MATH 350: Introduction to Computational Mathematics

Chapter IV: Locating Roots of Equations

Greg Fasshauer

Department of Applied Mathematics
Illinois Institute of Technology

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Outline

1. Motivation and Applications
2. Bisection
3. Newton's Method
4. Secant Method
5. Inverse Quadratic Interpolation
6. Root Finding in MATLAB: The Function `fzero`
7. Newton's Method for Systems of Nonlinear Equations
8. Optimization

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fasshauer@iit.edu

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Find the first positive root of the Bessel function

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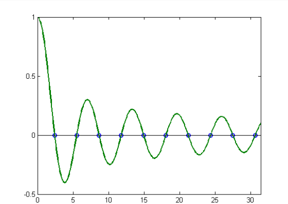

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Consider the skydive model of Chapter 1. We can use a numerical method to find the velocity at any time $t \geq 0$. At what time will the skydiver hit the ground?

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Solution

- First we need to find the position (altitude) for any time t from the initial position and calculated velocity (essentially the solution of another differential equation).
- Then we need to find the root of the position function — a rather complex procedure.

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Consider a missile M following the parametrized path

$$x_M(t) = t, \qquad y_M(t) = 1 - e^{-t},$$

and a missile interceptor I whose launch angle α we want to determine so that it will intersect the missile's path. Let the parametrized path for the interceptor be given as

$$x_I(t) = 1 - t\cos\alpha, \qquad y_I(t) = t\sin\alpha - \frac{t^2}{10}.$$

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Thus, we want to solve the nonlinear system

$$\left\{\begin{array}{rcl} t & = & 1 - t\cos\alpha \\ 1 - e^{-t} & = & t\sin\alpha - \frac{t^2}{10} \end{array}\right. \quad \text{or} \quad \left\{\begin{array}{rcl} f(t,\alpha) & = & t - 1 + t\cos\alpha = 0 \\ g(t,\alpha) & = & 1 - e^{-t} - t\sin\alpha + \frac{t^2}{10} = 0. \end{array}\right.$$

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  - Repeat entire procedure with either $[a, b] = [a, x]$ or $[a, b] = [x, b]$ (making sure that $f(a)$ and $f(b)$ have opposite signs).

