*CS 1678: Intro to Deep Learning*

# Neural Network Training (Part 2)

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# Plan for this lecture

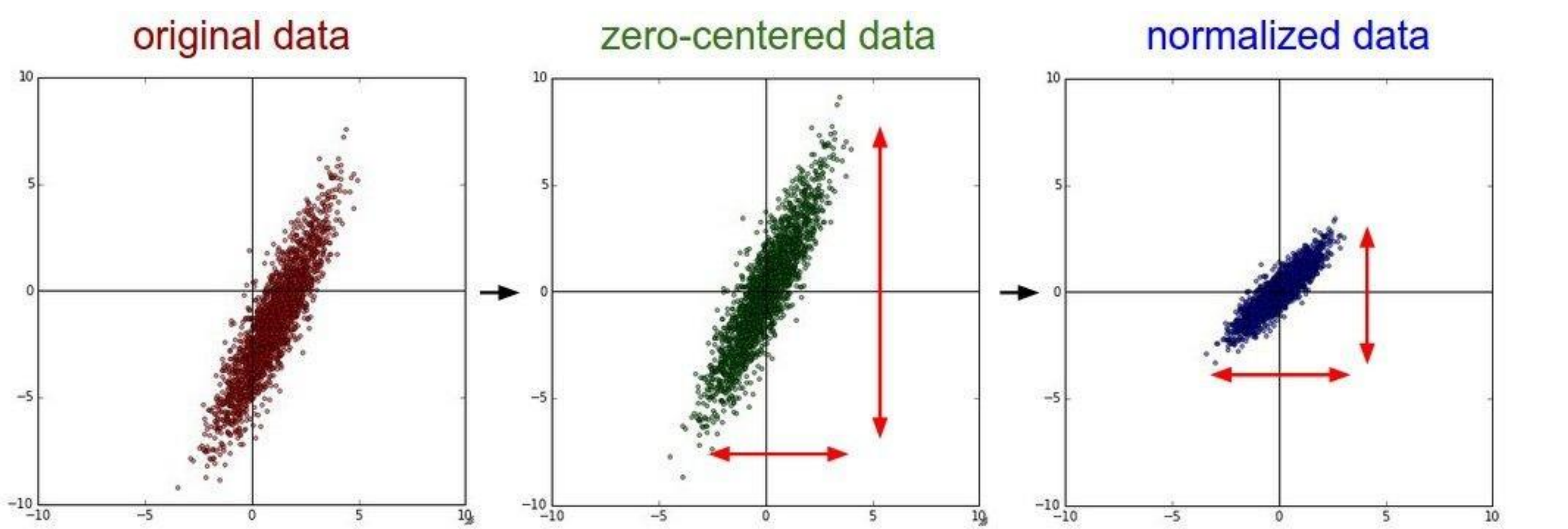
- Tricks of the trade
  - Preprocessing, initialization, normalization
  - Dealing with limited data
  - GPUs
- Convergence of gradient descent
  - How long will it take?
  - Will it work at all?
- Different optimization strategies
  - Alternatives to SGD
  - Learning rates
  - Choosing hyperparameters
- How to do the computation
  - Computation graphs
  - Vector notation (Jacobians)

# Tricks of the trade

# Practical matters

- Getting started: Preprocessing, initialization, normalization, choosing activation functions
- Improving performance and dealing with sparse data: regularization, augmentation, transfer learning
- Hardware and software
- Extra reading/visualization resources
  - https://www.deeplearning.ai/ai-notes/initialization/
  - https://www.deeplearning.ai/ai-notes/optimization/

# Preprocessing the Data



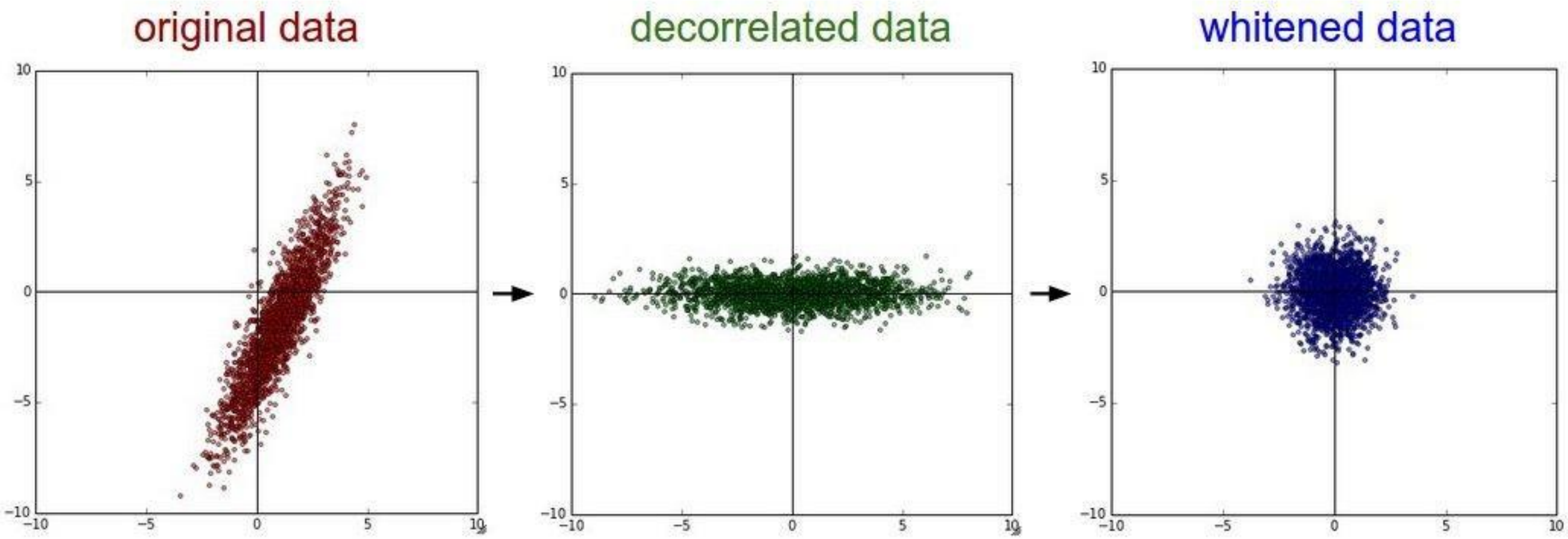

```
X -= np.mean(X, axis = 0)
```

```
X /= np.std(X, axis = 0)
```

(Assume X [NxD] is data matrix, each example in a row)

# Preprocessing the Data

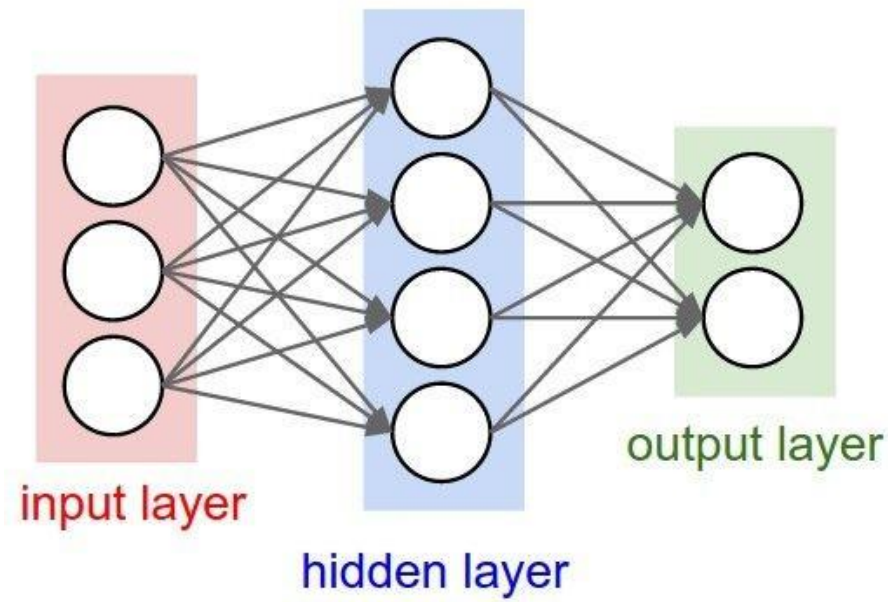
In practice, you may also see **PCA** and **Whitening** of the data




(data has diagonal covariance matrix)

(covariance matrix is the identity matrix)

# Weight Initialization




- Q: what happens when W=constant init is used?

# Weight Initialization

- Another idea: **Small random numbers**

(gaussian with zero mean and 1e-2 standard deviation)

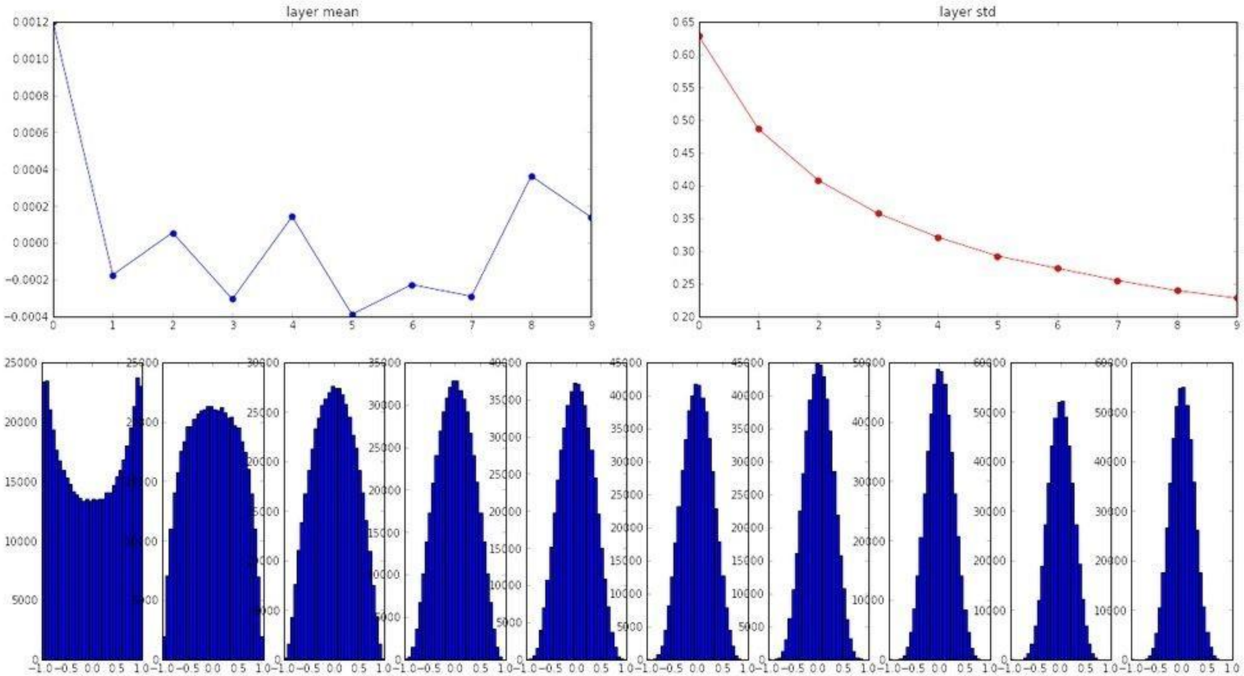
```
W = 0.01* np.random.randn(D,H)
```

Works ~okay for small networks, but problems with deeper networks.

```
input layer had mean 0.001800 and std 1.001311
hidden layer 1 had mean 0.001198 and std 0.627953
hidden layer 2 had mean -0.000175 and std 0.486051
hidden layer 3 had mean 0.000055 and std 0.407723
hidden layer 4 had mean -0.000306 and std 0.357108
hidden layer 5 had mean 0.000142 and std 0.320917
hidden layer 6 had mean -0.000389 and std 0.292116
hidden layer 7 had mean -0.000228 and std 0.273387
hidden layer 8 had mean -0.000291 and std 0.254935
hidden layer 9 had mean 0.000361 and std 0.239266
hidden layer 10 had mean 0.000139 and std 0.228008
```

```
W = np.random.randn(fan_in, fan_out) / np.sqrt(fan_in) # layer initialization
```

"Xavier initialization"
[Glorot et al., 2010]




**Reasonable initialization.**
(Mathematical derivation assumes linear activations)

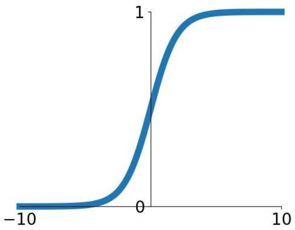


https://www.deeplearning.ai/ai-notes/initialization/#IV

# Activation Functions

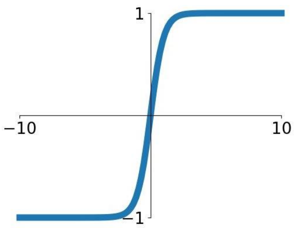
**Sigmoid**

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



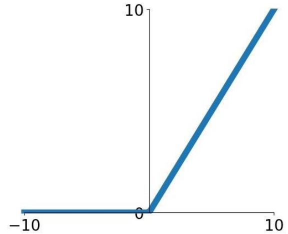

**tanh**

$\tanh(x)$



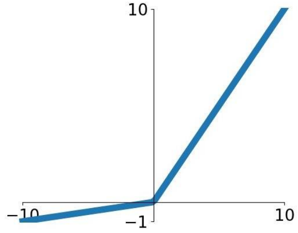

**ReLU**

$\max(0, x)$




**Leaky ReLU**

$\max(0.1x, x)$

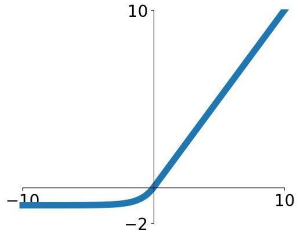



**Maxout**

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

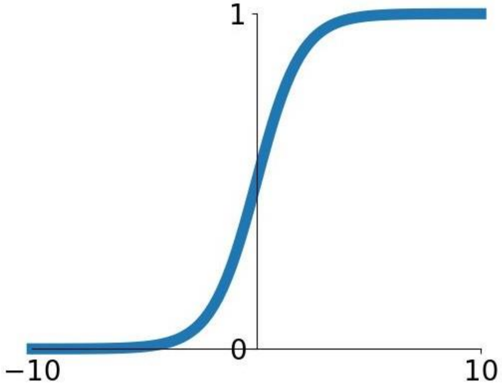
**ELU**

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



# Activation Functions

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




**Sigmoid**

- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron

# Activation Functions

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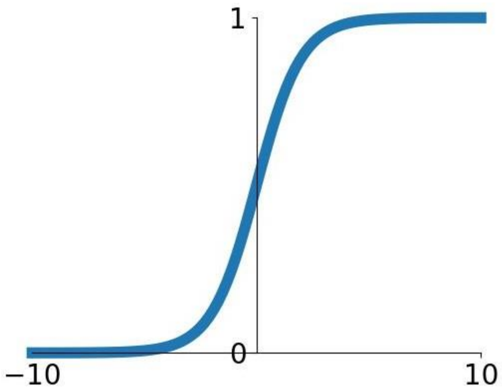


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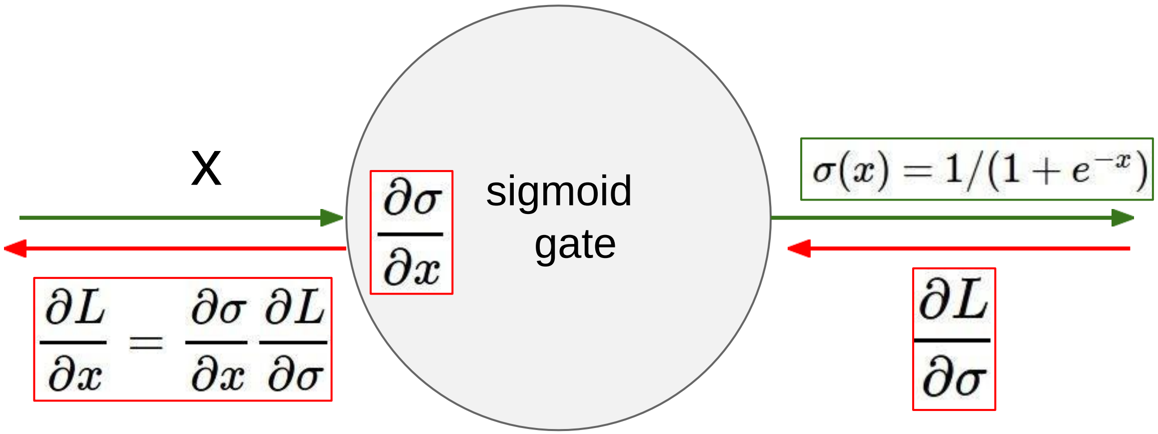
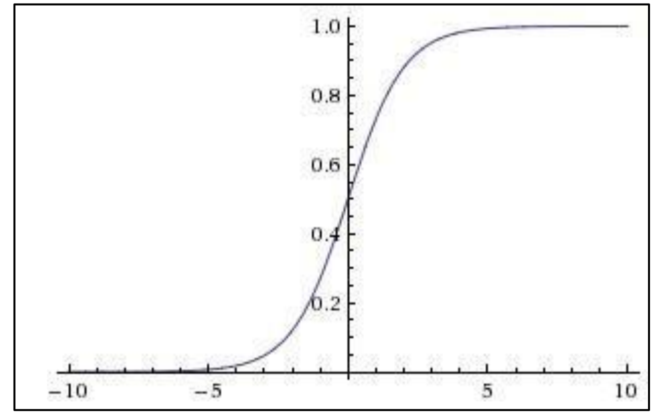
• 3 problems:

1. Saturated neurons “kill” the gradients




What happens when x = -10?
What happens when x = 0?
What happens when x = 10?

# Activation Functions

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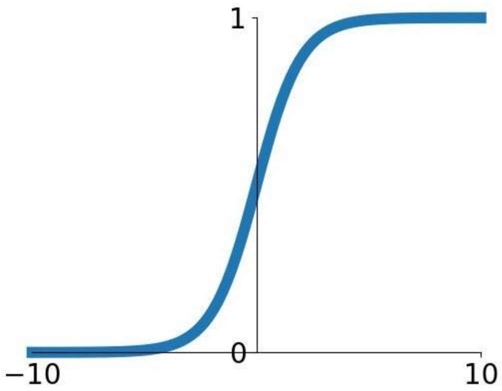


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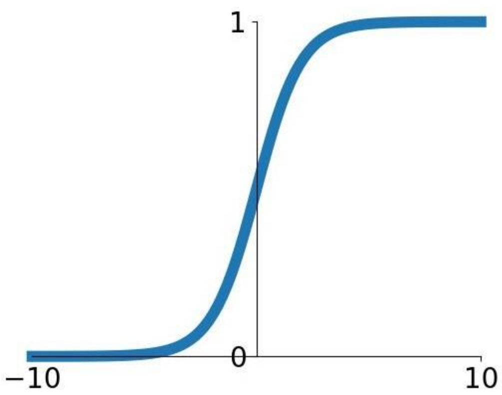


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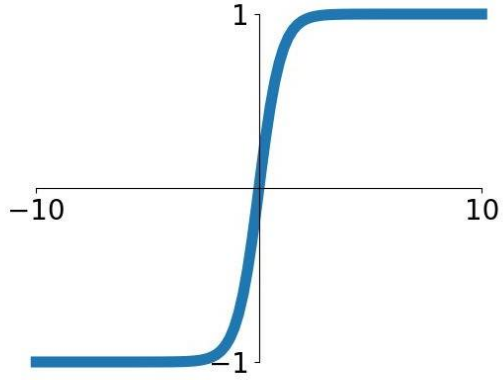
- 3 problems:

  1. Saturated neurons “kill” the gradients
  2. Sigmoid outputs are not zero-centered
  3. exp() is a bit compute expensive

# Activation Functions

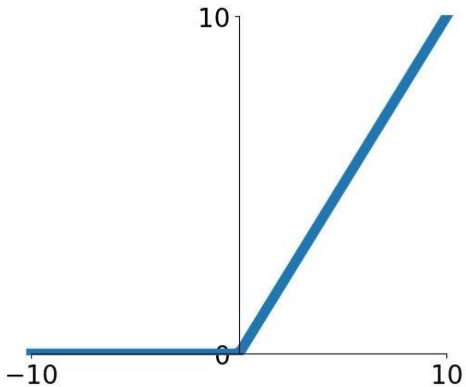



**tanh(x)**

- Squashes numbers to range [-1,1]
- zero centered (nice)
- still kills gradients when saturated :(

[LeCun et al., 1991]

# Activation Functions



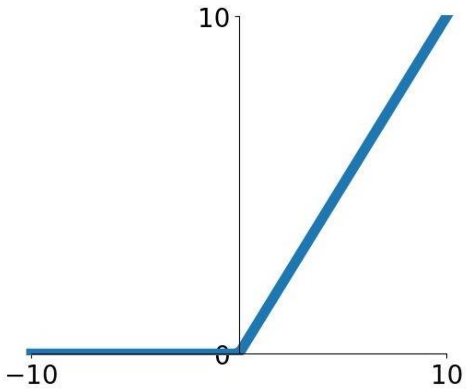

**ReLU**
(Rectified Linear Unit)

- Computes f(x) = max(0,x)

- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)

[Krizhevsky et al., 2012]

# Activation Functions

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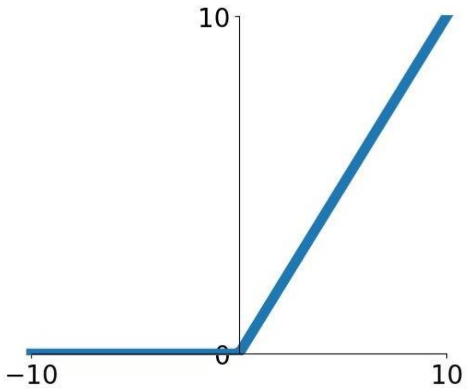
# Activation Functions

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- Does not saturate (in +region)
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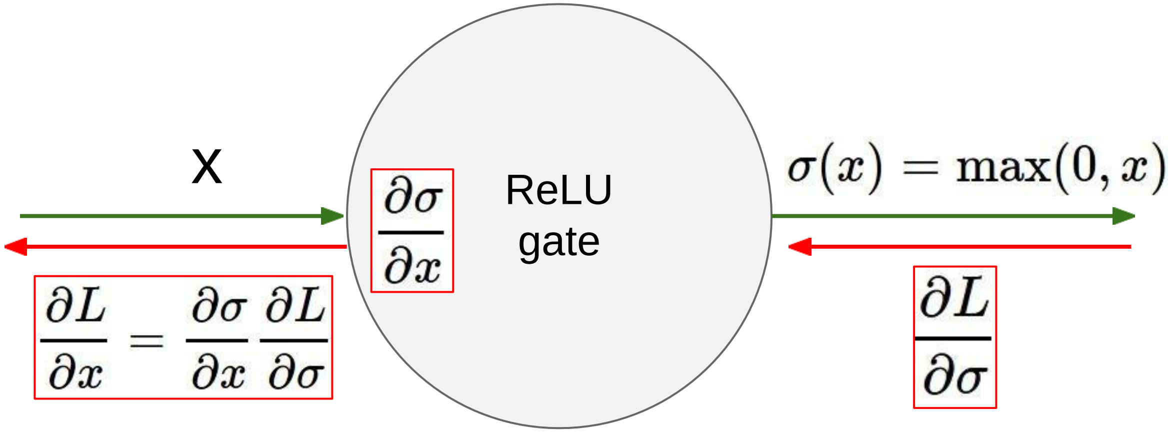
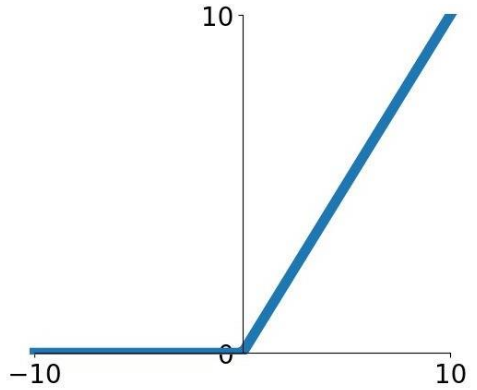
- Not zero-centered output
- An annoyance:

hint: what is the gradient when $x < 0$?

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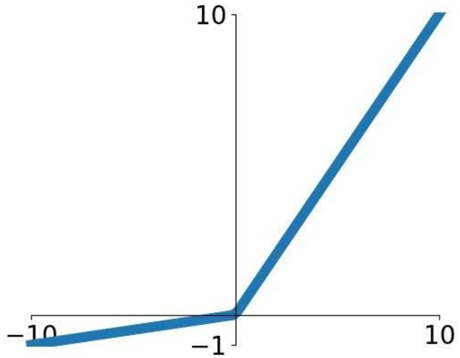
# Activation Functions

[Mass et al., 2013]
[He et al., 2015]




- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not "die".**

**Leaky ReLU**

$$f(x) = \max(0.01x, x)$$

# Activation Functions

[Mass et al., 2013]
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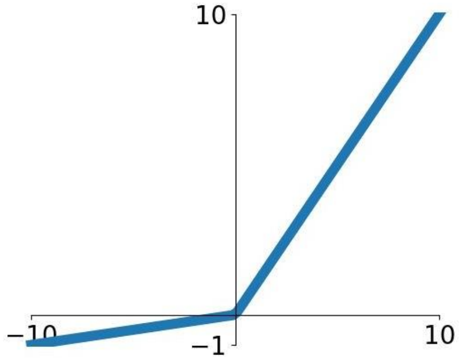


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**Leaky ReLU**

$$f(x) = \max(0.01x, x)$$

**Parametric Rectifier (PReLU)**

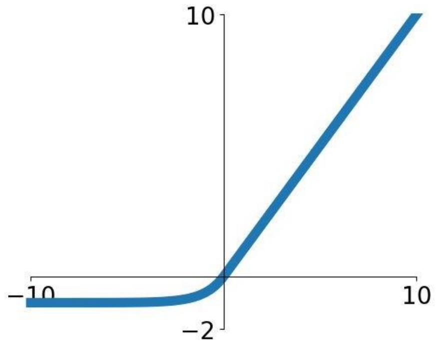
$$f(x) = \max(\alpha x, x)$$

backprop into alpha (parameter)

# Activation Functions

[Clevert et al., 2015]

## Exponential Linear Units (ELU)




- All benefits of ReLU
- Closer to zero mean outputs
- Negative saturation regime compared with Leaky ReLU adds some robustness to noise

$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha\,(\exp(x) - 1) & \text{if } x \le 0 \end{cases}$$

- Computation requires exp()

[Goodfellow et al., 2013]

# Maxout "Neuron"

- Does not have the basic form of dot product -> nonlinearity
- Generalizes ReLU and Leaky ReLU
- Linear Regime! Does not saturate! Does not die!

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

Problem: doubles the number of parameters/neuron :(

TLDR: In practice:

- Use ReLU. Be careful with your learning rates
- Try out Leaky ReLU / Maxout / ELU / PReLU
- Try out tanh but don't expect much
- Don't use sigmoid

# Batch Normalization

[Ioffe and Szegedy, 2015]

“you want zero-mean unit-variance activations? just make them so.”

consider a batch of activations at some layer. To make each dimension zero-mean unit-variance, apply:

$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

# Batch Normalization

[Ioffe and Szegedy, 2015]

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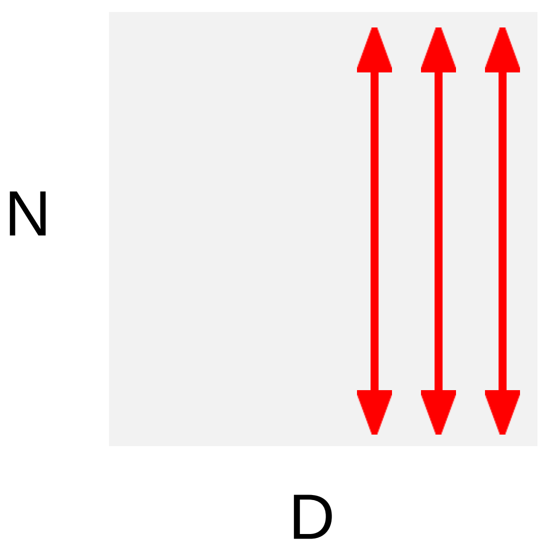


1. compute the empirical mean and variance independently for each dimension.

2. Normalize

$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

# Batch Normalization

[Ioffe and Szegedy, 2015]

Normalize:

$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

And then allow the network to squash the range if it wants to:

$$y^{(k)} = \gamma^{(k)} \widehat{x}^{(k)} + \beta^{(k)}$$

Note, the network can learn:

$$\gamma^{(k)} = \sqrt{\mathrm{Var}[x^{(k)}]}$$

$$\beta^{(k)} = \mathrm{E}[x^{(k)}]$$

to recover the identity mapping.

# Batch Normalization

[Ioffe and Szegedy, 2015]

**Input:** Values of $x$ over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: $\gamma$, $\beta$

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

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

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

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

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

- Improves gradient flow through the network
- Allows higher learning rates
- Reduces the strong dependence on initialization
- Acts as a form of regularization

# Batch Normalization

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**Note: at test time BatchNorm layer functions differently:**

The mean/std are not computed based on the batch. Instead, a single fixed empirical mean of activations during training is used.

