McGill initiative in Computational Medicine

Fundamentals of Machine Learning

Optimization

Workshop Lead: Tugce Gurbuz

Jul 24th, 2024

What is optimization?

What do we optimize?

How do we optimize?

What is optimization?

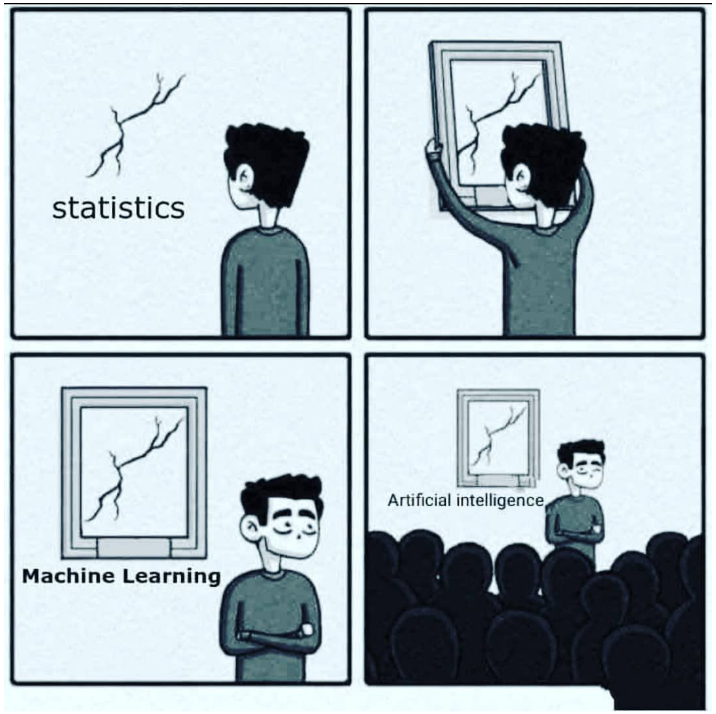
What do we optimize? **-> Parameters of the model to make the loss minimum**

How do we optimize?

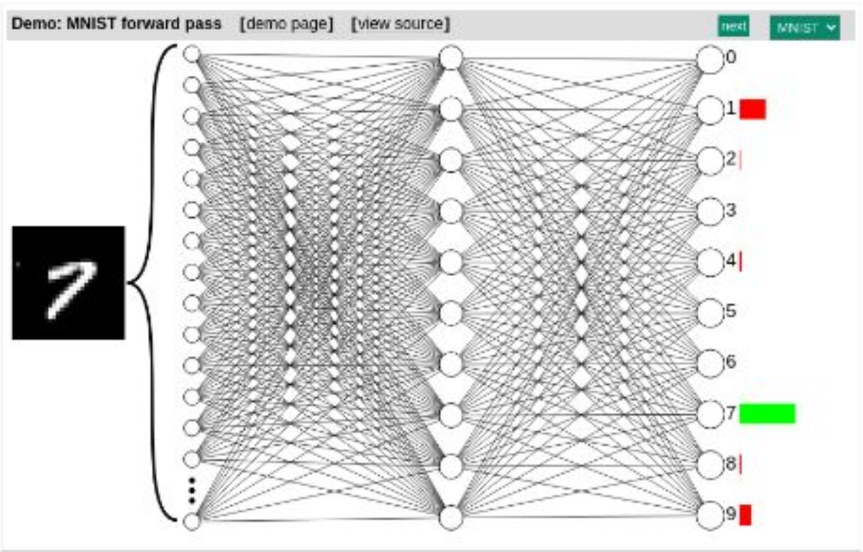
What is optimization?

