Outline

Recap: Interpolation

Starting point: Looking for a linear combination of functions φ_i to hit given data points (x_i, y_i).

Interpolation becomes solving the linear system:

$$y_i = f(x_i) = \sum_{j=0}^{N_{\text{func}}} \alpha_j \underbrace{\varphi_j(x_i)}_{V_{ij}} \qquad \leftrightarrow \qquad V\boldsymbol{\alpha} = \boldsymbol{y}.$$

Want unique answer: Pick $N_{\text{func}} = N \to V$ square.

V is called the (generalized) Vandermonde matrix.

Main lesson:

$$V\,(\text{coefficients}) = (\text{values at nodes})\,.$$

Outline

Rethinking Interpolation

We have so far always used monomials $(1, x, x^2, x^3, \ldots)$ and equispaced points for interpolation. It turns out that this has *significant problems*.

Demo: Monomial interpolation (click to visit)

Demo: Choice of Nodes for Polynomial Interpolation (click to visit)

Interpolation: Choosing Basis Function and Nodes

Both function basis and point set are under our control. What do we pick?

Ideas for basis functions:

- Monomials $1, x, x^2, x^3, x^4, \ldots$
- Functions that make $V = I \to$ 'Lagrange basis'
- Functions that make V triangular $\to$ 'Newton basis'
- Splines (piecewise polynomials)
- Orthogonal polynomials
- Sines and cosines
- 'Bumps' ('Radial Basis Functions')

Ideas for nodes:

- Equispaced
- 'Edge-Clustered' (so-called Chebyshev/Gauss/... nodes)

Better Conditioning: Orthogonal Polynomials

What caused monomials to have a terribly conditioned Vandermonde?

Being close to linearly dependent.

What's a way to make sure two vectors are *not* like that?

Orthogonality

But polynomials are functions!

How can those be orthogonal? Just need something like a dot product!

$$\begin{aligned} \boldsymbol{f} \cdot \boldsymbol{g} &= \sum_{i=1}^{n} f_i g_i \quad = \langle \boldsymbol{f}, \boldsymbol{g} \rangle \\ \langle f, g \rangle &= \int_{-1}^{1} f(x) g(x) dx \end{aligned}$$

Better Conditioning: Orthogonal Polynomials (II)

Orthogonal then just means $\langle f, g\rangle = 0$.
Q: How can we find an orthogonal basis?
A: Apply Gram-Schmidt to the monomials.
Obtained Legendre polynomials.
Demo: Orthogonal Polynomials (click to visit)

But how can I practically compute the Legendre polynomials?

$\rightarrow$ DLMF, Chapter on orthogonal polynomials
Main lessons:

- There exist three-term recurrences. Easy to apply if you know the first two.

Better Conditioning: Orthogonal Polynomials (III)

- There is a whole zoo of polynomials there, depending on the weight function w in the (generalized) inner product:

  $$\langle f, g \rangle = \int w(x) f(x) g(x) dx.$$

  Some sets of orthogonal polynomials live on intervals other than $(-1, 1)$.

Another Family of Orthogonal Polynomials: Chebyshev

Three equivalent definitions:

- Result of Gram-Schmidt with weight $1/\sqrt{1-x^2}$

  What is that weight?

  $1/$ (Half circle), i.e. $x^2+y^2=1$, with $y=\sqrt{1-x^2}$
- $T_k(x)=\cos(k\cos^{-1}(x))$
- $T_k(x)=2xT_{k-1}(x)-T_{k-2}(x)$

Demo: Chebyshev interpolation (click to visit) (Part 1)

What are good nodes to use with Chebyshev polynomials?

The answer would be particularly simple if the nodes were $\cos(*)$.
So why not $\cos$ (equispaced)?

Might get

$$x_i=\cos\left(\frac{i}{k}\pi\right) \qquad (i=0,1,\ldots,k)$$

Chebyshev Nodes

Might also consider zeros (instead of roots) of T_k:

$$x_i = \cos\left(\frac{2i-1}{2k}\pi\right) \quad (i = \dots, k).$$

The Vandermonde for these (with T_k) can be applied in $O(N \log N)$ time, too.

It turns out that we were still looking for a good set of interpolation nodes.

We came up with the criterion that the nodes should bunch towards the ends. Do these do that?

Yes.

