CS 760: Machine Learning
Optimization

University of Wisconsin-Madison

Outline

- **Optimization problems in machine learning**

- **Gradient descent**
  - idea, algorithm, convexity, convergence, nonconvexity

- **Drawbacks and other optimizers**
  - stochastic gradient descent, alternative optimizers

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Optimization in ML

- in supervised learning, we
- have a training dataset of $\left(x^{(i)}, y^{(i)}\right)$ pairs for $i = 1, \dots, n$
- search a hypothesis space H for a function h that
  - predicts well, i.e. $h\left(x^{(i)}\right) = y^{(i)}$ on most of the training data
  - satisfies other constraints, e.g. simplicity so as not to overfit

Optimization in ML

- often **searching the hypothesis space** is an **optimization problem**:

- decision trees

$$\min_{\substack{h(x^{(i)})=y^{(i)} \\ \forall i\in[n]}} \quad depth(h)$$

predicts well **is simple**

- parametric models

$$\min_{\theta\in\mathbb{R}^d} \sum_{i=1}^{n} loss\left(h_\theta\left(x^{(i)}\right), y^{(i)}\right) + penalty(\theta)$$

Optimization in ML

- often **searching the hypothesis** space is an **optimization problem**:

- decision trees

$$\min_{\substack{h(x^{(i)})=y^{(i)} \\ \forall i\in[n]}} depth(h)$$

- parametric models

$$\min_{\theta\in\mathbb{R}^d} \sum_{i=1}^{n} \underbrace{loss}_{\text{squared error}}\left(h_\theta\left(x^{(i)}\right), y^{(i)}\right) + \underbrace{penalty}_{\text{squared } \ell_2\text{-norm}}(\theta)$$

h_θ is a neural net

linear / Ridge regression
$\theta = (X^T X + \lambda I)^{-1} X^T y$

sometimes optimization is (NP) hard and we must use a heuristic

sometimes we have a closed-form solution

This lecture: sometimes there is an **efficient optimization algorithm** to get the solution

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Iterative Methods: Gradient Descent

- What if there's no closed-form solution?
- Use an iterative approach to gradually get closer to the solution.

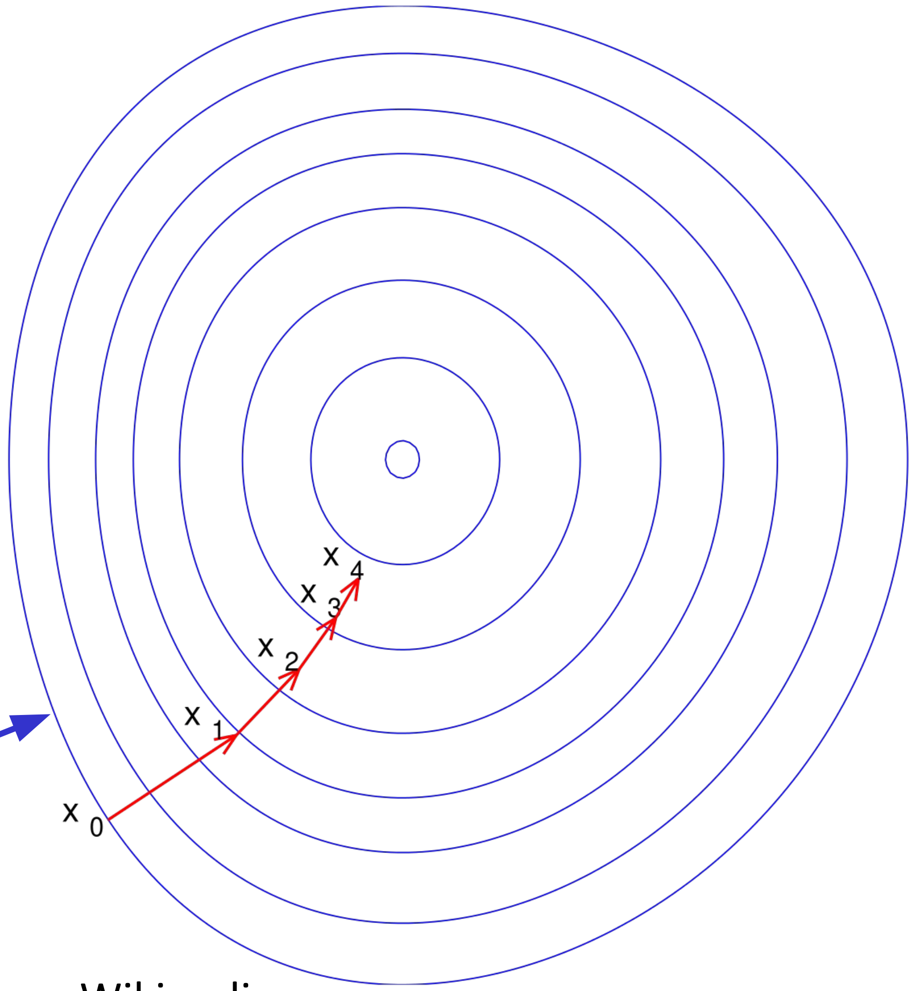
- Gradient descent:
  - Suppose we're computing $\min_{\theta} g(\theta)$
  - Start at some θ_0
  - Iteratively compute $\theta_{t+1} = \theta_t - \underset{\text{learning rate/step size}}{\alpha} \nabla g(\theta_t)$
  - Stop after some # of steps

