

Topics:

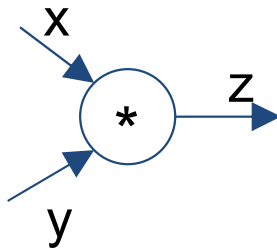
- Optimization

**CS 4644-DL / 7643-A**

**ZSOLT KIRA**

- **Assignment 1 – Due Friday!!!**
- **Assignment 2**
  - Implement convolutional neural networks
- **Piazza:** Start with public posts so that others can benefit!
  - Doesn't mean don't post!
- **Meta Lectures:** Data wrangling video available online, OH recordings available:
  - See dropbox link piazza @68 for lectures, @125 for first office hours **Thursday 4pm ET**
  - All OH are on the Canvas Zoom list!

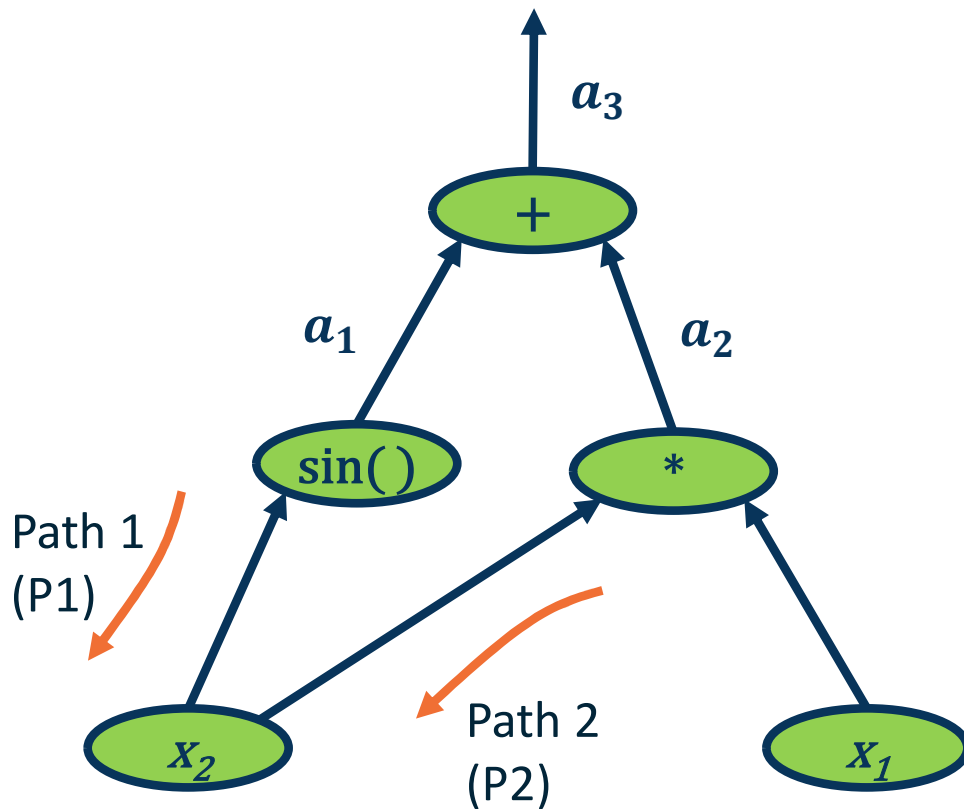
## Modularized implementation: forward / backward API



(x,y,z are scalars)

```
class MultiplyGate(object):  
    def forward(x,y):  
        z = x*y  
        self.x = x # must keep these around!  
        self.y = y  
        return z  
    def backward(dz):  
        dx = self.y * dz # [dz/dx * dL/dz]  
        dy = self.x * dz # [dz/dy * dL/dz]  
        return [dx, dy]
```

$$f(x_1, x_2) = x_1x_2 + \sin(x_2)$$



$$\bar{a}_3 = \frac{\partial f}{\partial a_3} = 1$$

$$\bar{a}_1 = \frac{\partial f}{\partial a_1} = \frac{\partial f}{\partial a_3} \frac{\partial a_3}{\partial a_1} = \frac{\partial f}{\partial a_3} \frac{\partial (a_1 + a_2)}{\partial a_1} = \frac{\partial f}{\partial a_3} \cdot 1 = \bar{a}_3$$

$$\bar{a}_2 = \frac{\partial f}{\partial a_2} = \frac{\partial f}{\partial a_3} \frac{\partial a_3}{\partial a_2} = \bar{a}_3$$

$$\bar{x}_2^{P1} = \frac{\partial f}{\partial a_1} \frac{\partial a_1}{\partial x_2} = \bar{a}_1 \cos(x_2)$$

$$\bar{x}_2^{P2} = \frac{\partial f}{\partial a_2} \frac{\partial a_2}{\partial x_2} = \frac{\partial f}{\partial a_2} \frac{\partial (x_1x_2)}{\partial x_2} = \bar{a}_2 x_1$$

$$\bar{x}_1 = \frac{\partial f}{\partial a_2} \frac{\partial a_2}{\partial x_1} = \bar{a}_2 x_2$$

Gradients from multiple paths summed

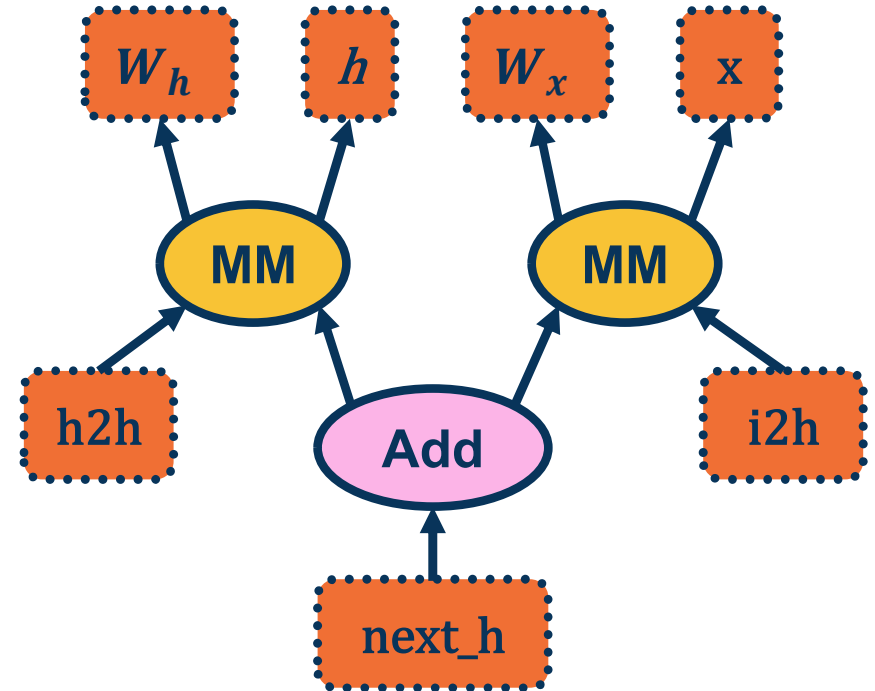
Example

## A graph is created on the fly

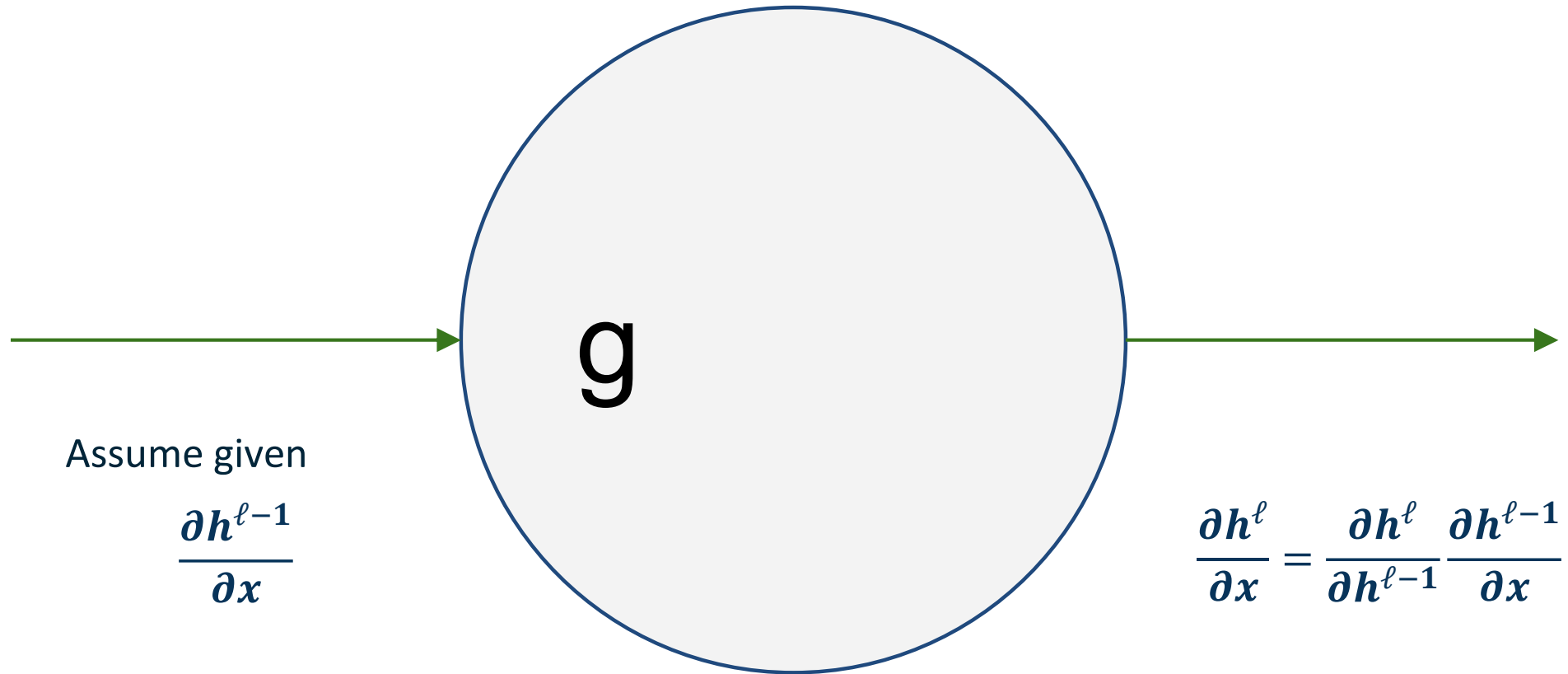
```
from torch.autograd import Variable

x = Variable(torch.randn(1, 20))
prev_h = Variable(torch.randn(1, 20))
W_h = Variable(torch.randn(20, 20))
W_x = Variable(torch.randn(20, 20))

i2h = torch.mm(W_x, x.t())
h2h = torch.mm(W_h, prev_h.t())
next_h = i2h + h2h
```

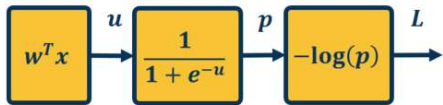


(Note above)



See [https://www.cc.gatech.edu/classes/AY2020/cs7643\\_spring/slides/autodiff\\_forward\\_reverse.pdf](https://www.cc.gatech.edu/classes/AY2020/cs7643_spring/slides/autodiff_forward_reverse.pdf)

## Forward Mode Autodifferentiation



$$L = \frac{1}{p}$$

$$\bar{p} = \frac{\partial L}{\partial p} = -\frac{1}{p^2}$$

where  $p = \sigma(w^T x)$  and  $\sigma(x) = \frac{1}{1+e^{-x}}$

$$\bar{u} = \frac{\partial L}{\partial u} = \frac{\partial L}{\partial p} \frac{\partial p}{\partial u} = \bar{p} \sigma(1-\sigma)$$

$$\bar{w} = \frac{\partial L}{\partial w} = \frac{\partial L}{\partial u} \frac{\partial u}{\partial w} = \bar{u} x^T$$