What do we optimize? **-> Parameters of the model tomake the loss minimum**

How do we optimize? **-> Math!**

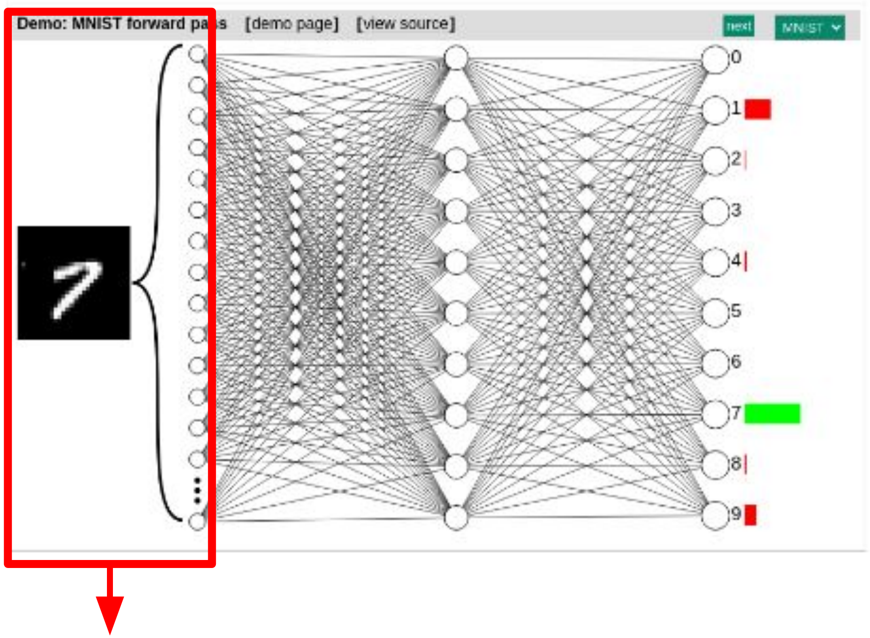


Task in tutorial: Classifying handwritten digits with MLP



Source:
https://ml4a.github.io/demos/forward_pass_mnist/

Task in tutorial: Classifying handwritten digits with MLP



28 x 28 image -> 784 vector

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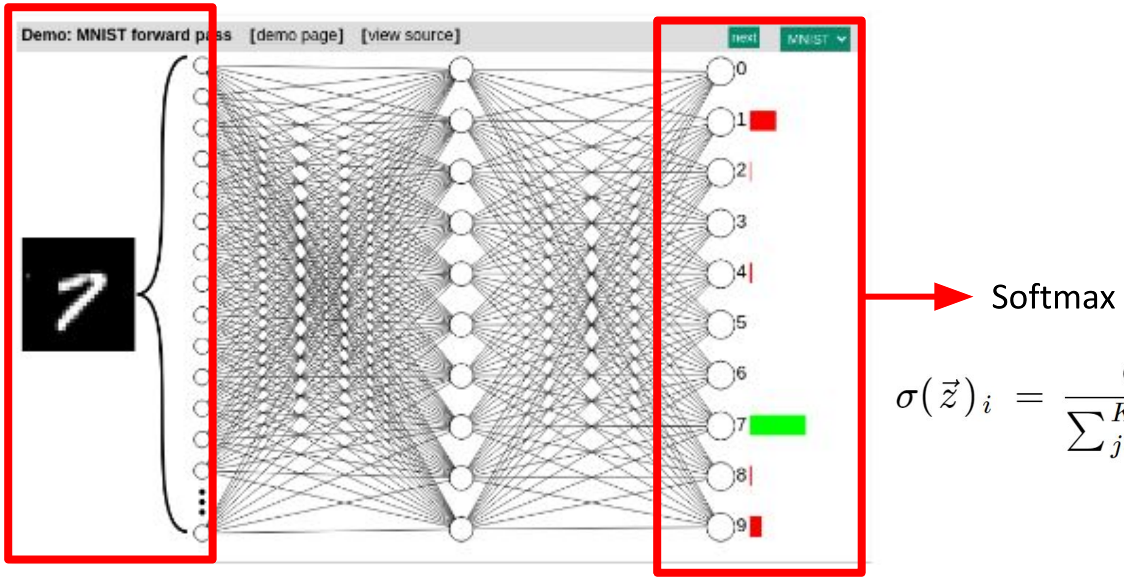
Task in tutorial: Classifying handwritten digits with MLP



$$\sigma(\vec{z})_i = \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}$$

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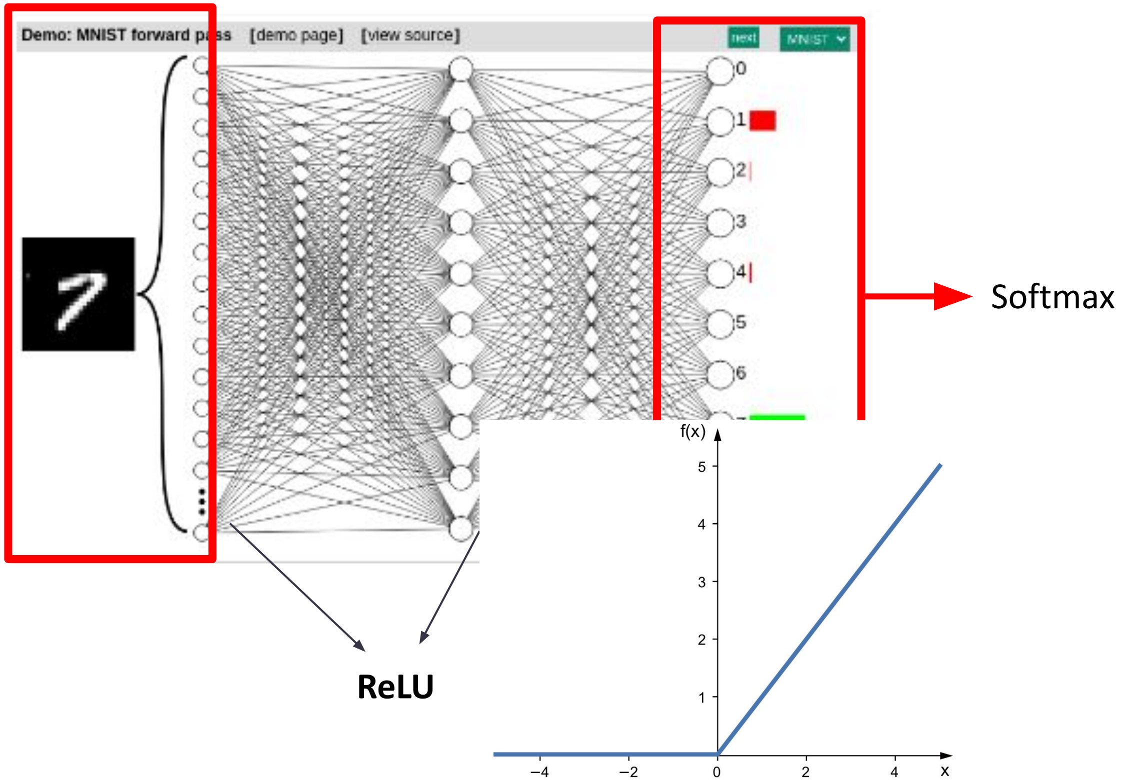
Task in tutorial: Classifying handwritten digits with MLP



