Computational Astrophysics

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Outline

Root Finding

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f could be a single equation or a system of equations).
f can either explicitly depend on x or have and implicit dependence on x.

Newton-Raphson Method

If we expand a function $f(x)$ about its root x_r, we get:

$$f(x_r) = f(x) + (x_r - x)f'(x) + \mathcal{O}((x_r - x)^2) = 0 \ . \qquad (1)$$

x_r can be seen a trial value for the root x_r at the n-th step of an iterative procedure. The $n + 1$-th step is then

$$f(x_{n+1}) = f(x_n) + \underbrace{(x_{n+1} - x_n)}_{\delta x} f'(x_n) \approx 0 \ , \qquad (2)$$

and, thus,

$$x_{n+1} = x_n + \delta x = x_n - \frac{f(x_n)}{f'(x_n)} \ . \qquad (3)$$

Newton-Raphson Method

The iteration is stopped when the fractional change between iteration n and $n+1$ is smaller than some small number: $|[f(x_{n+1}) - f(x_n)]/f(x_n)| < \epsilon$. One should not expect ϵ to be smaller than floating point accuracy.

Newton's Method as quadratic convergence, provided $f(x)$ is well behaved and that one has **a good initial guess for the root**. It also requires to know the derivative $f'(x_n)$ directly.

Secant Method

The Secant Method is just the Newton's method but evaluating the first derivative $f'(x_n)$ numerically. For example, with a backward difference, this is

$$x_{n+1} = x_n - f(x_n)\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})} \ . \tag{4}$$

This method will converge less rapidly than Newton's method because we have introduced a first-order derivative.
Note that it is needed to know two points to start the iteration.

Bisection Method

The intermediate-value theorem states that a continuous function $f(x)$ has at least one root in the interval $[a, b]$ if $f(a)$ and $f(b)$ are of opposite sign.

The bisection method exploits the intermediate-value theorem.

Bisection Method

1. Pick initial values of a and b so that $f(a)$ and $f(b)$ have opposite sign.
2. Compute the midpoint $c = \frac{a+b}{2}$. If $f(c) = 0$ or $|[f(c) - f(a)]/f(a)| < \epsilon$ or $|[f(c) - f(b)]/f(b)| < \epsilon$, then one is done!.
   If not:
   a. If $f(a)$ and $f(c)$ have opposite sign, then they bracket a root. Go to 1 with $a = a$, $b = c$.
   b. If $f(c)$ and $f(b)$ have opposite sign, then they bracket a root. Got to 1 with $a = c$, $b = b$.

Bisection Method

The bisection method is very effective, more robust, but generally not as fast as Newton's Method, requiring more iterations until a root is found.

Multi-Variate Root Finding

$\mathbf{f}(\mathbf{x})$ is a multi-variate vector function and we are looking for $\mathbf{f}(\mathbf{x}) = 0$.

Analogously to the scalar case, we write the multi-variate Newton's/Secant Method,

Multi-Variate Root Finding

$$\mathbf{f}(\mathbf{x}_{n+1}) \approx \mathbf{f}(\mathbf{x}_n) + \nabla \otimes \mathbf{f}(\mathbf{x}_n)(\mathbf{x}_{n+1} - \mathbf{x}_n) = 0 \ , \tag{5}$$

and

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \left[\nabla \otimes \mathbf{f}(\mathbf{x}_n)\right]^{-1} \mathbf{f}(\mathbf{x}) \ . \tag{6}$$

Here,

$$\mathbf{J} \equiv \nabla \otimes \mathbf{f}(\mathbf{x}_n) \ , \tag{7}$$

is the Jacobian matrix. In index notation, it is given by

$$J_{ij} = \frac{\partial f_i}{\partial x_j} \ . \tag{8}$$