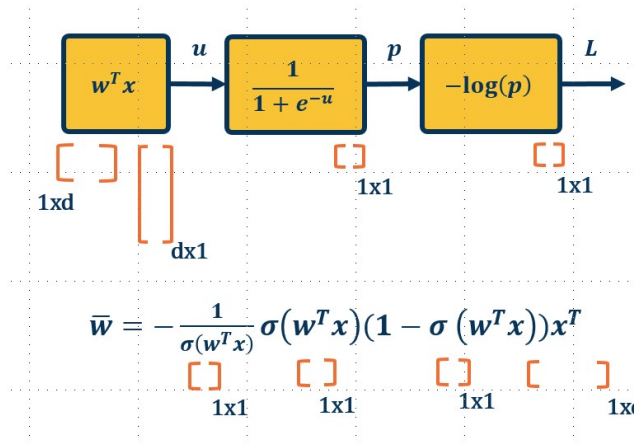
We can do this in a combined way to see all terms together:

$$\bar{w} = \frac{\partial L}{\partial p} \frac{\partial p}{\partial u} \frac{\partial u}{\partial w} = -\frac{1}{\sigma(w^T x)} \sigma(w^T x) (1 - \sigma(w^T x)) x^T$$

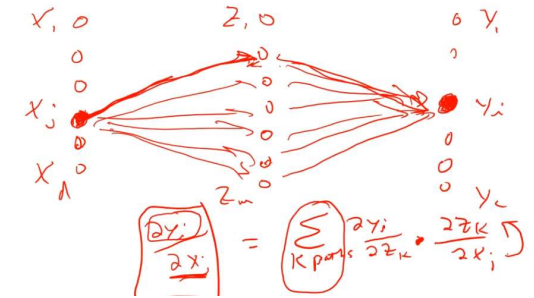
$$= -(1 - \sigma(w^T x)) x^T$$

This effectively shows gradient flow along path from  $L$  to  $w$

## Computation Graph / Global View of Chain Rule

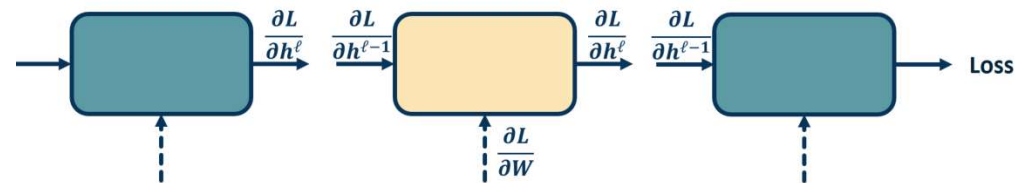


## Computational / Tensor View



## Graph View

● We want to compute:  $\left\{ \frac{\partial L}{\partial h^{\ell-1}}, \frac{\partial L}{\partial W} \right\}$

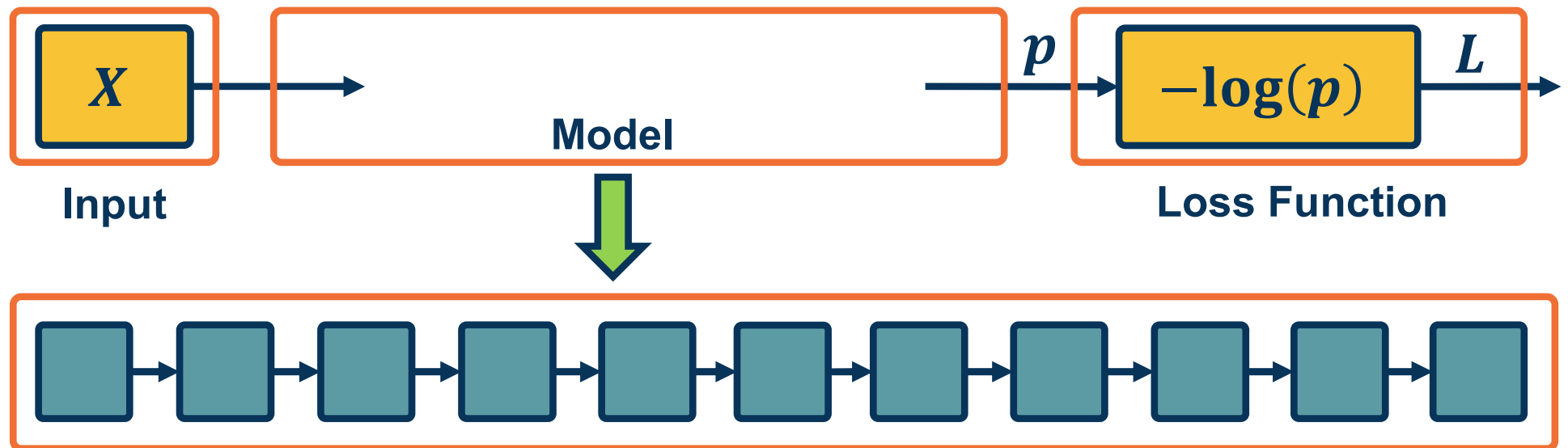


## Backpropagation View (Recursive Algorithm)

# Different Views of Equivalent Ideas

Backpropagation, and automatic differentiation, allows us to optimize **any** function composed of differentiable blocks

- ◆ **No need to modify** the learning algorithm!
- ◆ The complexity of the function is only limited by **computation and memory**

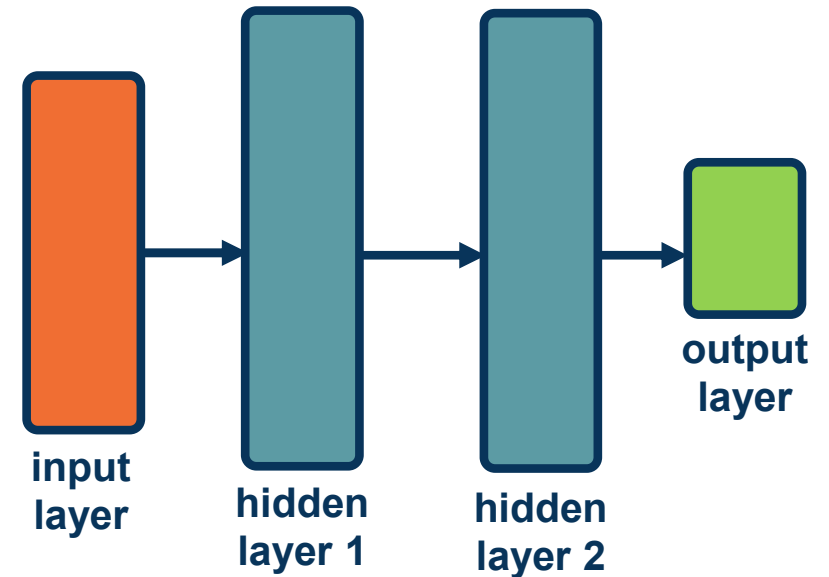




A network with two or more hidden layers is often considered a **deep** model

### Depth is important:

- Structure the model to represent an inherently compositional world
- Theoretical evidence that it leads to parameter efficiency
- Gentle dimensionality reduction (if done right)



# Convolutional network (AlexNet)

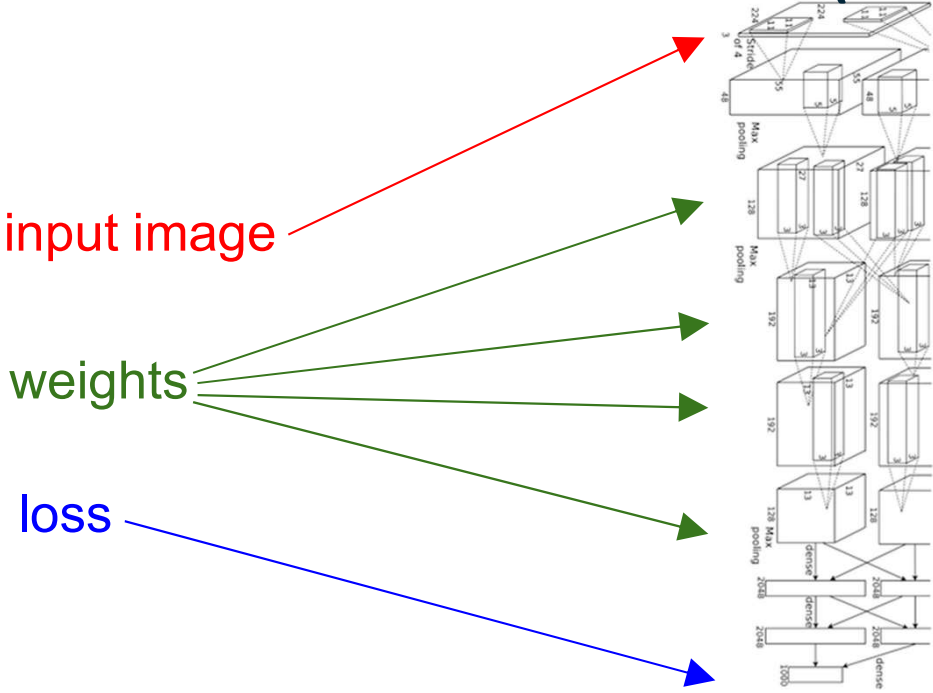


Figure copyright Alex Krizhevsky, Ilya Sutskever, and Geoffrey Hinton, 2012. Reproduced with permission.

