DSCI 565: OPTIMIZATION ALGORITHMS

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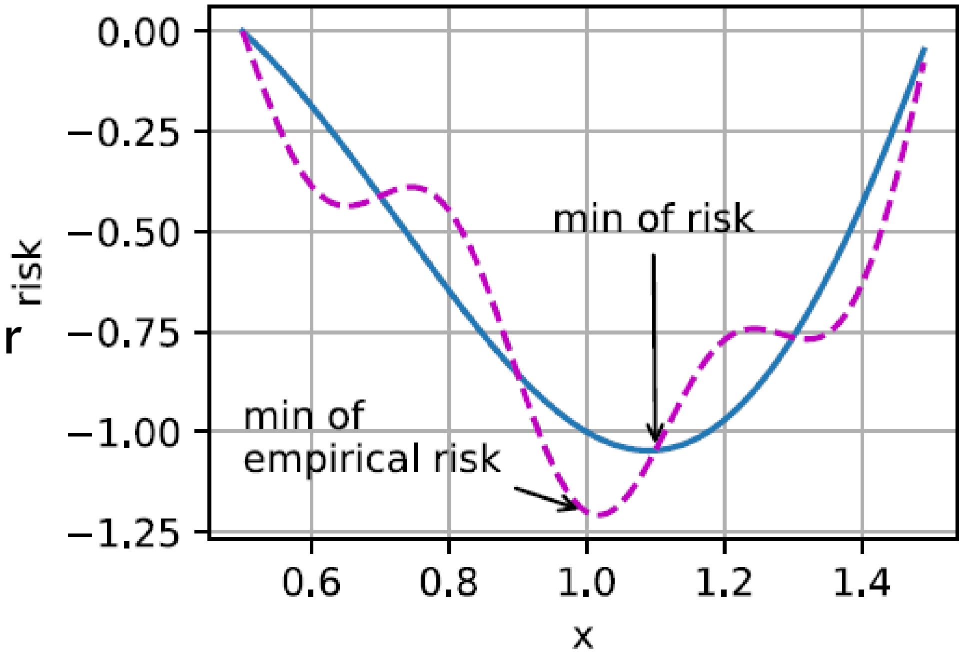
Lecture 20: 2025-10-20

Optimization and Deep Learning

- Goal of optimization:
  - Given objective function $f(x)$ find x that minimizes the objective function
- Goal of deep learning:
  - Finding a suitable model, given a finite amount of data

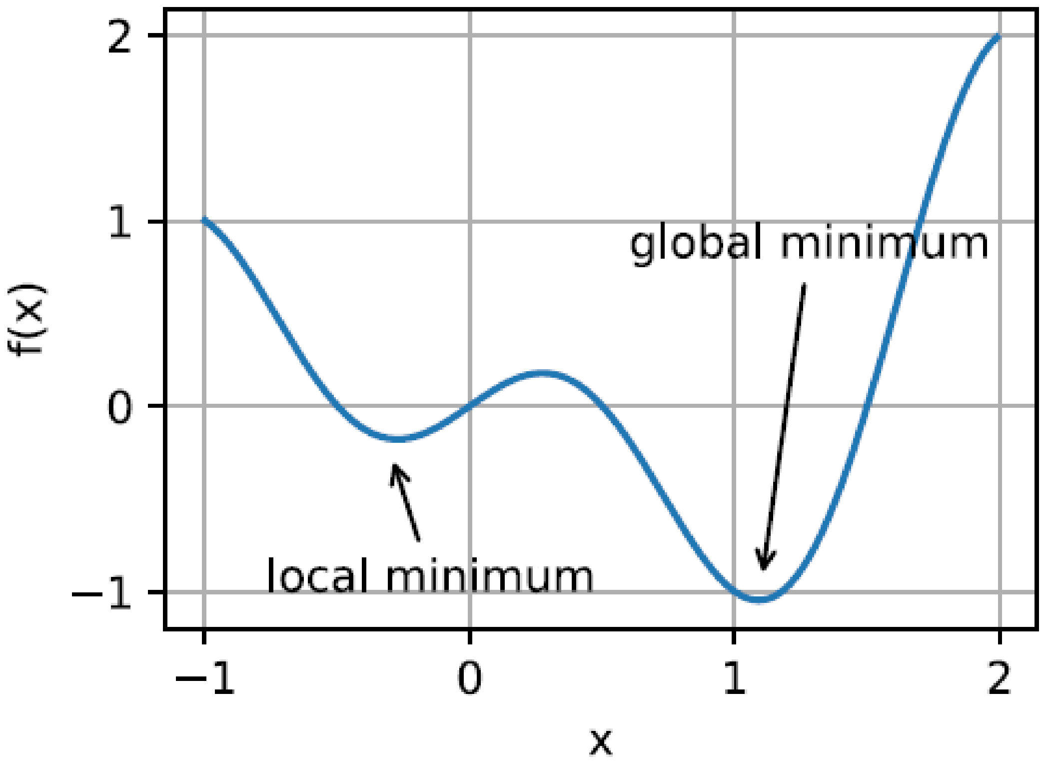
- These two goals are not the same
  - If we set objective function to be the loss function and find optimum parameter x^*, then we are minimizing the training error
  - For deep learning we care about generalization error
  - We want select the right model that neither overfits the data, nor underfits the data



