Machine Learning (CE 40717)

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Problem Definition

- **Goal**: Given a function $f(x)$ of some variable x, find the value of x where $f(x)$ is **minimum** or **maximum**
- In neural networks, the goal is to make the prediction error as small as possible
- We want to find the network weights W^* that result in the **lowest loss**:

$$w^* = \arg\min_{w} J(w)$$

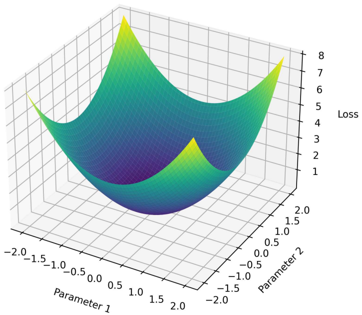
Problem Definition

- Simply put, we want to find the direction to step in that will **reduce our loss** as quickly as possible
- In other words, **which way is downhill?**

Figure 1: Visualization from CS231n, Stanford University

Convexity

- **Definition**: A function is **convex** if, for any two points on the curve, the line segment connecting them lies above or on the curve
  - **Example**: Bowl-shaped curves
- **Convex functions** are easier to optimize because they have only **one global minimum** (the lowest point)
  - Analytical solutions ($\nabla f(x) = 0$) and second-order methods ($\nabla^2 f(x) > 0$) can be used for faster and more accurate convergence
  - **Gradient descent** is guaranteed to converge to the global minimum in convex functions



Convexity

- **Definition**: a function is **non-convex** if it has multiple local minima and maxima
  - **Global Minimum**: The very lowest point across the whole curve
  - **Local Minimum**: A point that's lower than nearby points, but not the lowest overall
  - **Saddle Points**: A flat region where the slope is almost zero. It can go up in some directions and down in others
- Non-convex functions make finding the **global minimum** complicated

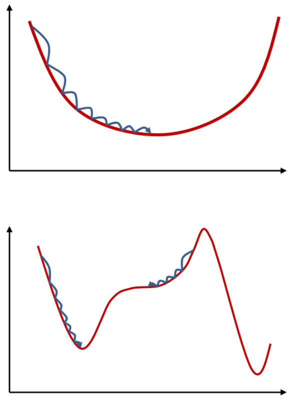


Figure 2: Convex (above) and non-convex (below) functions. From 11-785 Introduction to Deep Learning, CMU, Fall 2024

Definition

- The loss surface represents how the error changes based on the network's weights
- The loss surface of a neural network is typically **non-convex** due to multiple layers, nonlinear activation functions, and complex interactions between parameters, resulting in multiple local minima and saddle points
- In large networks, most local minima give similar error values and are close to the **global minimum**. This isn't true for smaller networks

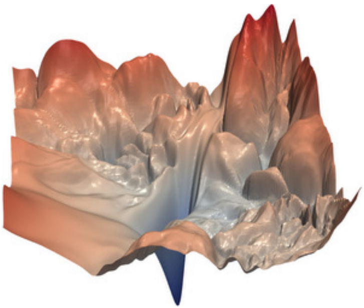


Figure 3: ResNet56 from `https://github.com/tomgoldstein/loss-landscape`

Loss Optimization

- How can we optimize a non-convex loss function?
- **Strategy**: Instead of randomly searching for a good direction, we calculate the **best direction** to reduce the loss
  - Mathematically, this is guaranteed to be the direction of the steepest descent

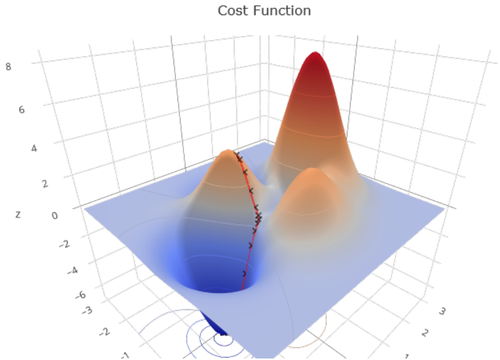


Figure 4: Gradient Descent visualization from `https://blog.skz.dev/gradient-descent`

Gradient Descent

- As introduced earlier, Gradient Descent is an iterative method for minimizing the error by updating network weights in the direction of the steepest descent (negative gradient)

$$w_{t+1} = w_t - \eta \nabla J(w_t)$$

  where:
  - η is called the 'learning rate' or 'step size'
- The goal is to keep adjusting the weights until we reach a point where the error is as low as possible (a local or global minimum)

Types of Gradient Descent

- **Batch Gradient Descent**: Uses the entire dataset to calculate the gradient. This gives smooth updates but can be slow
- **Stochastic Gradient Descent (SGD)**: Uses one data point at a time, leading to faster but noisier updates
- **Mini-batch Gradient Descent**: Uses small groups (batches) of data points. This is a balance between batch and stochastic, combining speed with more stable updates

