Scientific Computing: Solving Nonlinear Equations

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Outline

Fundamentals

- Simplest problem: **Root finding** in one dimension:

$$f(x) = 0 \text{ with } x \in [a, b]$$

- Or more generally, solving a **square system of nonlinear equations**

$$\mathbf{f}(\mathbf{x}) = \mathbf{0} \quad \Rightarrow f_i(x_1, x_2, \ldots, x_n) = 0 \textbf{ for } i = 1, \ldots, n.$$

- There can be no closed-form answer, so just as for eigenvalues, we need **iterative methods**.
- Most generally, starting from $m \geq 1$ **initial guesses** $x^0, x^1, \ldots, x^m$, iterate:

$$x^{k+1} = \phi(x^k, x^{k-1}, \ldots, x^{k-m}).$$

Order of convergence

- Consider one dimensional root finding and let the actual root be α, $f(\alpha) = 0$.
- A sequence of iterates x^k that converges to α has **order of convergence** $p \geq 1$ if as $k \to \infty$

$$\frac{\left|x^{k+1} - \alpha\right|}{\left|x^k - \alpha\right|^p} = \frac{\left|e^{k+1}\right|}{\left|e^k\right|^p} \to C = \text{const},$$

  where the constant C is a **convergence factor**, $C < 1$ for $p = 1$.
- A method should at least converge **linearly** ($p = 1$), that is, the error should at least be reduced by a constant factor every iteration, for example, the number of accurate digits increases by 1 every iteration.
- A good method for root finding coverges **quadratically** ($p = 2$), that is, the number of accurate digits **doubles** every iteration!

Local vs. global convergence

- A **good initial guess** is extremely important in nonlinear solvers!
- Assume we are looking for a **unique root** $a \leq \alpha \leq b$ starting with an initial guess $a \leq x_0 \leq b$.
- A method has **local convergence** if it converges to a given root α for any initial guess that is sufficiently close to α (in the **neighborhood of a root**).
- A method has **global convergence** if it converges to the root for any initial guess.
- General rule: Global convergence requires a **slower** (careful) method **but is safer**.
- It is best to combine a global method to first find a good initial guess close to α and then use a faster local method.

Conditioning of root finding

$$f(\alpha + \delta\alpha) \approx f(\alpha) + f'(\alpha)\delta\alpha = \delta f$$

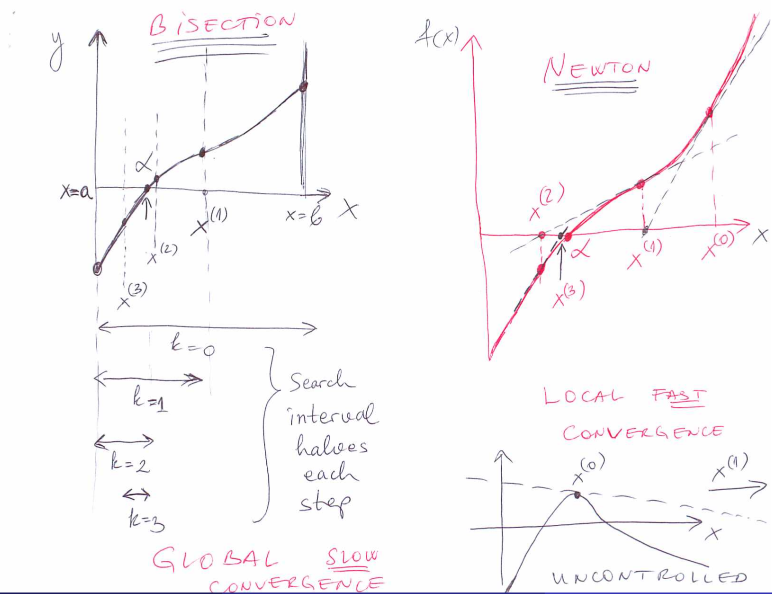
$$|\delta\alpha| \approx \frac{|\delta f|}{|f'(\alpha)|} \quad \Rightarrow \kappa_{abs} = \left|f'(\alpha)\right|^{-1}.$$

