McGill initiative in Computational Medicine

Introduction to Machine Learning

Module 1C: Optimization

Instructor: Tugce Gurbuz

July 14th 2022

What is optimization?

What do we optimize?

How do we optimize?

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How do we optimize?

Why optimization is important (at the societal level)?

What is optimization?

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

How do we optimize?

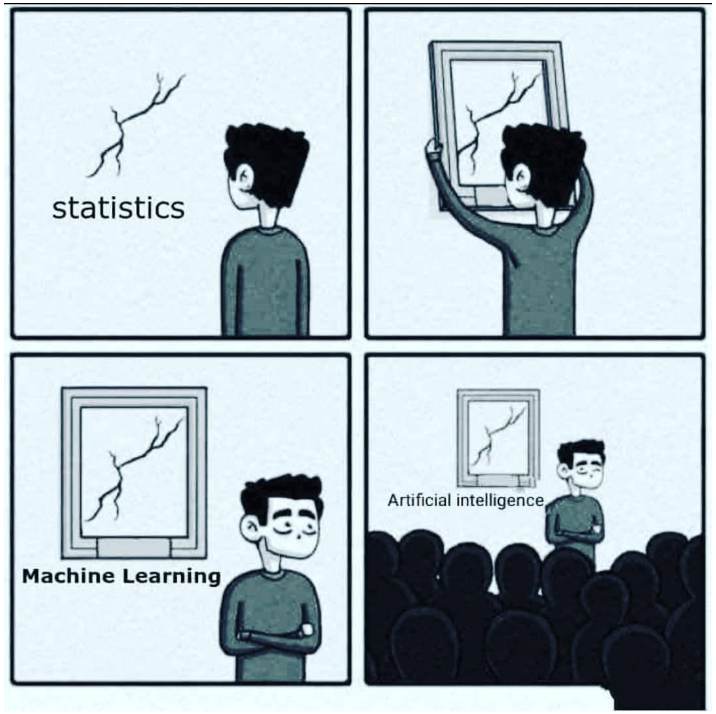
Why optimization is important (at the societal level)?

What is optimization?

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

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

Why optimization is important (at the societal level)?



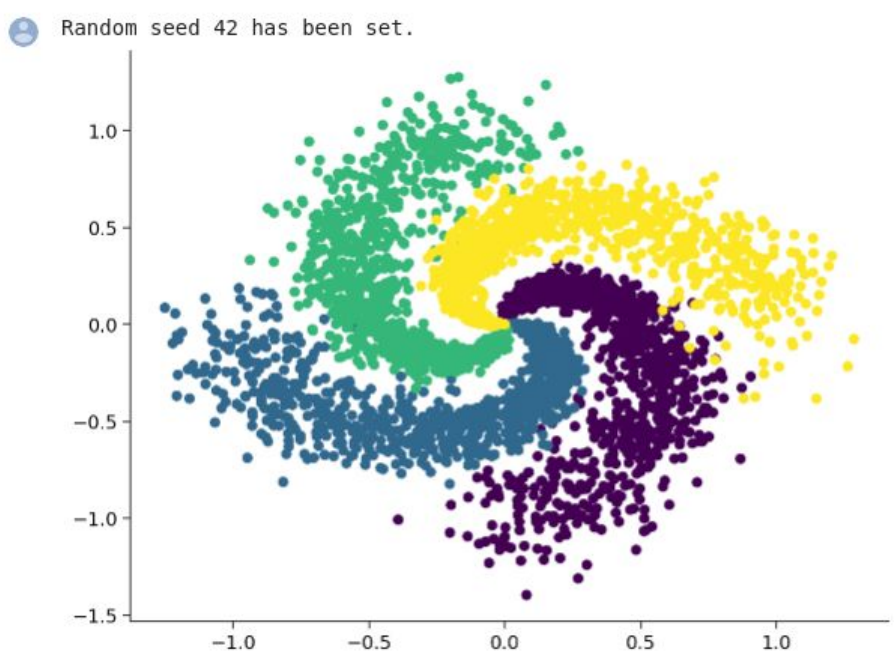
What is optimization?

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

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

Why optimization is important (at the societal level)? **-> Creating fair algorithms**

How to calculate the loss?



