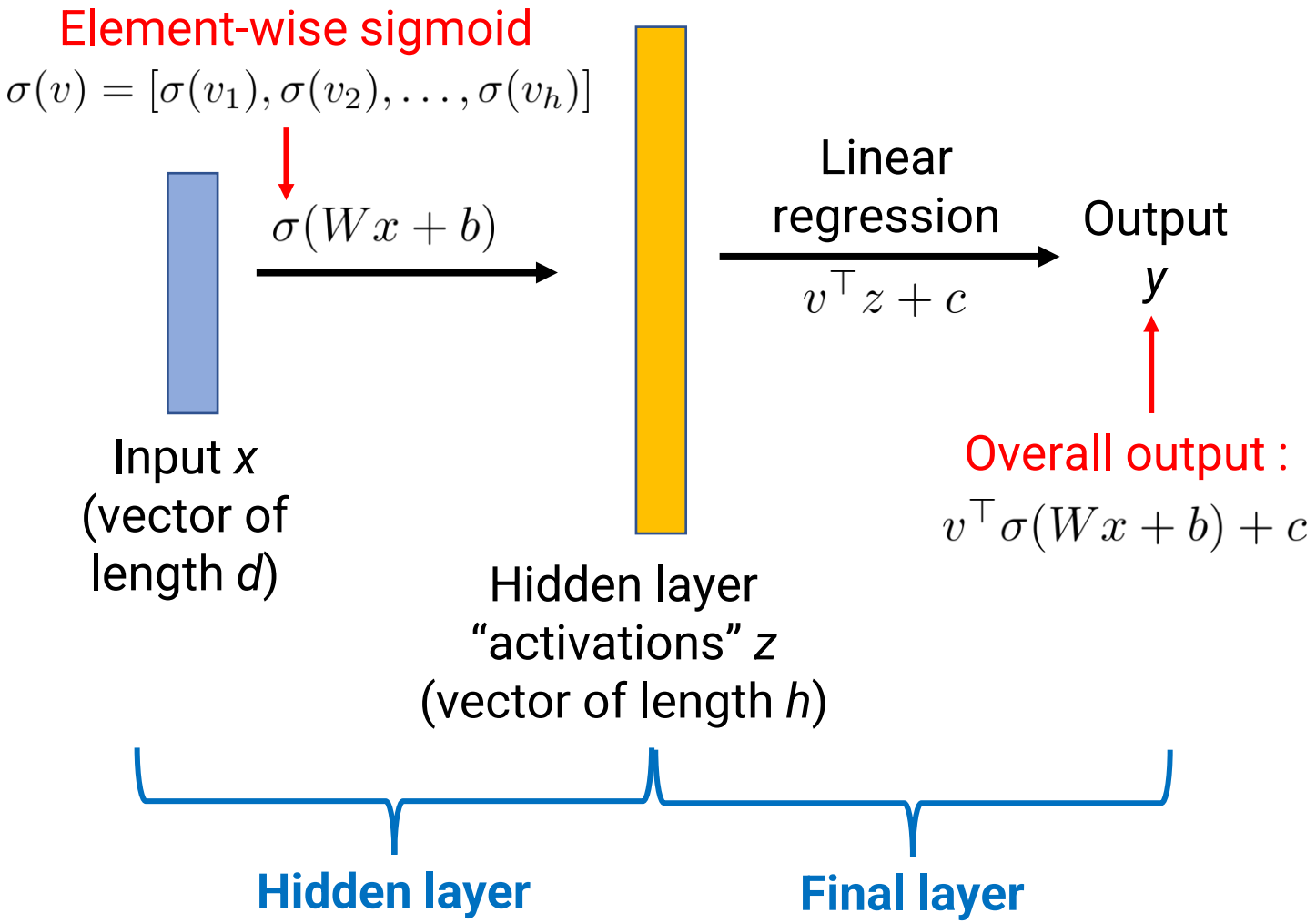
Neural Networks III: Optimization, Regularization

Robin Jia

USC CSCI 467, Spring 2024

February 15, 2024

Review: Neural Networks (2-layer MLP)



- Hidden layer = A bunch of logistic regression classifiers
  - Parameters: $\boldsymbol{w}_j$ and $\boldsymbol{b}_j$ for each classifier, for each $j=1, \ldots, h$
  - Equivalently: matrix $\boldsymbol{W}$ (h x d) and vector $\boldsymbol{b}$ (length h)
  - h = number of neurons in hidden layer ("hidden nodes")
  - Produces "activations"= learned feature vector
- Final layer = linear model
  - For regression: linear model with weight vector $\boldsymbol{v}$ and bias $\boldsymbol{c}$
- Parameters of model are $\boldsymbol{\theta = (W, b, v, c)}$

Review: Training Neural Networks

Linear Regression

- Model's output is

$$g(x) = w^\top x + b$$

- (Unregularized) loss function is

$$\frac{1}{n}\sum_{i=1}^{n}(g(x^{(i)}) - y^{(i)})^2$$

Regression w/ Neural Networks

- Model's output is

$$g(x) = v^\top \sigma(Wx + b) + c$$

- **Use same loss function**, in terms of g!

$$\frac{1}{n}\sum_{i=1}^{n}(g(x^{(i)}) - y^{(i)})^2$$

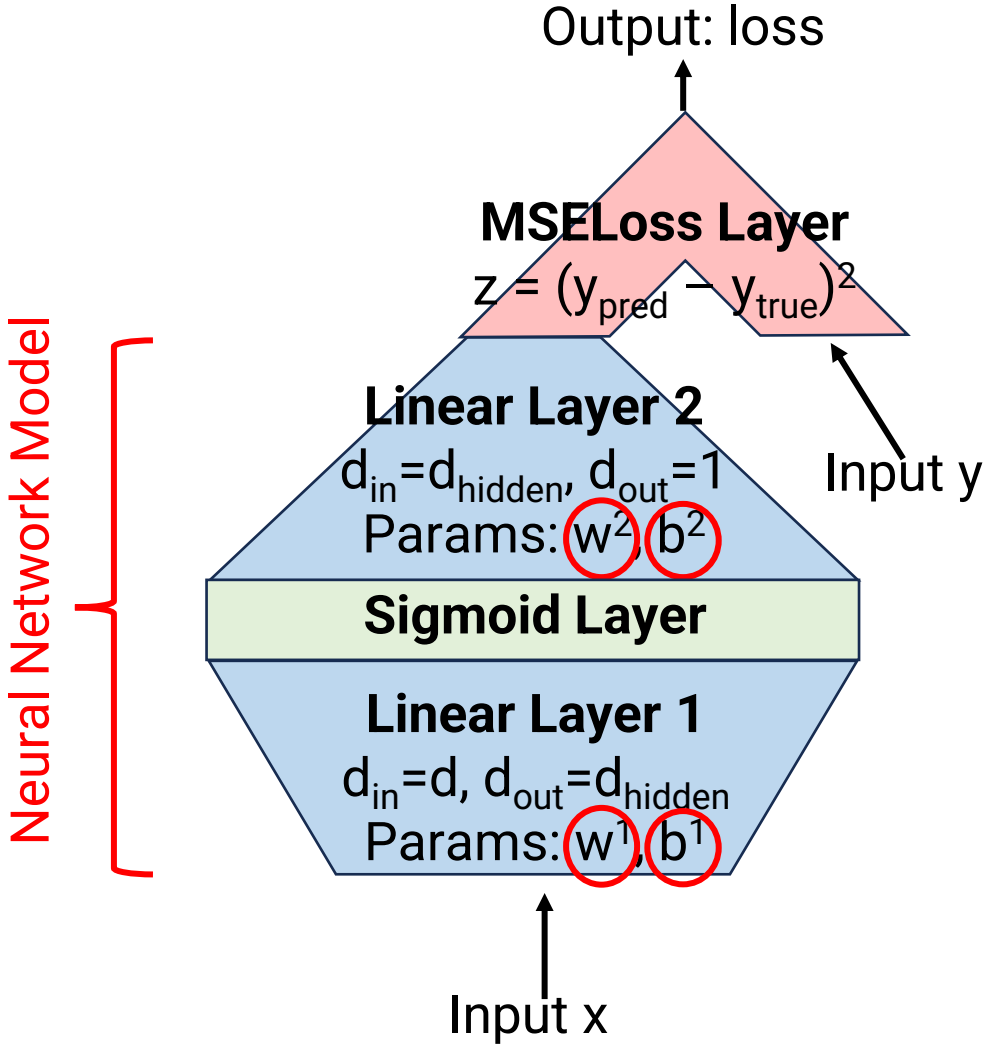
Training objective for both types of models:

$$\frac{1}{n}\sum_{i=1}^{n}\ell\left(y^{(i)}, g(x^{(i)})\right), \text{ where } \ell(y,u) = (y-u)^2$$

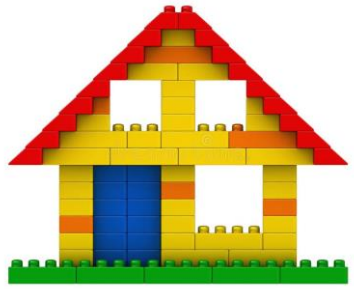
Also applies for logistic regression, softmax regression, etc.

Review: Neural Building Blocks

- Can build many different neural architectures from same set of building blocks
- To train any model, first build the computation graph that computes the loss
- With **backpropagation**, gradient of loss w.r.t. parameters can be computed automatically!
- Update all parameters with gradient descent update rule



Neural Network Hyperparameters (so far)



- Architecture
  - How many “neurons” (i.e., how big is hidden layer)?
  - How many layers?
  - Which activation function (sigmoid, tanh, ReLU)?
- Optimization [coming today]
- Regularization [coming today]

How to choose? Big grid search or random search, optimize for development set

Today's Plan

- Optimization (i.e., Training)
  - Stochastic gradient descent
  - Random initialization
  - Learning rate schedules
  - Momentum & Adam
- Regularization
  - Early stopping
  - Dropout

Stochastic gradient descent

General loss function: $\frac{1}{n}\sum_{i=1}^{n}\ell\left(y^{(i)}, g(x^{(i)})\right)$

Model's output, depends on parameters θ

Gradient Descent

$$\theta \leftarrow \theta - \eta \cdot \underbrace{\frac{1}{n}\sum_{i=1}^{n}\nabla_\theta \ell\left(y^{(i)}, g(x^{(i)})\right)}_{\text{Average of per-example gradients}}$$

- Disadvantage: 1 update is O(n) time
  - What if dataset is very large?
- Idea: Approximate with sample mean

Stochastic Gradient Descent

1. Sample a *batch* B of examples from the training dataset
2. Do the update

$$\theta \leftarrow \theta - \eta \cdot \underbrace{\frac{1}{|B|}\sum_{(x,y)\in B}\nabla_\theta \ell\left(y, g(x)\right)}_{\text{Sample mean within batch}}$$

Stochastic gradient descent

In practice, partition training set into batches:

```
for t = 1, …, T:
```

Each t (i.e., each pass over the dataset) is called one "epoch"

```
    Randomly partition training examples into batches B_1, …, B_k
    for i = 1, …, k:
```

$$\theta \leftarrow \theta - \eta \cdot \frac{1}{|B_i|} \sum_{(x,y) \in B_i} \nabla_\theta \ell\left(y, g(x)\right)$$

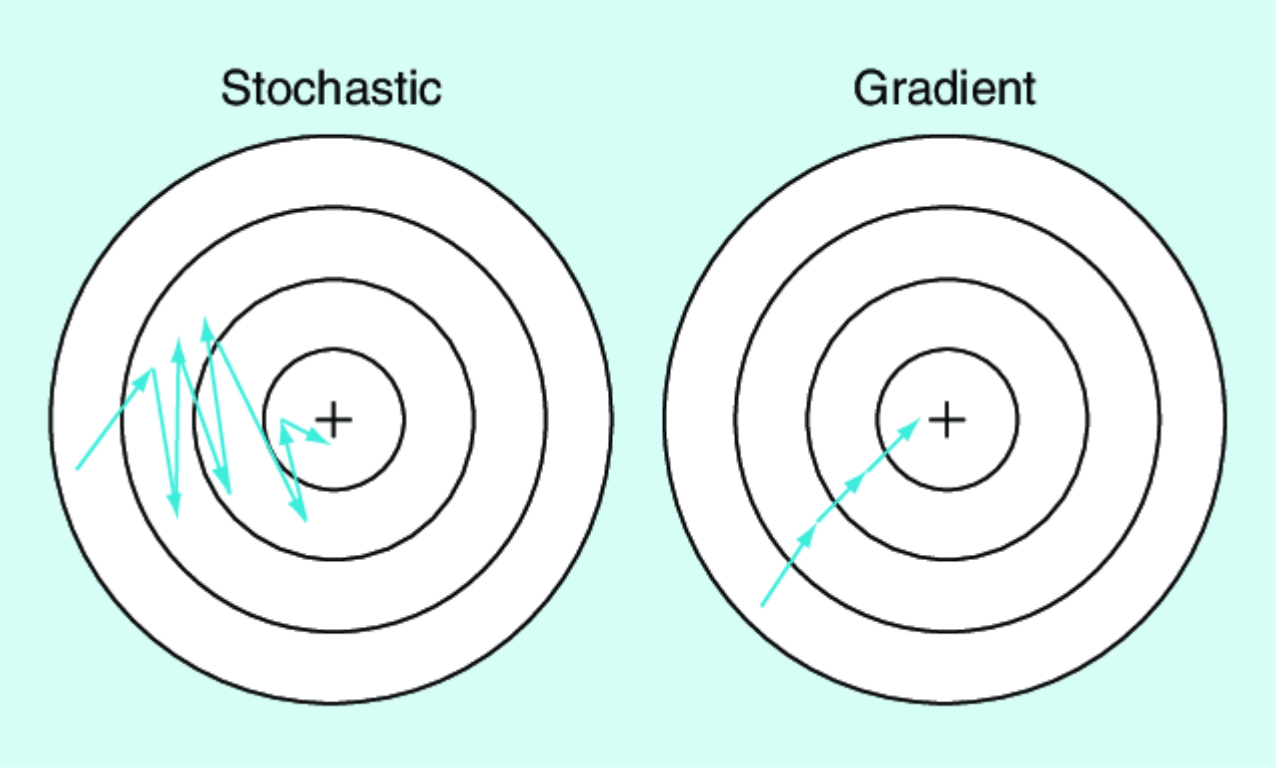
Update based on sample mean within current batch

How many batches? Desired "batch size" (# examples/batch) is another hyperparameter to tune

- Larger batch size = more accurate gradient, but slower
- Smaller batch size = faster, but may wander in suboptimal directions

- SGD is most useful when training data is large, computing full gradient is expensive
  - Can be used with any model

Stochastic gradient descent



- SGD: Each parameter update is only "approximately" going towards the minimum
- But given enough time, you'll end up in (almost) the same place
  - Plus each step is much faster!

