CS5489
Lecture 3.1: Gradient Descent and Its Variants

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Part of slides are borrowed from Stephen P. Boyd

Generative vs Discriminative Classifiers

显示地 对**建模

- The Bayes optimal classifier, NB and LDA are said to be *generative* classifiers because they explicitly model the joint distribution $p(\mathbf{x}, y)$ of the feature vectors $\mathbf{x}$ and the labels y
- To build a probabilistic classifier, all we really need to model is $p(y|\mathbf{x})$
- Classifiers based on directly estimating $p(y|\mathbf{x})$ are called *discriminative* classifiers because they don't care about the class conditional distribution $p(\mathbf{x}|y)$

Logistic Regression

- Logistic regression is a probabilistic discriminative classifier
- It directly models the decision boundary using a linear function:

$$p(y=+1|\mathbf{x}) = \frac{1}{1+\exp(-(\mathbf{w}^T\mathbf{x}+b))}$$

$$\log \frac{p(y=+1|\mathbf{x})}{p(y=-1|\mathbf{x})} = \mathbf{w}^T\mathbf{x}+b$$

那么P(y=-1|x)呢？

- The classification function is:

$$f_{\text{LR}}(\mathbf{x}) = \arg\max_{c\in\{1,\ldots,C\}} p(y=c|\mathbf{x})$$

什么叫分析方法，什么叫数值优化方法

- Learning the model parameters cannot be performed analytically and has to resort to numerical optimization methods

Optimization

- Much of machine learning can be written as an optimization problem:

$$\min_{\boldsymbol{\theta}} \ \ell(\mathcal{D};\boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \ \frac{1}{M}\sum_{i=1}^{M} \ell\left(\mathbf{x}^{(i)}, y^{(i)}; \boldsymbol{\theta}\right) + r(\boldsymbol{\theta})$$

  - $\boldsymbol{\theta}$ is a parameter vector to be optimized
  - $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)}), i = 1, \ldots, M\}$ is a finite training set
  - $r(\cdot)$ is a regularizer to prevent overfitting to $\mathcal{D}$

- In logistic regression ($\boldsymbol{\theta} = \{\mathbf{w}, b\}$)
  - $\ell(\mathbf{x}^{(i)}, y^{(i)}; \boldsymbol{\theta}) = \log\left(1 + \exp\left(-y^{(i)}(\mathbf{w}^T\mathbf{x}^{(i)} + b)\right)\right)$
  - $r(\boldsymbol{\theta}) = \frac{1}{C}\mathbf{w}^T\mathbf{w}$

这个log是logn还是log2？ 逻辑回归的公式怎么来的呢？有没有例子说明？

Types of Optimization

- Convex optimization 凸优化
  - The easy case
    - Includes logistic regression, linear regression, SVM
- Nonconvex optimization
  - Hard in general
    - Includes deep learning

Convex Set

- **Line segment** between $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$: all points

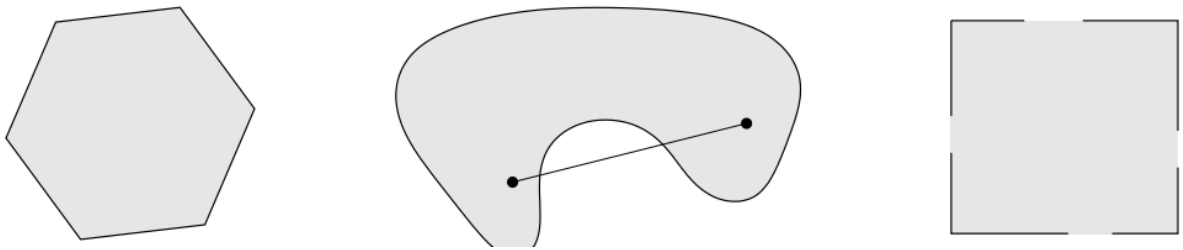
$$\mathbf{x} = \alpha\mathbf{x}^{(1)} + (1-\alpha)\mathbf{x}^{(2)}$$

with $0 \leq \alpha \leq 1$

- **Convex set**: contains line segment between any two points in the set

$$\mathbf{x}^{(1)}, \mathbf{x}^{(2)} \in \mathcal{X},\ 0 \leq \alpha \leq 1 \implies \alpha\mathbf{x}^{(1)} + (1-\alpha)\mathbf{x}^{(2)} \in \mathcal{X}$$

