EE 628 Deep Learning Fall 2019

Lecture 5

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STEVENS INSTITUTE of TECHNOLOGY
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Overview

- Last lecture we covered
    - Multilayer Perceptron
    - Overfitting/underfitting
- Today, we will cover
    - Backpropagation
    - Optimization Algorithms

Forward Propagation, Backward Propagation, and Computational Graphs

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- To start, we will focus our exposition on a simple multilayer perceptron with
  - a single hidden layer and
  - $\ell 2$ norm regularization.

Really simple example

- We want
  - $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$
  - for $\mathrm{f(x, y, z) = (x + y)z}$
  - where $x = -2, y = 5, z = -4$
- Draw the computation graph

Reference: http://cs231n.stanford.edu/slides/2019/cs231n_2019_lecture04.pdf

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- The regularization term is $s = \frac{\lambda}{2}(||\mathbf{W}^{(1)}||_F^2 + ||\mathbf{W}^{(2)}||_F^2)$
- Finally, the model's regularized loss (*objective function*) on a given data example is $J = L + s$

Computational Graph of Forward Propagation

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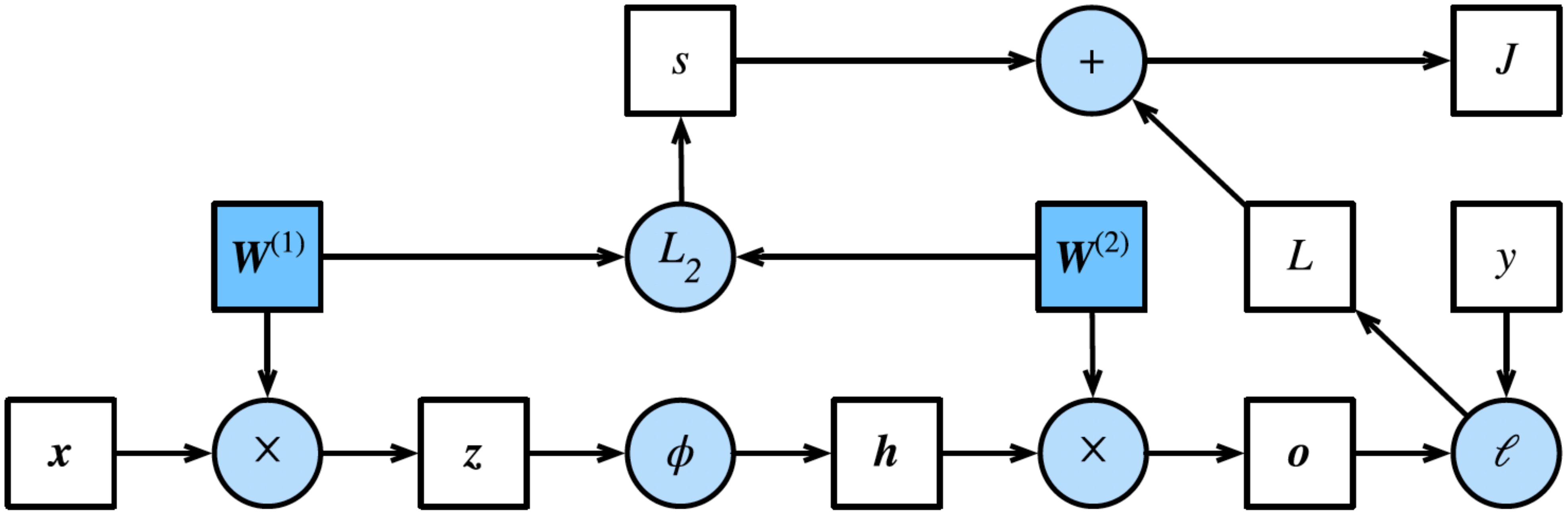

Fig. 6.7.1: Computational Graph

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- What gradients do we need in our example?

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- To obtain the gradient with respect to $\mathbf{W}^{(1)}$, we need to continue backpropagation along the output layer to the hidden layer $\frac{\partial J}{\partial \mathbf{h}} = prod\ \left(\frac{\partial J}{\partial \mathbf{o}}, \frac{\partial \mathbf{o}}{\partial \mathbf{h}}\right) = W^{(2)T} \frac{\partial J}{\partial \mathbf{o}}$. Calculating gradient with respect to $\mathbf{z}$, requires derivative of the activation function $\frac{\partial J}{\partial z} = prod\ \left(\frac{\partial J}{\partial \mathbf{h}}, \frac{\partial \mathbf{h}}{\partial z}\right) = \frac{\partial J}{\partial \mathbf{h}} \odot \phi'(\mathbf{z})$.