Training Objective Comparison

Linear Regression

- Model's output is

$$g(x) = w^\top x + b$$

- (Unregularized) loss function is

$$\frac{1}{n}\sum_{i=1}^{n}(g(x^{(i)}) - y^{(i)})^2$$

Convex loss function when g(x) is linear

Regression w/ Neural Networks

- Model's output is

$$g(x) = v^\top \sigma(Wx + b) + c$$

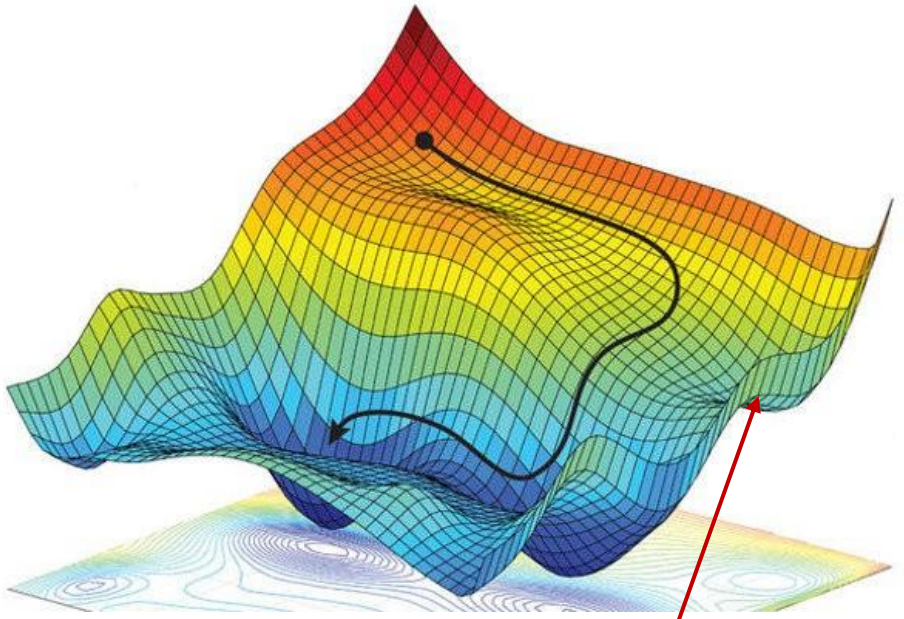
- **Use same loss function**, in terms of g!

$$\frac{1}{n}\sum_{i=1}^{n}(g(x^{(i)}) - y^{(i)})^2$$

Non-convex loss function when g(x) is neural network

Non-convexity During Training

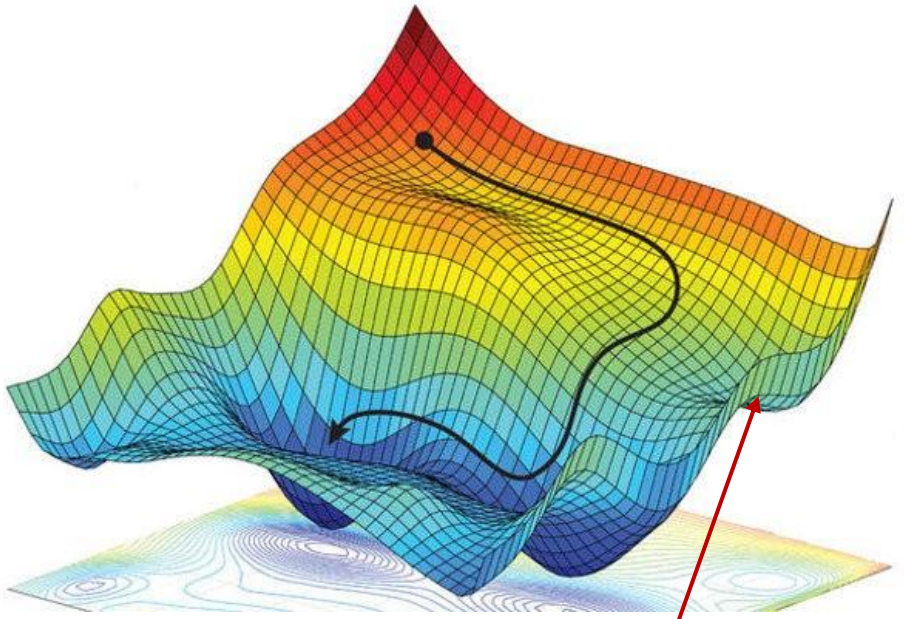
- Linear models were convex
  - All local optima are global optima
  - All reasonable optimization methods will find a global optimum
- Neural Networks are non-convex
  - Very hard to find global optimum
  - Different optimization techniques will converge to **different local optima**, some of which are much better than others
  - **Choice of optimization method really matters!**



Local minimum
Gradient descent can get stuck here!

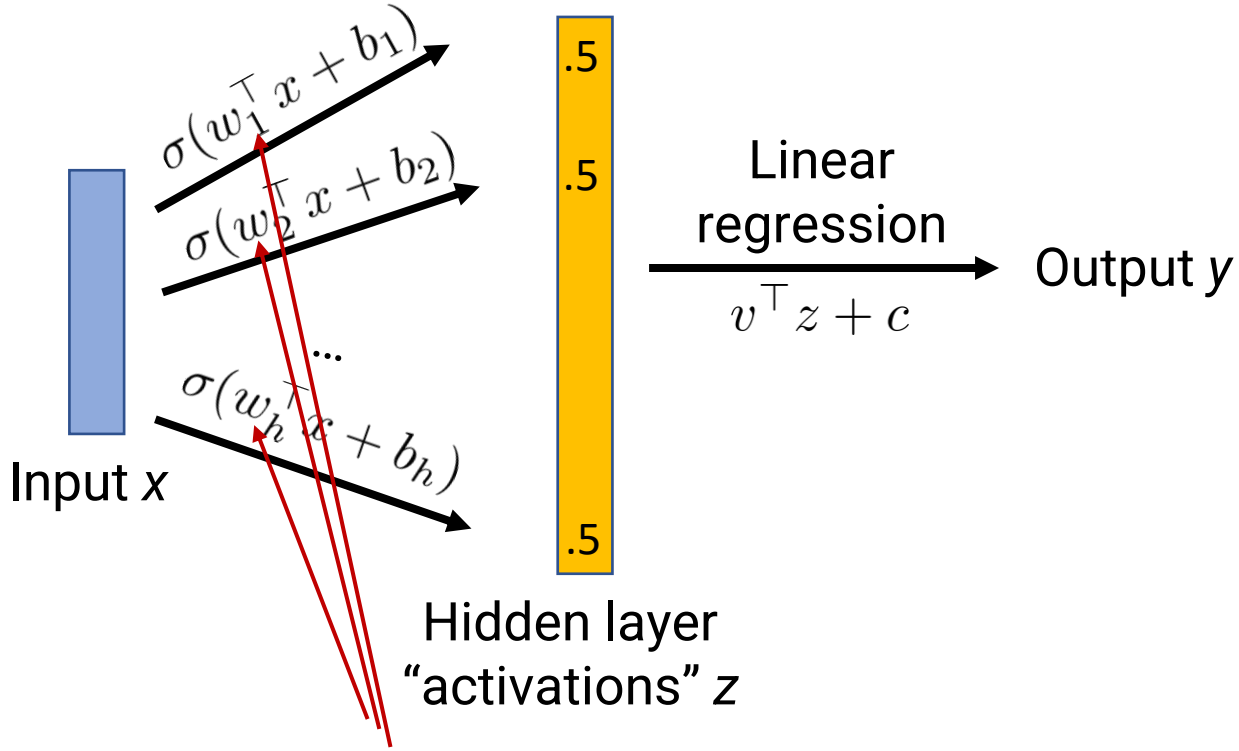
Initialization

- For convex problems (e.g. logistic regression), initialization doesn't matter much for final result
  - We just initialize parameters to all 0's
- For neural networks, initialization matters a lot!
  - Optimization problem is non-convex
  - Where you start determines what parameters you learn



Local minimum
If you initialize here, you get stuck here!