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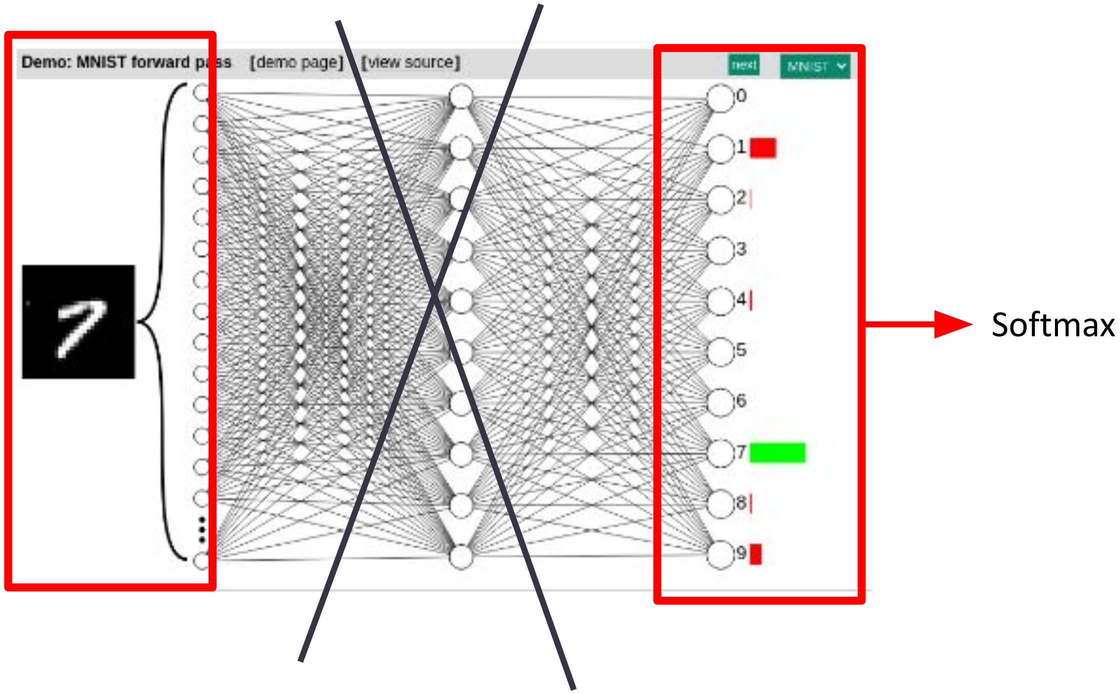

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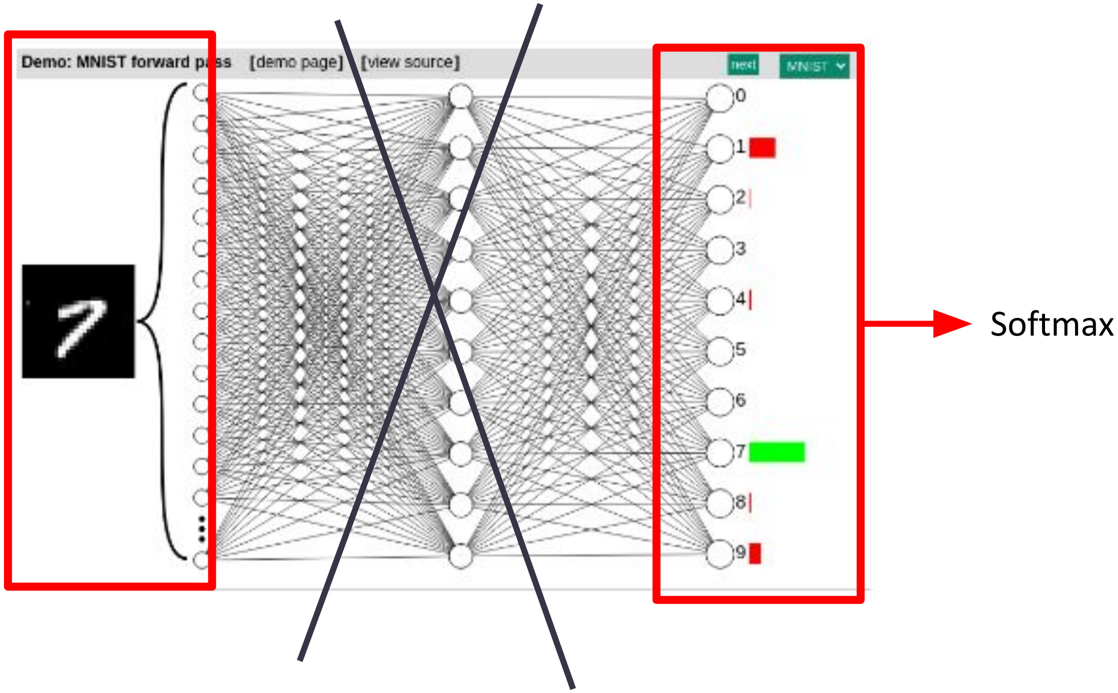
Task in tutorial: Classifying handwritten digits with MLP