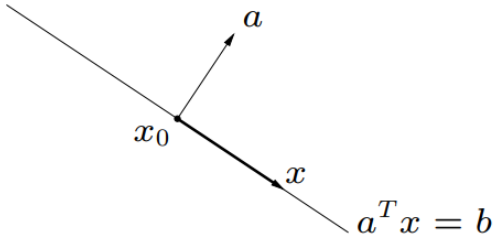
- Examples (one convex, two nonconvex sets)



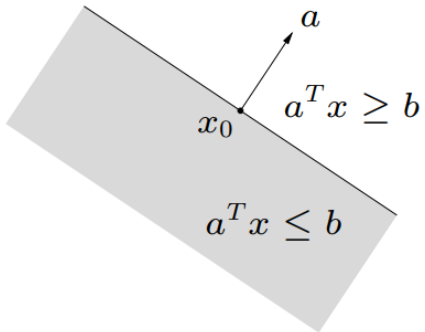
Hyperplanes and Halfspaces

- **Hyperplane**: set of the form $\{\mathbf{x}|\mathbf{a}^T\mathbf{x} = b\}$ $(\mathbf{a} \neq 0)$
  - **a** is the normal vector

超平面不一定是平面，其核心是边界。 平面中hyperplane是直线曲线。三维中hyperplane就是曲面了，以此类推（就好像逻辑回归不是回归是分类）



- **Halfspace**: set of the form $\{\mathbf{x}|\mathbf{a}^T\mathbf{x} \leq b\}$ $(\mathbf{a} \neq 0)$



- Hyperplanes and halfspaces are convex

Operations that Preserve Convexity

- Practical methods for establishing convexity of a set $\mathcal{X}$
  1. Apply definition

$$\mathbf{x}^{(1)}, \mathbf{x}^{(2)} \in \mathcal{X},\ 0 \leq \alpha \leq 1 \implies \alpha\mathbf{x}^{(1)} + (1-\alpha)\mathbf{x}^{(2)} \in \mathcal{X}$$

  2. Show that $\mathcal{X}$ is obtained from simple convex set (hyperplanes, halfspaces, etc.) by operations that preserve convexity
     - Intersection
     - Affine functions 仿射函数
     - ...

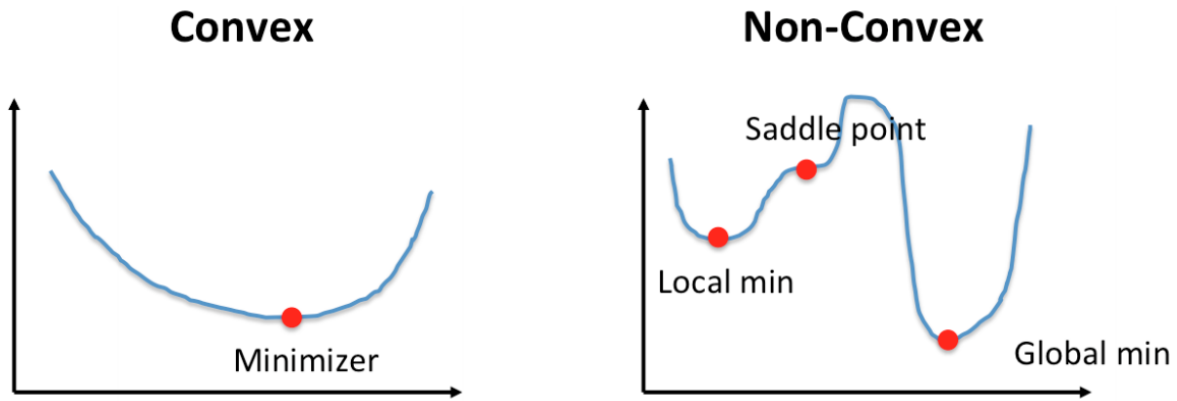
Convex Function

这一页应该是扩展了我们之前判断函数凹凸性的方法，引入了alpha ， dom(f)应该是domain，自变量取值范围的意思吧

- $f : \mathbb{R}^N \mapsto \mathbb{R}$ is convex if $\mathrm{dom}(f)$ is a convex set and

$$f(\alpha \mathbf{x}^{(1)} + (1-\alpha)\mathbf{x}^{(2)}) \leq \alpha f(\mathbf{x}^{(1)}) + (1-\alpha) f(\mathbf{x}^{(2)})$$

for all $\mathbf{x}^{(1)}, \mathbf{x}^{(2)} \in \mathrm{dom}(f)$, $0 \leq \alpha \leq 1$