Optimization Challenges in Deep Learning

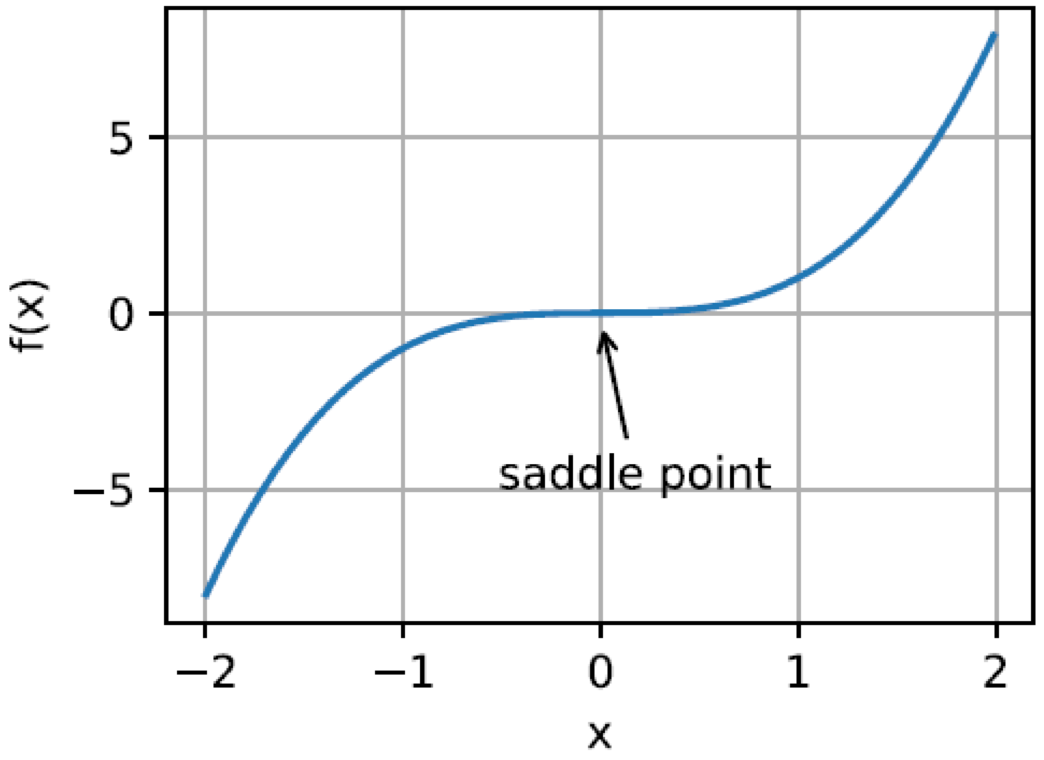
- In deep learning, the objective functions are complicated
- They do not have analytical solutions
- Optimization problems include
  - Local minima
  - Saddle points
  - Vanishing gradients

Local Minima



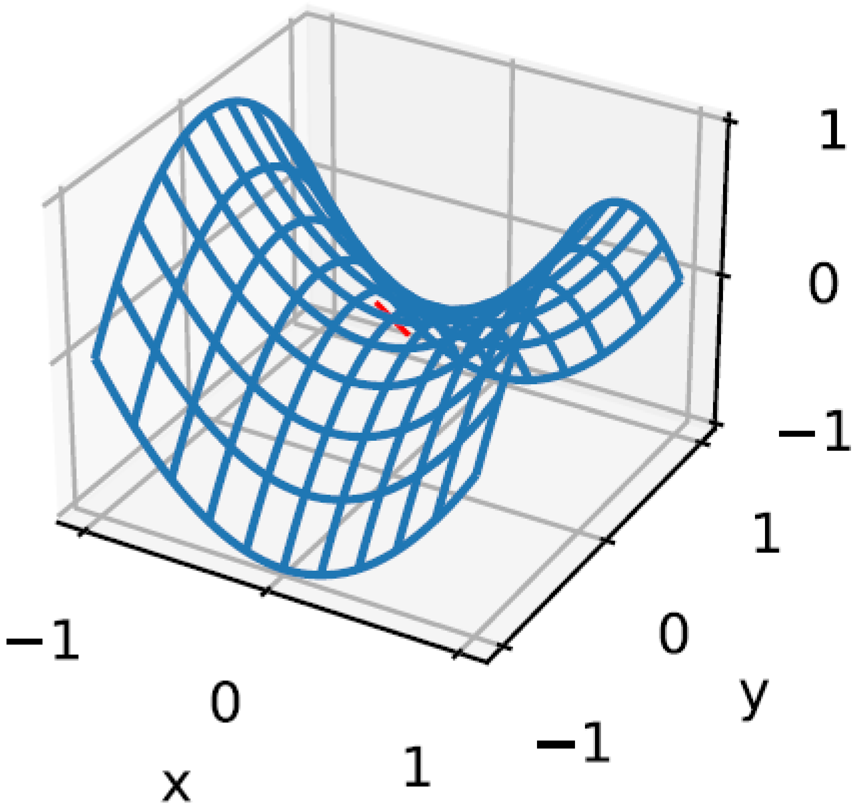
- For any objective function $f(x)$, x is a local minima if $f(x)$ is smaller than $f(x+\epsilon)$ for some ϵ
- At a local minima the gradient is zero
- For deep learning objective functions, there are many local minima

Saddle Points



- At a saddle point the gradient vanishes, but it is neither a minima nor a maxima
- Simply finding locations where the gradients vanish is not sufficient
- Consider the function $f(x) = x^3$

Saddle Points in Higher Dimensions



- In higher dimensions, a saddle point look like
  - A minima in one dimension
  - A maxima in another dimension
- Consider $f(x, y) = x^2 - y^2$
- Use Hessian matrix to determine type of critical point

