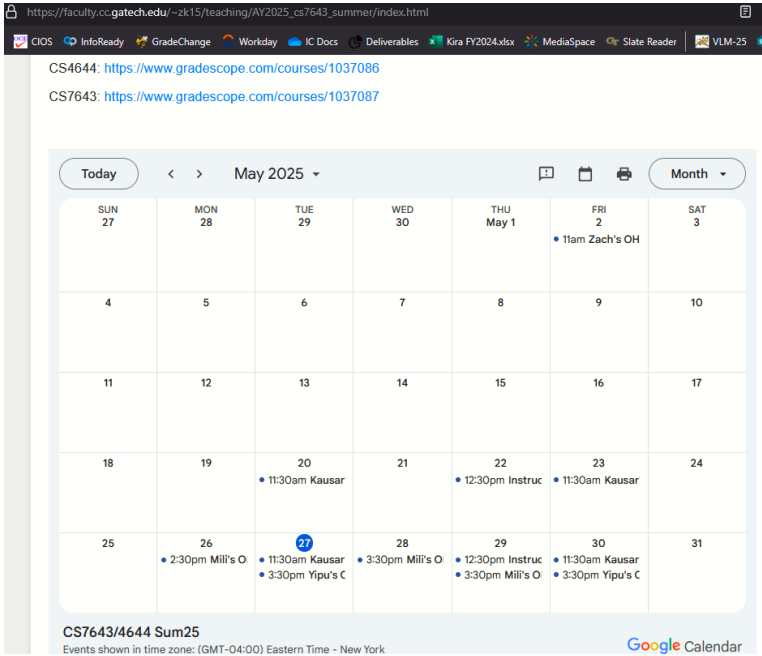
Topics:

- Autodiff
- Optimization

CS 4644-DL / 7643-A
ZSOLT KIRA

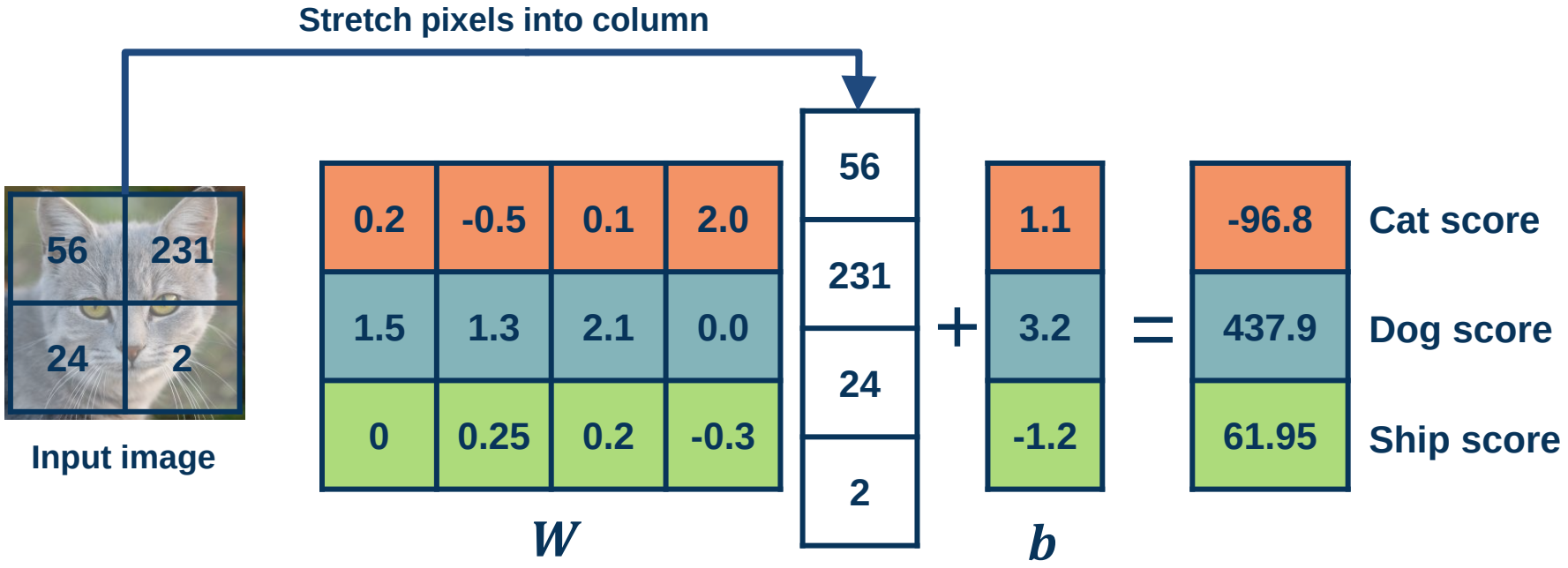
- **Assignment 1 out!**
  - **Due June 5th (with grace period June 7th)**
  - Start now, start now, start now!
  - Start now, start now, start now!
  - Start now, start now, start now!



- Resources:
  - These lectures
  - Matrix calculus for deep learning
  - Gradients notes and MLP/ReLU Jacobian notes.
  - **Topic OH:** Assignment 1 and matrix calculus (linked today)

- Piazza: Project teaming thread
  - **Project Proposal: June 15th, Project Check-in: July 1st .**
  - Project proposal reviewed last time

Example with an image with **4 pixels**, and **3 classes (cat/dog/ship)**



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

- We can find the steepest descent direction by computing the **derivative (gradient):**

$$f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}$$

- Steepest descent direction is the **negative gradient**
- **Intuitively:** Measures how the function changes as the argument a changes by a small step size
  - As step size goes to zero
- **In Machine Learning:** Want to know how the **loss function** changes **as weights** are varied
  - Can consider each parameter separately by taking **partial derivative** of loss function with respect to that parameter

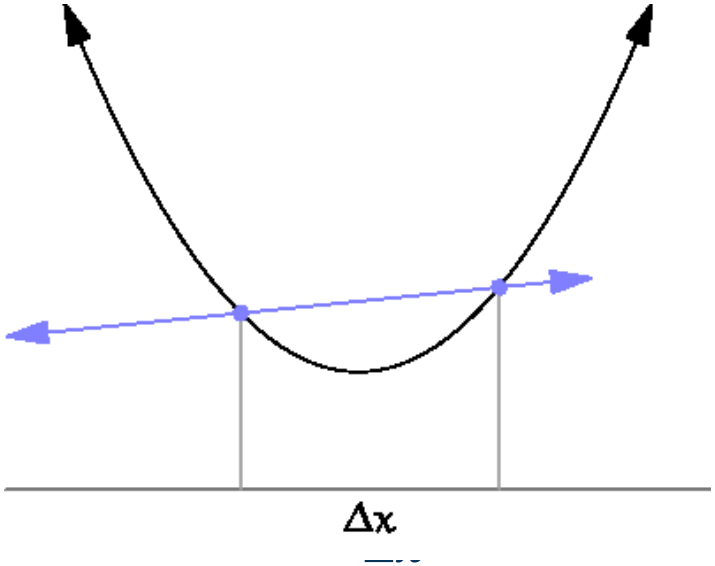


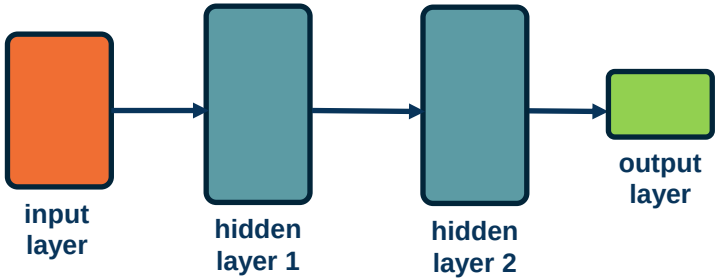
Image and equation from: https://en.wikipedia.org/wiki/Derivative#/media/File:Tangent_animation.gif

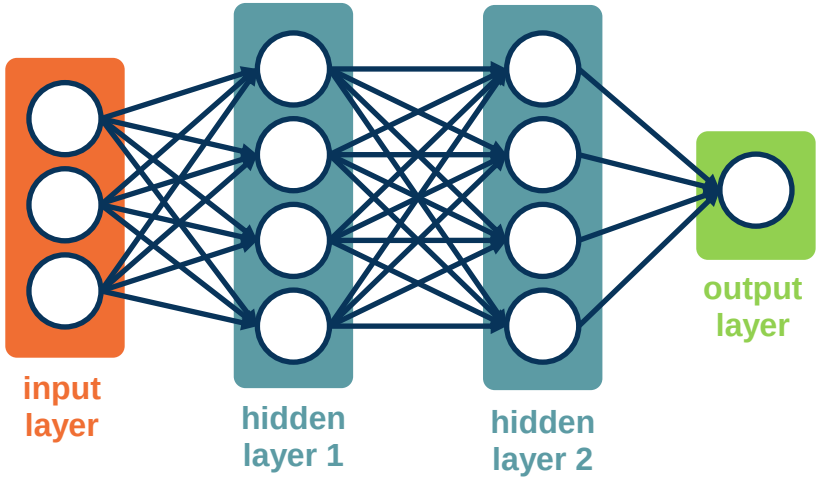
Large (deep) networks can be built by adding more and more layers

Three-layered neural networks can represent **any function**

- The number of nodes could grow unreasonably (exponential or worse) with respect to the complexity of the function

We will show them **without edges**:



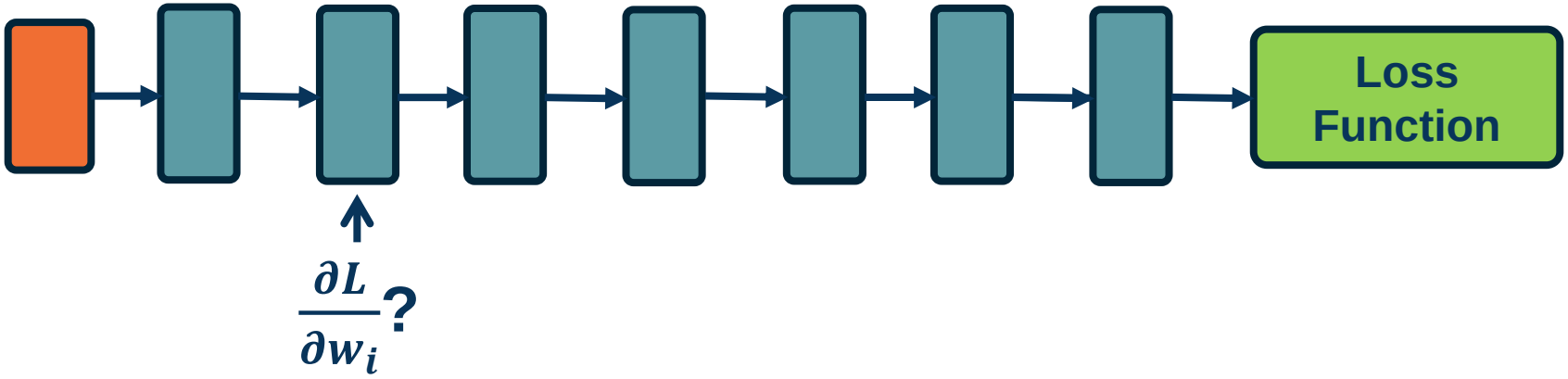


$$f(x, W_1, W_2, W_3) = \sigma(W_2\sigma(W_1 x))$$

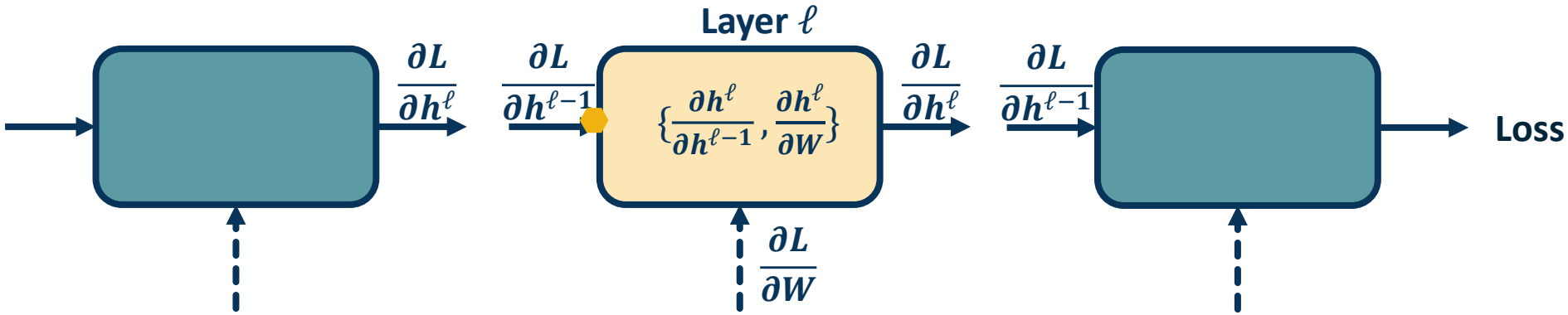
Figure adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Adding More Layers!