- The problem of finding a **simple root** is well-conditioned when $|f'(\alpha)|$ is far from zero.
- Finding **roots with multiplicity** $m > 1$ is **ill-conditioned**:

$$\left|f'(\alpha)\right| = \cdots = \left|f^{(m-1)}(\alpha)\right| = 0 \quad \Rightarrow \quad |\delta\alpha| \approx \left[\frac{|\delta f|}{|f^m(\alpha)|}\right]^{1/m}$$

- Note that finding **roots of algebraic equations** (polynomials) is a separate subject of its own that we skip.

The bisection and Newton algorithms



Bisection

- First step is to **locate a root** by searching for a **sign change**, i.e., finding a^0 and b^0 such that
$$f(a^0)f(b^0) < 0.$$
- The simply **bisect** the interval, for $k = 0, 1, \ldots$
$$x^k = \frac{a^k + b^k}{2}$$
and choose the half in which the function changes sign, i.e., either $a^{k+1} = x^k,\ b^{k+1} = b^k$ or $b^{k+1} = x^k,\ a^{k+1} = a^k$ so that $f(a^{k+1})f(b^{k+1}) < 0$.
- Observe that each step we need one **function evaluation**, $f(x^k)$, but only the sign matters.
- The **convergence is essentially linear** because
$$\left|x^k - \alpha\right| \leq \frac{b^k}{2^{k+1}} \quad \Rightarrow \frac{\left|x^{k+1} - \alpha\right|}{\left|x^k - \alpha\right|} \leq 2.$$

Newton's Method

- Bisection is a slow but sure method. It uses no information about the value of the function or its derivatives.
- Better convergence, of order $p = (1+\sqrt{5})/2 \approx 1.63$ (the golden ratio), can be achieved by using the value of the function at two points, as in the **secant method**.
- Achieving second-order convergence requires also evaluating the **function derivative**.
- **Linearize the function** around the current guess using Taylor series:

$$f(x^{k+1}) \approx f(x^k) + (x^{k+1} - x^k) f'(x^k) = 0$$

$$x^{k+1} = x^k - \frac{f(x^k)}{f'(x^k)}$$

Convergence of Newton's method

Use Taylor series with remainder and divide by $f'(x^k) \neq 0$:

$$\exists \xi \in [x_n, \alpha] : \quad f(\alpha) = 0 = f(x^k) + (\alpha - x^k) f'(x^k) + \frac{1}{2}(\alpha - x^k)^2 f''(\xi) = 0,$$

$$\left[x^k - \frac{f(x^k)}{f'(x^k)} \right] - \alpha = -\frac{1}{2}(\alpha - x^k)^2 \frac{f''(\xi)}{f'(x^k)}$$

$$x^{k+1} - \alpha = e^{k+1} = -\frac{1}{2} \left(e^k \right)^2 \frac{f''(\xi)}{f'(x^k)}$$

which shows **second-order convergence**

$$\frac{\left| x^{k+1} - \alpha \right|}{\left| x^k - \alpha \right|^2} = \frac{\left| e^{k+1} \right|}{\left| e^k \right|^2} = \left| \frac{f''(\xi)}{2f'(x^k)} \right| \to \left| \frac{f''(\alpha)}{2f'(\alpha)} \right|$$

Basin of attraction for Newton's method

- For convergence we want $\left|e^{k+1}\right| < \left|e^{k}\right|$ so we want

$$\left|e^{k}\right| \left|\frac{f''(\alpha)}{2f'(\alpha)}\right| < 1 \quad \Rightarrow \quad \left|e^{k}\right| < \left|\frac{2f'(\alpha)}{f''(\alpha)}\right|$$

- Newton's method **converges quadratically if we start sufficiently close to a simple root**, more precisely, if

$$\left|x^{0} - \alpha\right| = \left|e^{0}\right| \lesssim \left|\frac{2f'(\alpha)}{f''(\alpha)}\right|.$$

  This is just a **rough estimate**, not a precise bound!