Demo: Chebyshev interpolation (click to visit) (Part 2)

Outline

Calculus on Interpolants

Suppose we have an interpolant $\tilde{f}(x)$ with $f(x_i) = \tilde{f}(x_i)$ for $i = 1, \dots, n$:

$$\tilde{f}(x) = \alpha_1 \varphi_1(x) + \cdots + \alpha_n \varphi_n(x)$$

How do we compute the derivative of $\tilde{f}$?

$$\tilde{f}'(x) = \alpha_1 \varphi_1'(x) + \cdots + \alpha_n \varphi_n'(x).$$

Easy because interpolation basis (φ_i) is known.

Suppose we have function values at nodes $(x_i, f(x_i))$ for $i = 1, \dots, n$ for a function f. If we want $f'(x_i)$, what can we do?

$f'(x_i)$: Hard to get
$\tilde{f}'(x_i)$: Easy to get

Calculus on Interpolants (II)

So:

1. Compute coefficients $\boldsymbol{\alpha} = V^{-1}\boldsymbol{f}$, where $\boldsymbol{f} = (f(x_1), \dots, f(x_n))^T$.
2. Build generalized Vandermonde with *derivatives* of basis:

$$V' = \begin{pmatrix} \varphi_1'(x_1) & \cdots & \varphi_n'(x_1) \\ \vdots & & \vdots \\ \varphi_1'(x_n) & \cdots & \varphi_n'(x_n) \end{pmatrix}.$$

3. Compute

$$V'\boldsymbol{\alpha} = \begin{pmatrix} \alpha_1\varphi_1'(x_1) + \cdots + \alpha_n\varphi_n'(x_1) \\ \vdots \\ \alpha_1\varphi_1'(x_n) + \cdots + \alpha_n\varphi_n'(x_n) \end{pmatrix} = \underbrace{\begin{pmatrix} \tilde{f}'(x_1) \\ \vdots \\ \tilde{f}'(x_n) \end{pmatrix}}_{\tilde{\boldsymbol{f}'}}.$$

Calculus on Interpolants (III)

All in one step: $\widetilde{\boldsymbol{f}}' = V'V^{-1}\boldsymbol{f}$.
In other words: $V'V^{-1}$ is a matrix to apply a derivative!
We call $D = V'V^{-1}$ a differentiation matrix.

About Differentiation Matrices

How could you find coefficients of the derivative in the original basis (φ_i)?

$$\boldsymbol{\alpha}' = \underbrace{V^{-1}V' \quad \underbrace{V^{-1}\boldsymbol{f}}_{\text{coeff. in } (\varphi_i')}}_{\text{coeff. in } (\varphi_i)} \quad .$$

Give a matrix that finds the second derivative.

Using above, we can apply repeated derivatives using just V and V':

$$\mathbf{f}'' = \underbrace{V'V^{-1}V'V^{-1}}_{\text{matrix for double differentiation}} \mathbf{f}.$$

Demo: Taking Derivatives with Vandermonde Matrices (click to visit)

Finite Difference Formulas

It is possible to use the process above to find 'canned' formulas for taking derivatives. Suppose we use three points equispaced points $(x-h, x, x+h)$ for interpolation (i.e. a degree-2 polynomial).

- What is the resulting differentiation matrix?
- What does it tell us for the middle point?

$$D = V'V^{-1} = \begin{pmatrix} \dots & \dots & \dots \\ -\frac{1}{2h} & 0 & \frac{1}{2h} \\ \dots & \dots & \dots \end{pmatrix}$$

which we can check via

$$\underbrace{\begin{pmatrix} \dots & \dots & \dots \\ -\frac{1}{2h} & 0 & \frac{1}{2h} \\ \dots & \dots & \dots \end{pmatrix}}_{D} \underbrace{\begin{pmatrix} 1 & x-h & (x-h)^2 \\ 1 & x & x^2 \\ 1 & x+h & (x+h)^2 \end{pmatrix}}_{V} = \underbrace{\begin{pmatrix} \dots & \dots & \dots \\ 0 & 1 & 2x \\ \dots & \dots & \dots \end{pmatrix}}_{V'}$$

Finite Difference Formulas (II)

(Can find the dependence on h by varying h and watching the entries.) When we apply D, we get

$$V'V^{-1}\begin{pmatrix} f(x-h) \\ f(x) \\ f(x+h) \end{pmatrix} = \begin{pmatrix} \dots \\ \frac{f(x+h)-f(x-h)}{2h} \\ \dots \end{pmatrix}$$

So we can compute an approximate (second-order accurate!) derivative just by using this formula.
Generalizes to more (and non-center) points easily.