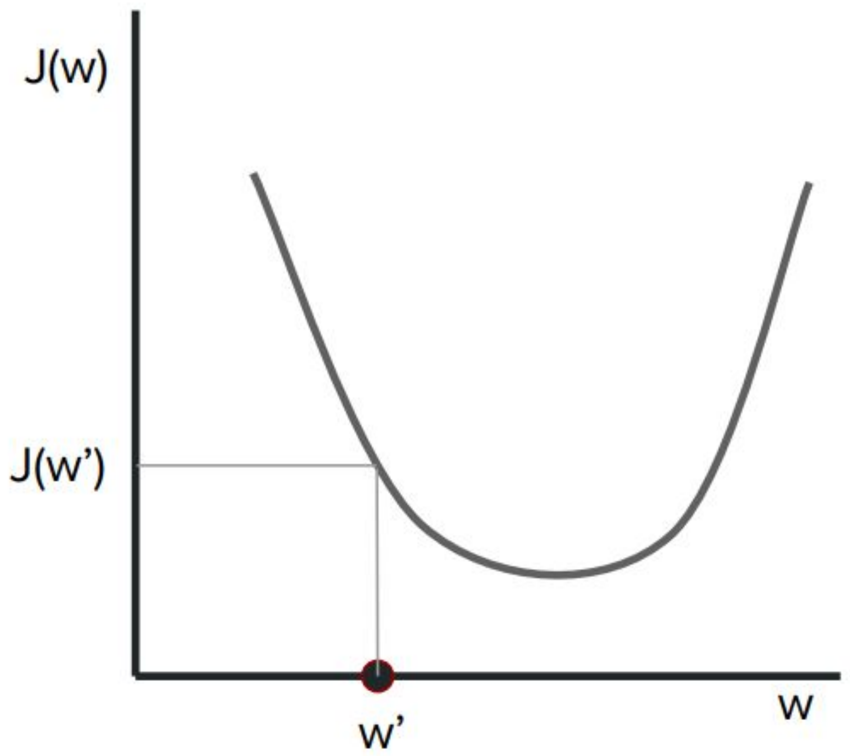
Multiclass classification: Cross-entropy vs. MSE?

Source: module1B-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

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

How to minimize the loss?

Gradient Descent

<u>Algorithm:</u>

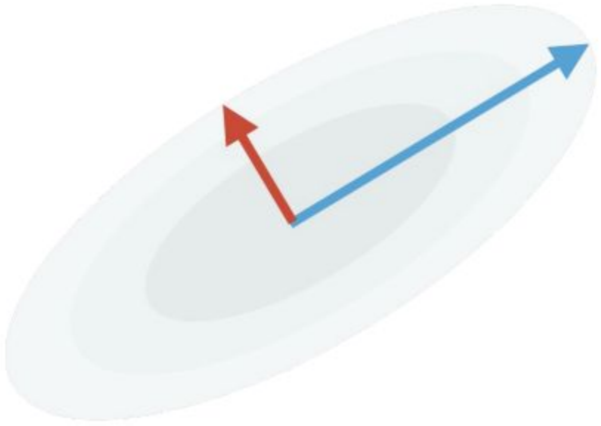
- Compute gradient (it points uphill)
- Do step in opposite direction of gradient
- Step size (learning rate), η

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

How to minimize the loss?

Gradient Descent

- How to choose learning rate?



How to minimize the loss?