Hessian Matrix

- For a function $f\colon \mathbb{R}^n \to \mathbb{R}$, the Hessian matrix $\mathbf{H}$ of f is all is second order partial derivatives:

$$\mathbf{H} \equiv \begin{bmatrix} \frac{\partial f}{\partial x_1^2} & \frac{\partial f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial f}{\partial x_1 \partial x_n} \\ \frac{\partial f}{\partial x_2 \partial x_1} & \frac{\partial f}{\partial x_2^2} & \cdots & \frac{\partial f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f}{\partial x_n \partial x_1} & \frac{\partial f}{\partial x_n \partial x_2} & \cdots & \frac{\partial f}{\partial x_n^2} \end{bmatrix}$$

Hessian Matrix Interpretation

- At a critical point of function f, i.e., gradient of f is zero
  - When the eigenvalues of the function's Hessian matrix are all positive, we have a local minimum for the function
  - When the eigenvalues of the function's Hessian matrix are all negative, we have a local maximum for the function
  - When the eigenvalues of the function's Hessian matrix are negative and positive, we have a saddle point for the function

Hessian Matrix Example

- For $f(x,y) = \frac{1}{2}(x^2 - y^2)$

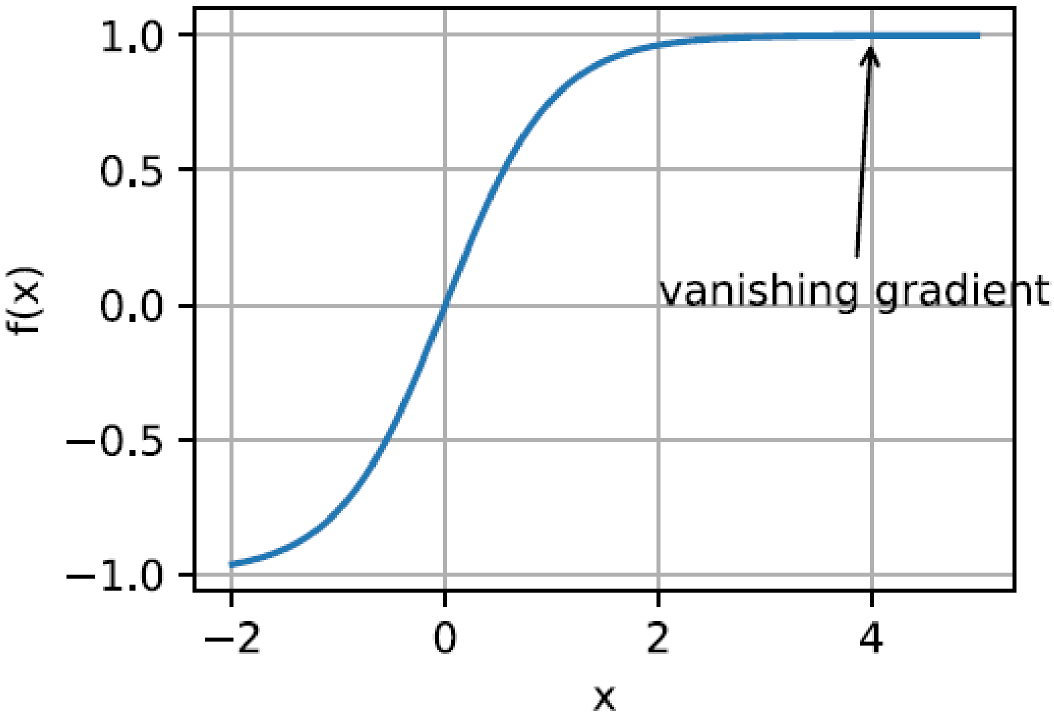
$$H = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

- The eigenvalues of its Hessian matrix is 1 and -1:

$$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 1 \begin{bmatrix} 1 \\ 0 \end{bmatrix} \text{ and } \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = -1 \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- Critical point $(0,0)$ is a saddle point

Vanishing Gradients



- At these points, the gradients become close to zero
- Optimization gets stuck and causes the learning to be slow