# Neural Turing Machine

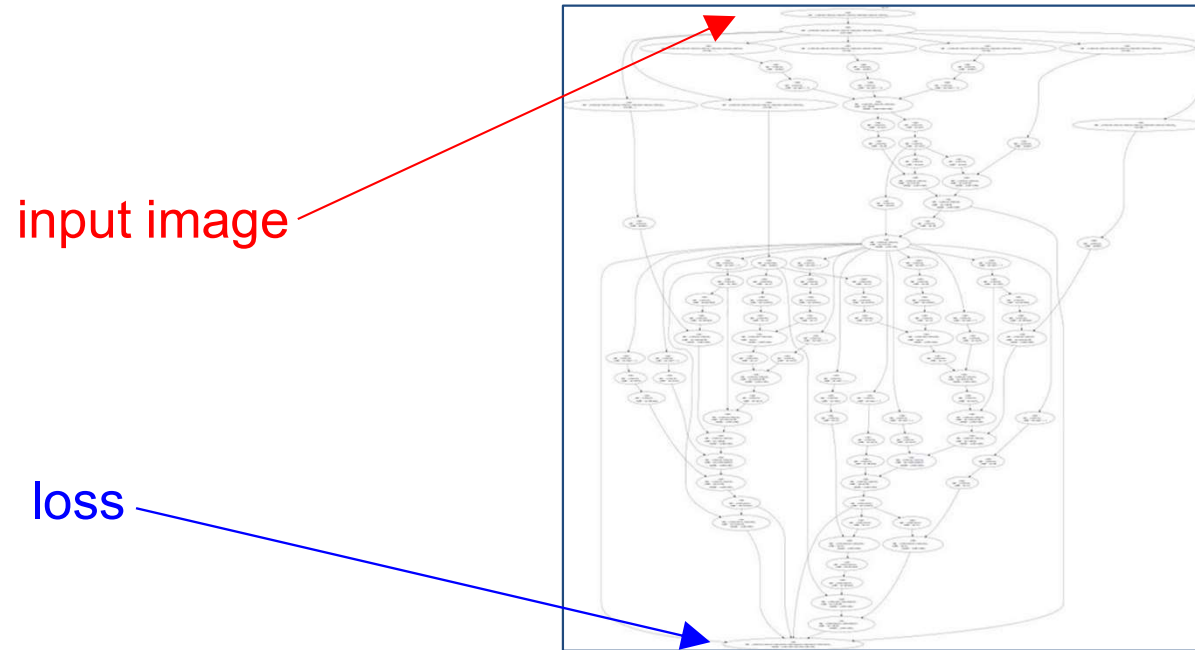
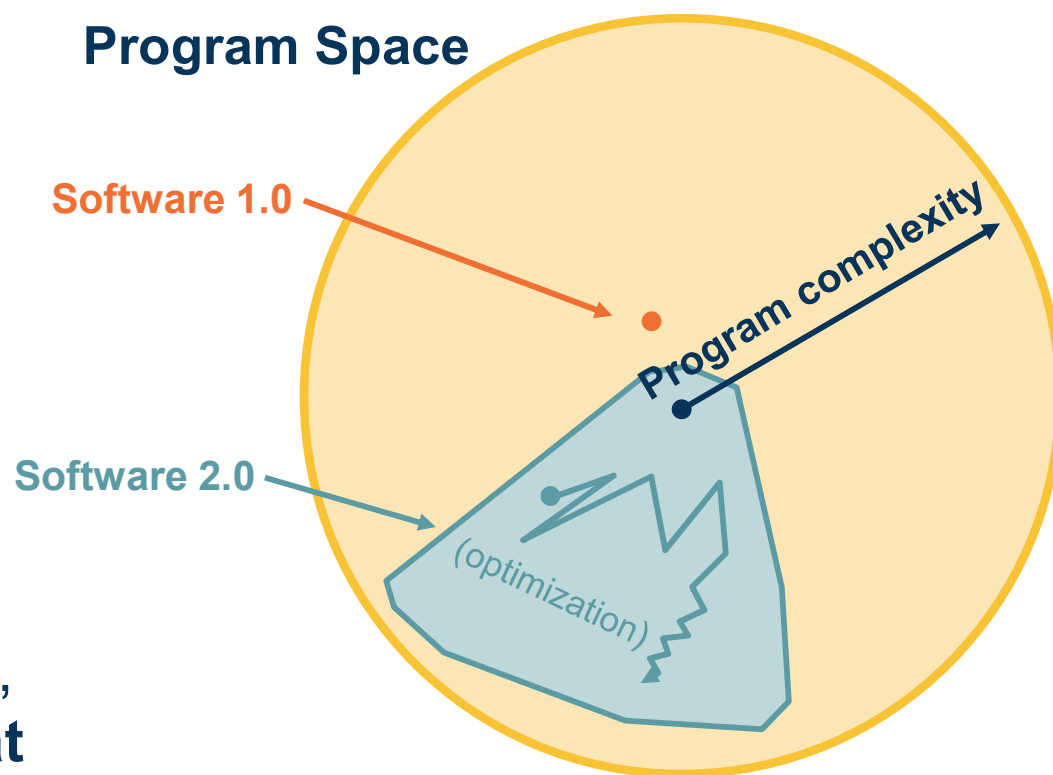


Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

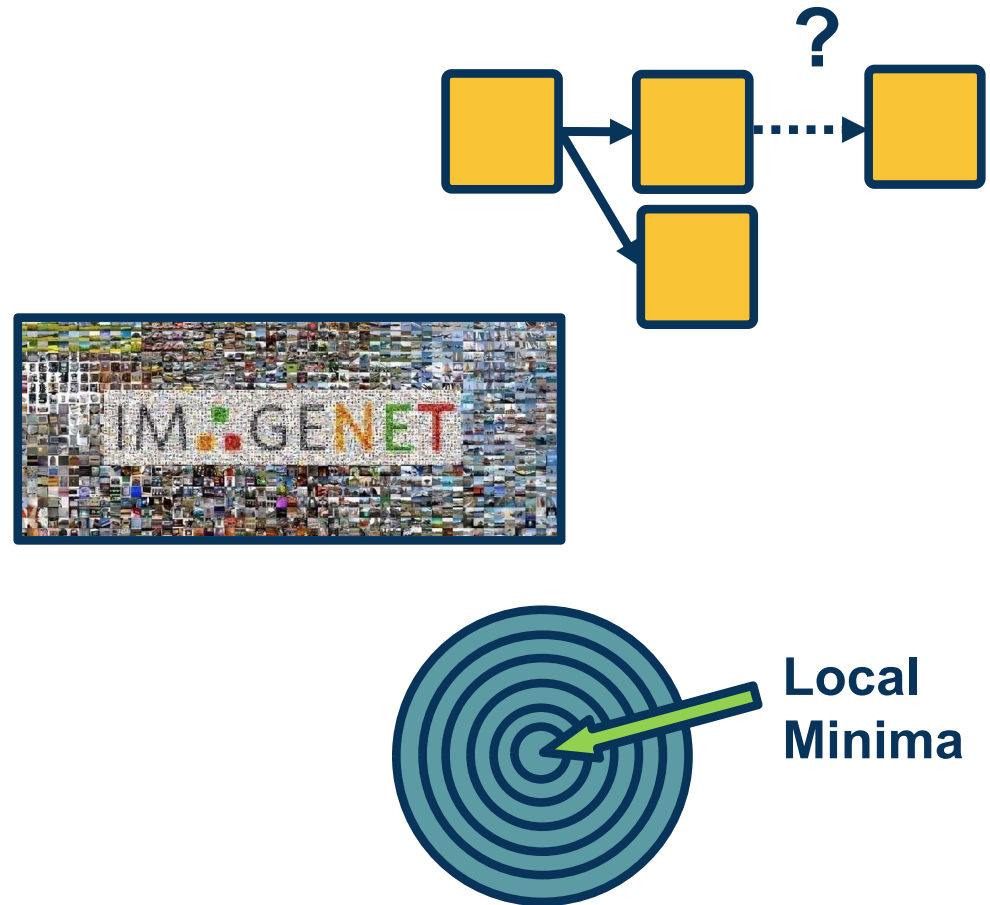
- Computation graphs are **not limited to mathematical functions!**
- Can have **control flows** (if statements, loops) and **backpropagate** through **algorithms!**
- Can be done **dynamically** so that **gradients are computed**, then **nodes are added**, repeat
- **Differentiable programming**



*Adapted from figure by Andrej Karpathy*

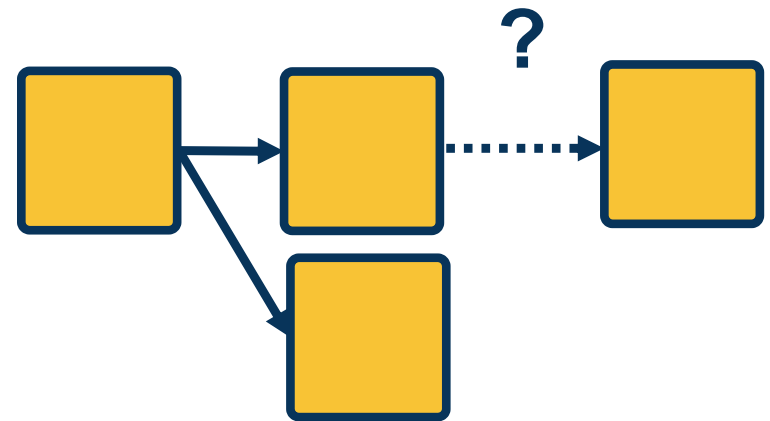
There are still many design decisions that must be made:

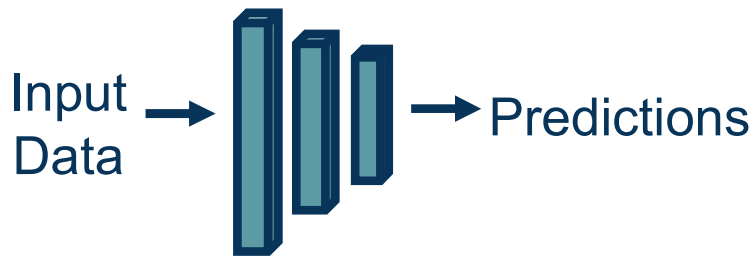
- ◆ **Architecture**
- ◆ **Data Considerations**
- ◆ **Training and Optimization**
- ◆ **Machine Learning Considerations**



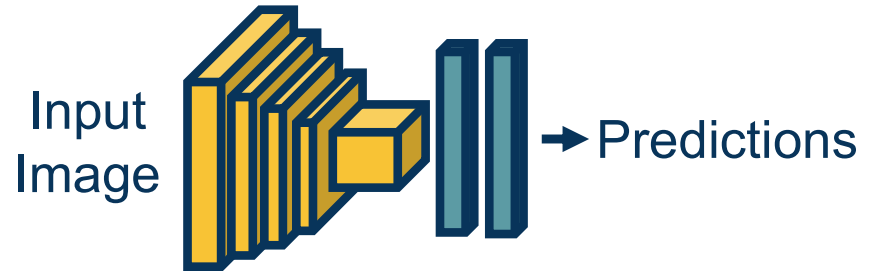
We must design the **neural network architecture**:

- ◆ What **modules (layers)** should we use?
- ◆ How should they **be connected together**?
- ◆ Can we use our **domain knowledge** to add architectural biases?

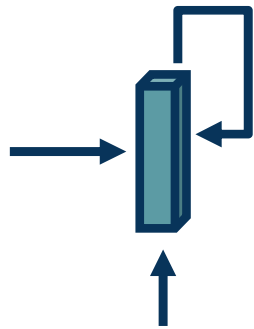




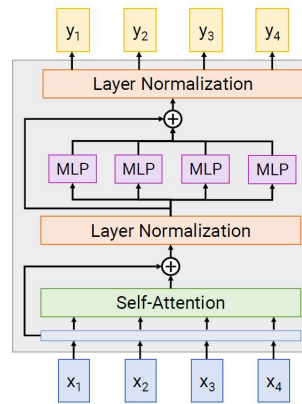
**Fully Connected Neural Network**



**Convolutional Neural Networks**



**Recurrent Neural Network**



**Transformers**

Different architectures are suitable for different applications or types of input

**Example Architectures**



As in traditional machine learning, **data** is key:

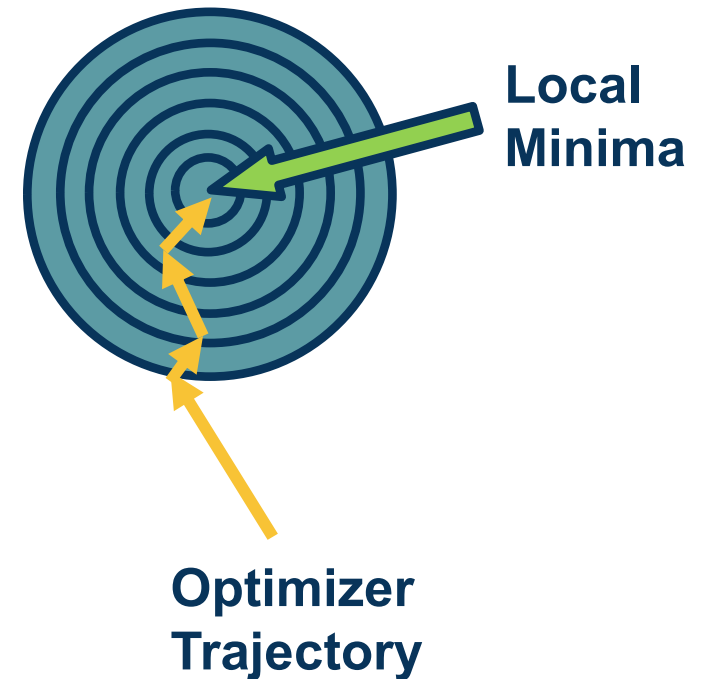
- ◆ Should we **pre-process** the data?
- ◆ Should we **normalize** it?
- ◆ Can we **augment** our data by adding noise or other perturbations?