(e.g. can be estimated during training with running averages)

# Babysitting the Learning Process

- Preprocess data
- Choose architecture
- Initialize and check initial loss with no regularization
- Increase regularization, loss should increase
- Then train – try small portion of data, check you can overfit
- Add regularization, and find learning rate that can make the loss go down
- Check learning rates in range [1e-3 … 1e-5]
- Coarse-to-fine search for hyperparameters (e.g. learning rate, regularization)

# Grid and Random Search

*Random Search for*
*Hyper-Parameter Optimization*
Bergstra and Bengio, 2012

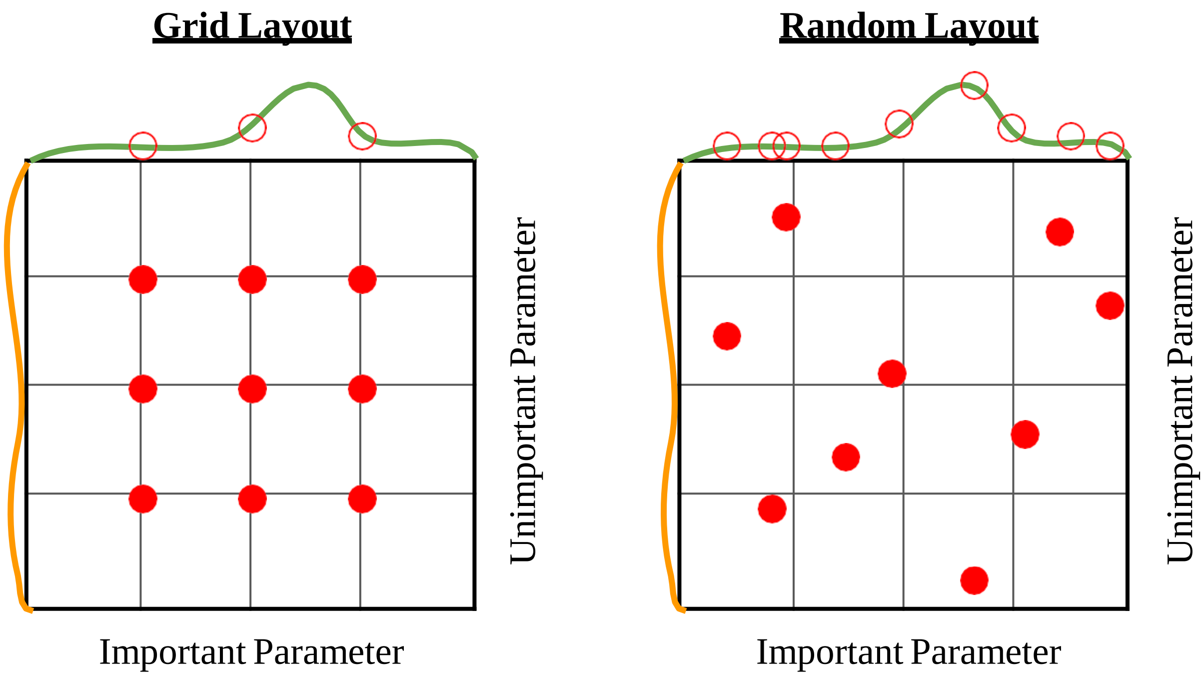
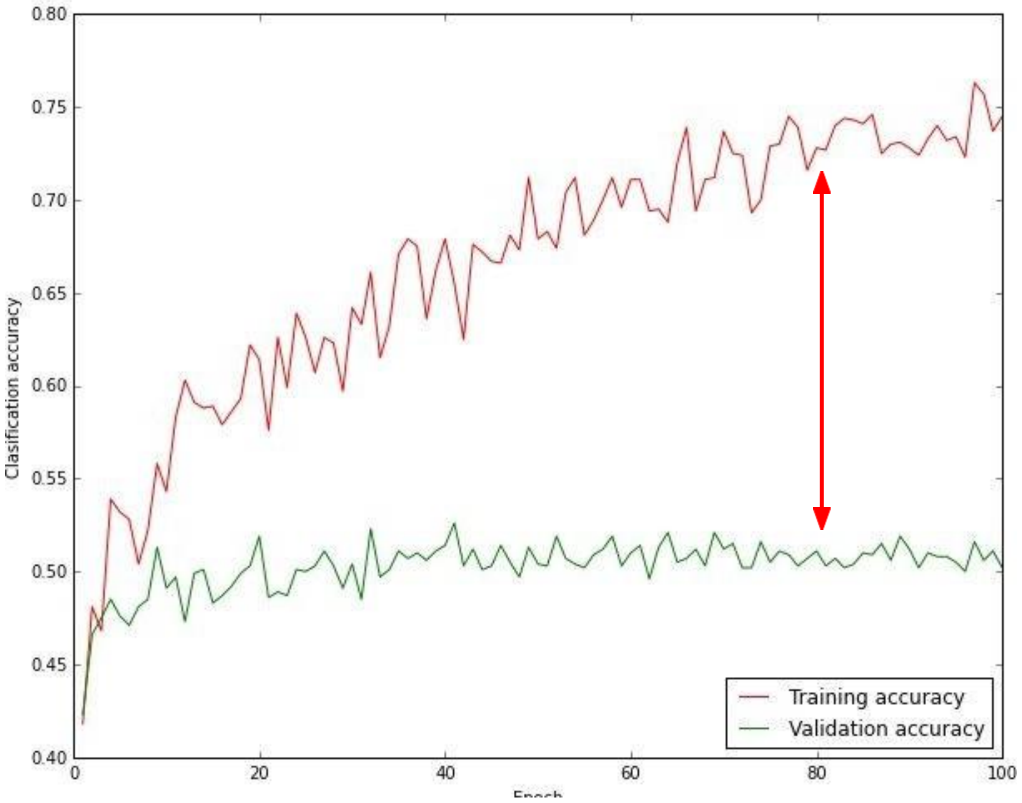



Illustration of Bergstra et al., 2012 by Shayne Longpre, copyright CS231n 2017

# Monitor and Visualize Accuracy




big gap = overfitting

=> increase regularization strength?

no gap

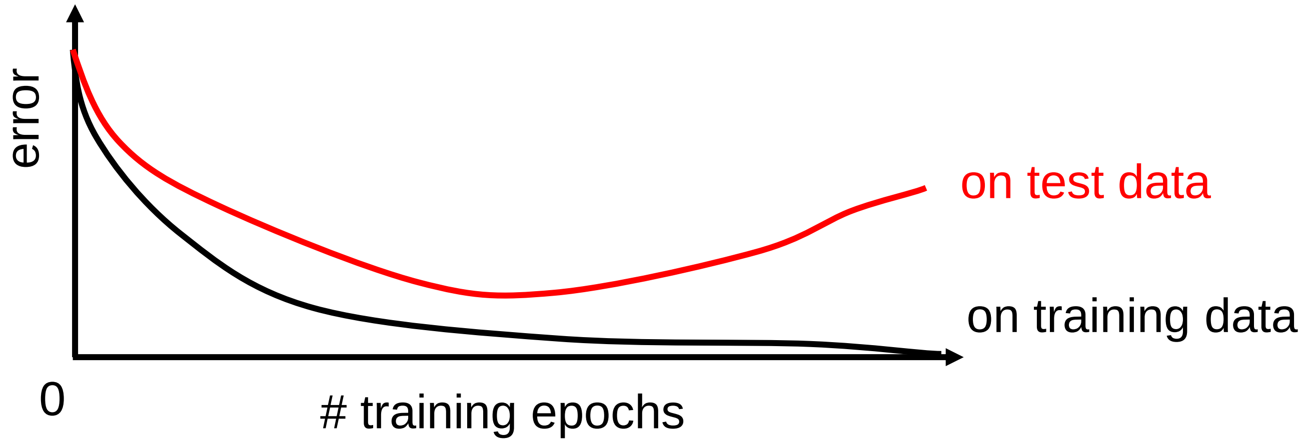
=> increase model capacity?

# Dealing with sparse data

- Deep neural networks require lots of data, and can overfit easily
- The more weights you need to learn, the more data you need
- That's why with a deeper network, you need more data for training than for a shallower network
- Ways to prevent overfitting include:
  - Using a validation set to stop training or pick parameters
  - Regularization
  - Data augmentation
  - Transfer learning

# Over-training prevention

- Running too many epochs can result in over-fitting.

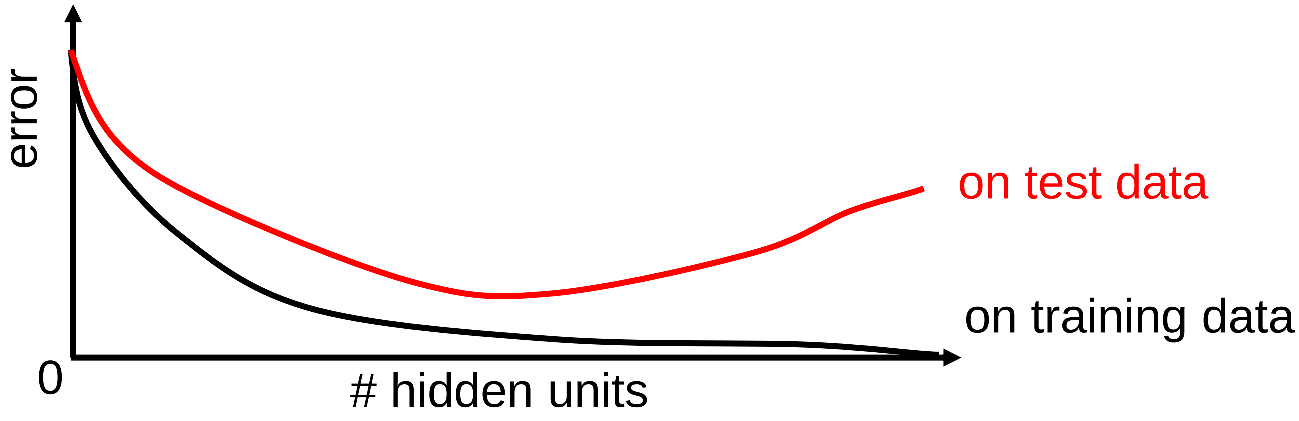



- Keep a hold-out validation set and test accuracy on it after every epoch. Stop training when additional epochs actually increase validation error.

Adapted from Ray Mooney

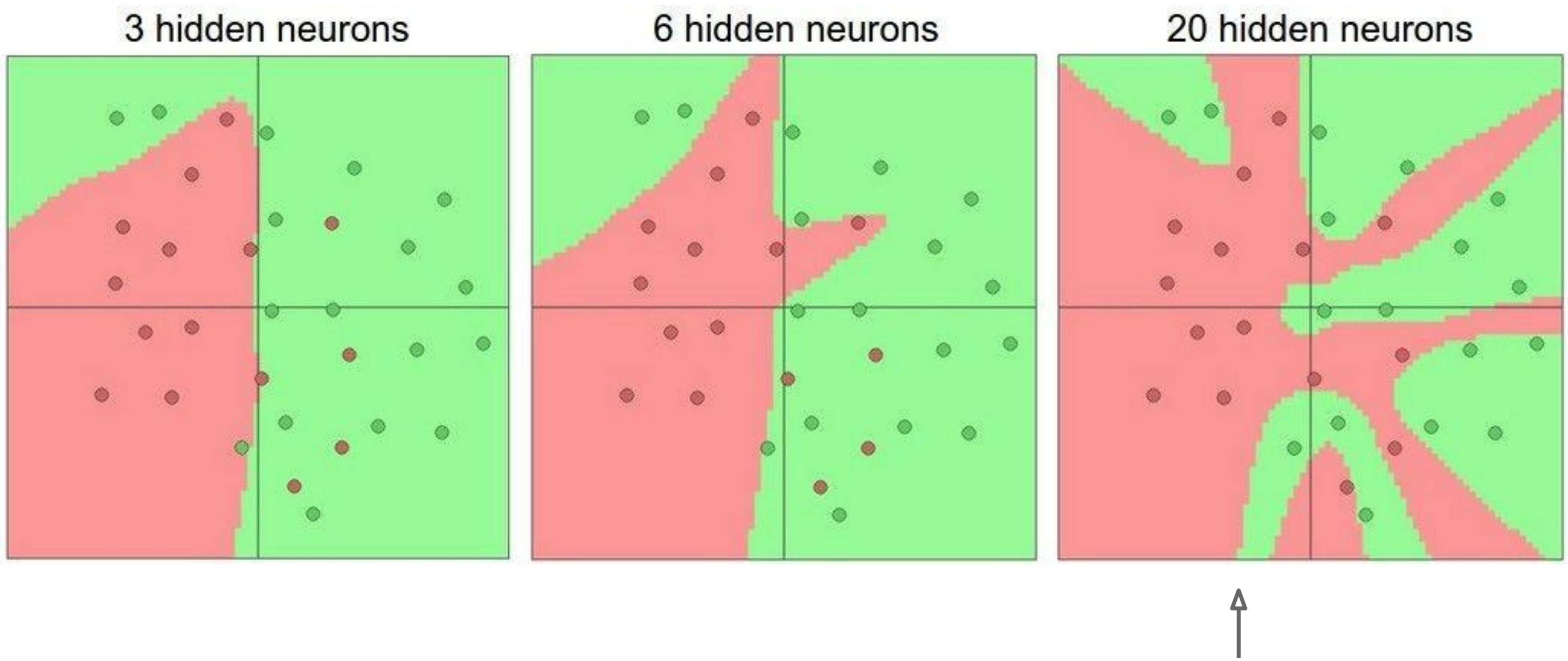
# Determining best number of hidden units

- Too few hidden units prevent the network from adequately fitting the data.
- Too many hidden units can result in over-fitting.




- Use internal cross-validation to empirically determine an optimal number of hidden units.

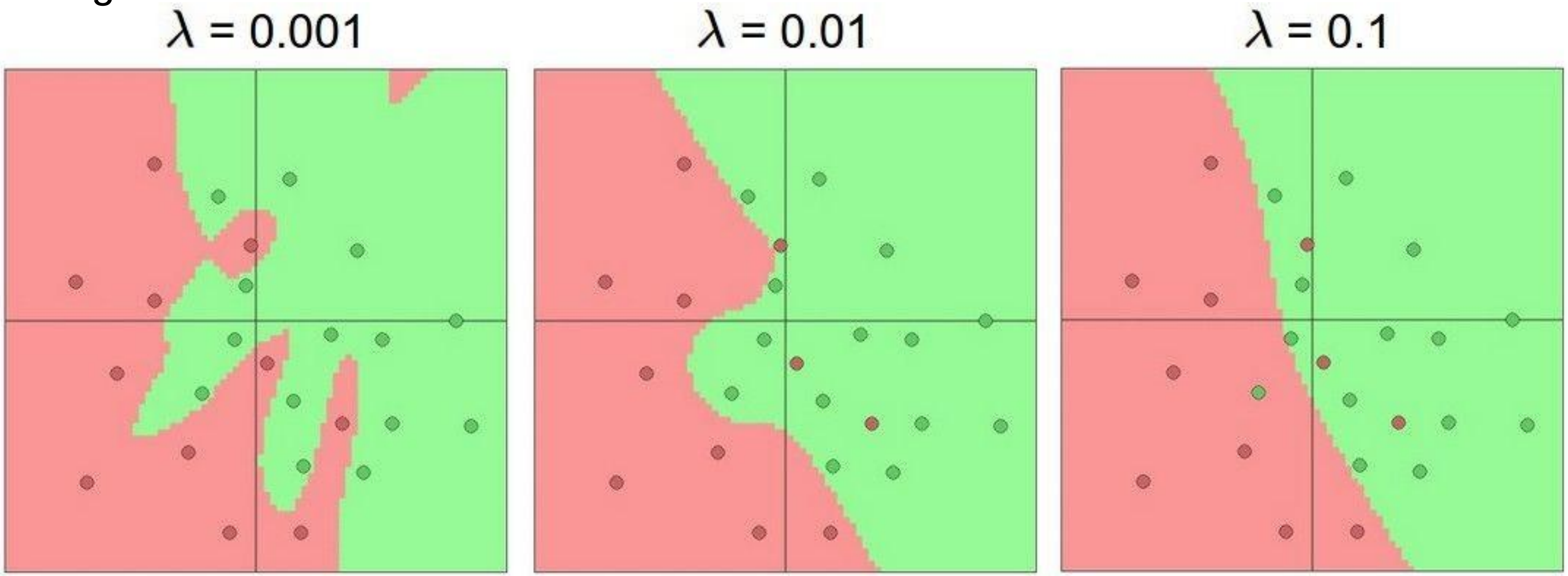
# Effect of number of neurons




more neurons = more capacity

# Effect of regularization

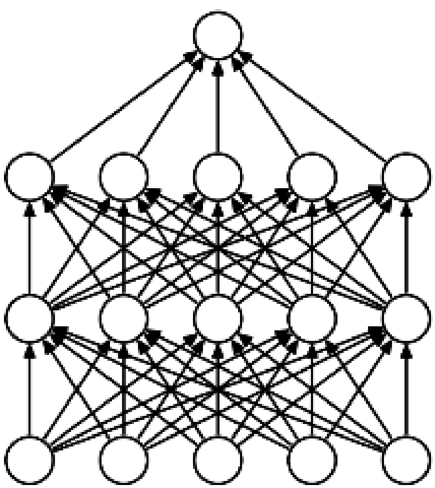
Do not use size of neural network as a regularizer. Use stronger regularization instead:



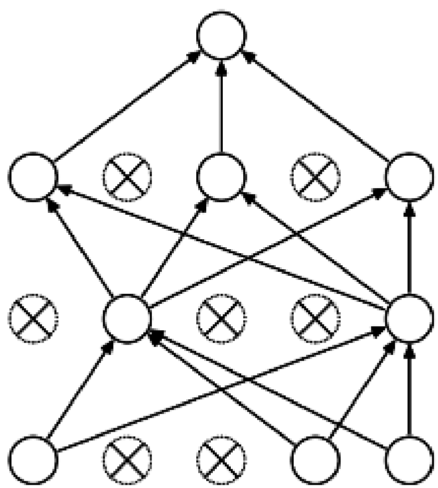

(you can play with this demo over at ConvNetJS: http://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html)

# Regularization

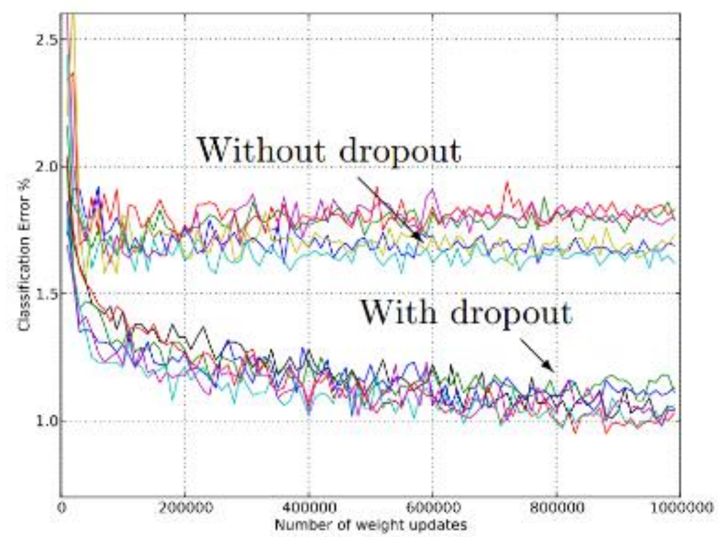
- L1, L2 regularization (*weight decay*)
- Dropout
  - Randomly turn off some neurons
  - Allows individual neurons to independently be responsible for performance



(a) Standard Neural Net



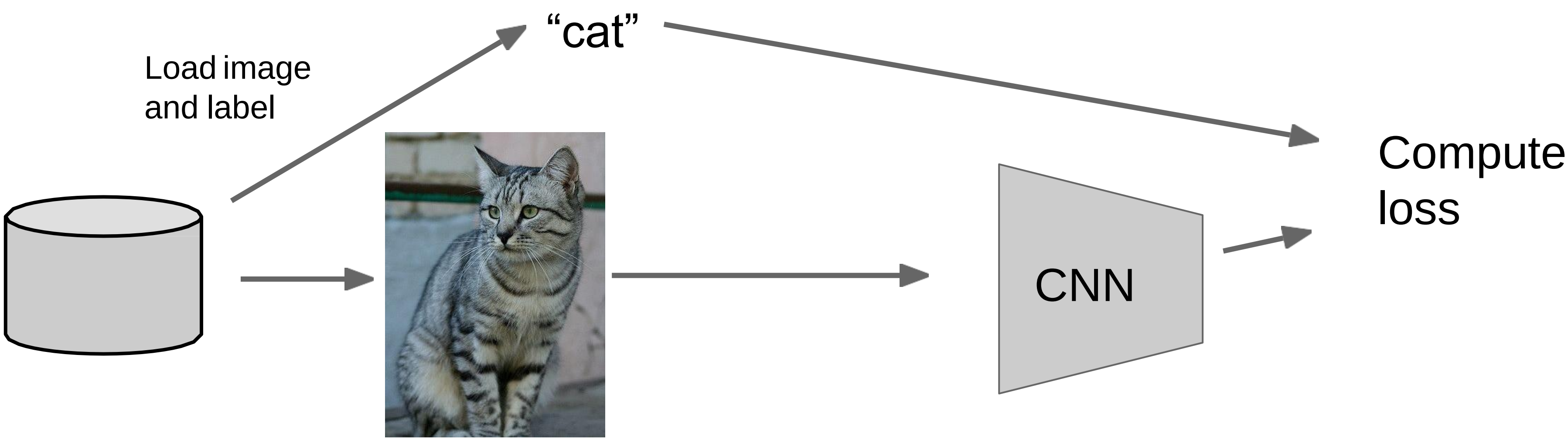
(b) After applying dropout.




Dropout: A simple way to prevent neural networks from overfitting [Srivastava JMLR 2014]

Adapted from Jia-bin Huang

# Data Augmentation



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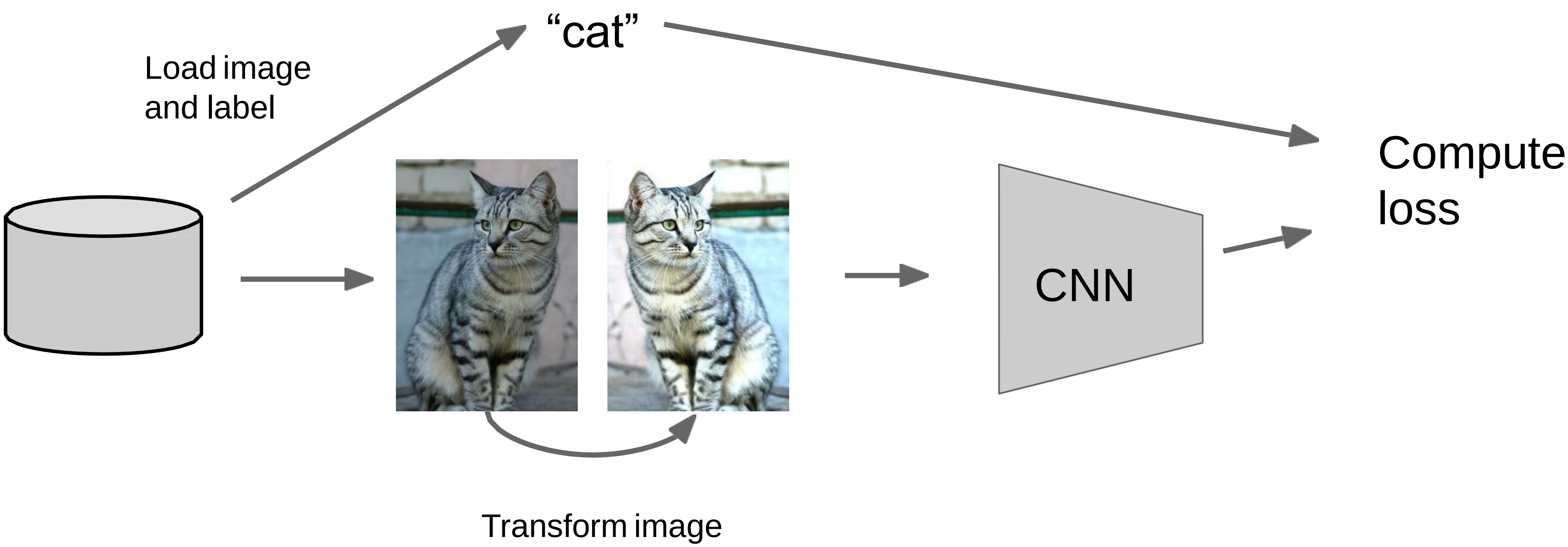
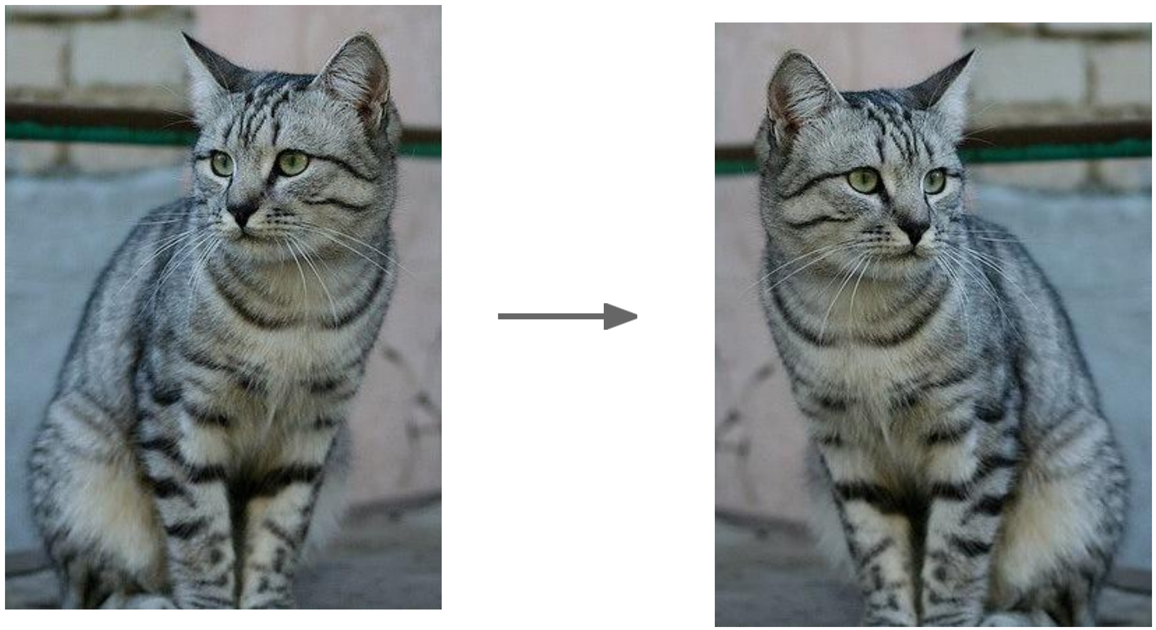


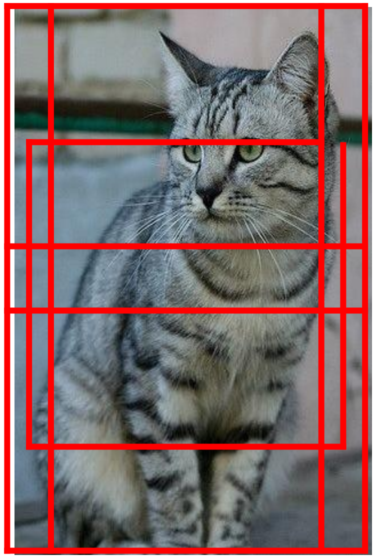
# Data Augmentation

## Horizontal Flips



# Data Augmentation

## Random crops and scales



**Training**: sample random crops / scales

ResNet:

1. Pick random L in range [256, 480]
2. Resize training image, short side = L
3. Sample random 224 x 224 patch

**Testing**: average a fixed set of crops

ResNet:

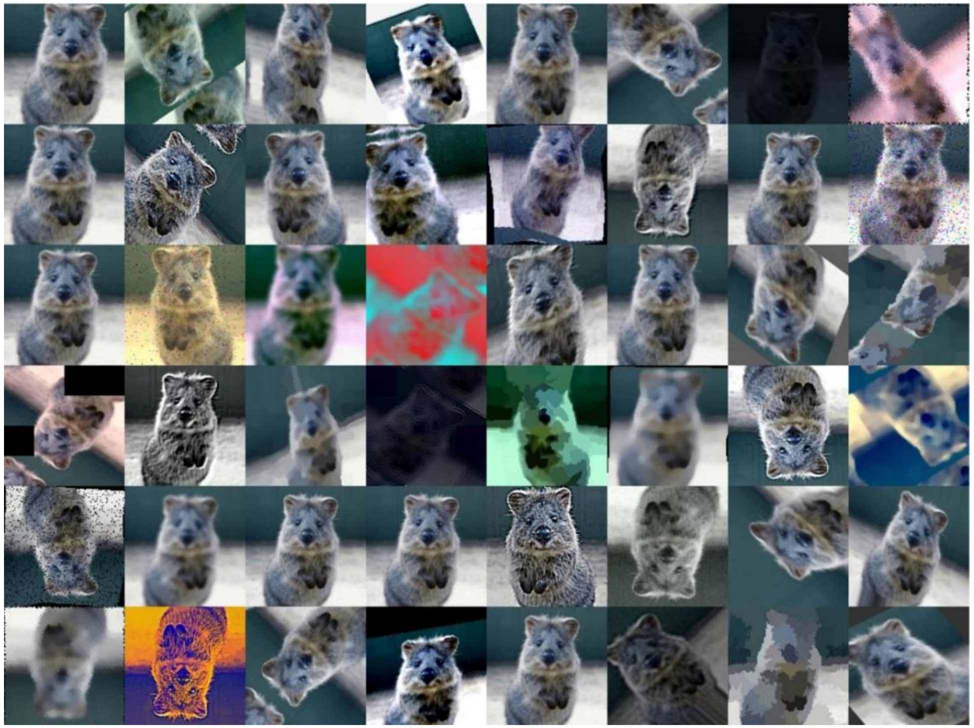
1. Resize image at 5 scales: {224, 256, 384, 480, 640}
2. For each size, use 10 224 x 224 crops: 4 corners + center, + flips

# Data Augmentation

Get creative for your problem!