Gradient Descent

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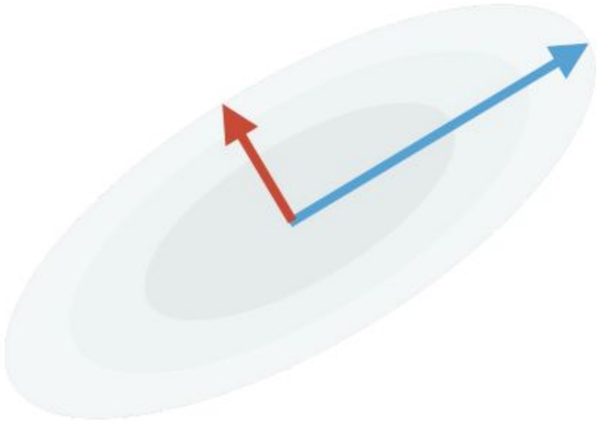
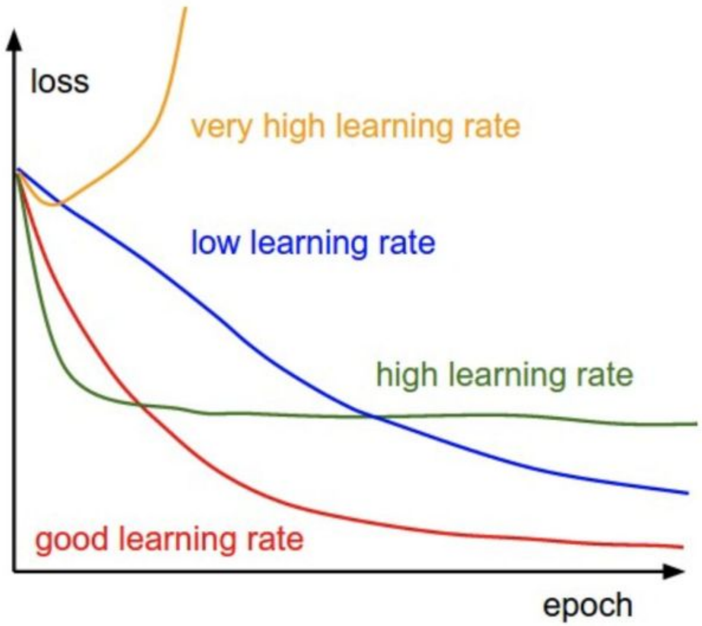
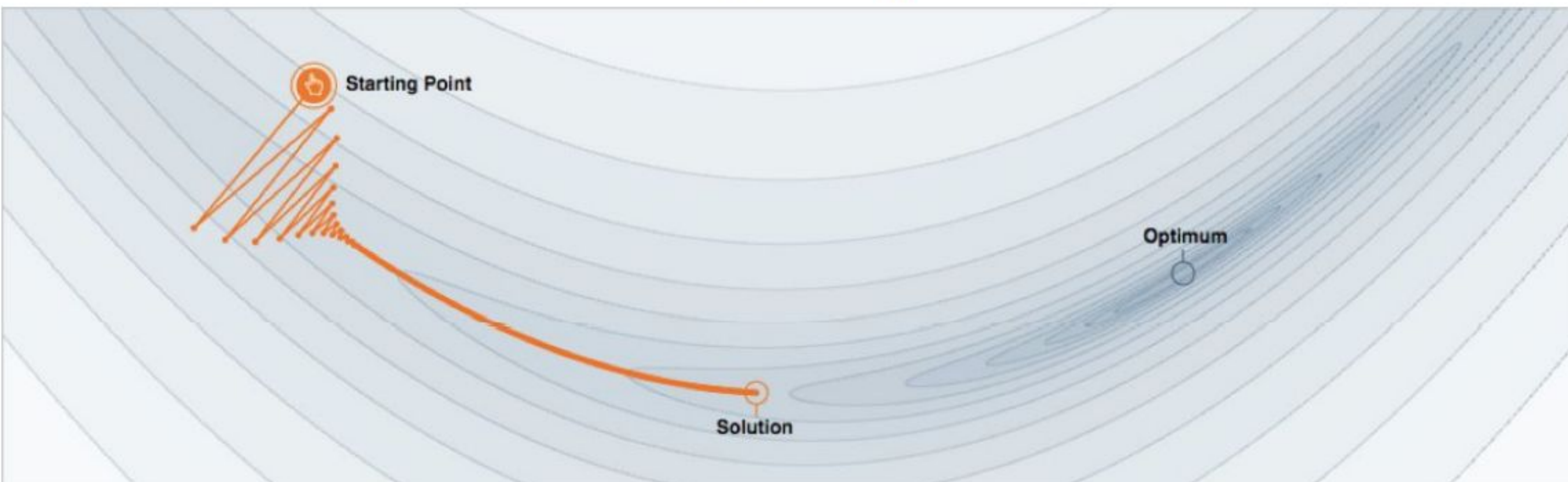




How to minimize the loss?



