

Improving on Newton?

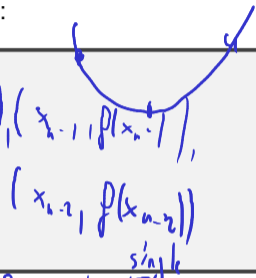
How would we do "Newton + 1" (i.e. even faster, even better)?

- Use another term in the Taylor series
- even more locally convergent
- possibly, 3rd order convergent
- parabola might not have roots
- need 2 derivatives

Root Finding with Interpolants

Secant method uses a linear interpolant based on points $f(x_k), f(x_{k-1})$, could use more points and higher-order interpolant:

- Could fit polynomial to $(x_0, f(x_0)), (x_{n-1}, f(x_{n-1})), (x_{n-2}, f(x_{n-2}))$
- Muller's method



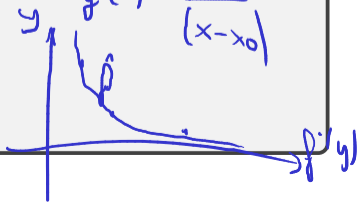
What about existence of roots in that case?

- Inverse quadratic interpolation fit inverse to $(f(x_0), x_0), (f(x_1), x_1), (f(x_2), x_2))$

Next guess is $\hat{f}(0)$

If x_0 is a ^{single} root of f ,

$$\hat{f}(x) = \frac{p(x)}{(x-x_0)}$$



Achieving Global Convergence

The linear approximations in Newton and Secant are only good locally.
How could we use that?

- Hybrid: bisection + Newton
 - ↳ Revert to bisection if Newton leaves the bisection bracket ✓
- "Trust region" method
- Limit step size

In-Class Activity: Nonlinear Equations

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Fixed Point Iteration

$$\|g(x) - g(y)\| \leq \delta \|x - y\|$$

$$\vec{x} = (x_1, \dots, x_n)$$

$$\vec{g} = (g_1, \dots, g_n)$$

$$x_0 = \langle \text{starting guess} \rangle$$

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

↳ n-dimensional

When does this converge?

$$J_g(x^*) = \begin{bmatrix} \partial_{x_1} g_1 & \dots & \partial_{x_n} g_1 \\ \vdots & & \vdots \\ \partial_{x_1} g_n & \dots & \partial_{x_n} g_n \end{bmatrix}$$

$$\|g(x) - g(x^*)\| \sim \|J_g(x^*) \cdot (x - x^*)\|$$

$$\leq \|J_g(x^*)\| \cdot \|x - x^*\|$$

$$\|J_g(x^*)\| \leq \rho(J_g(x^*)) + \epsilon < 1 \Rightarrow \text{convergence.}$$

↳ quadratic.

Newton's Method

What does Newton's method look like in n dimensions?

$$f(x+s) \approx f(x) + J_f(x) s$$

$$0 = f(x) + J_f(x) s \Rightarrow s = -J_f(x)^{-1} f(x)$$

$\left\{ \begin{array}{l} x_0 = \text{initial guess} \end{array} \right.$

$$\left\{ \begin{array}{l} x_{k+1} = x_k - J_f(x_k)^{-1} \cdot f(x_k) \end{array} \right.$$

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

Downsides of n -dim. Newton?

- locally convergent only
- computing / inverting J_f is expensive.

Demo: Newton's method in n dimensions [cleared]

Secant in n dimensions?

What would the secant method look like in n dimensions?

$$1D: f'(x) \approx \frac{f(x_{k+1}) - f(x_k)}{x_{k+1} - x_k}$$

$$nD: \underset{n \times n}{J_f(x)} \approx \tilde{J} \begin{bmatrix} \underset{\substack{n \\ f(x_{k+1})}}{f(x_{k+1})}, & \underset{\substack{n \\ f(x_k)}}{f(x_k)}, & \underset{\substack{n \\ x_{k+1}}}{x_{k+1}}, & \underset{\substack{n \\ x_k}}{x_k} \end{bmatrix}$$

$$\tilde{J} \cdot \Delta x = \Delta f$$

$4n$
Broyden's method etc.
 $\|J_{k+1} - J_k\|_F$

Outline

Introduction to Scientific Computing

Systems of Linear Equations

Linear Least Squares

Eigenvalue Problems

Nonlinear Equations

Optimization

Introduction

Methods for unconstrained opt. in one dimension

Methods for unconstrained opt. in n dimensions

Nonlinear Least Squares

Constrained Optimization

Interpolation

Numerical Integration and Differentiation

Initial Value Problems for ODEs

Boundary Value Problems for ODEs

Partial Differential Equations and Sparse Linear Algebra

Fast Fourier Transform

Additional Topics

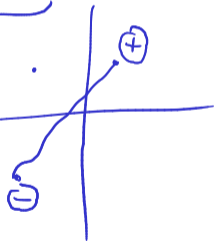
Optimization: Problem Statement

Have: Objective function $f : \mathbb{R}^n \rightarrow \mathbb{R}$

Want: Minimizer $\mathbf{x}^* \in \mathbb{R}^n$ so that

$$f(\mathbf{x}^*) = \min_{\mathbf{x}} f(\mathbf{x}) \quad \text{subject to } \mathbf{g}(\mathbf{x}) = 0 \quad \text{and} \quad \mathbf{h}(\mathbf{x}) \leq 0.$$

- ▶ $\mathbf{g}(\mathbf{x}) = 0$ and $\mathbf{h}(\mathbf{x}) \leq 0$ are called **constraints**.
They define the set of **feasible points** $\mathbf{x} \in S \subseteq \mathbb{R}^n$.
- ▶ If \mathbf{g} or \mathbf{h} are present, this is **constrained optimization**.
Otherwise **unconstrained optimization**.
- ▶ If \mathbf{f} , \mathbf{g} , \mathbf{h} are *linear*, this is called **linear programming**.
Otherwise **nonlinear programming**.



Optimization: Observations

Q: What if we are looking for a *maximizer* not a minimizer?

Give some examples:

... lots

$$\min \|F(x)\|$$

What about multiple objectives?

Pareto optimality
For us: combine into one

Existence/Uniqueness

Terminology: **global minimum** / **local minimum**

Under what conditions on f can we say something about existence/uniqueness?

If $f : S \rightarrow \mathbb{R}$ is continuous on a closed and bounded set $S \subseteq \mathbb{R}^n$, then

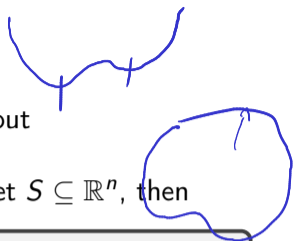
a minimum exists

$f : S \rightarrow \mathbb{R}$ is called *coercive* on $S \subseteq \mathbb{R}^n$ (which must be unbounded) if

$$\lim_{\|x\| \rightarrow \infty} f(x) = +\infty$$

If f is coercive, ...

a global minimum exists



Convexity

$S \subseteq \mathbb{R}^n$ is called **convex** if for all $\mathbf{x}, \mathbf{y} \in S$ and all $0 \leq \alpha \leq 1$

$f : S \rightarrow \mathbb{R}$ is called **convex on** $S \subseteq \mathbb{R}^n$ if for $\mathbf{x}, \mathbf{y} \in S$ and all $0 \leq \alpha \leq 1$

Q: Give an example of a convex, but not strictly convex function.