- We are learning **complex models** with significant amount of parameters (millions or billions)
- How do we compute the gradients of the **loss** (at the end) with respect to **internal** parameters?
- Intuitively, want to understand how **small changes** in weight deep inside **are propagated** to affect the **loss function** at the end



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



- We will use the *chain rule* to do this:

Chain Rule: $\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x}$

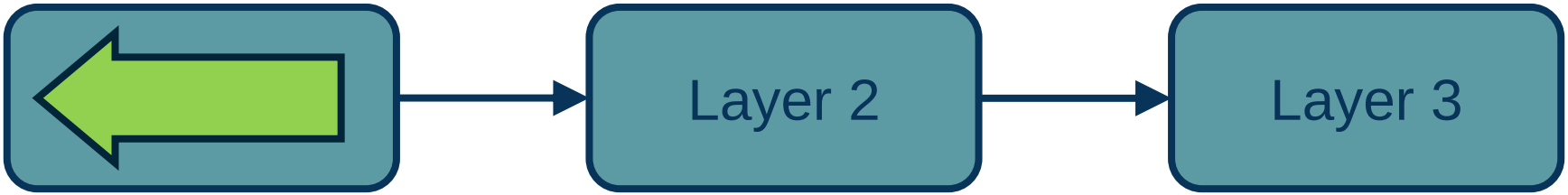
$$\frac{\partial L}{\partial h^{\ell-1}} = \frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial h^{\ell-1}}$$

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

Step 1: Compute Loss on Mini-Batch: **Forward Pass**

Step 2: Compute Gradients wrt parameters: **Backward Pass**

Step 3: Use **gradient** to update **all parameters** at the end



$$w_i = w_i - \alpha \frac{\partial L}{\partial w_i}$$

Backpropagation is the application of gradient descent to a computation graph via the chain rule!

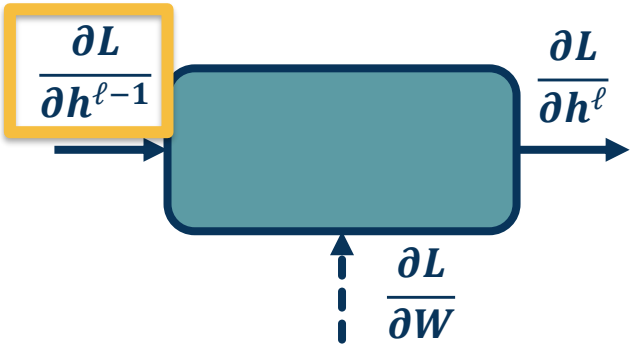
Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

$$h^{\ell} = W h^{\ell-1}$$

$$\frac{\partial h^{\ell}}{\partial h^{\ell-1}} = W$$

Define:

$$h_i^{\ell} = w_i^T h^{\ell-1}$$



$$\frac{\partial L}{\partial h^{\ell-1}} = \frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial h^{\ell-1}}$$

$$1 \times |h^{\ell-1}| \quad 1 \times |h^{\ell}| \quad |h^{\ell}| \times |h^{\ell-1}|$$

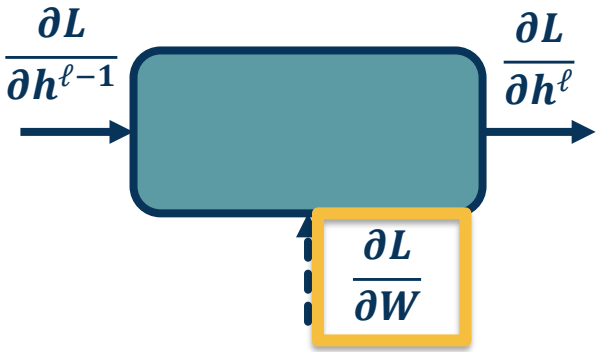
$$h^{\ell} = W h^{\ell-1}$$

$$\frac{\partial h^{\ell}}{\partial h^{\ell-1}} = W$$

Define:

$$h_i^{\ell} = w_i^T h^{\ell-1}$$

$$\frac{\partial h_i^{\ell}}{\partial w_i^T} = h^{(\ell-1),T}$$



Note doing this on full W matrix would result in Jacobian tensor!

But it is *sparse* – each output only affected by corresponding weight row

$$\frac{\partial L}{\partial w_i^T} = \frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial w_i^T}$$

$$\begin{bmatrix} 0 \\ \frac{\partial h_i^{\ell}}{\partial w_i^T} \\ 0 \end{bmatrix}$$

$$\frac{\partial L}{\partial W}$$

$1 \times |h^{\ell-1}|$ $1 \times |h^{\ell}|$ $|h^{\ell}| \times |h^{\ell-1}|$

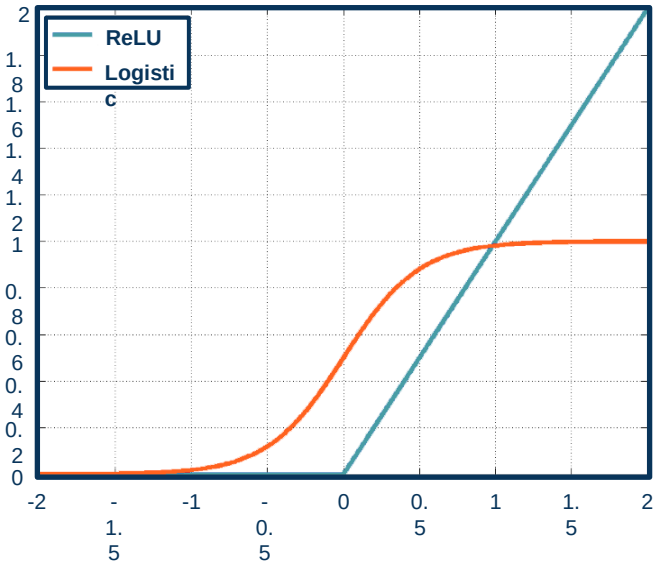
Iterate and populate
Note can simplify/vectorize!

We can employ **any differentiable (or piecewise differentiable) function**

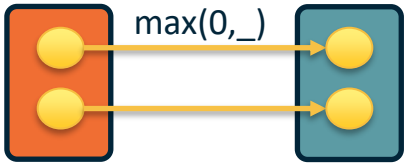
A common choice is the **Rectified Linear Unit**

- Provides non-linearity but better gradient flow than sigmoid
- Performed **element-wise**

How many parameters for this layer?



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

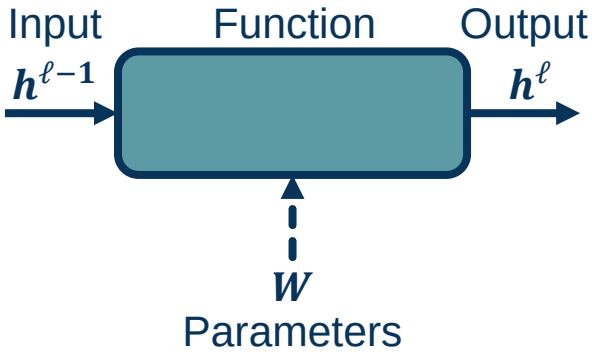


Full Jacobian of ReLU layer is **large** (output dim x input dim)

- But again it is **sparse**
- Only **diagonal values non-zero** because it is element-wise
- An output value affected only by **corresponding input value**

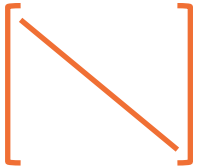
Max function **funnels gradients through selected max**

- Gradient will be **zero** if input **<= 0**



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

Backward: $\frac{\partial L}{\partial h^{\ell-1}} = \frac{\partial L}{\partial h^{\ell}} \frac{\partial h^{\ell}}{\partial h^{\ell-1}}$

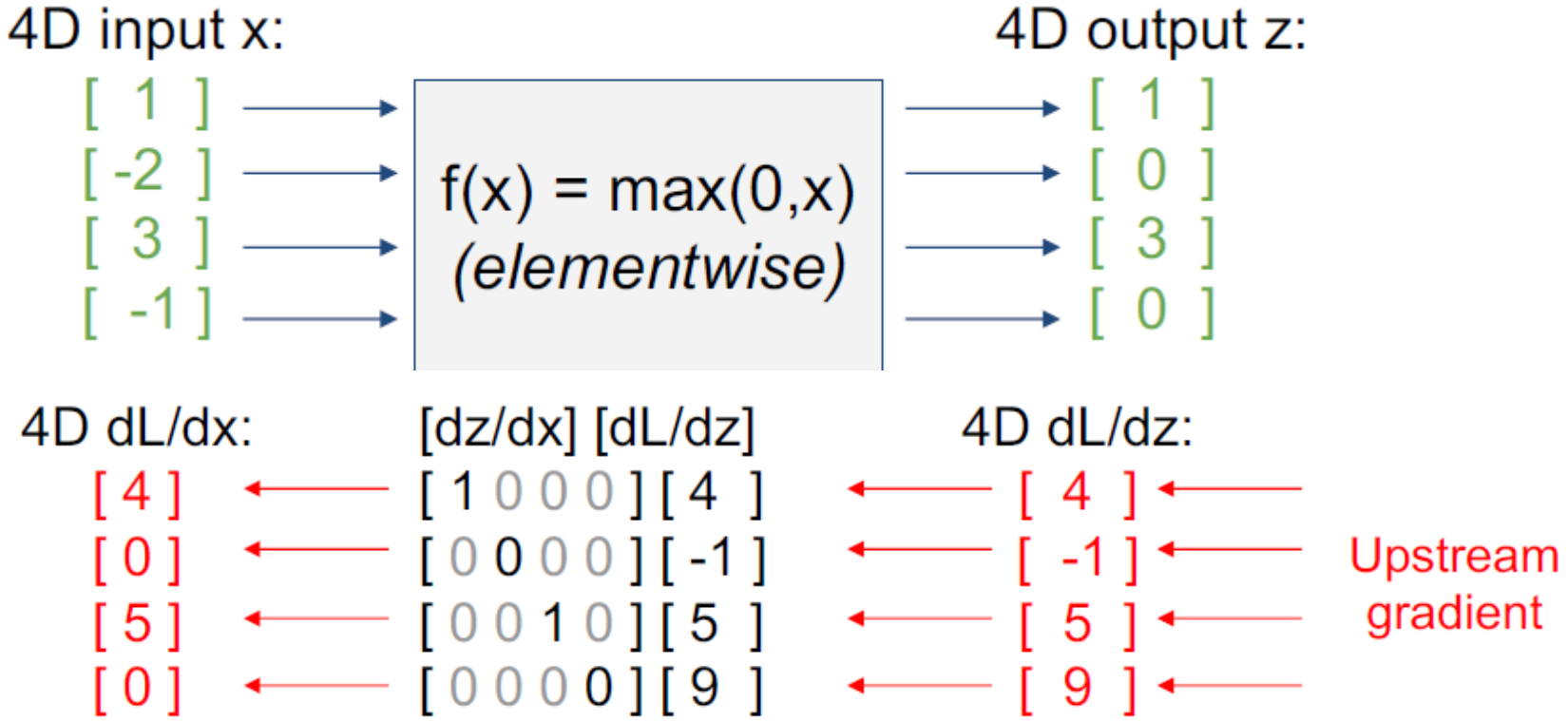


$|h^{\ell} \times h^{\ell-1}|$

For diagonal

$$\frac{\partial h^{\ell}}{\partial h^{\ell-1}} = \begin{cases} 1 & if\ h^{\ell-1} > 0 \\ 0 & otherwise \end{cases}$$

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



For element-wise ops, jacobian is **sparse**: off-diagonal entries always zero!
Never **explicitly** form Jacobian -- instead use elementwise multiplication

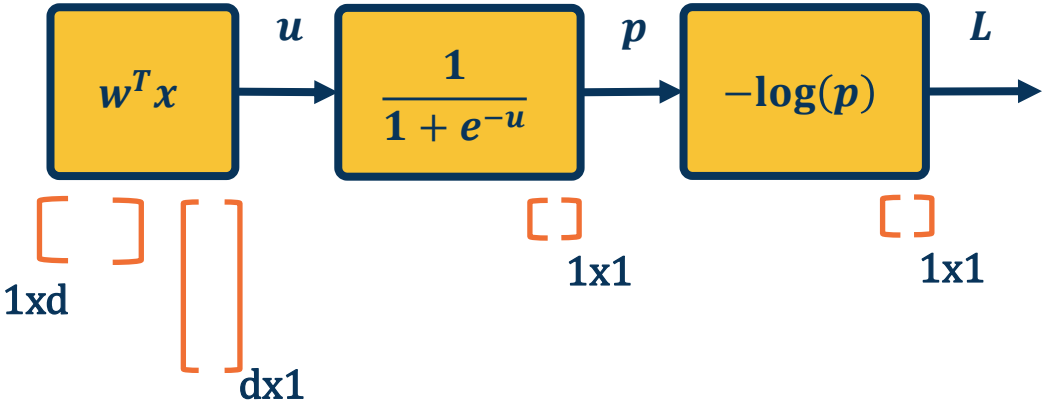
- Neural networks involves composing simple functions into a **computation graph**