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- Finally we obtain $\frac{\partial J}{\partial \mathbf{W}^{(1)}} = prod\left(\frac{\partial J}{\partial \mathbf{z}}, \frac{\partial \mathbf{z}}{\partial \mathbf{W}^{(1)}}\right) + prod\ \left(\frac{\partial J}{\partial s}, \frac{\partial s}{\partial \mathbf{W}^{(1)}}\right) = \frac{\partial J}{\partial \mathbf{z}} \mathbf{x}^T + \lambda \mathbf{W}^{(1)}$.

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- This is also one of the reasons why backpropagation requires significantly more memory

Numerical Stability and Initialization

- Which nonlinearity function we use
- How we decide to initialize our parameters
- can play important role in convergence

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- This product might be too large or too small!

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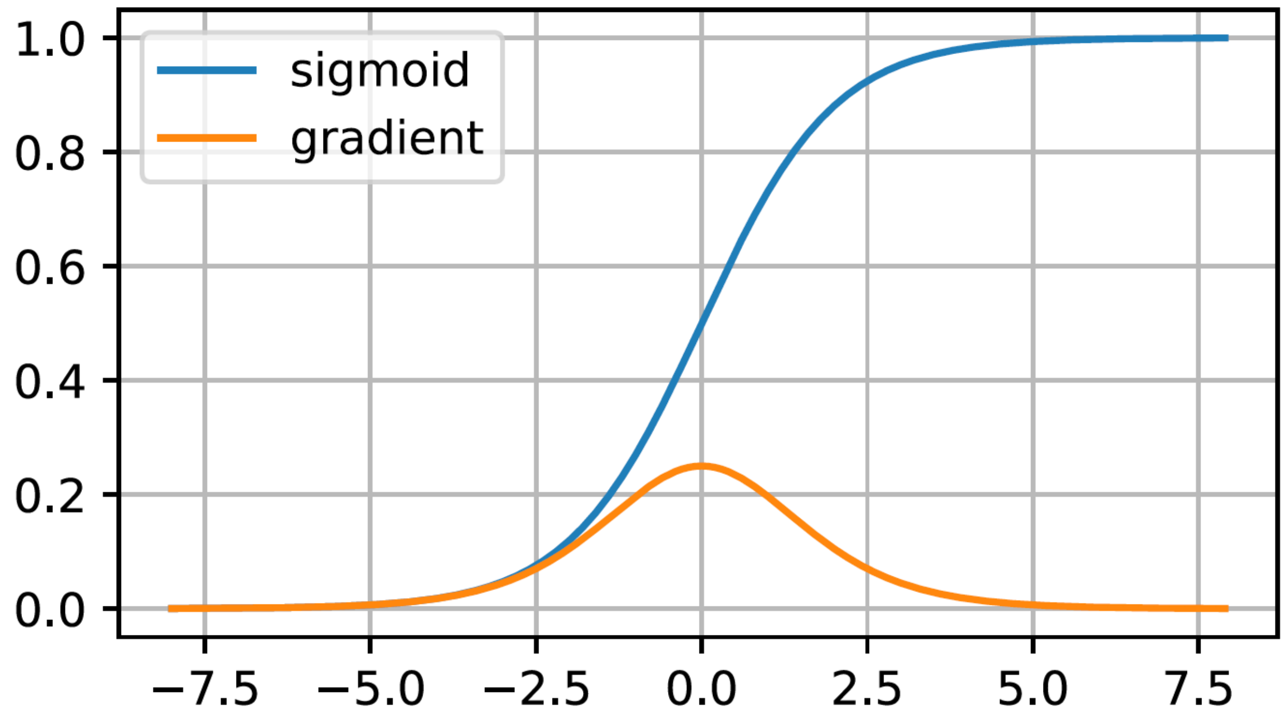
- That is why ReLUs have become the default choice !