The problem with all-0's initialization



If every w_j starts as 0 vector,
gradient update to each w_j will be the same

- What if we initialize with all 0's?
- Problem: Symmetry
  - All hidden units start out the same, so gradients will be the same for each
  - Thus, all hidden units will stay the same!
- **We must initialize in a way that breaks the symmetry**

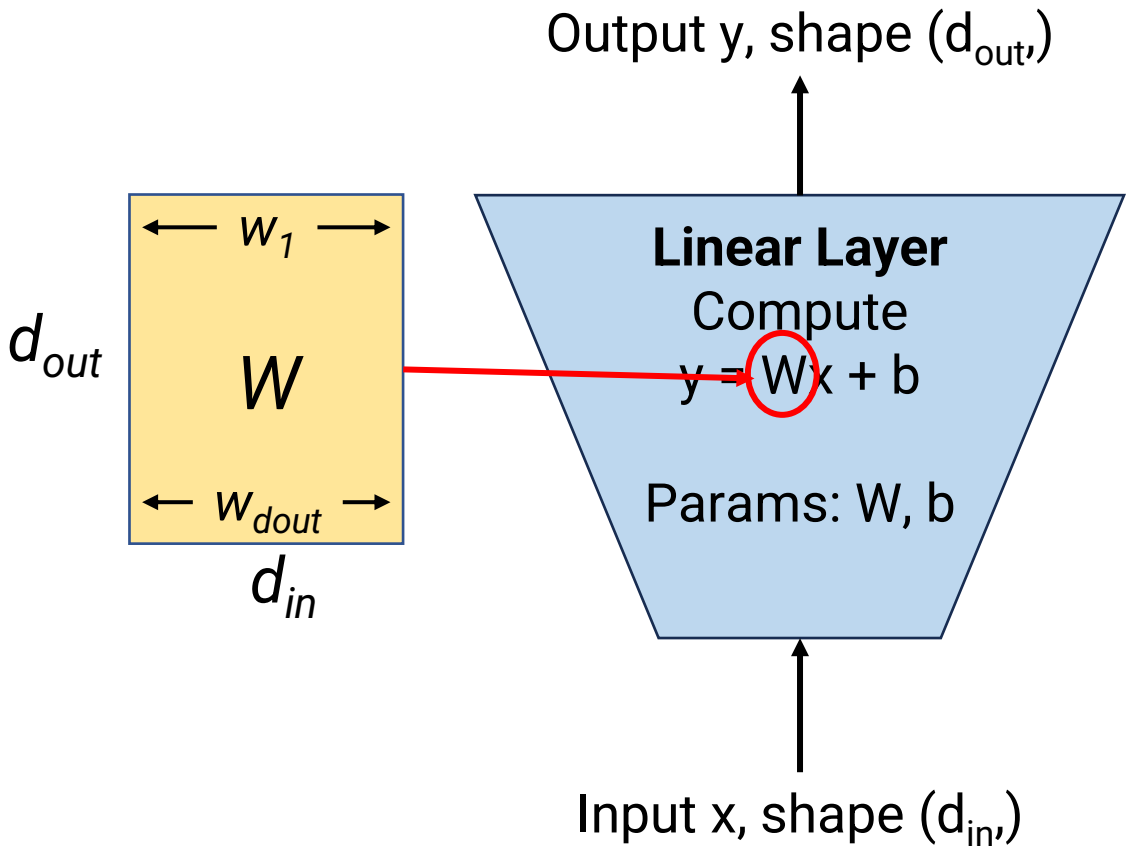
How to initialize neural networks?

- Solution: Initialize every parameter to be a small random number
- How small? Depends on "fan-in" d_{in} (# input features) and "fan-out" d_{out} (# output features)
  - Suppose input x_j's have variance γ^2 and w_{ij}'s have variance σ^2
  - For each row w_i of W:

$$\text{Variance}[w_i^\top x] = d_{in}\sigma^2\gamma^2.$$

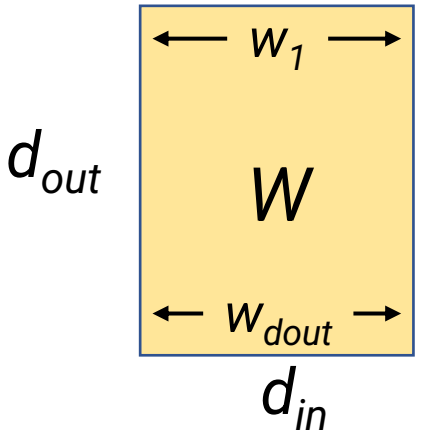
(Sum of d_{in} things, each with var. σ^2 γ^2)

  - This gets bigger as d_{in} gets bigger
  - So: choose σ^2 proportional to $1/d_{in}$



How to initialize neural networks

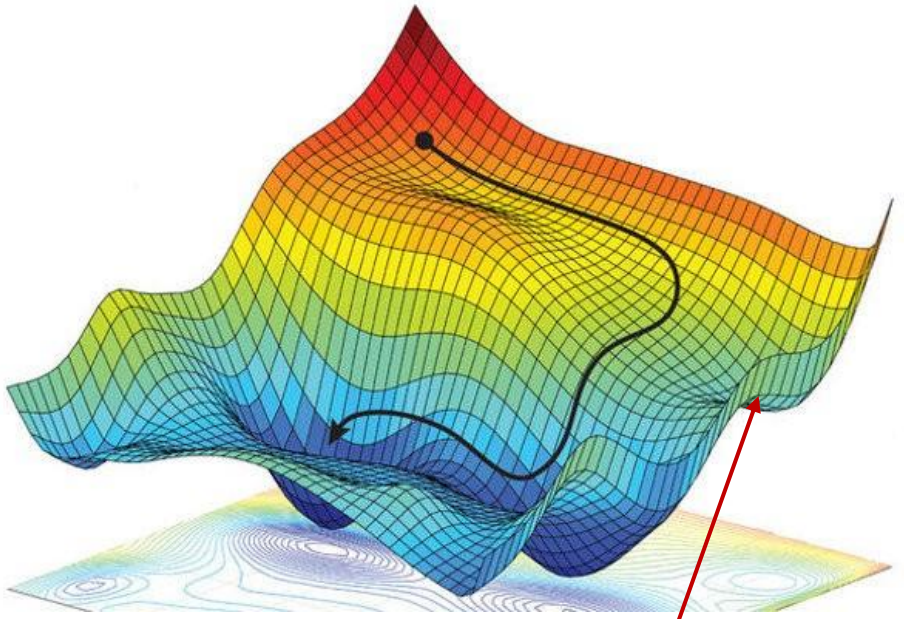
- As usual, you have many options…
  - He initialization: $\text{Normal}\left(0, \frac{2}{d_{in}}\right)$ (mean 0, variance $2/d_{in}$)
  - Xavier initialization: $\text{Normal}\left(0, \frac{2}{d_{in} + d_{out}}\right)$ Also divides by d_{out} (But usually d_{in} and d_{out} are similar size)
  - Pytorch default: $\text{Uniform}\left(-\frac{1}{\sqrt{d_{in}}}, \frac{1}{\sqrt{d_{in}}}\right)$ Uniform avoids large outliers Note: Variance is proportional to $1/d_{in}$



- Usually you don't tune these as hyperparameters, just use defaults

Importance of Learning Rate

- For convex problems (e.g. logistic regression), ***learning rate*** doesn't change final result very much
  - All reasonable values converge to the same final answer
- For neural networks, learning rate matters a lot!