Reusing Finite Difference Formulas

Suppose we have the following finite difference rule using M equispaced points to the left of x and N equispaced points to the right of x (say, from a row of a differentiation matrix):

$$f'(x) \approx \sum_{i=-M}^{N} \alpha_i f(x + ih).$$

How reusable is this rule?

Can we use this rule at a different $\tilde{x} \neq x$?

Yes, with unchanged 'coefficients':

$$f'(\tilde{x}) \approx \sum_{i=-M}^{N} \alpha_i f(\tilde{x} + ih).$$

Reusing Finite Difference Formulas (II)

This is true because if you consider a shifted function $g(x) = f(x-s)$ with s so that $\tilde{x} = x - s$, then the rule still applies:

$$\begin{aligned} f'(\tilde{x}) = f'(x-s) = g'(x) &\approx \sum_{i=-M}^{N} \alpha_i g(x+ih) \\ &= \sum_{i=-M}^{N} \alpha_i f(x-s+ih) \\ &= \sum_{i=-M}^{N} \alpha_i f(\tilde{x}+ih). \end{aligned}$$

Can we use this rule with a different point distance $\tilde{h} = \beta h \neq h$?

Yes, with scaled ‘coefficients’:

$$f'(x) \approx \sum_{i=-M}^{N} \frac{\alpha_i}{\beta} f(x+i\beta h).$$

Reusing Finite Difference Formulas (III)

This is true because if you consider a scaled function $g(x) = f(\beta x)$, then the rule still applies:

$$\beta f'(x) = g'(x) \approx \sum_{i=-M}^{N} \alpha_i g(ih) = \sum_{i=-M}^{N} \alpha_i f(\beta ih),$$

so

$$f'(x) \approx \sum_{i=-M}^{N} \frac{\alpha_i}{\beta} f(\beta ih).$$

Computing Integrals with Interpolation

Can we use a similar process to compute (approximate) integrals of a function f?

The process of computing approximate integrals is called 'quadrature'.

Same idea as derivatives: interpolate, then integrate.

Have: interpolant $\tilde{f}(x) = \alpha_1\varphi_1(x) + \cdots + \alpha_n\varphi_n(x)$
so that $\tilde{f}(x_i) = f(x_i) = y_i$. We'll call the x_i the quadrature nodes.

Want: Integral

$$\begin{aligned}\int_a^b f(x)dx &\approx \int_a^b \tilde{f}(x)dx = \int_a^b \alpha_1\varphi_1(x) + \cdots + \alpha_n\varphi_n(x)dx \\ &= \alpha_1 \int_a^b \varphi_1(x)dx + \cdots + \alpha_n \int_a^b \varphi_n(x)dx.\end{aligned}$$

Computing Integrals with Interpolation (II)

Idea: $d_i = \int_a^b \varphi_i(x)dx$ can be computed ahead of time, so that

$$\int_a^b \tilde{f}(x)dx = \alpha_1 d_1 + \cdots + \alpha_n d_n = \boldsymbol{d}^T\boldsymbol{\alpha} = \boldsymbol{d}^T(V^{-1}\boldsymbol{y}) = (\boldsymbol{d}^T V^{-1})\boldsymbol{y}.$$

Can call $\boldsymbol{w} := V^{-T}\boldsymbol{d}$ the quadrature weights and compute

$$\int_a^b \tilde{f}(x)dx = \boldsymbol{w}^T\boldsymbol{y} = \boldsymbol{w}\cdot\boldsymbol{y}.$$

Demo: Creating and Transforming Quadrature Rules (click to visit)

Example: Building a Quadrature Rule

Demo: Computing the Weights in Simpson's Rule (click to visit)

Suppose we know

$$f(x_0) = 2 \qquad f(x_1) = 0 \qquad f(x_2) = 3$$

$$x_0 = 0 \qquad x_1 = \frac{1}{2} \qquad x_2 = 1$$

How can we find an approximate integral?

1. Find coefficients

$$\boldsymbol{\alpha} = V^{-1} \begin{pmatrix} 2 \\ 0 \\ 3 \end{pmatrix}.$$

Example: Building a Quadrature Rule (II)

2. Compute integrals

$$
\begin{aligned}
\int_0^1 1 dx &= 1 \\
\int_0^1 x dx &= \frac{1}{2} \\
\int_0^1 x^2 dx &= \left[\frac{1}{3}x^3\right]_0^1 = \frac{1}{3}
\end{aligned}
$$

3. Combine it all together:

$$\int_0^1 \tilde{f}(x)dx = \underbrace{\begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{3} \end{pmatrix} V^{-1}}_{\text{weights } \boldsymbol{w}} \begin{pmatrix} 2 \\ 0 \\ 3 \end{pmatrix} = \begin{pmatrix} .167 \\ .667 \\ .167 \end{pmatrix} \cdot \begin{pmatrix} f(0) \\ f(1/2) \\ f(1) \end{pmatrix}.$$

These weights are dependent only on the choice of nodes and not the basis functions (the interpolant is unique, so its integral is unique). For equispaced points like above, the method defined by the quadrature weights is called Simpson's rule.