Bisection Algorithm

```
while abs(b-a) > eps*abs(b)
    x = (a + b)/2;
    if sign(f(x)) == sign(f(b))
        b = x;     % set [a,x] as new [a,b]
    else
        a = x;     % set [x,b] as new [a,b]
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See `BisectDemo.m` and `bisect.m` for an illustration.

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Remark

The algorithm as coded above should always — independent of f — converge in 52 iterations since the IEEE standard uses 52 bits for the mantissa, and we compute the answer with 1 bit accuracy.

Outline

By Taylor's theorem (assuming $f''(\xi)$ exists) we have

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + \frac{(x - x_0)^2}{2} f''(\xi).$$

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$$0 \approx f(x_0) + (x - x_0)f'(x_0) \quad \Longleftrightarrow \quad x - x_0 \approx -\frac{f(x_0)}{f'(x_0)}.$$

This motivates the Newton iteration formula

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \qquad n = 0, 1, \ldots,$$

where an initial guess x_0 is required to start the iteration.

Graphical Interpretation

Consider the tangent line to the graph of f at x_n:

$$y - f(x_n) = f'(x_n)(x - x_n) \quad \Longrightarrow \quad y = f(x_n) + (x - x_n)f'(x_n).$$

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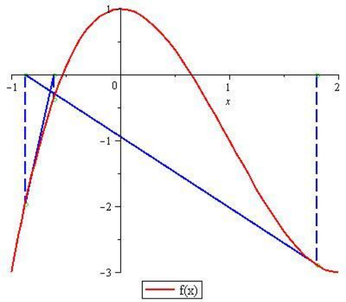

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Remark

Convergence of Newton's method depends quite a bit on the choice of the initial guess x_0*. If successful, the algorithm above converges very quickly to within machine accuracy.*

Problem

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Solution

Let's assume $f''(x)$ exists and $f'(x) \neq 0$ for all x of interest.

- Denote the root of f by x_*,
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This is known as quadratic convergence, and implies that the number of correct digits approximately doubles in each iteration.

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Then we get the iteration formula

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Remark

The secant method requires two initial guesses, x_0 and x_1.

Secant Method

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while abs(b-a) > eps*abs(b)
    c = a;
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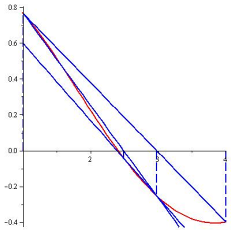
See `SecantDemo.m` and `secant.m` for an illustration. The Maple file `SecantDemo.mws` contains an animated graphical illustration of the algorithm.



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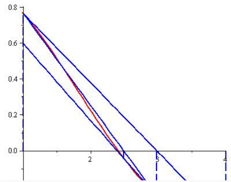

Remark

Convergence of the secant method also depends on the choice of initial guesses. If successful, the algorithm converges superlinearly, i.e., $e_{n+1} = \mathcal{O}(e_n^{\phi})$, *where* $\phi = (\sqrt{5}+1)/2$, *the golden ratio.*

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Answer

In principle, "yes". The resulting method is called inverse quadratic interpolation (IQI).

> *IQI is like an immature race horse. It moves very quickly when it is near the finish line, but its global behavior can be erratic [NCM].*

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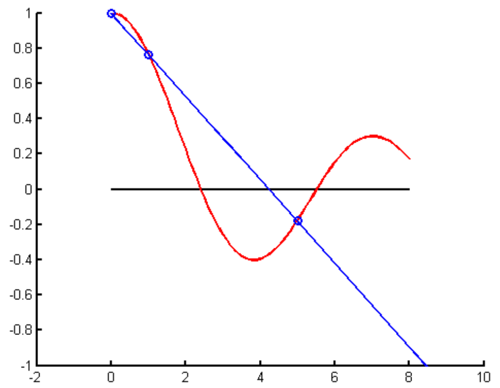

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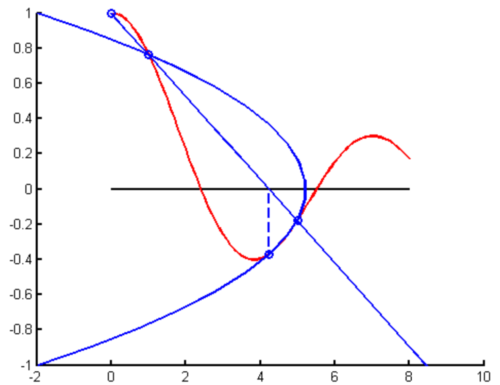
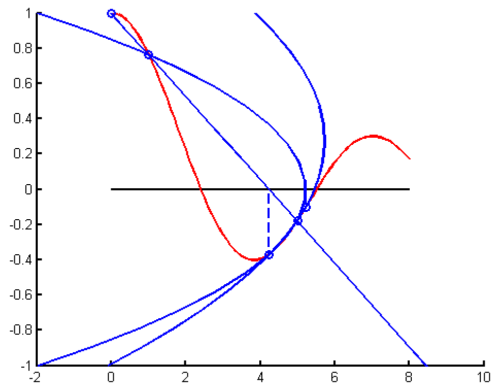


How does inverse quadratic interpolation work?

Assume we have 3 data points: $(a, f(a)), (b, f(b)), (c, f(c))$.
Instead of interpolating the data directly with a quadratic polynomial we reverse the roles of x and y since then we can evaluate the resulting polynomial at $y = 0$; and this gives an approximation to the root of f!



IQI Method

```
while abs(c-b) > eps*abs(c)
    x = polyinterp([f(a),f(b),f(c)],[a,b,c],0);
    a = b;
    b = c;
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See the MATLAB script `IQIDemo.m` which calls the function `iqi.m`.

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See the MATLAB script `IQIDemo.m` which calls the function `iqi.m`.

Remark

One of the major challenges for the IQI method is to ensure that the function values, i.e., $f(a)$, $f(b)$ and $f(c)$, are distinct — since we are using them as our interpolation nodes.

Outline

1. Motivation and Applications
2. Bisection
3. Newton's Method
4. Secant Method
5. Inverse Quadratic Interpolation
6. **Root Finding in MATLAB: The Function `fzero`**
7. Newton's Method for Systems of Nonlinear Equations
8. Optimization

The MATLAB code `fzerotx.m` from [NCM] is based on a combination of three of the methods discussed above: bisection, secant, and IQI.