- Optimization (updating weights) of this graph is through backpropagation
  - Recursive algorithm: Gradient descent (partial derivatives) plus chain rule

- Remaining questions:
  - How does this work with vectors, matrices, tensors?
    - Across a composed function? **Next!**
  - How can we implement this algorithmically to make these calculations automatic? **Automatic Differentiation**

Summary

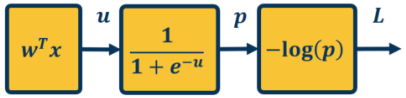
The chain rule can be computed as a **series of scalar, vector, and matrix linear algebra operations**



Extremely efficient in graphics processing units (GPUs)

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

1x1 1x1 1x1 1xd



$L = 1$

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

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

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

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

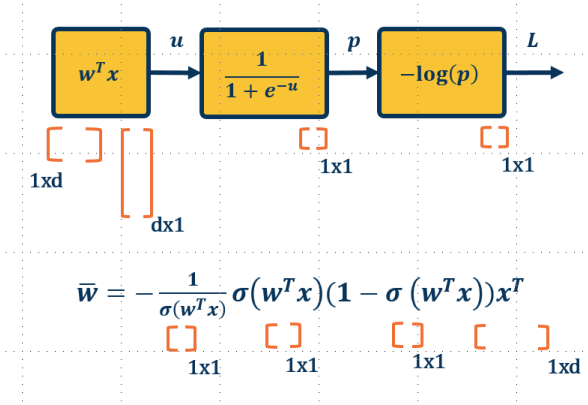
We can do this in a combined way to see all terms together:

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

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

This effectively shows gradient flow along path from L to w

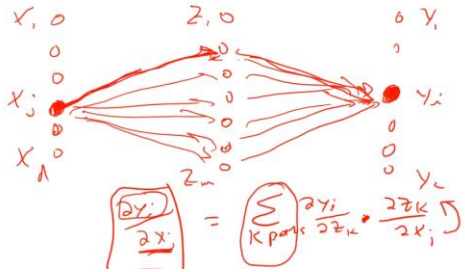
Computation Graph / Global View of Chain Rule



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

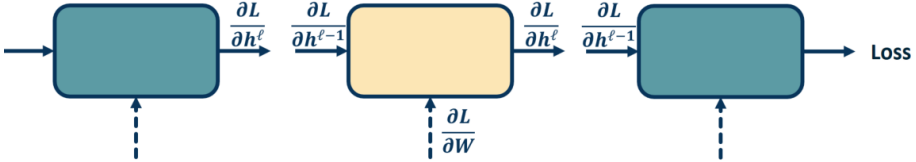
1x1 1x1 1x1 1xd

Computational / Tensor View



Graph View

- We want to 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

Georgia Tech

- **Backpropagation:** Recursive, modular algorithm for chain rule + gradient descent

- **When we move to vectors and matrices:**
  - Composition of functions (scalar)
  - Composition of functions (vectors/matrices)
  - Jacobian view of chain rule
  - Can view entire set of calculations as linear algebra operations (matrix-vector or matrix-matrix multiplication)

- **Automatic differentiation**:
  - Reduction of modules to simple operations we know (simple multiplication, etc.)
  - Automatically build computation graph in background as write code
  - Automatically compute gradients via backward pass

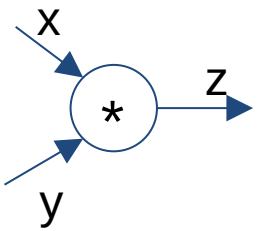
Automatic Differentiation

Deep Learning = Differentiable Programming

- Computation = Graph
  - Input = Data + Parameters
  - Output = Loss
  - Scheduling = Topological ordering

- What do we need to do?
  - Generic code for representing the graph of modules
  - Specify modules (both forward and backward function)

Modularized implementation: forward / backward API



(x,y,z are scalars)

```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        return z
    def backward(dz):
        # dx = ... #todo
        # dy = ... #todo
        return [dx, dy]
```

$\frac{\partial L}{\partial z}$

$\frac{\partial L}{\partial x}$

Backpropagation does not really spell out how to **efficiently** carry out the necessary computations

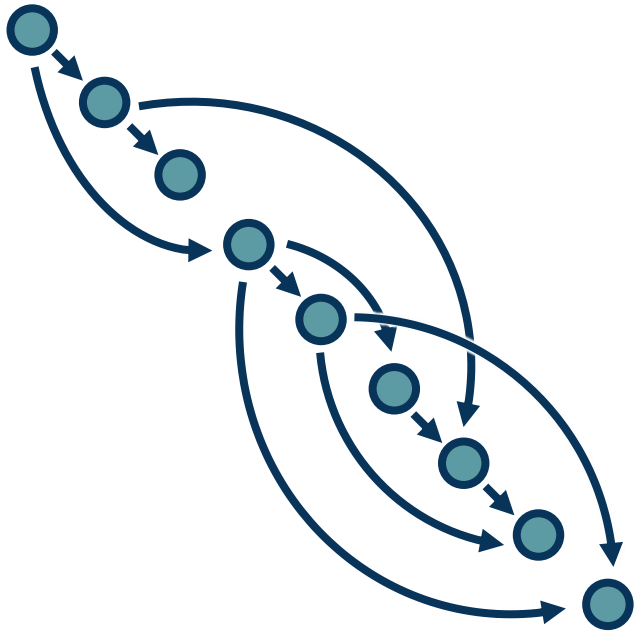
But the idea can be applied to **any directed acyclic graph (DAG)**

- Graph represents an **ordering constraining** which paths must be calculated first

Given an ordering, we can then iterate from the last module backwards, **applying the chain rule**

- We will store, for each node, its **local gradient function/computation for efficiency**
- We will do this **automatically** by computing backwards function for primitives and as you write code, express the function with them

This is called reverse-mode **automatic differentiation**



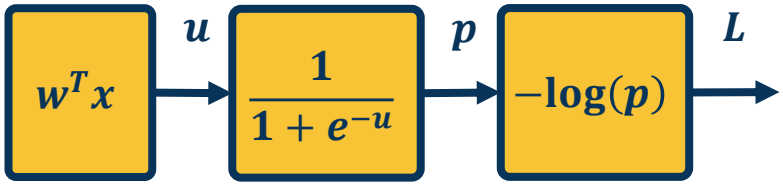
A General Framework

Computation = Graph

- Input = Data + Parameters
- Output = Loss
- Scheduling = Topological ordering

Auto-Diff

- A family of algorithms for implementing chain-rule on computation graphs



Automatic differentiation:

- Carries out this procedure for us on arbitrary graphs
- Knows derivatives of primitive functions
- As a result, we just define these (forward) functions **and don't even need to specify the gradient (backward) functions!**

$$\bar{L} = 1$$

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

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:

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

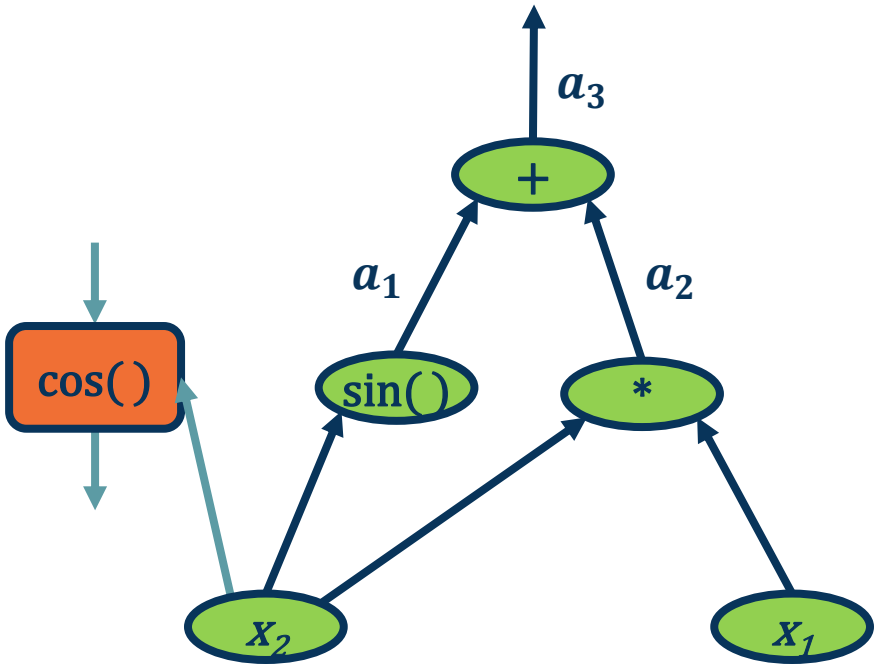
This effectively shows gradient flow along path from L to w

Example Gradient Computations

- Key idea is to **explicitly store computation graph** in memory and **corresponding gradient functions**

- **Nodes** broken down to **basic primitive computations** (addition, multiplication, log, etc.) for which **corresponding derivative is known**

$$\overline{x_2} = \frac{\partial f}{\partial a_1}\frac{\partial a_1}{\partial x_2} = \overline{a_1}\ \cos(x_2)$$



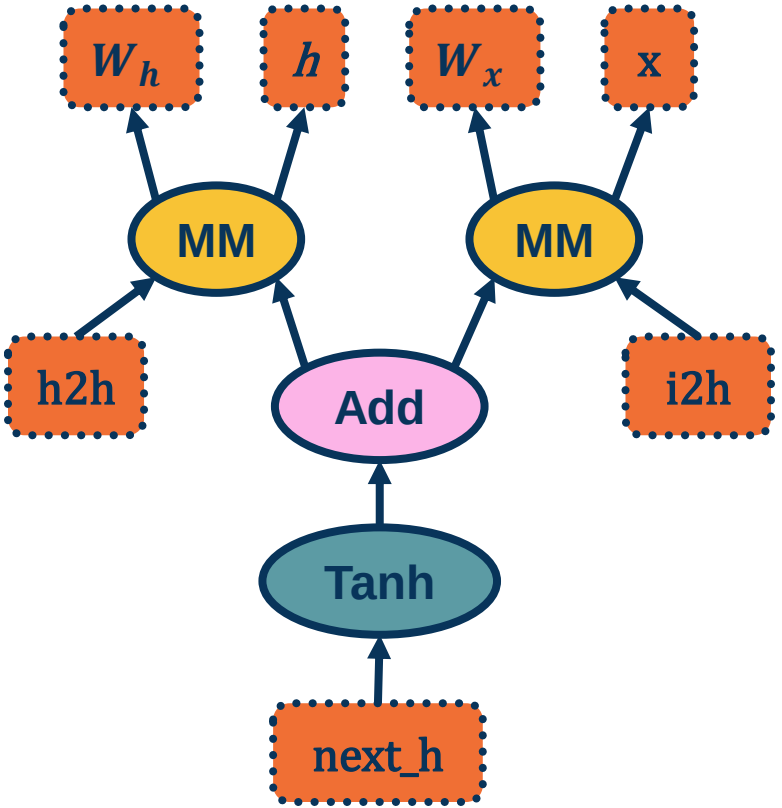
A graph is created on the fly

```
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)

Back-propagation uses the dynamically built graph

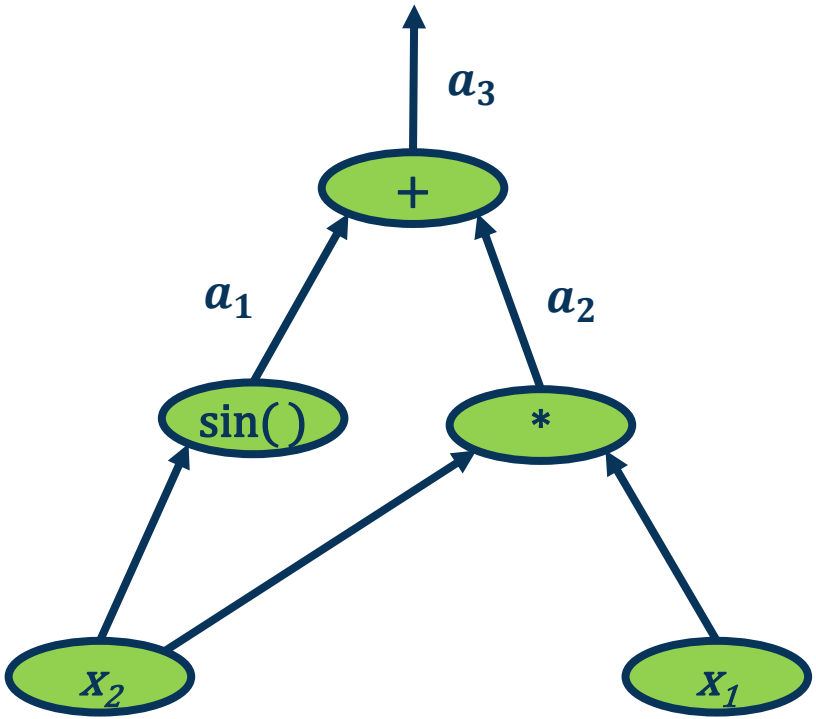
```
from torch.autograd import Variable