Even given a good neural network architecture, we need a **good optimization algorithm to find good weights**

- What **optimizer** should we use?
  - Different optimizers make **different weight updates** depending on the gradients
- How should we **initialize** the weights?
- What **regularizers** should we use?
- What **loss function** is appropriate?



## Machine Learning Considerations

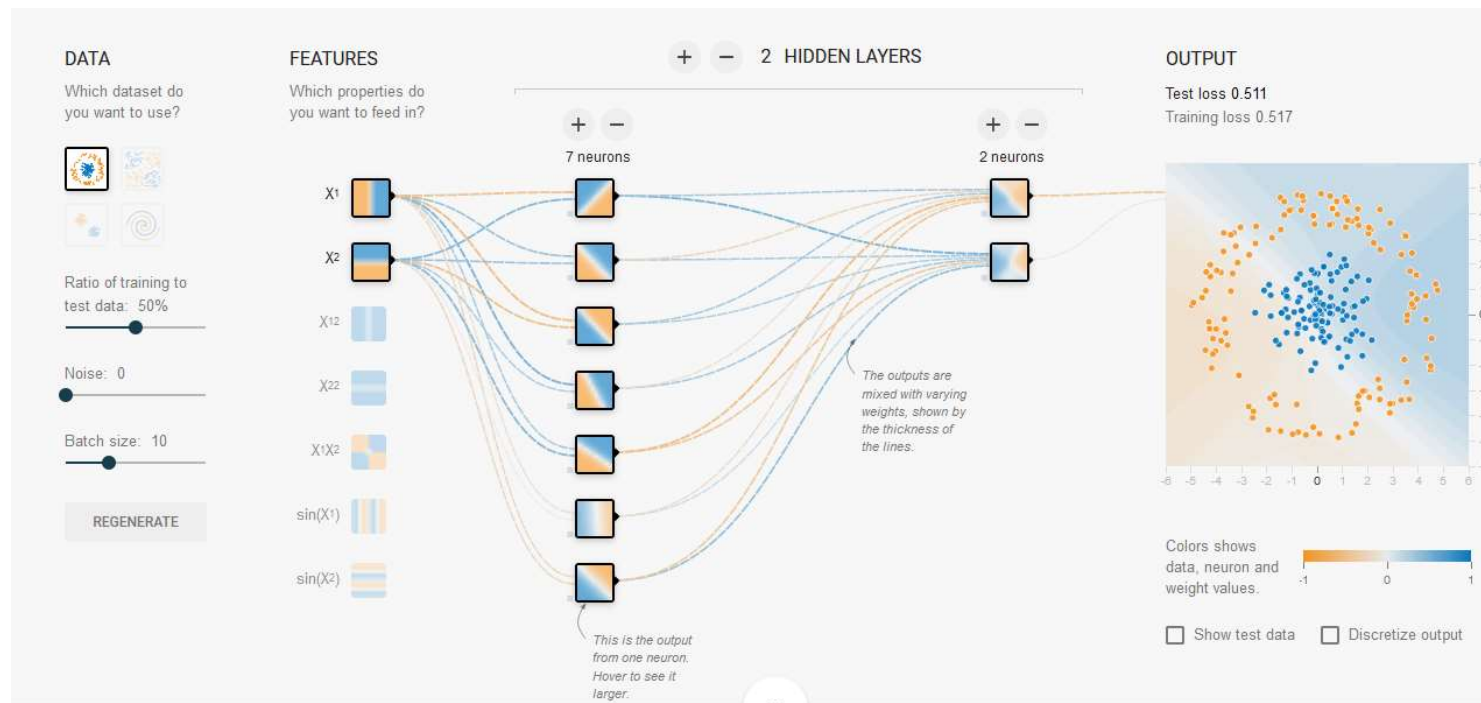
The practice of machine learning is **complex**: For your particular application you have to **trade off** all of the considerations together

- ◆ Trade-off between **model capacity** (e.g. measured by # of parameters) and **amount of data**
- ◆ Adding **appropriate biases** based on knowledge of the domain



# Demo

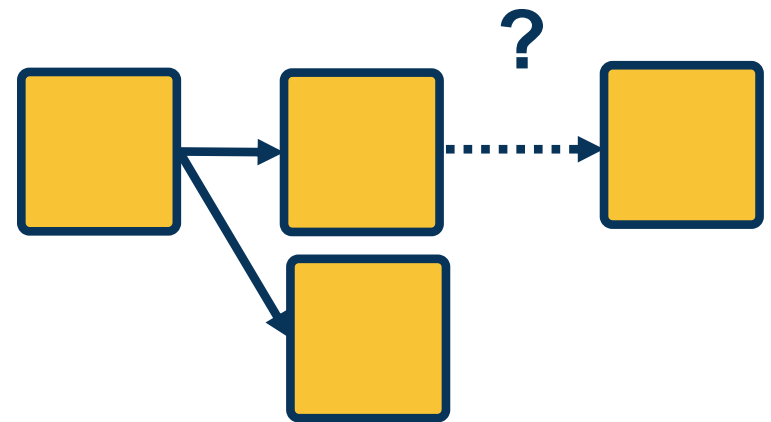
- <http://playground.tensorflow.org>



# Architectural Considerations

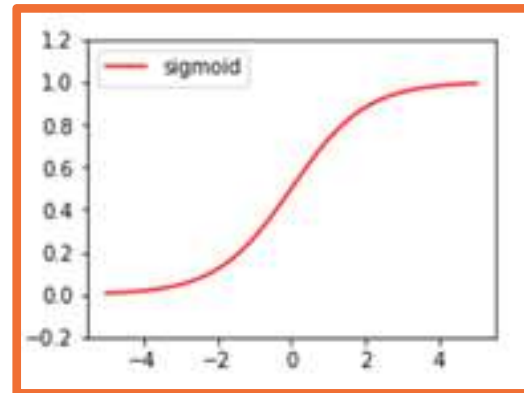
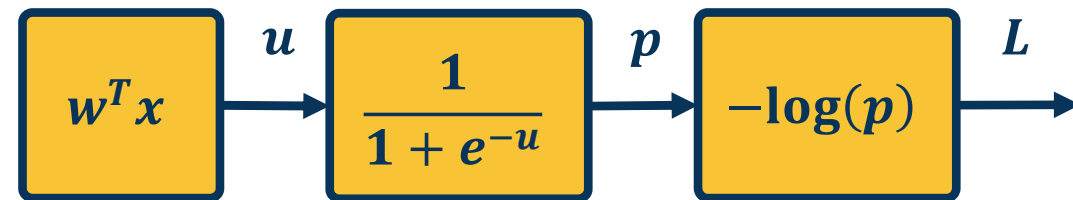
Determining what modules to use, and how to connect them is part of the **architectural design**

- ◆ Guided by the **type of data used** and its **characteristics**
  - ◆ Understanding your data is always the first step!
- ◆ **Lots of data types (modalities)** already have good architectures
  - ◆ Start with what others have discovered!
- ◆ **The flow of gradients** is one of the key principles to use when analyzing layers



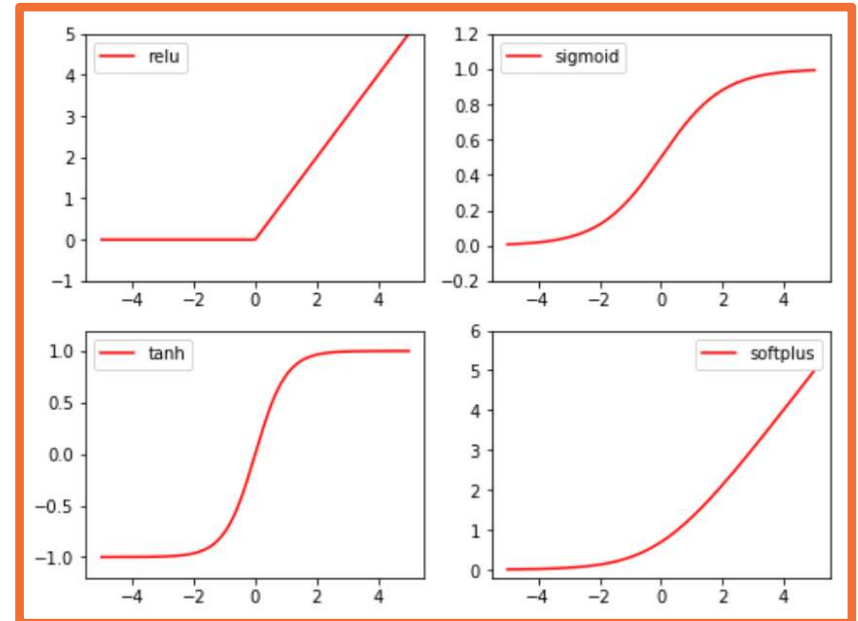
- ◆ **Combination** of linear and non-linear layers
- ◆ Combination of **only** linear layers has same representational power as one linear layer
- ◆ **Non-linear layers** are crucial
  - ◆ Composition of non-linear layers **enables complex transformations of the data**

$$w_1^T(w_2^T(w_3^T x)) = w_4^T x$$



Several aspects that we can **analyze**:

- Min/Max
- Correspondence between input & output statistics
- **Gradients**
  - At initialization (e.g. small values)
  - At extremes
- Computational complexity

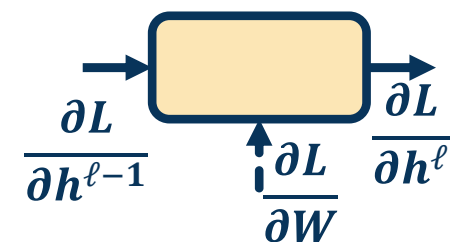


- Min: 0, Max: 1
- Output always positive
- Saturates at both ends
- Gradients
  - Vanishes at both end
  - Always positive
- Computation: Exponential term



$$h^\ell = \sigma(h^{\ell-1})$$

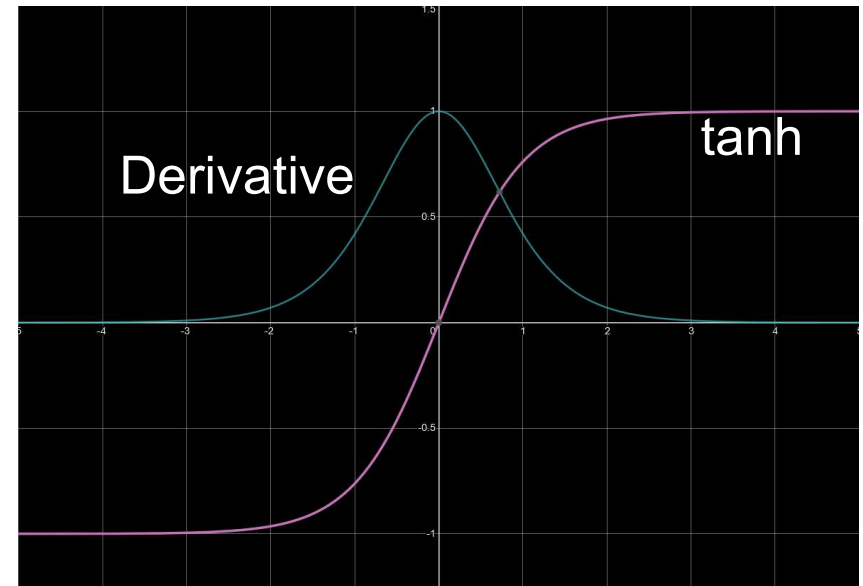
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



$$\frac{\partial L}{\partial W} = \frac{\partial L}{\partial h^\ell} \frac{\partial h^\ell}{\partial W}$$