Random mix/combinations of :

- translation
- rotation
- stretching
- shearing,
- lens distortions
- …

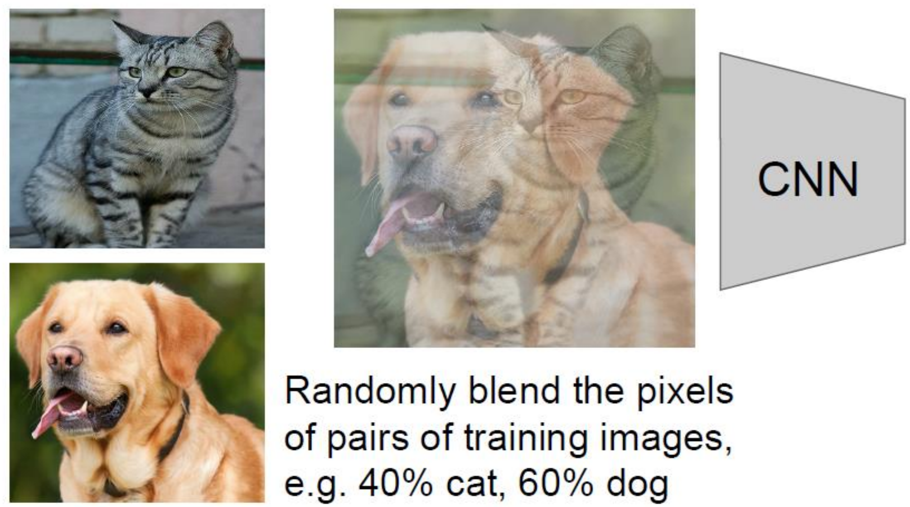


# Data Augmentation

## Regularization: Mixup

**Training**: Train on random blends of images

**Testing**: Use original images



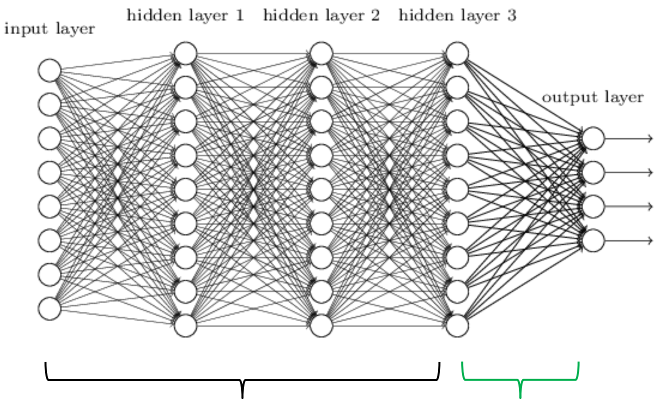

Target label:
cat: 0.4
dog: 0.6

Randomly blend the pixels of pairs of training images, e.g. 40% cat, 60% dog

Zhang et al, “*mixup*: Beyond Empirical Risk Minimization”, ICLR 2018

# Transfer learning

- If you have sparse data in your domain of interest *(target)*, but have rich data in a disjoint yet related domain *(source)*,
- You can train the early layers on the *source* domain, and only the last few layers on the *target domain:*

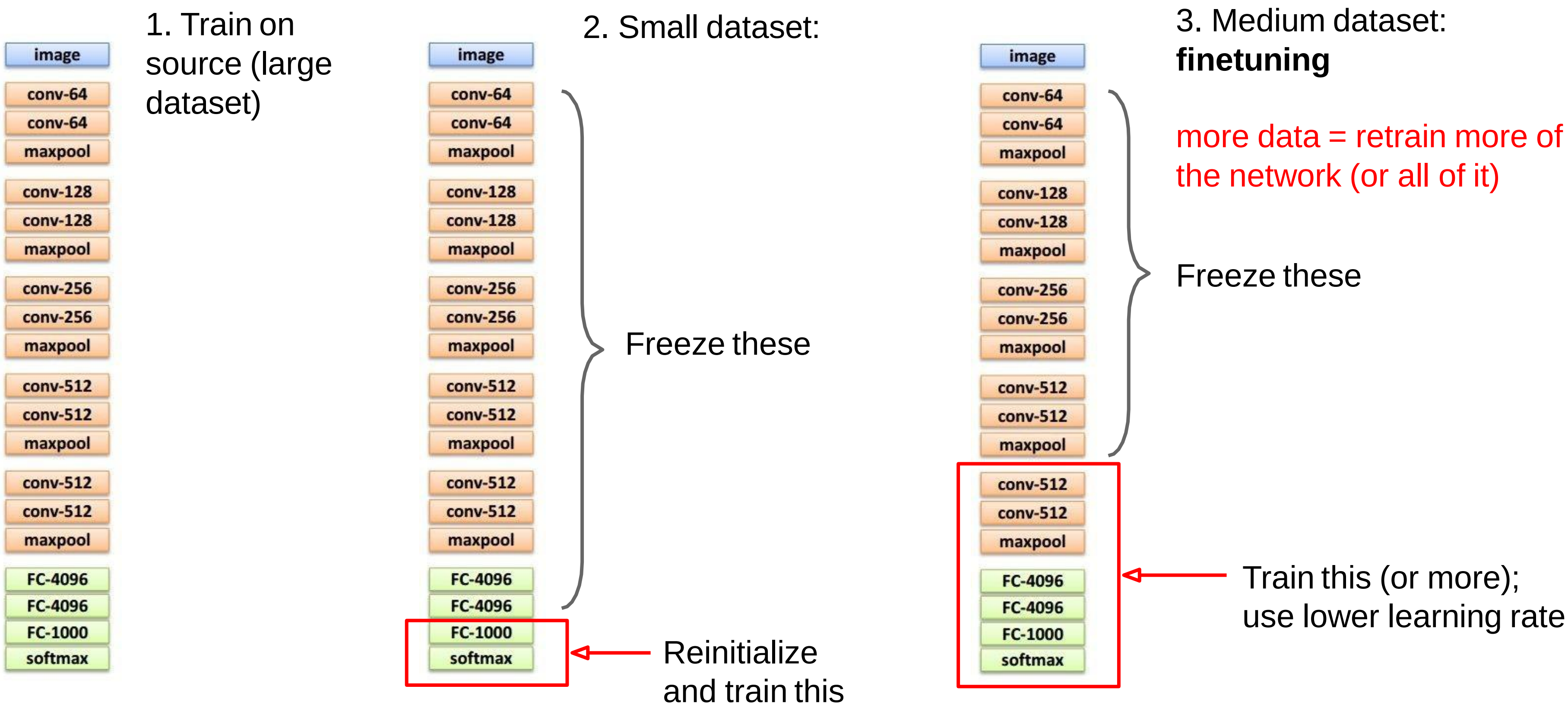



Set these to the already learned weights from another network

Learn these on your own task

# Transfer learning

Source: classify 20 animal classes　　Target: 10 car classes




Another option: use network as feature extractor, train SVM/LR on extracted features for target task

Adapted from Andrej Karpathy

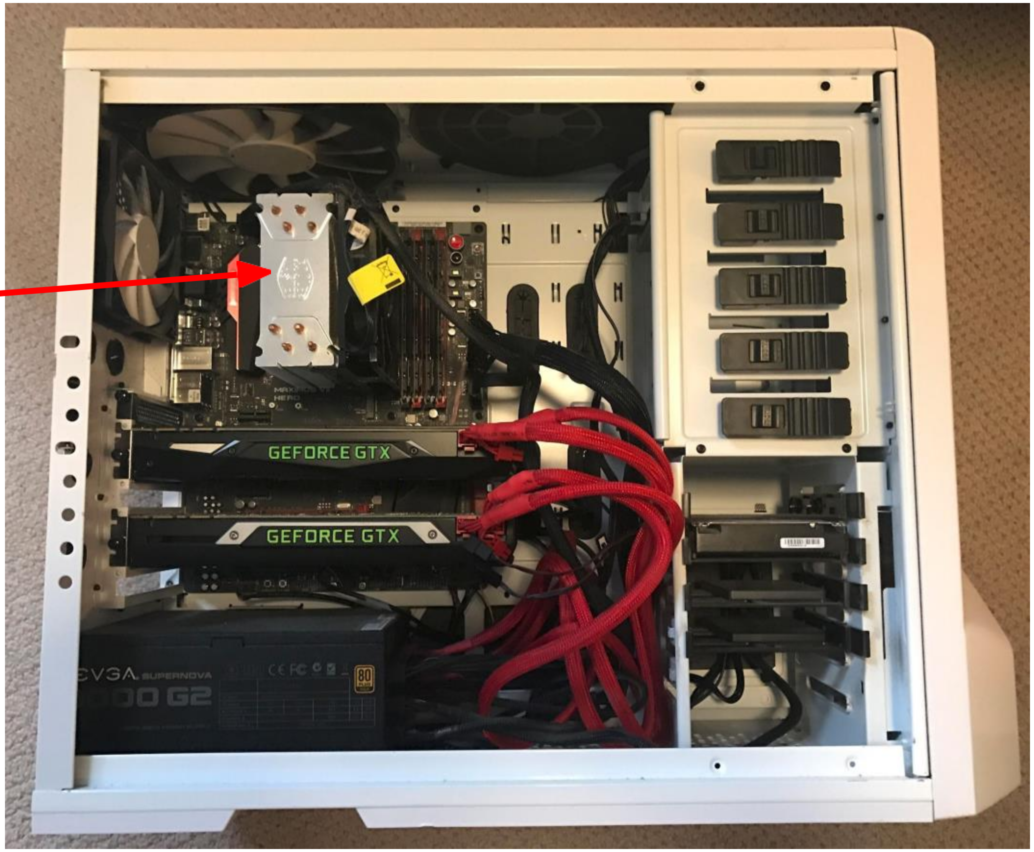
# Mini-batch gradient descent

- In classic gradient descent, we compute the gradient from the loss for all training examples
- Could also only use *some* of the data for each gradient update
- We cycle through all the training examples multiple times
- Each time we've cycled through all of them once is called an 'epoch'
- Allows faster training (e.g. on GPUs), parallelization

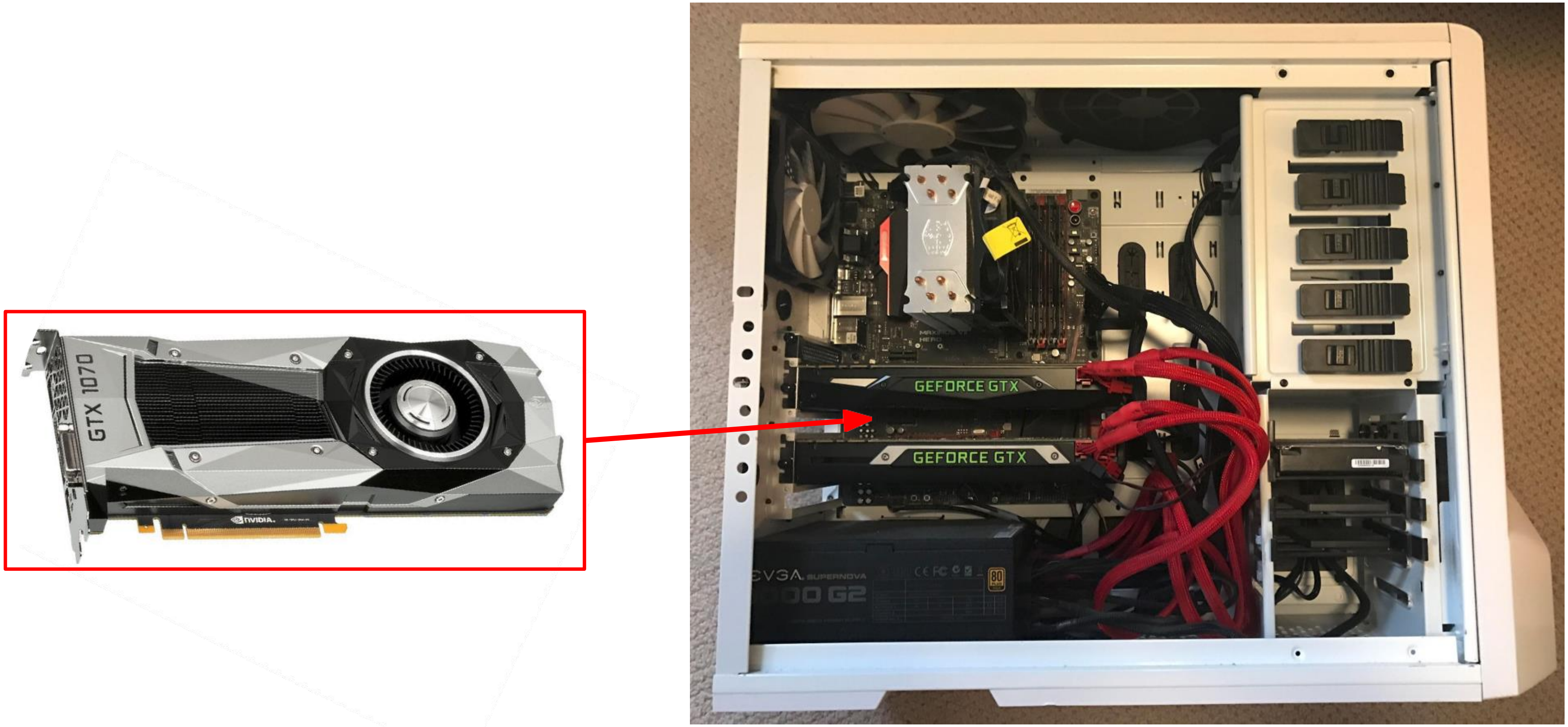
# Training: Best practices

- Center (subtract mean from) your data
- Use Xavier initialization for weights
- Use RELU or leaky RELU or ELU or PReLU
- Use batch normalization
- Use data augmentation
- Use regularization
- Use mini-batch
- Learning rate: too high? Too low?
- Use cross-validation for hyperparameters

# Spot the CPU! (central processing unit)



# Spot the GPUs! (graphics processing unit)



# CPU vs GPU

| | Cores | Clock Speed | Memory | Price* | Speed |
|---|---|---|---|---|---|
| **CPU** (Intel Core i7-7700k) | 4 | 4.2 GHz | System RAM | $385 | ~540 GFLOPs FP32 |
| **GPU** (NVIDIA RTX 2080 Ti) | 4352 | 1.6 GHz | 11 GB GDDR6 | $1,199 | ~13.4 TFLOPs FP32 |
| **GPU** (NVIDIA Quadro RTX 5000) | 3072 | 1.6 GHz | 16 GB GDDR6 | $2,299 | ~11.2 TFLOPs FP32 |
| **GPU** (NVIDIA RTX A5000) | 8192 CUDA, 256 tensor | 1.2 GHz | 24 GB GDDR6 | $2,500 | ~27.8 TFLOPS FP32 |
| **TPU** NVIDIA TITAN V | 5120 CUDA, 640 tensor | 1.5 GHz | 12GB HBM2 | $2,999 | ~14 TFLOPs FP32<br>~112 TFLOP FP16 |
| **TPU** Google Cloud TPU | ? | ? | 64 GB HBM | $4.50 / hr | ~180 TFLOP |

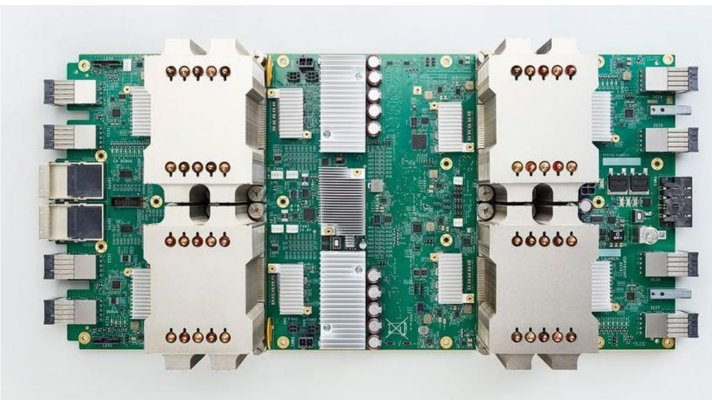
**CPU**: Fewer cores, but each core is much faster and much more capable; great at sequential tasks

**GPU**: More cores, but each core is much slower and "dumber"; great for parallel tasks

**TPU**: Specialized hardware for deep learning

Adapted from Fei-Fei Li, Andrej Karpathy, Justin Johnson, Serena Yeung; https://en.wikipedia.org/wiki/List_of_Nvidia_graphics_processing_units

# TensorFlow: Tensor Processing Units



Google Cloud TPU
= 180 TFLOPs of compute!

NVIDIA Tesla V100
= 125 TFLOPs of compute

NVIDIA Tesla P100 = 11 TFLOPs of compute
GTX 580 = 0.2 TFLOPs

# TensorFlow: Tensor Processing Units

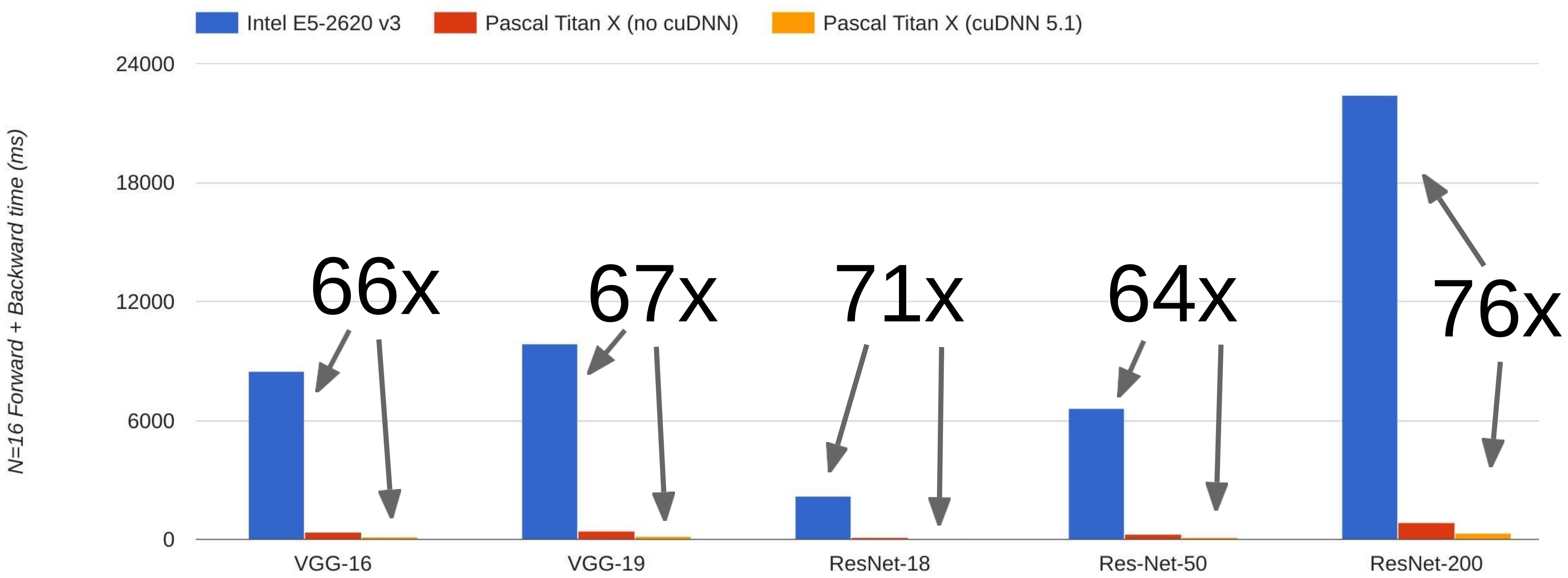
Google Cloud TPU
= 180 TFLOPs of compute!

Google Cloud TPU Pod
= 64 Cloud TPUs
= 11.5 PFLOPs of compute!

https://www.tensorflow.org/versions/master/programmers_guide/using_tpu

# CPU vs GPU in practice

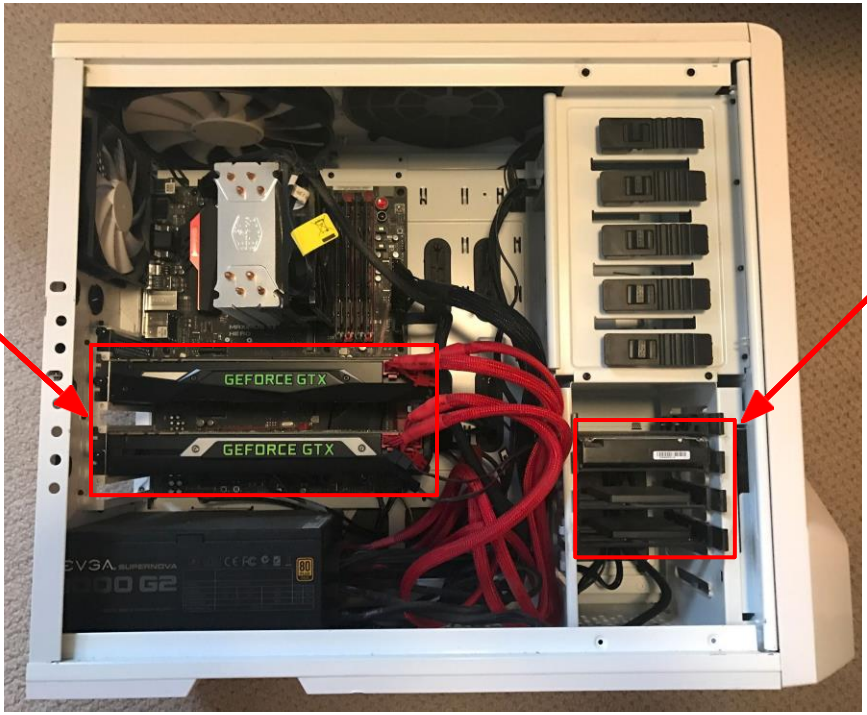
(CPU performance not well-optimized, a little unfair)




Data from https://github.com/jcjohnson/cnn-benchmarks

# CPU / GPU Communication

Model
is here




Data is here

If you aren't careful, training can bottleneck on reading data and transferring to GPU!

**Solutions**:

- Read all data into RAM
- Use SSD instead of HDD
- Use multiple CPU threads to prefetch data

# Software: A zoo of frameworks!

Caffe (UC Berkeley) → Caffe2 (Facebook)

Torch (NYU / Facebook) → PyTorch (Facebook)

Theano (U Montreal) → TensorFlow (Google)

PaddlePaddle (Baidu)

Chainer

MXNet (Amazon)

CNTK (Microsoft)

JAX (Google)

And others...

# Convergence of training

# Successful training

- We want training to converge (stop) at a reasonable place
- Stopping is not guaranteed – e.g. imagine taking larger and larger steps…
- Stopping in a good place is not guaranteed

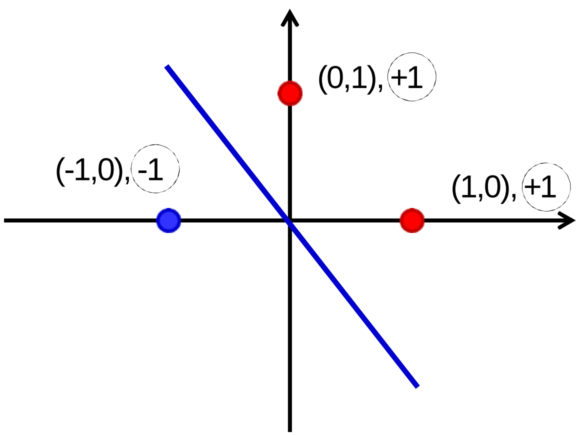
# Will backprop do the right thing?

- In classification problems, classification error is a non-differentiable function of weights
- The divergence function minimized (loss) is only a proxy for classification error
- Minimizing loss may not minimize classification error

Adapted from Bhiksha Raj

# Will backprop do the right thing?

- With these three points, backprop finds the right answer

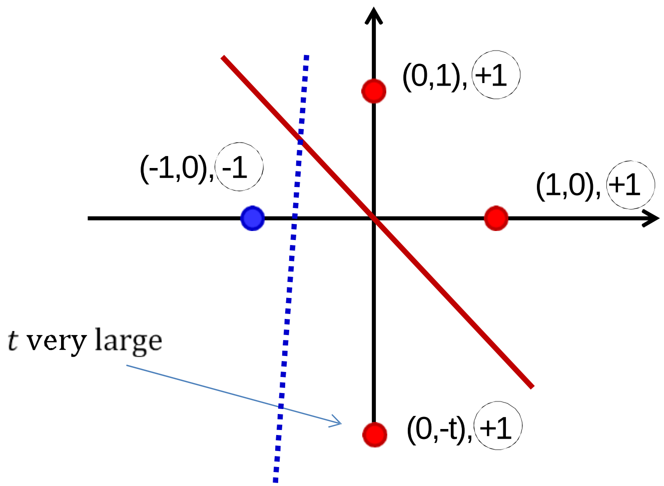



- From the three points we get three independent equations:

$$w_s\,.\,1 + w_y\,.\,0 + b = u$$
$$w_s\,.\,0 + w_y\,.\,1 + b = u$$
$$w_s\,.\,{-1} + w_y\,.\,0 + b = -u$$

- Unique solution $(w_s = u, w_s = u, b = 0)$ exists

# Will backprop do the right thing?

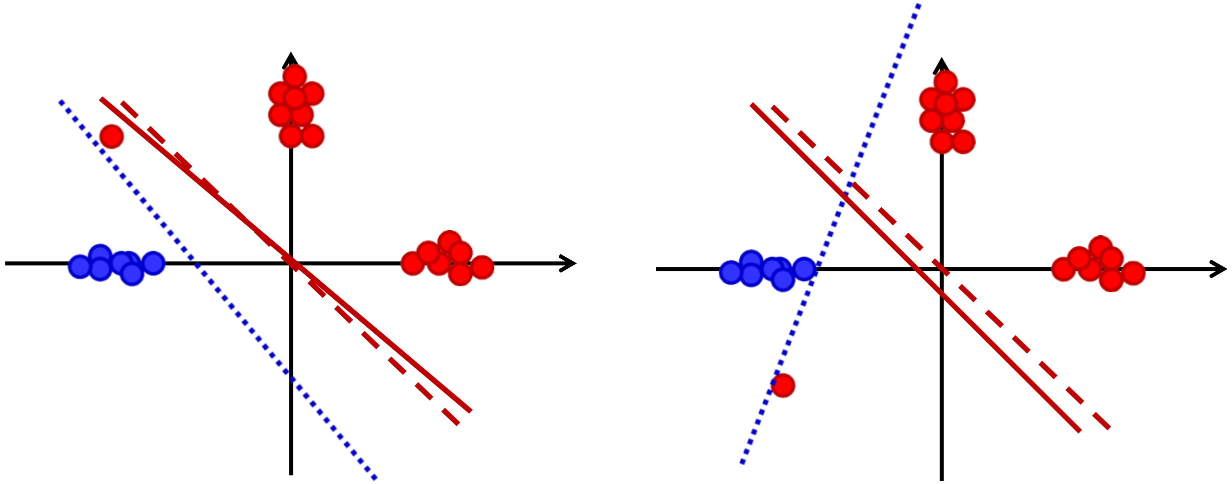



- Now add a fourth point
- With large enough t, 0 contribution of 4th point to derivative of $L_2$ error (e.g. if sigmoid/tanh used)
- Local optimum solution found by backprop
- Does not separate the points *even though they are linearly separable!*
- Another algorithm (perceptron, in blue) does find the optimal separator

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_{\mathrm{P}}(\mathbf{w}) = \mathbf{w}^{(\tau)} + \eta \boldsymbol{\phi}_n t_n$$

Adapted from Bhiksha Raj

# Will backprop do the right thing?



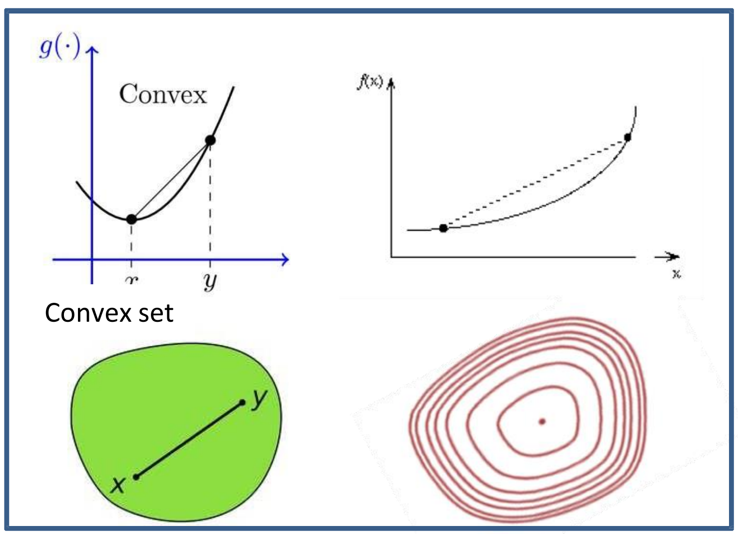
- Adding a "spoiler" (or a small number of spoilers)
  - Perceptron finds the linear separator
  - For bounded *w,* backprop does not find a separator
  - A single additional input does not change the loss function significantly
- Backprop is minimally changed by new training instances
  - Prefers consistency over perfection

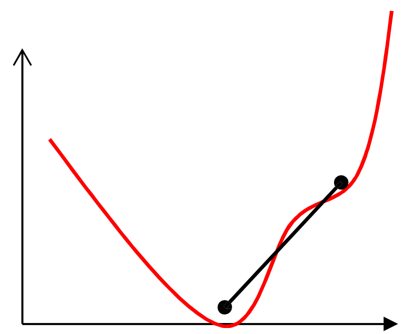
# Loss surfaces

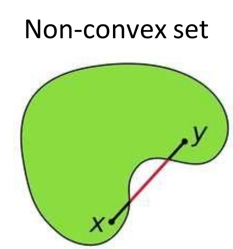
- Usually Loss(W) is not convex, so there are many local minima
- However, in deep networks, these minima are reasonably similar – not true in small networks
- What are desirable properties of the loss surface?

# Convexity

- A surface is "convex" if it continuously curves upward
  - We can connect any two points above the surface without intersecting it
  - Many mathematical definitions that are equivalent
- Caveat: Neural net loss surface generally not convex



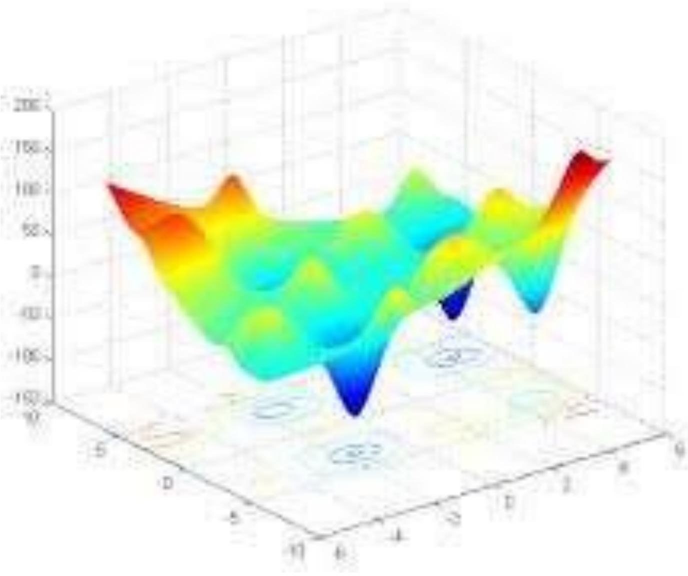






Adapted from Bhiksha Raj

# The loss surface

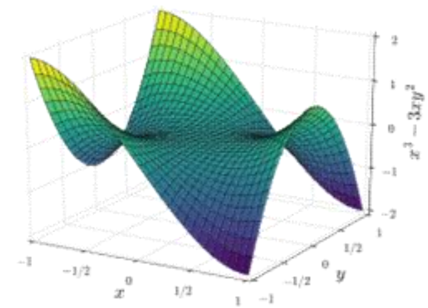
- Gradient descent makes the assumption that loss/objective has a single global optimum
- What about local optima?

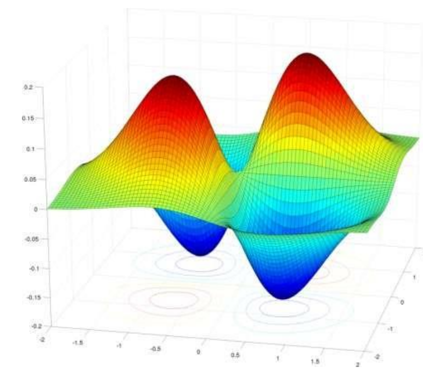


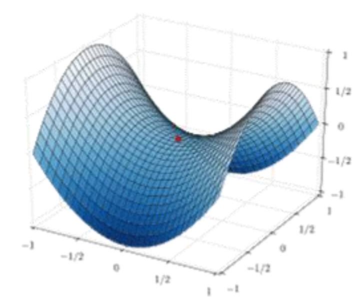
Adapted from Bhiksha Raj

# The loss surface

- Popular hypothesis:
  – Most local minima are equivalent
    - And close to global minimum
  – This is not true for small networks
  – In large networks, saddle points are far more common than local minima
    - Frequency exponential in network size
- Saddle point: A point where:
  – The slope is zero
  – The surface increases in some directions, but decreases in others
    - Some of the Eigenvalues of the Hessian are positive; others are negative
  – Gradient descent algs often get "stuck" in saddle points







# The *controversial* loss surface

- **Baldi and Hornik (89), "***Neural Networks and Principal Component Analysis: Learning from Examples Without Local Minima*" : An MLP with a *single* hidden layer has only saddle points and no local minima
- **Dauphin et. al (2015),** "*Identifying and attacking the saddle point problem in high-dimensional non-convex optimization*" : An exponential number of saddle points in large networks
- **Chomoranksa et. al (2015)**, "*The loss surface of multilayer networks*" : For large networks, most local minima lie in a band and are equivalent
- **Swirscz et. al. (2016)**, "Local minima in training of deep networks", In networks of finite size, trained on finite data, you *can* have horrible local minima
- *Watch this space…*

# Conditions for convergence

- So far we have assumed training arrives at a local minimum

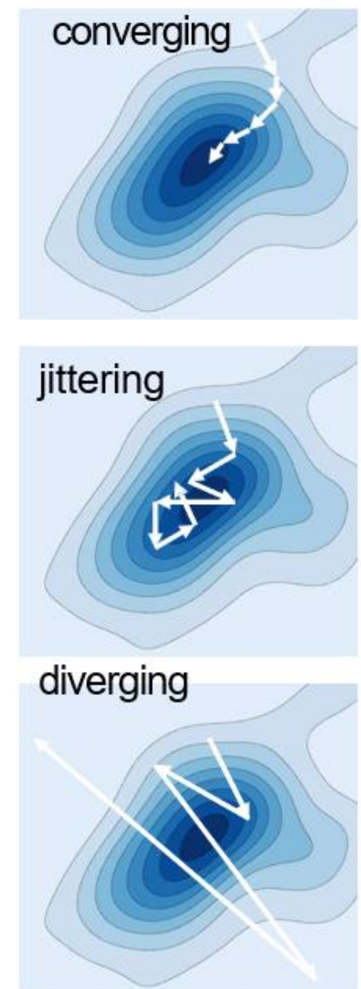
- Does it always converge?
- How long does it take?

- Hard to analyze for a neural network, but we can look at the problem through the lens of convex optimization

Adapted from Bhiksha Raj

# Convergence and convergence rate

- An iterative algorithm is said to *converge* to a solution if the value updates arrive at a fixed point
  - Where the gradient is 0 and further updates do not change the estimate
- The algorithm may not converge
  - It may jitter around the local minimum
  - It may even diverge
- Conditions for convergence?