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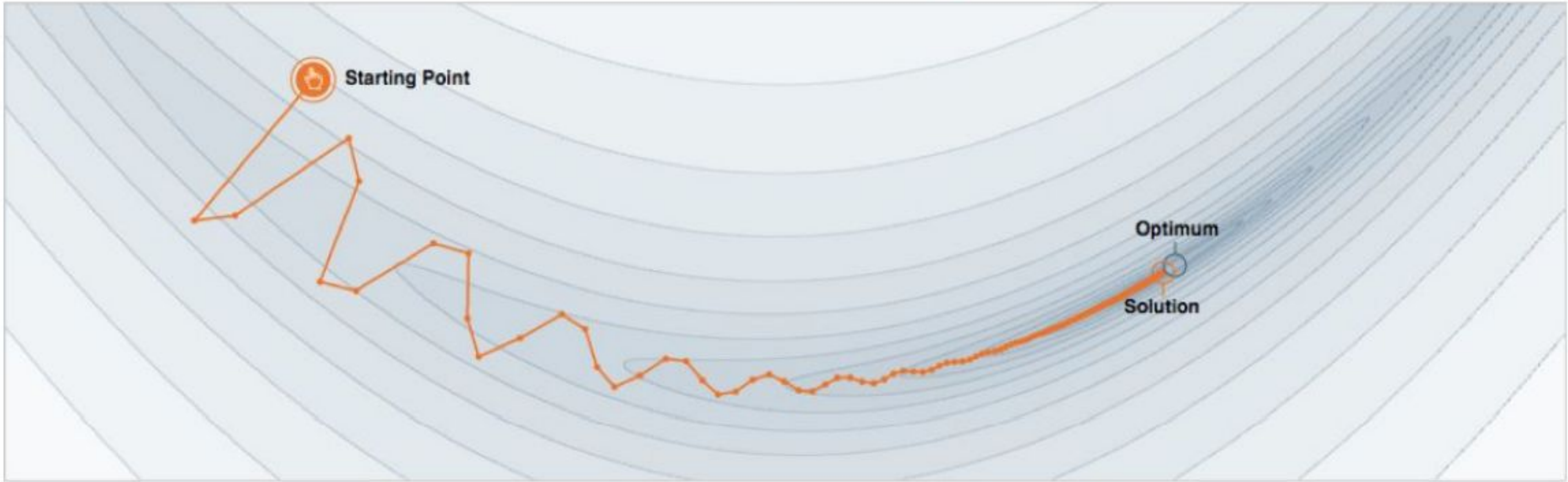
How to minimize the loss?

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?

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

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

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

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

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

$$[v_{t+1}]_i = \alpha[v_t]_i + (1-\alpha)[\nabla J(w_t)]_i^2$$

How to minimize the loss?

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- **Adam: RMSprop + momentum**

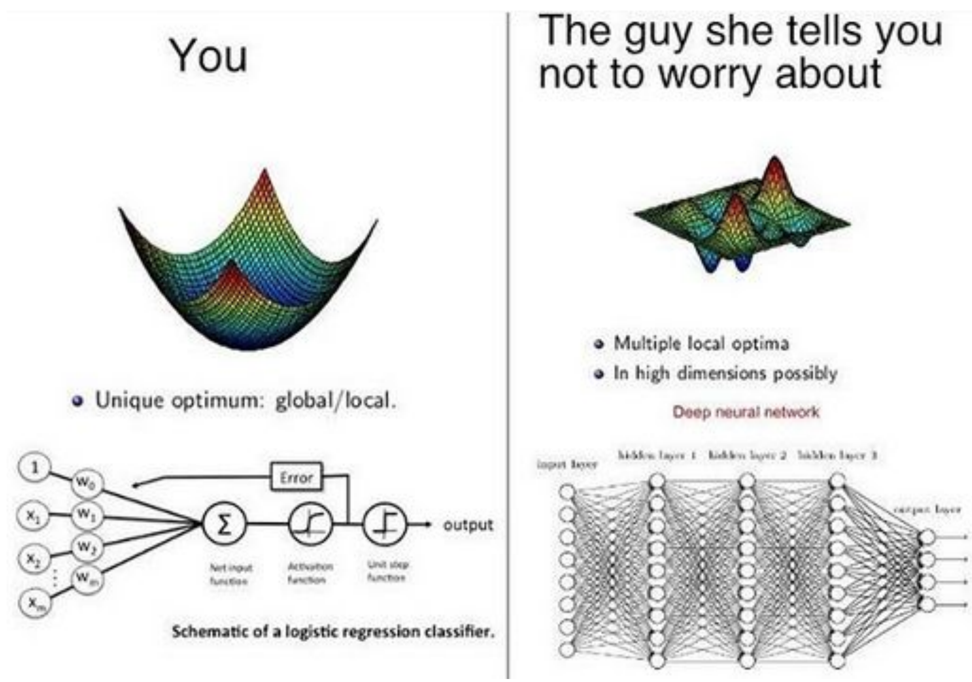
How to minimize the loss?