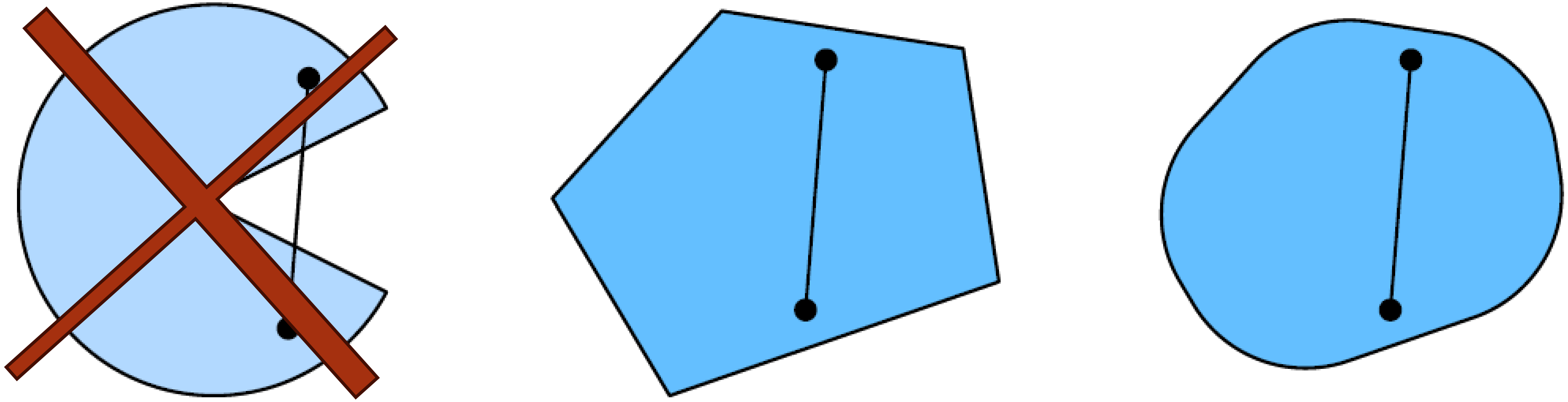
Convexity

- Optimization problems that obey convexity properties are easier to analyze and solve
- If an algorithm performs poorly for convex problems, then it is unlikely to do well for nonconvex problems
- Deep learning optimization problems are typically nonconvex, but near local optima they look like convex problems

Convex Sets

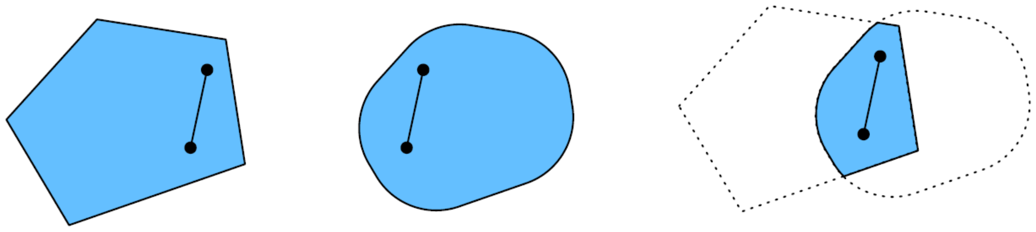
- A set $\mathcal{X}$ in a vector space is convex if for any $a, b \in \mathcal{X}$ the line segment connecting a and b is also in $\mathcal{X}$

$$\lambda a + (1-\lambda) b \in \mathcal{X}, \qquad \text{for } \lambda \in [0,1]$$

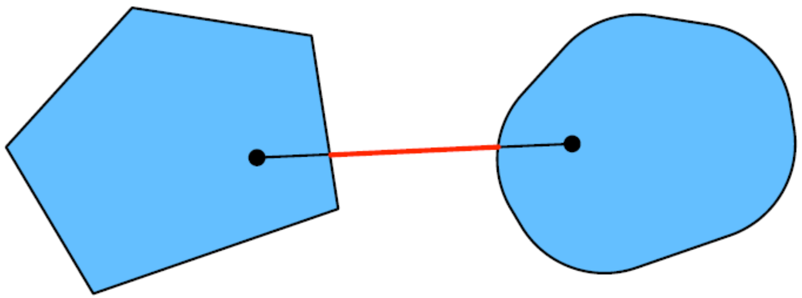


Convex Sets

- Intersection of convex sets is convex



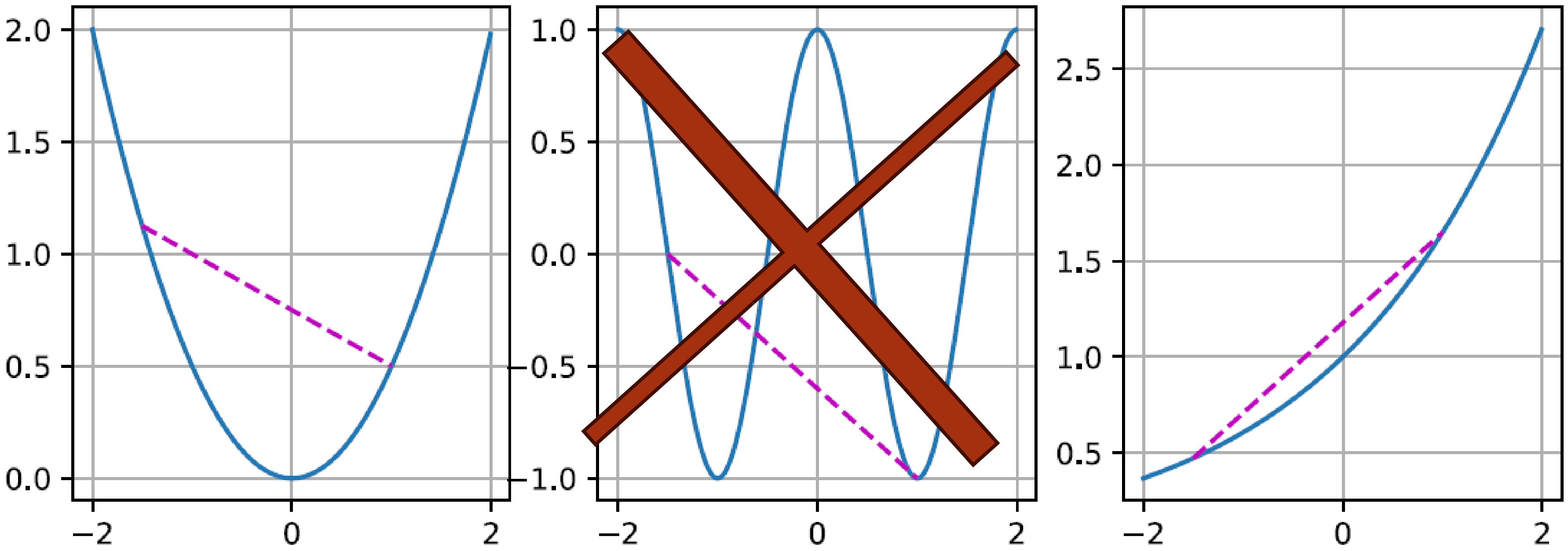
- Union of convex sets need not be convex