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- Let’s draw 100 Gaussian random matrices and multiply them with some initial matrix 100 times.
- The matrix product explodes

```
A single matrix
[[ 2.2122064   0.7740038   1.0434405   1.1839255 ]
 [ 1.8917114  -1.2347414  -1.771029   -0.45138445]
 [ 0.57938355 -1.856082   -1.9768796  -0.20801921]
 [ 0.2444218  -0.03716067 -0.48774993 -0.02261727]]
<NDArray 4x4 @cpu(0)>
After multiplying 100 matrices
[[ 3.1575275e+20 -5.0052276e+19  2.0565092e+21 -2.3741922e+20]
 [-4.6332600e+20  7.3445046e+19 -3.0176513e+21  3.4838066e+20]
 [-5.8487235e+20  9.2711797e+19 -3.8092853e+21  4.3977330e+20]
 [-6.2947415e+19  9.9783660e+18 -4.0997977e+20  4.7331174e+19]]
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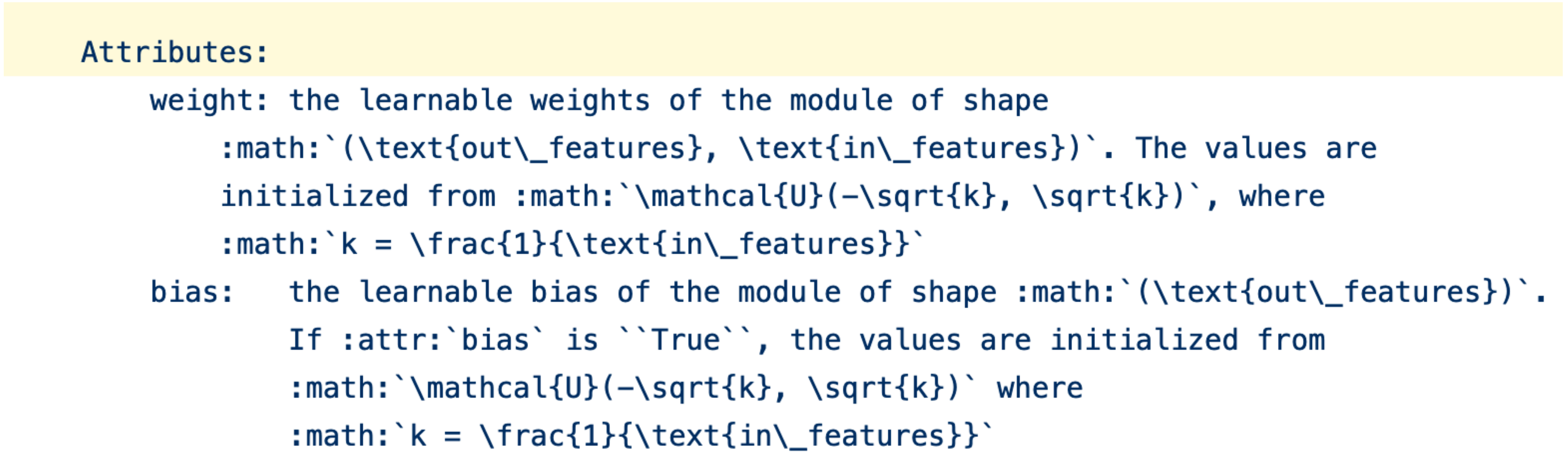
- In this case, the gradients for all dimensions are identical
- SGD would never break symmetry but dropout regularization would.

Parameter Initialization

- One way of addressing the issues raised above is through careful initialization of the weight vectors
- PyTorch uses uniform initialization by default for Linear layers



```
Attributes:
    weight: the learnable weights of the module of shape
        :math:`(\text{out\_features}, \text{in\_features})`. The values are
        initialized from :math:`\mathcal{U}(-\sqrt{k}, \sqrt{k})`, where
        :math:`k = \frac{1}{\text{in\_features}}`
    bias:   the learnable bias of the module of shape :math:`(\text{out\_features})`.
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- In this case, the mean and variance of h_i is:

$$\mathrm{E}[h_i] = \sum_{j=1}^{n_{in}} \mathrm{E}[W_{ij} x_j] = 0 \qquad \mathrm{E}[h_i^2] = \sum_{j=1}^{n_{in}} \mathrm{E}[W_{ij}^2 x_j^2] = \sum_{j=1}^{n_{in}} \mathrm{E}[W_{ij}^2] \mathrm{E}[x_j^2] = n_{in} \sigma^2 \gamma^2$$

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- Xavier initialization simply tries to satisfy: $\frac{1}{2}(n_{in} + n_{out})\sigma^2 = 1$

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- Almost all problems arising in deep learning are nonconvex
- However, analysis of the algorithms in the context of convex problems can be very instructive.

