Lecture 2: Function Minimization

STAT 545: Intro. to Computational Statistics

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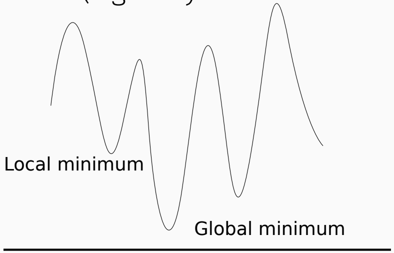
Global and local minima

Find minimum of some function $f : \mathbb{R}^D \to \mathbb{R}$.
(maximization is just minimizing $-f$).

No global information (e.g. only function values, derivatives).



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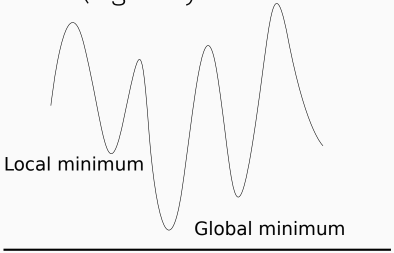

Finding global minima is hard! Usually settle for local minima.

Even finding local minima is not easy. Usually need iterative algorithms. (Exceptions?)

Gradient descent (iterative method)

Consider 1-d case. Let x_{old} be our current value.

Update x_{new} as $$x_{new} = x_{old} - \eta \, \frac{\mathrm{d}f}{\mathrm{d}x}\bigg|_{x_{old}}$$

The steeper the slope, the bigger the move.

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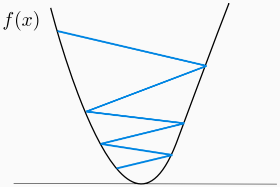

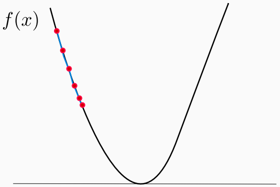

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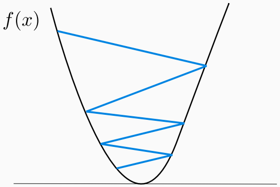
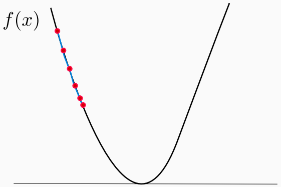




Better methods adapt step-size according to the curvature of f.

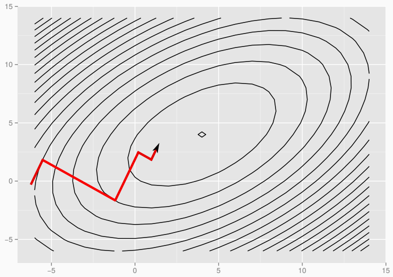
Gradient descent in higher-dimensions

Also applies to higher dimensions: $x_{new} = x_{old} - \eta \left.\nabla f\right|_{x_{old}}$

Again, need care choosing η

Alternately, at each step, set η by minimizing along ∇f

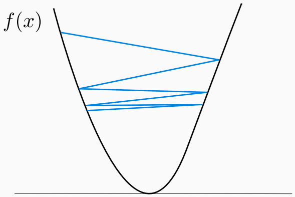
- Note: even the optimal step-size η can be inefficient:

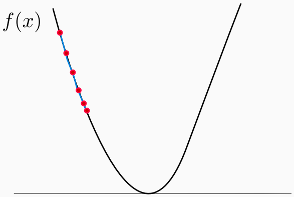


Rather than finding best step-size each step, save computation and find a decent solution

Wolfe conditions to decide step-size

Bad step sizes along direction **p** (for grad. descent, $\mathbf{p} = -\nabla f$):





1) Big steps with little decrease 2) Small steps getting nowhere

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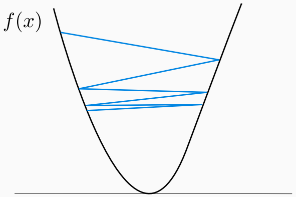

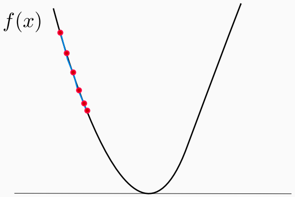

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Avoid (1): Avg. decrease at least some fraction of initial rate:

$$f(\mathbf{x} + \eta\mathbf{p}) \leq f(\mathbf{x}) + \eta c_1(\nabla f \cdot \mathbf{p}), \qquad c_1 \in (0, 1) \ \textit{e.g.}\ 0.9$$