- f is concave if $-f$ is convex

凹的

Examples on $\mathbb{R}$

- Convex:
  - Affine: $ax + b$ on $\mathbb{R}$, for any $a, b \in \mathbb{R}$
  - Exponential: e^{ax}, for any $a \in \mathbb{R}$
  - Powers: x^a on $\mathbb{R}_{++}$ for $a \geq 1$ or $a \leq 0$
  - Powers of absolute value: $|x|^p$ on $\mathbb{R}$, for $p \geq 1$
  - Negative entropy: $x \log x$ on $\mathbb{R}_{++}$

exponential是指数函数，
power应该是幂函数，

应该是逆熵

- Concave:
  - Affine: $ax + b$ on $\mathbb{R}$, for any $a, b \in \mathbb{R}$
  - Powers: x^a on $\mathbb{R}_{++}$ for $0 \leq a \leq 1$
  - Logarithm: $\log x$ on $\mathbb{R}_{++}$

Examples on $\mathbb{R}^N$ and $\mathbb{R}^{M\times N}$

- Examples on $\mathbb{R}^N$
  - Affine function: $\mathbf{a}^T\mathbf{x}+b$
  - Norms: $\|\mathbf{x}\|_p = (\sum_{j=1}^N |x_j|^p)^{1/p}$ for $p \geq 1$; $\|\mathbf{x}\|_\infty = \max_j |x_j|$

这个$\max_j$的j打错了？

- Examples on $\mathbb{R}^{M\times N}$ ($M \times N$ matrices)
  - Affine function:

$$f(\mathbf{X}) = \sum_{i=1}^M \sum_{j=1}^N A_{ij}X_{ij} + b = \mathrm{tr}(\mathbf{A}^T\mathbf{X}) + b$$

  - Spectral norm (maximum singular value):

光譜範數（最大奇異值）

$$f(\mathbf{X}) = \|\mathbf{X}\|_2 = \sigma_{\max}(\mathbf{X}) = (\lambda_{\max}(\mathbf{X}^T\mathbf{X}))^{1/2}$$

Example: Quadratic

- $f(x) = x^2$

- Proof of convexity:

$$
\begin{aligned}
(\alpha x + (1-\alpha)y)^2 &= \alpha^2 x^2 + 2\alpha(1-\alpha)xy + (1-\alpha)^2 y^2 \\
&= \alpha x^2 + (1-\alpha)y^2 - \alpha(1-\alpha)(x^2 - 2xy + y^2) \\
&\leq \alpha x^2 + (1-\alpha)y^2
\end{aligned}
$$

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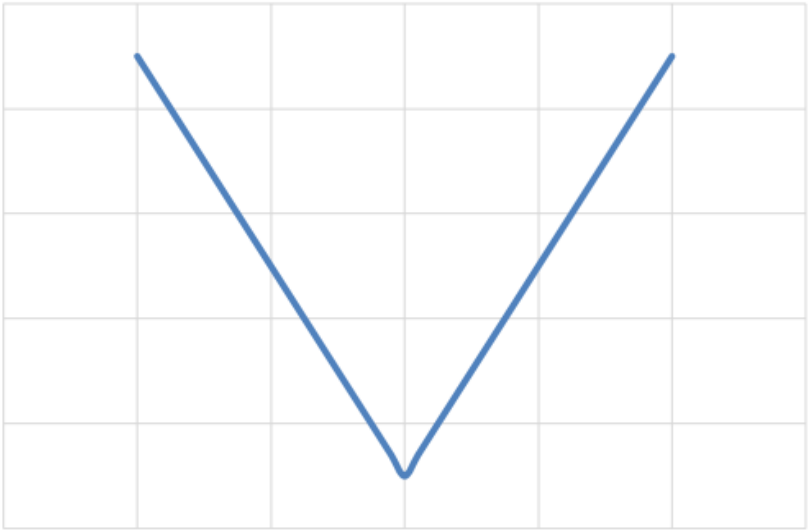
Example: Abs