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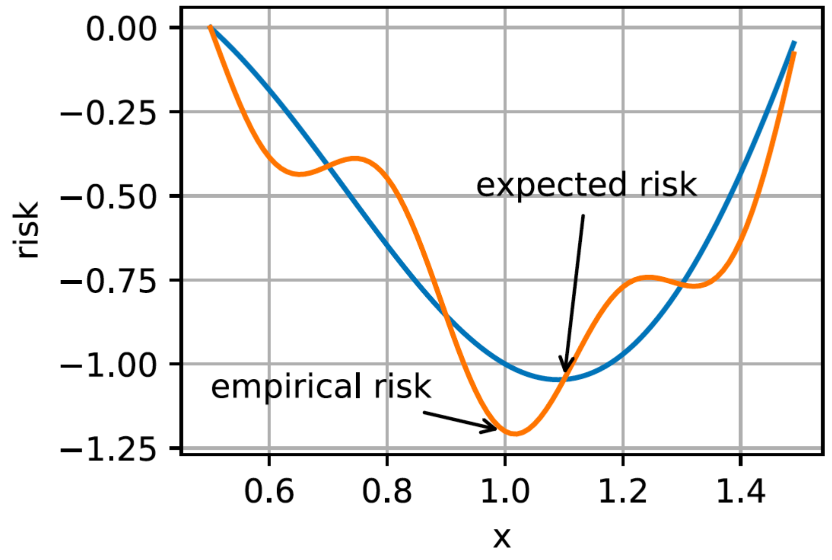

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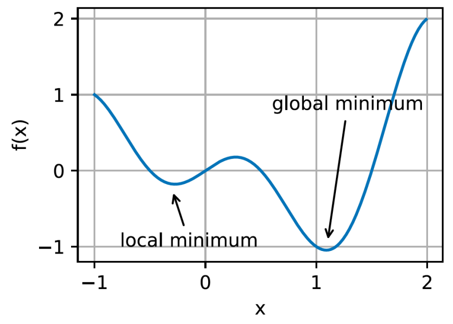

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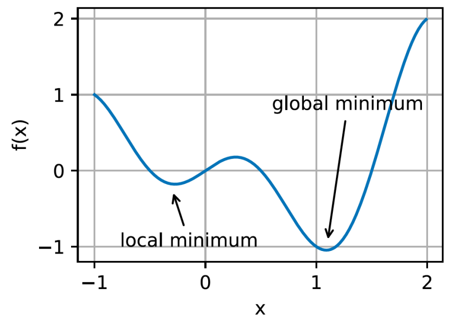
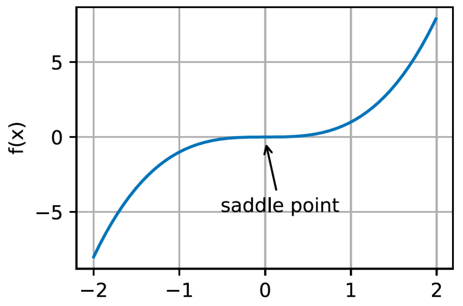
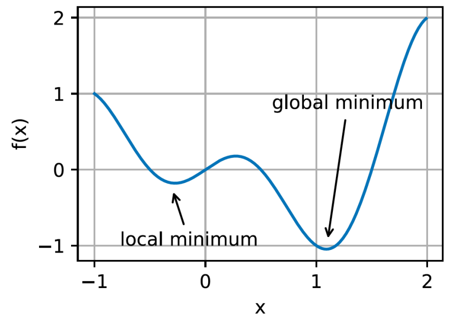


- **Saddle Points:** Any location where all gradients vanish but which is neither a global or a local minimum.
  - Optimization might stall at the point even though it is not a minimum.



Optimization Challenges in Deep Learning

- We are going to focus specifically on the performance of the optimization algorithm in minimizing the objective function
- **Local Minima**: The objective functions of deep learning models usually has many local minima.
  - Only some degree of noise might knock the parameter out of the local minimum.
  - This is one of the beneficial properties of SGD.