- A robust but fast algorithm for root finding would **safeguard Newton's method** with bisection: Eventually we will accept all Newton steps once close to the root, so we will get **quadratic convergence**, but also be **guaranteed to converge** to a root.

Fixed-Point Iteration

$$f(x) = 0 \quad \Rightarrow \quad x = f(x) + x = \phi(x)$$

- Then we can use **fixed-point iteration**

$$x^{k+1} = \phi(x^k)$$

- whose fixed point (limit), if it converges, is $x \to \alpha$. Taylor series estimate:

$$x^{k+1} = \alpha + e^{k+1} \approx \phi(\alpha) + \phi'(\alpha)\left(x^k - \alpha\right) = \alpha + \phi'(\alpha)e^k \quad \Rightarrow$$

$$e^{k+1} \approx \phi'(\alpha)e^k \quad \Rightarrow \quad \text{we want } \left|\phi'(\alpha)\right| < 1.$$

- It can be proven that the fixed-point iteration converges if $\phi(x)$ is a **contraction mapping**:

$$\left|\phi'(x)\right| \leq K < 1 \quad \forall x \in [a, b]$$

[If $\phi(x)$ is Lipschitz continuous with Lipschitz constant $L < 1$.]

Stopping Criteria

- A good library function for root finding has to implement careful termination criteria.
- An obvious option is to terminate when the **residual becomes small**

$$\left|f(x^k)\right| < \varepsilon,$$

  which **works for very well-conditioned problems**, $|f'(\alpha)| \sim 1$.
- Another option is to terminate when the **increment becomes small**

$$\left|x^{k+1} - x^k\right| < \varepsilon.$$

- For example, for fixed-point iteration this test would stop at step k:

$$x^{k+1} - x^k = e^{k+1} - e^k \approx \left[1 - \phi'(\alpha)\right] e^k \quad \Rightarrow \quad \left|e^k\right| \approx \frac{\varepsilon}{[1 - \phi'(\alpha)]},$$

  so we see that the increment test **works for rapidly converging iterations**, i.e., when $|1 - \phi'(\alpha)|$ is not small.

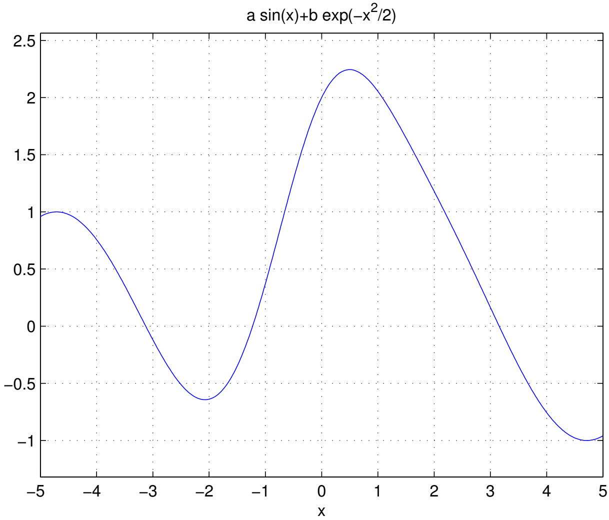
In practice

- A robust but fast algorithm for root finding would **combine (safeguard) bisection with Newton's method**: Given a current bisection interval $[a, b]$, if $x^{k+1} \in (a, b)$ then accept Newton step, otherwise just set $x^{k+1} = (a + b)/2$. Take new bisection interval to be either $\left[a, x^{k+1}\right]$ or $\left[x^{k+1}, b\right]$ the same way as in bisection where we always use $x^{k+1} = (a + b)/2$.
- Newton's method requires first-order derivatives so often other methods are preferred that require **function evaluation only**. Examples include secant method (based on linear interpolation) or **inverse quadratic interpolation** (fit a parabola through three past points $(f(x_i), x_i)$, $i = 1, 2, 3$, and evaluate for zero argument to give a new point).
- Matlab's function *fzero* combines bisection, secant and inverse quadratic interpolation and is "fail-safe". See, for example, "**Brent's method**" on Wikipedia.