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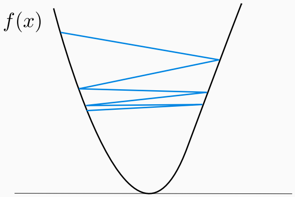

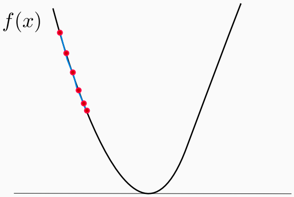

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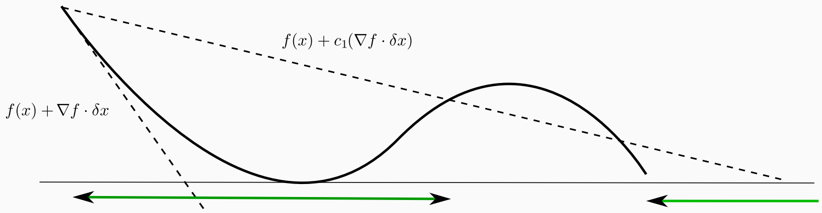
Avoid (2): Final rate is greater than some fraction of initial rate:

$$\nabla f(\mathbf{x} + \eta\mathbf{p}) \cdot \mathbf{p} \geq c_2 \nabla f(\mathbf{x}) \cdot \mathbf{p}, \qquad c_2 \in (0,1) \ e.g. \ 0.1$$

Wolfe conditions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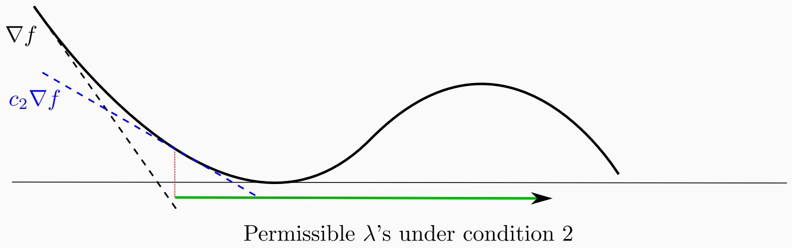
Permissible δx's under condition 1

Wolfe conditions



Wolfe conditions

A simple way to satisfy Wolfe conditions:

Set $\mathbf{p} = -\nabla f, c_1 = c_2 = .5$

Start with $\nu = 1$, and while condition i is not satisfied, set $\nu = \beta_i t$ (for $\beta_1 \in (0, 1), \beta_2 > 1$ and $\beta_1 * \beta_2 < 1$

Gradient flow

One way to understand/improve gradient descent is to view it as an approximation to ‘gradient flow’.

Write x_t for the position of a particle at time t, evolving as

$$\frac{\mathrm{d}\mathsf{x}_t}{\mathrm{d}t} = -\nabla f(\mathsf{x}_t), \quad \text{for some initialization at } t = 0.$$

x_t converges to x^*, the minimum of f as t increases

- At minimum, $\nabla f(\mathsf{x}^*) = 0$.

Typically, not easy to solve the differential eq. for x_t

Different algs can be seen as approximations to this ideal

Forward and backward methods

$$\frac{\Delta \mathsf{x}_t}{\Delta t} \approx \frac{\mathrm{d}\mathsf{x}_t}{\mathrm{d}t} = -\nabla f(\mathsf{x}_t) \quad \text{(forward Euler approximation)}$$

$$\implies \quad \mathsf{x}_{t+\Delta t} = \mathsf{x}_t - \Delta t \nabla f(\mathsf{x}_t)$$

This is just gradient descent with stepsize $\eta = \Delta t$

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Backward Euler approx $\implies \quad \mathbf{x}_{t+\Delta t} = \mathbf{x}_t - \Delta t \nabla f(\mathbf{x}_{t+\Delta t})$

For a step size η, the iterates are:

$$\mathbf{x}_{i+1} = \mathbf{x}_i - \eta \nabla f(\mathbf{x}_{i+1})$$

The updates are implicit ($\mathbf{x}_{i+1}$ is on both LHS and RHS).
Why do we care?