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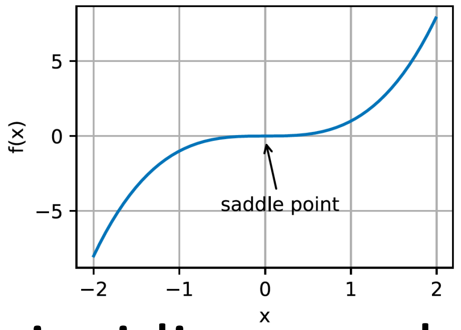

- Vanishing Gradients: Probably, the most insidious problem

Convexity

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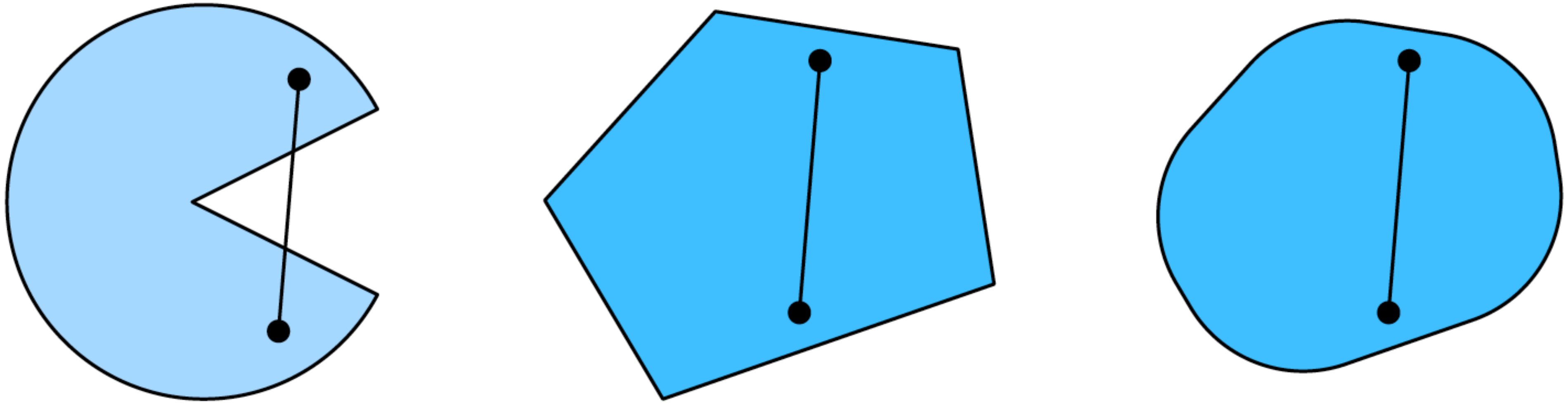

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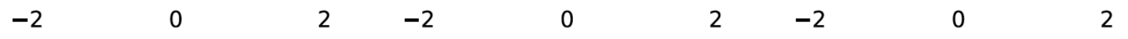

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  - For instance R^d is a convex set
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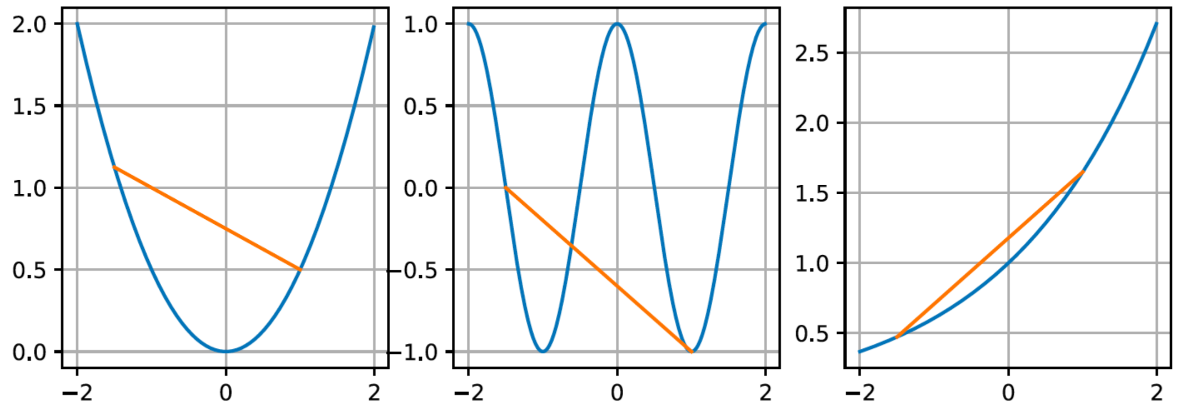
- **Functions**: Given a convex set X, a function defined on it $f: X \to R$ is convex if for all $x, x' \in X$ and for all $\lambda \in [0, 1]$ we have

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



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- Jensen's Inequality: It amounts to generalization of the definition of convexity. $\sum_i \alpha_i f(x_i) \geq f\left(\sum_i \alpha_i x_i\right)$ and $\mathrm{E}_x[f(x)] \geq f\left(\mathrm{E}_x[x]\right)$

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- In other words, the expectation of a convex function is larger than the convex function of an expectation.
- Can you prove this?