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

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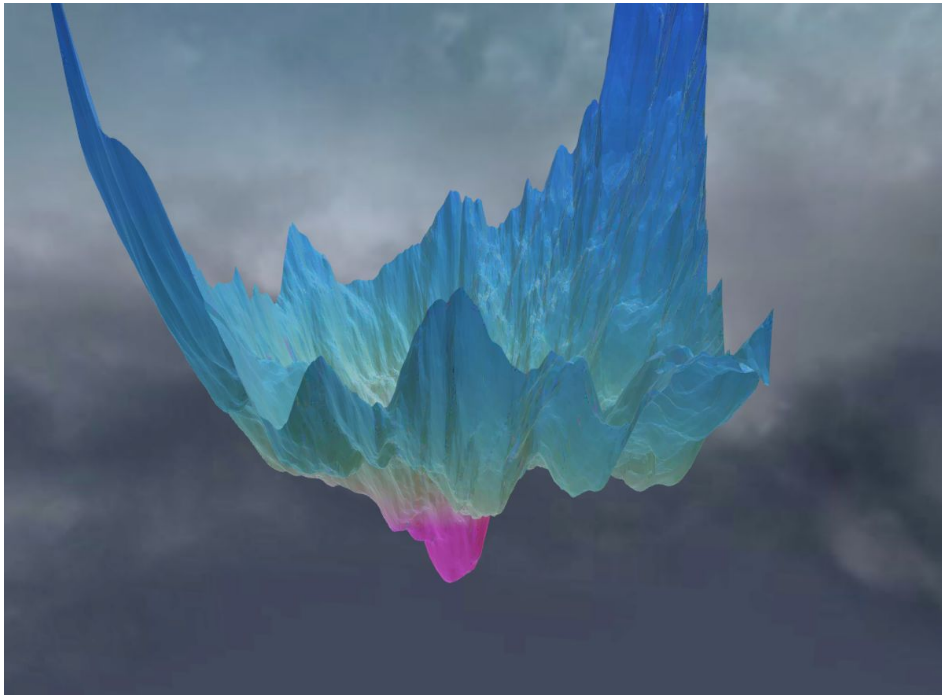
- Non-convex -> have different global and local minimum

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

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

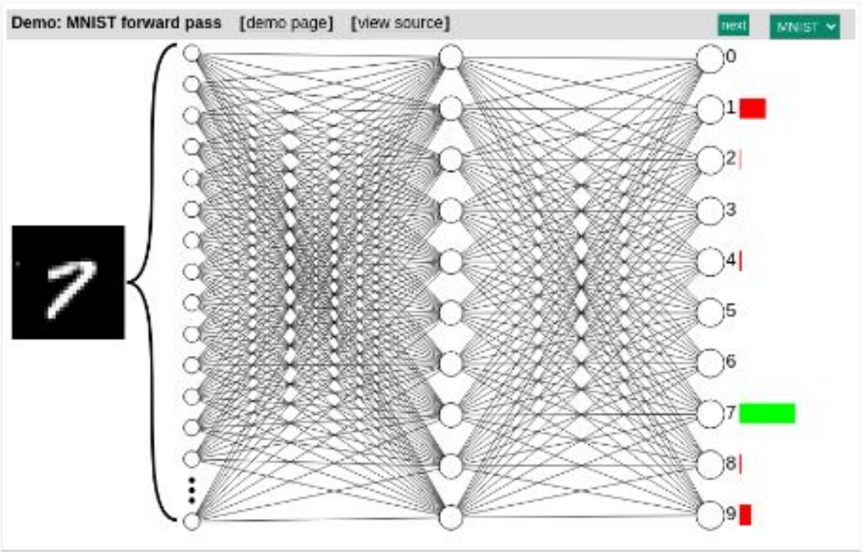
- Minibatch training <3 -> stochastic gradient descent

How to minimize the loss?