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- Start with a and b so that $f(a)$ and $f(b)$ have opposite signs.
- Use a secant step to give c between a and b.
- Repeat the following steps until $|b - a| < \epsilon|b|$ or $f(b) = 0$.
- Arrange a, b, and c so that
  - $f(a)$ and $f(b)$ have opposite signs,
  - $|f(b)| \leq |f(a)|$,
  - c is the previous value of b.
- If $c \neq a$, consider an IQI step.
- If $c = a$, consider a secant step.
- If the IQI or secant step is in the interval $[a, b]$, take it.
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The algorithm always works and combines the robustness of the bisection method and the speed of the secant and IQI methods.

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Root finding in MATLAB (cont.)

A step-by-step exploration of the `fzero` algorithm is possible with `fzerogui.m` from [NCM].
To find the first positive root of J_0 use

```
fzerogui(@(x) besselj(0,x),[0,4]),
```

where `@(x) besselj(0,x)` is an *anonymous function* of the one variable `x` (while the argument `@besselj` would be a *function handle* for a function of two variables – and therefore confuse the routine `fzerogui`).

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Example

We now want to solve a nonlinear system such as

$$\begin{aligned} f(t,\alpha) &= t - 1 + t\cos\alpha = 0 \\ g(t,\alpha) &= 1 - e^{-t} - t\sin\alpha + \frac{t^2}{10} = 0. \end{aligned}$$

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$$f(x) = f(c) + (x-c)f'(c) + \frac{(x-c)^2}{2}f''(\xi).$$

Then

$$f(x) \approx f(c) + (x-c)f'(c) \quad \overset{f(x)=0}{\Longleftrightarrow} \quad x \approx c - \frac{f(c)}{f'(c)}.$$

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where $\boldsymbol{x} = [t,\alpha]^T$ and $\boldsymbol{f} = [f,g]^T$.
We therefore need a multivariate version of Newton's method.

For a single function f of m variables we would need the expansion

$$f(\boldsymbol{x}) = f(\boldsymbol{c}) + ((\boldsymbol{x}-\boldsymbol{c})^T\nabla)f(\boldsymbol{c}) + \frac{1}{2}((\boldsymbol{x}-\boldsymbol{c})^T\nabla)^2 f(\xi),$$

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If we have only $m = 2$ variables, i.e., $\boldsymbol{x} = [x_1, x_2]^T$, this becomes

$$\begin{aligned} f(x_1,x_2) &= f(c_1,c_2) + \left((x_1-c_1)\frac{\partial}{\partial x_1} + (x_2-c_2)\frac{\partial}{\partial x_2}\right) f(c_1,c_2) \\ &\quad + \frac{1}{2}\left((x_1-c_1)\frac{\partial}{\partial x_1} + (x_2-c_2)\frac{\partial}{\partial x_2}\right)^2 f(\xi_1,\xi_2) \end{aligned}$$

fasshauer@iit.edu

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Example (cont.)

Therefore, we can approximate f by

$$f(x_1, x_2) \approx f(c_1, c_2) + (x_1 - c_1)\frac{\partial f}{\partial x_1}(c_1, c_2) + (x_2 - c_2)\frac{\partial f}{\partial x_2}(c_1, c_2)$$

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Note that this approximation is a linearization of f and in fact denotes the tangent plane to the graph of f at the point $\boldsymbol{c}$.

More generally, we have the multivariate Taylor expansion:

$$f(\boldsymbol{x}) = \sum_{k=0}^{n} \frac{1}{k!}((\boldsymbol{x}-\boldsymbol{c})^T\nabla)^k f(\boldsymbol{c}) + E_{n+1}(\boldsymbol{x}). \tag{3}$$

Here the remainder is

$$E_{n+1}(\boldsymbol{x}) = \frac{1}{(n+1)!}((\boldsymbol{x}-\boldsymbol{c})^T\nabla)^{n+1} f(\xi)$$

where $\xi = \boldsymbol{c} + \theta(\boldsymbol{x}-\boldsymbol{c})$ with $0 < \theta < 1$ a point somewhere on the line connecting $\boldsymbol{c}$ and $\boldsymbol{x}$, and $\nabla = \left[\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \ldots, \frac{\partial}{\partial x_m}\right]^T$ is the gradient operator as before.