- $f(x) = |x|$

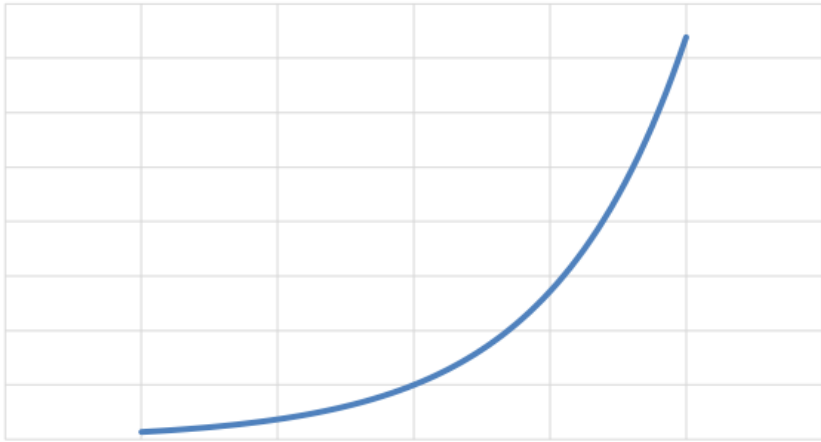


- Proof of convexity:

$$\begin{aligned} |\alpha x + (1-\alpha)y| &\leq |\alpha x| + |(1-\alpha)y| \\ &= \alpha|x| + (1-\alpha)|y| \end{aligned}$$

Example: Exponential

- $f(x) = e^x$



- Proof of convexity (assuming $x > y$):

$$e^{\alpha x+(1-\alpha)y} = e^y e^{\alpha(x-y)} = e^y \sum_{n=0}^{\infty} \frac{1}{n!}\alpha^n (x-y)^n$$ 泰勒

$$\leq e^y \left(1 + \alpha \sum_{n=1}^{\infty} \frac{1}{n!}(x-y)^n\right)$$

$$= e^y \left((1-\alpha) + \alpha e^{x-y}\right) = (1-\alpha)e^y + \alpha e^x$$

Properties of Convex Functions

- Any line segment we draw between two points lies above the curve
- Every local minimum is a **global** minimum
  - Why?
- This is what makes convex optimization easy
  - It suffices to find a local minimum because we know it will be global

足够

Properties of Convex Functions

- Non-negative combinations of convex functions are convex

$$h(\mathbf{x}) = af(\mathbf{x}) + bg(\mathbf{x})$$

- Affine scalings of convex functions are convex

$$h(\mathbf{x}) = f(\mathbf{A}\mathbf{x} + \mathbf{b})$$

- Pointwise maximum of convex functions are convex

$$h(\mathbf{x}) = \max\{f(\mathbf{x}), g(\mathbf{x})\}$$

- Compositions of convex functions are **NOT** generally convex
  - Neural nets are like this $h(\mathbf{x}) = f(g(\mathbf{x}))$

First-Order Condition

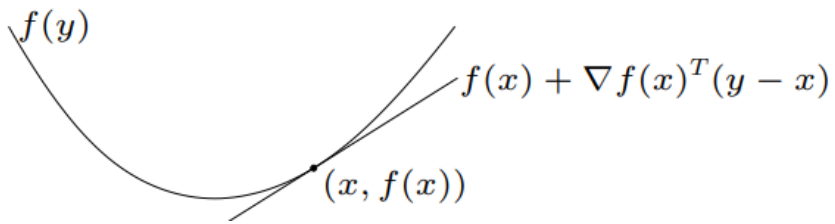
- f is **differentiable** if the gradient

$$\nabla f(\mathbf{x}) = \left[\frac{\partial f(\mathbf{x})}{\partial x_1}, \frac{\partial f(\mathbf{x})}{\partial x_2}, \ldots, \frac{\partial f(\mathbf{x})}{\partial x_N}\right]^T$$

  exists at each $\mathbf{x} \in \text{dom}(f)$

- **1st-order condition**: differentiable f with convex domain is convex iff

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^T(\mathbf{y} - \mathbf{x}), \quad \text{for all } \mathbf{x}, \mathbf{y} \in \text{dom}(f)$$



- First-order approximation of f is global underestimator

Second-Order Condition

- f is **twice differentiable** if the Hessian $\nabla^2 f(\mathbf{x}) \in \mathbb{S}^N$

$$\nabla^2 f(\mathbf{x})_{ij} = \frac{\partial^2 f(\mathbf{x})}{\partial x_i \partial x_j}$$

  exists at each $\mathbf{x} \in \text{dom}(f)$

- **2nd-order condition**: twice differentiable f with convex domain is convex iff

$$\nabla^2 f(\mathbf{x}) \succeq 0$$

  - This means that the Hessian matrix is positive semidefinite

$$\mathbf{A} \succeq 0 \iff \forall \mathbf{x}, \mathbf{x}^T \mathbf{A} \mathbf{x} \geq 0$$