# Convergence and convergence rate

- Convergence rate: how fast iterations arrive at the solution
- Generally quantified as:

$$R = \frac{\left|f\left(x^{(k+1)}\right) - f(x^*)\right|}{\left|f\left(x^{(k)}\right) - f(x^*)\right|}$$

  - $x^{(k+1)}$ is the k-th iteration
  - $x^*$ is the optimal value of $x$

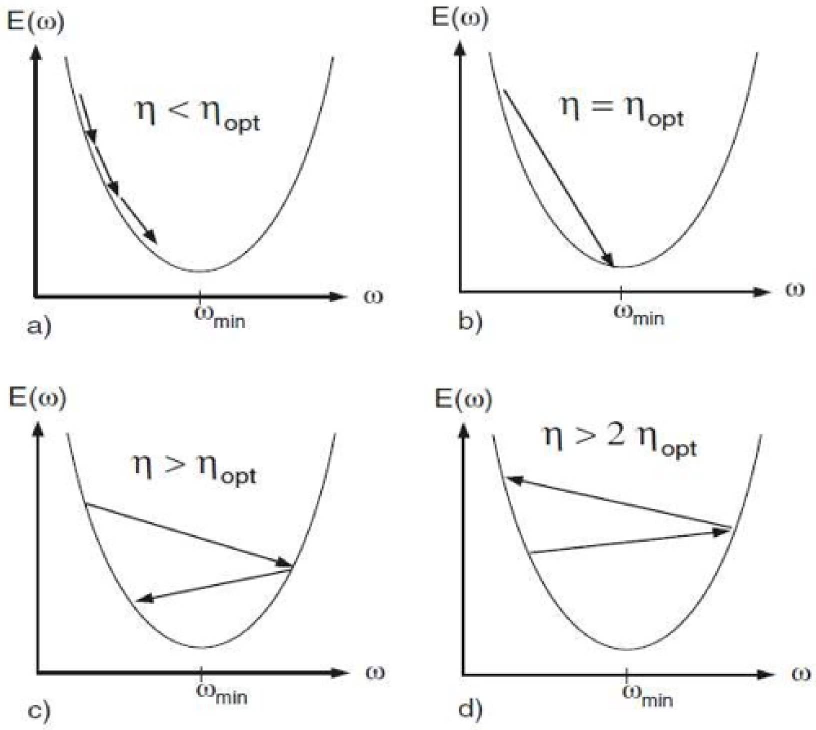
- If R is a constant (or upper-bounded): convergence is linear

Adapted from Bhiksha Raj

# With non-optimal step size

$$w^{(k+1)} = w^{(k)} - \eta \frac{dE\left(w^{(k)}\right)}{dw}$$

Gradient descent with fixed step size $\eta$ to estimate scalar parameter $w$



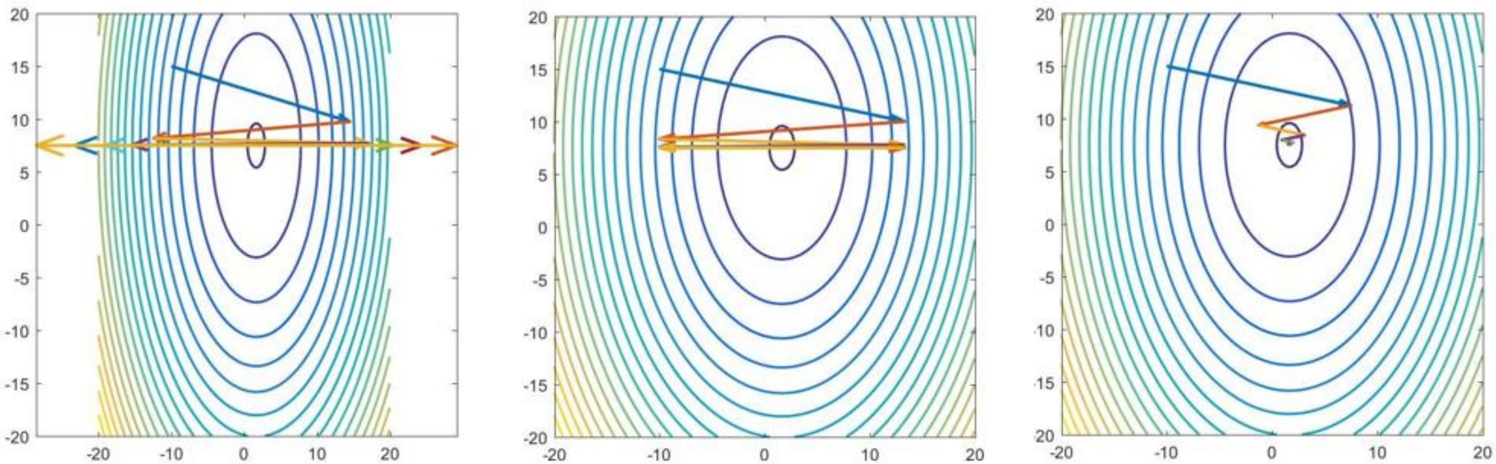

- For $\eta < \eta_{opt}$ the algorithm will converge monotonically
- For $2\eta_{opt} > \eta > \eta_{opt}$ we have oscillating convergence
- For $\eta > 2\eta_{opt}$ we get divergence

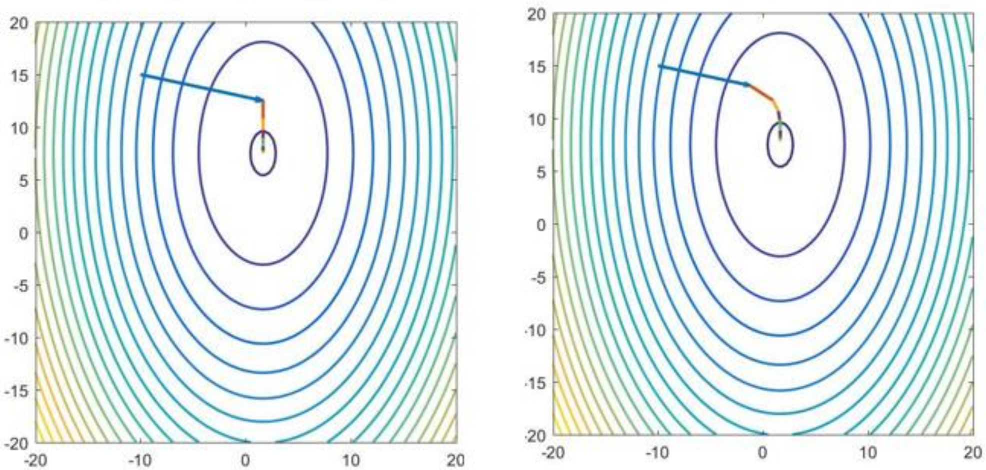
# Multivariate quadratic surface

- Optimal learning rate is different for the different coordinates
- The learning rate must be lower than twice the *smallest* optimal learning rate for any component $\eta < 2 \min_i \eta_{i,opt}$
  - Otherwise the learning will diverge
- This, however, makes the learning very slow
- Convergence is particularly slow if the following is large (the "condition" number is small)

$$\frac{\max_i \eta_{i,opt}}{\min_i \eta_{i,opt}}$$

# Dependence on learning rate




- $\eta_{1,opt} = 1;\ \eta_{2,opt} = 0.33$
- $\eta = 2.1\eta_{2,opt}$
- $\eta = 2\eta_{2,opt}$
- $\eta = 1.5\eta_{2,opt}$
- $\eta = \eta_{2,opt}$
- $\eta = 0.75\eta_{2,opt}$

# Optimization strategies

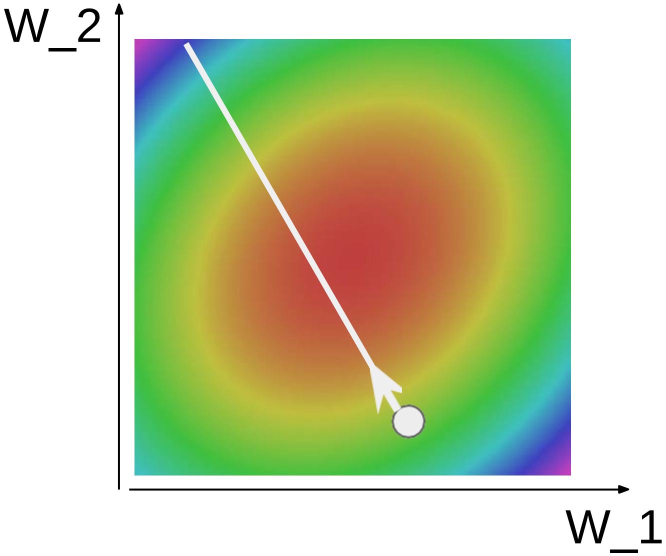
# Getting to the minimum

- Gradient descent is just one strategy, but has several problems
- What other “steps” can we take?
- How far in the direction of decreasing gradient do we go? With what speed/acceleration?
- What about overshooting minima?

# Optimization

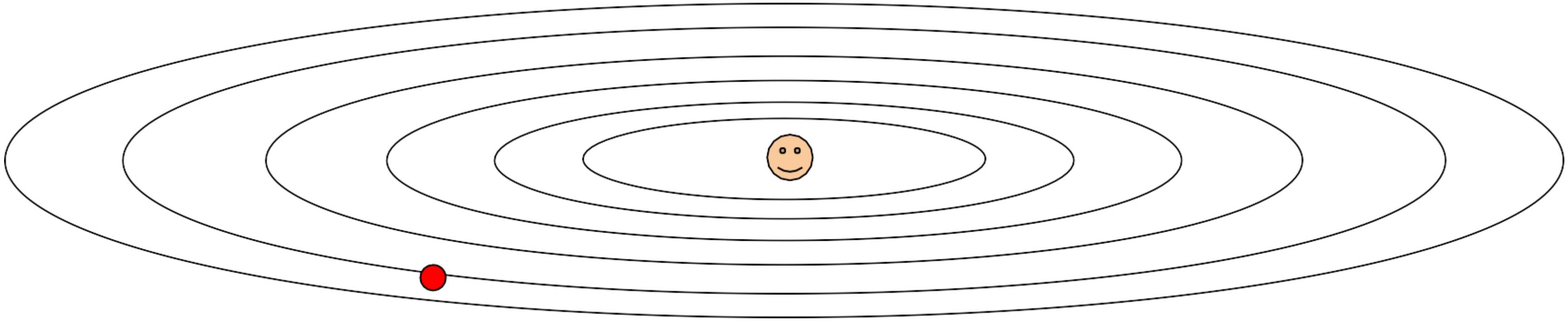
```
# Vanilla Gradient Descent

while True:
  weights_grad = evaluate_gradient(loss_fun, data, weights)
  weights += - step_size * weights_grad # perform parameter update
```



# Optimization: Problems with SGD

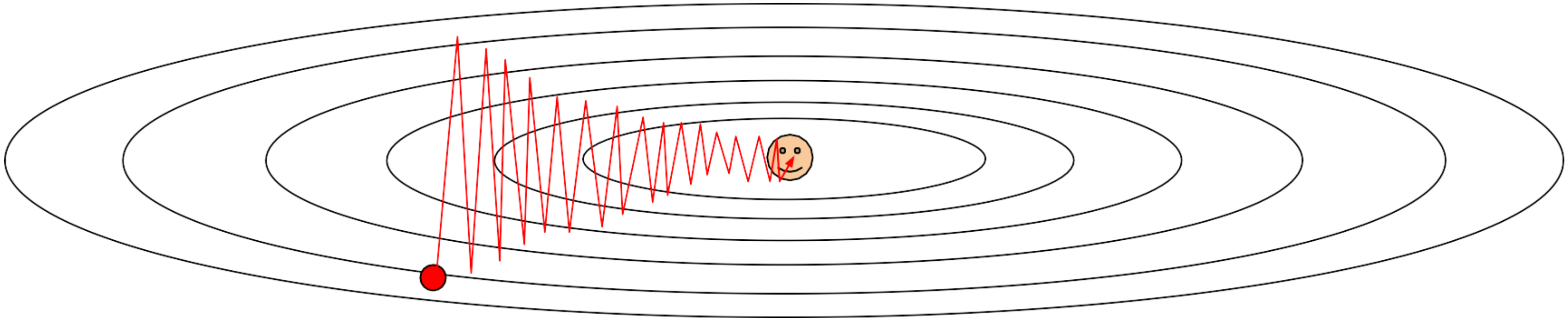
What if loss changes quickly in one direction and slowly in another?
What does gradient descent do?



Loss function has high **condition number**: ratio of largest to smallest singular value of the Hessian matrix is large

# Optimization: Problems with SGD

What if loss changes quickly in one direction and slowly in another?
What does gradient descent do?
Very slow progress along shallow dimension, jitter along steep direction

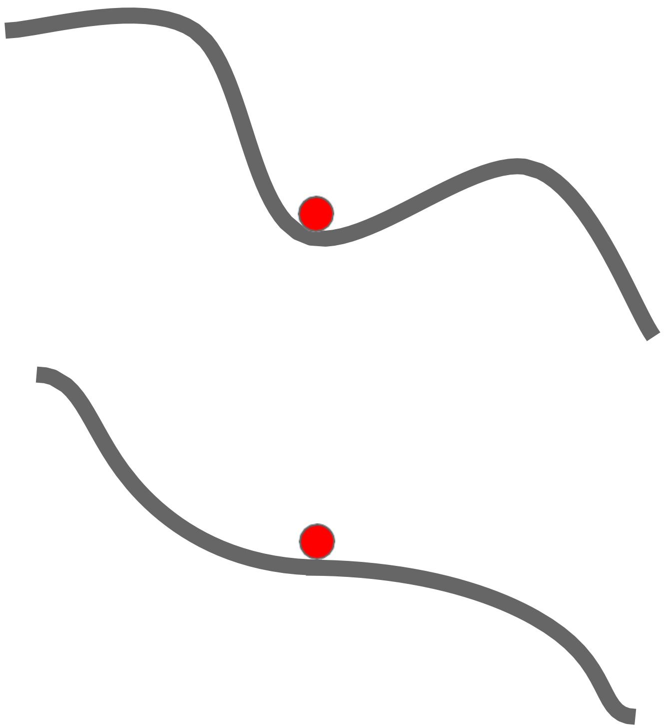


Loss function has high **condition number**: ratio of largest to smallest singular value of the Hessian matrix is large

# Optimization: Problems with SGD

What if the loss function has a **local minima** or **saddle point**?

Zero gradient, gradient descent gets stuck

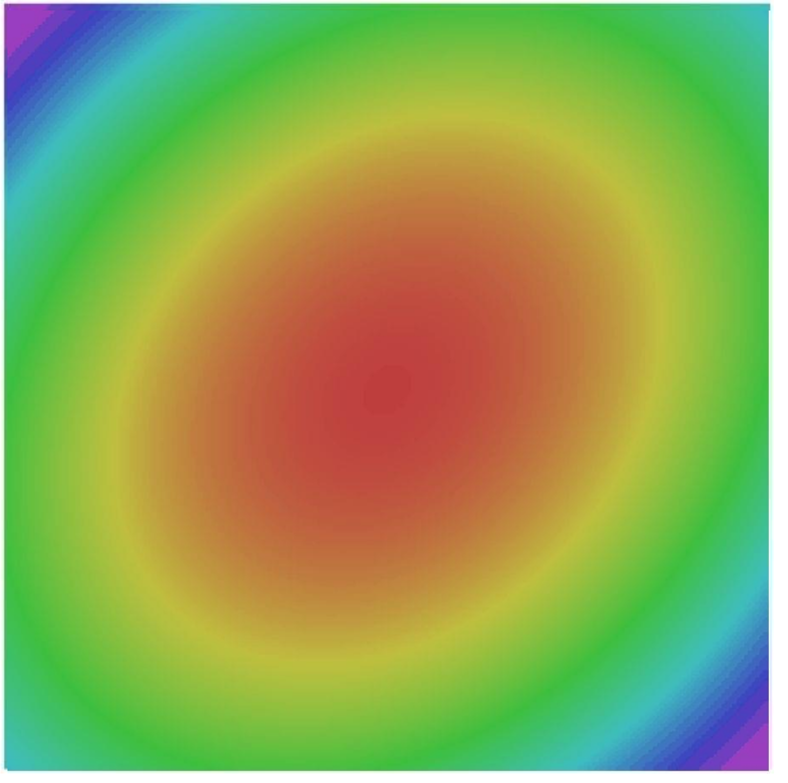


# Optimization: Problems with SGD

Our gradients come from minibatches so they can be noisy!

$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(x_i, y_i, W)$$

$$\nabla_W L(W) = \frac{1}{N} \sum_{i=1}^{N} \nabla_W L_i(x_i, y_i, W)$$



# SGD + Momentum

## SGD

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

```
while True:
  dx = compute_gradient(x)
  x -= learning_rate * dx
```

## SGD+Momentum

$$v_{t+1} = \rho v_t + \nabla f(x_t)$$
$$x_{t+1} = x_t - \alpha v_{t+1}$$

```
vx = 0
while True:
  dx = compute_gradient(x)
  vx = rho * vx + dx
  x -= learning_rate * vx
```

- Build up “velocity” as a running mean of gradients
- Rho gives “friction”; typically rho=0.9 or 0.99

Sutskever et al, “On the importance of initialization and momentum in deep learning”, ICML 2013

# AdaGrad

```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

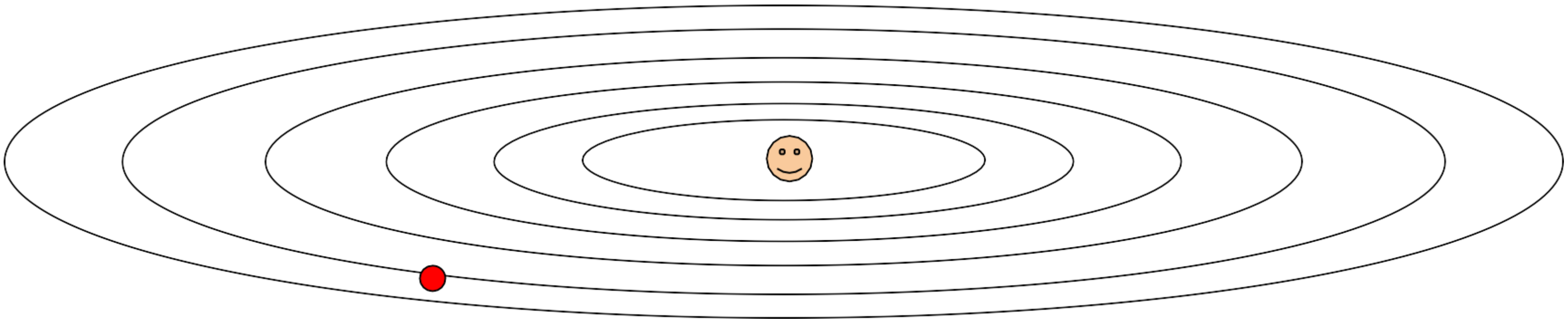
Added element-wise scaling of the gradient based on the historical sum of squares in each dimension

"Per-parameter learning rates"
or "adaptive learning rates"

Duchi et al, "Adaptive subgradient methods for online learning and stochastic optimization", JMLR 2011

# AdaGrad

```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

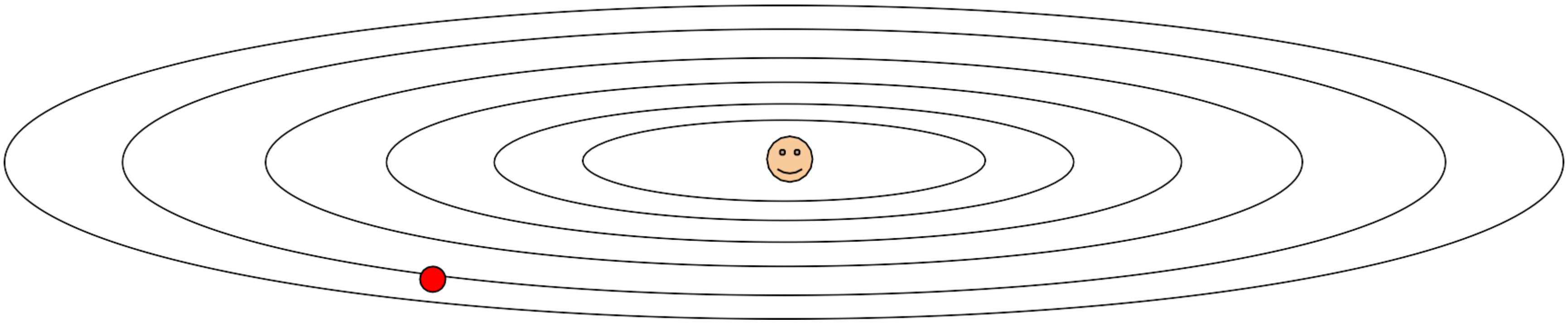


Q: What happens with AdaGrad?

Progress along “steep” directions is damped; progress along “flat” directions is accelerated

# AdaGrad

```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



Q2: What happens to the step size over long time?

# RMSProp

AdaGrad

```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

↓

RMSProp

```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared = decay_rate * grad_squared + (1 - decay_rate) * dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

Tieleman and Hinton, 2012

# Adam

