
- Based on nontrivial derivation using Lagrange interpolation, 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 is normally $r \approx 1.839$

< interactive example >

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

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

  is 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 is 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

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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 are 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 is much more difficult than scalar case because

- Wider variety of behavior is possible, so determining existence and number of solutions or good starting guess is much more complex
- There is 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

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

- 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
- Convergence rate is normally linear, with constant C given by spectral radius $\rho(\boldsymbol{G}(\boldsymbol{x}^*))$
- If $\boldsymbol{G}(\boldsymbol{x}^*) = \boldsymbol{O}$, then convergence rate is at least 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, we 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

$$\boldsymbol{f}(\boldsymbol{x}) = \begin{bmatrix} x_1 + 2x_2 - 2 \\ x_1^2 + 4x_2^2 - 4 \end{bmatrix} = \boldsymbol{0}$$

- Jacobian matrix is $\boldsymbol{J}_f(\boldsymbol{x}) = \begin{bmatrix} 1 & 2 \\ 2x_1 & 8x_2 \end{bmatrix}$
- If we take $\boldsymbol{x}_0 = \begin{bmatrix} 1 & 2 \end{bmatrix}^T$, 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 $\boldsymbol{s}_0 = \begin{bmatrix} -1.83 \\ -0.58 \end{bmatrix}$,

so $\boldsymbol{x}_1 = \boldsymbol{x}_0 + \boldsymbol{s}_0 = \begin{bmatrix} -0.83 & 1.42 \end{bmatrix}^T$

Example, continued

- Evaluating at new point,

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

- Solving system $\begin{bmatrix} 1 & 2 \\ -1.67 & 11.3 \end{bmatrix} \boldsymbol{s}_1 = \begin{bmatrix} 0 \\ -4.72 \end{bmatrix}$ gives $\boldsymbol{s}_1 = \begin{bmatrix} 0.64 & -0.32 \end{bmatrix}^T$, so $\boldsymbol{x}_2 = \boldsymbol{x}_1 + \boldsymbol{s}_1 = \begin{bmatrix} -0.19 & 1.10 \end{bmatrix}^T$
- Evaluating at new point,

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

- Iterations eventually convergence to solution $x^* = \begin{bmatrix} 0 & 1 \end{bmatrix}^T$

< interactive example >

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

- But it 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 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
- Secant updating methods often cost less overall than Newton's method because of lower cost per iteration

Broyden's Method

- *Broyden's method* is typical secant updating method
- Beginning with initial guess $\boldsymbol{x}_0$ for solution and initial approximate Jacobian $\boldsymbol{B}_0$, following steps are repeated until convergence

$\boldsymbol{x}_0$ = 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 $\boldsymbol{B}_k$ is 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

$$\boldsymbol{f}(\boldsymbol{x}) = \begin{bmatrix} x_1 + 2x_2 - 2 \\ x_1^2 + 4x_2^2 - 4 \end{bmatrix} = \boldsymbol{0}$$

- If $\boldsymbol{x}_0 = \begin{bmatrix} 1 & 2 \end{bmatrix}^T$, then $\boldsymbol{f}(\boldsymbol{x}_0) = \begin{bmatrix} 3 & 13 \end{bmatrix}^T$, 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 $\boldsymbol{s}_0 = \begin{bmatrix} -1.83 \\ -0.58 \end{bmatrix}$, so $\boldsymbol{x}_1 = \boldsymbol{x}_0 + \boldsymbol{s}_0 = \begin{bmatrix} -0.83 \\ 1.42 \end{bmatrix}$

Example, continued

- Evaluating at new point $\boldsymbol{x}_1$ gives $\boldsymbol{f}(\boldsymbol{x}_1) = \begin{bmatrix} 0 \\ 4.72 \end{bmatrix}$, so

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

- 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 $\boldsymbol{s}_1 = \begin{bmatrix} 0.59 \\ -0.30 \end{bmatrix}$, so $\boldsymbol{x}_2 = \boldsymbol{x}_1 + \boldsymbol{s}_1 = \begin{bmatrix} -0.24 \\ 1.120 \end{bmatrix}$

Example, continued

- Evaluating at new point $\boldsymbol{x}_2$ gives $\boldsymbol{f}(\boldsymbol{x}_2) = \begin{bmatrix} 0 \\ 1.08 \end{bmatrix}$, so

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

- 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 $\boldsymbol{x}^* = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

< interactive example >

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 will be given in Chapter 6