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Remark

Note, however, that this slide is added as a reference/reminder only and is not required for the derivation of the multivariate Newton method.

Now we want to tackle the full problem, i.e., we want to solve the following (square) *system of nonlinear equations*:

$$\begin{aligned} f_1(x_1, x_2, \ldots, x_m) &= 0, \\ f_2(x_1, x_2, \ldots, x_m) &= 0, \\ &\vdots \\ f_m(x_1, x_2, \ldots, x_m) &= 0. \end{aligned} \tag{4}$$

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To derive Newton's method for (4) we write it in the form,

$$f_i(\boldsymbol{x}) = 0, \qquad i = 1, \ldots, m.$$

By linearizing f_i, $i = 1, \ldots, m$, as discussed above we have

$$f_i(\boldsymbol{x}) \approx f_i(\boldsymbol{c}) + ((\boldsymbol{x} - \boldsymbol{c})^T \nabla) f_i(\boldsymbol{c}).$$

Since $f_i(\boldsymbol{x}) = 0$ we get

$$\begin{aligned} -f_i(\boldsymbol{c}) &\approx ((\boldsymbol{x}-\boldsymbol{c})^T\nabla)f_i(\boldsymbol{c}) \\ &= (x_1-c_1)\frac{\partial f_i}{\partial x_1}(\boldsymbol{c}) + (x_2-c_2)\frac{\partial f_i}{\partial x_2}(\boldsymbol{c}) + \ldots + (x_m-c_m)\frac{\partial f_i}{\partial x_m}(\boldsymbol{c}). \end{aligned}$$

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\end{aligned}$$

Therefore, we have a linear system for the unknown approximate root $\boldsymbol{x}$ of (4):

$$\begin{aligned}
-f_1(c_1,\ldots,c_m) &= (x_1 - c_1)\frac{\partial f_1}{\partial x_1}(c_1,\ldots,c_m) + \ldots + (x_m - c_m)\frac{\partial f_1}{\partial x_m}(c_1,\ldots,c_m), \\
-f_2(c_1,\ldots,c_m) &= (x_1 - c_1)\frac{\partial f_2}{\partial x_1}(c_1,\ldots,c_m) + \ldots + (x_m - c_m)\frac{\partial f_2}{\partial x_m}(c_1,\ldots,c_m), \\
&\vdots \\
-f_m(c_1,\ldots,c_m) &= (x_1 - c_1)\frac{\partial f_m}{\partial x_1}(c_1,\ldots,c_m) + \ldots + (x_m - c_m)\frac{\partial f_m}{\partial x_m}(c_1,\ldots,c_m).
\end{aligned} \tag{5}$$

To simplify notation a bit we now introduce $\boldsymbol{h} = [h_1, \ldots, h_m]^T = \boldsymbol{x} - \boldsymbol{c}$, and note that (5) is a linear system for $\boldsymbol{h}$ of the form

$$\mathsf{J}(\boldsymbol{c})\boldsymbol{h} = -\boldsymbol{f}(\boldsymbol{c}),$$

where $\boldsymbol{f} = [f_1, \ldots, f_m]^T$ and

$$\mathsf{J} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_m} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_m} \end{bmatrix}$$

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Since $\boldsymbol{h} = \boldsymbol{x} - \boldsymbol{c}$ or $\boldsymbol{x} = \boldsymbol{c} + \boldsymbol{h}$ we see that $\boldsymbol{h}$ is an update to the previous approximation $\boldsymbol{c}$ of the root $\boldsymbol{x}$.