```
first_moment = 0
second_moment = 0
for t in range(1, num_iterations):
  dx = compute_gradient(x)
  first_moment = beta1 * first_moment  + (1 - beta1) * dx
  second_moment = beta2 * second_moment + (1 - beta2) * dx * dx
  first_unbias = first_moment / (1 - beta1 ** t)
  second_unbias = second_moment / (1 - beta2 ** t)
  x -= learning_rate * first_unbias / (np.sqrt(second_unbias) + 1e-7))
```

Momentum

Bias correction

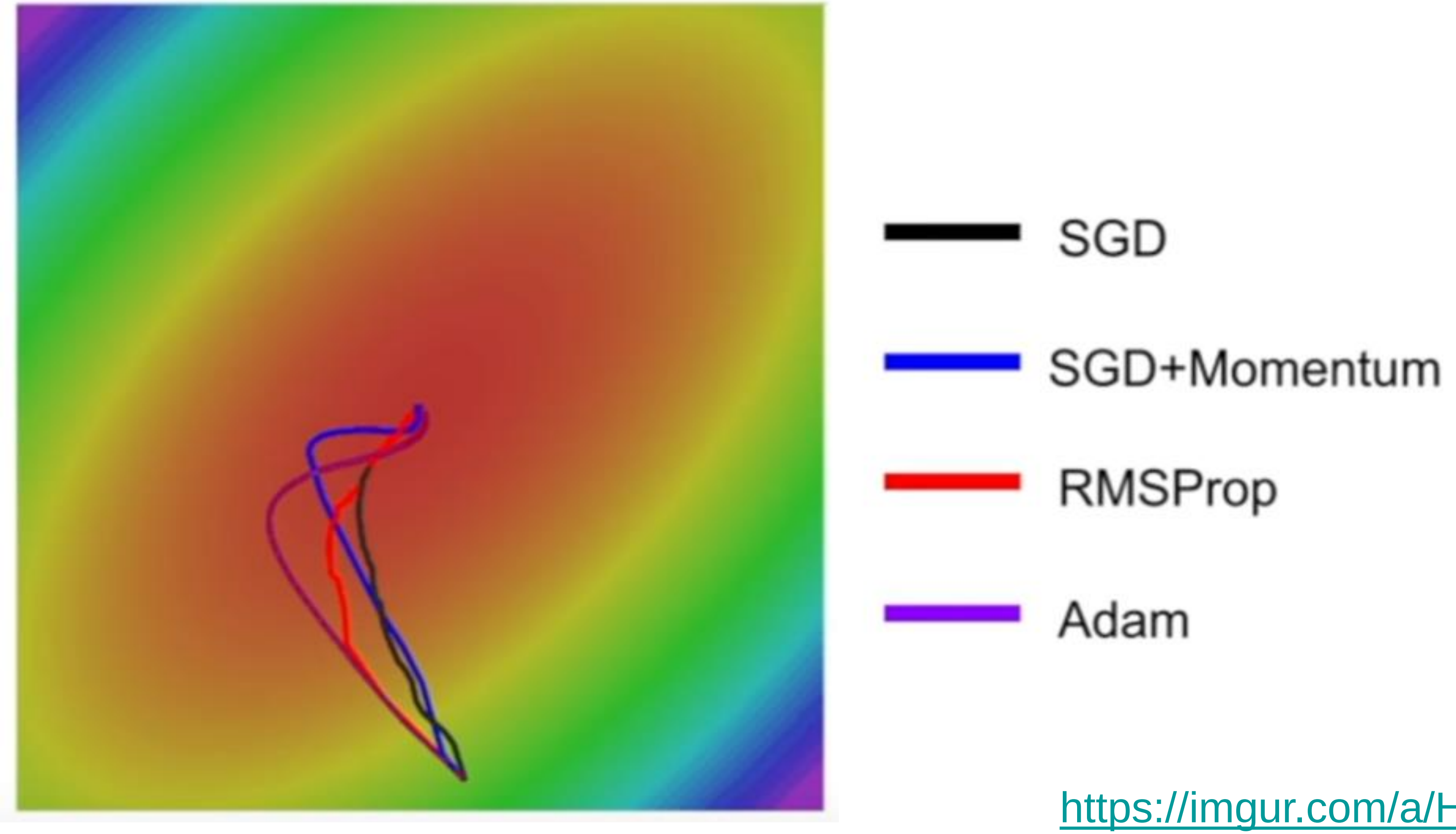
AdaGrad / RMSProp

Bias correction for the fact that first and second moment estimates start at zero

Adam with beta1 = 0.9,
beta2 = 0.999, and learning_rate = 1e-3 or 5e-4
is a great starting point for many models!

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

# Optimizers comparison




https://imgur.com/a/Hqolp

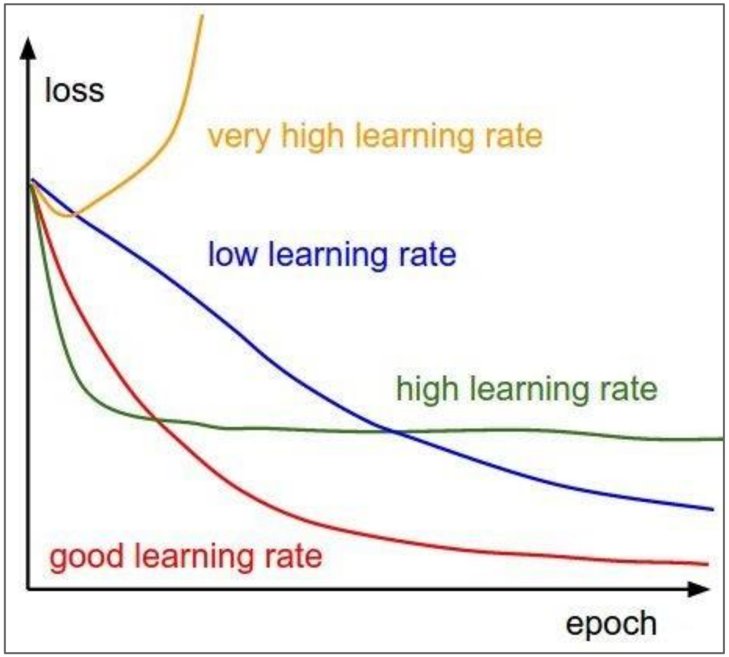
# Visualization

https://www.deeplearning.ai/ai-notes/optimization/

(bottom of page)

“In this visualization, you can compare optimizers applied to different cost functions and initialization. For a given cost landscape (**1**) and initialization (**2**), you can choose optimizers, their learning rate and decay (**3**). Then, press the play button to see the optimization process (**4**). There's no explicit model, but you can assume that finding the cost function's minimum is equivalent to finding the best model for your task.”

SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a hyperparameter.




**=> Learning rate decay over time!**

**step decay:**
e.g. decay learning rate by half every few epochs.

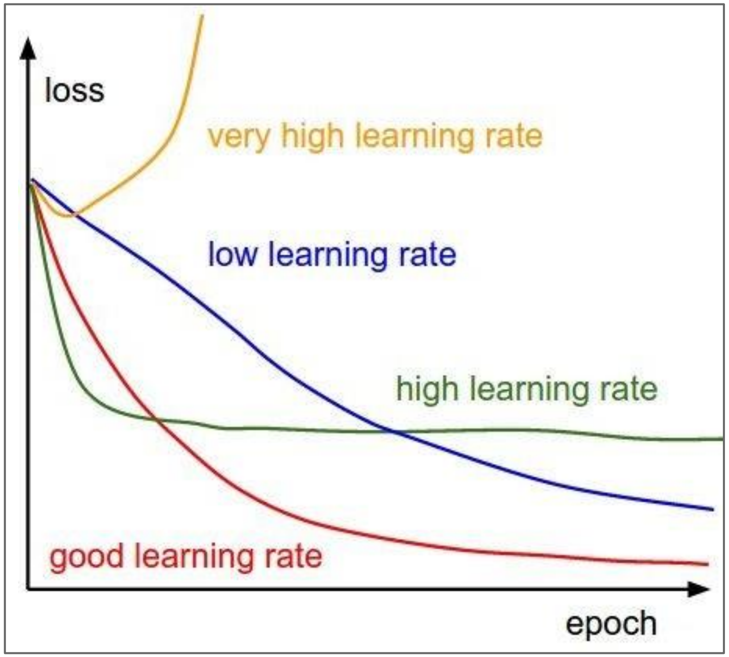
**exponential decay:**

$$\alpha = \alpha_0 e^{-kt}$$

**1/t decay:**

$$\alpha = \alpha_0 / (1 + kt)$$

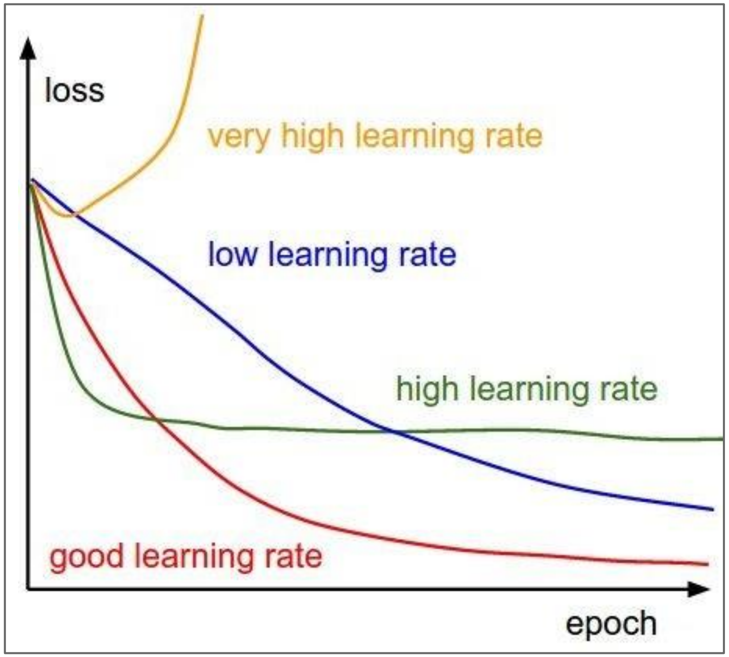
SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a hyperparameter.

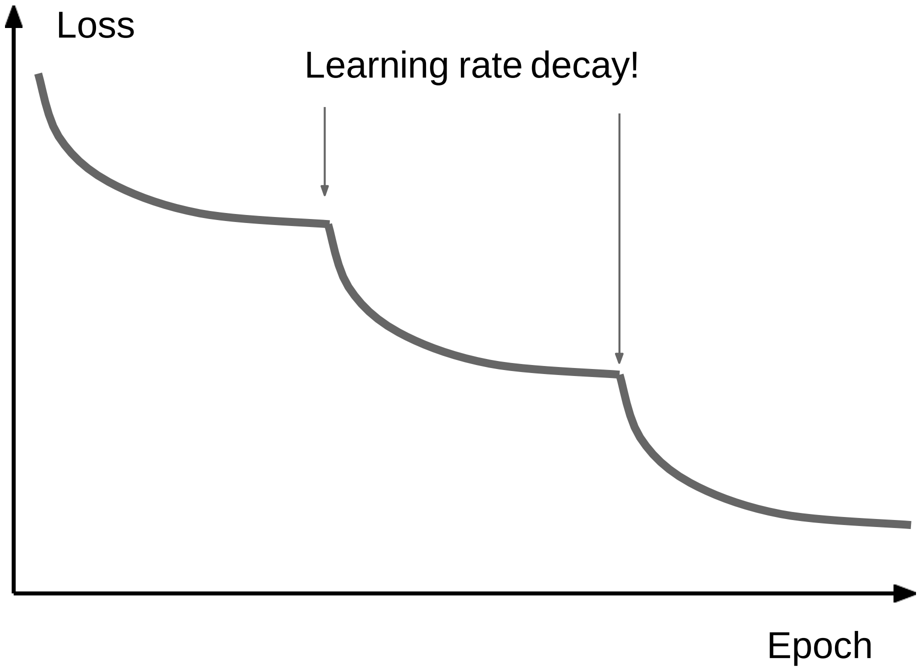



Q: Which one of these learning rates is best to use?

A: All of them! Start with large learning rate and decay over time

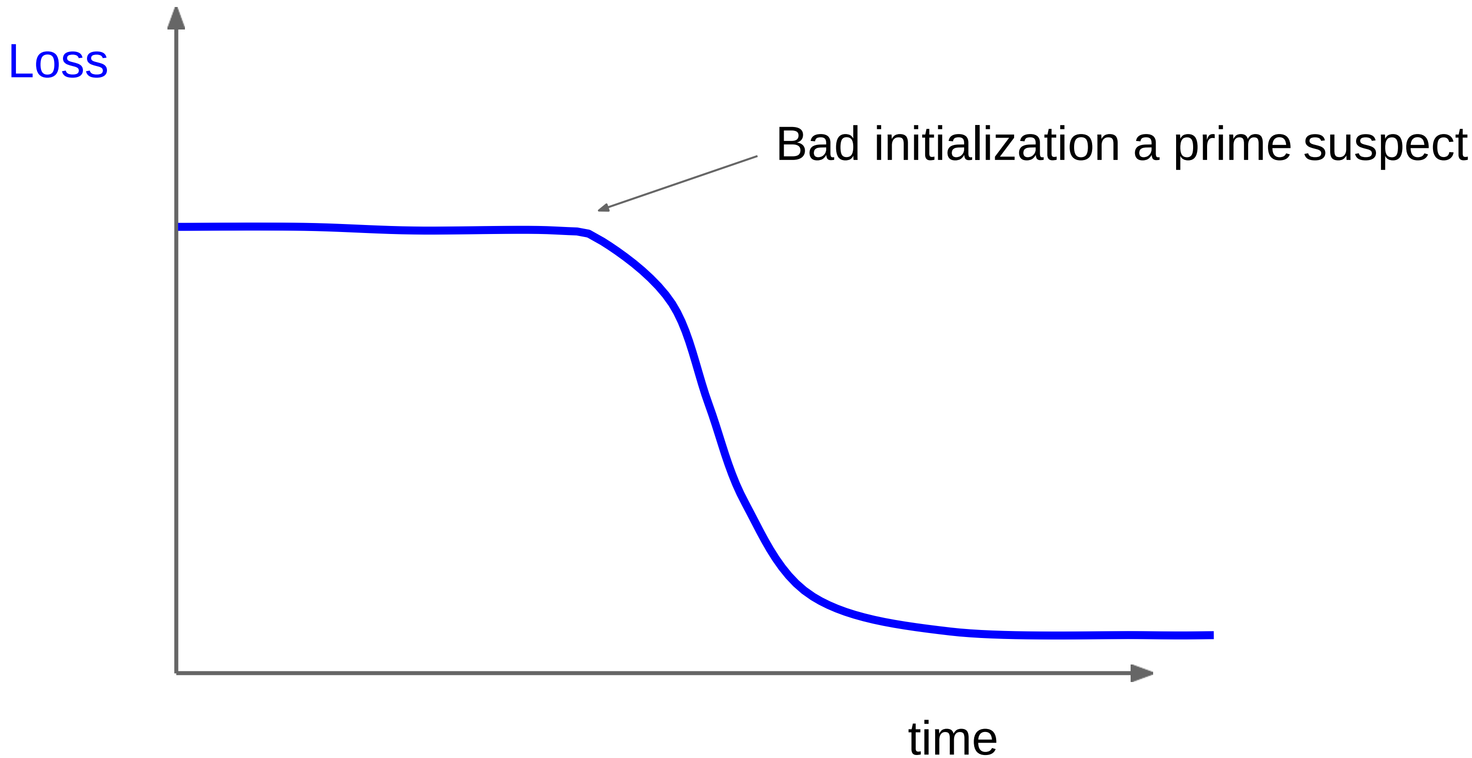
SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a hyperparameter.

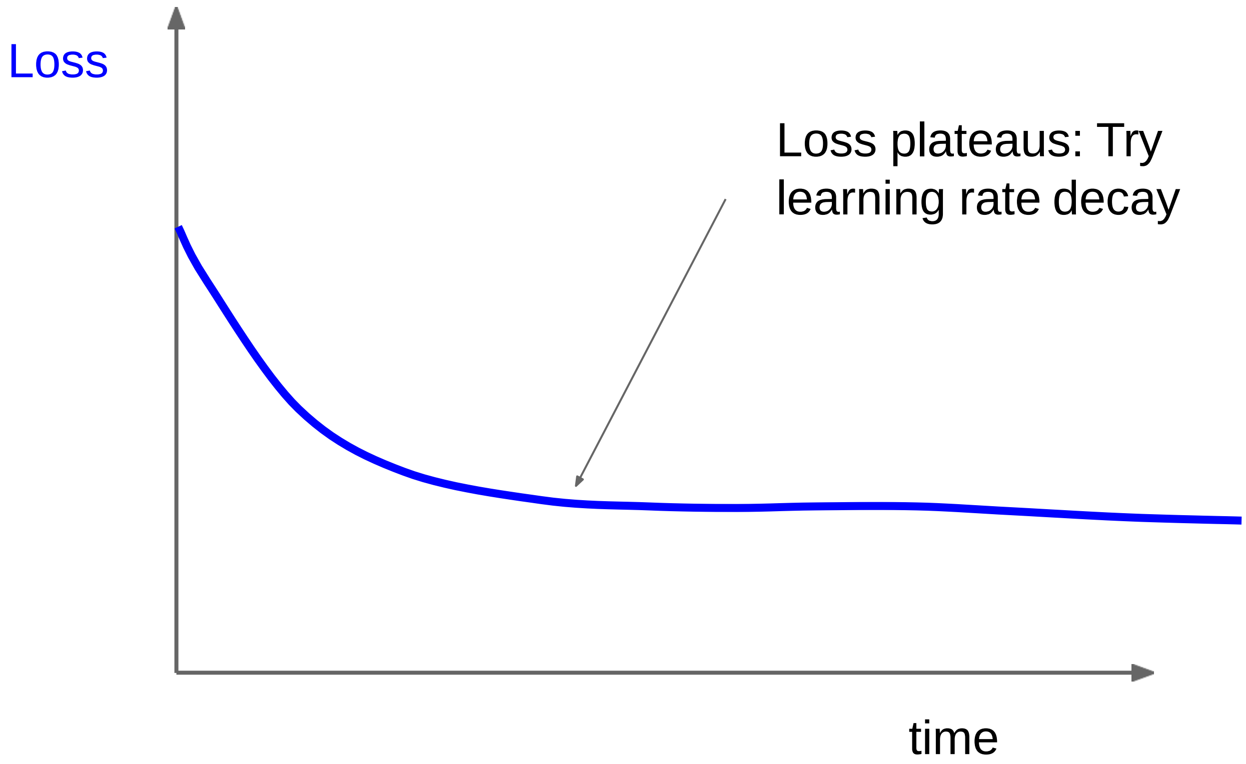


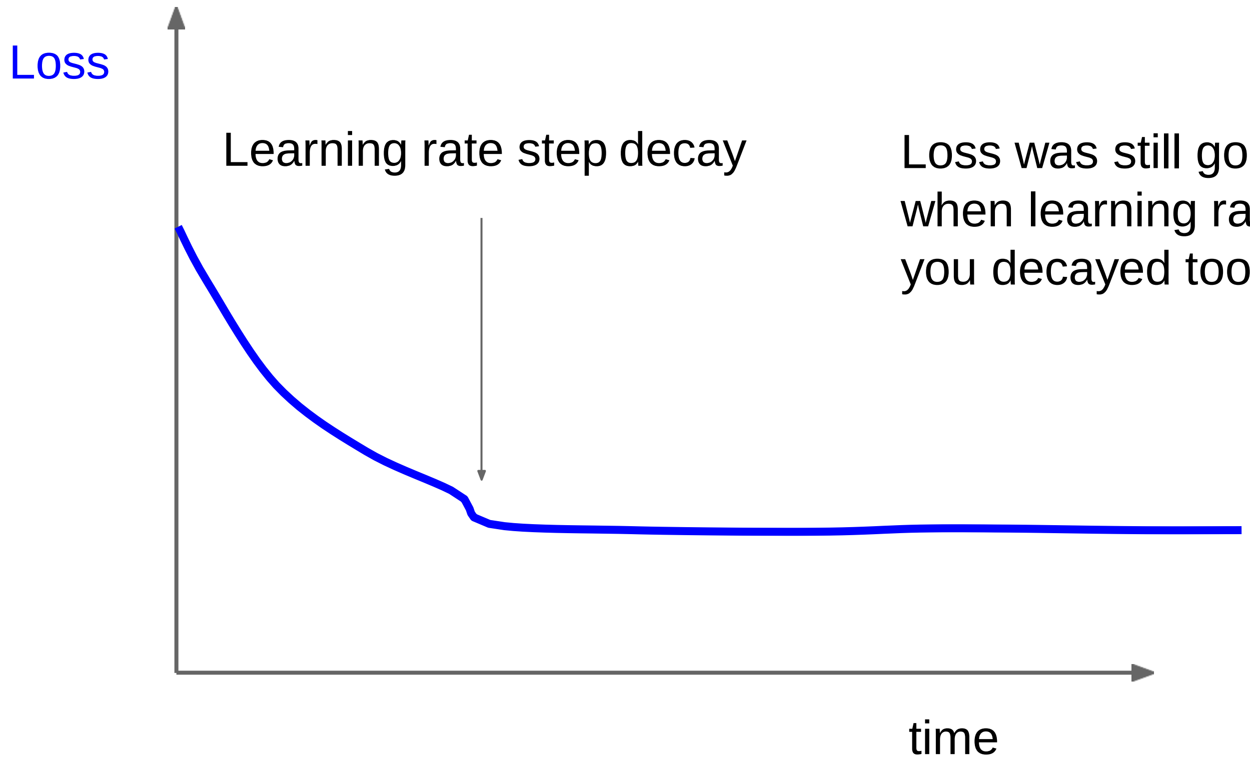




Also see https://openreview.net/pdf?id=r1eOnh4YPB

Adapted from Fei-Fei Li, Andrej Karpathy, Justin Johnson, Serena Yeung

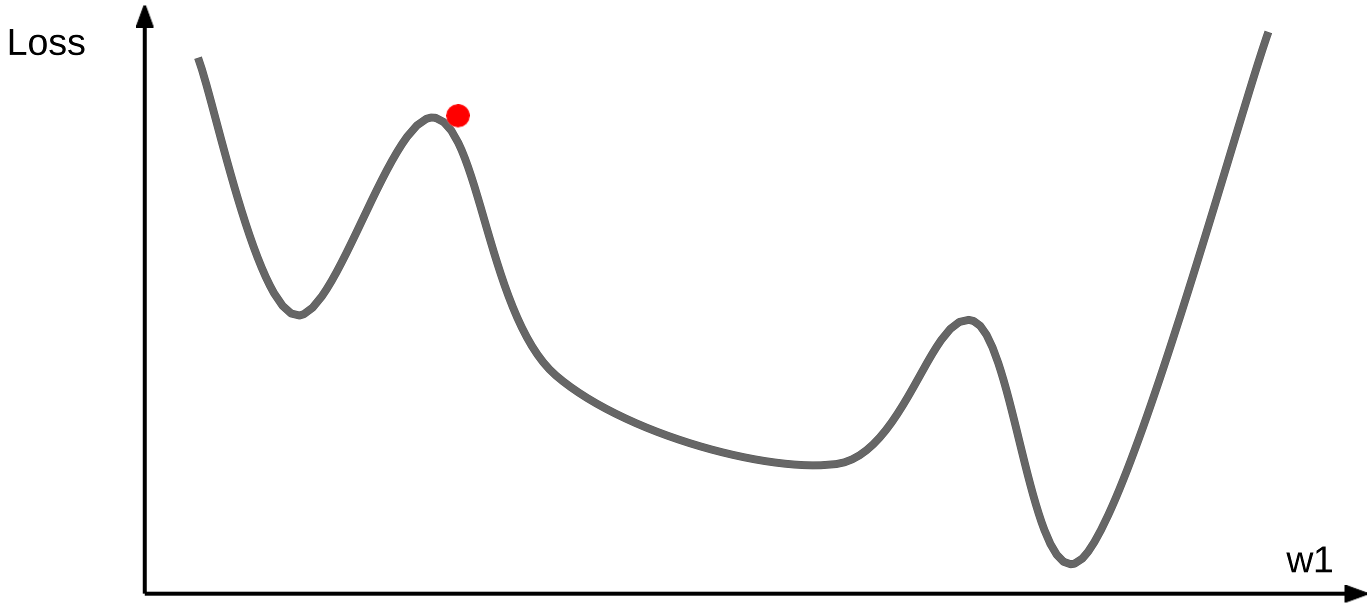

Loss
Bad initialization a prime suspect
time


Loss
Loss plateaus: Try learning rate decay
time



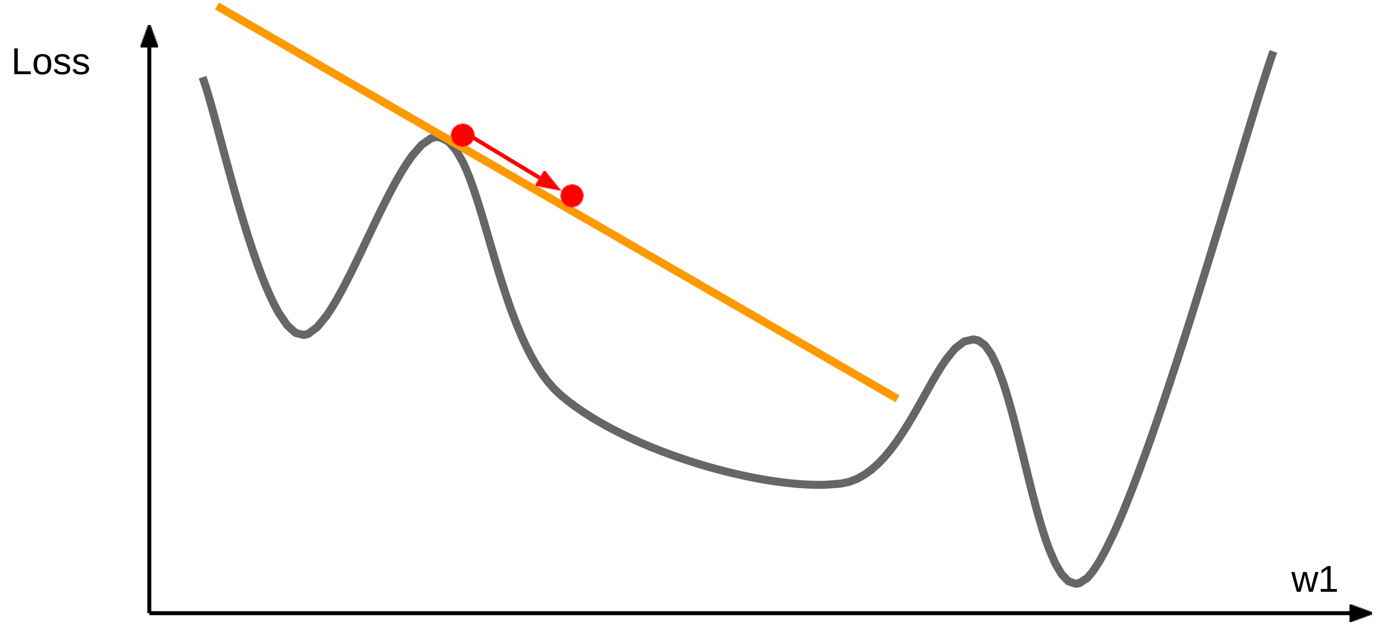

Loss was still going down when learning rate dropped, you decayed too early!

# First-Order Optimization



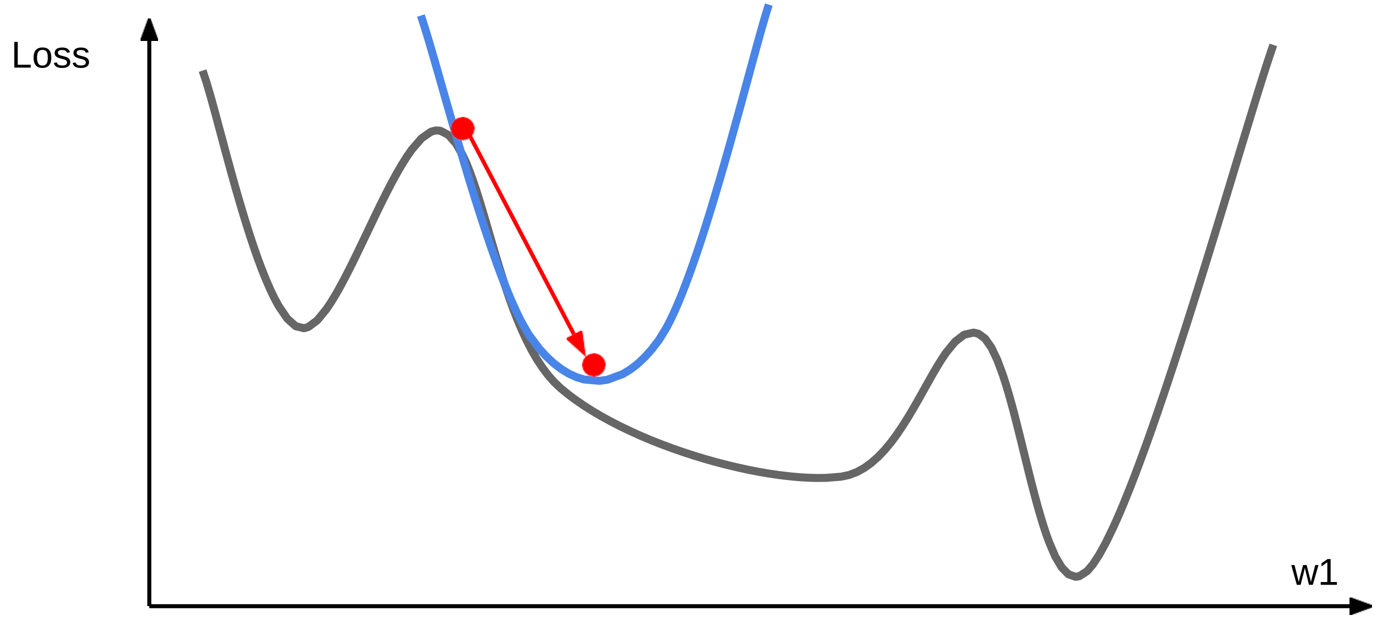
# First-Order Optimization

(1) Use gradient form linear approximation
(2) Step to minimize the approximation



# Second-Order Optimization

(1) Use gradient **and Hessian** to form **quadratic** approximation
(2) Step to the **minima** of the approximation



# Second-Order Optimization

$$H(\mathbf{w}) = \begin{pmatrix} \frac{\partial^2 \ell}{\partial w_1^2} & \frac{\partial^2 \ell}{\partial w_1 \partial w_2} & \cdots & \frac{\partial^2 \ell}{\partial w_1 \partial w_n} \\ \vdots & \cdots & \cdots & \vdots \\ \frac{\partial^2 \ell}{\partial w_n \partial w_1} & \cdots & \cdots & \frac{\partial^2 \ell}{\partial w_n^2} \end{pmatrix},$$

second-order Taylor expansion:

$$J(\boldsymbol{\theta}) \approx J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \boldsymbol{H}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)$$

Solving for the critical point we obtain the Newton parameter update:

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \boldsymbol{H}^{-1} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

Hessian has O(N^2) elements
Inverting takes O(N^3)
N = (Tens or Hundreds of) Millions

Q: Why is this bad for deep learning?

Partial solution: Quasi-Newton methods (e.g. **BGFS**) approximate inverse Hessian

# Choosing Hyperparameters

**Step 1**: Check initial loss

Without weight decay (regularization), sanity check loss at initialization
e.g. log(C) for softmax with C classes

# Choosing Hyperparameters

**Step 1**: Check initial loss
**Step 2**: Overfit a small sample

Try to train to 100% training accuracy on a small sample of training data (~5-10 minibatches); fiddle with architecture, learning rate, weight initialization

Loss not going down? LR too low, bad initialization
Loss explodes to Inf or NaN? LR too high, bad initialization

# Choosing Hyperparameters

**Step 1**: Check initial loss
**Step 2**: Overfit a small sample
**Step 3**: Find LR that makes loss go down

Use the architecture from the previous step, use all training data, turn on small weight decay, find a learning rate that makes the loss drop significantly within ~100 iterations

Good learning rates to try: 1e-1, 1e-2, 1e-3, 1e-4
Good weight decay to try: 1e-4, 1e-5, 0

# Choosing Hyperparameters

**Step 1**: Check initial loss
**Step 2**: Overfit a small sample
**Step 3**: Find LR that makes loss go down
**Step 4**: Coarse grid search, train for ~1-5 epochs

Choose a few values of learning rate and weight decay around what worked from Step 3, train a few models for ~1-5 epochs.

# Choosing Hyperparameters

**Step 1**: Check initial loss
**Step 2**: Overfit a small sample
**Step 3**: Find LR that makes loss go down
**Step 4**: Coarse grid, train for ~1-5 epochs
**Step 5**: Refine grid, train longer

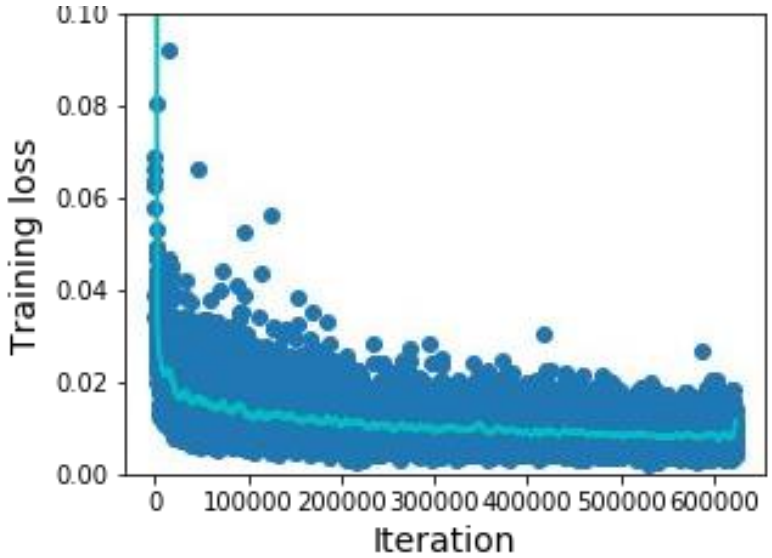
Pick best models from Step 4, train them for longer (~10-20 epochs) without learning rate decay

# Choosing Hyperparameters

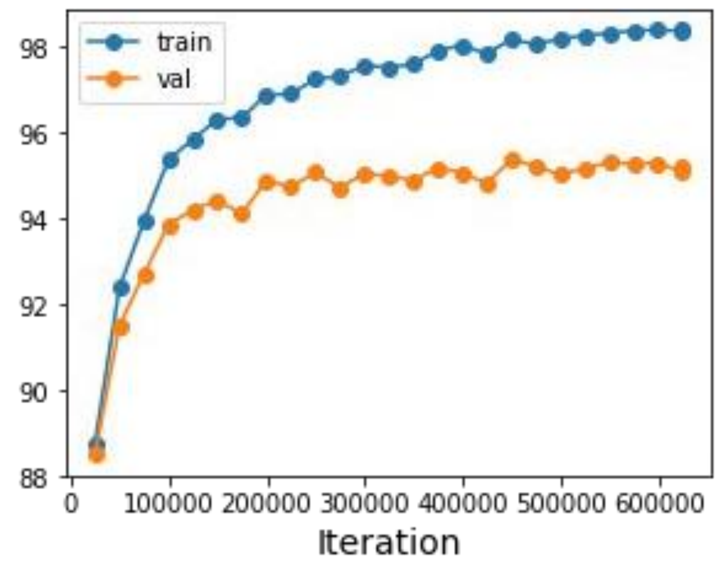
**Step 1**: Check initial loss
**Step 2**: Overfit a small sample
**Step 3**: Find LR that makes loss go down
**Step 4**: Coarse grid, train for ~1-5 epochs
**Step 5**: Refine grid, train longer
**Step 6**: Look at loss curves

# Look at learning curves!

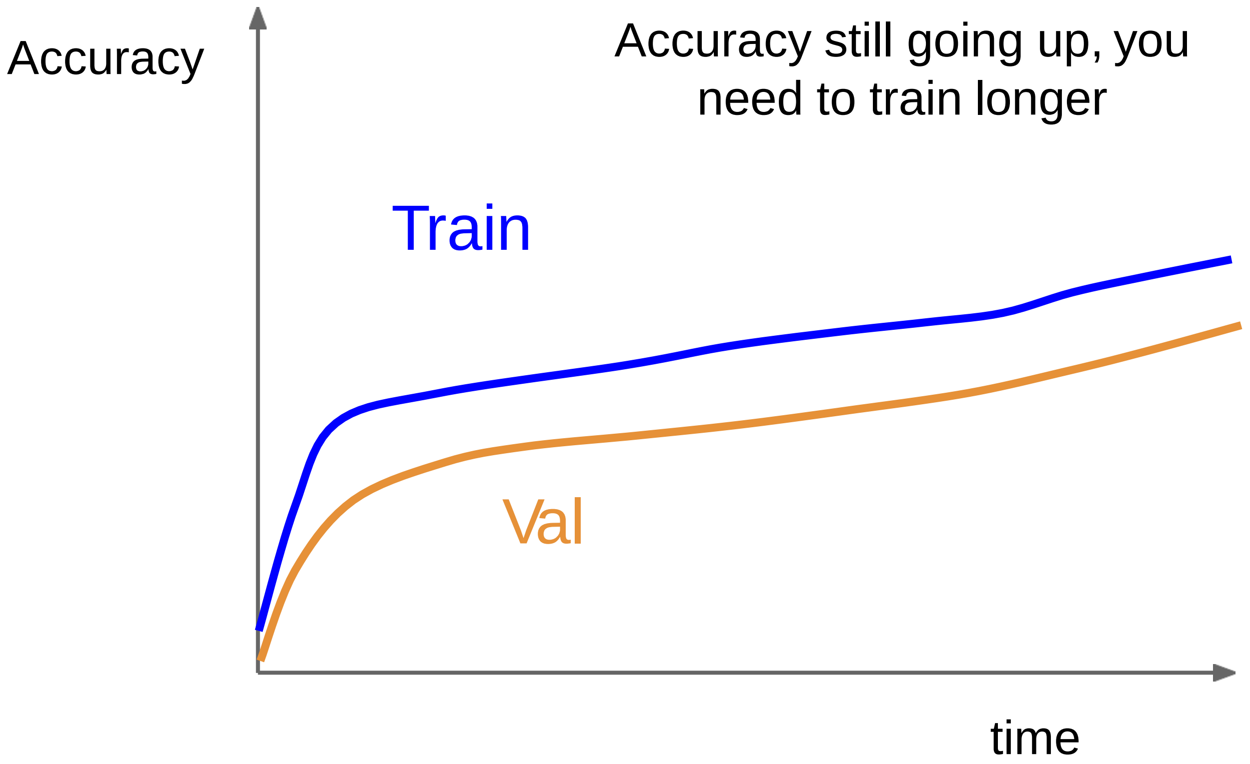
Training Loss

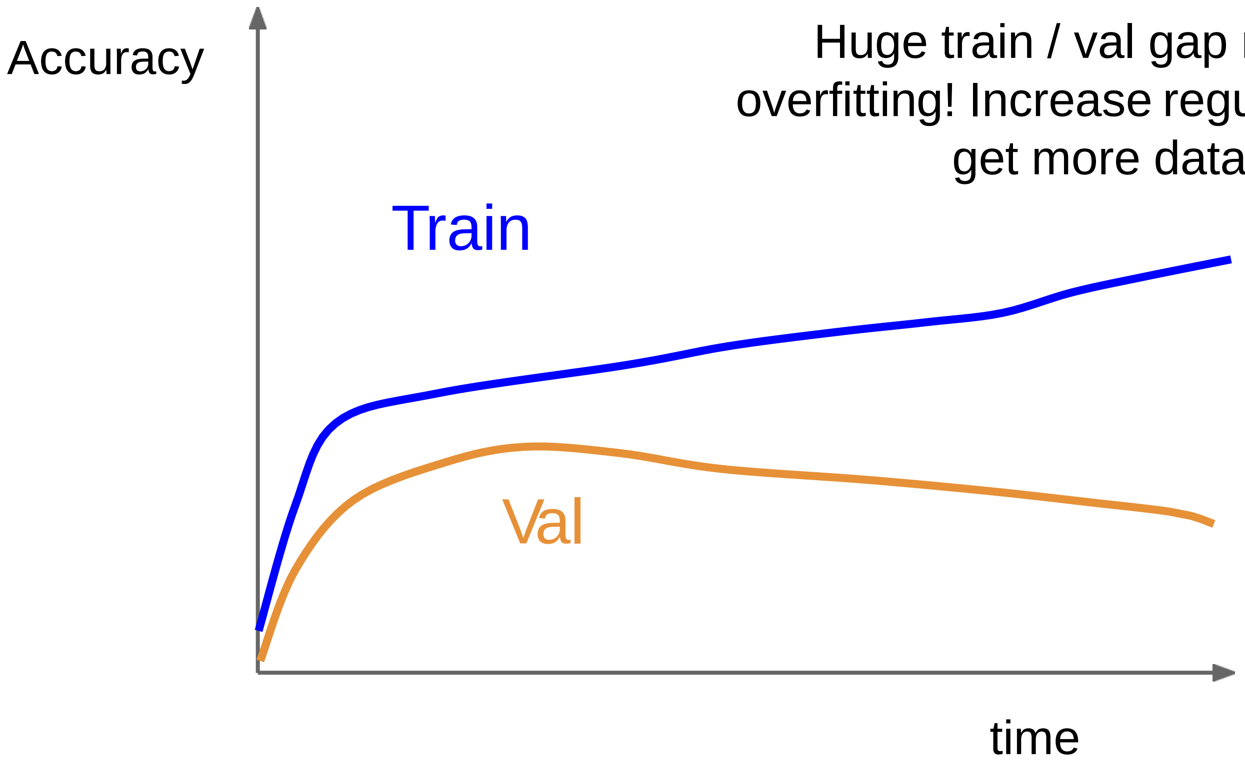



Train / Val Accuracy

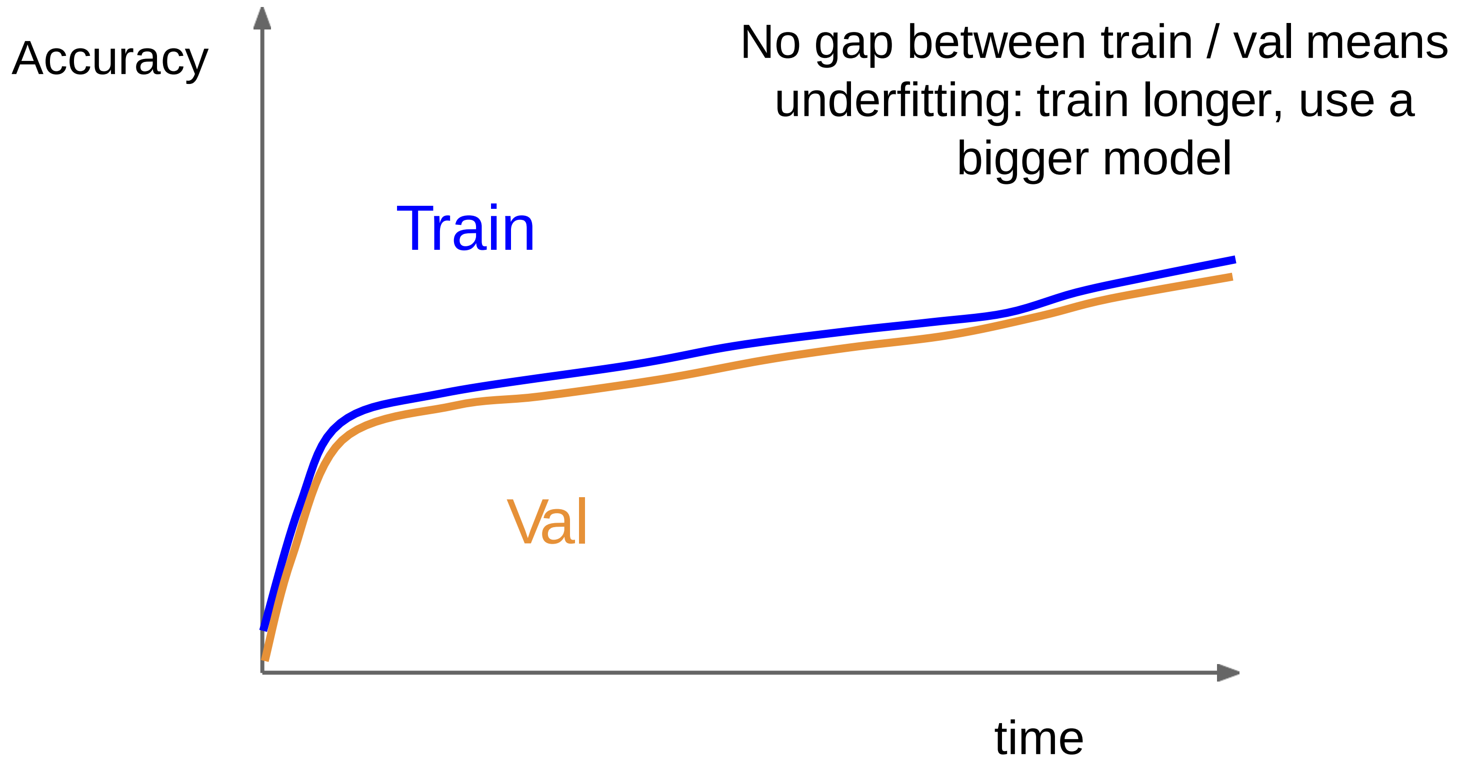



Losses may be noisy, use a scatter plot and also plot moving average to see trends better


Accuracy
Accuracy still going up, you need to train longer
Train
Val
time




Huge train / val gap means overfitting! Increase regularization, get more data



Accuracy
No gap between train / val means underfitting: train longer, use a bigger model
Train
Val
time

# Track the ratio of weight updates / weight magnitudes:

```
# assume parameter vector W and its gradient vector dW
param_scale = np.linalg.norm(W.ravel())
update = -learning_rate*dW # simple SGD update
update_scale = np.linalg.norm(update.ravel())
W += update # the actual update
print update_scale / param_scale # want ~1e-3
```

ratio between the updates and values: ~ 0.0002 / 0.02 = 0.01 (about okay)
**want this to be somewhere around 0.001 or so**

# Model Ensembles

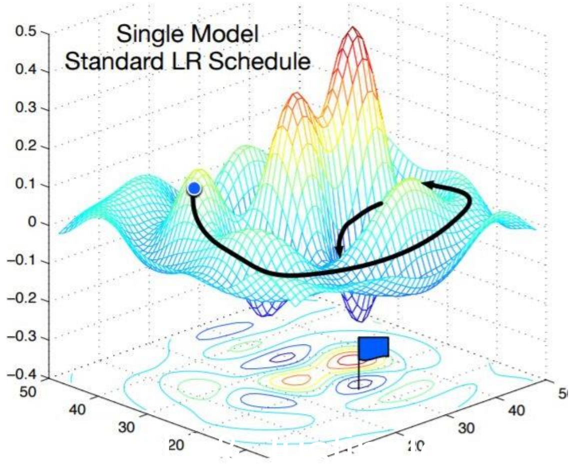
1. Train multiple independent models
2. At test time average their results

   (Take average of predicted probability distributions, then choose argmax)

Enjoy 2% extra performance

# Model Ensembles: Tips and Tricks

Instead of training independent models, use multiple snapshots of a single model during training!




Loshchilov and Hutter, "SGDR: Stochastic gradient descent with restarts", arXiv 2016
Huang et al, "Snapshot ensembles: train 1, get M for free", ICLR 2017
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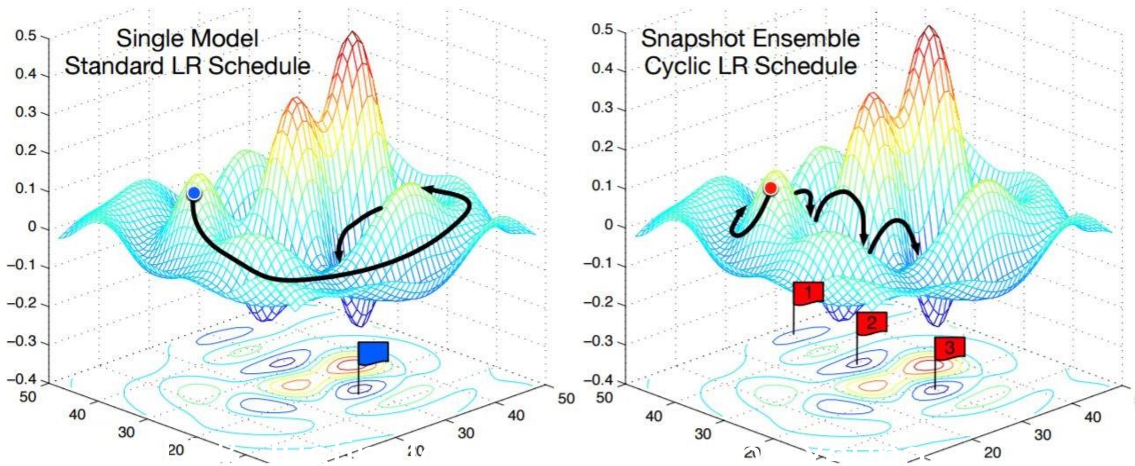
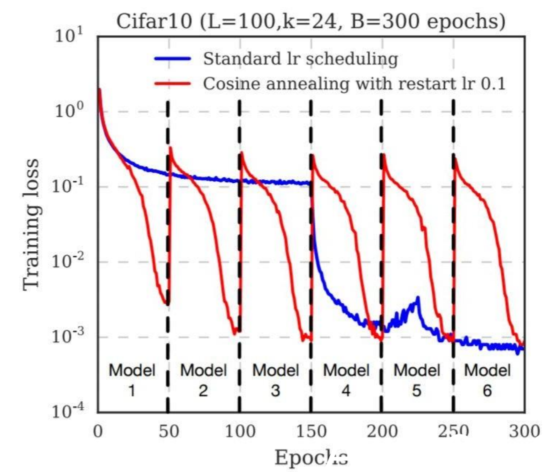
# Model Ensembles: Tips and Tricks

Instead of training independent models, use multiple snapshots of a single model during training!

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Cyclic learning rate schedules can make this work even better!

# Summary

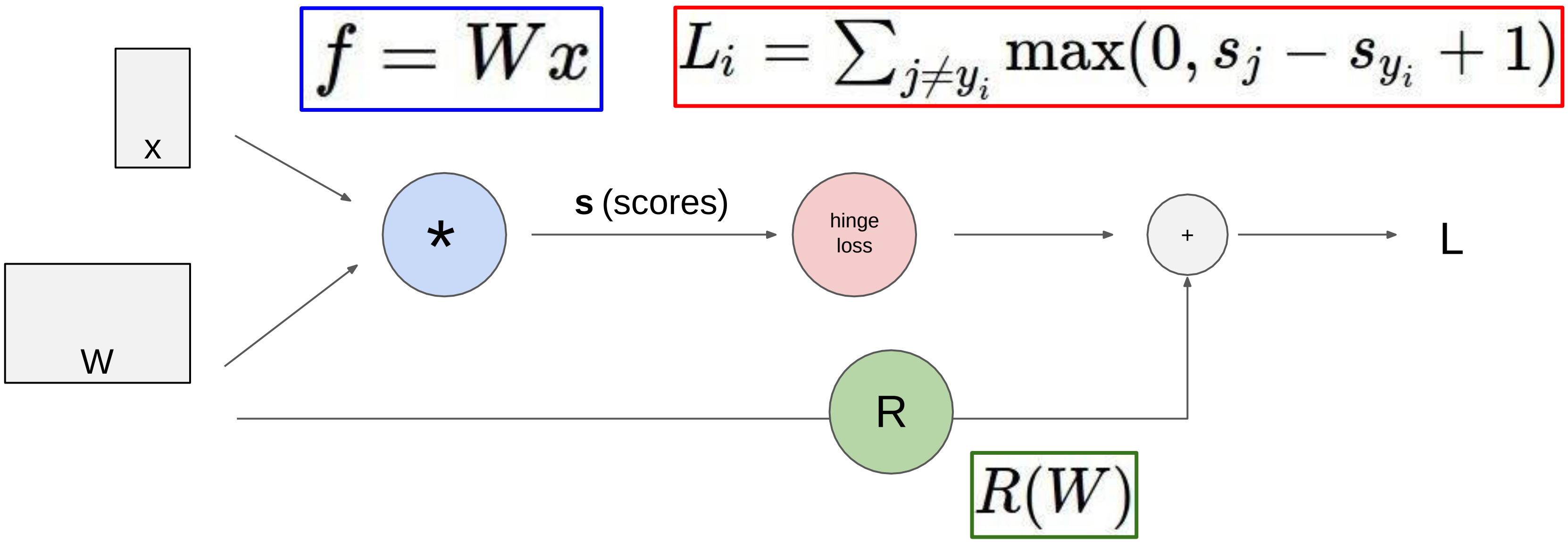
- Improve your training error:
  - Optimizers
  - Learning rate schedules
- Improve your test error:
  - Regularization
  - Choosing hyperparameters
  - Model ensembles

# Computation graphs

# How do we compute the gradient?

- Derive on paper? Tedious
- What about vector-valued functions?

# Computational graphs



# Backpropagation: a simple example

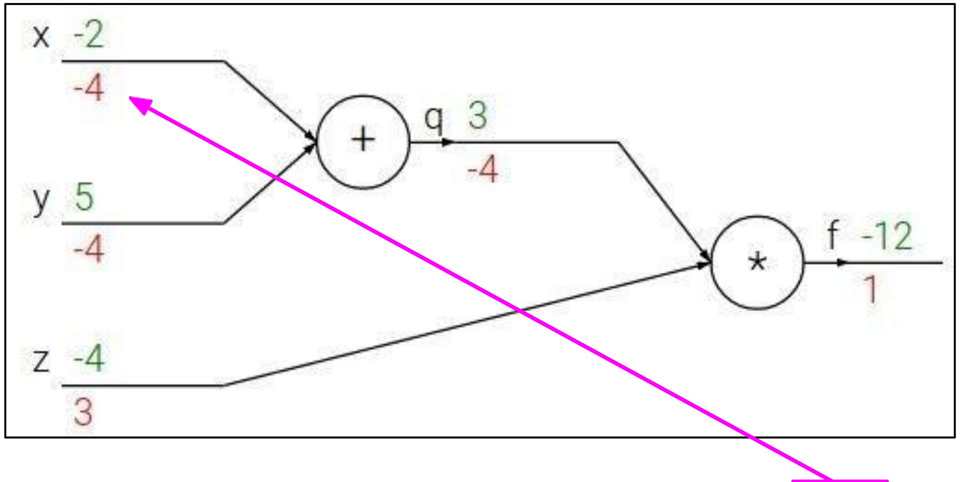
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



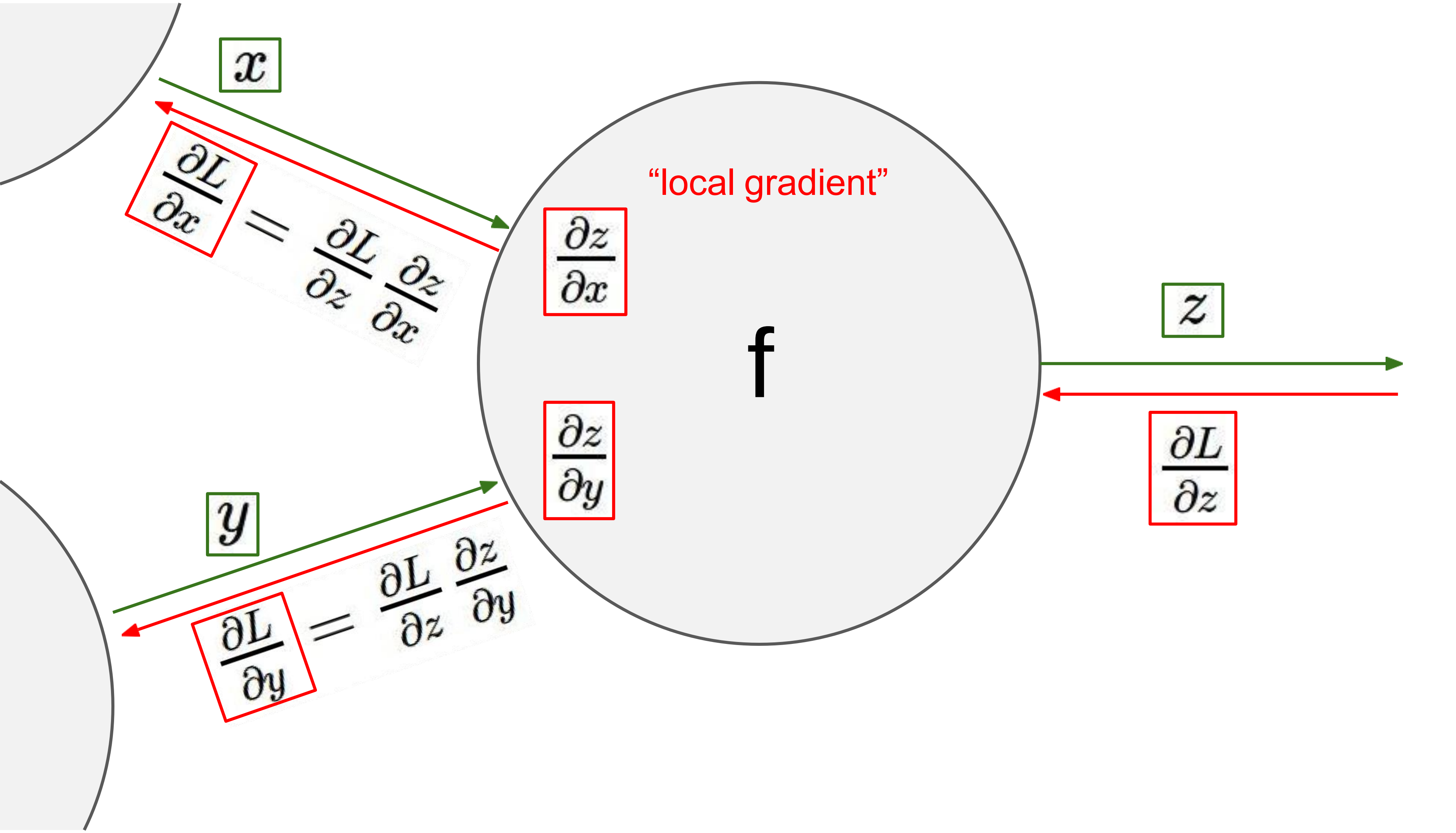

$$\frac{\partial f}{\partial x}$$

Chain rule:

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

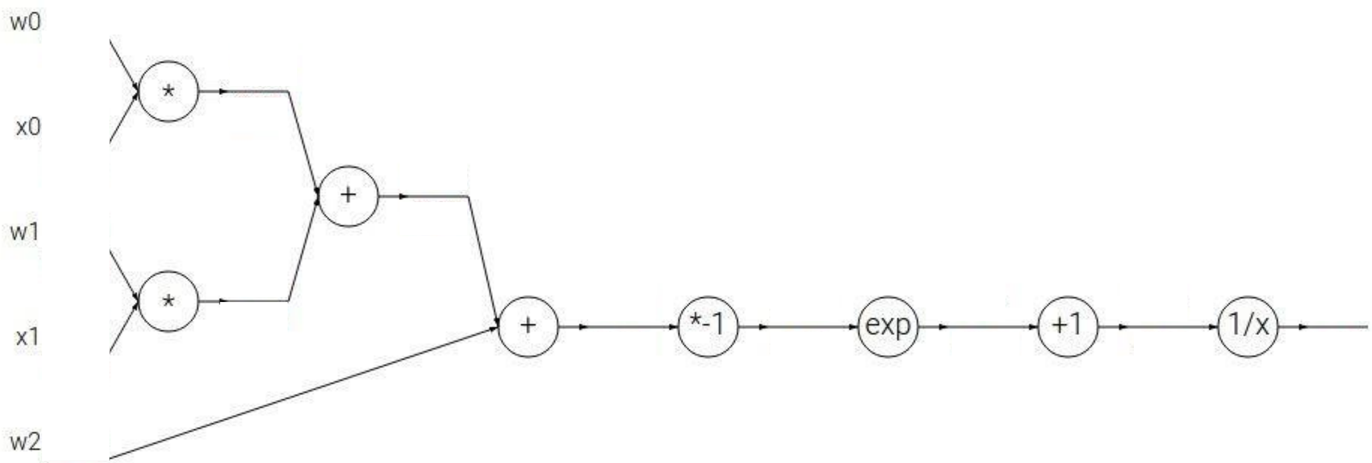
Upstream gradient

Local gradient

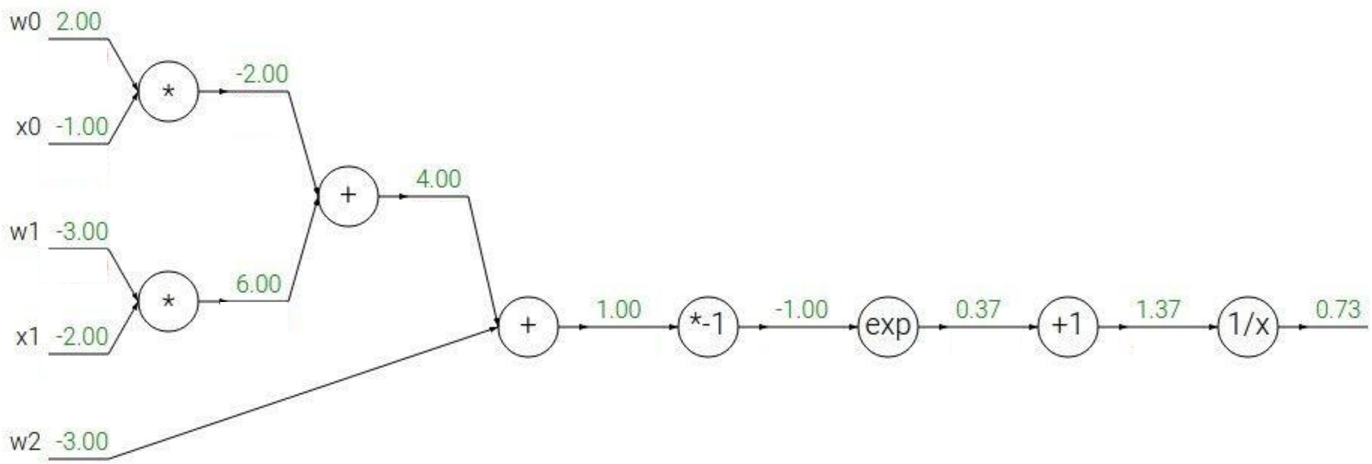



Adapted from Fei-Fei Li, Justin Johnson, Serena Yeung

Another example: $$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



Another example: $f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$



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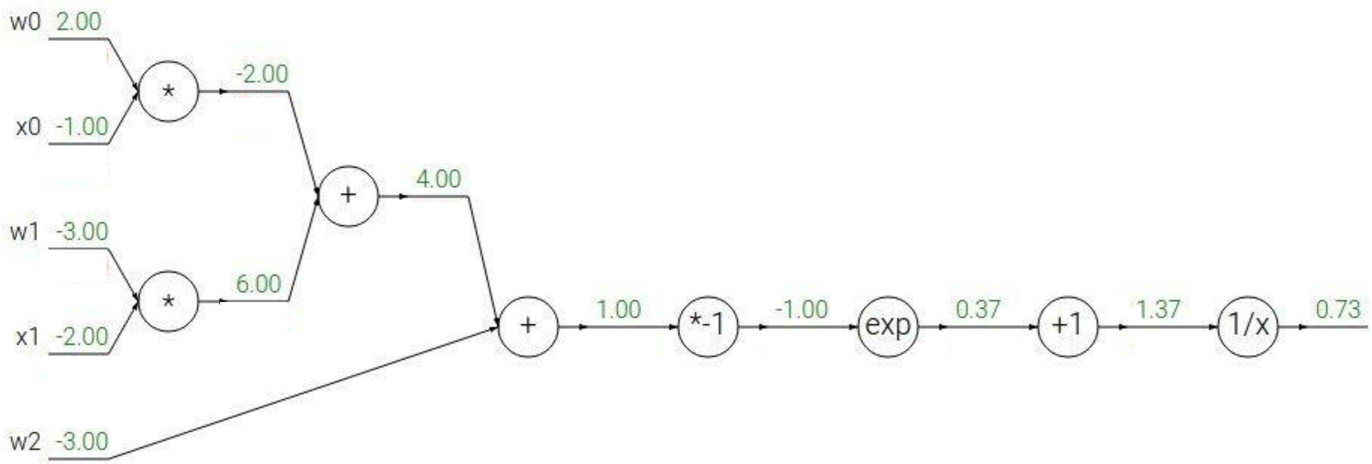


$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

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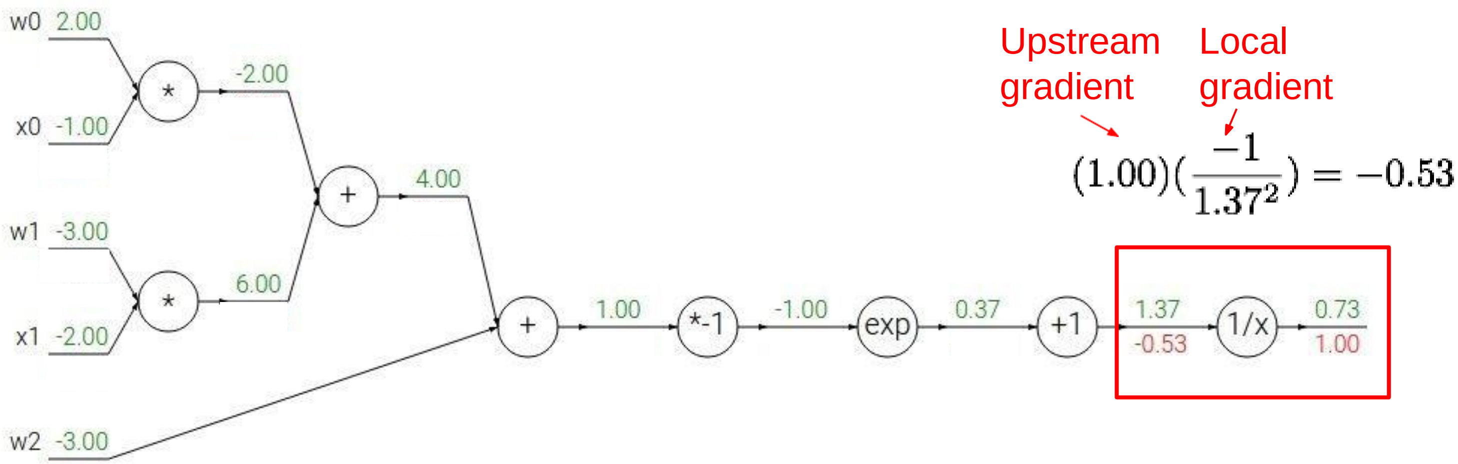


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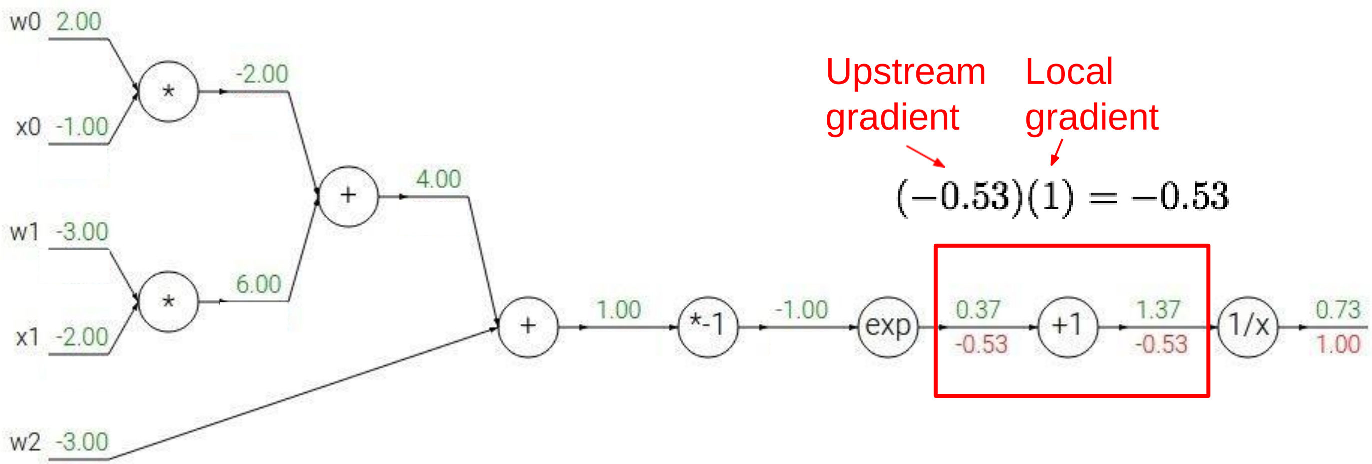


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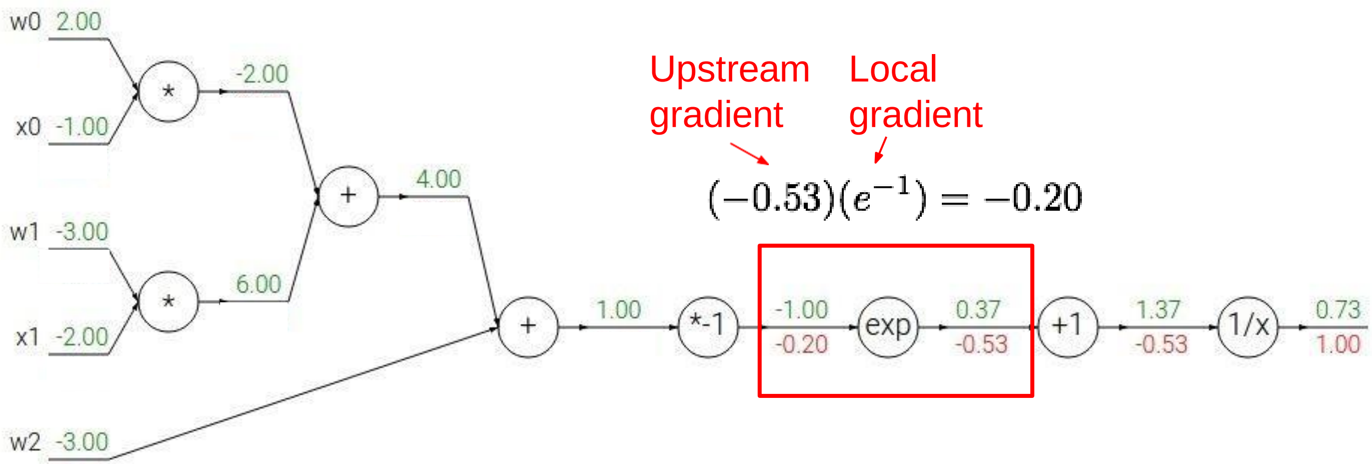


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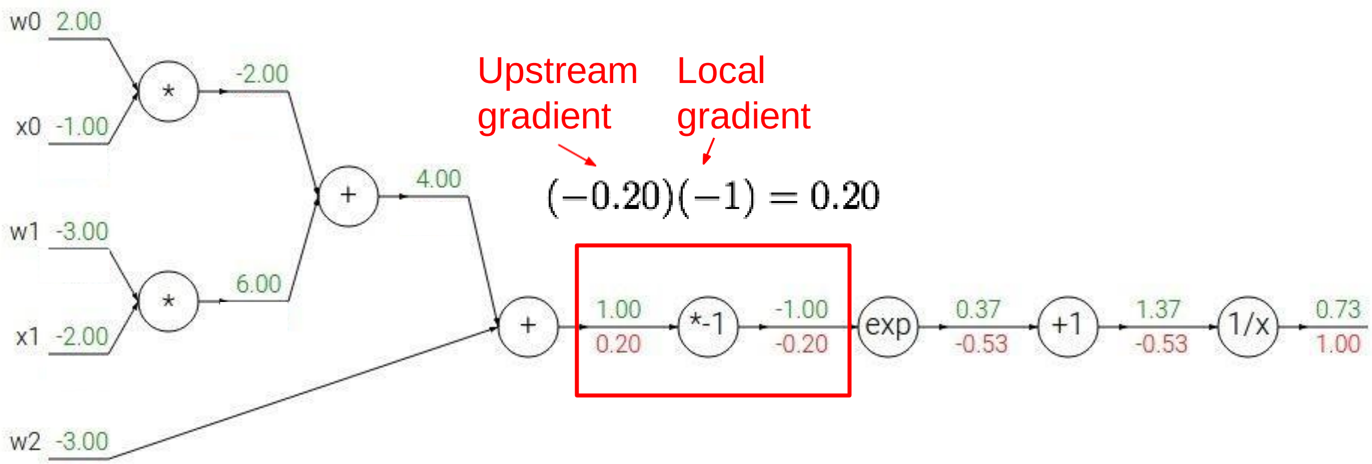


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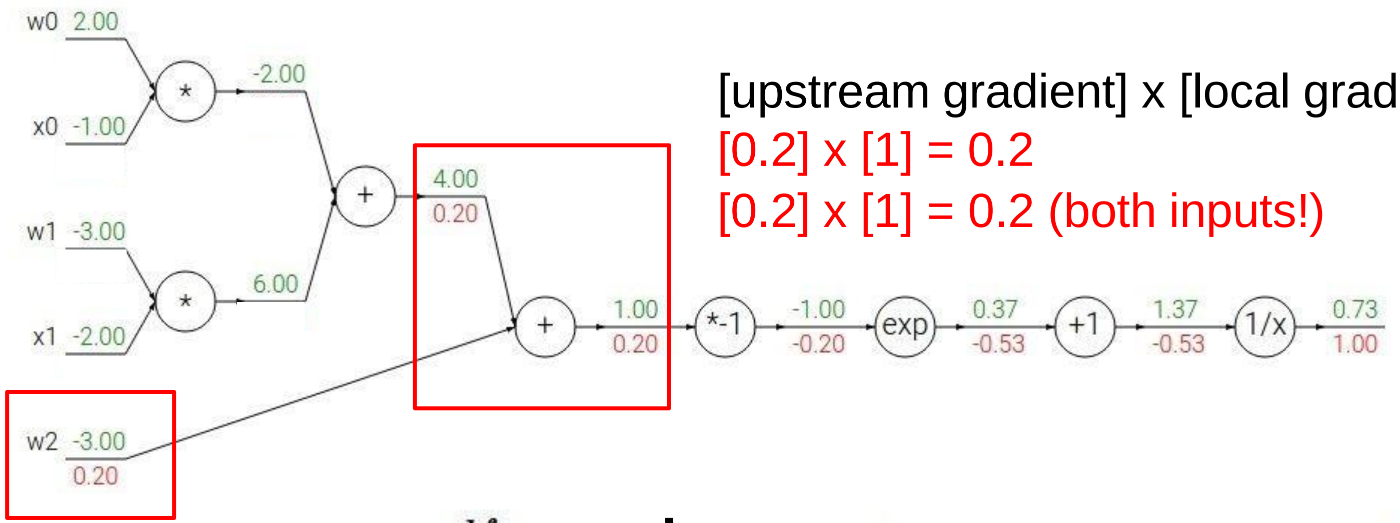
# Another example:

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

[upstream gradient] x [local gradient]

[0.2] x [1] = 0.2

[0.2] x [1] = 0.2 (both inputs!)

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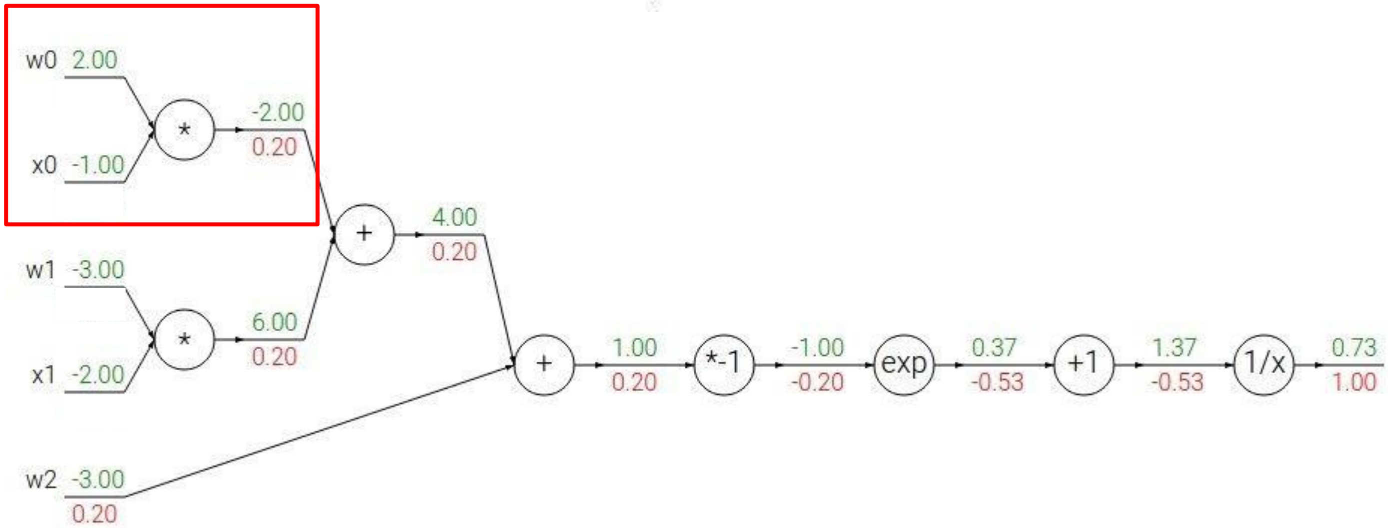


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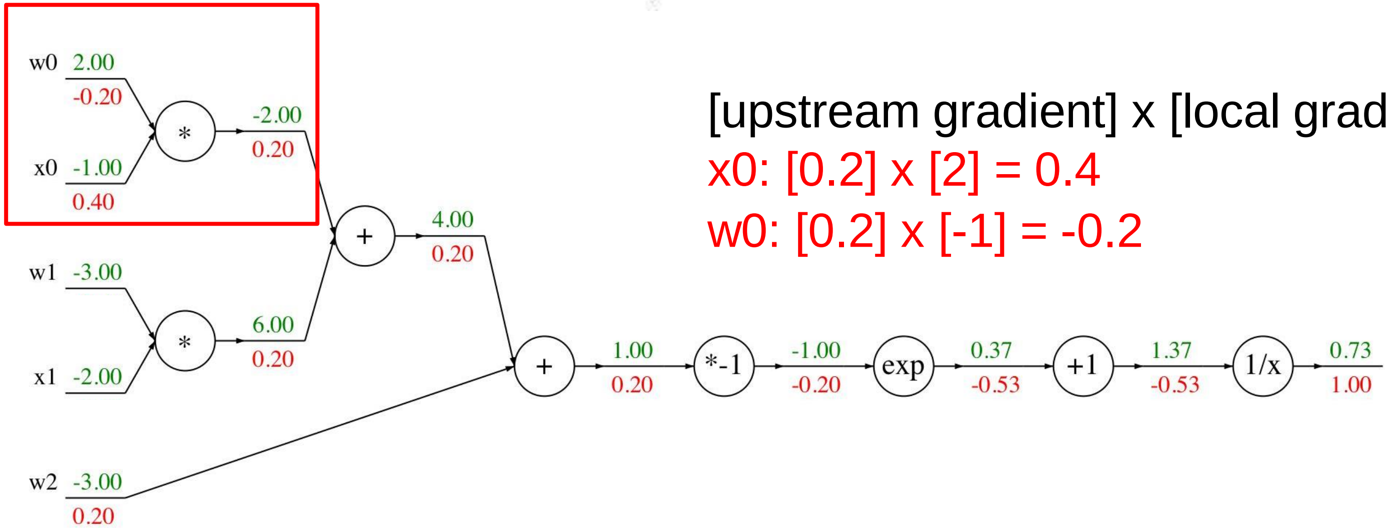


[upstream gradient] x [local gradient]

x0: [0.2] x [2] = 0.4

w0: [0.2] x [-1] = -0.2

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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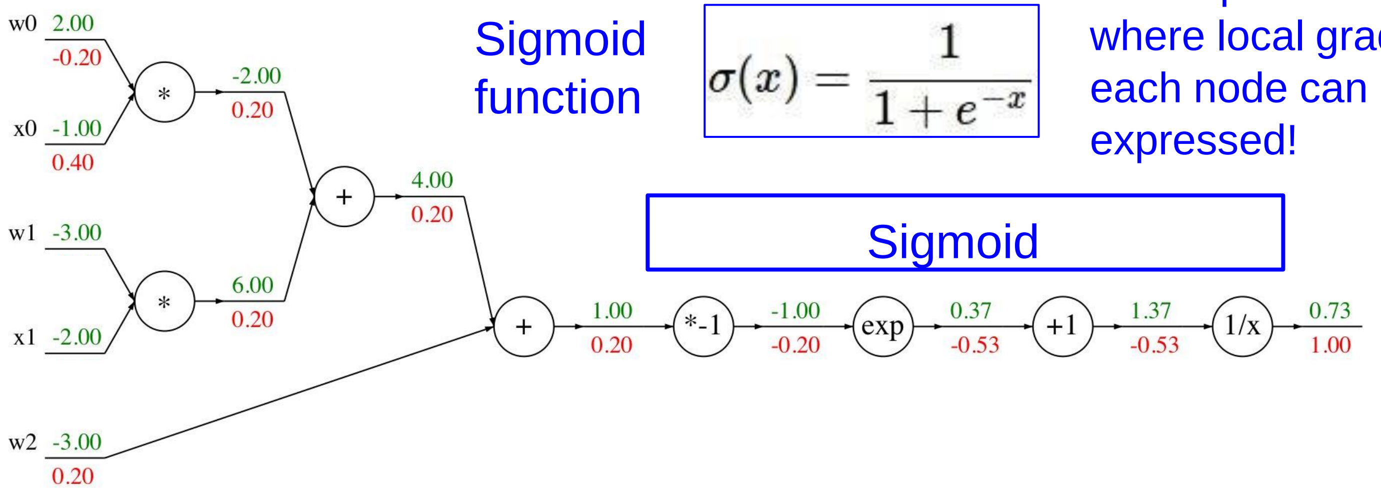
# Another example:

$$f(w,x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$

Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!

Sigmoid function

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



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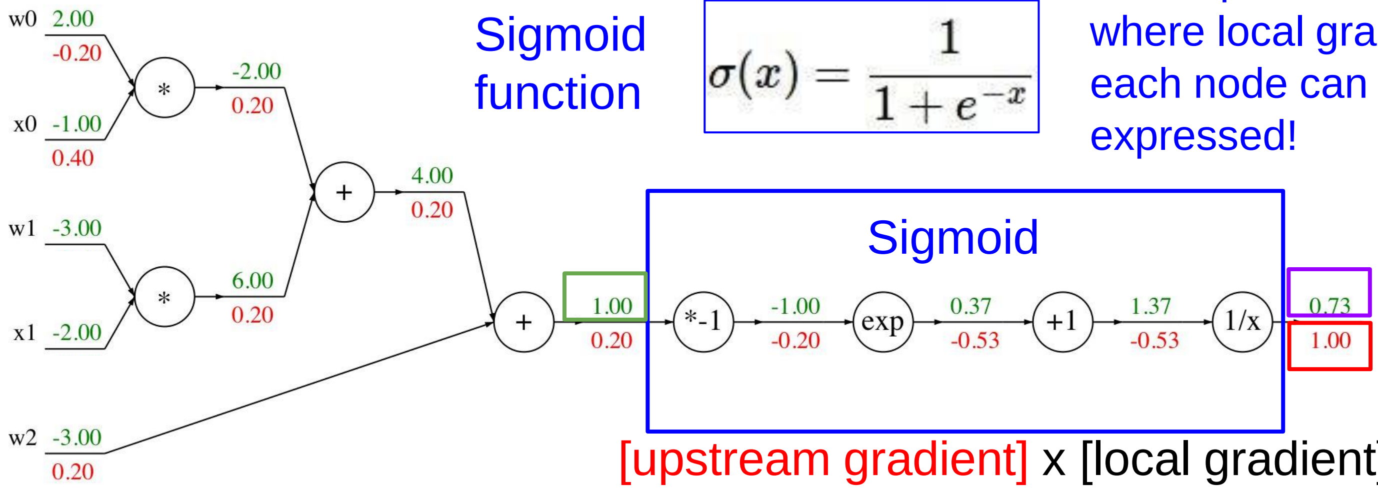



[upstream gradient] x [local gradient]

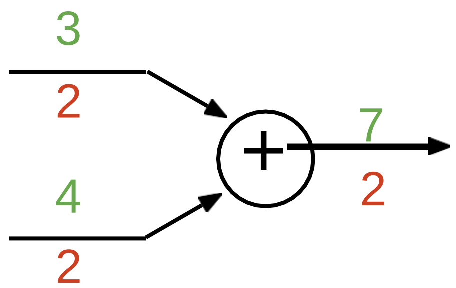
[1.00] x [(1 - 0.73) (0.73)] = 0.2

Sigmoid local gradient:

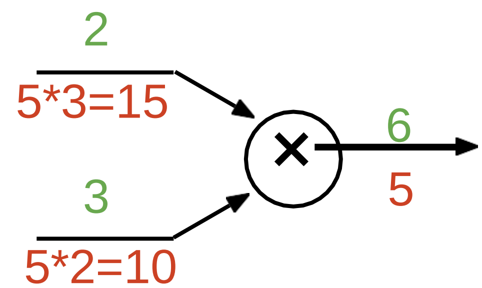
$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$

# Patterns in gradient flow

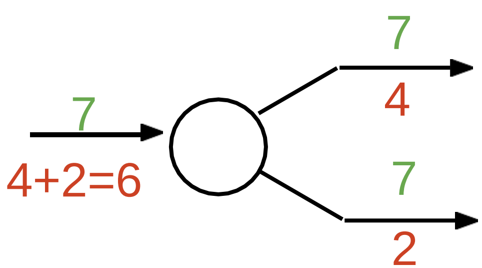
**add** gate: gradient distributor



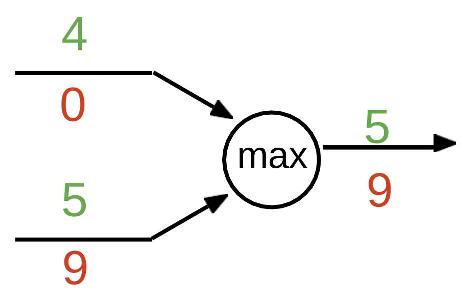

**mul** gate: “swap multiplier”



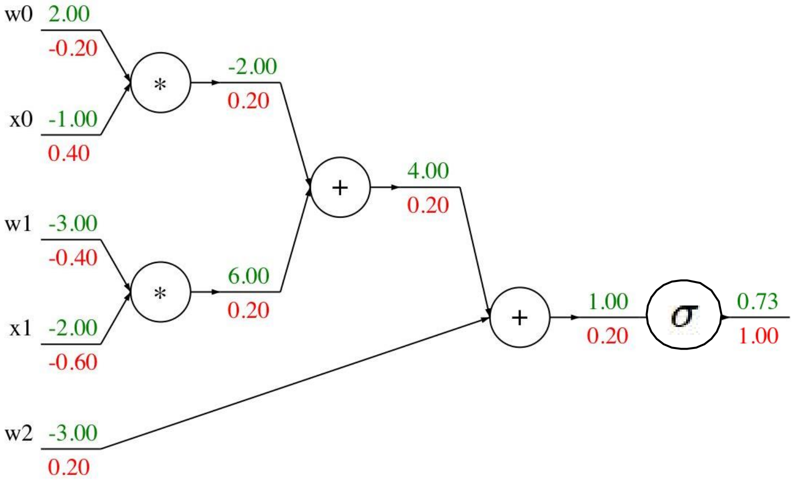

**copy** gate: gradient adder




**max** gate: gradient router



# Backprop Implementation: “Flat” code



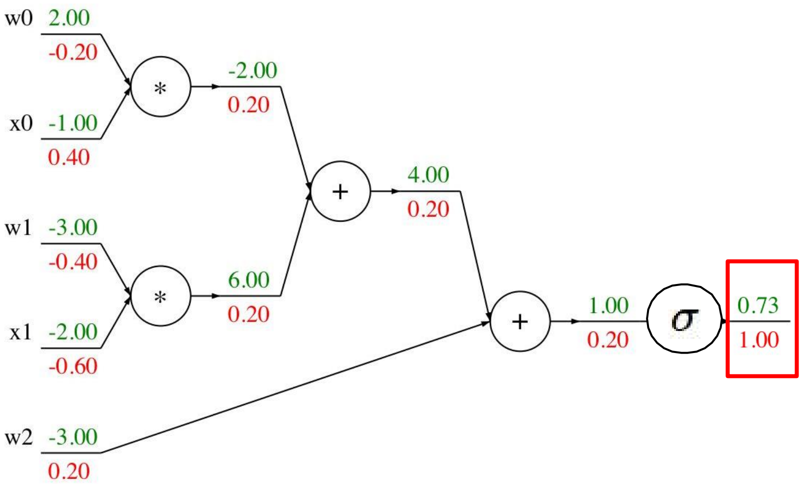

Forward pass:
Compute output

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

Backward pass:
Compute grads