Example: Quadratic

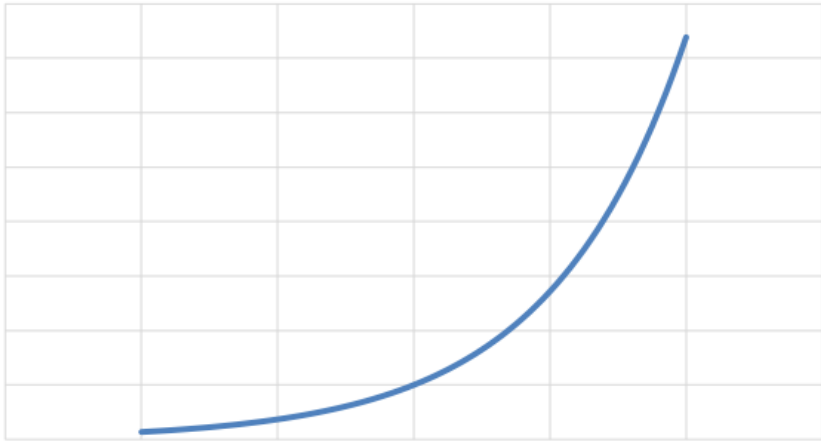
- $f(x) = x^2$

  - Proof of convexity:

$$f''(x) = 2 \geq 0$$

Example: Exponential

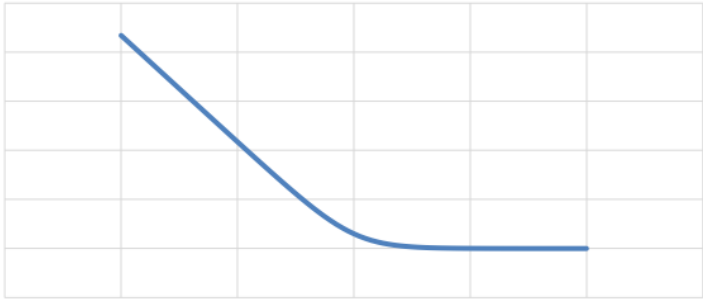
- $f(x) = e^x$



  - Proof of convexity:

$$f''(x) = e^x \geq 0$$

Example: Logistic Loss



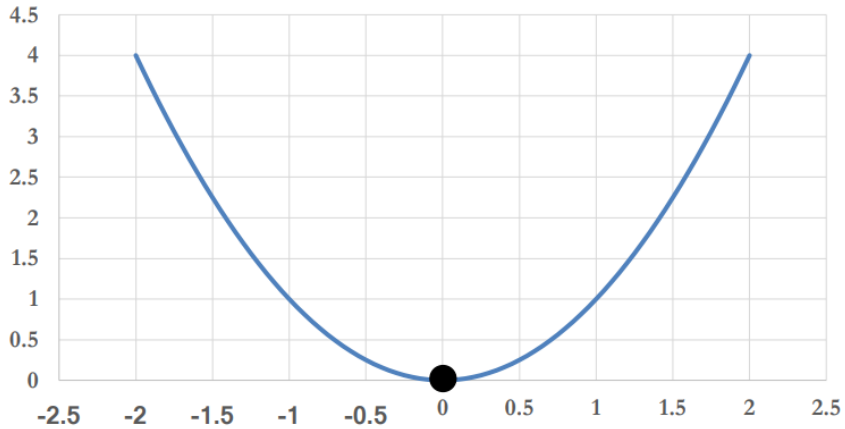
- $f(x) = \log(1 + e^{-x})$
  - Proof of convexity:

$$f'(x) = \frac{-e^{-x}}{1 + e^{-x}} = -\frac{1}{1 + e^{x}}$$

$$f''(x) = \frac{1}{(1 + e^{x})(1 + e^{-x})} \geq 0$$

Parameter Estimation

- Optimization in machine learning
  - Goal is to optimize a loss function defined in a machine learning problem for parameter estimation
- Convex optimization in machine learning
  - Goal is to minimize a convex loss function with respect to parameters
  - Example: $\ell(\theta) = \theta^2$