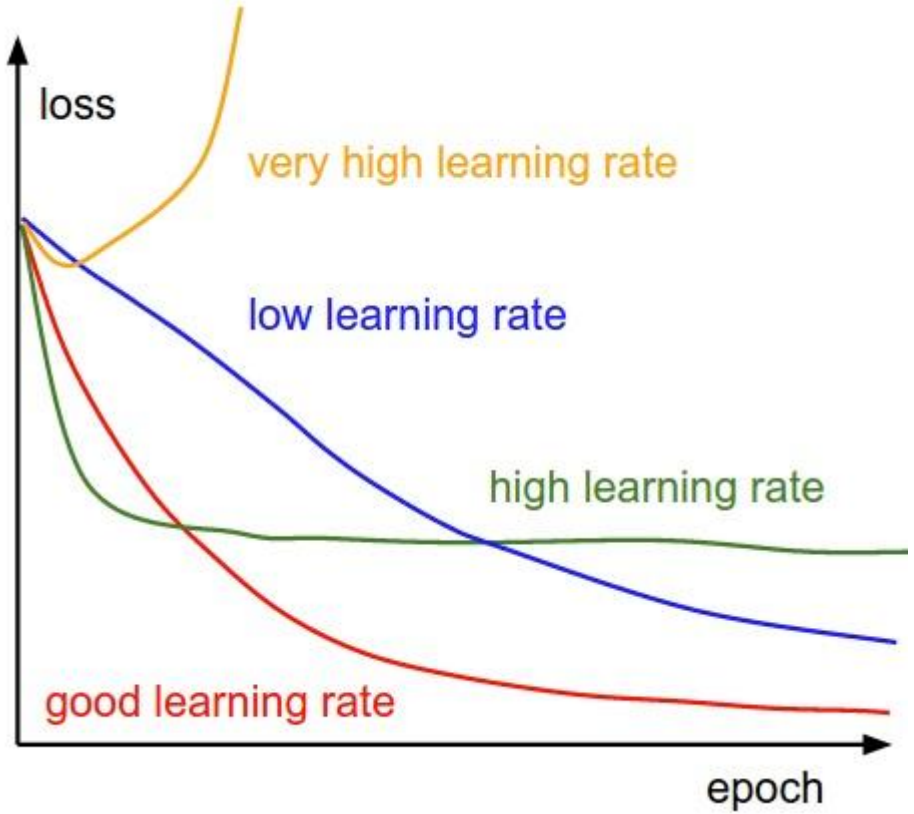


Local minimum
Get stuck here if learning rate is too small

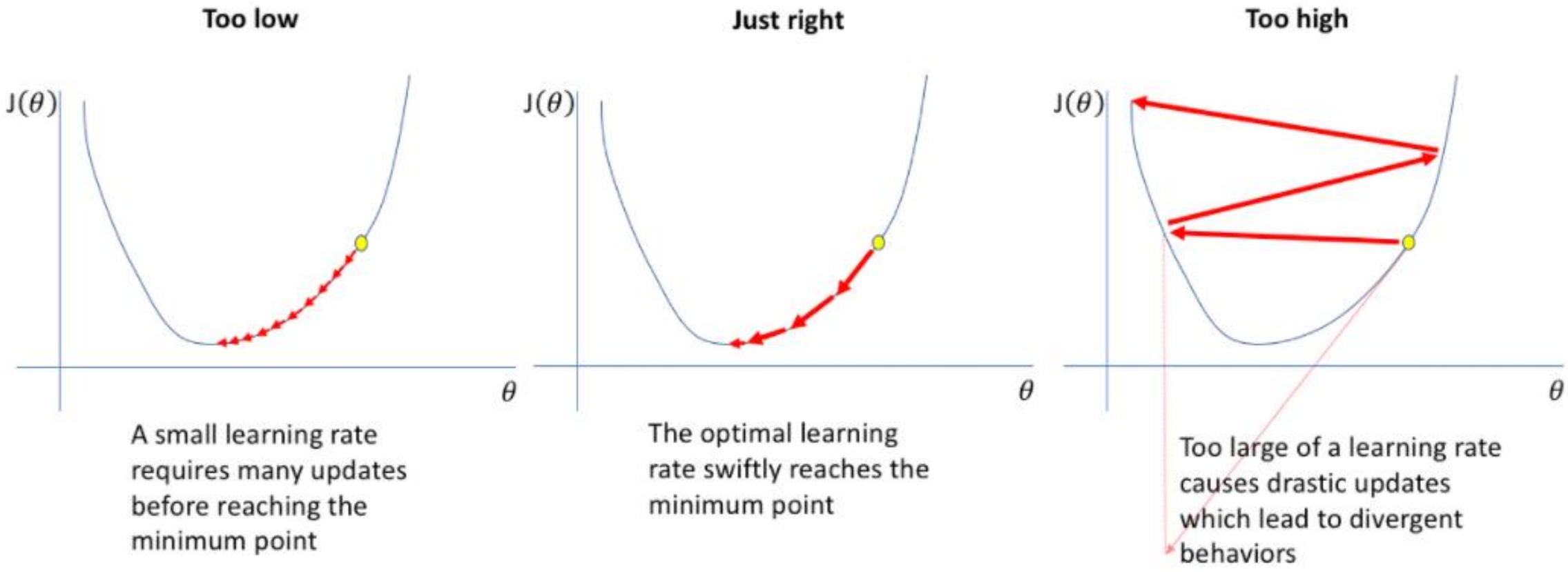
Importance of Learning Rate

$$\theta \leftarrow \theta - \eta \cdot \frac{1}{|B|} \sum_{(x,y) \in B} \nabla_\theta \ell\left(y, g(x)\right)$$

- Too small: Can't take big enough steps, don't converge fast enough, can get stuck in "flat" regions
- Too large: Steps are too large, too erratic and doesn't converge
- Need to carefully tune learning rate