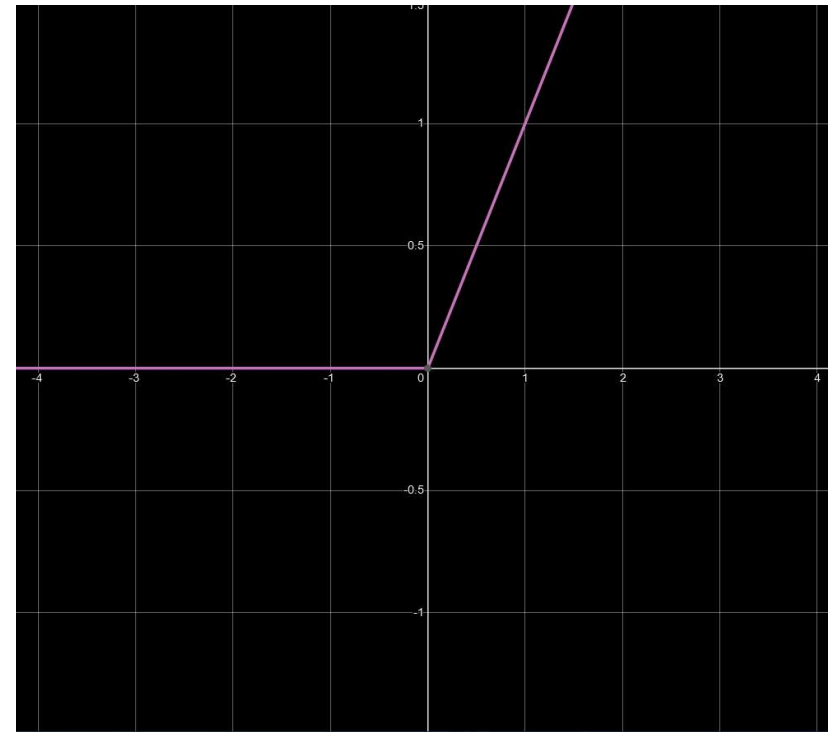


- **Min: -1, Max: 1**
- **Centered**
- **Saturates at both ends**
- **Gradients**
  - Vanishes at both end
  - Always positive
- **Still somewhat computationally heavy**



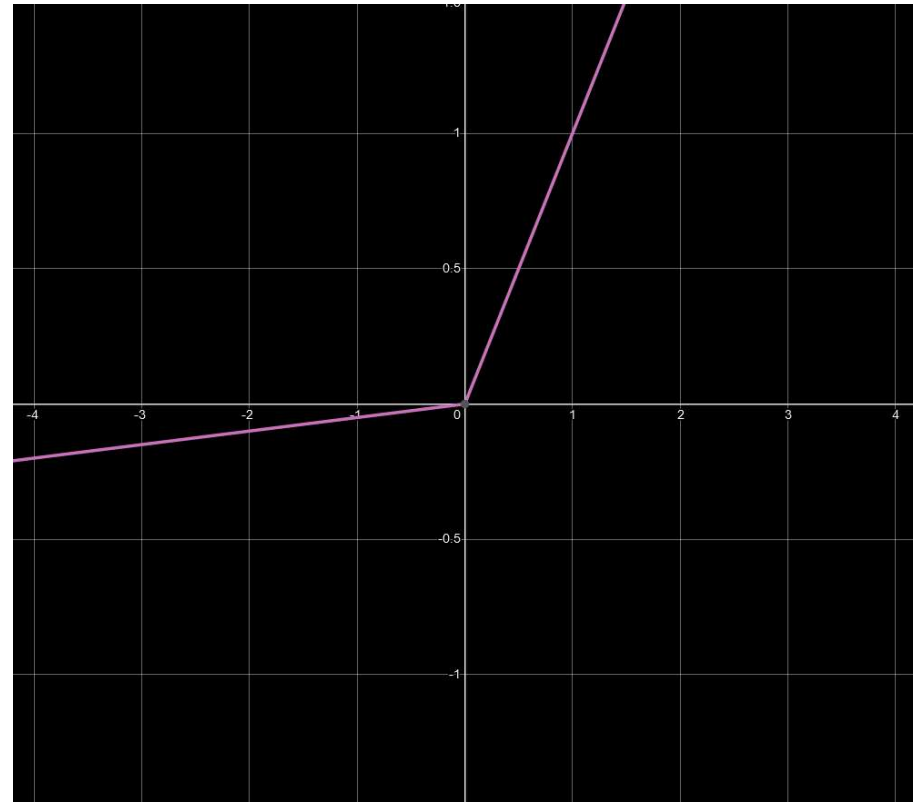
$$h^{\ell} = \tanh(h^{\ell-1})$$

- **Min: 0, Max: Infinity**
- Output always **positive**
- **No saturation** on positive end!
- **Gradients**
  - 0 if  $x \leq 0$  (dead ReLU)
  - Constant otherwise (does not vanish)
- **Cheap to compute (max)**



$$h^\ell = \max(0, h^{\ell-1})$$

- **Min: -Infinity, Max: Infinity**
- **Learnable parameter!**
- **No saturation**
- **Gradients**
  - No dead neuron
- **Still cheap to compute**



$$h^l = \max(\alpha h^{l-1}, h^{l-1})$$

**Leaky ReLU**

## Selecting a Non-Linearity

Which **non-linearity** should you select?

- ◆ Unfortunately, **no one activation function is best** for all applications
- ◆ **ReLU** is most common starting point
  - ◆ Sometimes leaky ReLU can make a big difference
- ◆ **Sigmoid** is typically avoided unless clamping to values from  $[0,1]$  is needed



# Initialization

## Initializing the Parameters

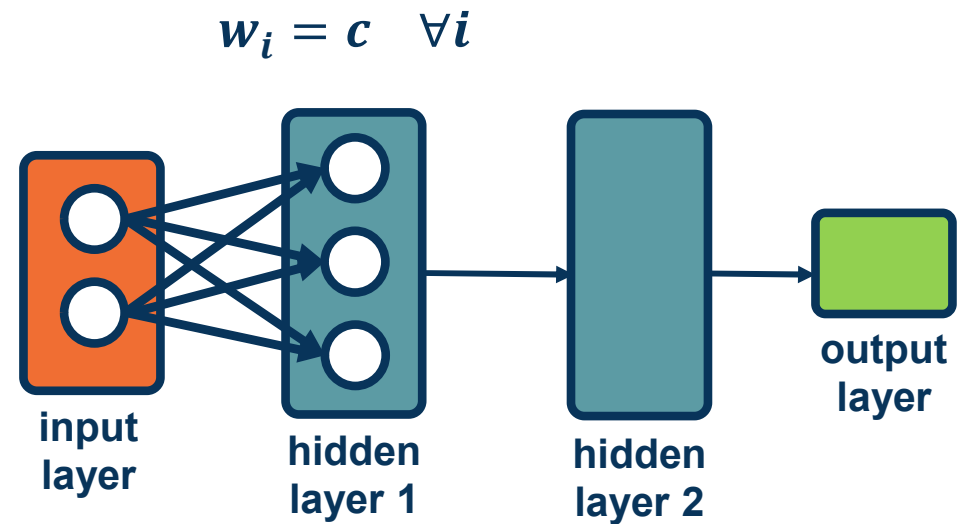
The parameters of our model must be **initialized to something**

- ◆ Initialization is **extremely important!**
  - ◆ Determines how **statistics of outputs** (given inputs) behave
  - ◆ Determines how well **gradients flow** in the beginning of training (important)
  - ◆ Could **limit use of full capacity** of the model if done improperly
- ◆ Initialization that is **close to a good (local) minima** will converge faster and to a better solution



Initializing values to a constant value leads to a **degenerate solution!**

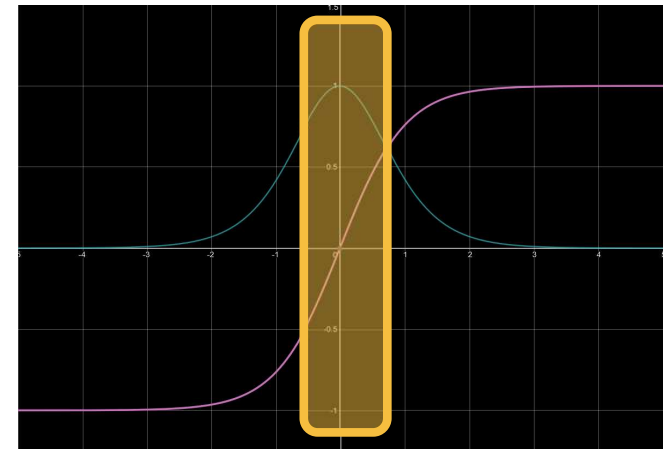
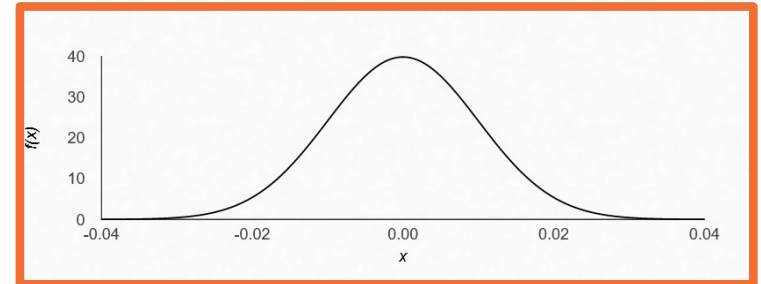
- What happens to the **weight updates**?
- Each node has the same input from previous layers so gradients **will be the same**
- As a results, **all weights will be updated** to the same exact values



**A Poor Initialization**

Common approach is **small normally distributed random numbers**

- E.g.  $N(\mu, \sigma)$  where  $\mu = 0, \sigma = 0.01$
- **Small weights** are preferred since no feature/input has prior importance
- Keeps the model within the **linear region of most activation functions**

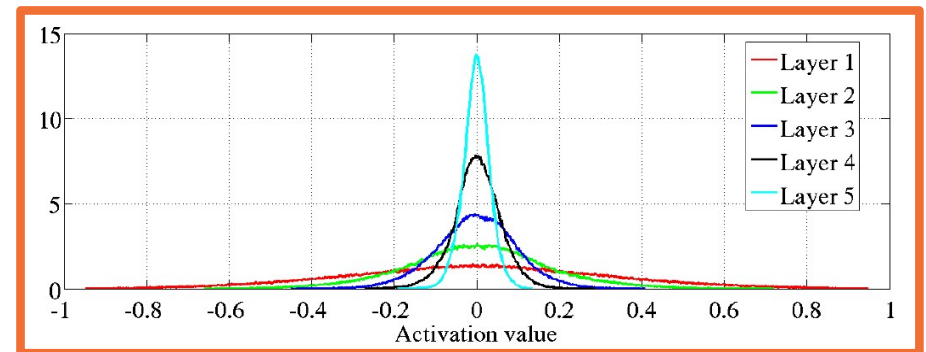


**Gaussian/Normal Initialization**



## Deeper networks (with many layers) are more sensitive to initialization

- With a deep network, **activations (outputs of nodes) get smaller**
- Standard deviation reduces significantly
- Leads to small updates** – smaller values multiplied by upstream gradients



**Distribution of activation values of a network with tanh nonlinearities, for increasingly deep layers**

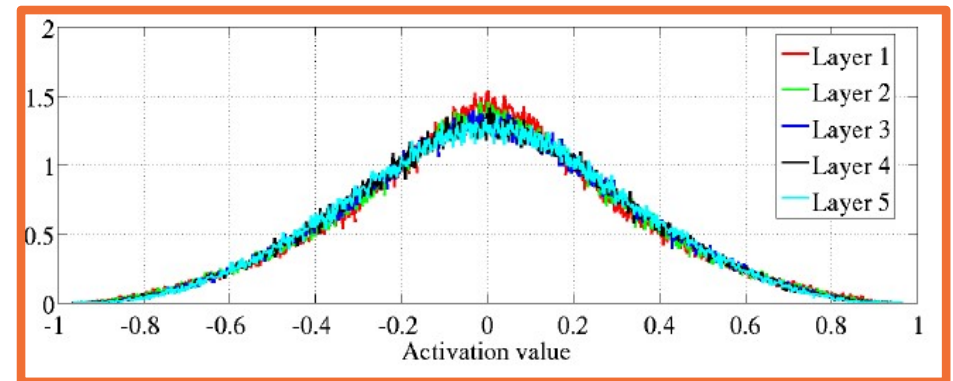
*From "Understanding the difficulty of training deep feedforward neural networks." AISTATS, 2010.*

Ideally, we'd like to maintain the variance at the output to be similar to that of input!