$$f(x) = \mathrm{softmax}(Wx + b)$$

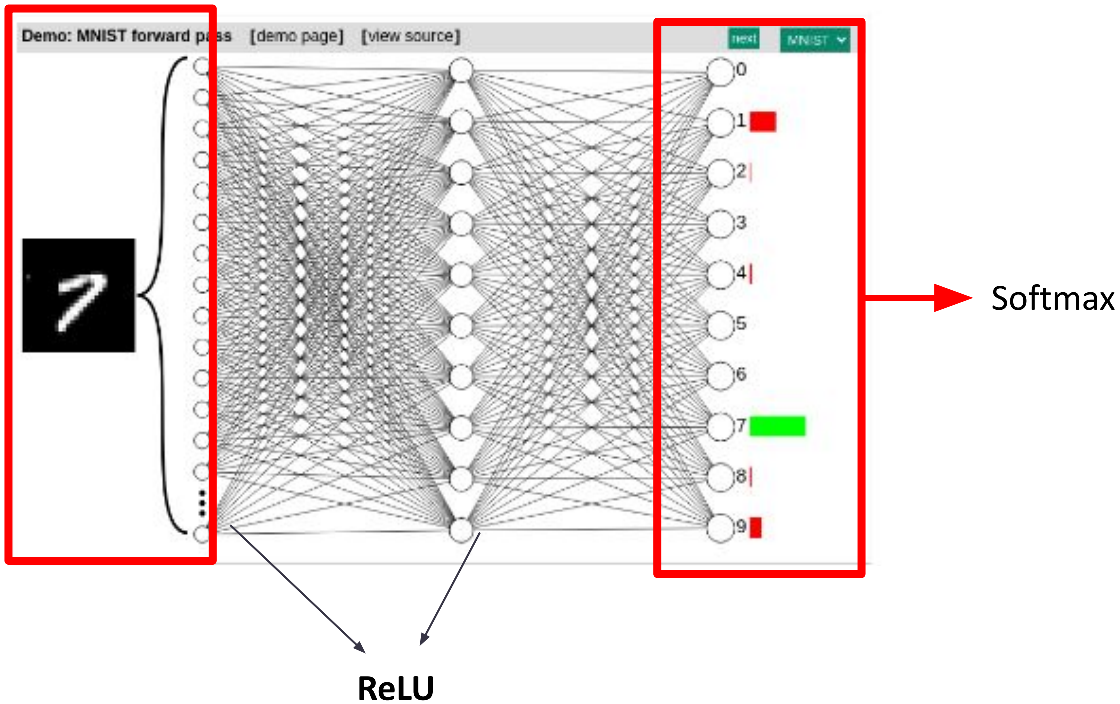
$x \in \mathbb{R}^{784}$,

$W \in \mathbb{R}^{10 \times 784}$

$b \in \mathbb{R}^{10}$

Source:
https://ml4a.github.io/demos/forward_pass_mnist/

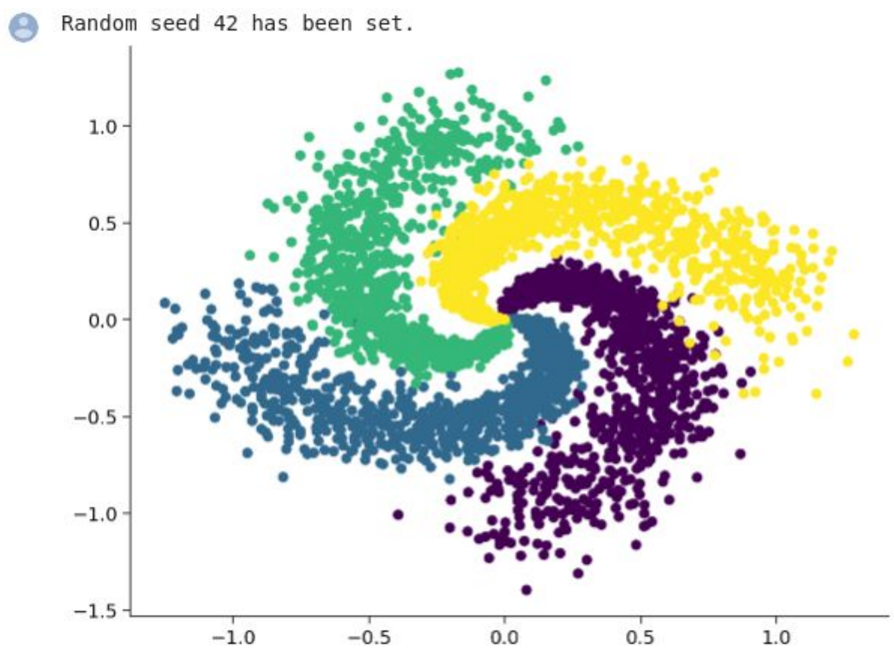
Task in tutorial: Classifying handwritten digits with MLP



Let's go to tutorial to implement our classification model!

Source:
https://ml4a.github.io/demos/forward_pass_mnist/

How to calculate the loss?



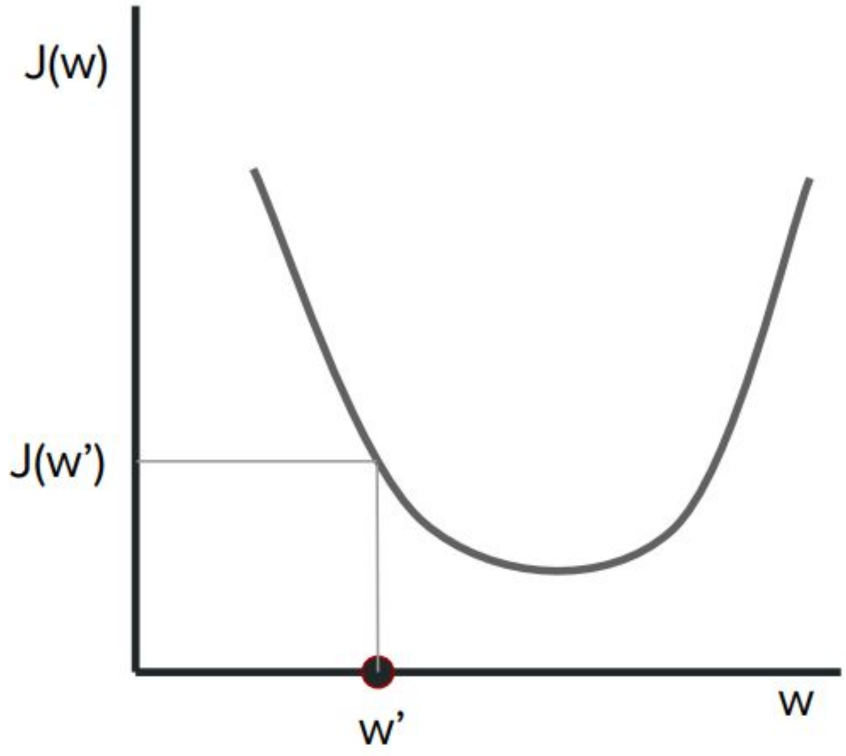
Multiclass classification: Cross-entropy vs. MSE?

Source: tutorial1

How to decide the loss function?

- Identify your problem (e.g., classification, regression?)
- Check the literature

How to minimize the loss?



How to minimize the loss?

Random search?

Algorithm:

sample random points around current w

if random point, w', yields lower objective (i.e. $J(w')<J(w)$):

Accept w' as new position and store it in w

How to minimize the loss?

Random search?

Source: https://miro.medium.com/max/1200/1*DuFS854z2avtDs3VciPp9w.jpeg

How to minimize the loss?

Gradient Descent <3

Algorithm:

- Compute gradient (it points uphill)
- Do step in opposite direction of gradient
- Step size (learning rate), η

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How to minimize the loss?

Gradient Descent

<u>Algorithm:</u>

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

How to minimize the loss?

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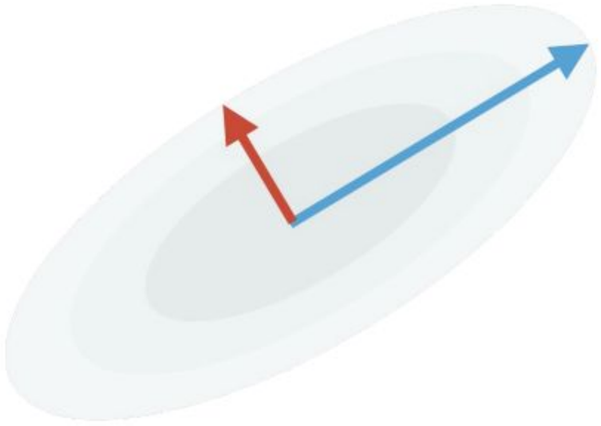
Let's go to our tutorial to implement Gradient Descent!!