Computation Cost Problem

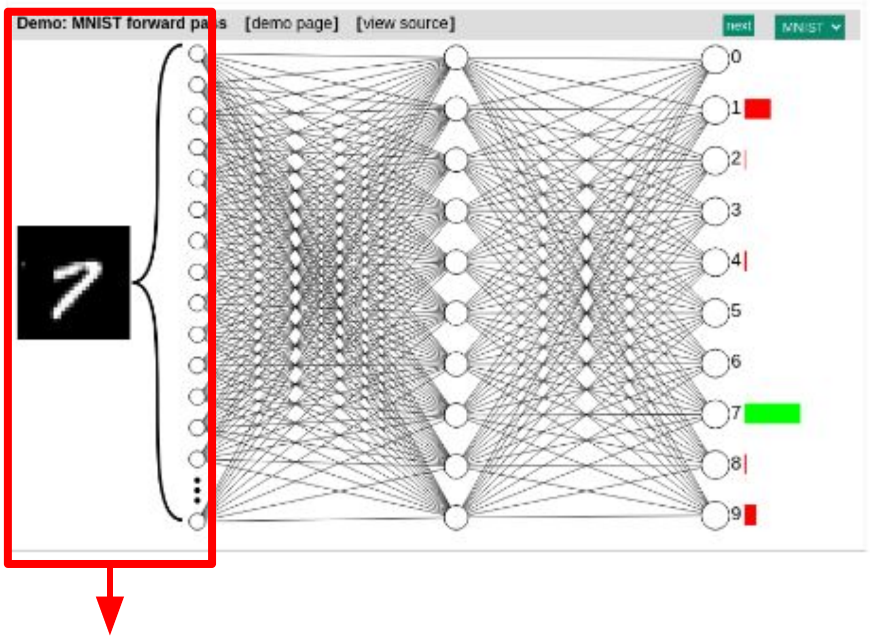
- Minibatch training <3 -> stochastic gradient descent
  - Minibatch size:
    - Too small batch size: optimization bounces around alot, and can lead to slower convergence to a minimum.
    - Too big batch size: won’t fit on GPU
    - Rule of thumb -> pick the largest batch size that fits in the GPU

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

Source:
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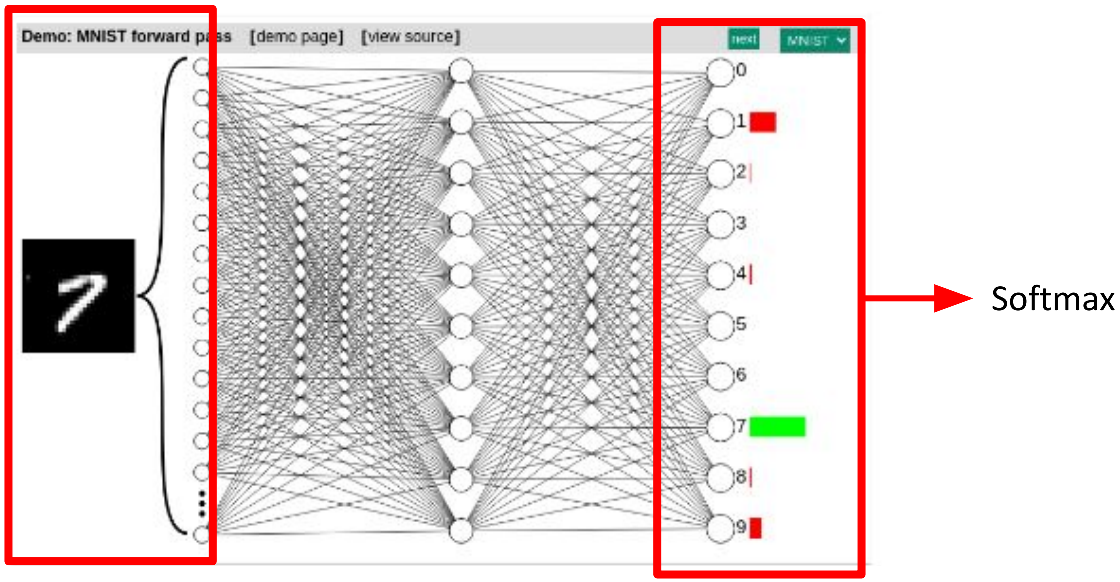