Gradient Descent: Illustration

- **Goal**: steps get closer to minimizer

- Some notes:
  - Step size can be fixed or varying
  - Under certain conditions, will converge to global minimum

level sets



Wikipedia

Gradient Descent: Efficiency

- Back to our linear regression problem

- Want to find $\min_{\theta} \ell(f_\theta) = \min_{\theta} \frac{1}{n} \|X\theta - y\|_2^2$
  - What's our gradient? $\nabla \ell(f_\theta) = \frac{1}{n}(2X^T X\theta - 2X^T y)$
  - So, plugging in , we get

$$\theta_{t+1} = \theta_t - \alpha \frac{1}{n}(2X^T X\theta_t - 2X^T y)$$

Linear Regression: Normal Equations vs GD

- Why do this for a setting with a closed-form solution?
- **Consider its computational cost:**

$$\theta = (\underbrace{X^T X}_{d \times d})^{-1} \underset{\overset{\uparrow}{d \times n}}{X^T} \underset{\overset{\uparrow}{n \times 1}}{y}$$

- Cost: (i) invert matrix, $\Theta(d^3)$. (ii) multiplication, $\Theta(d^2 n)$.
- **Total**: $\Theta(d^2 n + d^3)$.

Recall: by standard methods, inverting an *m* x *m* matrix is $\Theta(m^3)$.

Multiplying a *m* x *p* with a *p* x *q* matrix is $\Theta(mpq)$

Linear Regression: Normal Equations vs GD

Now let's compare to the cost of gradient descent

- Normal Equations $\theta = (X^T X)^{-1} X^T y$
  - **Total Cost**: $\Theta(d^2 n + d^3)$.

- Gradient Descent: t iterations

$$\theta_{t+1} = \theta_t - \alpha \frac{1}{n} (2X^T X \theta_t - 2X^T y)$$

  - Cost: $\Theta(dn)$ at each step.
  - **Total Cost**: $\Theta(dnt)$.

If we do "few" steps t, then **GD is cheaper**: $t < \max\{d, d^2/n\}$

Gradient Descent: Convergence

- Even if GD is cheaper, what does it give us?
- Let's analyze it. We'll need some **assumptions**
  - convex and differentiable objective f
  - f has L-Lipschitz-continuous gradients