Convex Functions

- Given a convex set $\mathcal{X}$, a function $\mathrm{f}: \mathcal{X} \rightarrow \mathbb{R}$ is convex if for all $\mathrm{x}, \mathrm{x}' \in \mathcal{X}$ and for all $\lambda \in [0,1]$

$$\lambda f(x) + (1-\lambda) f(x') \geq f(\lambda x + (1-\lambda) x')$$



Convex functions

- Examples of convex functions
  - $f(\mathbf{x}) = \mathbf{a}^T\mathbf{x} + \mathbf{b}$
  - $f(\mathbf{x}) = \mathbf{x}^T\mathbf{x}$
  - $f(\mathbf{x}) = \|\mathbf{x}\|_1$

Jensen's Inequality

- For convex functions, Jensen's inequality states

$$\sum_i \alpha_i f(x_i) \geq f\left(\sum_i \alpha_i x_i\right) \text{ and } E_X[f(X)] \geq f\left(E_X[X]\right),$$

- Where $\alpha_i \geq 0$ such that $\sum_i \alpha_i = 1$, and X is random variable
- Jensen's inequality provides a lower bound, which is usually simpler than original expression

Properties of Convex Functions

- Local minima are global minima
- Below sets of convex functions are convex
- A function is convex if its Hessian matrix H is semi-positive definite

Convexity: Local Minima is Global Minima

- Let f be a convex function defined on a convex set $\mathcal{X}$
  If $\mathrm{x}^* \in \mathcal{X}$ is local minima, then x^* is a global minima
- Proof by contradiction
  - Suppose there exists $\mathrm{x}' \in \mathcal{X}$, where $f(x') < f(x^*)$
  - If x^* is local minima, then there is a neighbor near x^*, $0 < \left|x - x^*\right| \leq P$, such that $\mathrm{f(x^*)} \ < f(x)$
  - We can find a λ such that $\lambda x^* + (1-\lambda)x'$ is in this neighborhood
  - But this contradicts that x^* is a local minima

$$
\begin{aligned}
f(\lambda x^* + (1-\lambda)x') &\leq \lambda f(x^*) + (1-\lambda) f(x') \\
&< \lambda f(x^*) + (1-\lambda) f(x^*) \\
&= f(x^*),
\end{aligned}
$$

Below Sets of Convex Functions are Convex

- We can define convex sets using *below sets* of convex functions
- Given a convex function f defined on a convex set $\mathcal{X}$, any below set

$$\mathcal{S}_b \equiv \{x | x \in \mathcal{X} \text{ and } f(x) \leq b\}$$

  is convex.
- Proof:
  - For any $x, x' \in \mathcal{S}_b$ we need to show $\lambda x + (1-\lambda)x' \in \mathcal{S}_b$ for $\lambda \in [0,1]$
  - But $f(\lambda x + (1-\lambda)x') \leq \lambda f(x) + (1-\lambda)f(x') \leq b$
    - By definition of convexity and $f(x) \leq b$ and $f(x') \leq b$

Convexity and Second Derivative

- A function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is convex if and only if the Hessian H of f is positive semi-definite

- A matrix H is positive semi-definite if for all $\mathbf{x} \in \mathbb{R}^n$

$$\mathbf{x}^{\mathrm{T}}\mathrm{H}\mathbf{x} \geq 0$$

- Proof is in Section 12.2.2

Constrained Optimization

- Constrained optimization problems

$$\min_{\boldsymbol{x}} f(\boldsymbol{x})$$
$$\text{subject to } c_i(\boldsymbol{x}) \leq 0 \text{ for all } i \in \{1, \dots, n\}$$

where f is the objective function and c_i are constraint functions

- Convex optimization: If f is convex and c_i define convex sets then there are polynomial algorithms to find optimal $\boldsymbol{x}$
- Example convex constraints: $c_1(\boldsymbol{x}) = \|\boldsymbol{x}\|_2 - 1$ or $c_2(x) = \boldsymbol{v}^T\boldsymbol{x} + b$
- In general optimization problems are NP-hard

One-Dimensional Gradient Descent

- Let $f: \mathbb{R} \to \mathbb{R}$ be continuously differentiable, using Taylor expansion