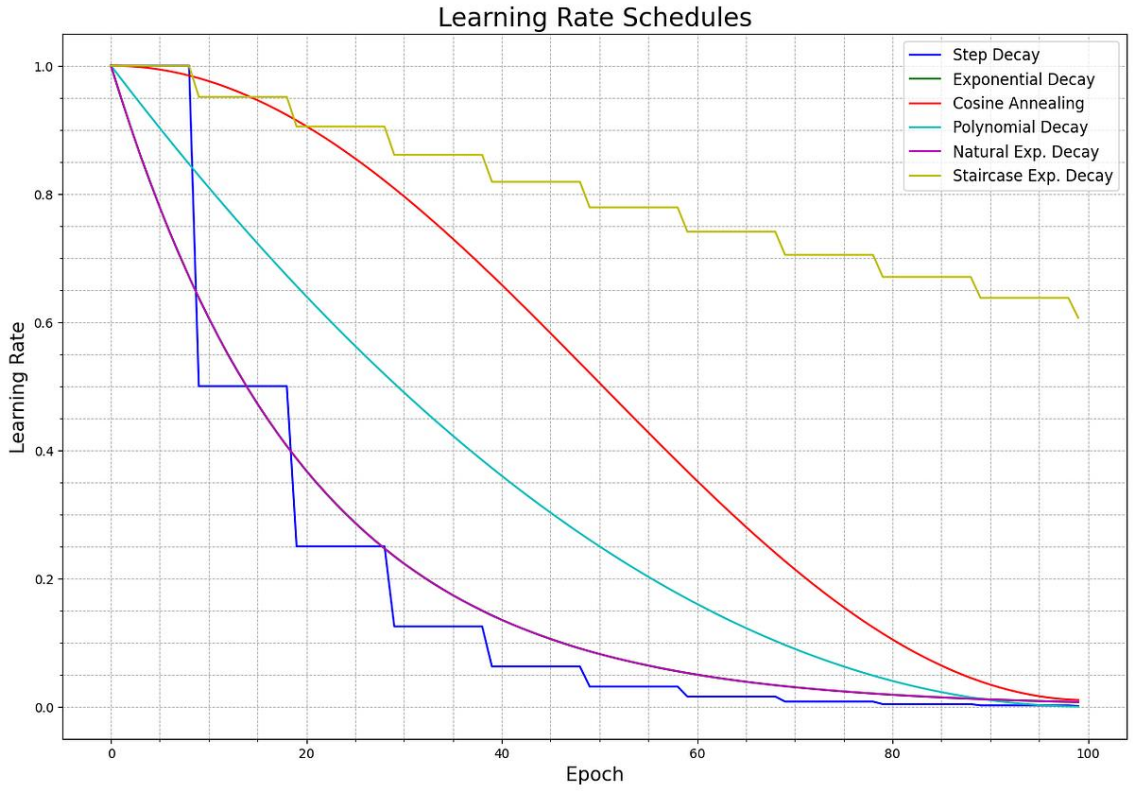


Importance of Learning Rate



Learning Rate Schedules

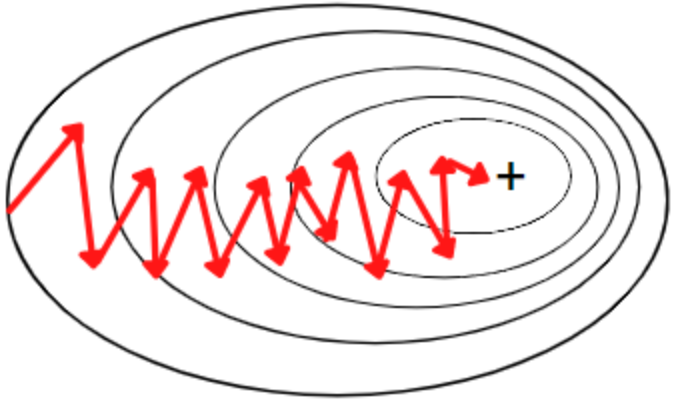
- Early on: We're far from the optimum, want to take large steps
- Later on: We're close to the optimum, take small steps so we don't "overshoot"
- Solution: Start with large learning rate, make it smaller over time ("decay")



Challenges for SGD

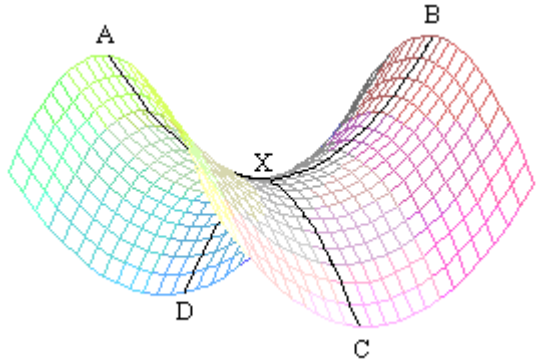
Problem #1: Ill-Conditioned loss

- Surface is very curved/steep in some directions, but shallow in others
- High learning rate: Zig-zag along steep direction
- Low learning rate: Move slowly along shallow direction



Problem #2: Saddle Points

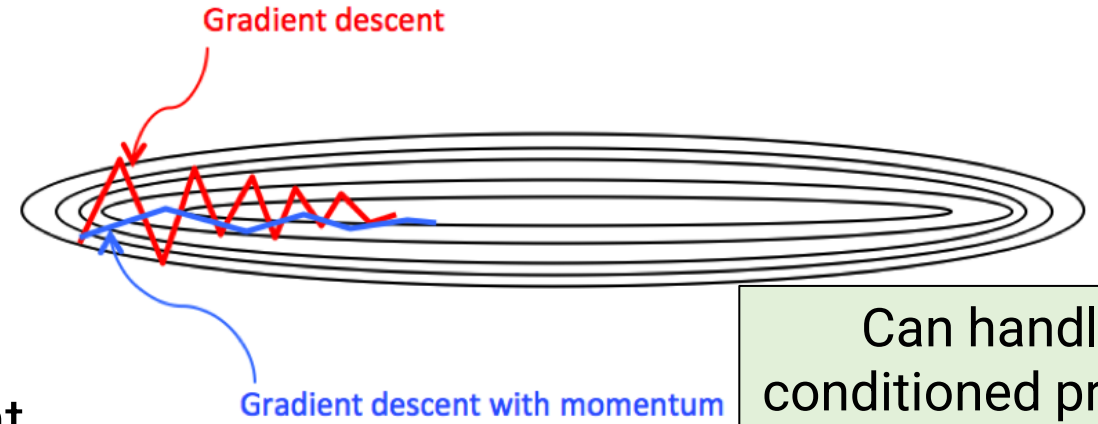
- Saddle Point = Area that is locally flat, but neither minimum nor maximum
- SGD can get stuck here because gradient is close to 0 -> take small steps



Idea #1: Momentum

SGD

```
w = w - lr * grad
```



Can handle ill-conditioned problems! Velocities cancel out in vertical direction, but build up in horizontal direction

SGD + Momentum

Momentum builds in direction of gradient

```
v = beta1 * v + (1-beta1) * grad
```

"velocity" or "momentum"

Keep momentum, with some "friction" beta1

Apply a "force" in direction of gradient

```
w = w - lr * v
```

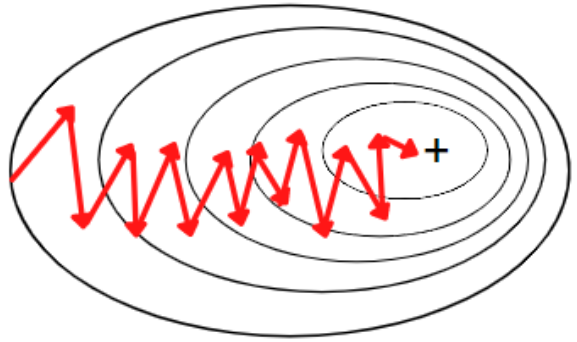
Parameters w are "position", they move in the direction of momentum