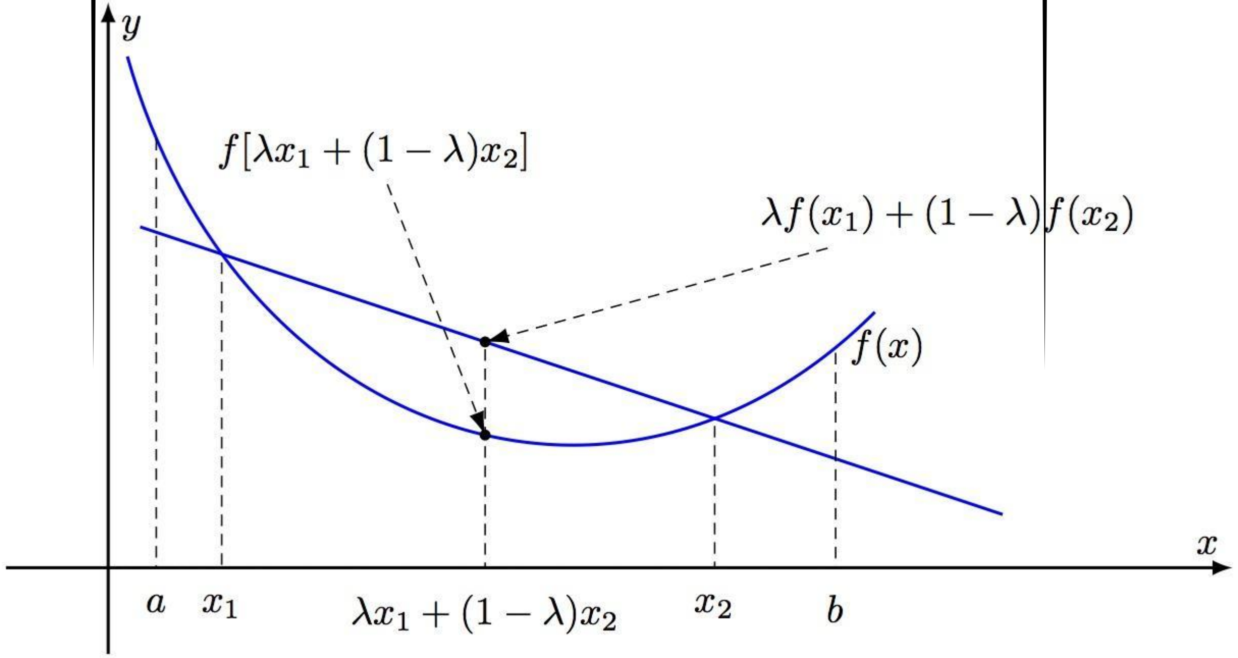
- Under these assumptions, we have the following guarantee:
  - if we run T steps of GD with fixed step size $\alpha \leq 1/L$ starting at x_0, then the Tth iterate x_T satisfies

$$f(x_T) - f(\underset{\uparrow\atop\text{minimizer}}{x^*}) \leq \frac{||x_0 - x^*||_2^2}{2T\alpha}$$

Gradient Descent Analysis : Convexity

A function f with convex domain X is called convex if for all x_1, x_2 in the domain and all $\lambda \in [0, 1]$ we have

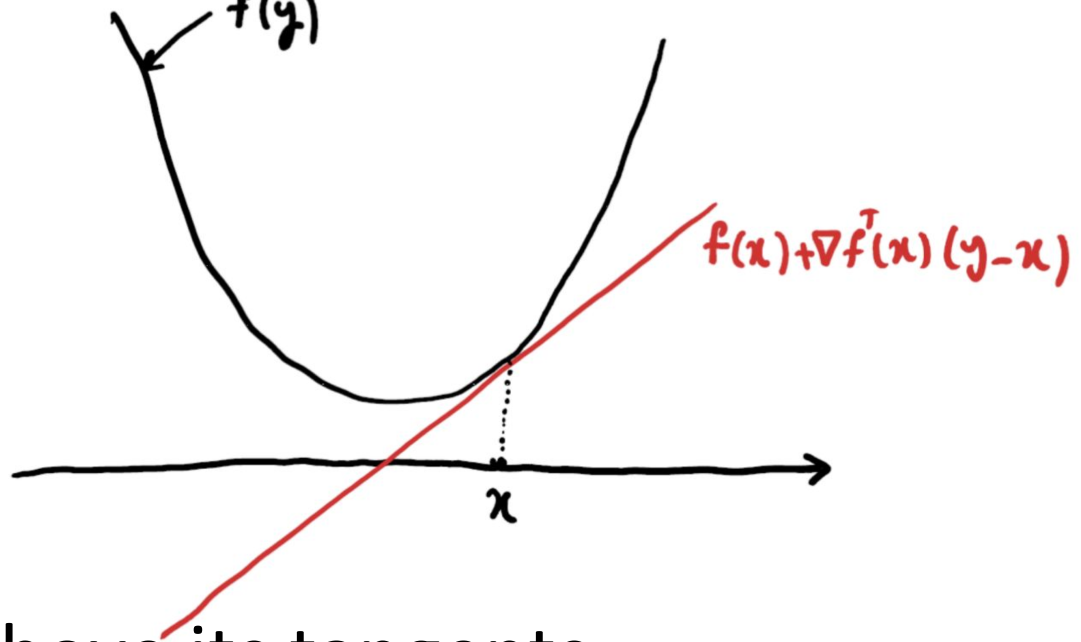
$$f(\underbrace{\lambda x_1 + (1-\lambda)x_2}_{\text{Convex combination}}) \le \underbrace{\lambda f(x_1) + (1-\lambda) f(x_2)}_{\text{Line segment joining } f(x_1) \text{ and } f(x_2)}$$