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
next_h = next_h.tanh()

next_h.backward(torch.ones(1, 20))
```



From pytorch.org

Example

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



We want to find the **partial derivative of output f** (output) with respect to **all intermediate variables**

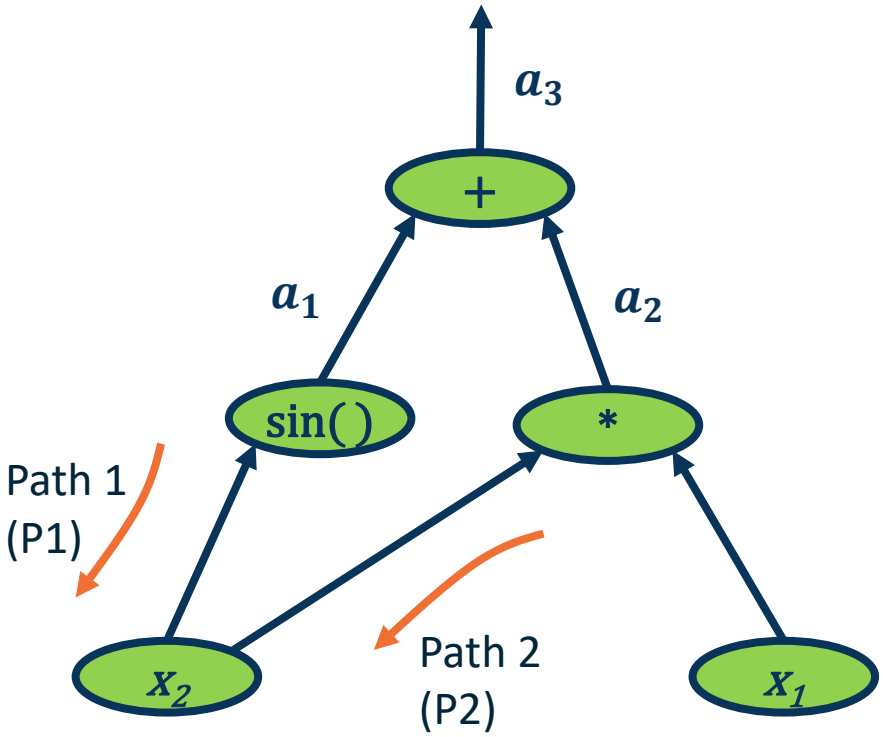
- Assign intermediate variables

  Simplify notation:

  Denote bar as: $\overline{a_3} = \frac{\partial f}{\partial a_3}$

- Start at **end** and move **backward**

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



$$\overline{a_3} = \frac{\partial f}{\partial a_3} = 1$$

$$\overline{a_1} = \frac{\partial f}{\partial a_1} = \frac{\partial f}{\partial a_3}\frac{\partial a_3}{\partial a_1} = \frac{\partial f}{\partial a_3}\frac{\partial (a_1+a_2)}{\partial a_1} = \frac{\partial f}{\partial a_3}\,1 = \overline{a_3}$$

$$\overline{a_2} = \frac{\partial f}{\partial a_2} = \frac{\partial f}{\partial a_3}\frac{\partial a_3}{\partial a_2} = \overline{a_3}$$

$$\overline{x_2^{P1}} = \frac{\partial f}{\partial a_1}\frac{\partial a_1}{\partial x_2} = \overline{a_1}\,\cos(x_2)$$

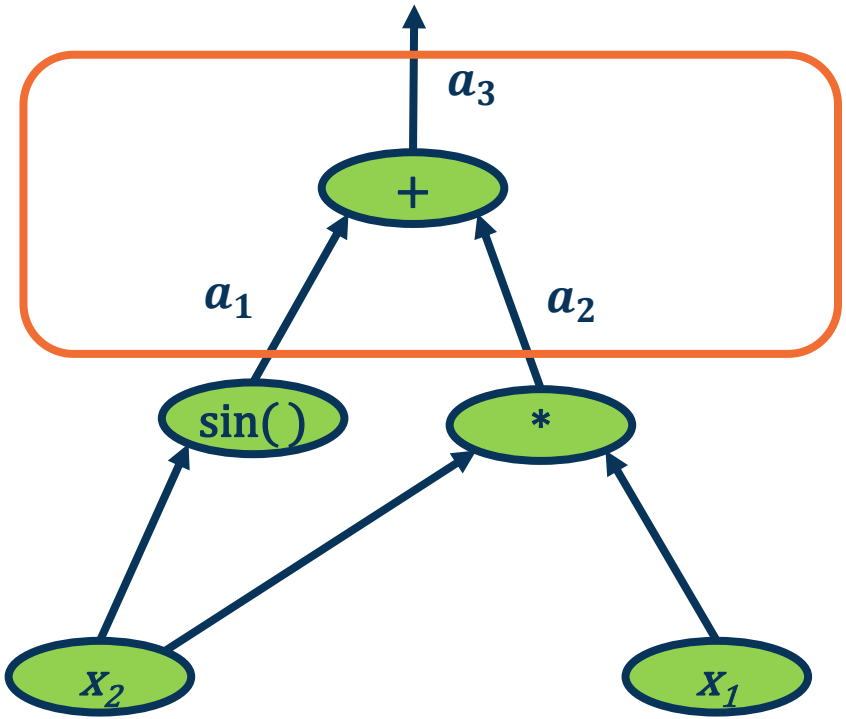
$$\overline{x_2^{P2}} = \frac{\partial f}{\partial a_2}\frac{\partial a_2}{\partial x_2} = \frac{\partial f}{\partial a_2}\frac{\partial (x1x2)}{\partial x_2} = \overline{a_2} x_1$$

Gradients from multiple paths **summed**

$$\overline{x_1} = \frac{\partial f}{\partial a_2}\frac{\partial a_2}{\partial x_1} = \overline{a_2} x_2$$

Example

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



$$\overline{a_1} = \frac{\partial f}{\partial a_1} = \frac{\partial f}{\partial a_3}\frac{\partial a_3}{\partial a_1} = \frac{\partial f}{\partial a_3}\frac{\partial (a_1 + a_2)}{\partial a_1} = \frac{\partial f}{\partial a_3}\,1 = \overline{a_3}$$

$$\overline{a_2} = \frac{\partial f}{\partial a_2} = \frac{\partial f}{\partial a_3}\frac{\partial a_3}{\partial a_2} = \overline{a_3}$$

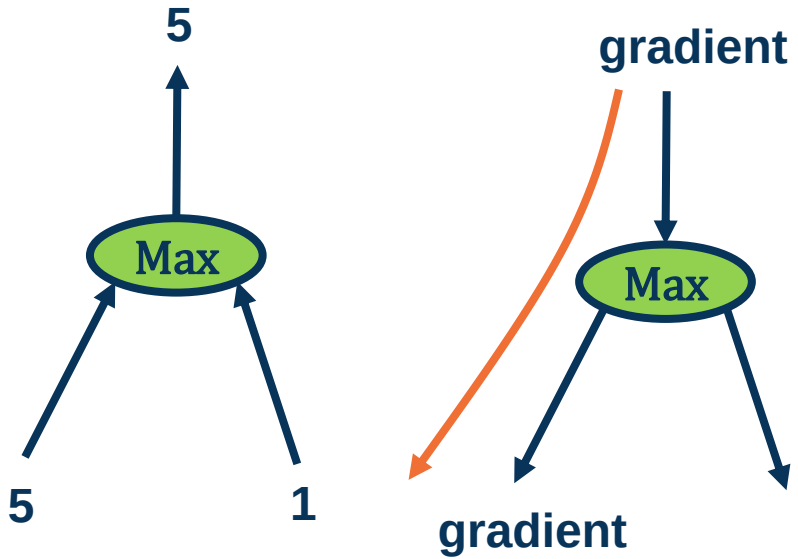
Addition operation distributes gradients along all paths!

Patterns of Gradient Flow: Addition

Several other patterns as well, e.g.:

Max operation **selects** which path to push the gradients through

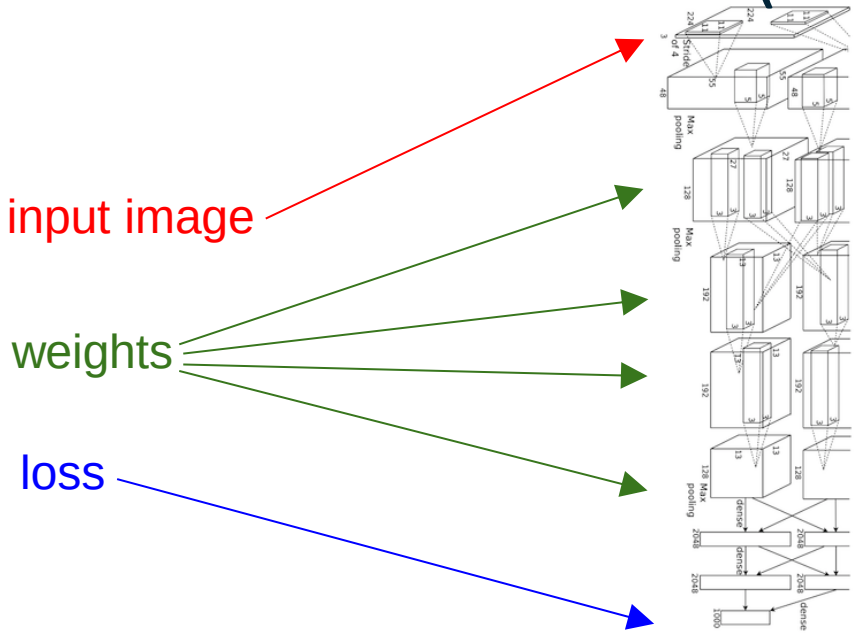
- Gradient flows along the path that was “selected” to be max
- This information must be recorded in the forward pass



The flow of gradients is one of the **most important aspects** in deep neural networks

- If gradients **do not flow backwards properly,** learning slows or stops!

Convolutional network (AlexNet)



Neural Turing Machine

input image

loss

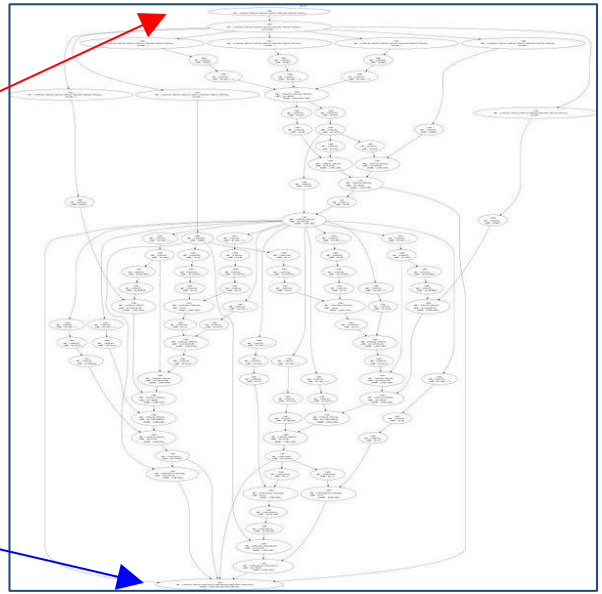
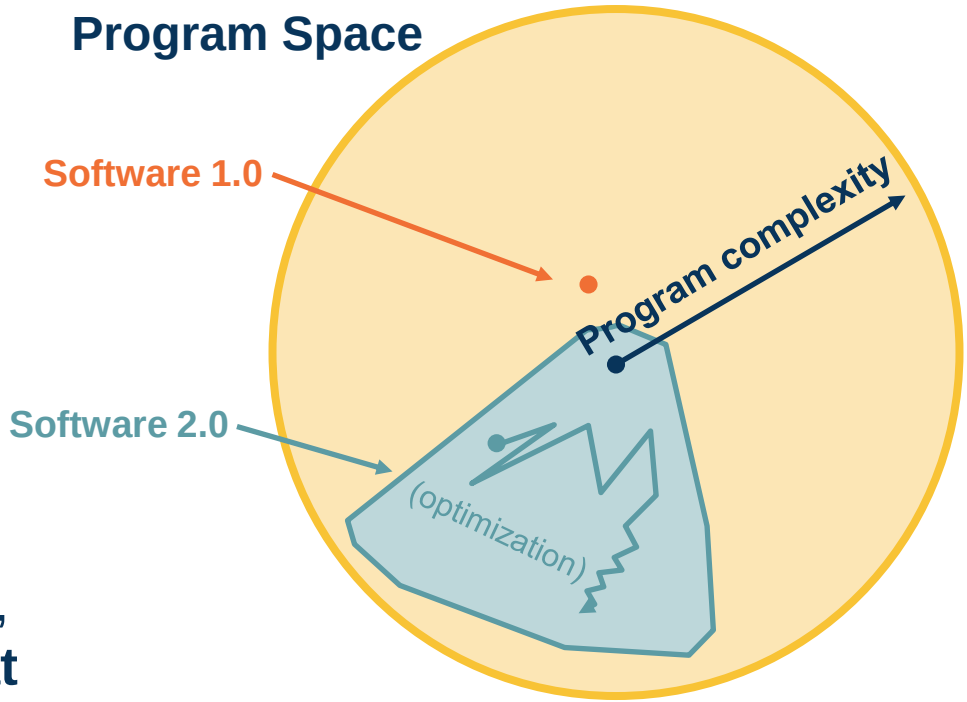


Figure reproduced with permission from a Twitter post by Andrej Karpathy.

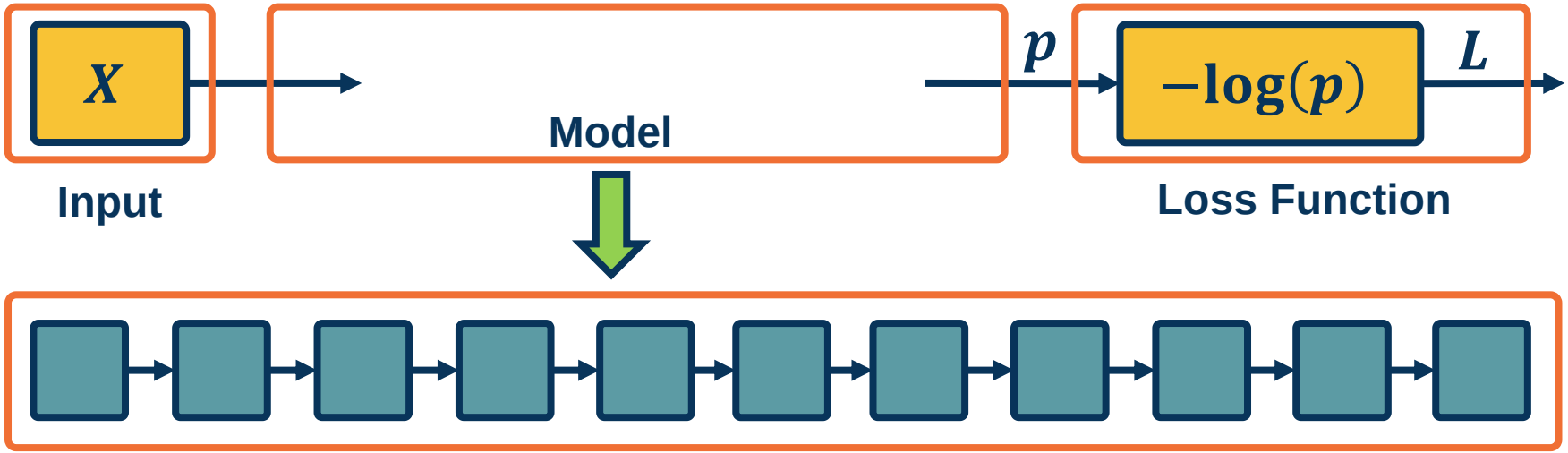
- Computation graphs are **not limited to mathematical functions!**