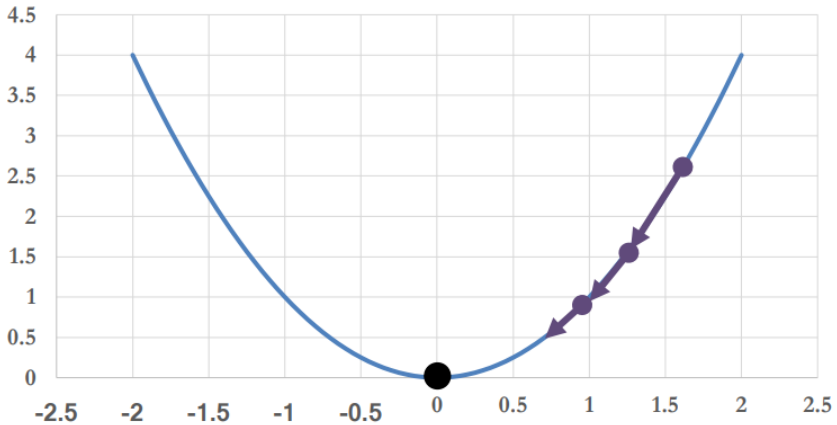
Gradient Descent

- Gradient descent (GD) uses the following update formula

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \nabla \ell(\boldsymbol{\theta})$$

  - α is the learning rate
  - $\nabla \ell(\boldsymbol{\theta})$ is the gradient of $\ell(\boldsymbol{\theta})$ evaluated at $\boldsymbol{\theta}$

- Example: $\ell(\theta) = \theta^2$, $\nabla \ell(\theta) = 2\theta$, and $\alpha = 0.125$



Gradient Descent

- GD first chooses an initial point $\boldsymbol{\theta}^{(0)}$ and repeats:

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \alpha \nabla \ell(\mathcal{D}; \boldsymbol{\theta}^{(t)}) = \boldsymbol{\theta}^{(t)} - \alpha \frac{1}{M} \sum_{i=1}^{M} \nabla \ell(\mathbf{x}^{(i)}, y^{(i)}; \boldsymbol{\theta}^{(t)})$$

- How to stop?
  - $\|\boldsymbol{\theta}^{(t+1)} - \boldsymbol{\theta}^{(t)}\|_2 \leq \epsilon$
  - $\|\nabla \ell(\mathcal{D}; \boldsymbol{\theta}^{(t)})\|_2 \leq \epsilon$
    - $\|\boldsymbol{\theta}\|_2 = \sqrt{\sum_j |\theta_j|^2}$ is the ℓ_2-norm of $\boldsymbol{\theta}$
    - ϵ is a small positive constant, *e.g.*, 10^{-6}

Gradient Descent

- A negative gradient step can decrease the loss function

  Proof. Let $\boldsymbol{\theta}^{(0)}$ be any initial point. Using the first-order Taylor expansion for the next point $\boldsymbol{\theta}^{(1)} = \boldsymbol{\theta}^{(0)} - \alpha \nabla \ell(\boldsymbol{\theta}^{(0)})$, we have

$$\begin{aligned}
\ell(\boldsymbol{\theta}^{(1)}) &= \ell(\boldsymbol{\theta}^{(0)}) + \nabla \ell(\boldsymbol{\theta}^{(0)})^T (\boldsymbol{\theta}^{(1)} - \boldsymbol{\theta}^{(0)}) \\
&= \ell(\boldsymbol{\theta}^{(0)}) + \nabla \ell(\boldsymbol{\theta}^{(0)})^T (-\alpha \nabla \ell(\boldsymbol{\theta}^{(0)})) \\
&= \ell(\boldsymbol{\theta}^{(0)}) - \alpha \|\nabla \ell(\boldsymbol{\theta}^{(0)})\|_2^2
\end{aligned}$$

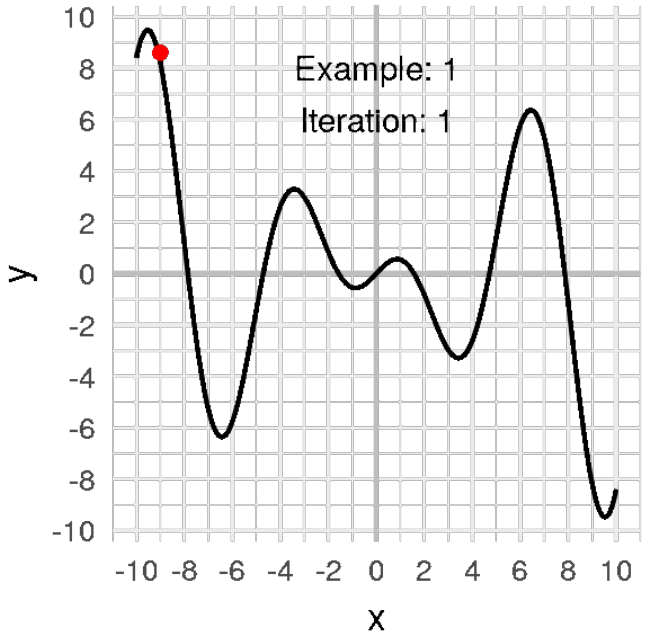
  Hence, if $\nabla \ell(\boldsymbol{\theta}^{(0)}) \neq 0$ and α is sufficiently small, we have