Idea #2: Per-Parameter Learning Rates

SGD

```
w = w - lr * grad
```

RMSProp: Normalize gradient for each parameter



```
s = beta2 * s + (1-beta2) * grad**2
```

Tracks how big grad usually is for each parameter

Weighted average of elementwise squares

Elementwise square
Measures size of grad for each parameter

```
w = w - lr * grad / (sqrt(s) + eps)
```

Elementwise sqrt

Avoid divide by 0

For each parameter, divide gradient by the size of its gradient on average
Result: parameters with large average gradient (steeper directions) get smaller effective learning rate

Adam = Momentum + Per-Parameter LR

Momentum: Build momentum in direction of gradient

```
v = beta1 * v + (1 - beta1) * grad  # Add momentum
w = w - lr * v                      # Move in direction of momeutm
```

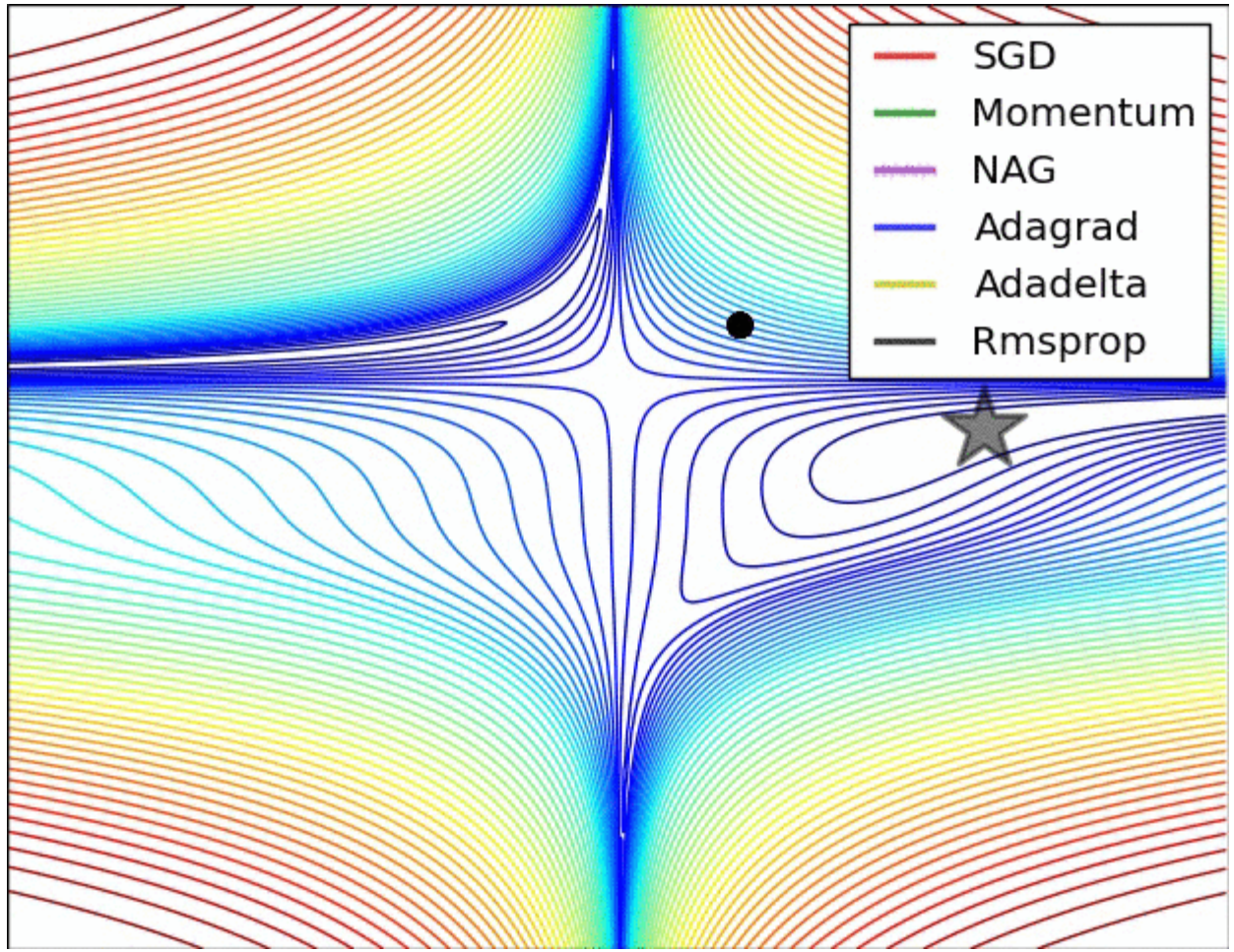
RMSProp: Adapt learning rate for each parameter separately

```
s = beta2 * s + (1-beta2) * grad**2   # Per-parameter scale
w = w - lr * grad / (sqrt(s) + eps)   # Divide by scale
```

Adam: Combine Momentum and RMSProp, commonly used!

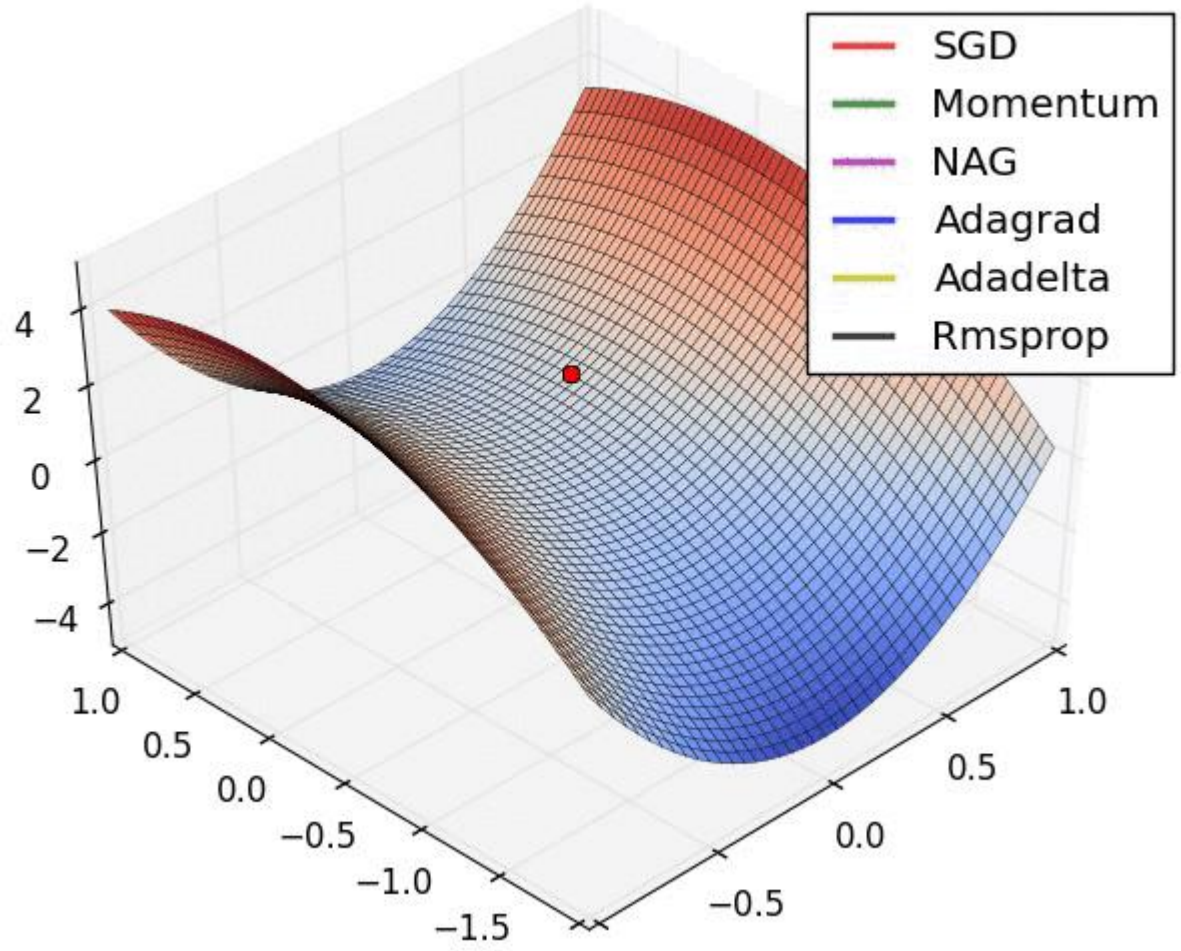
```
v = beta1 * v + (1 - beta1) * grad    # Momentum
s = beta2 * s + (1-beta2) * grad**2   # RMSProp
w = w - lr * v / (sqrt(s) + eps)      # Mix both update rules
```