Gradient Descent

- Let’s start with an example in one dimension to explain why the gradient descent algorithm may reduce the value of the objective function.
  - Prove
  - Hint: Use Taylor’s series expansion around $x + \epsilon$ and then replace ϵ with $-\eta f'(x)$.

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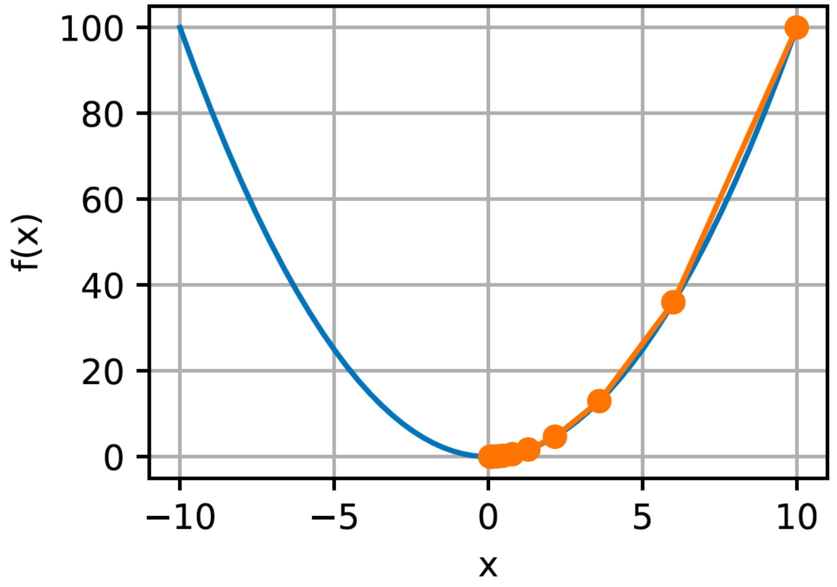
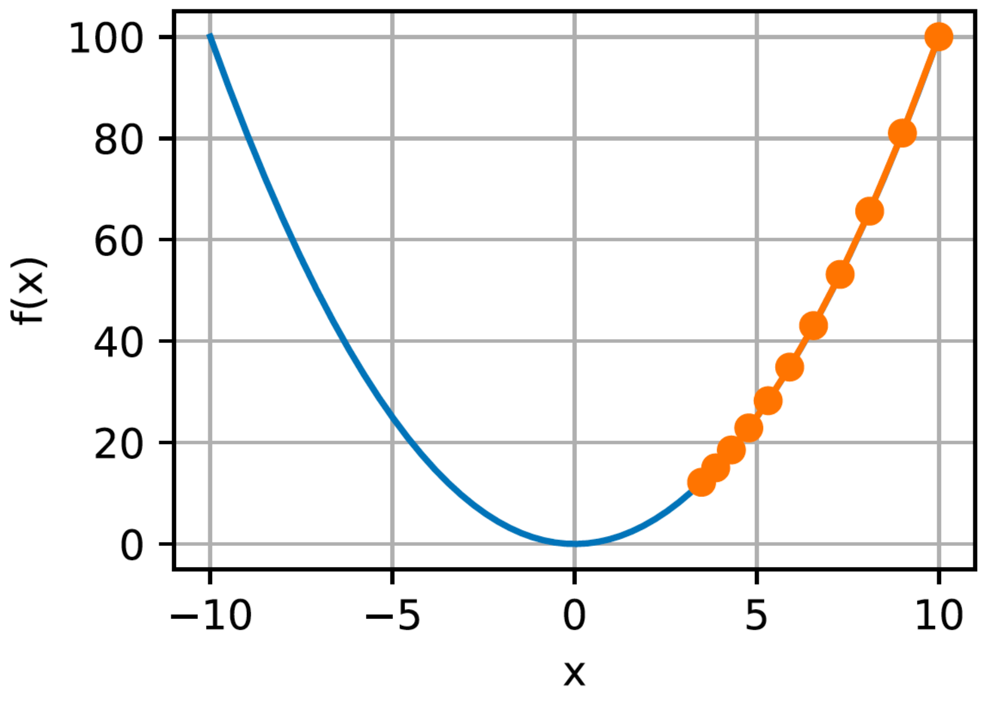
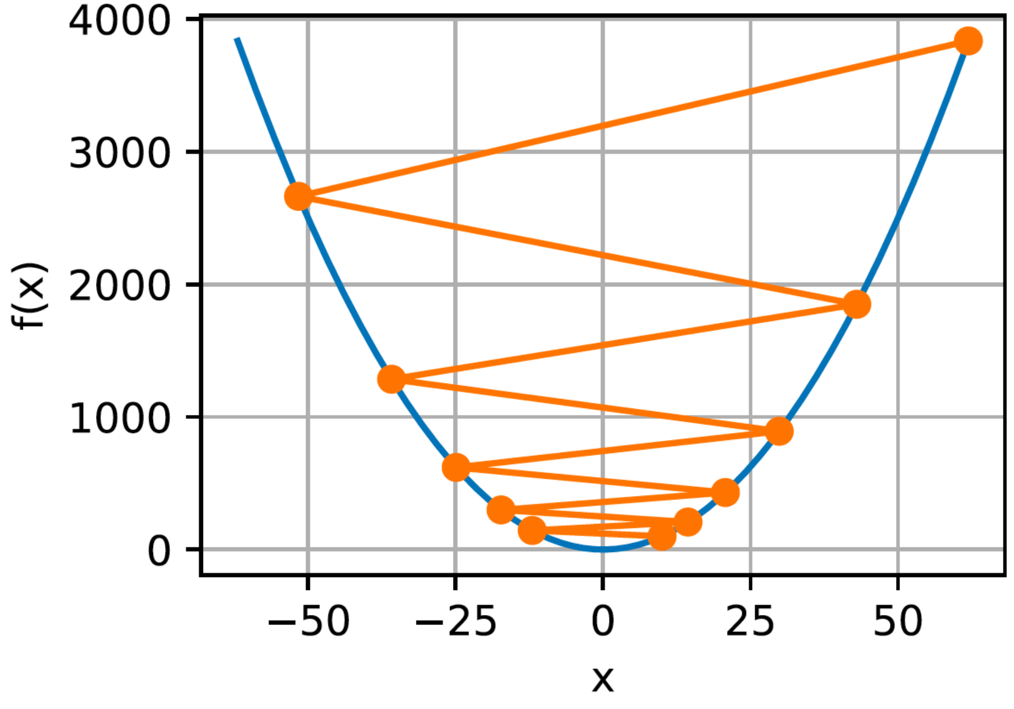