Using Quadrature Rules

To estimate an integral over an arbitrary interval $[a, b]$ we can use a quadrature rule with weights derived by integrating over $[0, 1]$, since

$$\int_a^b f(x)dx \underbrace{=}_{x=(b-a)\bar{x}+a} (b-a)\int_0^1 f((b-a)\bar{x}+a)d\bar{x}.$$

Thus, given weights $\mathbf{w} = V^{-T}\mathbf{d}$ computed from integrating n basis functions on $[0, 1]$ (to get $\mathbf{d}$) and V defined based on points $\bar{x}_1, \ldots, \bar{x}_n \in [0, 1]$, we can use the same weights for the above integral as

$$\int_a^b f(x)dx \approx (b-a)\mathbf{w}^T\mathbf{y}.$$

Above $\mathbf{y}$ corresponds to f evaluated at points $(b-a)\bar{x}_1 + a, \ldots, (b-a)\bar{x}_n + a$.

Facts about Quadrature

What does Simpson's rule look like on $[0, 1/2]$?

$$\frac{1}{2}\begin{pmatrix} .167 \\ .667 \\ .167 \end{pmatrix} \cdot \begin{pmatrix} f(0) \\ f(1/4) \\ f(1/2) \end{pmatrix}$$

What does Simpson's rule look like on $[5, 6]$?

$$\begin{pmatrix} .167 \\ .667 \\ .167 \end{pmatrix} \cdot \begin{pmatrix} f(5) \\ f(5.5) \\ f(6) \end{pmatrix}$$

How accurate is Simpson's rule with polynomials of degree n?

Demo: Accuracy of Simpson's rule (click to visit)

Facts about Quadrature (II)

- Quadrature:

$$\left|\int_a^b f(x)dx - \int_a^b \tilde{f}(x)dx\right| \leqslant C \cdot h^{n+2}$$

(where $h = b - a$)
(Side note: due to a happy accident, even n produce an even smaller error.)

- Interpolation:

$$\max_{x\in[a,b]} \left|f(x) - \tilde{f}(x)\right| \leqslant C \cdot h^{n+1}$$

- Differentiation:

$$\max_{x\in[a,b]} \left|f'(x) - \tilde{f}'(x)\right| \leqslant C \cdot h^{n}$$

General lesson: More derivatives $\Rightarrow$ Worse accuracy.

Outline

What is linear convergence? quadratic convergence?

Let $\boldsymbol{e}_k = \widehat{\boldsymbol{x}}_k - \boldsymbol{x}$ be the error in the kth estimate $\widehat{\boldsymbol{x}}_k$ of a desired solution $\boldsymbol{x}$.

An iterative method converges with rate r if

$$\lim_{k\to\infty} \frac{\|\boldsymbol{e}_{k+1}\|}{\|\boldsymbol{e}_k\|^r} = C \begin{cases} > 0, \\ < \infty. \end{cases}$$

$r = 1$ is called linear convergence.
$r > 1$ is called superlinear convergence.
$r = 2$ is called quadratic convergence.

Examples:

- Power iteration is linearly convergent.
- Rayleigh quotient iteration is quadratically convergent.

About Convergence Rates

Demo: Rates of Convergence (click to visit)

Characterize linear, quadratic convergence in terms of the 'number of accurate digits'.

- Linear convergence gains a constant number of digits each step:

  $$\|\boldsymbol{e}_{k+1}\| \leqslant C \|\boldsymbol{e}_k\|$$

  (and $C < 1$ matters!)
- Quadratic convergence doubles the number of digits each step:

  $$\|\boldsymbol{e}_{k+1}\| \leqslant C \|\boldsymbol{e}_k\|^2$$

  (Only starts making sense once $\|\boldsymbol{e}_k\|$ is small. C doesn't matter much.)

Outline

Solving Nonlinear Equations

What is the goal here?

Solve $f(x) = 0$ for $f : \mathbb{R} \to \mathbb{R}$.
If looking for solution to $f(x) = y$, simply consider $f(x) = \tilde{f}(x) - y$.