```
  grad_L = 1.0
  grad_s3 = grad_L * (1 - L) * L
  grad_w2 = grad_s3
  grad_s2 = grad_s3
  grad_s0 = grad_s2
  grad_s1 = grad_s2
  grad_w1 = grad_s1 * x1
  grad_x1 = grad_s1 * w1
  grad_w0 = grad_s0 * x0
  grad_x0 = grad_s0 * w0
```

# Backprop Implementation: "Flat" code



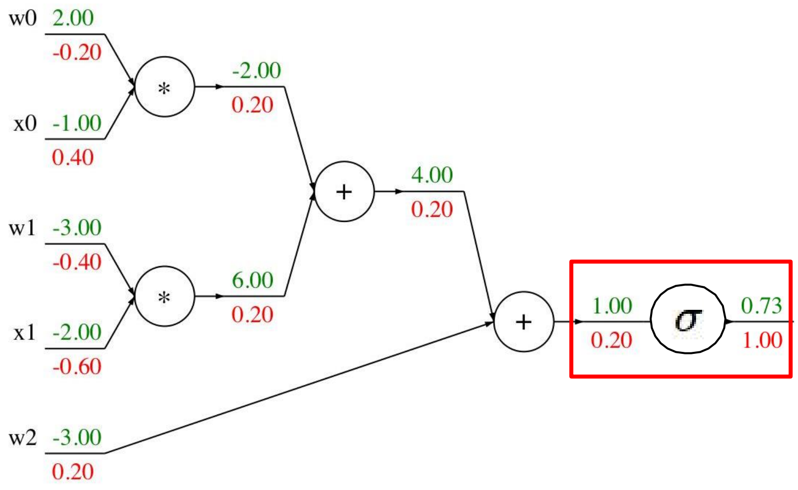

Forward pass: Compute output

Base case

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)

  grad_L = 1.0
  grad_s3 = grad_L * (1 - L) * L
  grad_w2 = grad_s3
  grad_s2 = grad_s3
  grad_s0 = grad_s2
  grad_s1 = grad_s2
  grad_w1 = grad_s1 * x1
  grad_x1 = grad_s1 * w1
  grad_w0 = grad_s0 * x0
  grad_x0 = grad_s0 * w0
```

# Backprop Implementation: “Flat” code




Forward pass: Compute output

Sigmoid

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)

  grad_L = 1.0
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  grad_w2 = grad_s3
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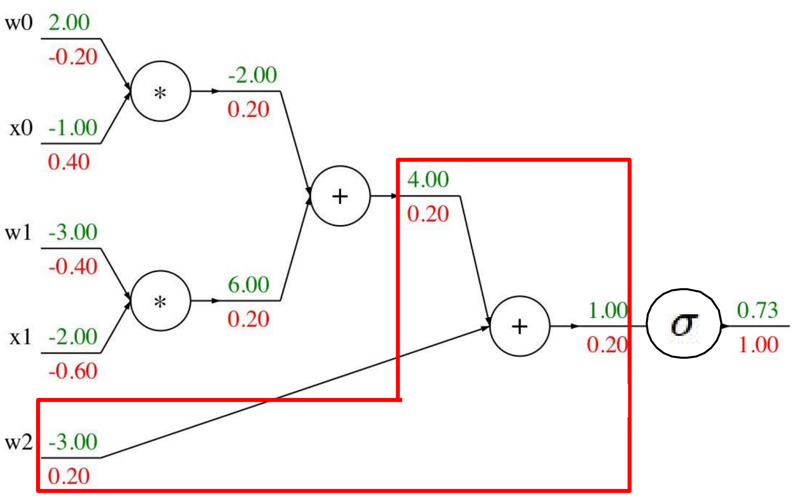
# Backprop Implementation: "Flat" code




Forward pass:
Compute output

```
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Add gate

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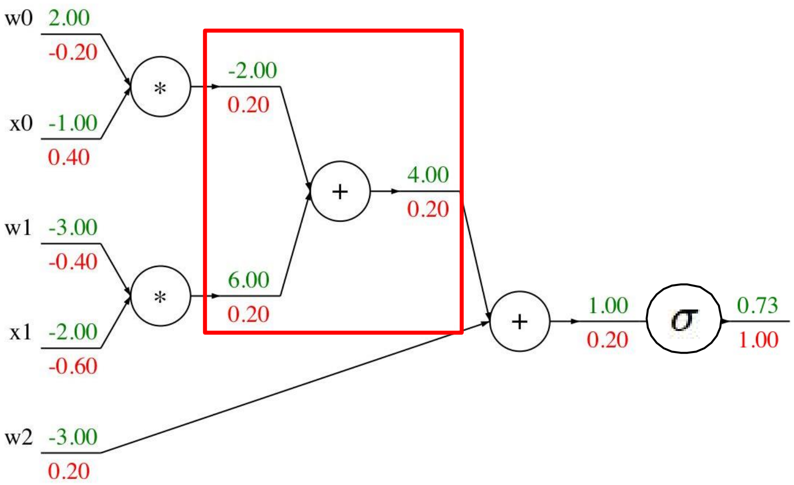


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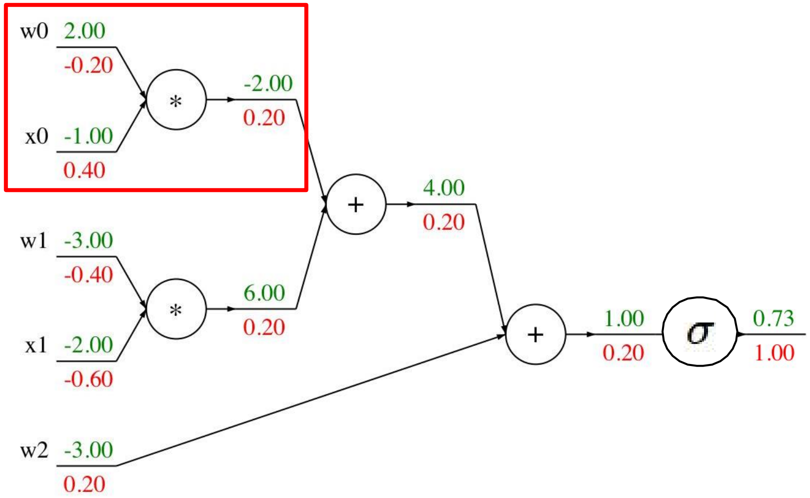


Forward pass: Compute output

Multiply gate

```
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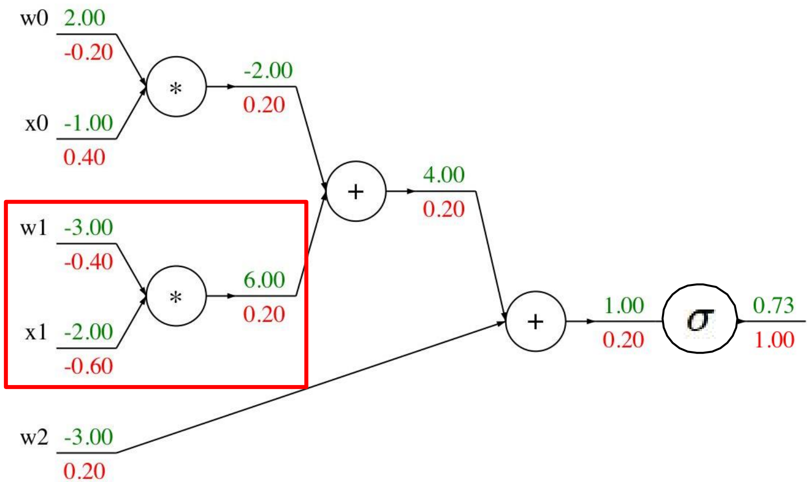


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Multiply gate

So far: backprop with scalars

What about vector-valued functions?

# Recap: Vector derivatives

## Scalar to Scalar

$$x \in \mathbb{R}, y \in \mathbb{R}$$

Regular derivative:

$$\frac{\partial y}{\partial x} \in \mathbb{R}$$

If x changes by a small amount, how much will y change?

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## Vector to Scalar

$$x \in \mathbb{R}^N, y \in \mathbb{R}$$

Derivative is **Gradient**:

$$\frac{\partial y}{\partial x} \in \mathbb{R}^N \quad \left(\frac{\partial y}{\partial x}\right)_n = \frac{\partial y}{\partial x_n}$$

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## Vector to Vector

$$x \in \mathbb{R}^N, y \in \mathbb{R}^M$$

Derivative is **Jacobian**:

$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M} \quad \left(\frac{\partial y}{\partial x}\right)_{n,m} = \frac{\partial y_m}{\partial x_n}$$

For each element of x, if it changes by a small amount then how much will each element of y change?

# Gradients

- Given a function with 1 output and *n* inputs

$$f(\boldsymbol{x}) = f(x_1, x_2, ..., x_n)$$

- Its gradient is a vector of partial derivatives with respect to each input

$$\frac{\partial f}{\partial \boldsymbol{x}} = \left[ \frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, ..., \frac{\partial f}{\partial x_n} \right]$$

# Jacobian Matrix: Generalization of Gradient

- Given a function with ***m* outputs** and *n* inputs

$$\boldsymbol{f}(\boldsymbol{x}) = [f_1(x_1, x_2, ..., x_n), ..., f_m(x_1, x_2, ..., x_n)]$$

- Its Jacobian is an ***m* x *n* matrix** of partial derivatives

$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

$$\left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right)_{ij} = \frac{\partial f_i}{\partial x_j}$$

# Chain Rule

- For one-variable functions: **multiply derivatives**

$$z = 3y$$

$$y = x^2$$

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx} = (3)(2x) = 6x$$

- For multiple variables at once: **multiply Jacobians**

$$\boldsymbol{h} = f(\boldsymbol{z})$$

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

$$\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}}\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}} = \ldots$$

# Example Jacobian: Elementwise activation Function

$$\boldsymbol{h} = f(\boldsymbol{z}), \text{what is } \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}}? \qquad \boldsymbol{h}, \boldsymbol{z} \in \mathbb{R}^n$$

$$h_i = f(z_i)$$

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Function has *n* outputs and *n* inputs → *n* by *n* Jacobian

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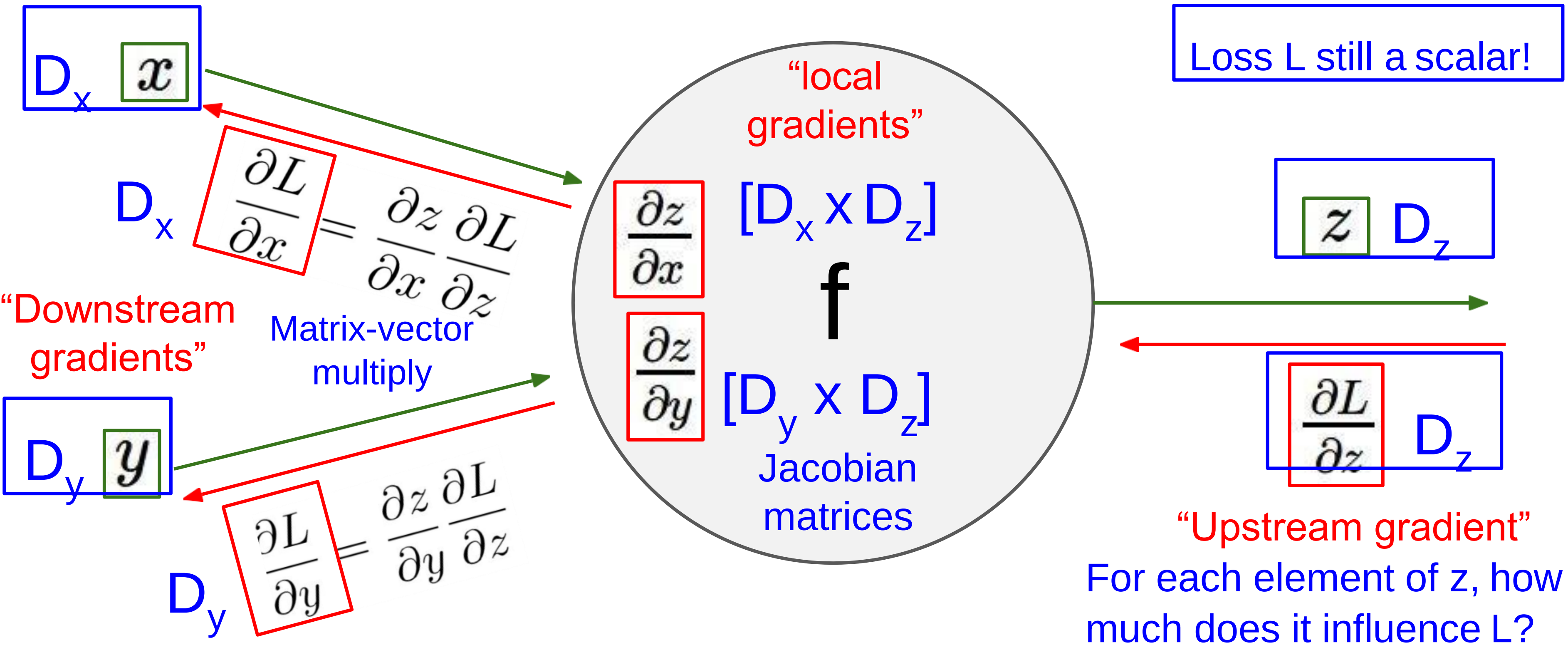
$$\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} = \begin{pmatrix} f'(z_1) & & 0 \\ & \ddots & \\ 0 & & f'(z_n) \end{pmatrix} = \text{diag}(\boldsymbol{f}'(\boldsymbol{z}))$$

# Backprop with Vectors



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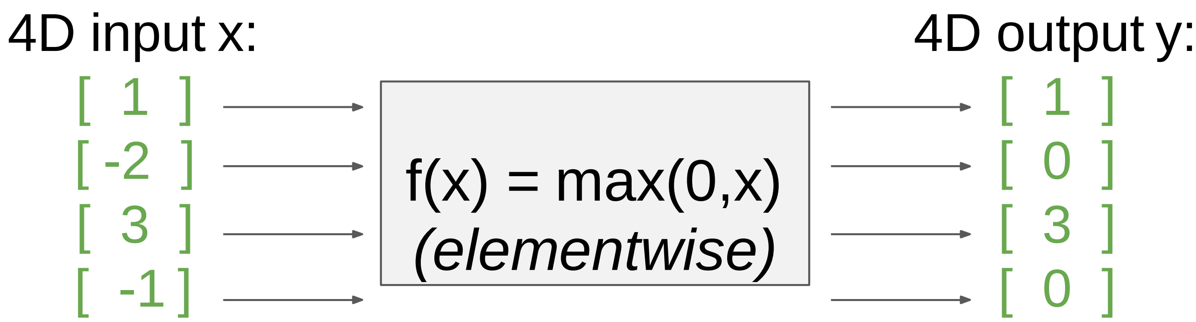

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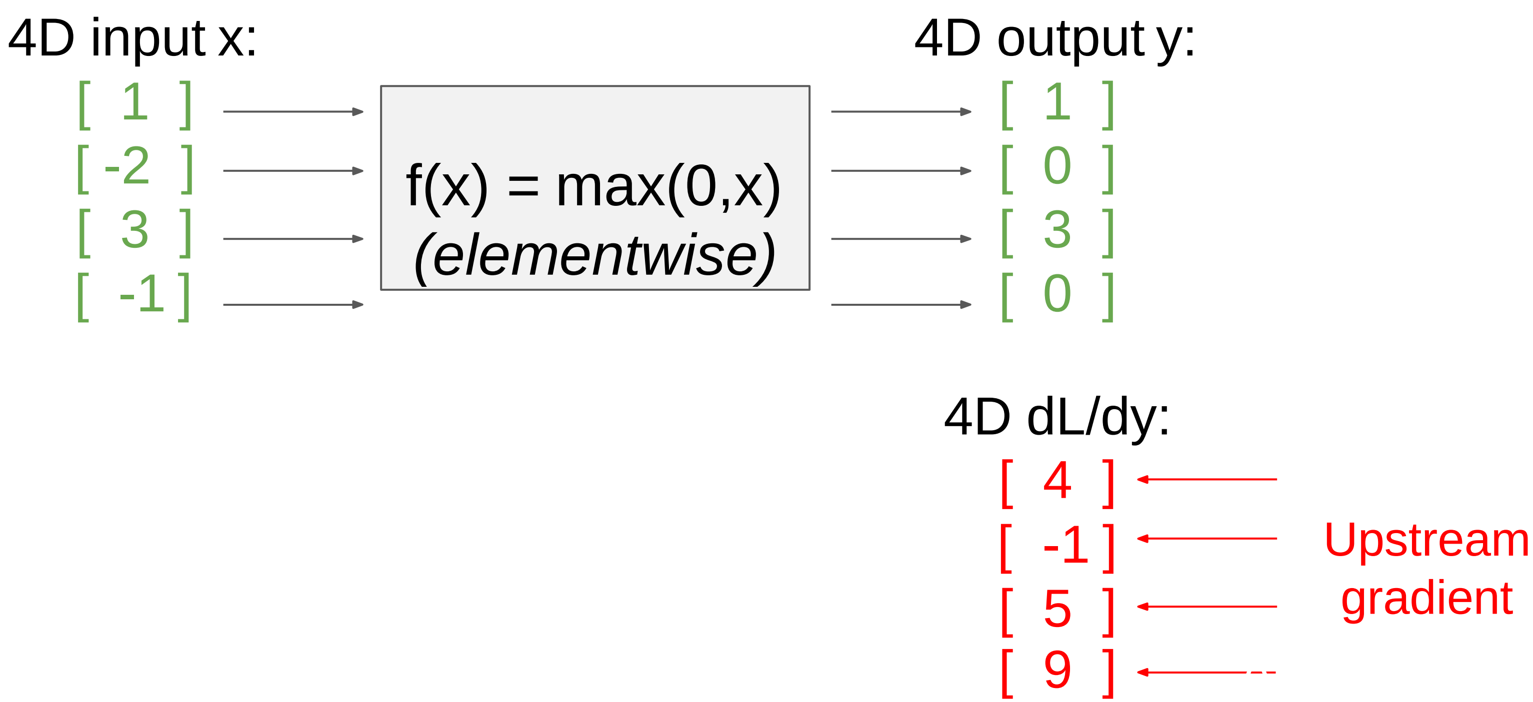