- This condition leads to a **simple initialization rule**, sampling from uniform distribution:

$$\text{Uniform}\left(-\frac{\sqrt{6}}{n_j+n_{j+1}}, +\frac{\sqrt{6}}{n_j+n_{j+1}}\right)$$

- Where  $n_j$  is **fan-in** (number of input nodes) and  $n_{j+1}$  is **fan-out** (number of output nodes)



**Distribution of activation values of a network with tanh nonlinearities, for increasingly deep layers**

*From "Understanding the difficulty of training deep feedforward neural networks." AISTATS, 2010.*

**Xavier Initialization**

In practice, **simpler versions** perform empirically well:

$$N(\mathbf{0}, \mathbf{1}) * \sqrt{\frac{1}{n_j}}$$

- ◆ This analysis holds for **tanh or similar activations**.
- ◆ Similar analysis for **ReLU activations** leads to:

$$N(\mathbf{0}, \mathbf{1}) * \sqrt{\frac{1}{n_j/2}}$$

*"Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification", ICCV, 2015.*

**(Simpler) Xavier and Xavier2 Initialization**



## Summary

Key takeaway: **Initialization matters!**

- ◆ Determines the **activation** (output) statistics, and therefore **gradient statistics**
- ◆ If gradients are **small**, no learning will occur and no improvement is possible!
- ◆ Important to reason about **output/gradient statistics** and analyze them for new layers and architectures



# **Normalization, Preprocessing, and Augmentation**

## Importance of Data

In deep learning, **data drives learning** of features and classifier

- ◆ Its **characteristics** are therefore extremely important
- ◆ Always **understand your data!**
- ◆ **Relationship** between output statistics, layers such as non-linearities, and gradients is important



Just like initialization, **normalization** can improve gradient flow and learning

Typically **normalization methods** apply:

- ◆ Subtract mean, divide by standard deviation (**most common**)
  - ◆ This can be done **per dimension**
- ◆ Whitening, e.g. through Principle Component Analysis (PCA) (**not common**)

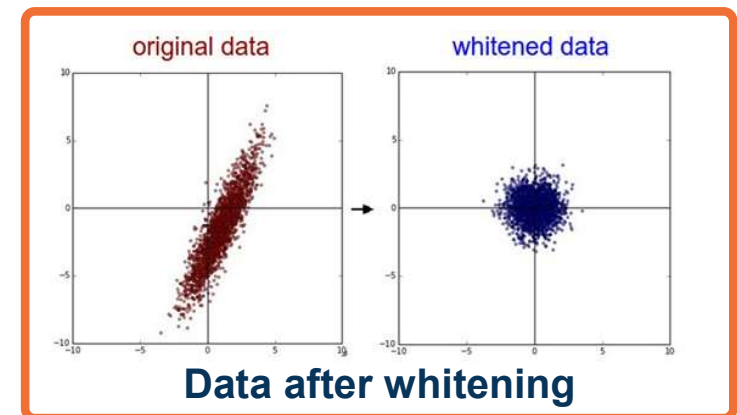
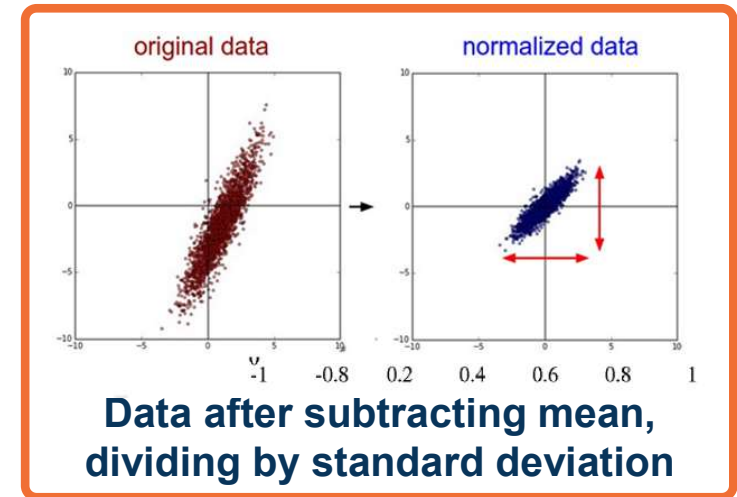


Figure from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

- We can try to come up with a *layer* that can normalize the data across the neural network
- **Given:** A mini-batch of data  $[B \times D]$  where  $B$  is batch size
- Compute mean and variance **for each dimension  $d$**

**Input:** Values of  $x$  over a mini-batch:  $\mathcal{B} = \{x_{1\dots m}\}$ ;

Parameters to be learned:  $\gamma, \beta$

**Output:**  $\{y_i = \text{BN}_{\gamma, \beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^m x_i \quad // \text{ mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2 \quad // \text{ mini-batch variance}$$

From: *Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift*, Sergey Ioffe, Christian Szegedy

## Making Normalization a Layer



## Normalize data

$$\hat{x}_i = \frac{x_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

**Note:** This part does not involve new parameters

**Input:** Values of  $x$  over a mini-batch:  $\mathcal{B} = \{x_1 \dots x_m\}$ ;  
Parameters to be learned:  $\gamma, \beta$

**Output:**  $\{y_i = \text{BN}_{\gamma, \beta}(x_i)\}$

$$\mu_B \leftarrow \frac{1}{m} \sum_{i=1}^m x_i \quad // \text{ mini-batch mean}$$

$$\sigma_B^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_B)^2 \quad // \text{ mini-batch variance}$$

$$\hat{x}_i \leftarrow \frac{x_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}} \quad // \text{ normalize}$$

From: *Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift*, Sergey Ioffe, Christian Szegedy

Normalizing the Data



- ◆ We can give the model flexibility through **learnable parameters  $\gamma$  (scale) and  $\beta$  (shift)**
- ◆ Network can learn to **not normalize** if necessary!
- ◆ This layer is called a **Batch Normalization (BN) layer**

**Input:** Values of  $x$  over a mini-batch:  $\mathcal{B} = \{x_{1\dots m}\}$ ;

Parameters to be learned:  $\gamma, \beta$

**Output:**  $\{y_i = \text{BN}_{\gamma, \beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^m x_i \quad // \text{ mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2 \quad // \text{ mini-batch variance}$$

$$\hat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \quad // \text{ normalize}$$

$$y_i \leftarrow \gamma \hat{x}_i + \beta \equiv \text{BN}_{\gamma, \beta}(x_i) \quad // \text{ scale and shift}$$

*From: Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift, Sergey Ioffe, Christian Szegedy*

## Learnable Scaling and Offset

## Some Complexities of BN

**During inference**, stored mean/variances calculated on training set are used

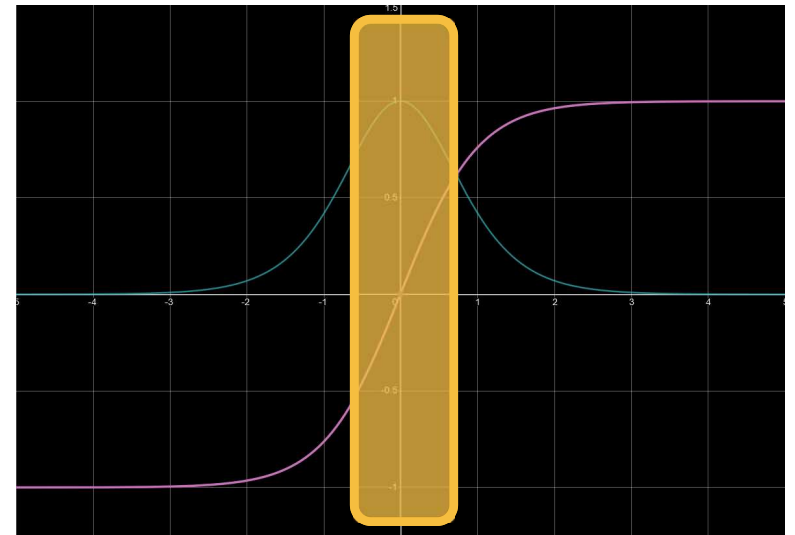
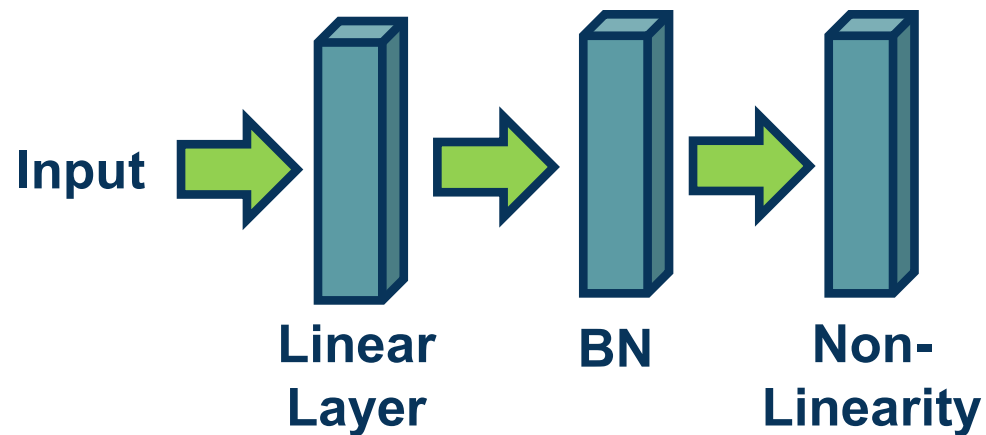
**Sufficient batch sizes** must be used to get stable per-batch estimates during training

- ◆ This is especially an issue when **using multi-GPU or multi-machine training**
- ◆ **Use `torch.nn.SyncBatchNorm`** to estimate batch statistics in these settings



Normalization especially important before **non-linearities!**

- Very low/high values (un-normalized/imbalanced data) cause **saturation**



Where to Apply BN

## Generalization of BN

There are many variations of batch normalization

- ◆ See Convolutional Neural Network lectures for an example

Resource:

- ◆ [ML Explained - Normalization](#)