- Can have **control flows** (if statements, loops) and **backpropagate** through **algorithms**!
- Can be done **dynamically** so that **gradients are computed**, then **nodes are added, repeat**
- **Differentiable programming**



Adapted from figure by Andrej Karpathy

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

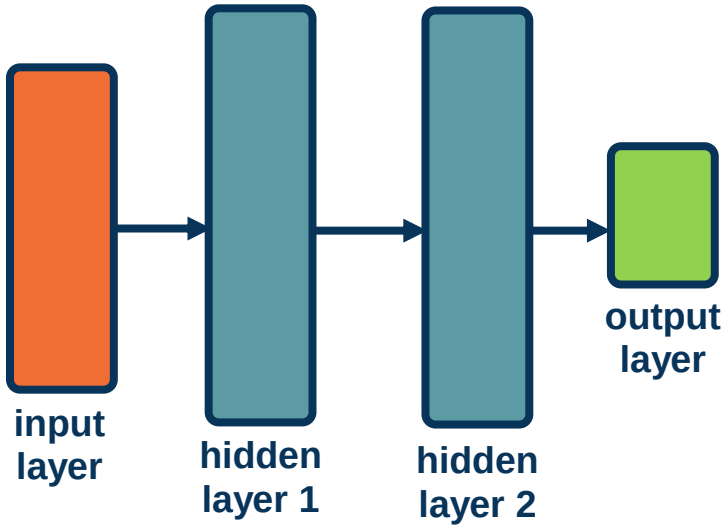
- **No need to modify** the learning algorithm!
- The complexity of the function is only limited by **computation and memory**



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

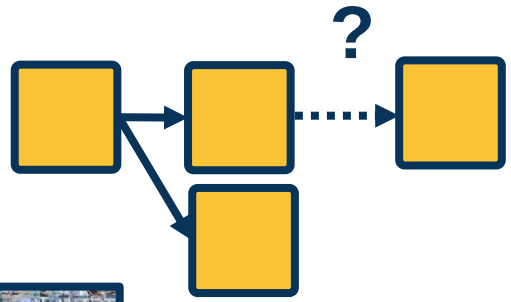
Depth is important:

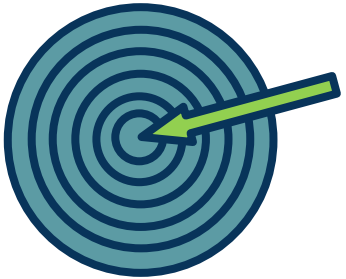
- Structure the model to represent an inherently compositional world
- Theoretical evidence that it leads to parameter efficiency
- Gentle dimensionality reduction (if done right)



There are still many design decisions that must be made:

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



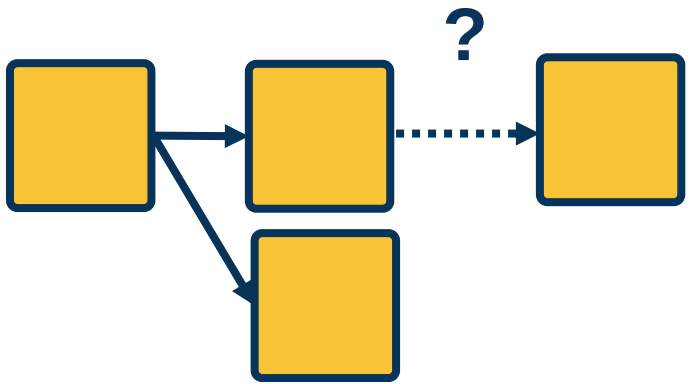


Local Minima

Architectural Considerations

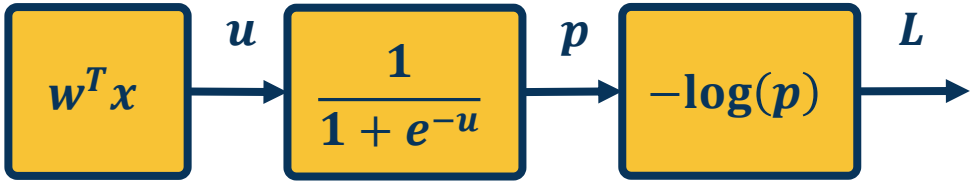
Determining what modules to use, and how to connect them is part of the **architectural design**

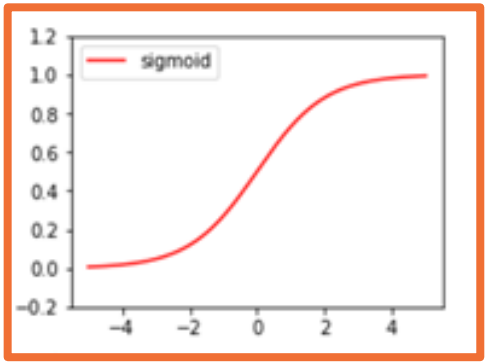
- Guided by the **type of data used** and its **characteristics**
  - Understanding your data is always the first step!
- **Lots of data types (modalities)** already have good architectures
  - Start with what others have discovered!
- **The flow of gradients** is one of the key principles to use when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

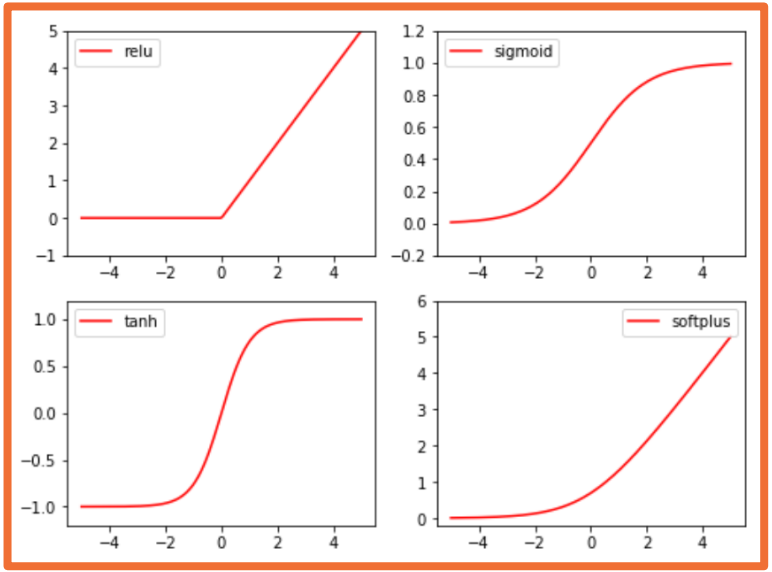
$$w_1^T(w_2^T(w_3^T x)) = w_4^T \mathbf{x}$$



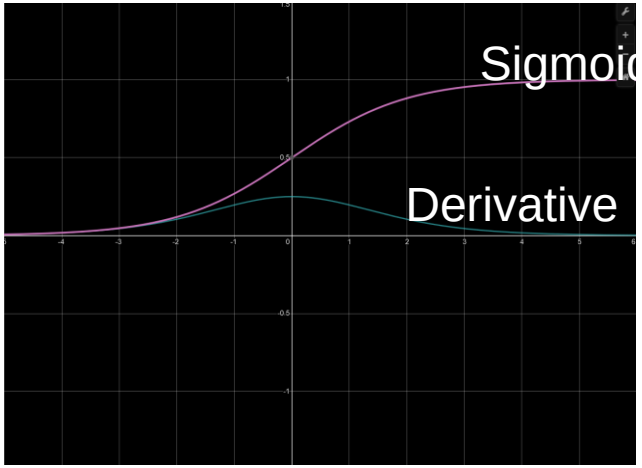


Several aspects that we can **analyze**:

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

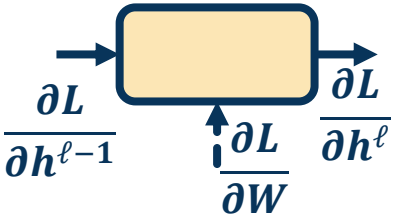


- **Min:** 0, **Max:** 1
- Output **always positive**
- Saturates at **both ends**
- **Gradients**
  - Vanishes at both end
  - Always positive
- **Computation: Exponential term**



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

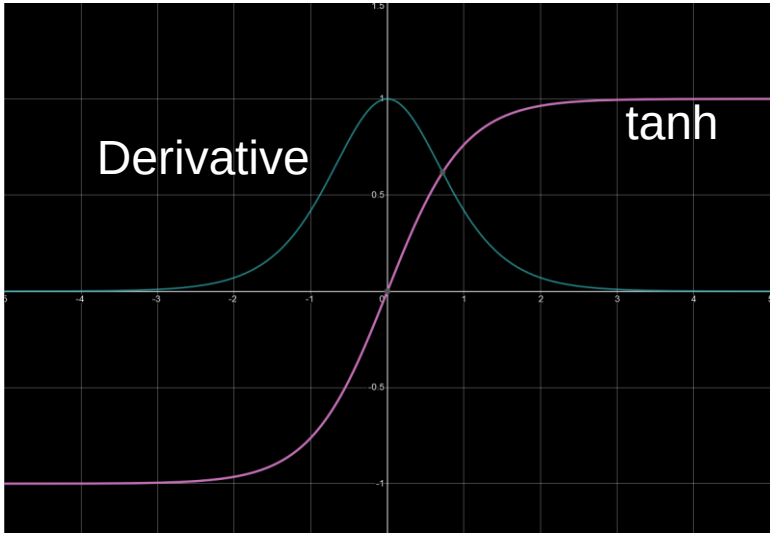
$$\sigma(x) = \frac{1}{1+e^{-x}}$$



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

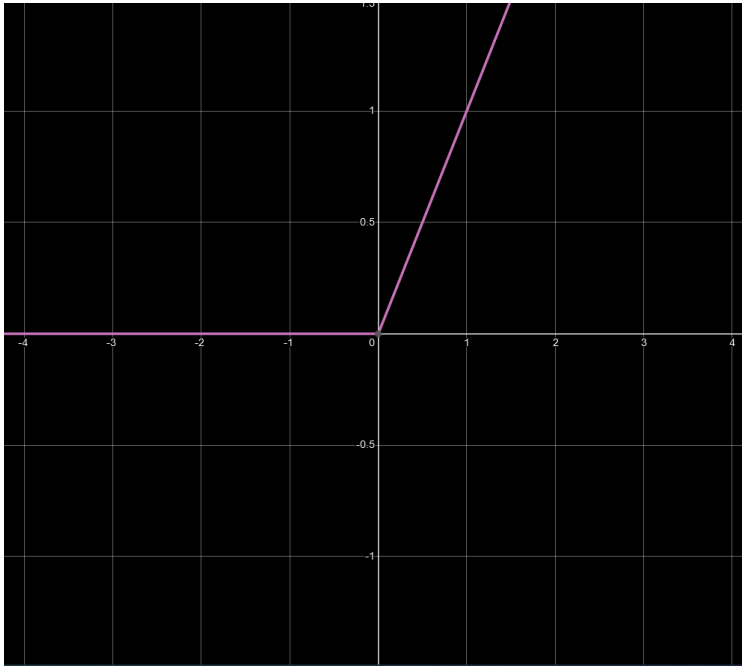
Sigmoid Function

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



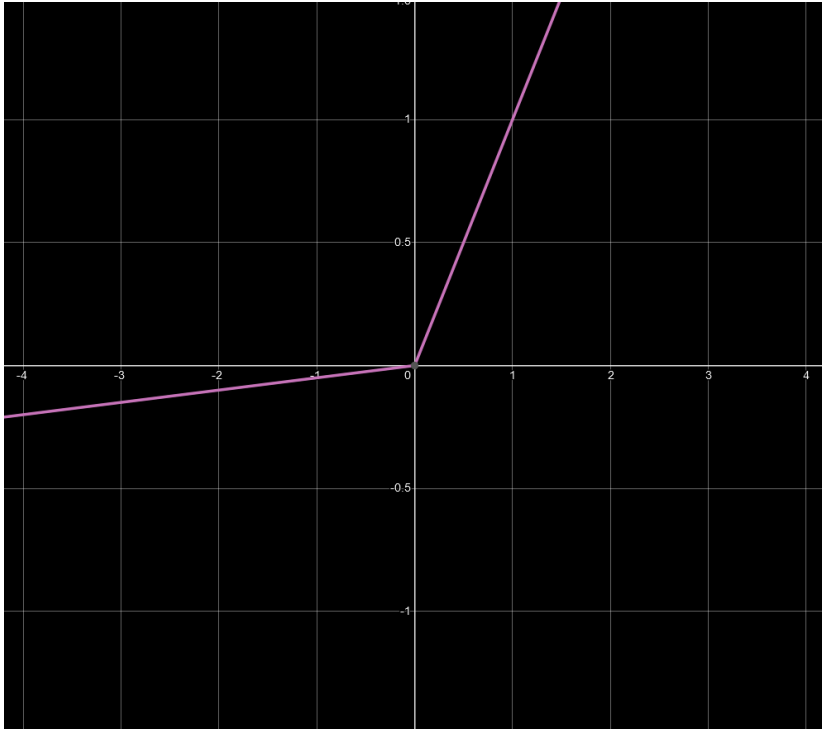
$$h^{\ell} = tanh(h^{\ell-1})$$

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



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

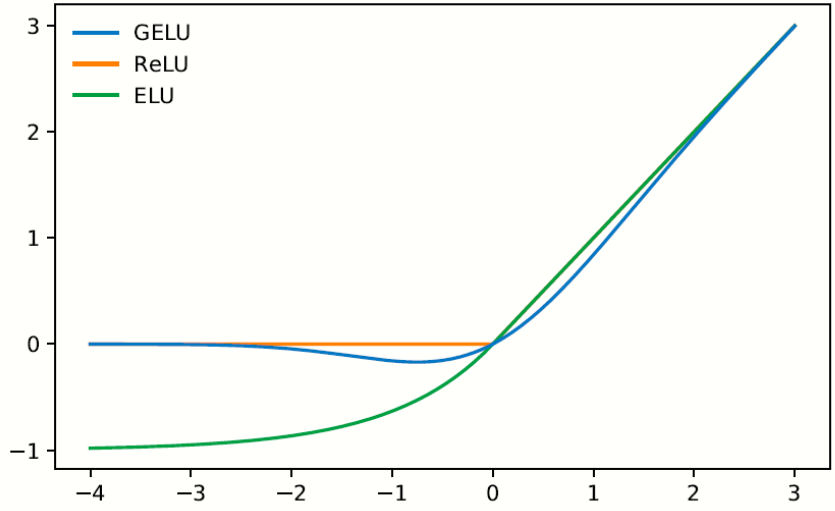
- **Min:** -Infinity, **Max:** Infinity
- **Learnable parameter!**
- **No saturation**
- **Gradients**
  - No dead neuron
- **Still cheap to compute**



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

Leaky ReLU

- **Activation functions is still area of research!**
  - Though many don't catch on
- **In Transformer architectures, other activations such as GeLU is common**