Learning Rate in Gradient Descent

- Which one has large learning rate and which one has small?





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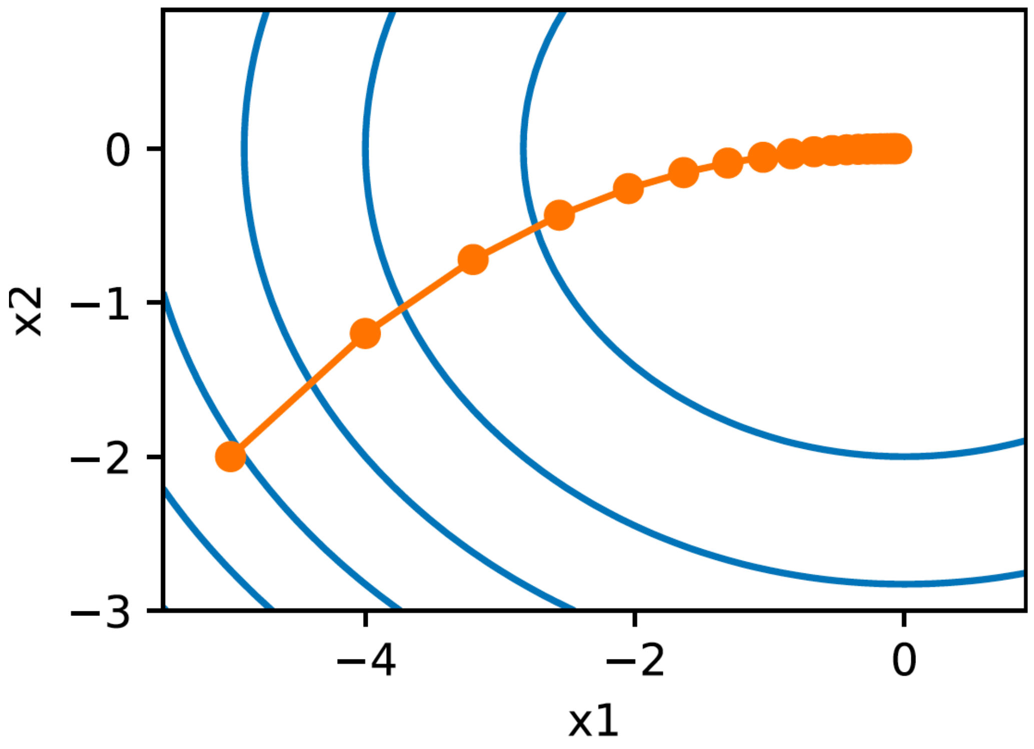