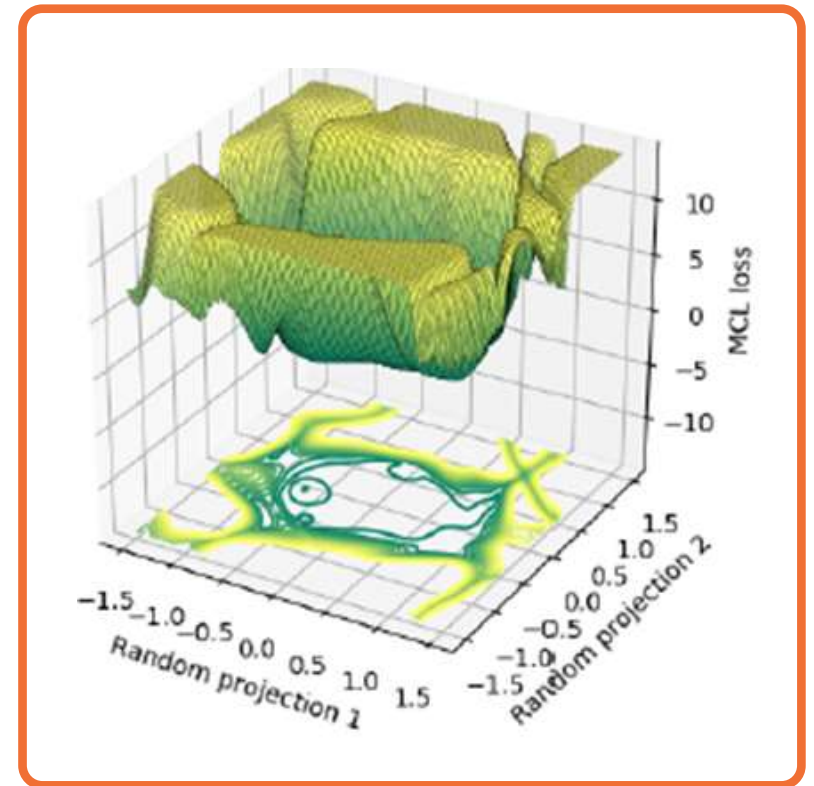
# Optimizers

Deep learning involves **complex, compositional, non-linear functions**

The **loss landscape** is extremely **non-convex** as a result

There is **little direct theory** and a **lot of intuition/rules of thumbs** instead

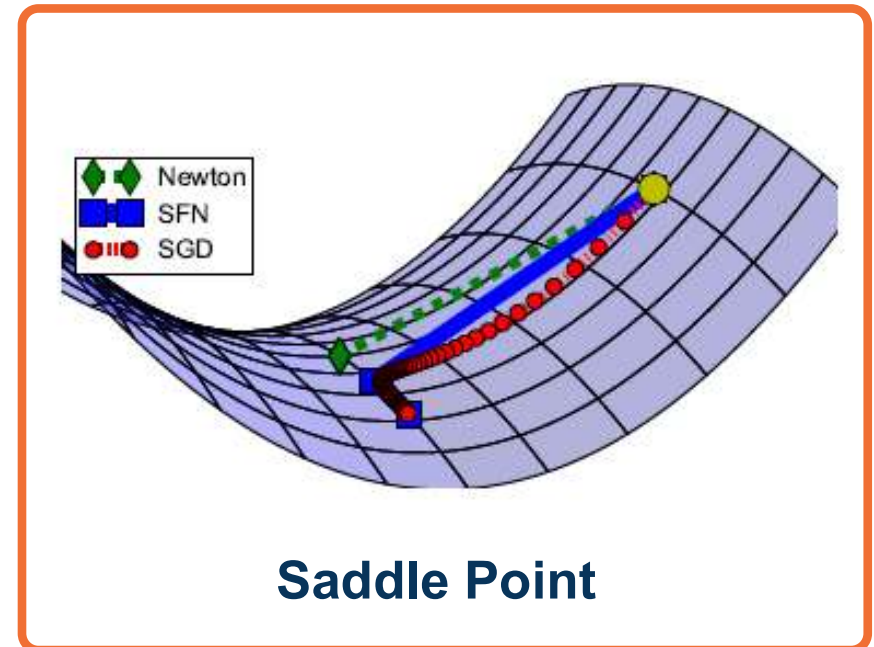
- Some insight can be gained via theory for simpler cases (e.g. convex settings)



It used to be thought that **existence of local minima is the main issue** in optimization

There are other **more impactful issues**:

- ◆ Noisy gradient estimates
- ◆ Saddle points
- ◆ Ill-conditioned loss surface

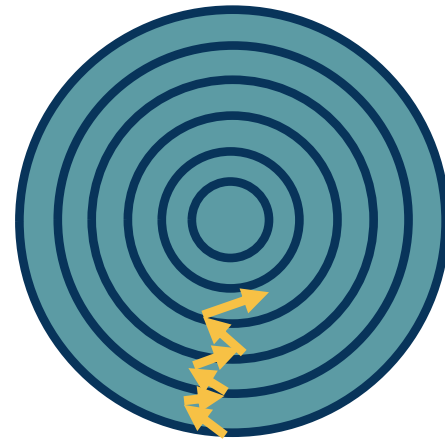


*From: Identifying and attacking the saddle point problem in high-dimensional non-convex optimization, Dauphi et al., 2014.*



- ◆ We use a **subset of the data at each iteration** to calculate the loss (& gradients)
- ◆ This is an **unbiased** estimator but can have high variance
- ◆ This results in **noisy steps** in gradient descent

$$L = \frac{1}{M} \sum L(f(x_i, W), y_i)$$

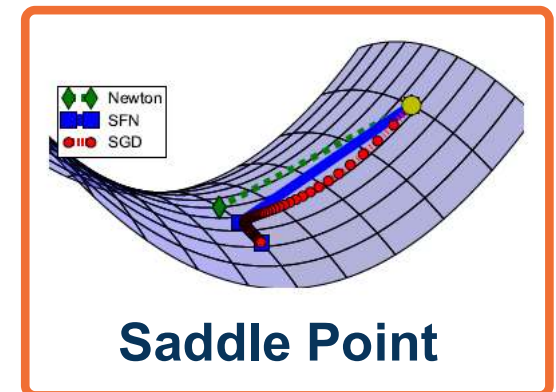
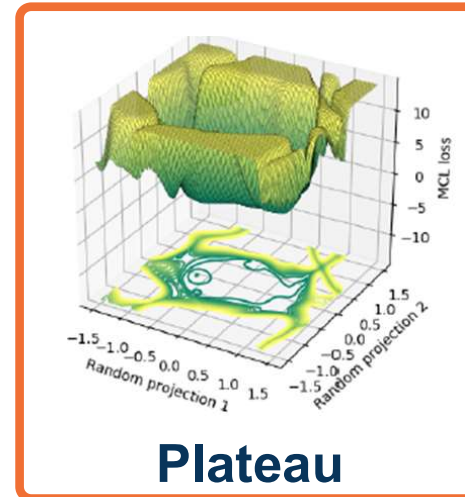


Several **loss surface geometries** are difficult for optimization

Several **types of minima**: Local minima, plateaus, saddle points

**Saddle points** are those where the gradient of orthogonal directions are zero

- But they **disagree** (it's min for one, max for another)



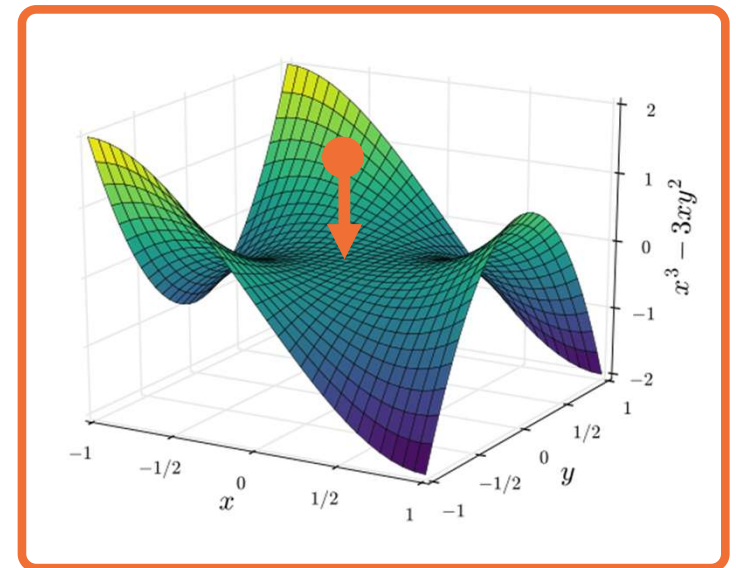
- Gradient descent takes a step in the **steepest direction** (negative gradient)
- Intuitive idea:** Imagine a ball rolling down loss surface, and use **momentum** to pass flat surfaces

$$w_i = w_{i-1} - \alpha \frac{\partial L}{\partial w_i}$$

$$v_i = \beta v_{i-1} + \frac{\partial L}{\partial w_{i-1}} \quad \text{Update Velocity (starts as 0, } \beta = 0.99)$$

$$w_i = w_{i-1} - \alpha v_i \quad \text{Update Weights}$$

- Generalizes SGD ( $\beta = 0$ )



## Adding Momentum

- Velocity term is an **exponential moving average** of the gradient

$$v_i = \beta v_{i-1} + \frac{\partial L}{\partial w_{i-1}}$$

$$v_i = \beta \left( \beta v_{i-2} + \frac{\partial L}{\partial w_{i-2}} \right) + \frac{\partial L}{\partial w_{i-1}}$$

$$= \beta^2 v_{i-2} + \beta \frac{\partial L}{\partial w_{i-2}} + \frac{\partial L}{\partial w_{i-1}}$$

- There is a **general class of accelerated gradient methods**, with some theoretical analysis (under assumptions)

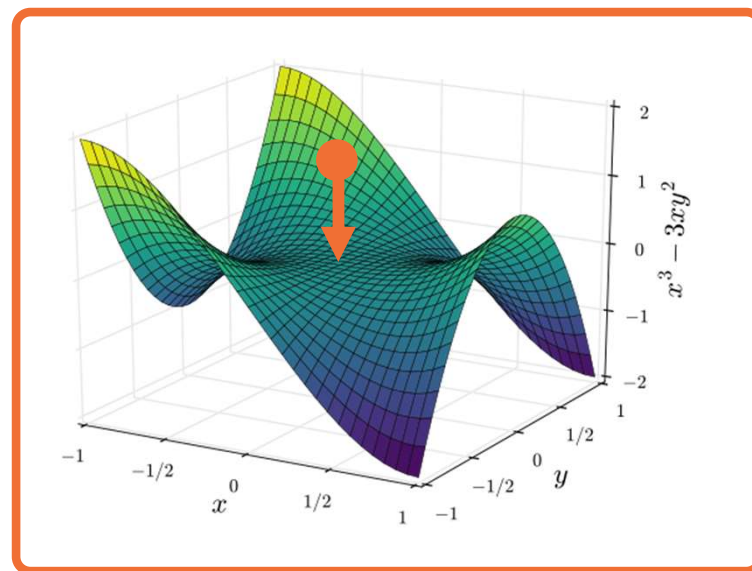
## Equivalent formulation:

$$v_i = \beta v_{i-1} - \alpha \frac{\partial L}{\partial w_{i-1}}$$

Update Velocity  
(starts as 0)

$$w_i = w_{i-1} + v_i$$

Update Weights



Equivalent Momentum Update

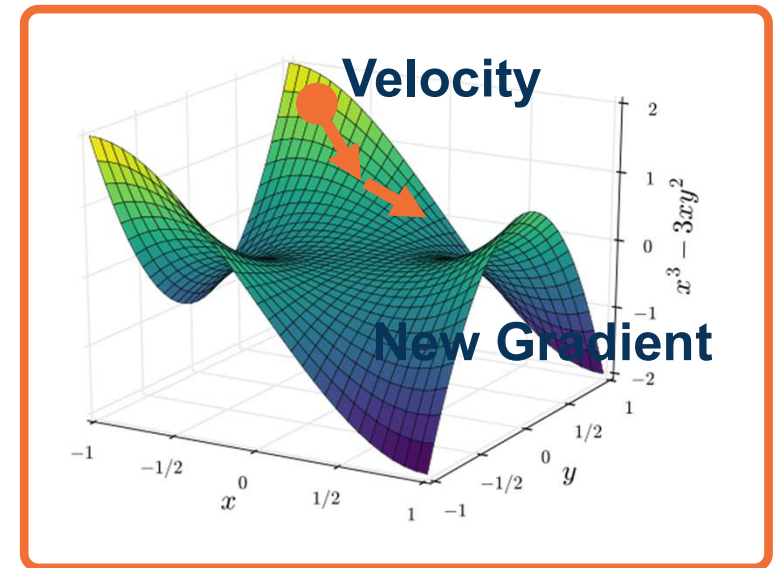
**Key idea:** Rather than combining velocity with current gradient, go along velocity **first** and then calculate gradient at new point

- ◆ We know velocity is probably a **reasonable direction**

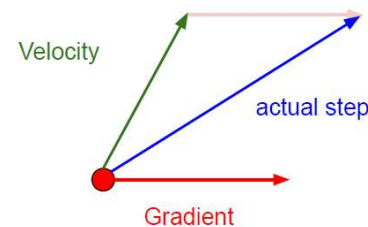
$$\hat{w}_{i-1} = w_{i-1} + \beta v_{i-1}$$

$$v_i = \beta v_{i-1} + \frac{\partial L}{\partial \hat{w}_{i-1}}$$

$$w_i = w_{i-1} - \alpha v_i$$



Momentum update:



Nesterov Momentum

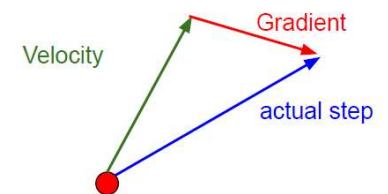


Figure Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

**Nesterov Momentum**

## Momentum

Note there are **several equivalent formulations** across deep learning frameworks!