This is called root finding. A related task is optimization, where one looks to find an x^* so that $f(x^*)$ is minimal.
There are flavors of both root finding and optimization in one and n dimensions.

Root Finding, Optimization: Applications

- *FPUs*: Assume you have built a floating point unit that can add, subtract and multiply. At this point, division and square root seem like obvious next steps to implement. Newton's method (see below) for finding $1/\sqrt{y}$ can be implemented with just add/subtract/multiply. This in turn can be used to implement both division and square root. See `https://en.wikipedia.org/wiki/Fast_inverse_square_root` for some related computer game nostalgia.
- *GPS*: GPS measures signal run time between satellites and a receiver device. The receiver must solve the navigation equations to determine latitude/longitude/elevation/time. `https://en.wikipedia.org/wiki/Global_Positioning_System#Navigation_equations`

Root Finding, Optimization: Applications (II)

- *Inverse kinematics*: Given the desired position of the end of a kinematic chain (such as the manipulator at the end of a robot arm), finding the joint angles (i.e. the information needed to drive the robot) requires solving $\mathbf{f}(\theta) = \mathbf{y}$, where $\mathbf{f}$ is the *forward kinematic model* based on the joint angles θ.
- *Data fitting*: Just like in our discussion of least squares, as soon as a system of equations is non-square (such as when there is more data than unknowns–think more than four satellites in view for GPS), achieving $\mathbf{f}(\mathbf{x}) = \mathbf{y}$ becomes unlikely. A natural idea is to consider the optimization problem $\|\mathbf{f}(\mathbf{x}) - \mathbf{y}\|_2^2$ instead. (This specifically is called nonlinear least squares).

Bisection Method

Assume continuous function f has a zero on the interval $[a, b]$ and

$$\operatorname{sign}(f(a)) = -\operatorname{sign}(f(b)).$$

Perform binary search: check sign of $f((a+b)/2)$ and define new search interval so that ends have opposite sign.
Demo: Bisection Method (click to visit)

What's the rate of convergence? What's the constant?

Linear with constant $1/2$.

Newton's Method

Derive Newton's method.

Idea: Approximate f at current iterate using Taylor.

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

Now find root of this linear approximation in terms of h:

$$f(x_k) + f'(x_k)h = 0 \quad \Leftrightarrow \quad h = -\frac{f(x_k)}{f'(x_k)}.$$

So

$$\begin{aligned} x_0 &= \langle\text{starting guess}\rangle \\ x_{k+1} &= x_k - \frac{f(x_k)}{f'(x_k)} = g(x_k) \end{aligned}$$

Demo: Newton's Method (click to visit)
Demo: Convergence of Newton's Method (click to visit)

What are some **drawbacks** of Newton?

- Convergence argument only good *locally*
  Will see: convergence only local (near root)
- Have to have derivative!

Secant Method

What would Newton without the use of the derivative look like?

Approximate

$$f'(x_k) \approx \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}.$$

So

$$\begin{aligned} x_0 &= \langle \text{starting guess} \rangle \\ x_{k+1} &= x_k - \frac{f(x_k)}{\frac{f(x_k)-f(x_{k-1})}{x_k - x_{k-1}}}. \end{aligned}$$

Rate of convergence (not shown) is $\left(1+\sqrt{5}\right)/2 \approx 1.618$.

Secant Method Drawbacks

What are some **drawbacks** of Secant?

- Convergence argument only good *locally*
  Will see: convergence only local (near root)
- Slower convergence
- Need two starting guesses

Demo: Secant Method (click to visit)
In-class activity: Secant Method

Outline

Solving Nonlinear Equations

What is the goal here?

Solve $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ for $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n$
In other words, $\mathbf{f}(\mathbf{x})$ is now a vector-valued function

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) \\ \vdots \\ f_n(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} f_1(x_1, \dots, x_n) \\ \vdots \\ f_n(x_1, \dots, x_n) \end{bmatrix}$$

If looking for solution to $\tilde{\mathbf{f}}(\mathbf{x}) = \mathbf{y}$, simply consider $\mathbf{f}(\mathbf{x}) = \tilde{\mathbf{f}}(\mathbf{x}) - \mathbf{y}$.