y
$f[\lambda x_1 + (1-\lambda)x_2]$
$\lambda f(x_1) + (1-\lambda) f(x_2)$
$f(x)$
x
a
x_1
$\lambda x_1 + (1-\lambda)x_2$
x_2
b

Gradient Descent Analysis : Convexity

- An equivalent definition:

$$f(x_2) \geq f(x_1) + \nabla f(x_1)^T (x_2 - x_1)$$



- Function sits above its tangents

Gradient Descent Analysis : Lipschitzness

- A function has L-Lipschitz gradients if

$$\|\nabla f(x_1) - \nabla f(x_2)\|_2 \leq L\|x_1 - x_2\|_2$$

- Equivalent to $\nabla^2 f(x) \preceq LI$

- Recall: $A \preceq B$ means that $B - A$ is positive semidefinite

- Recall some more: C is positive semidefinite if $x^T C x \geq 0$

Gradient Descent: Convergence Proof p. 1

- We'll use our **two assumptions**.
- Let's start with a Taylor expansion:

$$f(y) = f(x) + \nabla f(x)^T (y - x) + 1/2 (y - x)^T \nabla^2 f(z) (y - x)$$

- Next, our gradient Lipschitz condition means $\nabla^2 f(x) \preceq LI$

$$\boxed{\implies f(y) \leq \underbrace{f(x) + \nabla f(x)^T (y - x)}_{\text{Linear Approximation}} + \underbrace{1/2 L \|y - x\|^2}_{\text{Remainder: at most a quadratic}}}$$

Gradient Descent: Convergence Proof p. 2

- Let’s plug in our GD relationship $y \leftarrow x_{t+1} = x_t - \alpha \nabla f(x_t)$

$$\boxed{\implies f(y) \leq f(x) + \nabla f(x)^T (y - x) + 1/2L \|y - x\|^2}$$

- Start with some algebra

$$f(x_{t+1}) \leq f(x_t) + \nabla f(x_t)^T (x_{t+1} - x_t) + 1/2L \|x_{t+1} - x_t\|_2^2$$

$$= f(x_t) - \nabla f(x_t)^T \alpha \nabla f(x_t) + 1/2L \|\alpha \nabla f(x_t)\|_2^2$$

$$= f(x_t) - \alpha \|\nabla f(x_t)\|_2^2 + 1/2L\alpha^2 \|\nabla f(x_t)\|_2^2$$

$$\boxed{= f(x_t) - \alpha(1 - 1/2L\alpha) \|\nabla f(x_t)\|_2^2}$$

Gradient Descent: Convergence Proof p. 3

- So, we now have

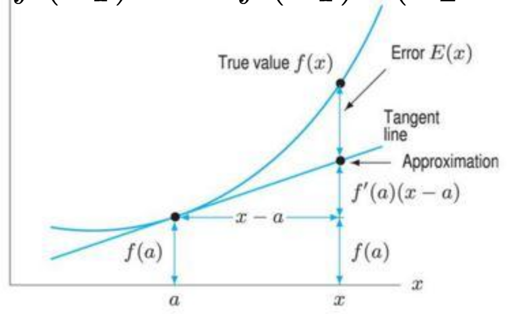
$$f(x_{t+1}) \leq f(x_t) - \underbrace{1/2\alpha\|\nabla f(x_t)\|_2^2}_{\text{Positive except at minimum (where it's 0)}}$$

- Promising! Our estimates are getting better.