### Resource:

<https://medium.com/the-artificial-impostor/sgd-implementation-in-pytorch-4115bcb9f02c>

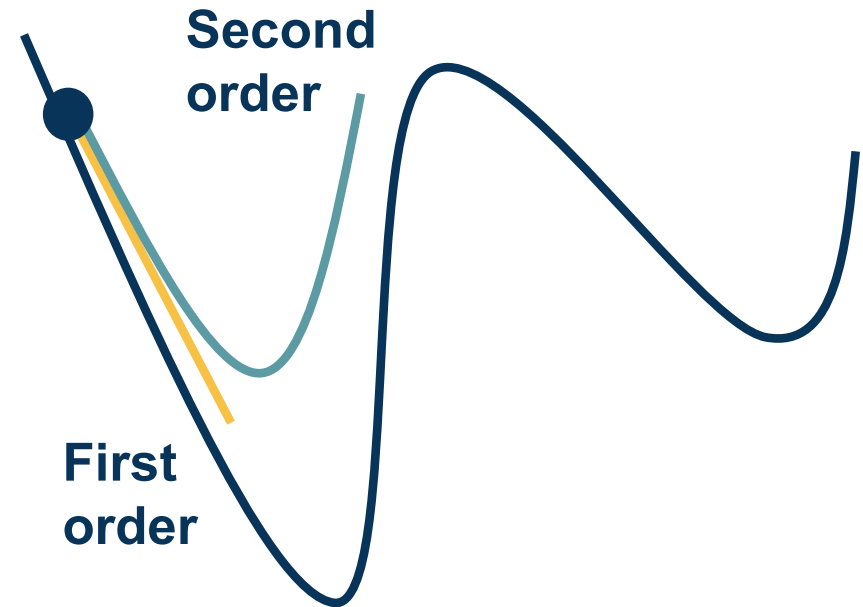


- Various mathematical ways to **characterize the loss landscape**

- If you liked **Jacobians**... meet:

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

- Gives us information about the **curvature of the loss surface**



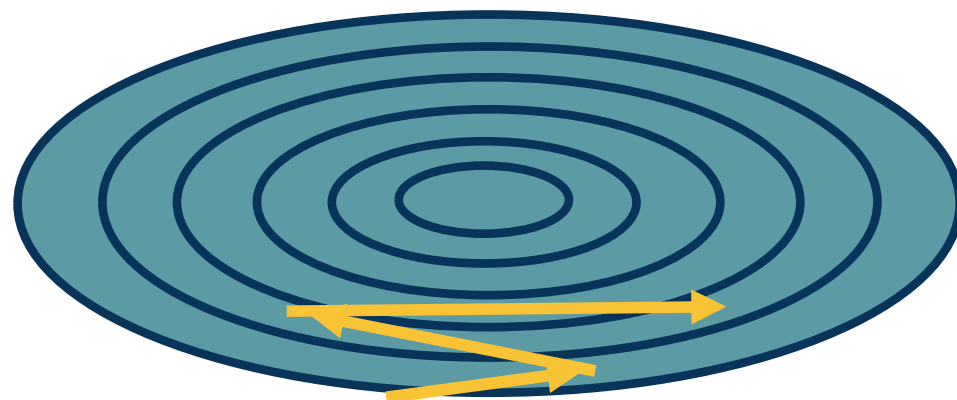


**Condition number** is the ratio of the largest and smallest eigenvalue

- ◆ Tells us how different the curvature is along different dimensions

If this is high, SGD will make **big** steps in some dimensions and **small** steps in other dimension

Second-order optimization methods divide steps by curvature, but expensive to compute



## Per-Parameter Learning Rate

**Idea:** Have a dynamic learning rate for each weight

Several flavors of **optimization algorithms:**

- ◆ RMSProp
- ◆ Adagrad
- ◆ Adam
- ◆ ...

**SGD can achieve similar results** in many cases but with much more tuning



**Idea:** Use gradient statistics to reduce learning rate across iterations

**Denominator:** Sum up gradients over iterations

Directions with **high curvature will have higher gradients**, and learning rate will reduce

$$G_i = G_{i-1} + \left( \frac{\partial L}{\partial w_{i-1}} \right)^2$$
$$w_i = w_{i-1} - \frac{\alpha}{\sqrt{G_i} + \epsilon} \frac{\partial L}{\partial w_{i-1}}$$

**As gradients are accumulated learning rate will go to zero**

*Duchi, et al., "Adaptive Subgradient Methods for Online Learning and Stochastic Optimization"*

**Solution:** Keep a moving average of squared gradients!

Does not saturate the learning rate

$$G_i = \beta G_{i-1} + (1 - \beta) \left( \frac{\partial L}{\partial w_{i-1}} \right)^2$$

$$w_i = w_{i-1} - \frac{\alpha}{\sqrt{G_i + \epsilon}} \frac{\partial L}{\partial w_{i-1}}$$

**Combines ideas** from above algorithms

**Maintains both first and second moment** statistics for gradients

$$v_i = \beta_1 v_{i-1} + (1 - \beta_1) \left( \frac{\partial L}{\partial w_{i-1}} \right)$$

$$G_i = \beta_2 G_{i-1} + (1 - \beta_2) \left( \frac{\partial L}{\partial w_{i-1}} \right)^2$$

$$w_i = w_{i-1} - \frac{\alpha v_i}{\sqrt{G_i + \epsilon}}$$

**But unstable in the beginning**  
(one or both of moments will be tiny values)

*Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015*

**Solution:** Time-varying bias correction

Typically  $\beta_1 = 0.9$ ,  $\beta_2 = 0.999$

So  $\hat{v}_i$  will be small number divided by  $(1-0.9=0.1)$  resulting in more reasonable values (and  $\hat{G}_i$  larger)

$$v_i = \beta_1 v_{i-1} + (1 - \beta_1) \left( \frac{\partial L}{\partial w_{i-1}} \right)$$
$$G_i = \beta_2 G_{i-1} + (1 - \beta_2) \left( \frac{\partial L}{\partial w_{i-1}} \right)^2$$

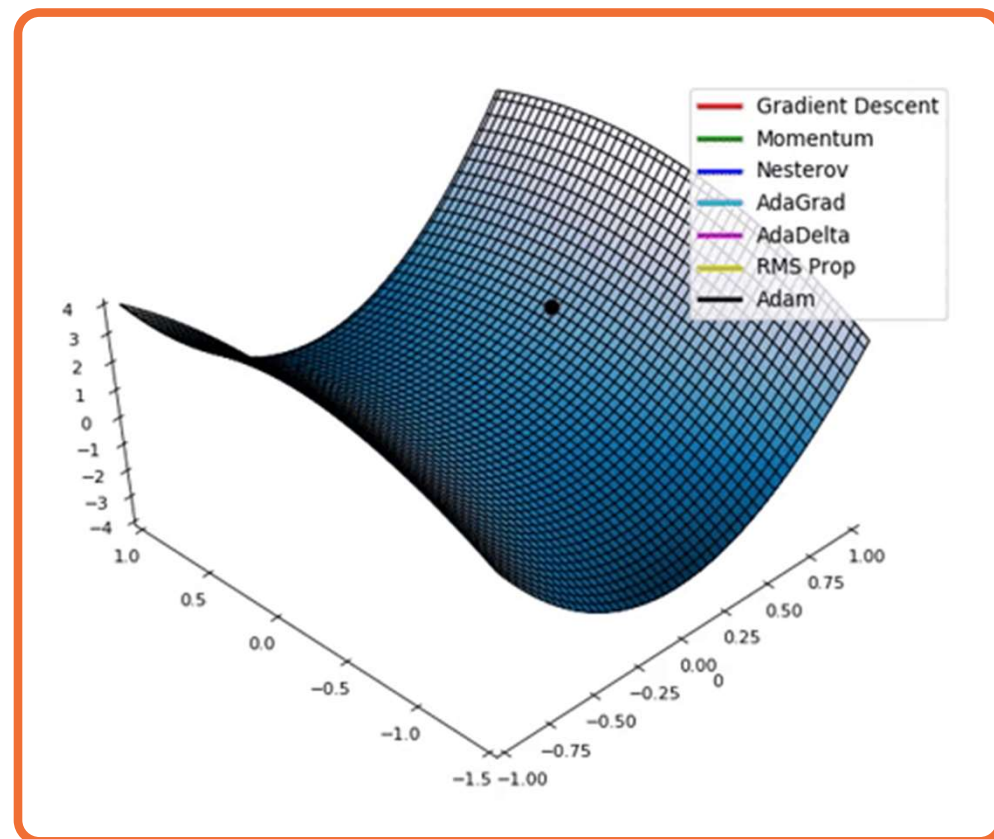
$$\hat{v}_i = \frac{v_i}{1 - \beta_1^t} \quad \hat{G}_i = \frac{G_i}{1 - \beta_2^t}$$
$$w_i = w_{i-1} - \frac{\alpha \hat{v}_i}{\sqrt{\hat{G}_i + \epsilon}}$$

Optimizers behave differently  
**depending on landscape**

Different behaviors such as  
**overshooting, stagnating, etc.**

**Plain SGD+Momentum** can  
generalize better than adaptive  
methods, but requires more tuning

- **See:** *Luo et al., Adaptive Gradient Methods with Dynamic Bound of Learning Rate, ICLR 2019*



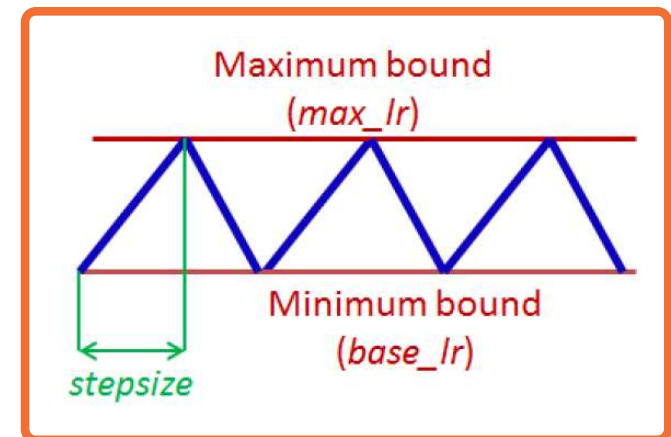
From: <https://mlfromscratch.com/optimizers-explained/#/>

First order optimization methods have **learning rates**

Theoretical results rely on **annealed learning rate**

**Several schedules that are typical:**

- ◆ Graduate student!
- ◆ Step scheduler
- ◆ Exponential scheduler
- ◆ Cosine scheduler



From: Leslie Smith, "Cyclical Learning Rates for Training Neural Networks"