From "Gaussian Error Linear Units (GELUs)", Hendrycks & Gimpel

Variations: ELU, GeLU, etc.

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

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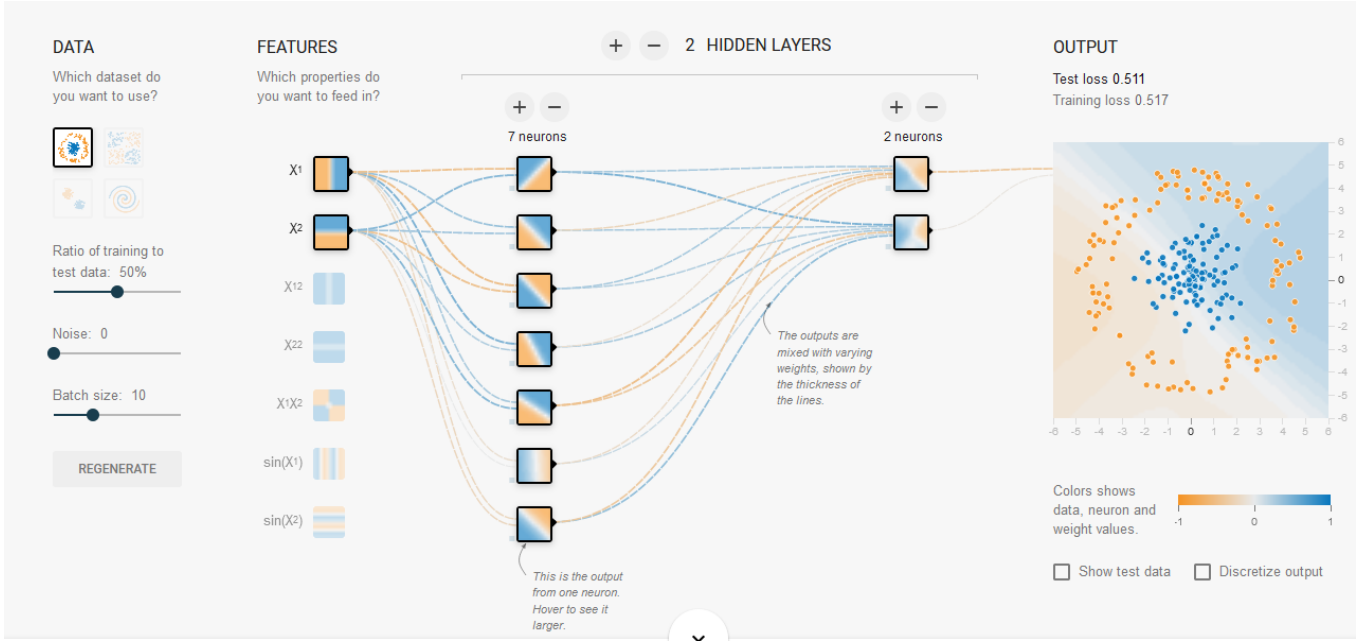
Demo

- http://playground.tensorflow.org



Initialization

Initializing the Parameters

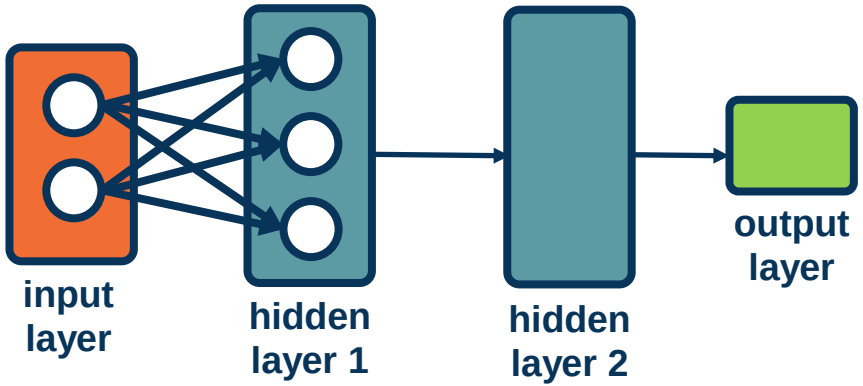
The parameters of our model must be **initialized to something**

- 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**!

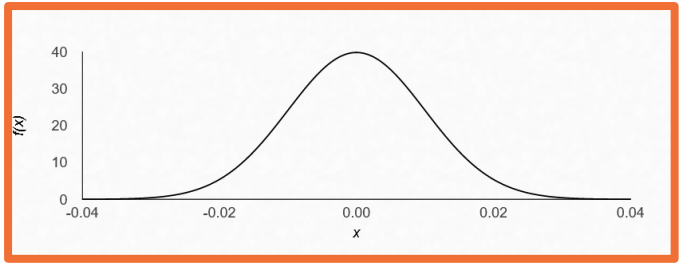
- What happens to the **weight updates?**
- Each node has the same input from previous layers so gradients **will be the same**
- As a results**, all weights will be updated** to the same exact values

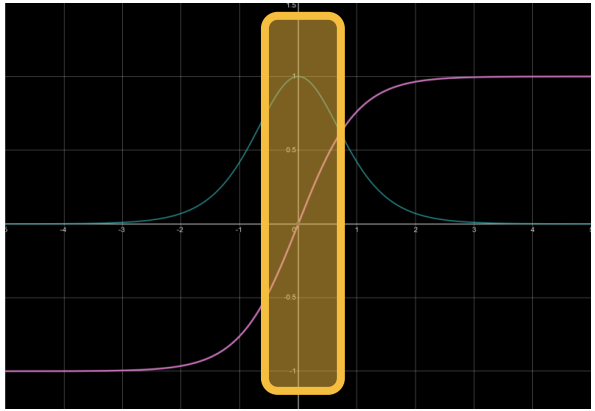
$$w_i = c \quad \forall i$$



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

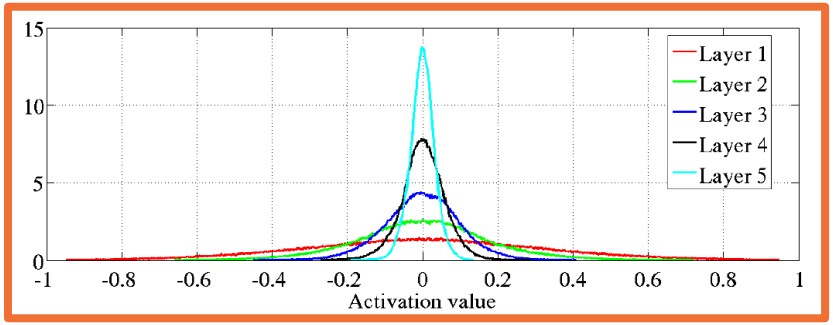
- E.g. $N(\mu, \sigma)$ $where$ $\mu = 0, \sigma = 0.01$
- **Small weights** are preferred since no feature/input has prior importance
- Keeps the model within the **linear region of most activation functions**





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 non-linearities, for increasingly deep layers

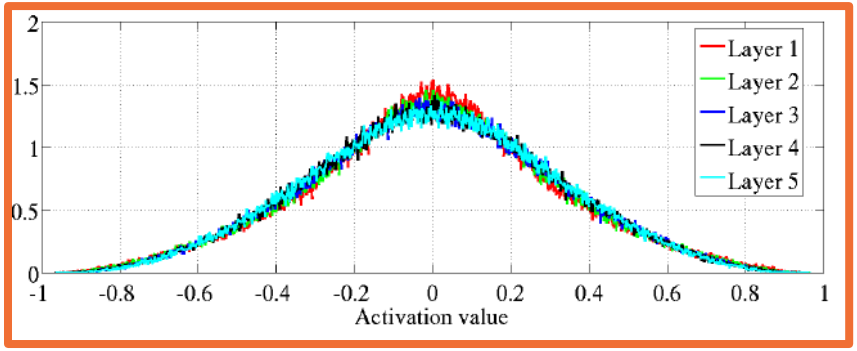
From "Understanding the difficulty of training deep feedforward neural networks." AISTATS, 2010.

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 non-linearities, for increasingly deep layers

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

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

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

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

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

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

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

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Regularization

Many **standard regularization methods** still apply!

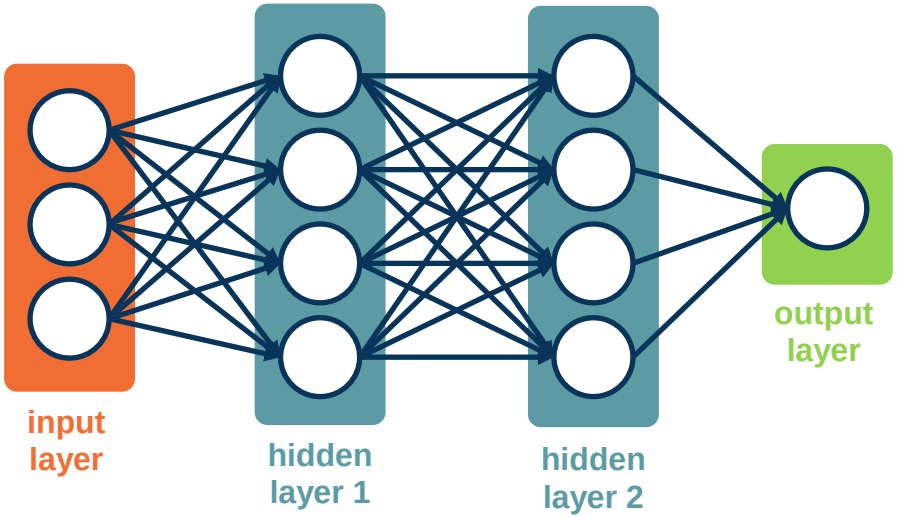
L1 Regularization

$$L = |y - Wx_i|^2 + \lambda|W|$$

where $|W|$ is element-wise

Example regularizations:

- L1/L2 on weights (encourage small values)
- L2: $L = |y - Wx_i|^2 + \lambda|W|^2$ (weight decay)
- Elastic L1/L2: $|y - Wx_i|^2 + \alpha|W|^2 + \beta|W|$

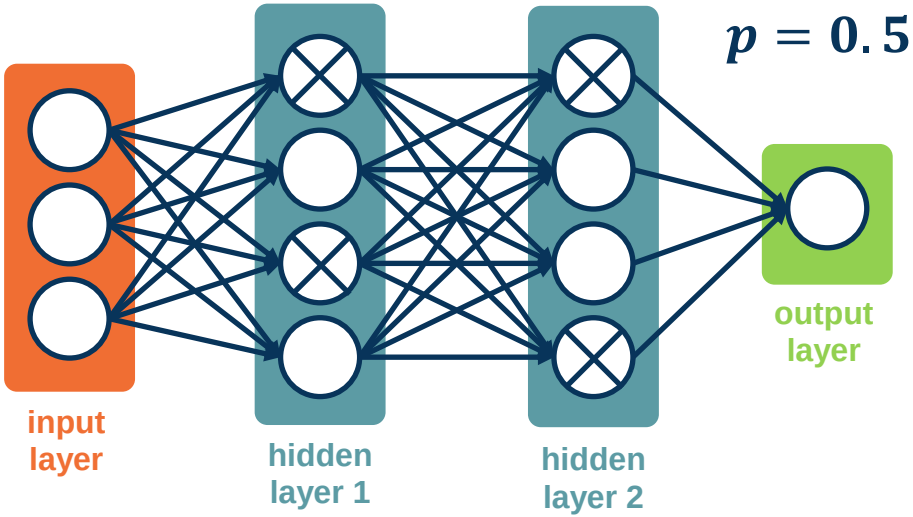


Problem: Network can learn to rely strong on a few features that work really well

- May cause **overfitting** if not representative of test data

From: Dropout: A Simple Way to Prevent Neural Networks from Overfitting, Srivastava et al.

Preventing Co-Adapted Features



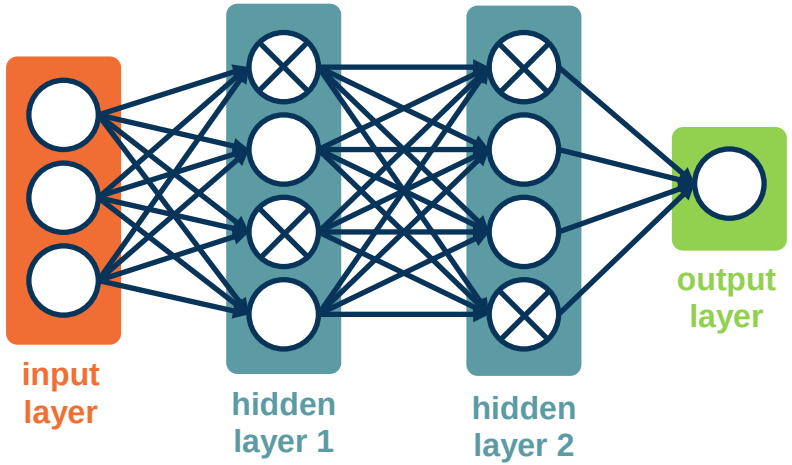
An idea: For each node, keep its output with probability p

- Activations of deactivated nodes are essentially zero

Choose whether to mask out a particular node **each iteration**

From: Dropout: A Simple Way to Prevent Neural Networks from Overfitting, Srivastava et al.