$$\ell(\boldsymbol{\theta}^{(1)}) - \ell(\boldsymbol{\theta}^{(0)}) = -\alpha \|\nabla \ell(\boldsymbol{\theta}^{(0)})\|_2^2 < 0$$

  For sufficiently small α, $\boldsymbol{\theta}^{(1)}$ is an improvement over $\boldsymbol{\theta}^{(0)}$

Gradient Descent

- Initial point matters
  - Consider $y = f(x) = x\cos(x)$



  - The final convergence point depends a lot on the initial point
  - To improve optimization, run GD multiple times with different initializations, and keep the best minimum of all times (may take a long time to run)

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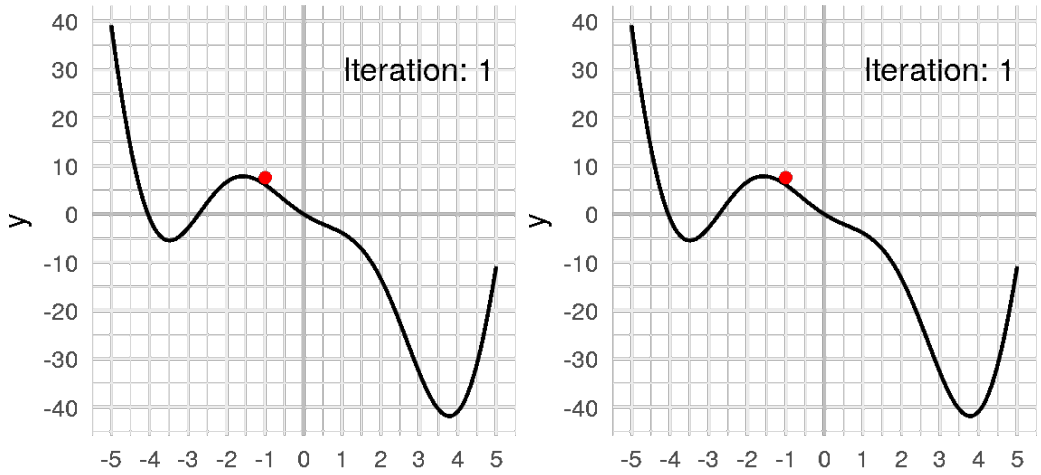
Gradient Descent

- Learning rate matters
  - If α is too big, GD moves more quickly with a high risk that the algorithm will never converge
  - If α is too small, GD moves slowly...so slowly that you might just lose patience and never reach the minimum
  - Consider $y = f(x) = 2x^2 \cos(x) - 5x$



  - Unfortunately, no magic bullet exists to find the perfect learning rate, and you have to test several values and pick the best