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- Second order methods that also look at the value of *curvature* can help.
- They cannot be applied directly to DL due to computational cost
- But they provide useful intuition into how to design advanced optimization algorithms

Newton’s method

- Reviewing the Taylor expansion of f there is no need to stop after the first term. In fact, we can write it as

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

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- Preconditioning: computing the inverse of Hessian is expensive. So only use the diagonal entries of Hessian

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- Computation cost of each update is $\mathcal{O}(n)$
- SGD reduces the computational cost at each iteration
    - At each iteration of SGD, we uniformly sample an index $i \in \{1, \dots, n\}$ for data instances at random
    - Compute the gradient $\nabla f_i(\mathbf{x})$ to update $\mathbf{x}$

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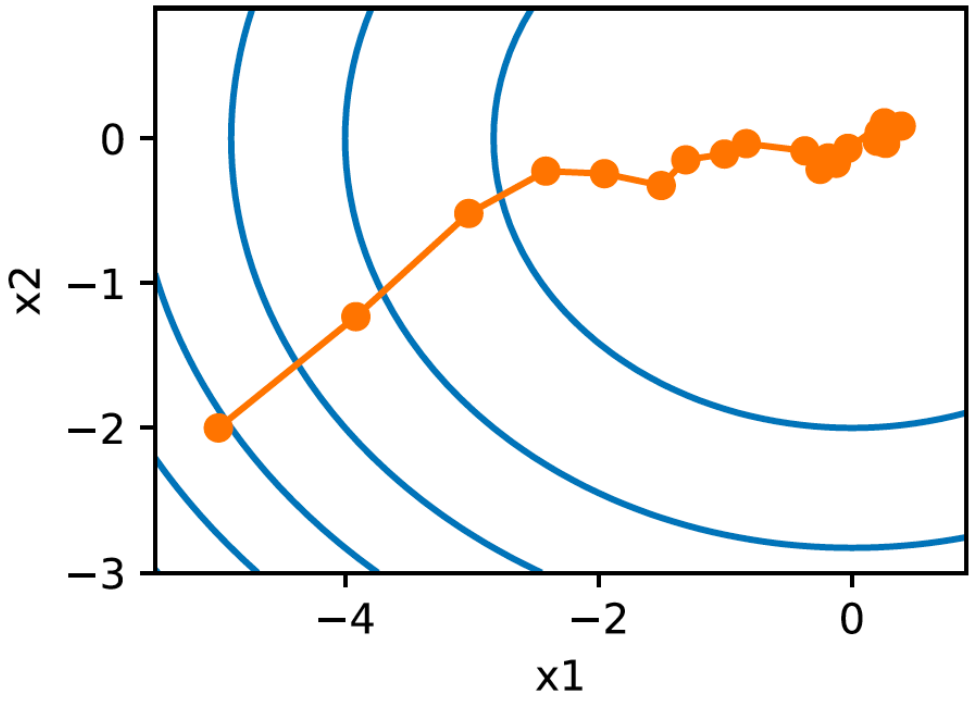

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- SGD can self-decay itself by using $\eta_t = \eta t^{\alpha}$ (usually $\alpha = -1$ or $\alpha = -0.5$), $\eta_t = \eta \alpha^t$ (e.g. $\alpha = 0.95$)