Find zeros of $a\sin(x) + b\exp(-x^2/2)$

```
% f=@mfile uses a function in an m-file

% Parameterized functions are created with:
a = 1; b = 2;
f = @(x)    a*sin(x) + b*exp(-x^2/2) ; % Handle

figure(1)
ezplot(f,[-5,5]); grid

x1=fzero(f, [-2,0])
[x2, f2]=fzero(f, 2.0)

x1 =    -1.227430849357917
x2 =     3.155366415494801
f2 =    -2.116362640691705e-16
```

Figure of $f(x)$



Multi-Variable Taylor Expansion

- It is convenient to focus on one of the equations, i.e., consider a **scalar function** $f(\mathbf{x})$.
- The usual Taylor series is replaced by

$$f(\mathbf{x}+\Delta\mathbf{x}) = f(\mathbf{x}) + \mathbf{g}^T(\Delta\mathbf{x}) + \frac{1}{2}(\Delta\mathbf{x})^T\mathbf{H}(\Delta\mathbf{x})$$

where the **gradient vector** is

$$\mathbf{g} = \boldsymbol{\nabla}_{\mathbf{x}} f = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \cdots, \frac{\partial f}{\partial x_n}\right]^T$$

and the **Hessian matrix** is

$$\mathbf{H} = \boldsymbol{\nabla}^2_{\mathbf{x}} f = \left\{\frac{\partial^2 f}{\partial x_i \partial x_j}\right\}_{ij}$$

Vector Functions of Vectors

- We are after solving a **square system of nonlinear equations** for some variables $\mathbf{x}$:

$$\mathbf{f}(\mathbf{x}) = \mathbf{0} \quad \Rightarrow f_i(x_1, x_2, \ldots, x_n) = 0 \textbf{ for } i = 1, \ldots, n.$$

- The first-order Taylor series is

$$\mathbf{f}\left(\mathbf{x}^k + \Delta\mathbf{x}\right) \approx \mathbf{f}\left(\mathbf{x}^k\right) + \left[\mathbf{J}\left(\mathbf{x}^k\right)\right] \Delta\mathbf{x} = \mathbf{0}$$

where the Jacobian $\mathbf{J}$ has the gradients of $f_i(\mathbf{x})$ as rows:

$$\left[\mathbf{J}\left(\mathbf{x}\right)\right]_{ij} = \frac{\partial f_i}{\partial x_j}$$

Newton's Method for Systems of Equations

- It is much harder if not impossible to do globally convergent methods like bisection in higher dimensions!
- A good initial guess is therefore a must when solving systems, and Newton's method can be used to refine the guess.
- The basic idea behind Newton's method is to **linearize** the equation around the current guess:

$$\mathbf{f}\left(\mathbf{x}^k + \Delta\mathbf{x}\right) \approx \mathbf{f}\left(\mathbf{x}^k\right) + \left[\mathbf{J}\left(\mathbf{x}^k\right)\right]\Delta\mathbf{x} = \mathbf{0}$$

$$\left[\mathbf{J}\left(\mathbf{x}^k\right)\right]\Delta\mathbf{x} = -\mathbf{f}\left(\mathbf{x}^k\right) \text{ but denote } \mathbf{J} \equiv \mathbf{J}\left(\mathbf{x}^k\right)$$

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \Delta\mathbf{x} = \mathbf{x}^k - \mathbf{J}^{-1}\mathbf{f}\left(\mathbf{x}^k\right).$$

- This method requires computing a whole **matrix of derivatives**, which can be expensive or hard to do (differentiation by hand?)!