- In practice, implement with a **mask** calculated each iteration
- During testing, no nodes are dropped

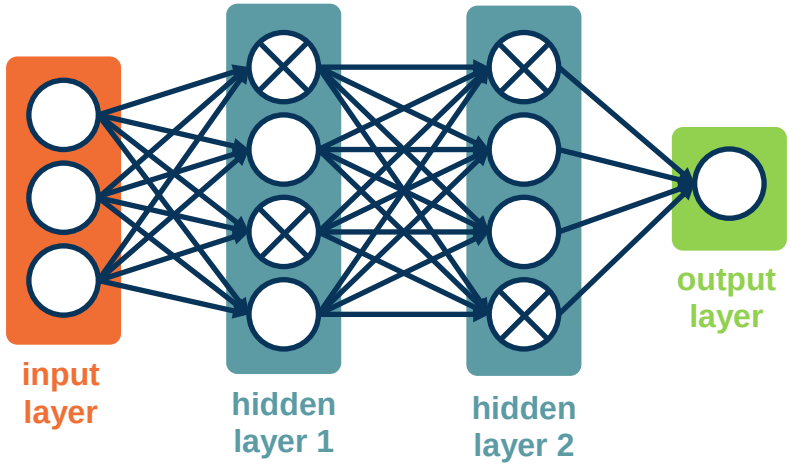


$$\begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ a_{41} \end{bmatrix} \cdot \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}$$

From: Dropout: A Simple Way to Prevent Neural Networks from Overfitting, Srivastava et al.

Dropout Implementation

- During training, each node has an expected $\boldsymbol{p} * \boldsymbol{fan\_in}$ nodes
- During test all nodes are activated
- **Principle:** Always try to have similar train and test-time input/output distributions!



Solution: During test time, scale outputs (or equivalently weights) by $\boldsymbol{p}$

- i.e. $\boldsymbol{W_{test} = pW}$

$$\begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ a_{41} \end{bmatrix} \cdot \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}$$

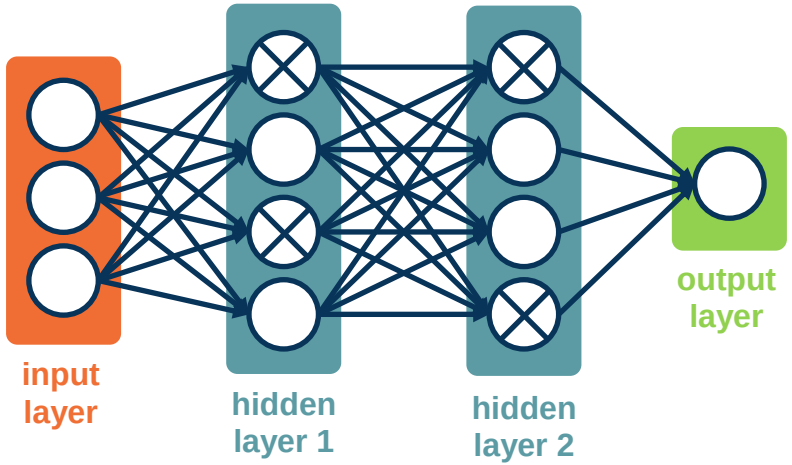
- Alternative: Scale by $\frac{1}{p}$ at train time

From: Dropout: A Simple Way to Prevent Neural Networks from Overfitting, Srivastava et al.

Inference with Dropout

Interpretation 1: The model should not rely too heavily on particular features

- If it does, it has probability $\mathbf{1} - \boldsymbol{p}$ of losing that feature in an iteration



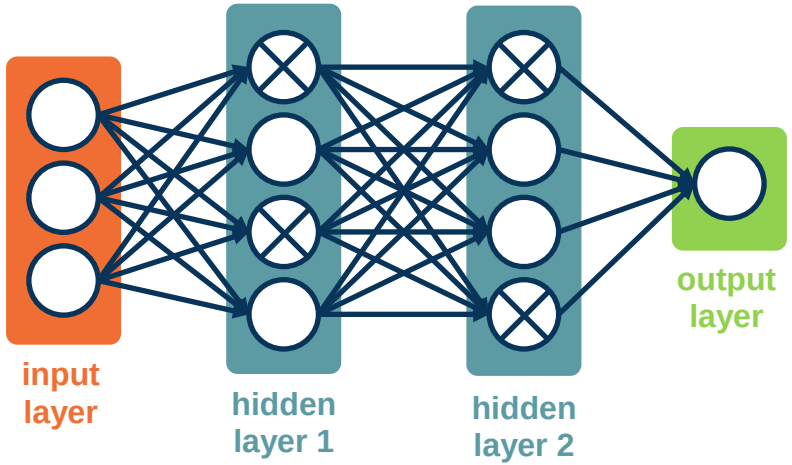
From: Dropout: A Simple Way to Prevent Neural Networks from Overfitting, Srivastava et al.

Interpretation 1: The model should not rely too heavily on particular features

- If it does, it has probability $\mathbf{1} - \boldsymbol{p}$ of losing that feature in an iteration

Interpretation 2: Training $\mathbf{2}^{\boldsymbol{n}}$ networks:

- Each configuration is a network
- Most are trained with 1 or 2 mini-batches of data



From: Dropout: A Simple Way to Prevent Neural Networks from Overfitting, Srivastava et al.

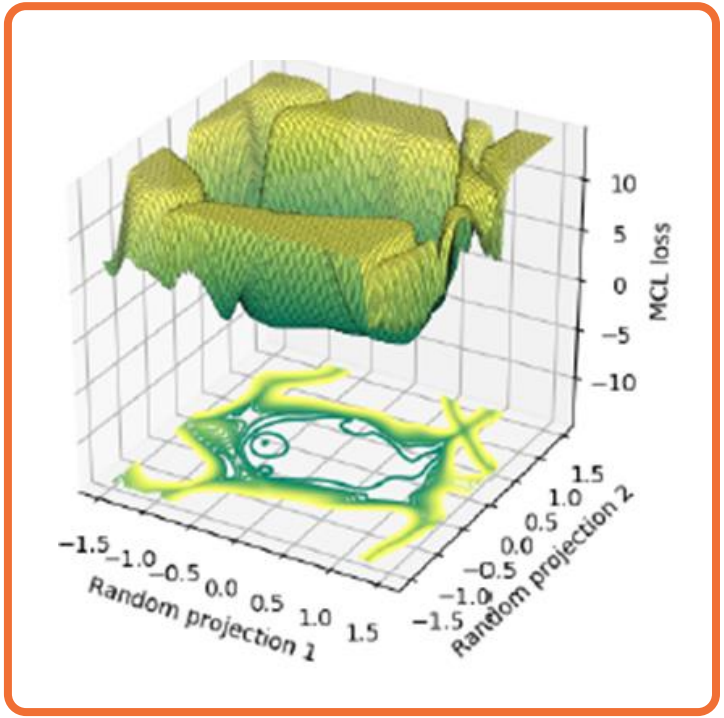
Optimizers

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

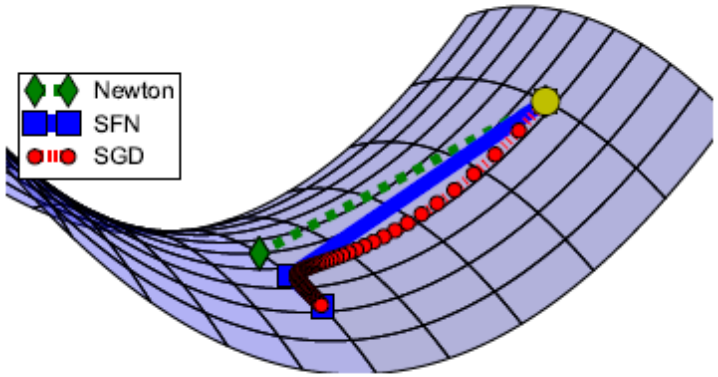
- Some insight can be gained via theory for simpler cases (e.g. convex settings)



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

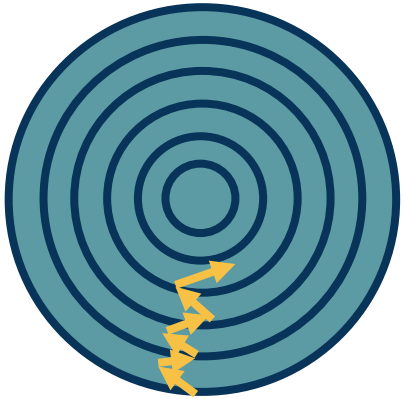


Saddle Point

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

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



Noisy Gradients

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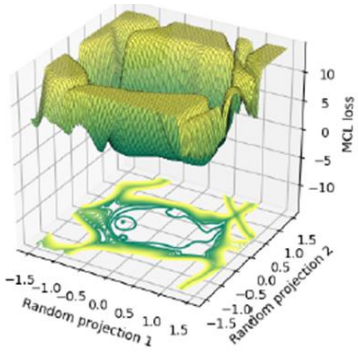
Several **loss surface geometries** are difficult for optimization

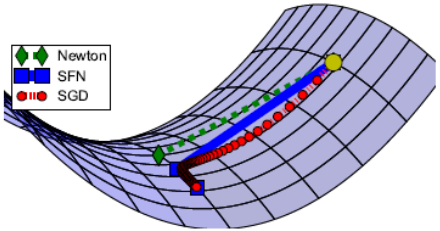
Several types of minima: Local minima, plateaus, saddle points

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

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



Plateau



Saddle Point

- Gradient descent takes a step in the **steepest direction** (negative gradient)

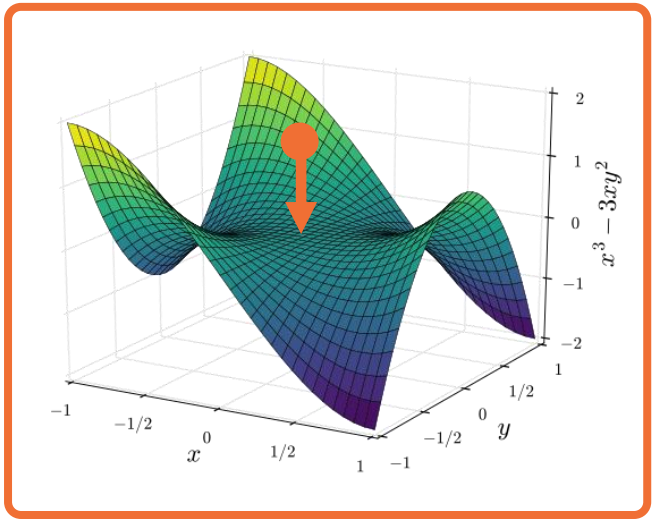
$$w_i = w_{i-1} - \alpha \frac{\partial L}{\partial w_i}$$