$$f(x+\epsilon) = f(x) + \epsilon f'(x) + \mathcal{O}(\epsilon^2)$$

- If we take a "small" step, $\eta > 0$, in the negative gradient direction

$$f(x - \eta f'(x)) = f(x) - \eta f'^2(x) + \mathcal{O}(\eta^2 f'^2(x))$$

- If the derivative $f'(x) \neq 0$, then $\eta f'^2(x) > 0$. For small enough η

$$f(x - \eta f'(x)) \lessapprox f(x)$$

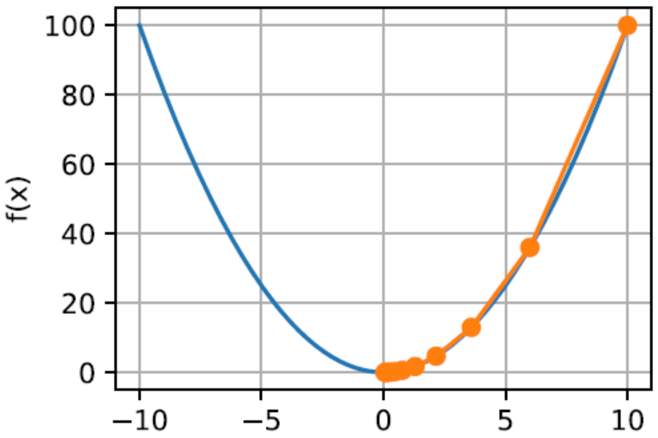
- Gradient descent iterate using

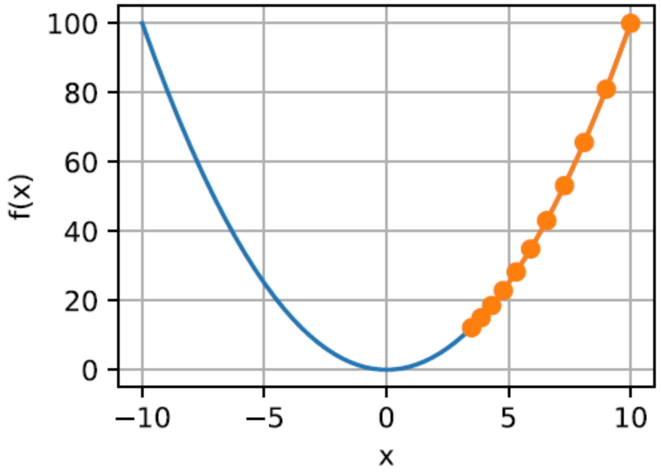
$$x \leftarrow x - \eta f'(x)$$

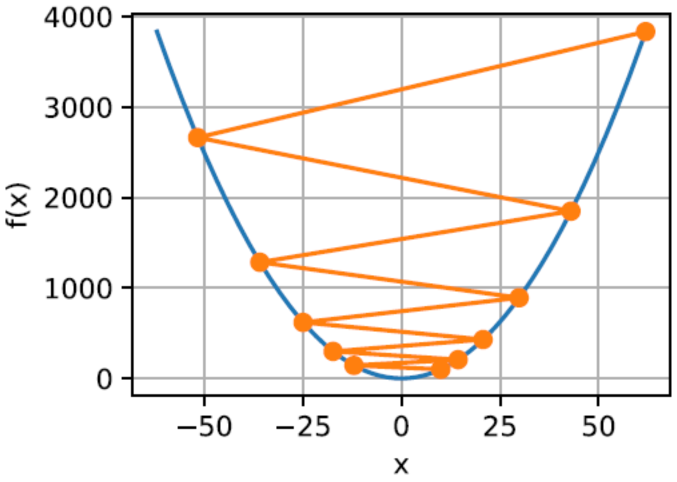
Learning Rate

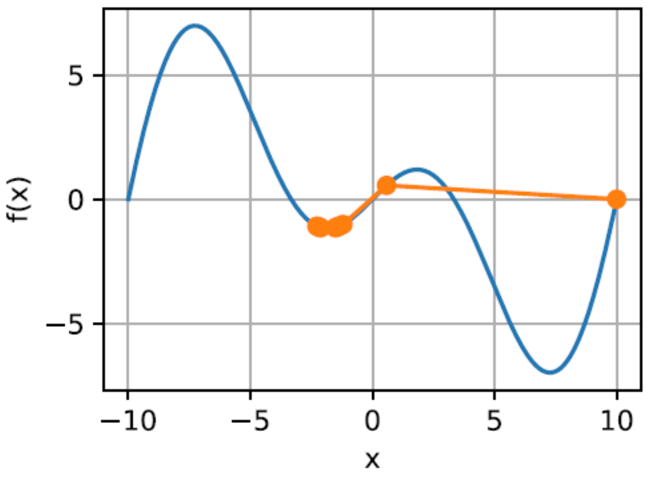
- The learning rate η controls the size of the step
- If η is too small, then convergence to local minima is slow
- If η is too large, then higher order terms of the Taylor expansion $\mathcal{O}(\eta^2 f'^2(x))$ may become significant
  - The gradient descent may overshoot and diverge

Learning Rate and Convergence









Multivariate Gradient Descent

- Let $f: \mathbb{R}^d \to \mathbb{R}$, then the gradient of f is

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

- The Taylor expansion is

$$f(\mathbf{x} + \boldsymbol{\epsilon}) = f(\mathbf{x}) + \boldsymbol{\epsilon}^T \nabla f(\mathbf{x}) + \mathcal{O}(||\boldsymbol{\epsilon}||^2)$$

- Gradient descent iterate using

$$\mathbf{x} \leftarrow \mathbf{x} - \eta \nabla f(\mathbf{x})$$

Newton's Method

- For function $f\colon \mathbb{R}^d \to \mathbb{R}$, we add another term to the Taylor expansion

$$f(\mathbf{x}+\boldsymbol{\epsilon}) = f(\mathbf{x}) + \boldsymbol{\epsilon}^T \nabla f(\mathbf{x}) + \frac{1}{2}\boldsymbol{\epsilon}^T \nabla^2 f(\mathbf{x}) + \mathcal{O}(\|\boldsymbol{\epsilon}\|^3)$$

- Where Hessian $\mathbf{H} \equiv \nabla^2 f(\mathbf{x})$
- Take derivative with respect to $\boldsymbol{\epsilon}$, then $\nabla f(\mathbf{x}) + \mathbf{H}\boldsymbol{\epsilon} = 0$

$$\boldsymbol{\epsilon} = -\mathbf{H}^{-1}\nabla f(\mathbf{x})$$

- For $f(x) = \frac{1}{2}x^2$, gradient is $\nabla f(x) = x$ and $H = 1$
  - For any x, $\epsilon = -\frac{f'}{f''} = -x$
  - Only need one step to reach the global minimum