Types of Gradient Descent

Type	**Advantages**	**Disadvantages**
Batch	Stable convergence Accurate gradient estimate	Computationally expensive Slow for large datasets
Stochastic (SGD)	Fast updates Can escape local minima	Noisy updates May not converge smoothly
Mini-Batch	Faster than batch gradient descent, more stable than stochastic gradient descent (SGD) Efficient for larger datasets	Requires tuning batch size Some noise remains

Table 1: Comparison of Gradient Descent Types

Problem 1

- **SGD** is fast and can escape local minima, but it faces some issues
- What if the loss changes quickly in one direction but slowly in another?
  - **Slow** progress along the shallow dimension, **jitter** along the steep direction

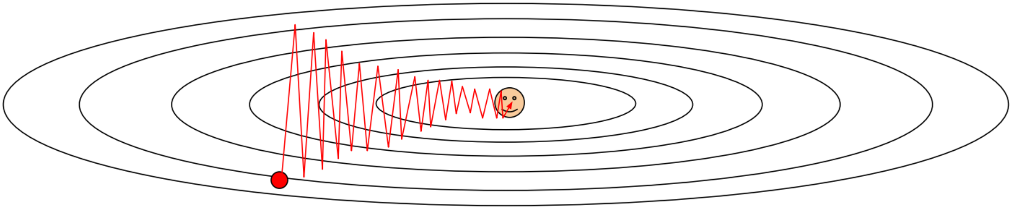


Figure 5: SGD visualization from CS231n, Stanford University

Problem 2

- What if the loss function has a local minima or saddle point?
  - The algorithm may settle for **sub-optimal solutions** or take a **long time** to make significant progress

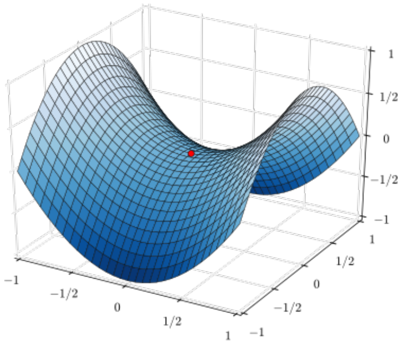


Figure 6: Saddle point from `https://en.wikipedia.org/wiki/Saddle_point`

Problem 3

- Gradients that come from single data points or mini-batches can be **noisy**

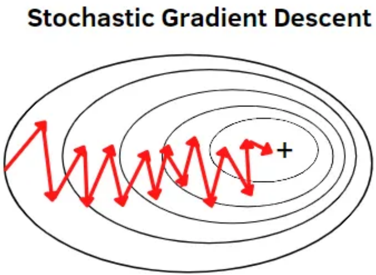


Figure 7: SGD visualization from `https://laptrinhx.com/understanding-optimization-algorithms-3818430905/`

Problem 4

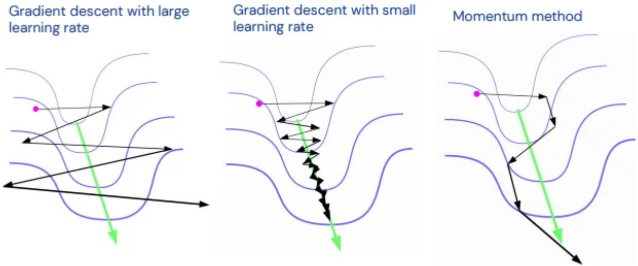
- Why not just use mini-batches?
  - Even though mini-batch gradient descent helps **reduce the noise**, It can still converge **slowly** and might **get stuck** in regions where the gradients are small (like plateaus or valleys), which makes learning inefficient
- In addition, using the same learning rate for all dimensions can lead to:
  - Smooth convergence in some directions
  - Oscillations or divergence in other directions

Problem Definition

- So, how can we improve the vanilla Gradient Descent algorithm?
- **Proposal**:
  - Track oscillations in each direction
  - Increase steps in stable directions
  - Decrease steps in oscillating directions

Problem Definition

- **Goal**: Choose an appropriate learning rate to avoid slow convergence and getting stuck in local minima while not overshooting or becoming unstable
- **Naive Approach**: Test many different learning rates to find the one that works "just right"
  - This can be inefficient and time-consuming
- **Smarter Approach**: Design an adaptive learning rate that adapts to the loss surface
  - We can achieve this by incorporating **Momentum**



Momentum

- **Goal**: Speed up convergence by using past gradients to smooth out oscillations and avoid getting stuck
  - Continue moving in the same general direction as the previous steps
- **Benefit**: It accelerates learning in significant directions while reducing oscillations in less important ones

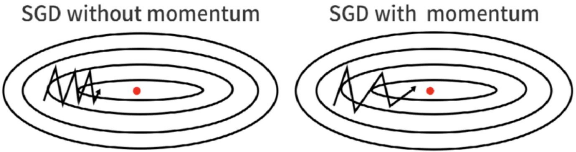


Figure 8: SGD comparison from `https://paperswithcode.com/method/sgd-with-momentum`

First Momentum

- The first momentum, denoted as m_t, is essentially **the moving average of the gradients**. The update rule is:

$$m_{t+1} = \beta_1 m_t + (1 - \beta_1)\nabla_w J(w_t)$$

$$w_{t+1} = w_t - \eta m_{t+1}$$

where:

  - m_{t+1} is the first moment at time step $t+1$
  - β_1 is the decay rate, controlling how much of the past gradients to include (typically 0.9 or 0.99)
  - $\nabla_w J(w_t)$ is the gradient at time step t

Why use the first moment?