Intuition: Each of the n equations describes a surface. Looking for intersections.
Demo: Three quadratic functions (click to visit)

Newton's method

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

Approximate by linear function:

$$\mathbf{f}(\mathbf{x}+\mathbf{s}) = \mathbf{f}(\mathbf{x}) + J_{\mathbf{f}}(\mathbf{x})\mathbf{s}$$

where $J_{\mathbf{f}}$ is the Jacobian matrix of $\mathbf{f}$:

$$J_{\mathbf{f}}(\mathbf{x}) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \cdots & \frac{\partial f_n}{\partial x_n} \end{pmatrix}(\mathbf{x}).$$

Set to $\mathbf{0}$:

$$J_{\mathbf{f}}(\mathbf{x})\mathbf{s} = -\mathbf{f}(\mathbf{x}) \quad \Rightarrow \quad \mathbf{s} = -(J_{\mathbf{f}}(\mathbf{x}))^{-1}\mathbf{f}(\mathbf{x})$$

That's a linear system! (Surprised?)

Newton's method (II)

So

$$\begin{aligned} \mathbf{x}_0 &= \langle \text{starting guess} \rangle \\ \mathbf{x}_{k+1} &= \mathbf{x}_k - (J_{\mathbf{f}}(\mathbf{x}_k))^{-1}\mathbf{f}(\mathbf{x}_k) \end{aligned}$$

Downsides:

- Still only locally convergent
- Computing and inverting $J_{\mathbf{f}}$ is expensive.

Newton: Example

Set up Newton's method to find a root of

$$\mathbf{f}(x,y) = \begin{pmatrix} x + 2y - 2 \\ x^2 + 4y^2 - 4 \end{pmatrix}.$$

Mostly just need the Jacobian:

$$J_{\mathbf{f}}(x,y) = \begin{pmatrix} 1 & 2 \\ 2x & 8y \end{pmatrix}.$$

Demo: Newton's method in n dimensions (click to visit)

Secant in n dimensions?

What would the secant method look like in n dimensions?

Need an 'approximate Jacobian' satisfying

$$\tilde{J}(\mathbf{x}_{k+1} - \mathbf{x}_k) = \mathbf{f}(\mathbf{x}_{k+1}) - \mathbf{f}(\mathbf{x}_k).$$

Suppose we have *already taken* a step to $\mathbf{x}_{k+1}$. Could we 'reverse engineer' $\tilde{J}$ from that equation?

- Solution non-unique: n^2 unknowns in $\tilde{J}$, but only n equations
- Better to 'update' $\tilde{J}$ with information from current guess.

One choice: Broyden's method (minimizes change to $\tilde{J}$)

Outline

Optimization

State the problem.

Have: Objective function $f : \mathbb{R}^n \to \mathbb{R}$
Want: Minimizer $\boldsymbol{x}^* \in \mathbb{R}^n$ so that

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

- $\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{0}$ and $\boldsymbol{h}(\boldsymbol{x}) \leqslant \boldsymbol{0}$ are called constraints.
  They define the set of feasible points $\boldsymbol{x} \in S \subseteq \mathbb{R}^n$.
- If $\boldsymbol{g}$ or $\boldsymbol{h}$ are present, this is constrained optimization.
  Otherwise unconstrained optimization.
- If $\boldsymbol{f}$, $\boldsymbol{g}$, $\boldsymbol{h}$ are *linear*, this is called linear programming.
  Otherwise nonlinear programming.
- **Q:** What if we are looking for a maximizer?
  A: Minimize $-f$ instead.

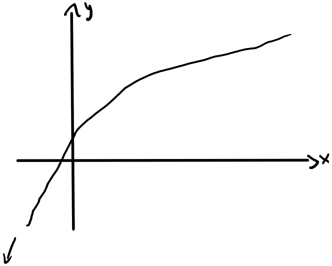
Optimization (II)

- Examples:
  - What is the fastest/cheapest/shortest... way to do...?
    Q: What about multiple objectives?
    A: Make up your mind–decide on one (or build a combined objective). Then we'll talk.
  - Solve a (nonlinear!) system of equations 'as well as you can' (if no exact solution exists)–similar to what least squares does for linear systems:
$$\min \|F(\boldsymbol{x})\|$$

Optimization: What could go wrong?

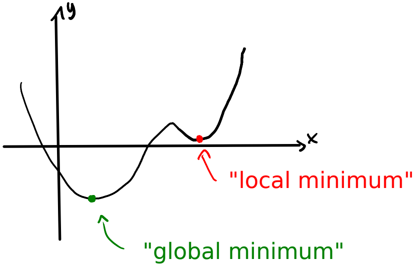
What are some potential problems in optimization?

- No minimum exists: Function just 'keeps going'.



Optimization: What could go wrong? (II)

- Find a local minimum when we meant to find a global minimum.