Algorithm

Newton's method for square nonlinear systems is performed by

```
Input $\boldsymbol{f}$, J, $\boldsymbol{x}^{(0)}$
for $n = 0, 1, 2, \ldots$ do
    Solve $\mathrm{J}(\boldsymbol{x}^{(n)})\boldsymbol{h} = -\boldsymbol{f}(\boldsymbol{x}^{(n)})$ for $\boldsymbol{h}$
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Remark

If we symbolically write $\mathbf{f}'$ *instead of* J*, then the Newton iteration becomes*

$$\boldsymbol{x}^{(n+1)} = \boldsymbol{x}^{(n)} - \underbrace{\left[\boldsymbol{f}'(\boldsymbol{x}^{(n)})\right]^{-1}}_{\text{matrix}} \boldsymbol{f}(\boldsymbol{x}^{(n)}),$$

which looks just like the Newton iteration formula for the single equation/single variable case.

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Solve the missile intercept problem

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This example is illustrated in the MATLAB script `NewtonmvDemo.m` which requires `newtonmv.m`, `missile_f.m` and `missile_j.m`.

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$$\begin{aligned} x^2 + y^2 &= 4 \\ xy &= 1, \end{aligned}$$

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This example is also illustrated in the MATLAB script `NewtonmvDemo.m`. The files `circhyp_f.m` and `circhyp_j.m` are also needed.

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4. *Also, there is no built-in* MATLAB *code for nonlinear systems. However, the Optimization Toolbox (part of the student version) has a function* `fsolve` *that can be used for this purpose (note that it does not require the Jacobian of f). Try, e.g.,*
   `fsolve(@circhyp_f, [-3 1.5]).`

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2. *In each iteration an $m \times m$ (dense) linear system has to be solved. This makes Newton's method very expensive and slow.*
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4. *Also, there is no built-in* MATLAB *code for nonlinear systems. However, the Optimization Toolbox (part of the student version) has a function* `fsolve` *that can be used for this purpose (note that it does not require the Jacobian of f). Try, e.g.,* `fsolve(@circhyp_f, [-3 1.5])`.
5. *More details for nonlinear systems are provided in MATH 477 and/or MATH 478.*

Outline

1. Motivation and Applications
2. Bisection
3. Newton's Method
4. Secant Method
5. Inverse Quadratic Interpolation