- Inspired by physics, it maintains movement due to accumulated momentum, similar to a ball rolling down a frictionless bowl

Second Momentum

- The second momentum, denoted as v_t, is a **moving average of the squared gradients**.
- It helps track the magnitude of the gradients over time. The update rule is:

$$v_{t+1} = \beta_2 v_t + (1 - \beta_2)(\nabla_w J(w_t))^2$$

$$w_{t+1} = w_t - \eta v_{t+1}$$

where:

  - v_{t+1} is the second moment at time step $t+1$
  - β_2 is the decay rate
  - $\nabla_w J(w_t)$ is the gradient at time step t

Why use the second moment?

- The second moment helps **regulate update sizes** by adjusting for consistently large or small gradients, preventing overshooting or slow learning

Moment Bias Correction

- **Problem**: When we start training, both m_t and v_t are initialized to zero, causing their estimates to be biased toward zero in the early steps, especially when gradients are small.
- **Solution**: We use bias-corrected versions of m_t and v_t to address this:

$$\hat{m}_t = \frac{m_t}{1-\beta_1^t}, \quad \hat{v}_t = \frac{v_t}{1-\beta_2^t}$$

- These corrections compensate for the bias by scaling m_t and v_t upward, especially in the early steps when t is small, ensuring more accurate estimates of the moments.

Adam

- **Adaptive Moment Estimation (Adam)** combines **momentum** and **adaptive learning rates** by maintaining an exponentially decaying average of both past gradients and squared gradients
- Adam adjusts the learning rate for each parameter based on the gradient history
  - Larger gradients result in smaller update steps, and vice versa

Adam

- The update rule for the Adam optimizer at step $t+1$ is denoted by w_{t+1}:

$$m_{t+1} = \beta_1 m_t + (1-\beta_1)\nabla_w J(w_t)$$

$$v_{t+1} = \beta_2 v_t + (1-\beta_2)(\nabla_w J(w_t))^2$$

$$\hat{m}_{t+1} = \frac{m_{t+1}}{1-\beta_1^{t+1}}, \quad \hat{v}_{t+1} = \frac{v_{t+1}}{1-\beta_2^{t+1}}$$

$$w_{t+1} = w_t - \eta \frac{\hat{m}_t}{\sqrt{\hat{v}_t}+\epsilon}$$

where:

- m_{t+1} and v_{t+1} are the first and second moments at step $t+1$
- β_1 and β_2 are the decay rates for the first and second moments
- $\hat{m}_{t+1}$ and $\hat{v}_{t+1}$ are bias-corrected estimates of the first and second moments
- ϵ is a small constant to prevent division by zero

Comparison of Momentum Methods

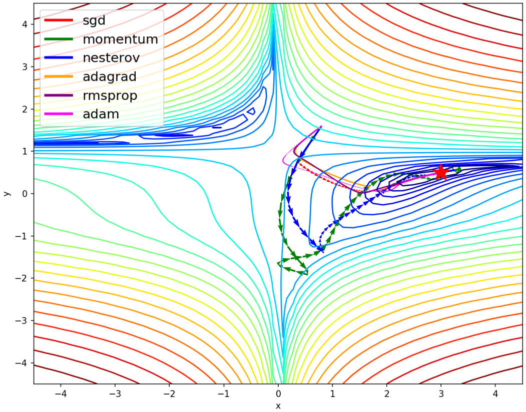


Figure 9: GD comparison from `https://github.com/ilguyi/optimizers.numpy`

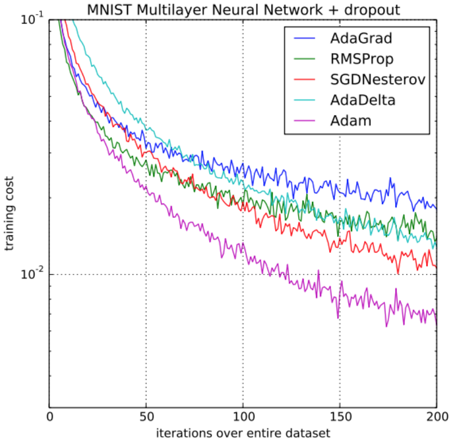


Figure 10: GD comparison on MNIST from `kingma2014adam`