How to minimize the loss?

Gradient Descent

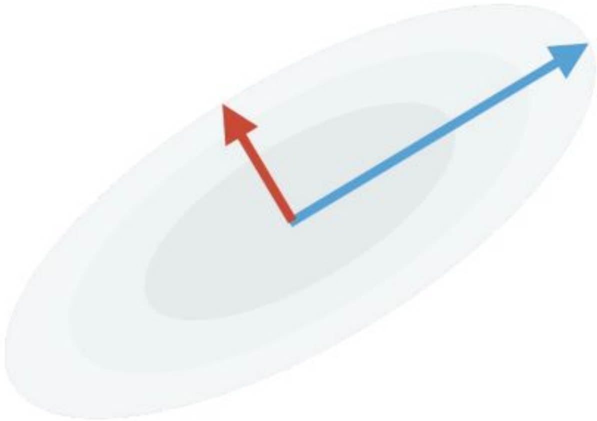
- How to choose learning rate?

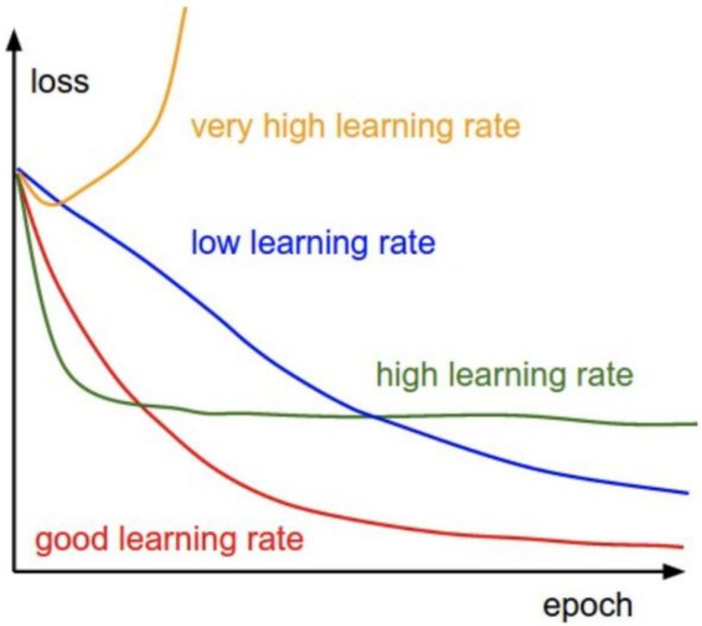


How to minimize the loss?

Gradient Descent

- How to choose learning rate?