Optimization: What is a solution?

How can we tell that we have a (at least local) minimum? (Remember calculus!)

- Necessary condition: $f'(x) = 0$
- Sufficient condition: $f'(x) = 0$ *and* $f''(x) > 0$.

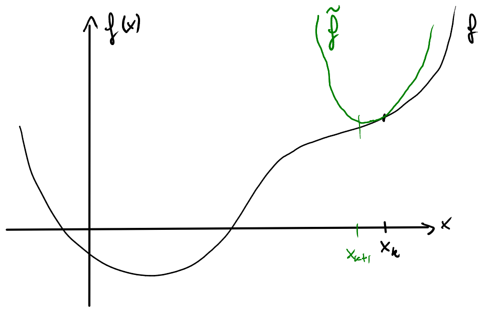
Newton's Method

Let's steal the idea from Newton's method for equation solving:
Build a simple version of f and minimize that.

Use Taylor approximation–with what degree?

Note: Line (i.e. degree 1 Taylor) wouldn't suffice–lines have no minimum. Must use at least parabola. (degree 2)

Newton's Method (II)



$$f(x+h) \approx f(x) + f'(x)h + f''(x)\frac{h^2}{2} =: \tilde{f}(h)$$

Solve $0 = \tilde{f}'(h) = f'(x) + f''(x)h$:

$$h = -\frac{f'(x)}{f''(x)}$$

Newton's Method (III)

1. $x_0 = \langle$some starting guess$\rangle$
2. $x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}$

Q: Notice something? Identical to Newton for solving $f'(x) = 0$. Because of that: locally quadratically convergent.

Demo: Newton's Method in 1D (click to visit)
In-class activity: Optimization Methods

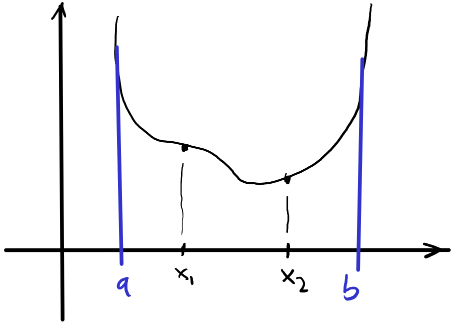
Golden Section Search

Would like a method like bisection, but for optimization.
In general: No invariant that can be preserved.
Need *extra assumption.*

f is called unimodal if for all $x_1 < x_2$

- $x_2 < x^* \Rightarrow f(x_1) > f(x_2)$
- $x^* < x_1 \Rightarrow f(x_1) < f(x_2)$

Suppose we have an interval with f unimodal:



Golden Section Search (II)

Would like to maintain unimodality.

1. Pick x_1, x_2
2. If $f(x_1) > f(x_2)$, reduce to (x_1, b)
3. If $f(x_1) \leqslant f(x_2)$, reduce to (a, x_2)

Remaining question: Where to put x_1, x_2?

- Want symmetry:
  $x_1 = a + (1 - \tau)(b - a)$
  $x_2 = a + \tau(b - a)$
- Want to reuse function evaluations: $\tau^2 = 1 - \tau$
  Find: $\tau = \left(\sqrt{5} - 1\right)/2$. Also known as the ‘golden section’.
- Hence golden section search.

Linearly convergent. Can we do better?

Demo: Golden Section Search Proportions (click to visit)

Outline

Optimization in n dimensions: What is a solution?

How can we tell that we have a (at least local) minimum? (Remember calculus!)

- Necessary condition: $\nabla f(\boldsymbol{x}) = 0$
  ∇f is a vector, the gradient:

$$\nabla f(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

- Sufficient condition: $\nabla f(\boldsymbol{x}) = 0$ *and* $H_f(\boldsymbol{x})$ positive definite.

$$H_f(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n} \end{pmatrix}$$

is called the Hessian matrix.

Steepest Descent

Given a scalar function $f : \mathbb{R}^n \to \mathbb{R}$ at a point $\boldsymbol{x}$, which way is down?

Direction of steepest descent: $-\nabla f$

Q: How far along the gradient should we go?

Unclear–do a line search. For example using Golden Section Search.

1. $\boldsymbol{x}_0 = \langle$some starting guess$\rangle$
2. $\boldsymbol{s}_k = -\nabla f(\boldsymbol{x}_k)$
3. Use line search to choose α_k to minimize $f(\boldsymbol{x}_k + \alpha_k \boldsymbol{s}_k)$
4. $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{s}_k$
5. Go to 2.