- Still need how big these gradient magnitudes are

Gradient Descent: Convergence Proof p. 4

$$f(x_2) \geq f(x_1) + \nabla f(x_1)^T (x_2 - x_1)$$



- Haven't used convexity yet, so let's:

$$f(x_t) \leq f(x^*) + \nabla f(x_t)^T (x_t - x^*)$$

- Combine with $\boxed{f(x_{t+1}) \leq f(x_t) - 1/2\alpha \|\nabla f(x_t)\|_2^2}$

$$f(x_{t+1}) \leq f(x^*) + \nabla f(x_t)^T (x_t - x^*) - \alpha/2 \|\nabla f(x_t)\|_2^2$$

$$f(x_{t+1}) - f(x^*) \leq \frac{1}{2\alpha}(2\alpha \nabla f(x_t)^T (x_t - x^*) - \alpha^2 \|\nabla f(x_t)\|_2^2)$$

$$\|b-a\|_2^2 = \|a\|_2^2 - 2a^\top b + \|b\|_2^2 \;\Rightarrow\; 2a^\top b - \|a\|_2^2 = \|b\|_2^2 - \|b-a\|_2^2$$

$$\boxed{f(x_{t+1}) - f(x^*) \leq \frac{1}{2\alpha}(\|x_t - x^*\|_2^2 - \|x_t - \alpha \nabla f(x_t) - x^*\|_2^2)}$$

Gradient Descent: Convergence Proof p. 5

- Now, simplify

$$f(x_{t+1}) - f(x^*) \leq \frac{1}{2\alpha}\left(\|x_t - x^*\|_2^2 - \|\underbrace{x_t - \alpha\nabla f(x_t)}_{\text{This part is just } x_{t+1}} - x^*\|_2^2\right)$$

$$f(x_{t+1}) - f(x^*) \leq \frac{1}{2\alpha}\left(\|x_t - x^*\|_2^2 - \|x_{t+1} - x^*\|_2^2\right)$$

Gradient Descent: Convergence Proof p. 6

- So, we have something familiar…

$$\boxed{f(x_{t+1}) - f(x^*) \leq \frac{1}{2\alpha}\underbrace{(\|x_t - x^*\|_2^2 - \|x_{t+1} - x^*\|_2^2)}_{\text{Can telescope!}}}$$

$$\sum_{t=0}^{T-1} f(x_{t+1}) - f(x^*) \leq \sum_{t=0}^{T-1} \frac{1}{2\alpha}(\|x_t - x^*\|_2^2 - \|x_{t+1} - x^*\|_2^2)$$

$$\boxed{\sum_{t=0}^{T-1} f(x_{t+1}) - f(x^*) \leq \frac{1}{2\alpha}(\|x_0 - x^*\|_2^2 - \|x_T - x^*\|_2^2)}$$

Gradient Descent: Convergence Proof p. 7

- Now we have

$$\boxed{\sum_{t=0}^{T-1} f(x_{t+1}) - f(x^*) \leq \frac{1}{2\alpha}(\|x_0 - x^*\|_2^2 - \|x_T - x^*\|_2^2)}$$

- Can ignore the rightmost term (we're just making the RHS same or bigger)

$$\boxed{\sum_{t=0}^{T-1} \underbrace{f(x_{t+1}) - f(x^*)}_{\text{Value gap for all steps}} \leq \frac{1}{2\alpha}(\underbrace{\|x_0 - x^*\|_2^2}_{\text{Initial guess gap to minimizer}})}$$

Gradient Descent: Convergence Proof p. 7

- Continue,

$$\sum_{t=0}^{T-1} f(x_{t+1}) - f(x^*) \leq \frac{1}{2\alpha}(\|x_0 - x^*\|_2^2)$$

- But, recall that each iterate has a smaller value, i.e.,

$$f(x_{t+1}) \leq f(x_t) - 1/2\alpha\|\nabla f(x_t)\|_2^2$$

- So

$$\sum_{t=0}^{T-1} f(x_T) \leq \sum_{t=0}^{T-1} f(x_{t+1})$$

Gradient Descent: Convergence Proof p. 8

- Almost there! We have $$\sum_{t=0}^{T-1} f(x_T) \leq \sum_{t=0}^{T-1} f(x_{t+1})$$
- Divide by T,

$$\implies f(x_T) - f(x^*) \leq \frac{1}{T} \sum_{t=0}^{T-1} f(x_{t+1}) - f(x^*)$$

- Combine with $$\boxed{\sum_{t=0}^{T-1} f(x_{t+1}) - f(x^*) \leq \frac{1}{2\alpha}(\|x_0 - x^*\|_2^2)}$$