Convergence of Newton's method

- Near the root the Jacobian and Hessian don't change much so just approximate $\mathbf{J} \approx \mathbf{J}(\boldsymbol{\alpha})$ and $\mathbf{H} \approx \mathbf{H}(\boldsymbol{\alpha})$.
- Next order term in Taylor series indicates error

$$\mathbf{f}\left(\mathbf{x}^k\right) = \mathbf{f}(\boldsymbol{\alpha}) + \mathbf{J}\mathbf{e}^k + \frac{1}{2}\left(\mathbf{e}^k\right)^T \mathbf{H}\mathbf{e}^k = \mathbf{J}\mathbf{e}^k + \frac{1}{2}\left(\mathbf{e}^k\right)^T \mathbf{H}\mathbf{e}^k \quad \Rightarrow$$

$$\mathbf{e}^{k+1} = \mathbf{x}^{k+1} - \boldsymbol{\alpha} = \mathbf{e}^k - \mathbf{J}^{-1}\mathbf{f}\left(\mathbf{x}^k\right) = \frac{1}{2}\mathbf{J}^{-1}\left(\mathbf{e}^k\right)^T \mathbf{H}\mathbf{e}^k$$

- Newton's method converges **quadratically** if started sufficiently close to a root $\boldsymbol{\alpha}$:

$$\left\|\mathbf{e}^{k+1}\right\| \leq \frac{\left\|\mathbf{J}^{-1}\right\| \left\|\mathbf{H}\right\|}{2} \left\|\mathbf{e}^k\right\|^2$$

- Newton's method converges fast **if the Jacobian $\mathbf{J}(\boldsymbol{\alpha})$ is well-conditioned**.
- Newton's method requires solving **many linear systems**, which can be expensive for many variables.

Quasi-Newton methods

- For large systems one can use so called **quasi-Newton** methods to estimate derivatives using finite-differences and to speed up by using rank-1 matrix updates (see Woodbury formula in homework 2):
  - Approximate the Jacobian with another matrix $\widetilde{\mathbf{J}}^k$ and solve $\widetilde{\mathbf{J}}^k \mathbf{d} = \mathbf{f}(\mathbf{x}^k)$.
  - Damp the step by a step length $\alpha_k \lesssim 1$,

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \alpha_k \mathbf{d} = \mathbf{x}^k + \Delta \mathbf{x}^k.$$

  - Update Jacobian by a rank-1 update, e.g., one of **Broyden's methods**:

$$\widetilde{\mathbf{J}}^{k+1} = \widetilde{\mathbf{J}}^k + \left(\mathbf{f}(\mathbf{x}^{k+1}) - \left(\mathbf{f}(\mathbf{x}^k) + \widetilde{\mathbf{J}}^k \Delta \mathbf{x}^k \right) \right) \frac{\left(\Delta \mathbf{x}^k \right)^T}{\|\Delta \mathbf{x}^k\|_2^2},$$

which ensures the desired **secant condition**

$$\mathbf{f}(\mathbf{x}^{k+1}) - \mathbf{f}(\mathbf{x}^k) = \widetilde{\mathbf{J}}^{k+1} \Delta \mathbf{x}^k.$$

Continuation methods

- To get a good initial guess for Newton's method and ensure that it converges fast we can use **continuation methods** (also called **homotopy methods**).
- The basic idea is to solve

$$\tilde{\mathbf{f}}_{\lambda}(\mathbf{x}) = \lambda \mathbf{f}(\mathbf{x}) + (1-\lambda)\,\mathbf{f}_{\mathbf{a}}(\mathbf{x}) = \mathbf{0}$$

  instead of the original equations, where $0 \leq \lambda \leq 1$ is a parameter.
- If $\lambda = 1$, we are solving the original equation $\mathbf{f}(\mathbf{x}) = \mathbf{0}$, which is hard because we do not have a good guess for the initial solution.
- If $\lambda = 0$, we are solving $\mathbf{f}_{\mathbf{a}}(\mathbf{x}) = \mathbf{0}$, and we will assume that this is **easy to solve**. For example, consider making this a linear function,

$$\mathbf{f}_{\mathbf{a}}(\mathbf{x}) = \mathbf{x} - \mathbf{a},$$

  where $\mathbf{a}$ is a vector of parameters that need to be chosen somehow. One can also take a more general $\mathbf{f}_{\mathbf{a}}(\mathbf{x}) = \mathbf{A}\mathbf{x} - \mathbf{a}$ where $\mathbf{A}$ is a matrix of parameters, so that solving $\mathbf{f}_{\mathbf{a}}(\mathbf{x}) = \mathbf{0}$ amounts to a linear solve which we know how to do already.