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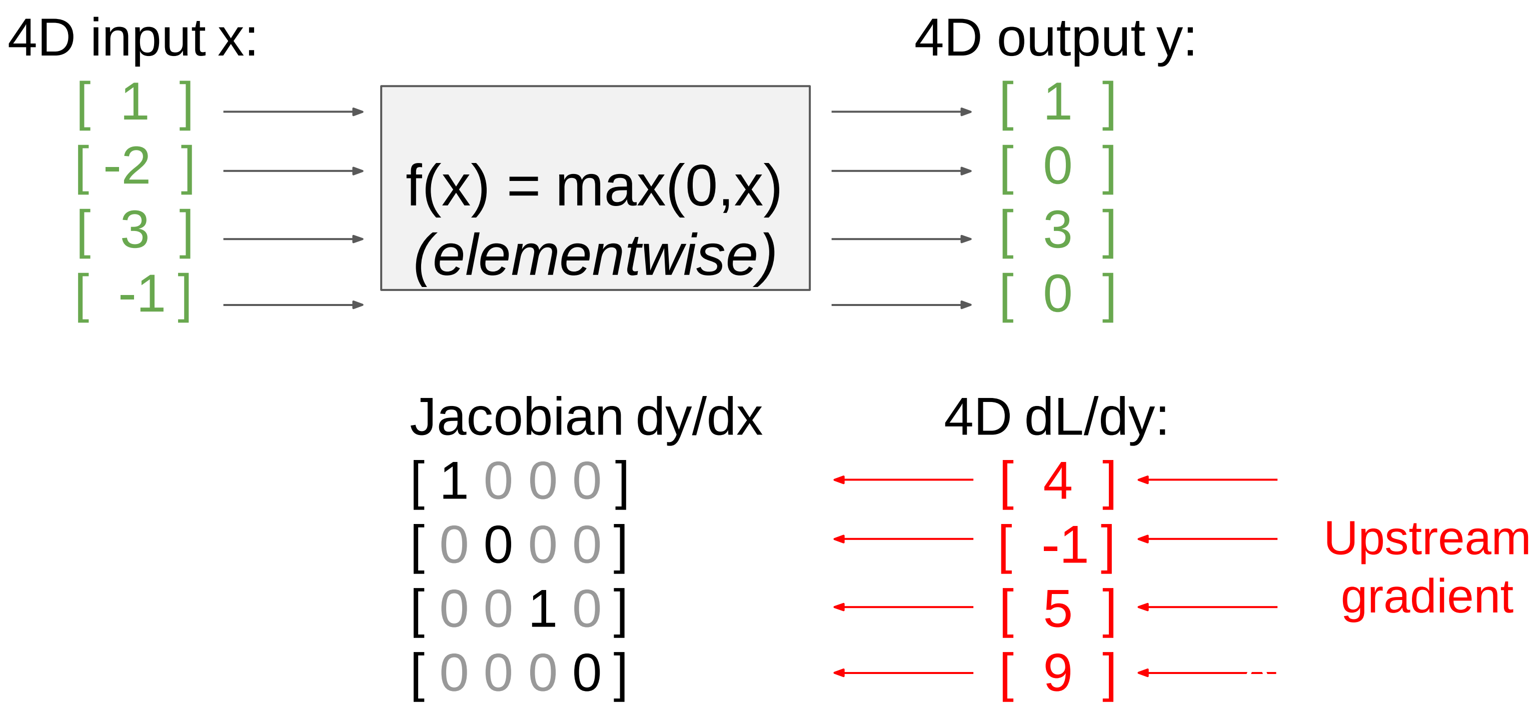

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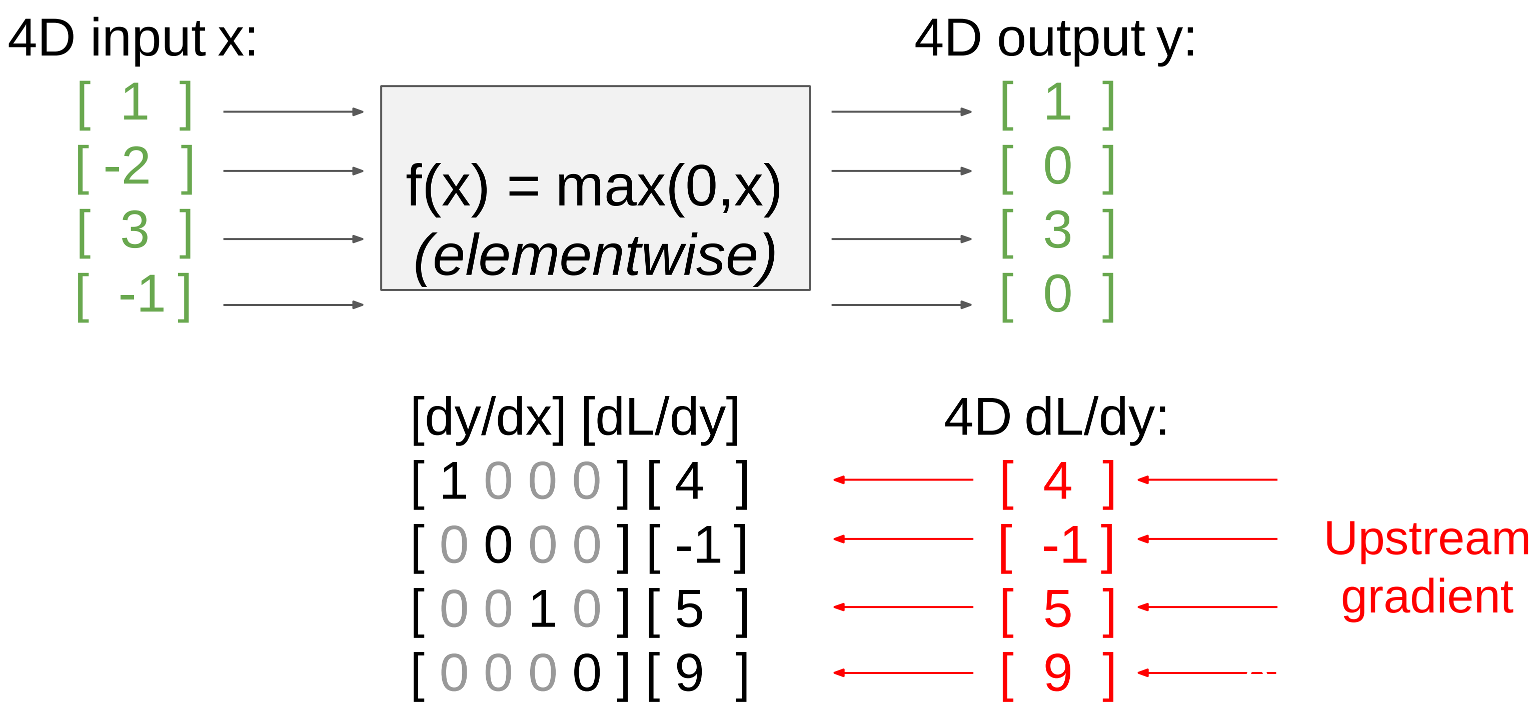

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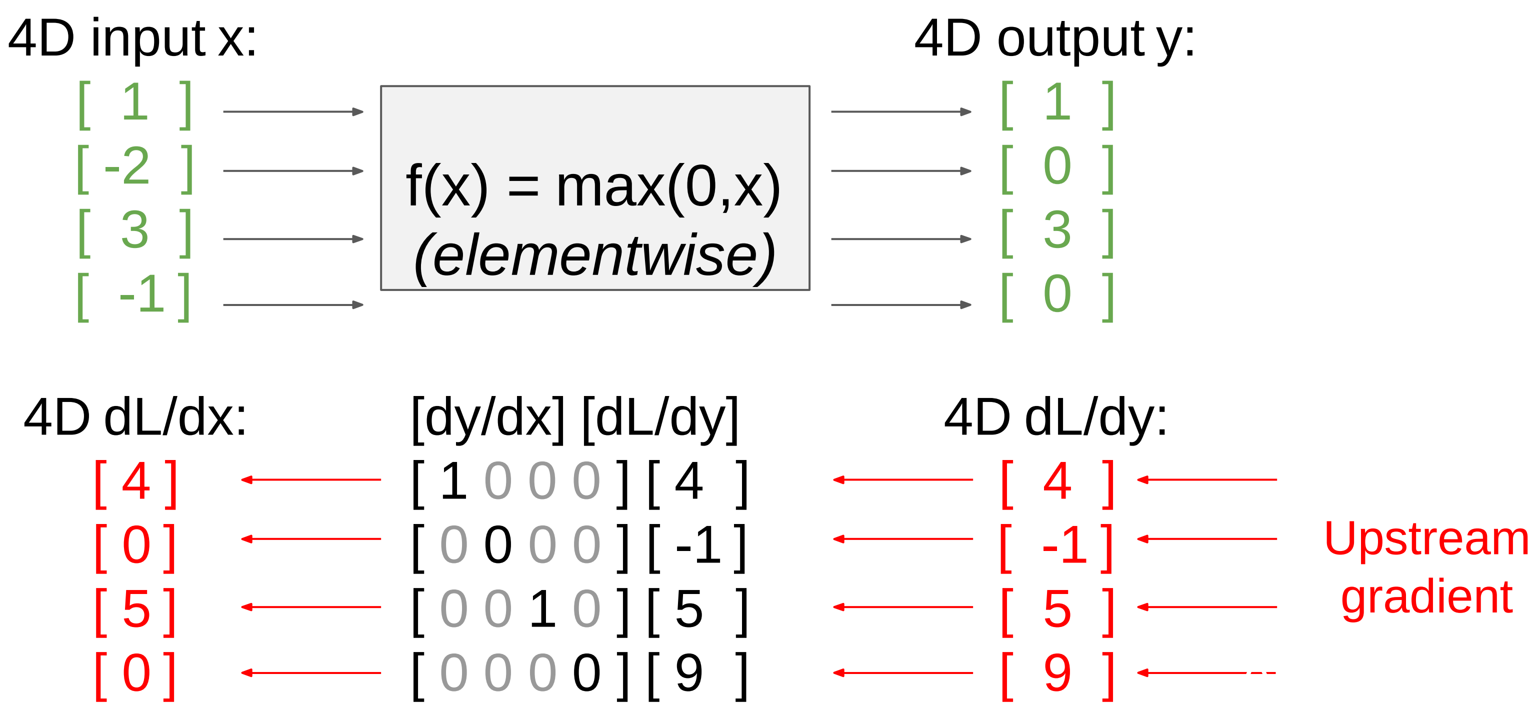
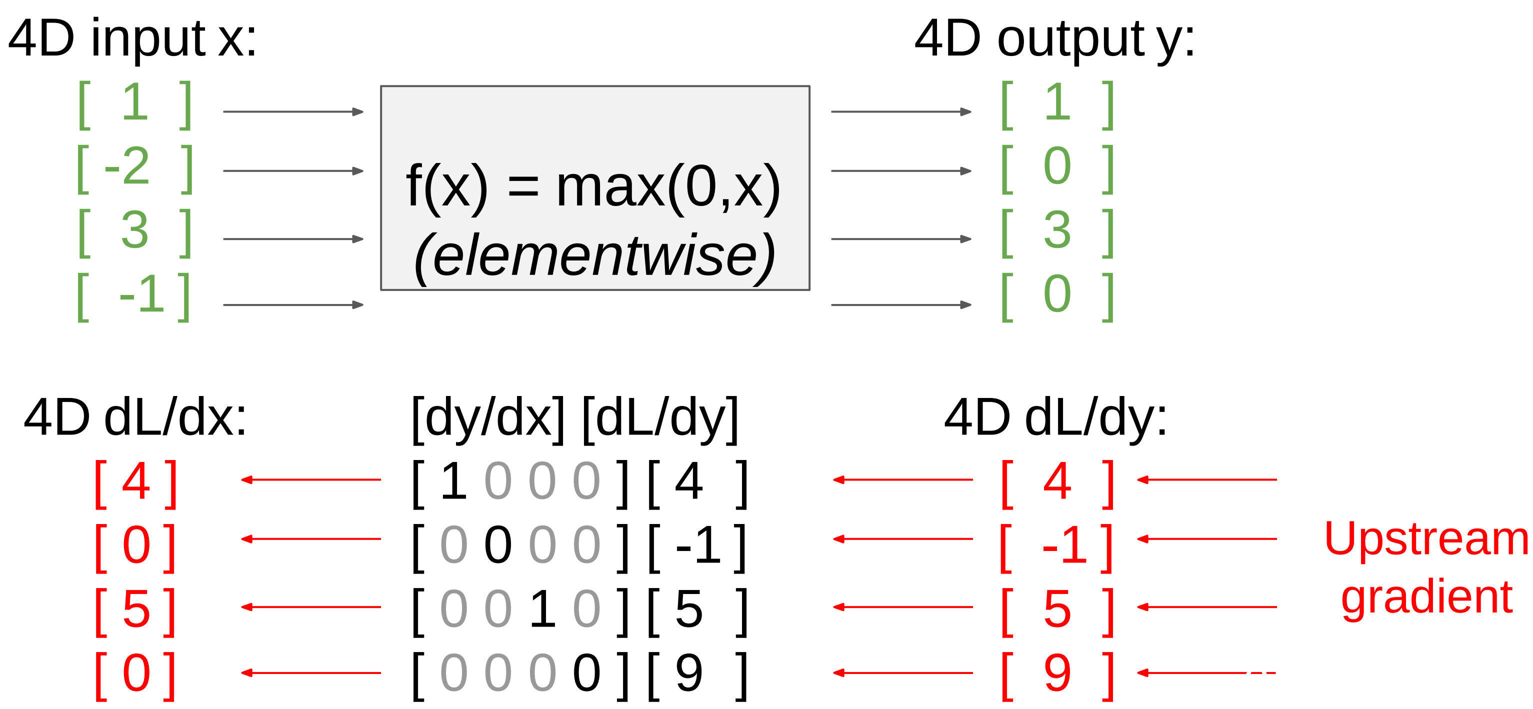


# Backprop with Vectors

Jacobian is **sparse**: off-diagonal entries always zero! Never **explicitly** form Jacobian -- instead use **implicit** multiplication



A vectorized example: $f(x,W) = ||W \cdot x||^2 = \sum_{i=1}^{n} (W \cdot x)_i^2$

$\in \mathbb{R}^n$ $\in \mathbb{R}^{n \times n}$

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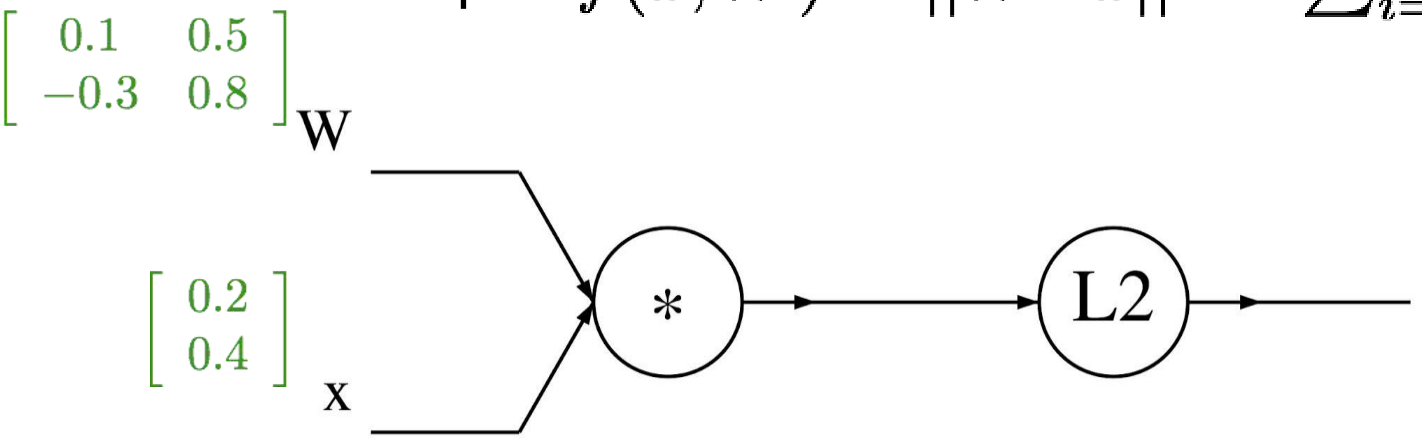


$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \cdots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \cdots + W_{n,n}x_n \end{pmatrix}$$

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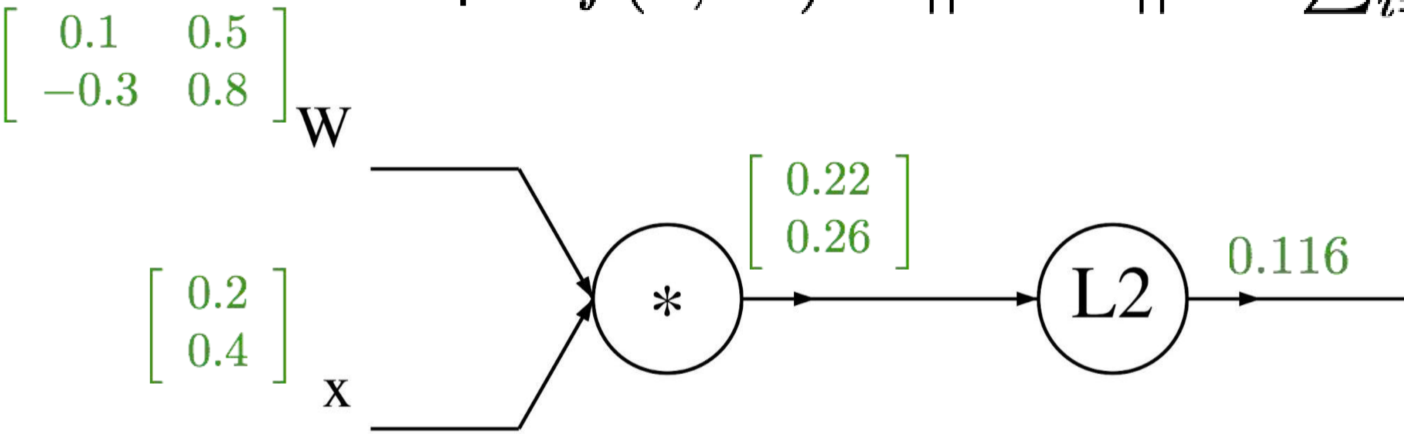


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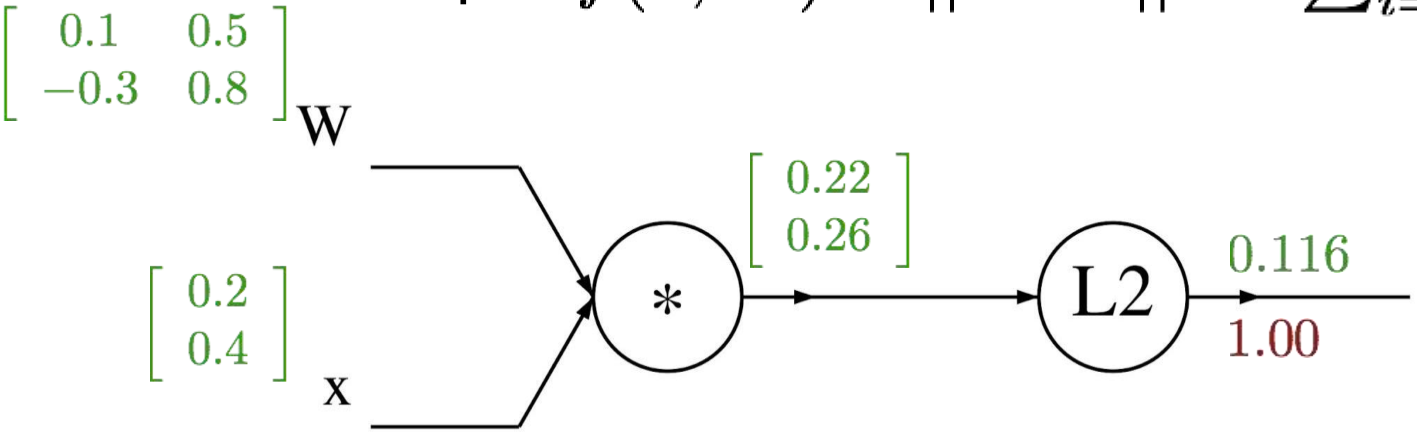


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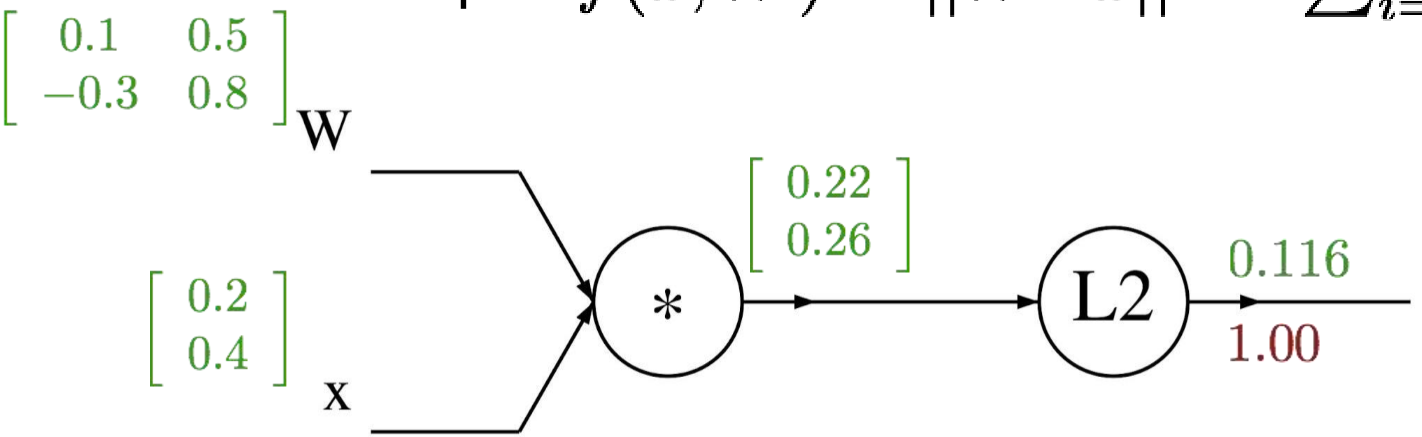


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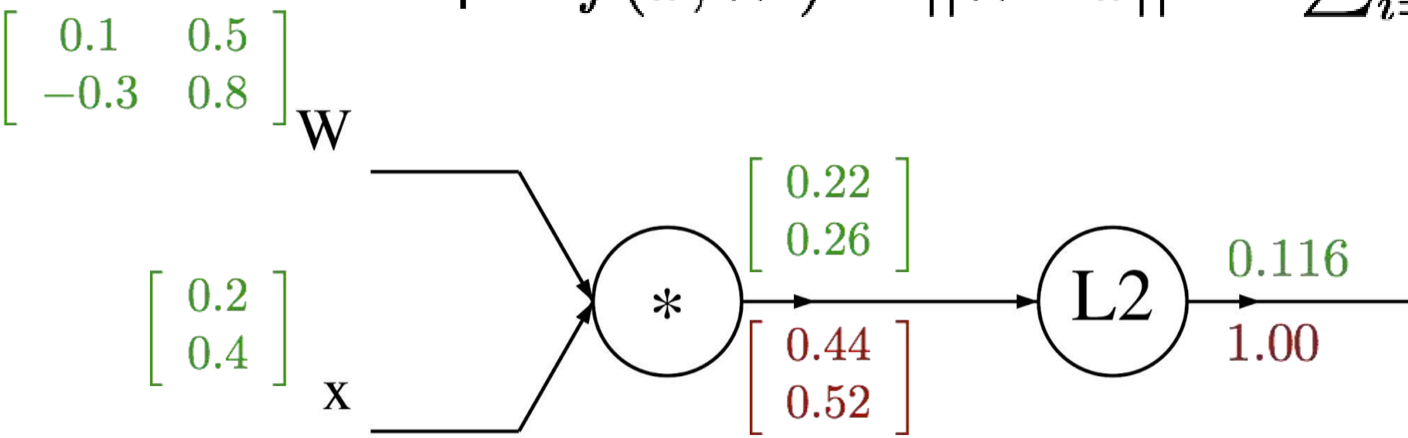


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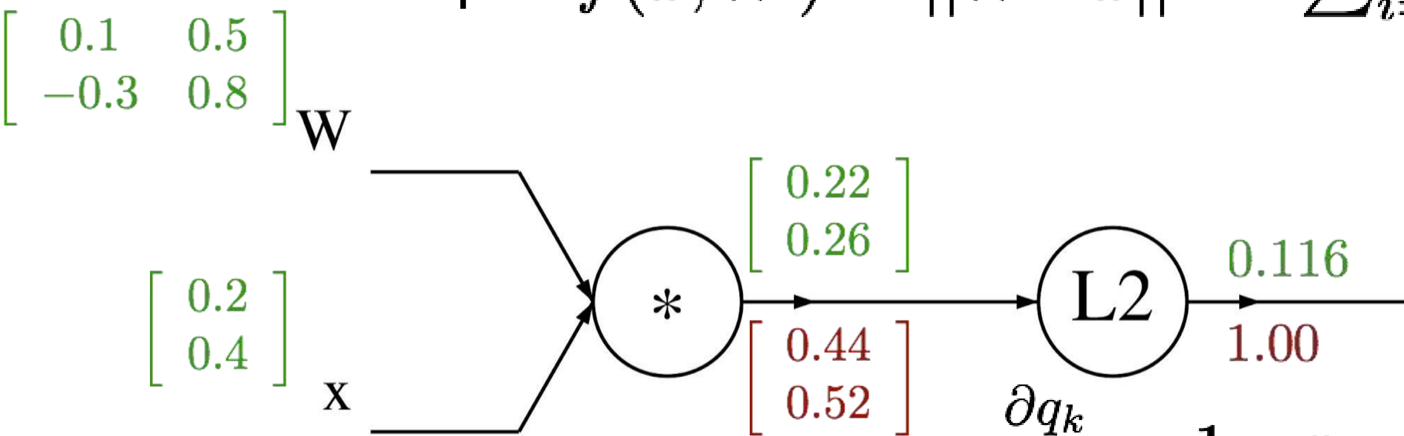


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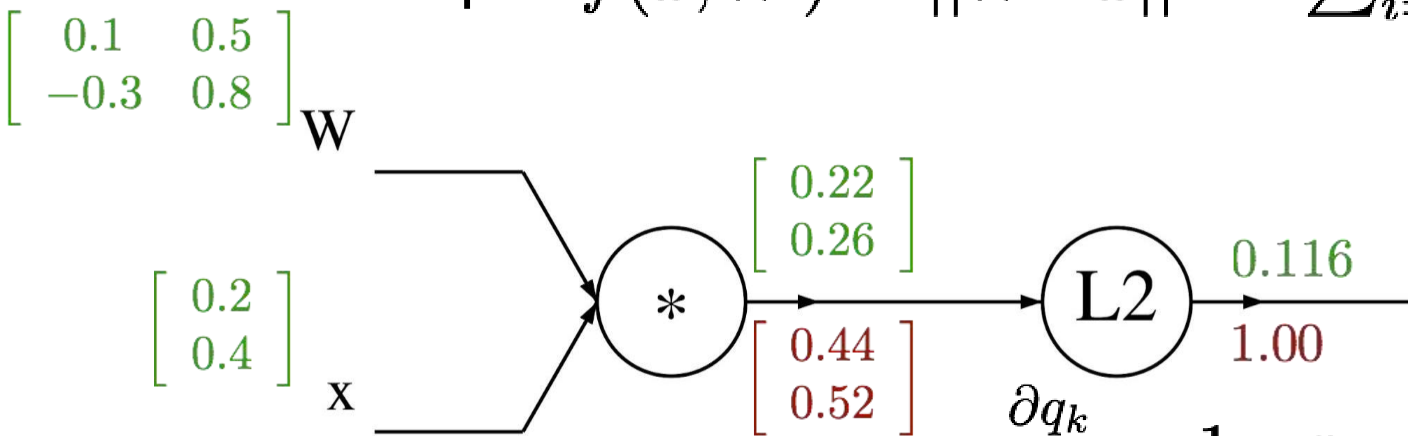


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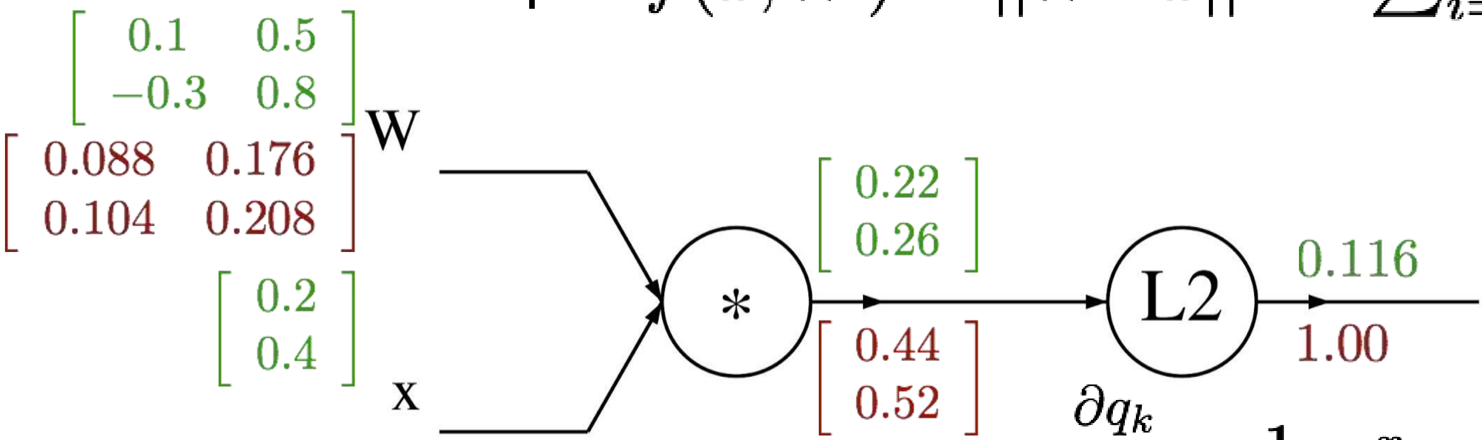


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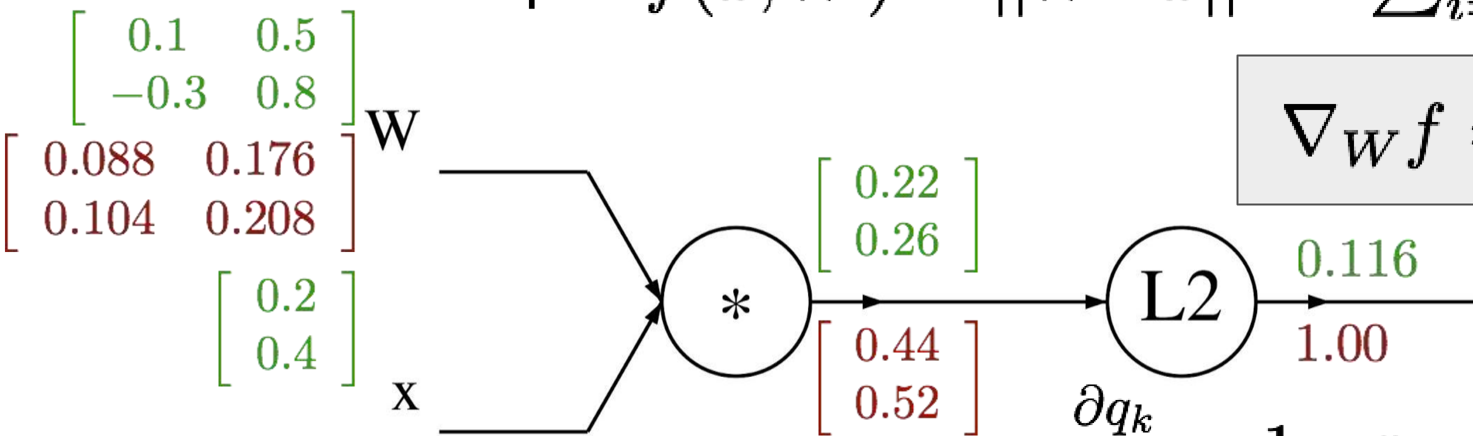


$$\nabla_W f = 2q \cdot x^T$$

Always check: The gradient with respect to a variable should have the same shape as the variable

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# Recap

- Tricks of the trade
  - Preprocessing, initialization, normalization
  - Dealing with limited data
- Convergence of gradient descent
  - How long will it take?
  - Will it work at all?
- Different optimization strategies
  - Alternatives to SGD
  - Learning rates
  - Choosing hyperparameters
- How to do the computation
  - Computation graphs
  - Vector notation (Jacobians)