- **Intuitive idea:** Imagine a ball rolling down loss surface, and use **momentum** to pass flat surfaces

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

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

- Generalizes SGD ($\beta = 0$)



Adding Momentum

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

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

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

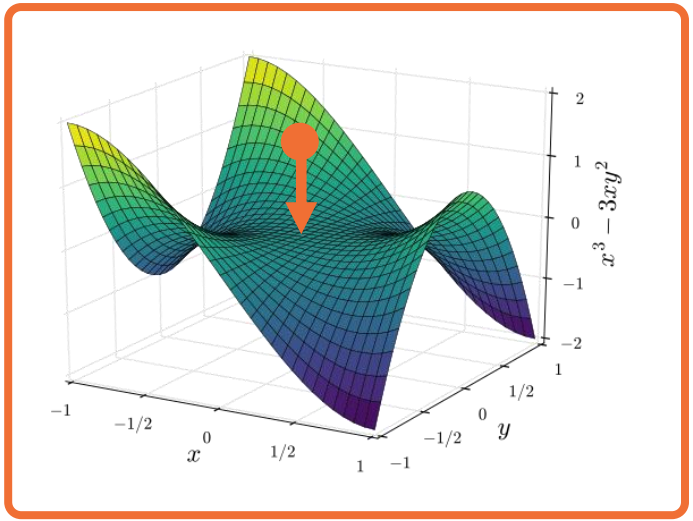
$$= \beta^2 v_{i-2} + \beta \frac{\partial L}{\partial w_{i-2}} + \frac{\partial L}{\partial w_{i-1}}$$

- 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**



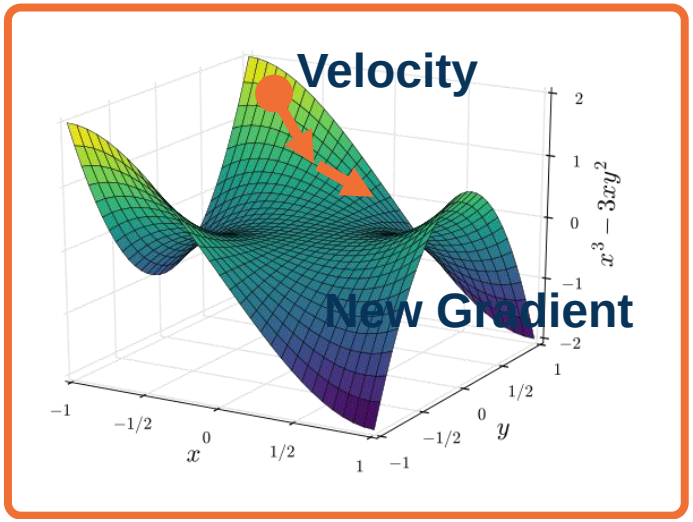
Key idea: Rather than combining velocity with current gradient, go along velocity **first** and then calculate gradient at new point

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

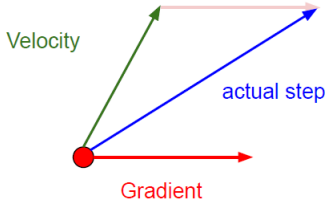
$$\hat{\boldsymbol{w}}_{\boldsymbol{i-1}} = \boldsymbol{w}_{\boldsymbol{i-1}} + \boldsymbol{\beta v}_{\boldsymbol{i-1}}$$

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

$$\boldsymbol{w}_{\boldsymbol{i}} = \boldsymbol{w}_{\boldsymbol{i-1}} - \boldsymbol{\alpha}\, \boldsymbol{v}_{\boldsymbol{i}}$$



Momentum update:



Nesterov Momentum

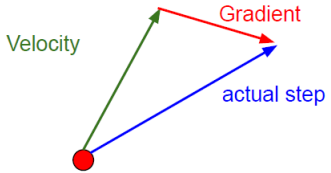


Figure Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Momentum

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

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

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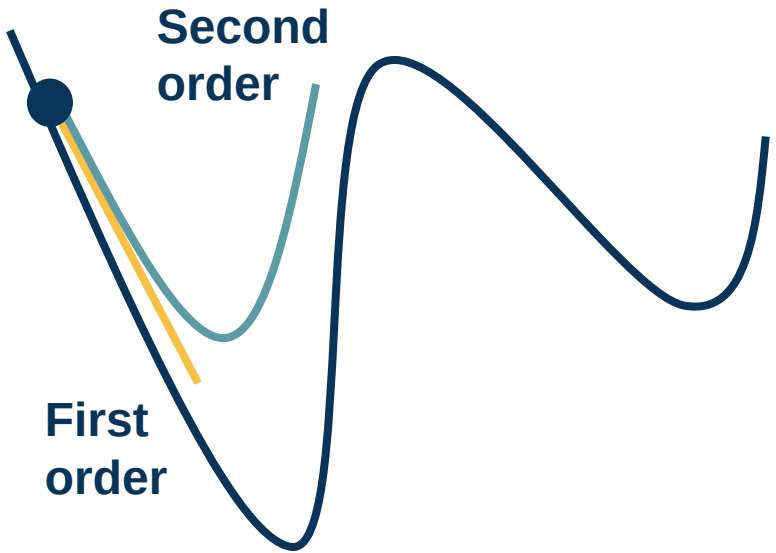
- **Activation Functions**: Use ReLU, GeLU, etc.
- **Initialization:** Important for initial activation and gradient statistics
- **Normalization:** Use dynamic normalization with learnable parts
- **Optimization:** Use momentum (helps w/ local minima, etc.)
  - **Next:** More sophisticated gradient history/statistics in update rule

- Various mathematical ways to **characterize the loss landscape**
- If you liked **Jacobians**… meet:

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



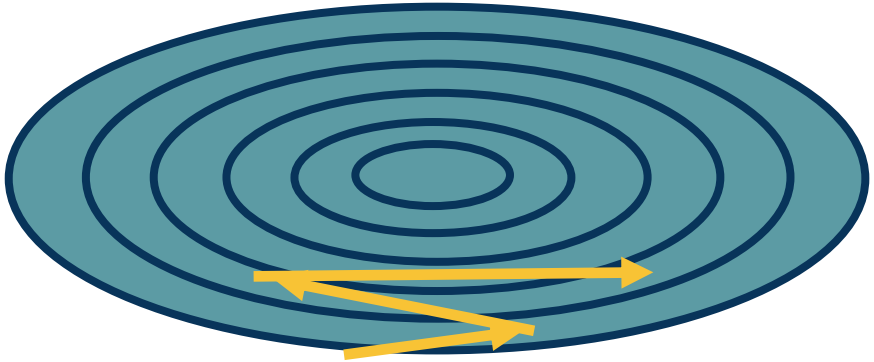
- Gives us information about the **curvature of the loss surface**

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"

Adagrad

Georgia Tech

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 $\boldsymbol{\beta_1 = 0.9,\ \ \beta_2 = 0.999}$

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)

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

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

$$\hat{v}_i = \frac{v_i}{1-\beta_1^t} \qquad \widehat{G_i} = \frac{G_i}{1-\beta_2^t}$$

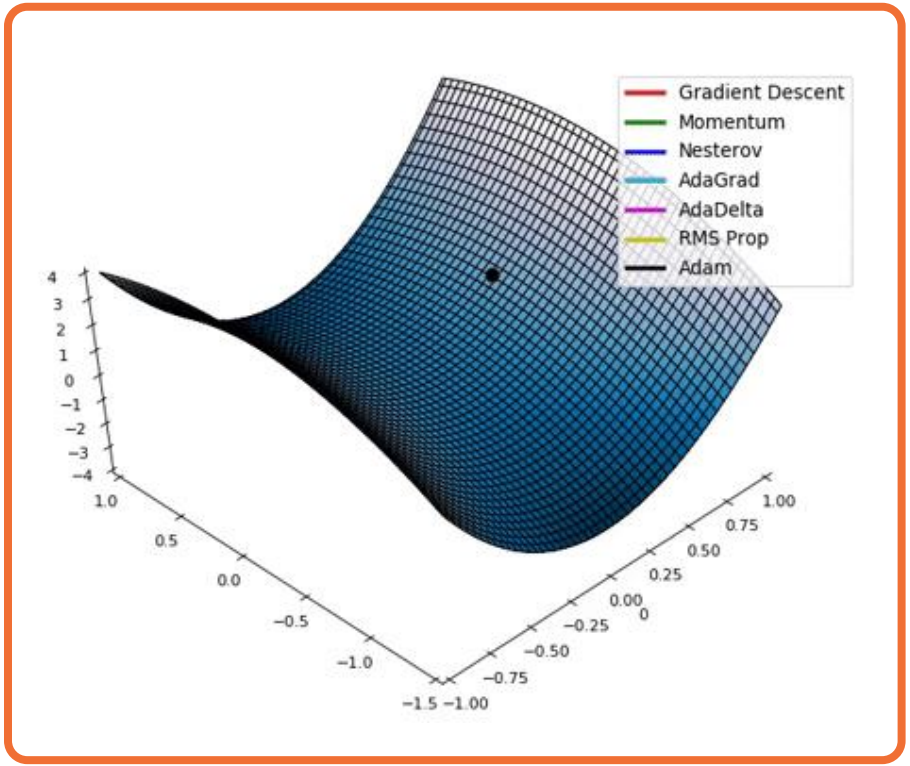
$$w_i = w_{i-1} - \frac{\alpha\, \hat{v}_i}{\sqrt{\widehat{G_i} + \epsilon}}$$

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*



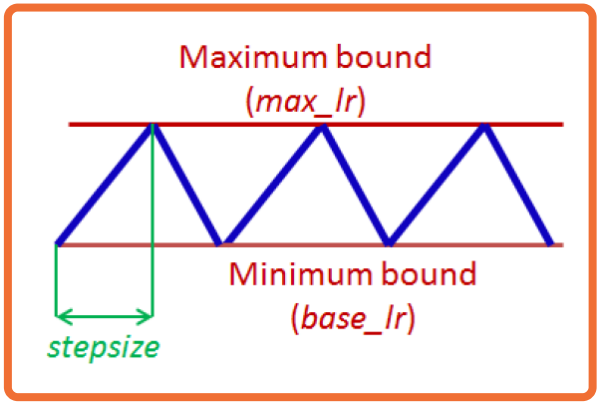
From: https://mlfromscratch.com/optimizers-explained/#/

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"