Path Following

- The basic idea of continuation methods is to start with $\lambda = 0$, and solve $\tilde{\mathbf{f}}_{\lambda}(\mathbf{x}) = 0$. This gives us a solution $\mathbf{x}_0$.
- Then increment λ by a little bit, say $\lambda = 0.05$, and solve $\tilde{\mathbf{f}}_{\lambda}(\mathbf{x})$ using Newton's method starting with $\mathbf{x}_0$ as an initial guess.
  Observe that this is a good initial guess under the assumption that the solution has not changed much because λ has not changed much.
- We can repeat this process until we reach $\lambda = 1$, when we get the actual solution we are after:
  - Choose a sequence $\lambda_0 = 0 < \lambda_1 < \lambda_2 < \cdots < \lambda_{n-1} < \lambda_n = 1$.
  - For $k = 0$ solve $\mathbf{f}_{\mathbf{a}}(\mathbf{x}_0) = \mathbf{0}$ to get $\mathbf{x}_0$.
  - For $k = 1, \ldots, n$, solve a nonlinear system to get $\mathbf{x}_k$,

$$\tilde{\mathbf{f}}_{\lambda_k}(\mathbf{x}_k) = \mathbf{0}$$

  using **Newton's method starting from $\mathbf{x}_{k-1}$ as an initial guess**.

Path Following

- Observe that if we change λ very slowly we have hope that the solution will trace a **continuous path of solutions**.
- That is, we can think of $\mathbf{x}(\lambda)$ as a continuous function defined on $[0, 1]$, defined implicitly via

$$\lambda \mathbf{f}(\mathbf{x}(\lambda)) + (1 - \lambda) \mathbf{f_a}(\mathbf{x}(\lambda)) = \mathbf{0}.$$

- This rests on the assumption that this path will **not have turning points, bifurcate or wonder to infinity**, and that there is a solution for every λ.
- It turns out that by a judicious choice of $\mathbf{f_a}$ one can insure this is the case. For example, choosing a random $\mathbf{a}$ and taking $\mathbf{f_a}(\mathbf{x}) = \mathbf{x} - \mathbf{a}$ works.
- The trick now becomes how to choose the sequence λ_k to make sure λ changes not too much but also not too little (i.e., not too slowly), see HOMPACK library for an example.

In practice

- It is much harder to construct general robust solvers in higher dimensions and some **problem-specific knowledge** is required.
- There is no built-in function for solving nonlinear systems in MATLAB, but the **Optimization Toolbox** has *fsolve*.
- In many practical situations there is some continuity of the problem so that **a previous solution can be used as an initial guess**.
- For example, **implicit methods for differential equations** have a time-dependent Jacobian $\mathbf{J}(t)$ and in many cases the solution $\mathbf{x}(t)$ evolves smootly in time.
- For large problems specialized **sparse-matrix solvers** need to be used.
- In many cases derivatives are not provided but there are some techniques for **automatic differentiation**.

Conclusions/Summary

- Root finding is well-conditioned for **simple roots** (unit multiplicity), ill-conditioned otherwise.
- Methods for solving nonlinear equations are always iterative and the **order of convergence** matters: second order is usually good enough.
- A good method uses a higher-order unsafe method such as **Newton method** near the root, but **safeguards** it with something like the **bisection** method.
- Newton's method is second-order but requires derivative/Jacobian evaluation. In **higher dimensions** having a **good initial guess** for Newton's method becomes very important.
- **Quasi-Newton** methods can aleviate the complexity of solving the Jacobian linear system.