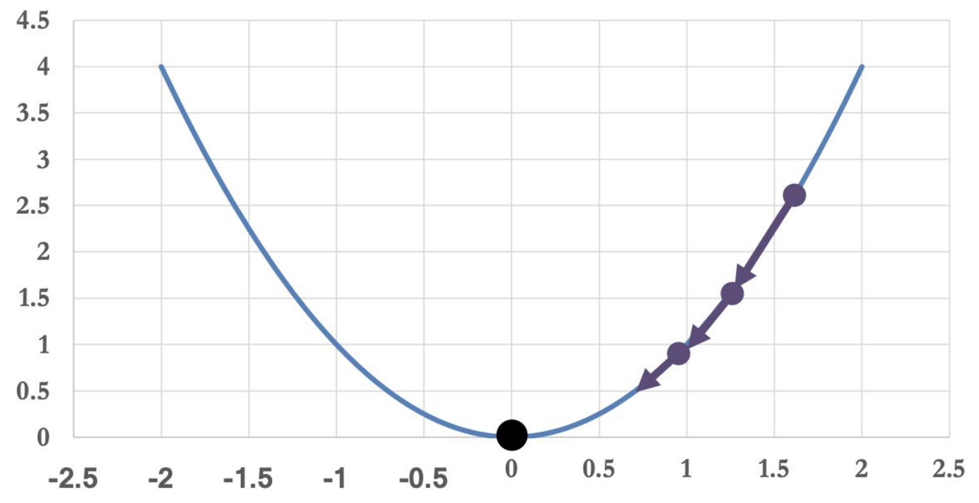
$$\boxed{\implies f(x_T) - f(x^*) \leq \frac{\|x_0 - x^*\|_2^2}{2T\alpha}}$$

Done!

Gradient Descent: Convergence Proof Recap

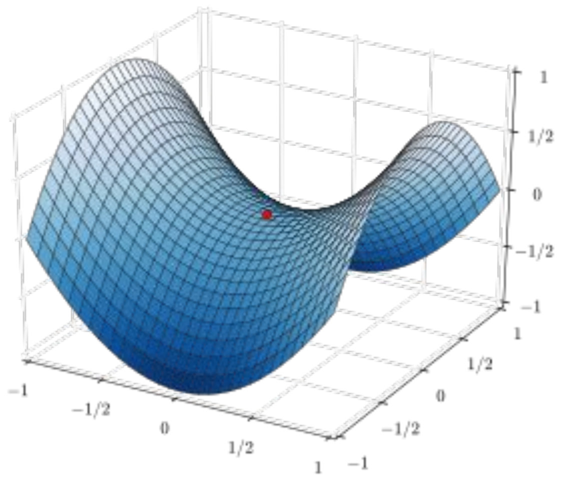
- **Note**: used all conditions in one or more places in the proof.
  - If you don't use an assumption, either your result is stronger than you thought or (more likely) you are making a mistake

- Other assumptions that lead to varying proofs/rates:
  - **Strong convexity**
  - **Non-convexity**
  - **Non-differentiability**



Gradient Descent as a heuristic

- If a function is non-convex, gradient descent
  - can still be applied so long as it is differentiable
  - is only guaranteed to reach a **stationary point**, not necessarily a global minimum



Wikipedia

- Nevertheless, neural networks are commonly fit using (extensions of) gradient descent:
  - objectives are non-convex AND non-smooth
  - often get parameters that **are optimal** (low training loss) AND **generalize well** (high test accuracy)
  - required decades hacking and experimentation
  - should be viewed as a poorly understood heuristic like information gain for decision trees

Break & quiz

Q: True or False: gradient descent is always a more efficient way of computing linear regression than the normal equations.

Q: True or False: gradient descent is always a more efficient way of computing linear regression than the normal equations.

False: depending on the number of data points, feature dimension, and number of steps taken, gradient descent can be more expensive.

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- **Drawbacks and other optimizers**
  - stochastic gradient descent, alternative optimizers

Gradient Descent: Drawbacks

- Why would we use anything but GD?
- Let's go back to ERM. $$\arg\min_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(h(x^{(i)}, y^{(i)})$$
- For GD, need to compute $\nabla \ell(h(x^{(i)}, y^{(i)})$
    - Each step: n gradient computations
    - ImageNet: 10^6 samples… so for 100 iterations, **10^8 gradients**

Solution: **Stochastic** Gradient Descent

- Simple modification to GD.
- Let’s use some notation: ERM:

$$\arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \ell(f(\theta; x^{(i)}), y^{(i)})$$

Note: this is what we’re optimizing over!
x’s are fixed samples.

