

LECTURE 2: FUNCTION MINIMIZATION

STAT 545: INTRO. TO COMPUTATIONAL STATISTICS

Vinayak Rao

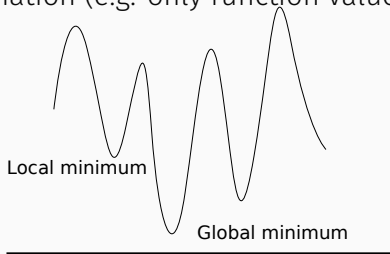
Purdue University

August 20, 2019

GLOBAL AND LOCAL MINIMA

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

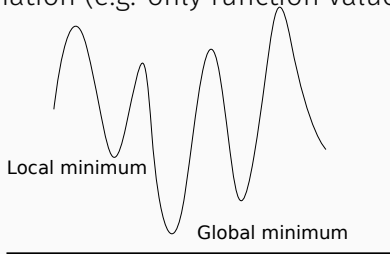
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Finding global minima is hard! Usually settle for local minima.
Even finding local minima is not easy. Usually need iterative algorithms. (Exceptions?)

GRADIENT DESCENT (ITERATIVE METHOD)

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

Update x_{new} as
$$x_{new} = x_{old} - \eta \left. \frac{df}{dx} \right|_{x_{old}}$$

The steeper the slope, the bigger the move.

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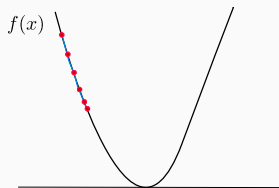
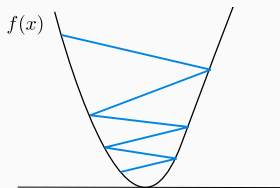
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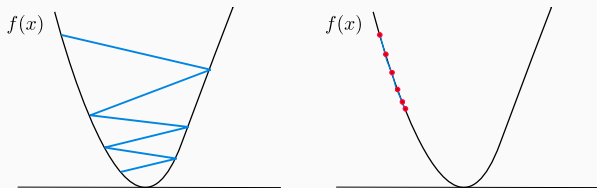
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Better methods adapt step-size according to the curvature of f .

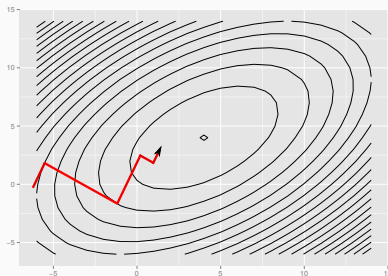
GRADIENT DESCENT IN HIGHER-DIMENSIONS

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

Again, need care choosing η

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

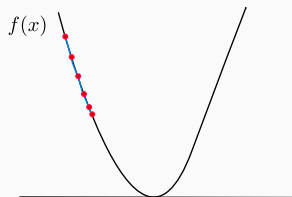
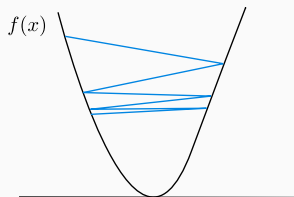
• Note: even the optimal step-size η can be inefficient:



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

WOLFE CONDITIONS TO DECIDE STEP-SIZE

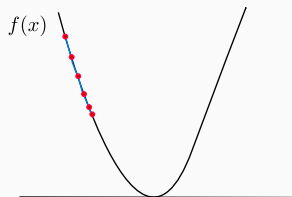
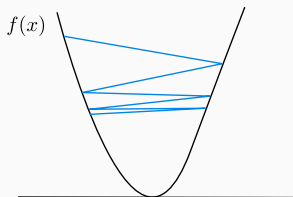
Bad step sizes along direction \mathbf{p} (for grad. descent, $\mathbf{p} = -\nabla f$):



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

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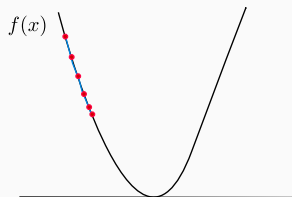
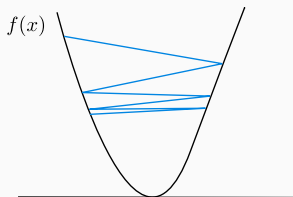
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Avoid (1): Avg. decrease at least some fraction of initial rate:

$$f(\mathbf{x} + \eta \mathbf{p}) \leq f(\mathbf{x}) + \eta c_1 (\nabla f \cdot \mathbf{p}), \quad c_1 \in (0, 1) \text{ e.g. } 0.1$$

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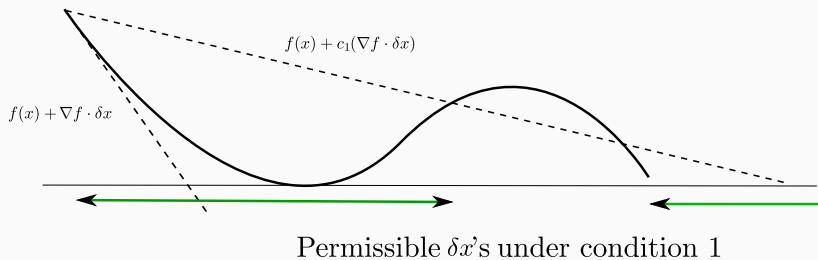
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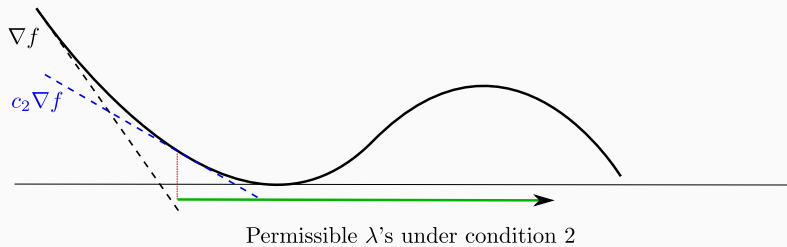
Avoid (2): Final rate is greater than some fraction of initial rate:

$$\nabla f(\mathbf{x} + \eta \mathbf{p}) \cdot \mathbf{p} \geq c_2 \nabla f(\mathbf{x}) \cdot \mathbf{p}, \quad c_2 \in (0, 1) \text{ e.g. } 0.9$$

WOLFE CONDITIONS



WOLFE CONDITIONS



A simple way to satisfy Wolfe conditions:

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

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

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

Write \mathbf{x}_t for the position of a particle at time t , evolving as

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

\mathbf{x}_t converges to \mathbf{x}^* , the minimum of f as t increases

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

Typically, not easy to solve the differential eq. for \mathbf{x}_t

Different algs can be seen as approximations to this ideal

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

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

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

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

FORWARD AND BACKWARD METHODS

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

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

Claim: this is the same as solving

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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:

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

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 $\mathbf{H}f(\mathbf{x}_i)$ for the Hessian of f at \mathbf{x}_i ,

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

Intuition:

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

MLE: maximum likelihood estimation

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

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

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

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Starting with an initial θ_0 , iterate:

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

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

Cons:

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

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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

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

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

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

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

STOCHASTIC GRADIENT DESCENT WITH MOMENTUM

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

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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 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.

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

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

Examples are AdaGrad, Adam etc.