Backward Euler method

Backward method: $\mathsf{x}_{i+1} = \mathsf{x}_i - \eta \nabla f(\mathsf{x}_{i+1})$

Claim: this is the same as solving

$$\mathsf{x}_{i+1} = \arg\min \; f(\mathsf{x}) + \frac{1}{2\eta}(\mathsf{x} - \mathsf{x}_i)^2$$

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Now, we see that:

- $\mathbf{x}_{i+1} \leq \mathbf{x}_i$, unlike gradient descent. Has faster convergence.
- This works even if ∇f is not defined!
- Can be generalized to different distance functions:

$$\mathbf{x}_{i+1} = \arg\min \; f(\mathbf{x}) + \frac{1}{2\eta} d(\mathbf{x}, \mathbf{x}_i)$$

Other approaches to improving convergence

Newton's method: uses second derivatives/Hessians:

$$x_{i+1} = x_i - f'(x_i)/f''(x_i)$$

For vector-valued $\mathbf{x}$, writing $\mathrm{H}f(\mathbf{x}_i)$ for the Hessian of f at $\mathbf{x}_i$,

$$\mathbf{x}_{i+1} = \mathbf{x}_i - [\mathrm{H}f(\mathbf{x}_i)]^{-1}\nabla f(\mathbf{x}_i)$$

Intuition:

- Stepsize is small when gradient is changing rapidly
- Each iteration uses $f(\mathbf{x}_i)$, $\nabla f(\mathbf{x}_i)$ and $\mathrm{H}f(\mathbf{x}_i)$ to construct a quadratic approximation to f, which is then minimized

Back to simple gradient descent

MLE: maximum likelihood estimation

Consider a set of observations $X = (x_1, \cdots, x_N)$.

Assume $x_i \sim p(x|\theta)$

$$\theta_{MLE} = \text{argmax}\, \ell(\theta) := \text{argmax} \sum_{i=1}^{N} \log p(x_i|\theta)$$

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Starting with an initial θ_0, iterate:

$$\theta_{i+1} = \theta_i + \eta_i \nabla \ell(\theta_i)$$

Gradient descent (contd.)

$$\nabla \ell(\theta) = \sum_{i=1}^{N} \nabla \log p(x_i|\theta)$$

Cons:

- Calculating gradient requires evaluating likelihood N times. (Each iteration must cycle through all datapoints.)
- *Lots* of redundancy, esp. for large N.

Gradient descent (contd.)

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Cons:

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Pros:

- Convergence is better understood.

Stochastic gradient descent

Use a noisy gradient $\widehat{\nabla \ell}$.

Typically split data into N/B batches of size B.
Each iteration, calculate gradient on one of the batches B_i:

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Pros:

- Calculating the gradient is $O(B)$.
  (Often, each batch is just a single datapoint)
- Much faster convergence (just one sweep through the data can get you a decent solution).
- Often, you get better solutions.
- Useful for online systems, tracking θ that varies over time .

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Cons:

- Convergence analysis is harder.
- Noisy gradients mean the algorithm will never converge.
  Typically need to reduce the step size every iteration.
  We want

$$\eta_i \to 0, \quad \sum_{i=1}^{\infty} \eta_i = \infty$$

  E.g. $\eta_i = \frac{a}{b+i}$

Stochastic gradient descent with momentum

One way to accelarate convergence is to include a momentum term:

$$\theta_{i+1} = \theta_i + \eta_i \widehat{\nabla \ell}(\theta_i) + \beta_i \underbrace{(\theta_i - \theta_{i-1})}_{\text{momentum}}$$

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More generally,

$$\theta_{i+1} = \theta_i + \eta_i \widehat{\nabla} \ell(\theta_i + \gamma(\theta_i - \theta_{i-1})) + \beta_i(\theta_i - \theta_{i-1})$$

Include many popular algorithms:

- Polyak's heavy ball method (HB): $\gamma = 0$
- Nesterov's accelerated gradient (NAG): $\gamma_i = \beta_i$

Adaptive methods

Adaptive methods accelerate convergence by using the entire history of iterates to determine step-sizes.

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Often take the general form

$$\theta_{i+1} = \theta_i + \eta_i H_i^{-1} \widehat{\nabla \ell}(\theta_i + \gamma(\theta_i - \theta_{i-1})) + \beta_i H_i^{-1} H_{i-1}(\theta_i - \theta_{i-1})$$

where H_i is some combination of all previous gradients. E.g.

$$H_i = \mathrm{diag}\left(\sum_{j=1}^{i} g_j \circ g_j\right),$$

with $g_j = \widehat{\nabla \ell}(\theta_j + \gamma(\theta_j - \theta_{j-1}))$, and $\circ$ element-wise product.

Examples are AdaGrad, Adam etc.