6. Root Finding in MATLAB: The Function `fzero`
7. Newton's Method for Systems of Nonlinear Equations
8. Optimization

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The final MATLAB function will again be a robust hybrid method.

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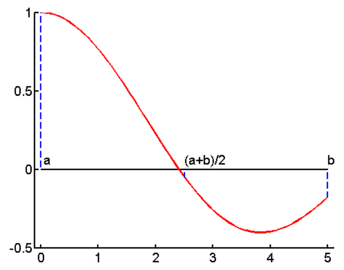

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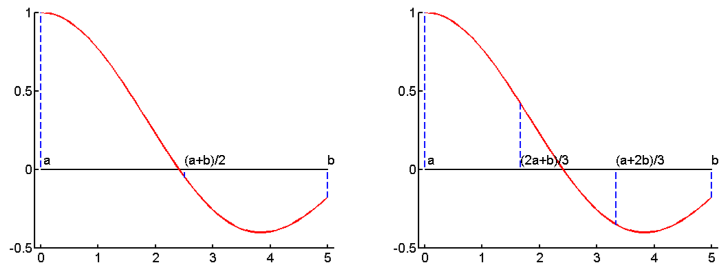

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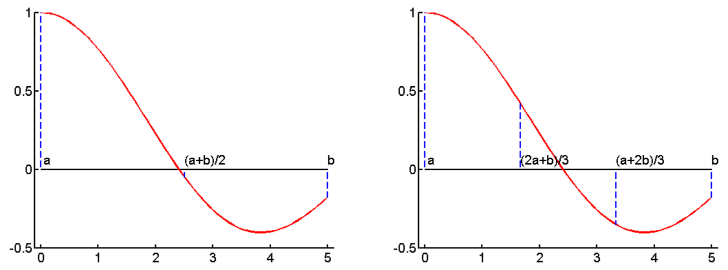

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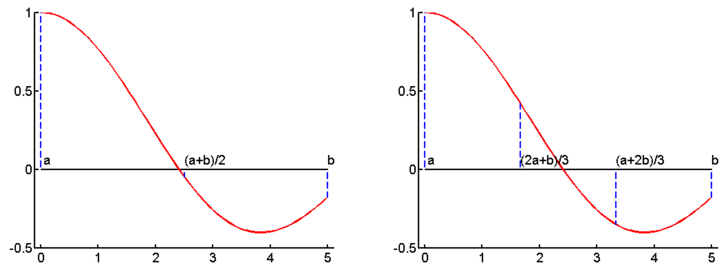

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This strategy would work, but is inefficient since $(a+2b)/3$ can't be used for the next trisection step.

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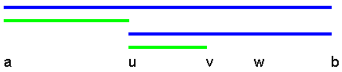
If, for example, the interval in the next iteration is $[u, b]$ with interior point v, then we want ρ to be such that the position of v relative to u and b is the same as that of u was to a and b in the previous iteration.



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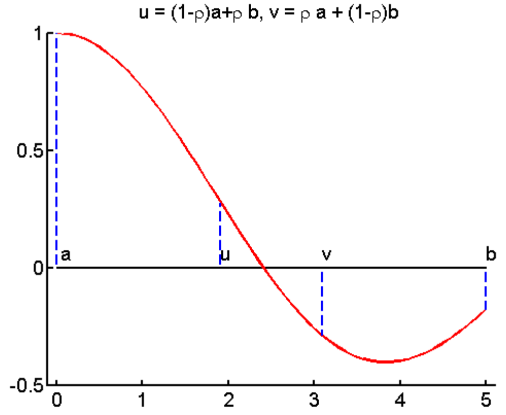
Since $\rho = 2-\phi$, where $\phi = \tfrac{1+\sqrt{5}}{2} \approx 1.618034$ is the golden ratio, the method is called the golden section search.

Golden Section Search (cont.)



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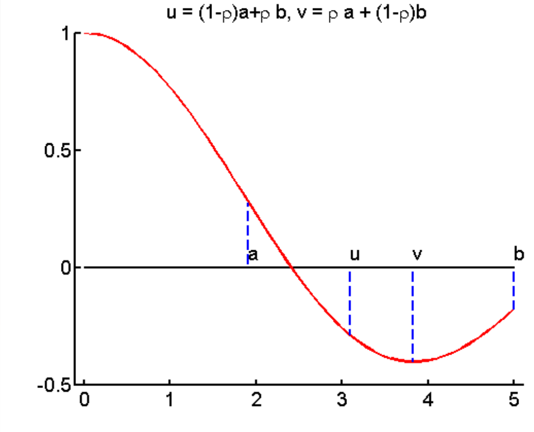

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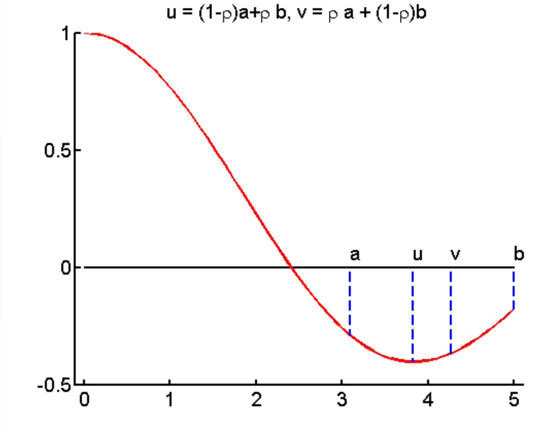

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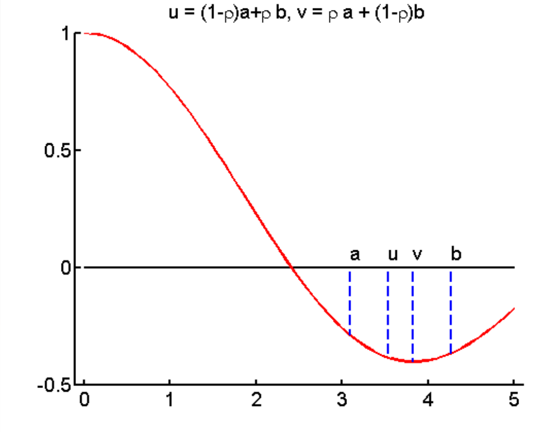

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For an illustration see the MATLAB script `FminDemo.m` which calls `fmintx.m` from [NCM].

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One could also use Newton's method to find the critical points of f. However, then not only f' needs to be known, but also f''.

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Minimization of functions of more than one variable can be attempted with `fminsearch` in basic MATLAB, and with other — more powerful — functions provided in the optimization toolbox.

References I

C. Moler.
Numerical Computing with MATLAB.
SIAM, Philadelphia, 2004.
Also http://www.mathworks.com/moler/.