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Stochastic Gradient Descent

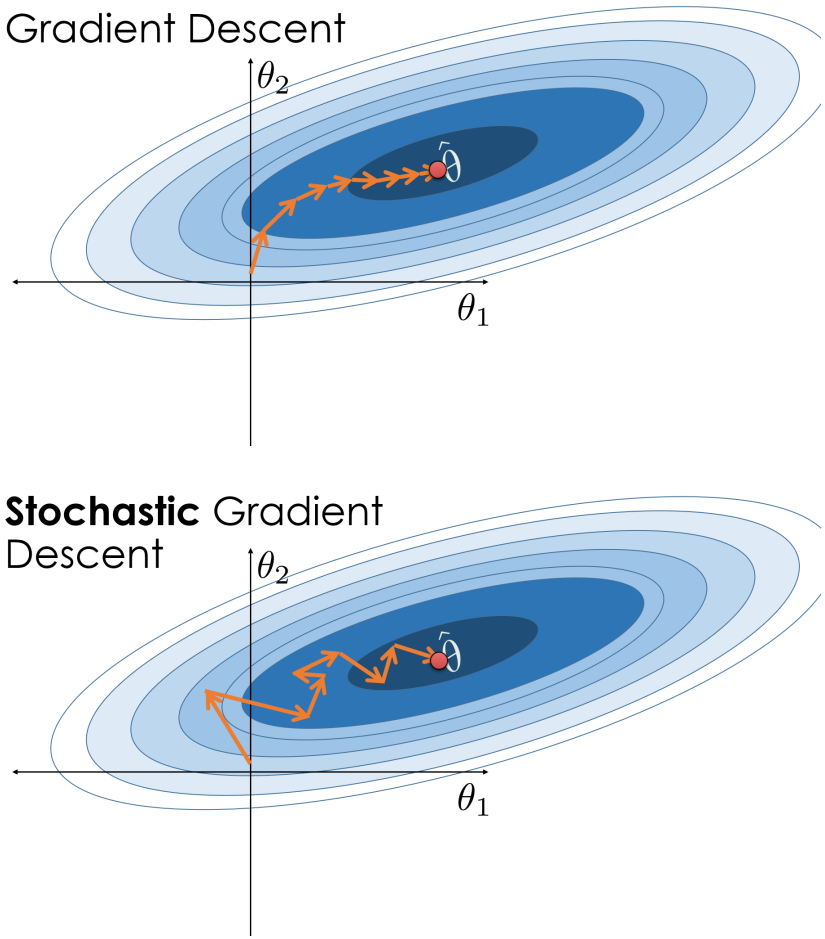
- The computational cost for GD at each iteration is $\mathcal{O}(M)$, which grows linearly with M
  - It is prohibitive to scale up to huge datasets
- Stochastic gradient descent (SGD)
  - Reduces the computational cost at each iteration to $\mathcal{O}(1)$
    - At t-th iteration, randomly sample a single training example and compute the gradient to update $\boldsymbol{\theta}^{(t)}$

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \alpha \nabla \ell(\mathbf{x}^{(i)}, y^{(i)}; \boldsymbol{\theta}^{(t)})$$

  - In expectation, SGD is just GD

$$\mathbb{E}[\nabla \ell(\mathbf{x}, y; \boldsymbol{\theta})] = \frac{1}{M} \sum_{i=1}^{M} \nabla \ell(\mathbf{x}^{(i)}, y^{(i)}; \boldsymbol{\theta}) = \nabla \ell(\mathcal{D}; \boldsymbol{\theta})$$

Stochastic Gradient Descent



Stochastic Gradient Descent

- **Advantages**:
  - It is easy to fit into memory and computationally fast due to a single training sample being processed at each iteration
  - The steps have oscillations, which may help the algorithm get out of bad local minima
- **Disadvantages**:
  - The steps are noisy. The objective does not always decrease for each step and it may take longer to achieve convergence
  - It loses the advantage of vectorized operations as it deals with only a single example at a time

Mini-Batch Gradient Descent: A Compromise

- Unlike SGD, mini-batch gradient descent randomly samples a small subset of training data $\mathcal{B} \subset \mathcal{D}$ at t-th iteration, and compute the gradient to update $\boldsymbol{\theta}^{(t)}$

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \alpha \nabla \ell(\mathcal{B}; \boldsymbol{\theta}^{(t)}) = \boldsymbol{\theta}^{(t)} - \alpha \frac{1}{|\mathcal{B}|} \sum_{(\mathbf{x},y)\in\mathcal{B}} \nabla \ell(\mathbf{x}, y; \boldsymbol{\theta}^{(t)})$$

- Mini-batch gradient descent and its variants are extremely popular and extensively used in deep learning

Summary

- Convex optimization
  - Convex set:
    - $\mathbf{x}^{(1)}, \mathbf{x}^{(2)} \in \mathcal{X}, 0 \leq \alpha \leq 1 \implies \alpha\mathbf{x}^{(1)} + (1-\alpha)\mathbf{x}^{(2)} \in \mathcal{X}$
  - Convex function:
    - $\text{dom}(f)$ is convex
    - $f(\alpha\mathbf{x} + (1-\alpha)\mathbf{y}) \leq \alpha f(\mathbf{x}) + (1-\alpha)f(\mathbf{y})$
  - Establish convexity
    - By definition
    - First-order condition: $f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^T(\mathbf{y}-\mathbf{x})$
    - Second-order condition: $\nabla^2 f(\mathbf{x}) \succeq 0$
- Numerical optimization methods
  - GD - guarantee to decrease loss; not scalable to large datasets
  - SGD - super fast to compute with noisy gradients
  - Mini-batch GD - a compromise between GD and SGD; the de facto method in deep learning