Notebook

- chapter_optimization/gd.ipynb

Newton's Method Convergence

- If we are sufficiently close to the minimum, then the error decreases quadratically with each iteration
- Let $x^{(k)}$ be the value of x at the k^{th} iteration, and let error $e^{(k)} \equiv x^{(k)} - x^*$, where x^* is the minimum, then

$$\left| e^{(k+1)} \right| \leq c\left(e^{(k)}\right)^2$$

- Where $\frac{\left| f'''\left(\xi^{(k)}\right) \right|}{2f''\left(x^{(k)}\right)} \leq c$, $\xi^{(k)} \in \left[x^{(k)} - e^{(k)}, x^{(k)}\right]$

Preconditioning

- Storing the full Hessian is very expensive, especially for deep learning
- One workaround is to only compute the diagonal of the Hessian

$$\mathbf{x} \leftarrow \mathbf{x} - \eta \mathrm{diag}(\mathbf{H})^{-1} \nabla f(\mathbf{x})$$

- This is called preconditioning
- Effectively preconditioning selects a different learning rate for each variable
- For example, consider if one variable is in millimeters and another in meters

Gradient Descent with Line Search

- Instead of fixing the learning rate η, at each step find the best rate by performing a binary search on η that minimized

$$f(\mathbf{x} - \eta \nabla f(\mathbf{x}))$$

- This approach has good convergence
- But it is very expensive for gradient descent, since each step of binary search requires evaluating the entire dataset

Stochastic Gradient Descent

- Let $f_i(\boldsymbol{x})$ be the loss with respect to training example $i \in [1, n]$ and $\boldsymbol{x}$ is the parameter vector
- The objective function and its gradient are:

$$f(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{n} f_i(\mathbf{x}) \qquad \nabla f(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(\mathbf{x})$$

- Stochastic gradient update:

$$\mathbf{x} \leftarrow \mathbf{x} - \eta \nabla f_i(\mathbf{x}).$$

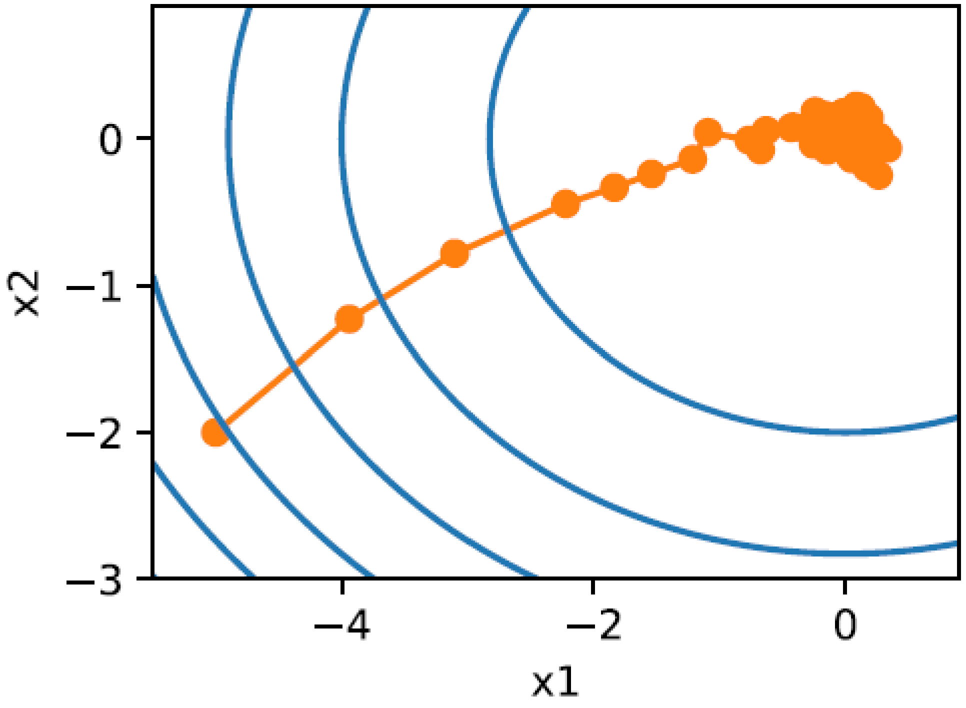
Stochastic Gradient Descent

- On average, $\nabla f_i(x)$ is a good estimate of the gradient

$$\mathbb{E}_i \nabla f_i(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(\mathbf{x}) = \nabla f(\mathbf{x}).$$

- But it has too much variance

- See notebook
  - chapter_optimization/sgd.ipynb
  - Tend to wander, especially near optima



Dynamic Learning Rate for Stochastic Gradient Descent

- Adjust learning rate $\eta(t)$

$$
\begin{aligned}
\eta(t) &= \eta_i \text{ if } t_i \leq t \leq t_{i+1} && \text{piecewise constant} \\
\eta(t) &= \eta_0 \cdot e^{-\lambda t} && \text{exponential decay} \\
\eta(t) &= \eta_0 \cdot (\beta t + 1)^{-\alpha} && \text{polynomial decay}
\end{aligned}
$$

- Piecewise constant drop rate when progress stalls
  - Popular choice for deep learning
- Exponential decay maybe to drastic
- For polynomial decay, $\alpha = 0.5$ is a popular choice