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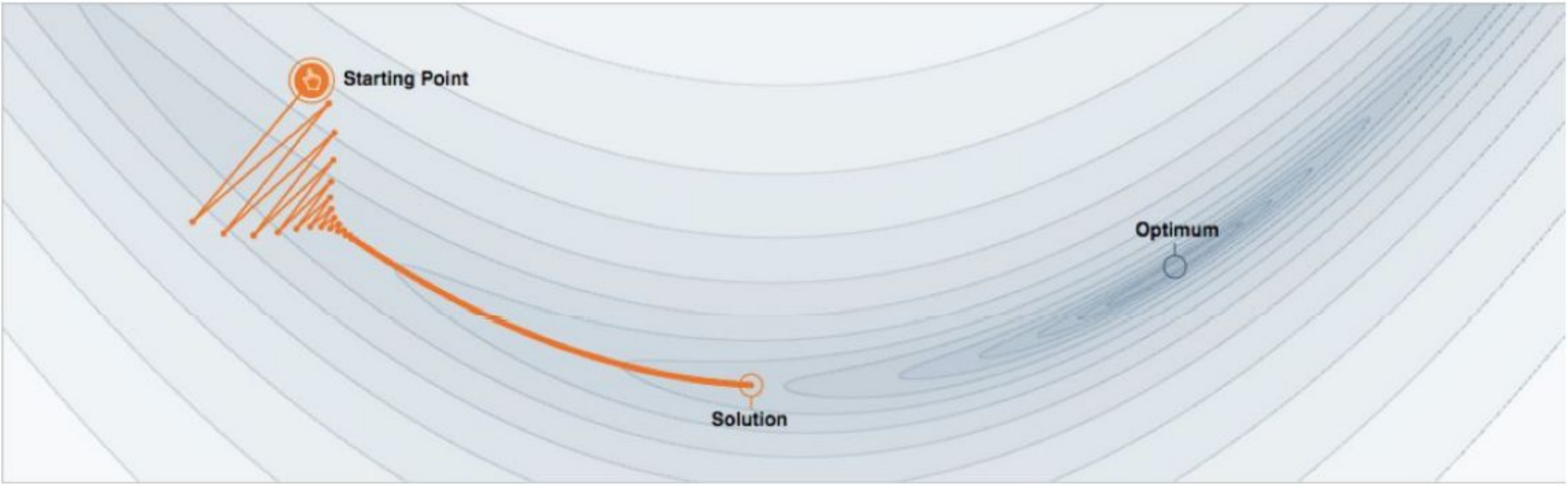
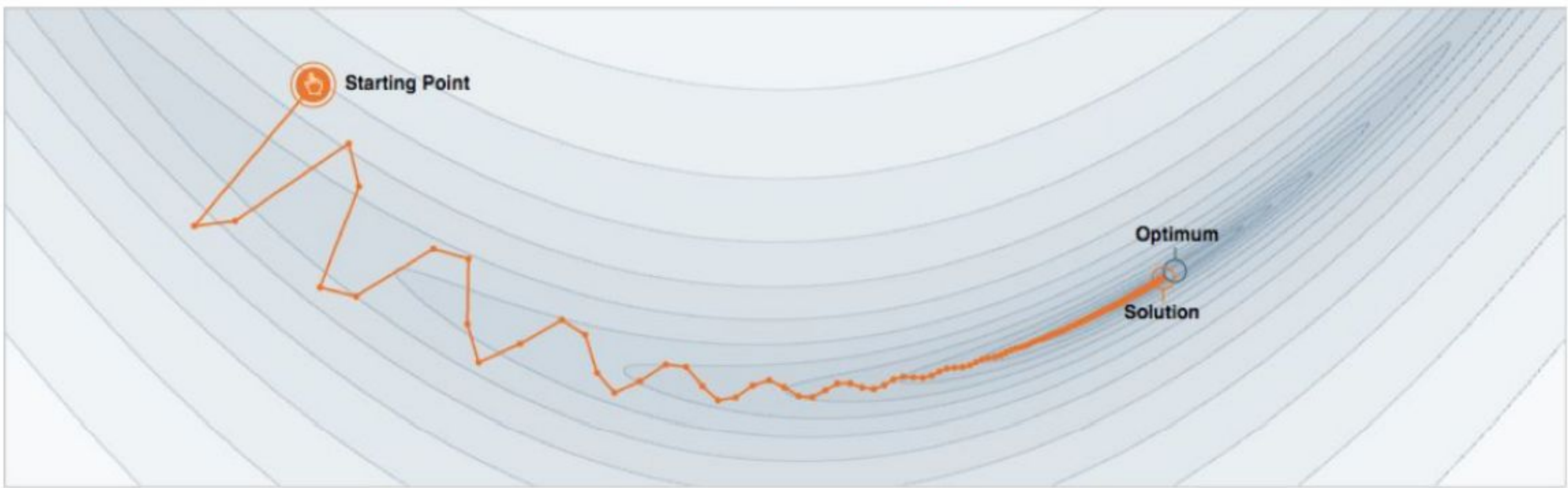


[Distill.pub]

How to minimize the loss?

Momentum <3

- Accelerates along flat directions
- Slows down along sharp directions



[Distill.pub]

How to minimize the loss?

How does the momentum work?

Momentum algorithm:

- Do a gradient descent step
- Apply the update from the last iteration, only smaller (momentum step)

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

How to minimize the loss?

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Let's go to our tutorial to implement Momentum!

How to minimize the loss?

Adaptive Methods <3

- Learning rate schedules

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

How to minimize the loss?

Adaptive Methods <3

- Learning rate schedules

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

Polynomial schedules, e.g. → $\eta_t = \frac{\alpha}{c+t}, \ \eta_t = \frac{\alpha}{c+\sqrt{t}}$

Exponential

Stepwise decay

Cosine/cyclical schedules

How to minimize the loss?

Adaptive Methods <3

- **Adagrad (Duchi et al., 2011)**
  - Adapts the learning rate for each parameter
  - Using running sum squares of past gradients
  - Typically used in stochastic form:
    - Instead of full gradient, use gradient from mini-batch

$$[w_{t+1}]_i = [w_t]_i - \frac{\eta}{\sqrt{[v_{t+1}]_i + \epsilon}} [\nabla J(w_t)]_i$$

$$[v_{t+1}]_i = \sum_{s=1}^{t} [\nabla J(w_s)]_i^2$$

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How to minimize the loss?

Adaptive Methods <3

- **RMSprop**
    - Uses a moving average instead of sum used by Adagrad
    - Moving average can be useful on non-convex objectives

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- **Adam: RMSprop + momentum**

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- **Adam: RMSprop + momentum**

Let’s go to our tutorial to implement RMSprop!

