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:

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

Rethinking Interpolation

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

Demo: Monomial interpolation

Demo: Choice of Nodes for Polynomial Interpolation

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 $V = I \rightarrow$ 'Lagrange basis'
- Functions that make V triangular $\rightarrow$ '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

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 $y=\sqrt{1-x^2}$
- $T_k(x)=\cos(k\cos^{-1}(x))$
- $T_k(x)=2xT_k(x)-T_{k-1}(x)$

Demo: Chebyshev interpolation part I

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:

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

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 part II

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

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

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?

$\boldsymbol{\alpha}' = V^{-1}V'V^{-1}\boldsymbol{f}$.

Give a matrix that finds the second derivative.

$V'V^{-1}V'V^{-1}$.

Demo: Taking derivatives with Vandermonde matrices

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?

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

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

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

Finite Difference Formulas (II)

So we can compute an approximate (second-order accurate!) derivative just by using this formula.

Generalizes to more (and non-center) points easily.

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

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

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

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

Example: Building a Quadrature Rule

Demo: Computing the Weights in Simpson's Rule

Suppose we know

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

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

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:

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

It turns out that this rule has someone's name attached to it. It's called Simpson's rule.

Facts about Quadrature

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

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

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?

Facts about Quadrature (II)

Demo: Accuracy of Simpson's rule

- Quadrature:

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

(where $h = b - a$)
(Due to a happy accident, odd 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

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 $f(x) = \tilde{f}(x) - y$.

Intuition: Each of the n equations describes a surface. Looking for intersections.

Bisection Method

Demo: Bisection Method

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
Demo: Convergence of Newton's Method

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 $\left(1+\sqrt{5}\right)/2 \approx 1.618$.

Drawbacks of Secant:

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

Demo: Secant Method
In-class activity: Nonlinear equations in 1D

Outline

Solving Nonlinear Equations

What is the goal here?

Solve $\boldsymbol{f}(\boldsymbol{x}) = \mathbf{0}$ for $f : \mathbb{R}^n \to \mathbb{R}^n$.

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

Intuition: Each of the n equations describes a surface. Looking for intersections.
Demo: Intersection of quadratics

Newton's method

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

Approximate by linear function:

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

where J_f is the Jacobian matrix of f:

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

Set to $\mathbf{0}$:

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

That's a linear system! (Surprised?)

Newton's method (II)

So

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

Downsides:

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

Newton: Example

Set up Newton's method to find a root of

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

Mostly just need the Jacobian:

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

Demo: Newton's method in n dimensions

Secant in n dimensions?

What would the secant method look like in n dimensions?

Need an ‘approximate Jacobian’ satisfying

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

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

- No: n^2 unknowns in $\tilde{J}$, but only n equations
- Can only hope 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)

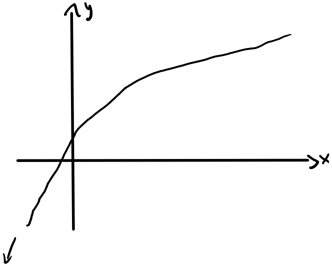
- Examples:
  - What is the fastest/cheapest/shortest... way to do...?
    Q: What about multiple objectives?
    A: Make up your mind–decide on one (or build a combined objective). Then we'll talk.
  - Solve a (nonlinear!) system of equations 'as well as you can' (if no exact solution exists)–similar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

$$\min \|F(\boldsymbol{x})\|$$

Optimization: What could go wrong?

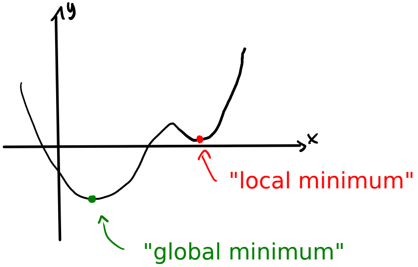
What are some potential problems in optimization?

- 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* $f''(x) > 0$.

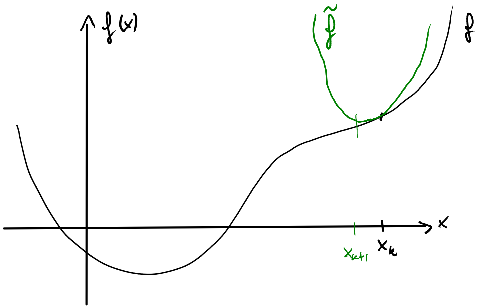
Newton's Method

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
In-class activity: Optimization Methods

Golden Section Search

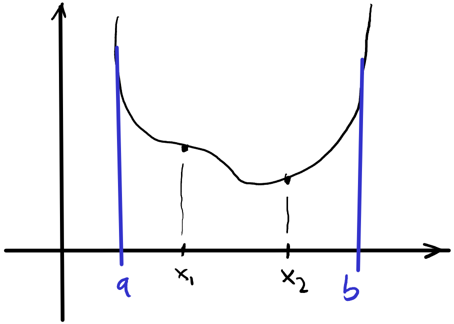
Would like a method like bisection, but for optimization.
In general: No invariant that can be preserved.
Need *extra assumption.*

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

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

Golden Section Search (II)

Suppose we have an interval with f unimodal:



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?

Golden Section Search (III)

- 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

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

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

Demo: Nelder-Mead Method

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