- GD:

$$\theta_{t+1} = \theta_t - \frac{\alpha}{n} \sum_{i=1}^{n} \nabla \ell(f(\theta_t; x^{(i)}), y^{(i)})$$

Solution: **Stochastic** Gradient Descent

- Simple modification to GD:

$$\theta_{t+1} = \theta_t - \frac{\alpha}{n}\sum_{i=1}^{n} \nabla \ell(f(\theta_t; x^{(i)}), y^{(i)})$$

- SGD:

$$\theta_{t+1} = \theta_t - \alpha \nabla \ell(f(\theta_t; x^{(a)}), y^{(a)})$$

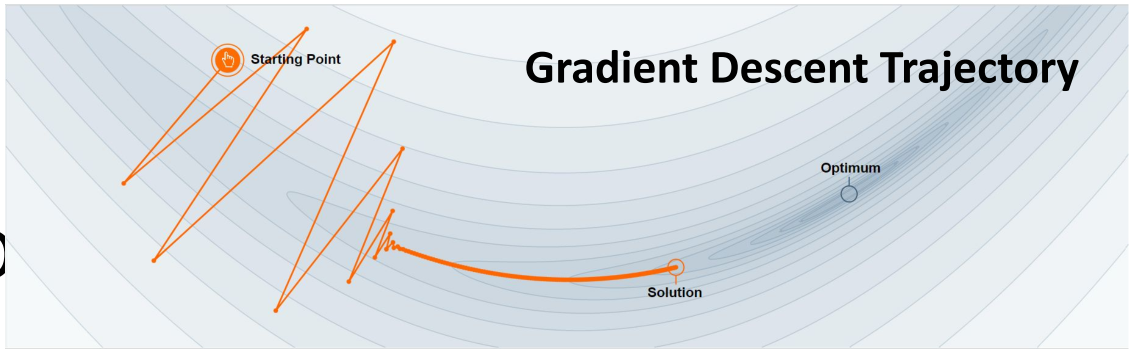
  - Here a is selected uniformly from 1,…,n ("**stochastic**" bit)
  - Note: **no sum**!
  - In expectation, same gradient as GD.
  - In practice we often update using **minibatches** of data to take advantage of (GPU) parallelism

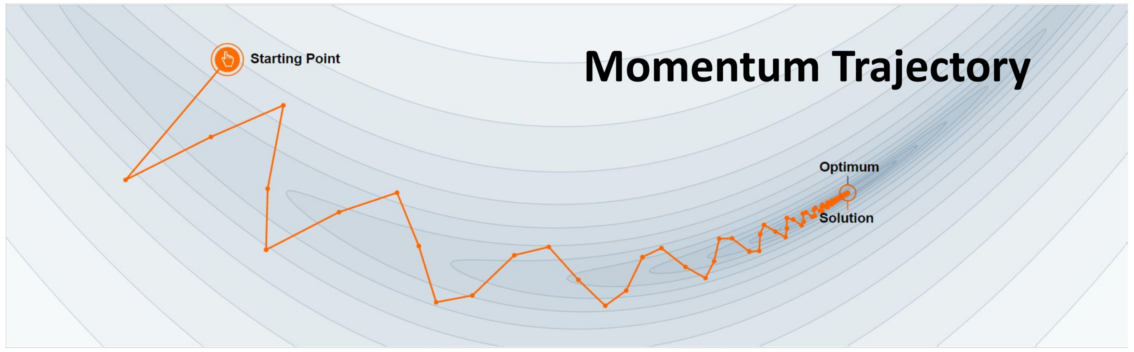
Other drawbacks of gradient descent

Behaves poorly on many important functions:

- e.g. LASSO is convex but non-differentiable, so we use coordinate descent or proximal methods

- on poorly conditioned problems, GD struggles to make progress down narrow valleys. Alternatives:
  - momentum methods
  - second-order methods (Newton)
  - approximate second-order methods (includes widely used deep net optimizers such as Adam)





Source: Goh. *Why Momentum Really Works*. Distill 2017.

Thanks Everyone!

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