Observation: (from demo)

- Linear convergence

Demo: Steepest Descent (click to visit)

Newton's method (nD)

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

Build a Taylor approximation:

$$f(\boldsymbol{x}+\boldsymbol{s}) \approx f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T \boldsymbol{s} + \frac{1}{2}\boldsymbol{s}^T H_f(\boldsymbol{x})\boldsymbol{s} =: \hat{f}(\boldsymbol{s})$$

Then solve $\nabla \hat{f}(\boldsymbol{s}) = \boldsymbol{0}$ for $\boldsymbol{s}$ to find

$$H_f(\boldsymbol{x})\boldsymbol{s} = -\nabla f(\boldsymbol{x}).$$

1. $x_0 = \langle$some starting guess$\rangle$
2. Solve $H_f(\boldsymbol{x}_k)\boldsymbol{s}_k = -\nabla f(\boldsymbol{x}_k)$ for $\boldsymbol{s}_k$
3. $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \boldsymbol{s}_k$

Drawbacks: (from demo)

Newton's method (nD) (II)

- Need second (!) derivatives
  (addressed by Conjugate Gradients, later in the class)
- local convergence
- Works poorly when H_f is nearly indefinite

Demo: Newton's Method in n dimensions (click to visit)
Demo: Nelder-Mead Method (click to visit)

Nonlinear Least Squares/Gauss-Newton

What if the f to be minimized is actually a 2-norm?

$$f(\boldsymbol{x}) = \|\boldsymbol{r}(\boldsymbol{x})\|_2\,, \qquad \boldsymbol{r}(\boldsymbol{x}) = \boldsymbol{y} - \boldsymbol{f}(\boldsymbol{x})$$

Define 'helper function'

$$\varphi(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{r}(\boldsymbol{x})^T\boldsymbol{r}(\boldsymbol{x}) = \frac{1}{2}f^2(\boldsymbol{x})$$

and minimize that instead.

$$\frac{\partial}{\partial x_i}\varphi = \frac{1}{2}\sum_{j=1}^{n}\frac{\partial}{\partial x_i}[r_j(\boldsymbol{x})^2] = \sum_j\left(\frac{\partial}{\partial x_i}r_j\right)r_j,$$

or, in matrix form:

$$\nabla\varphi = J_{\boldsymbol{r}}(\boldsymbol{x})^T\boldsymbol{r}(\boldsymbol{x}).$$

Nonlinear Least Squares/Gauss-Newton (II)

For brevity: $J := J_{\boldsymbol{r}}(\boldsymbol{x})$. Can show similarly:

$$H_\varphi(\boldsymbol{x}) = J^T J + \sum_i r_i H_{r_i}(\boldsymbol{x}).$$

Newton step $\boldsymbol{s}$ can be found by solving

$$H_\varphi(\boldsymbol{x})\boldsymbol{s} = -\nabla\varphi$$

Observation: $\sum_i r_i H_{r_i}(\boldsymbol{x})$ is inconvenient to compute *and* unlikely to be large (since it's multiplied by components of the residual, which is supposed to be small) $\rightarrow$ forget about it.

Gauss-Newton method: Find step $\boldsymbol{s}$ by

$$J^T J\boldsymbol{s} = -\nabla\varphi = -J^T\boldsymbol{r}(\boldsymbol{x})$$

Does that remind you of the *normal equations*?

$$J\boldsymbol{s} \cong -\boldsymbol{r}(\boldsymbol{x})$$

Nonlinear Least Squares/Gauss-Newton (III)

Solve that using our existing methods for least-squares problems.

Observations: (from demo)

- Newton on its own is only locally convergent
- Gauss-Newton is clearly similar
- It's worse because the step is only approximate
  $\rightarrow$ Much depends on the starting guess.

If Gauss-Newton on its own is poorly, conditioned, can try **Levenberg-Marquardt**:

$$(J_{\boldsymbol{r}}(\boldsymbol{x}_k)^T J_{\boldsymbol{r}}(\boldsymbol{x}_k) + \mu_k I)\boldsymbol{s}_k = -J_{\boldsymbol{r}}(\boldsymbol{x}_k)^T \boldsymbol{r}(\boldsymbol{x}_k)$$

for a 'carefully chosen' μ_k. This makes the system matrix 'more invertible' but also less accurate/faithful to the problem. Can also be translated into a least squares problem (see book).

What Levenberg-Marquardt does is generically called 'Regularization': Make H more positive definite.

Demo: Gauss-Newton (click to visit)