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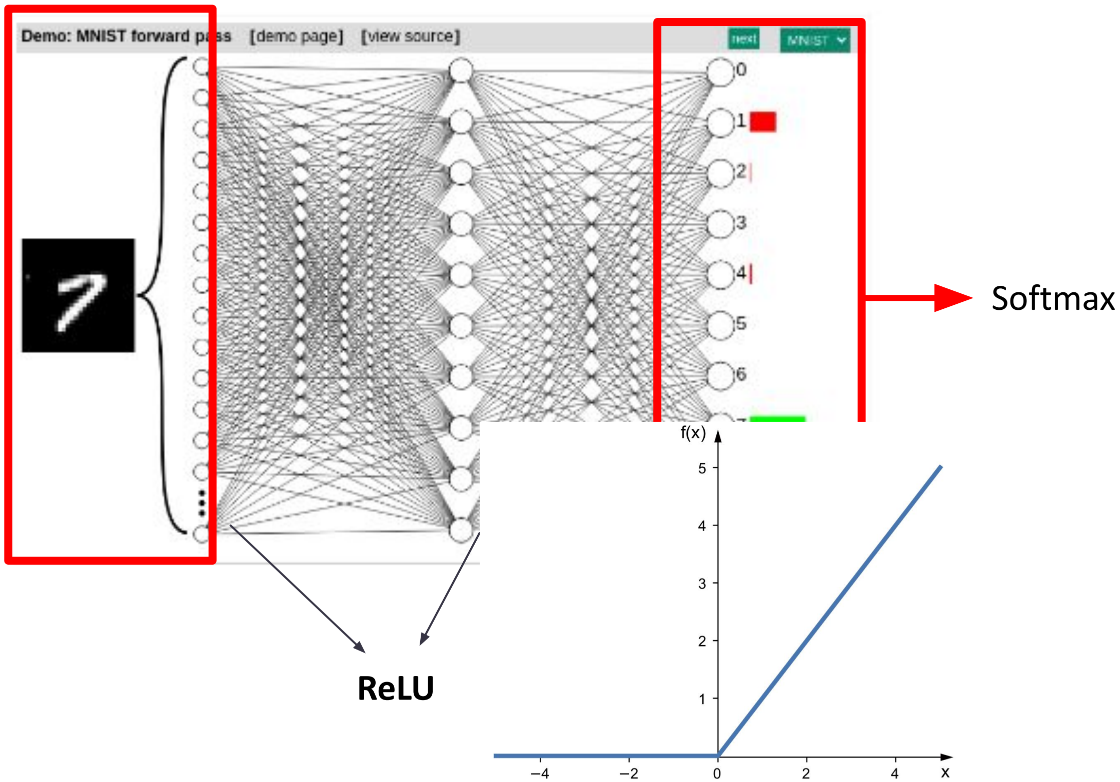

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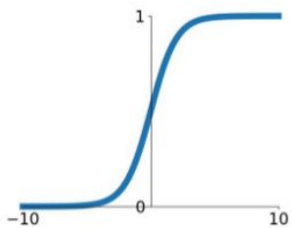
Activation Functions

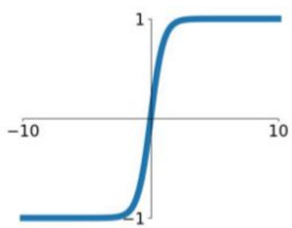
Sigmoid

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



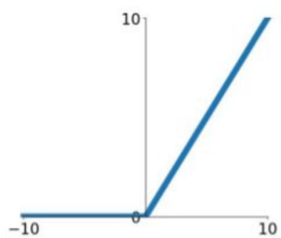
tanh

$\tanh(x)$



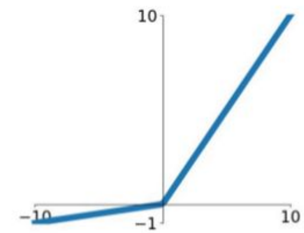
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

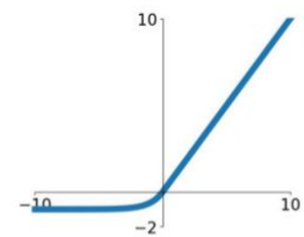


Maxout

$\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Source:
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