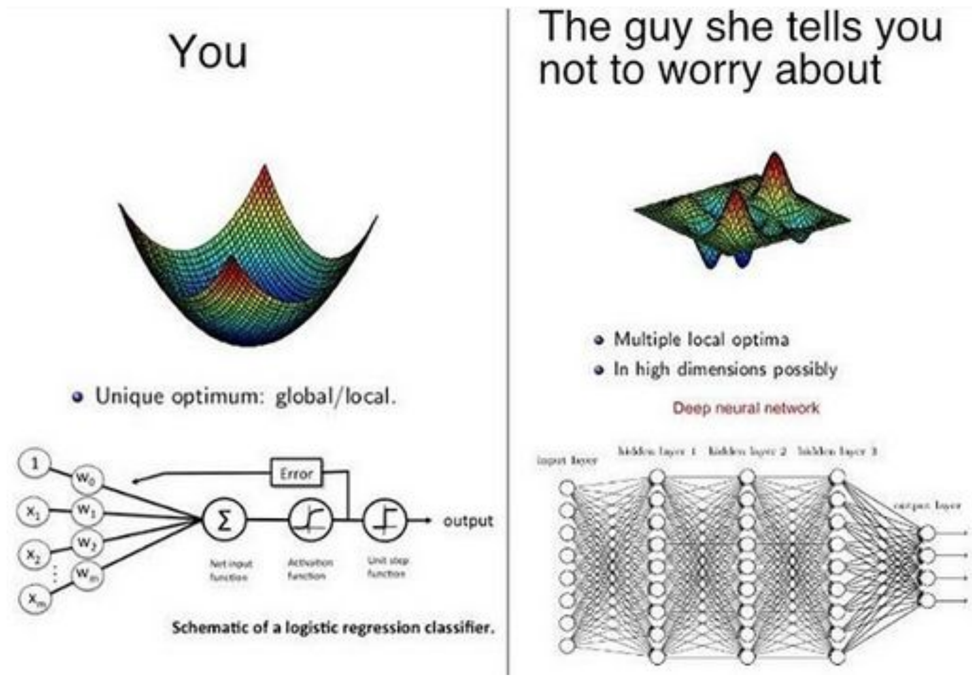
How to minimize the loss?

Non-convexity Problem

How to minimize the loss?

Non-convexity Problem

- Convex <3 -> have the same global and local minimum
- Non-convex -> have different global and local minimum



How to minimize the loss?

Non-convexity Problem

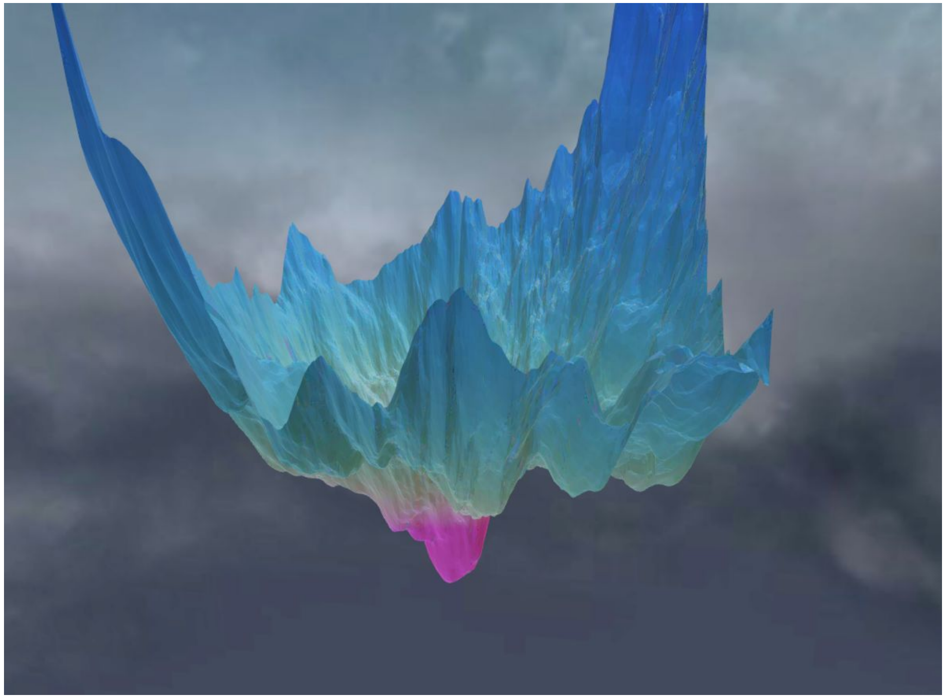
- Convex <3 -> have the same global and local minimum
- Non-convex -> have different global and local minimum

Great non-convexity, comes with great responsibility!

How to minimize the loss?

Non-convexity Problem

- Initialization matters!!
  https://losslandscape.com/explorer



How to minimize the loss?

Non-convexity Problem

- Overparameterization to rescue!

Let’s go to tutorial and overparameterize our MLP!

How to minimize the loss?

Computation Cost Problem

How to minimize the loss?

Computation Cost Problem

- Minibatch training <3

How to minimize the loss?

Computation Cost Problem

- Minibatch training <3 -> stochastic gradient descent

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How to minimize the loss?

Computation Cost Problem

- Minibatch training <3 -> stochastic gradient descent
  - Minibatch size:
    - Too small batch size: optimization bounces around alot, and can lead to slower convergence to a minimum.
    - Too big batch size: won’t fit on GPU
    - Rule of thumb -> pick the largest batch size that fits in the GPU

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Let’s go to our tutorial and implement Mini Batch Training!!!