Minibatch Stochastic Gradient Descent

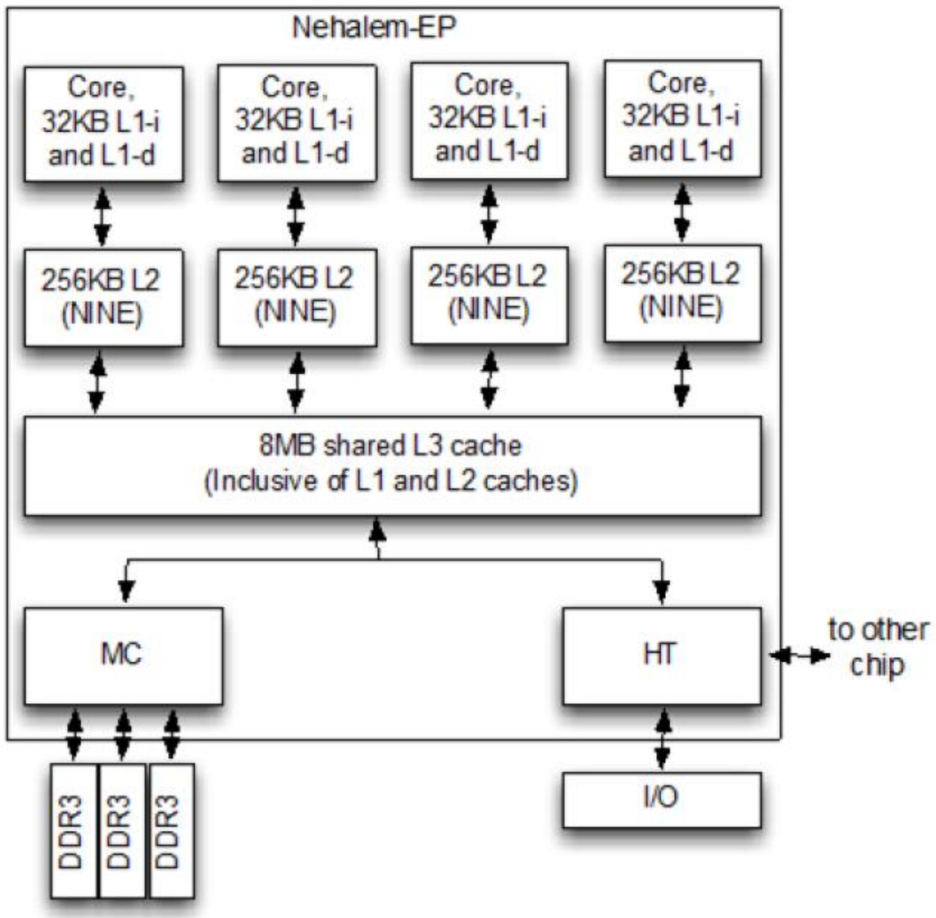
- Instead of training one example at a time, train in small batches of examples of size b
- If we draw batches uniformly at random from training set, then
  - The expectation of the gradient is unchanged
  - The variance is reduced by a factor of $b^{-\frac{1}{2}}$
- In practice choose batch size that fits into GPU memory

Memory Bottleneck

- CPUs and GPUs can process faster than memory can deliver the data
- Using vectorization (Single Instruction Multiple Data, SIMD), 2GHz CPU with 16 cores can process $2 * 10^9 * 16 * 32 = 10^{12} = 1000$ GB/s
- Main memory of a midrange server can only deliver 100 GB/s
- With just main memory CPU is idle 90% of the time
- GPUs have many more cores

Cache Hierarchy

- Cache hierarchy provides multiple levels of memory stores, with varying access speed and size
- Level-one (L1) cache is fast but small
- L2 cache is slower and larger
- L3 cache is even slower and larger



https://en.wikipedia.org/wiki/Cache_hierarchy

Notebook

- chapter_optimization/minibatch-sgd.ipynb
  - Vectorization and caches
  - https://en.wikipedia.org/wiki/Cache_hierarchy

Momentum

- Instead of using $\mathbf{g}_{t,t-1}$, the gradient of the minibatch at time t, use a leaky average (aka exponentially weighted average, aka exponential moving average) of the past gradients
- Let $\mathbf{v}_t$ be the velocity, $\mathbf{v}_t = \beta\mathbf{v}_{t-1} + \mathbf{g}_{t,t-1}$

$$\mathbf{v}_t = \beta^2\mathbf{v}_{t-2} + \beta\mathbf{g}_{t-1,t-2} + \mathbf{g}_{t,t-1} = \ldots, = \sum_{\tau=0}^{t-1}\beta^\tau\mathbf{g}_{t-\tau,t-\tau-1}.$$

- Up

$$\mathbf{x}_t \leftarrow \mathbf{x}_{t-1} - \eta_t\mathbf{v}_t.$$

- Advan
  - Reduction in variance beyond a single batch
  - “Rolling down hill”
  - Helps with ill-conditioned problems

Ill-Conditioned Problem

- For $f(x, y) = 0.1x^2 + 2y^2$, the Hessian matrix is

$$H = \begin{bmatrix} 0.2 & 0 \\ 0 & 4 \end{bmatrix}$$

- The eigenvalues of its Hessian matrix is 0.2 and 4:

$$\begin{bmatrix} 0.2 & 0 \\ 0 & 4 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 0.2 \begin{bmatrix} 1 \\ 0 \end{bmatrix} \text{ and } \begin{bmatrix} 0.2 & 0 \\ 0 & 4 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 4 \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- The condition number is $\frac{4}{0.2} = 20$
- Gradient much larger direction y than direction x
- Larger number implies ill-conditioned

Notebook

- See chapter_optimization/momentum.ipynb