Comparison of SGD Variants



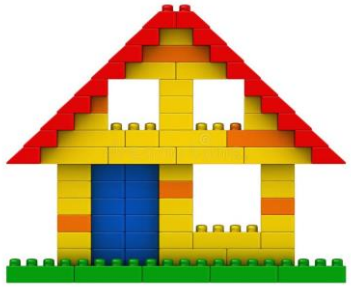
- SGD: Converges slowly
- Momentum: Moves much faster, although can overshoot
- Adagrad, RMSProp: Converge quickly here

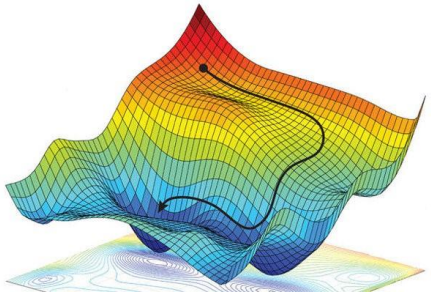
Comparison of SGD Variants



- One problem for non-convex optimization: **Saddle points**
  - Function is locally flat but is neither local minimum nor local maximum
  - Need to “escape” these to find a minimum
- SGD gets stuck, other methods can escape

Neural Network Hyperparameters





- Architecture
  - How many “neurons” (i.e., how big is hidden layer)?
  - How many layers?
  - Which activation function (sigmoid, tanh, ReLU)?
- Optimization
  - Learning rate (initial & decay)
  - Batch size
  - Optimizer (momentum? Adam?)
- Regularization [Next!]

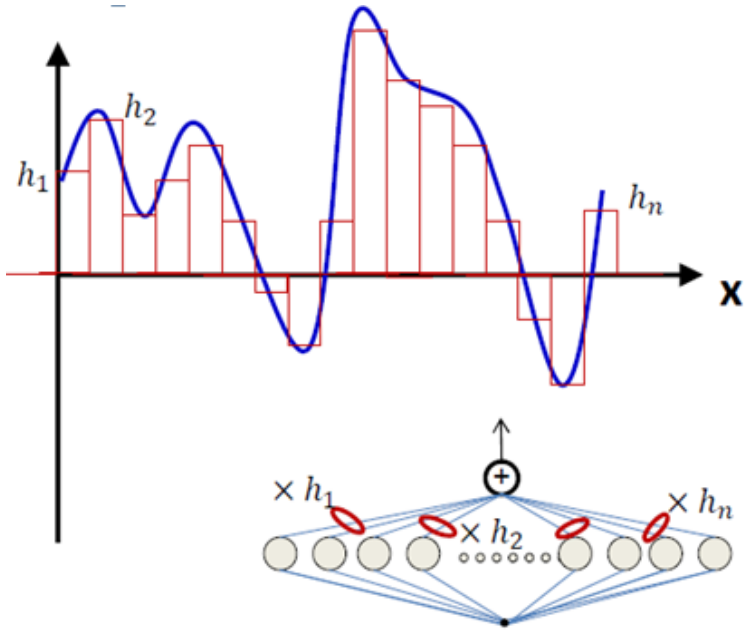
Announcements

- HW2 released, due Thursday, February 29
- Midterm exam Thursday, March 7
  - In-class, 80 minutes in SLH 100
  - Allowed one double-sided 8.5x11 sheet of notes
- Section Friday: Pytorch

Today's Plan

- Optimization (i.e., Training)
  - Stochastic gradient descent
  - Random initialization
  - Learning rate schedules
  - Momentum & Adam
- Regularization
  - Early stopping
  - Dropout

Regularization & Neural Networks



- Recall: Neural networks are universal approximators
- This means they are prone to overfitting!
  - Low bias, high variance
- How to avoid overfitting too badly?

Weight decay (AKA L2 Regularization)

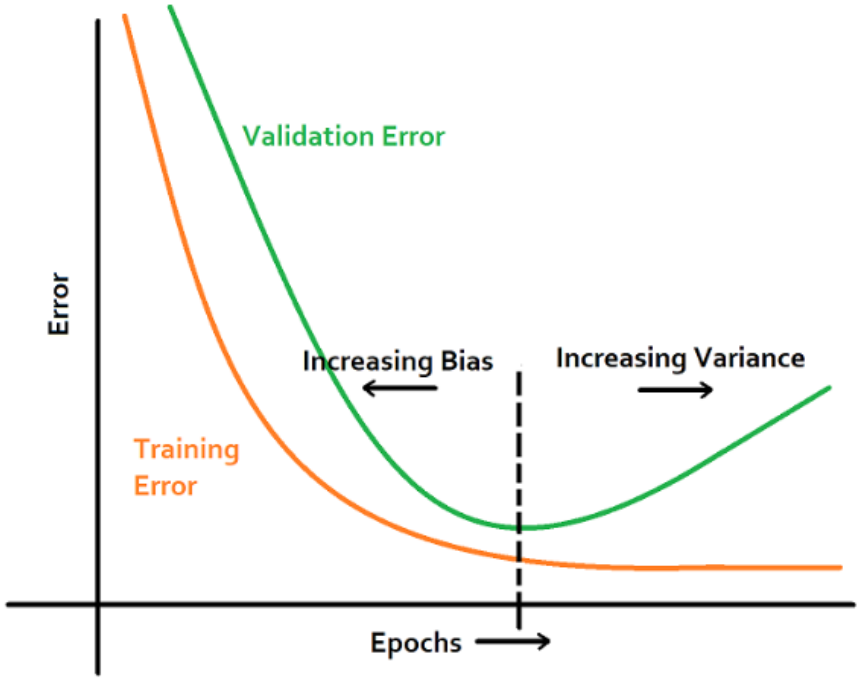
- L2 regularization is a valid strategy!
  - Add an L2 penalty for every parameter in the model
- Often called “weight decay” when used with neural networks
  - Because every gradient step, you add the update

$$\theta \leftarrow \theta - \eta \cdot \lambda \cdot \theta$$

Weights literally “decay” by factor of (1 – ηλ)

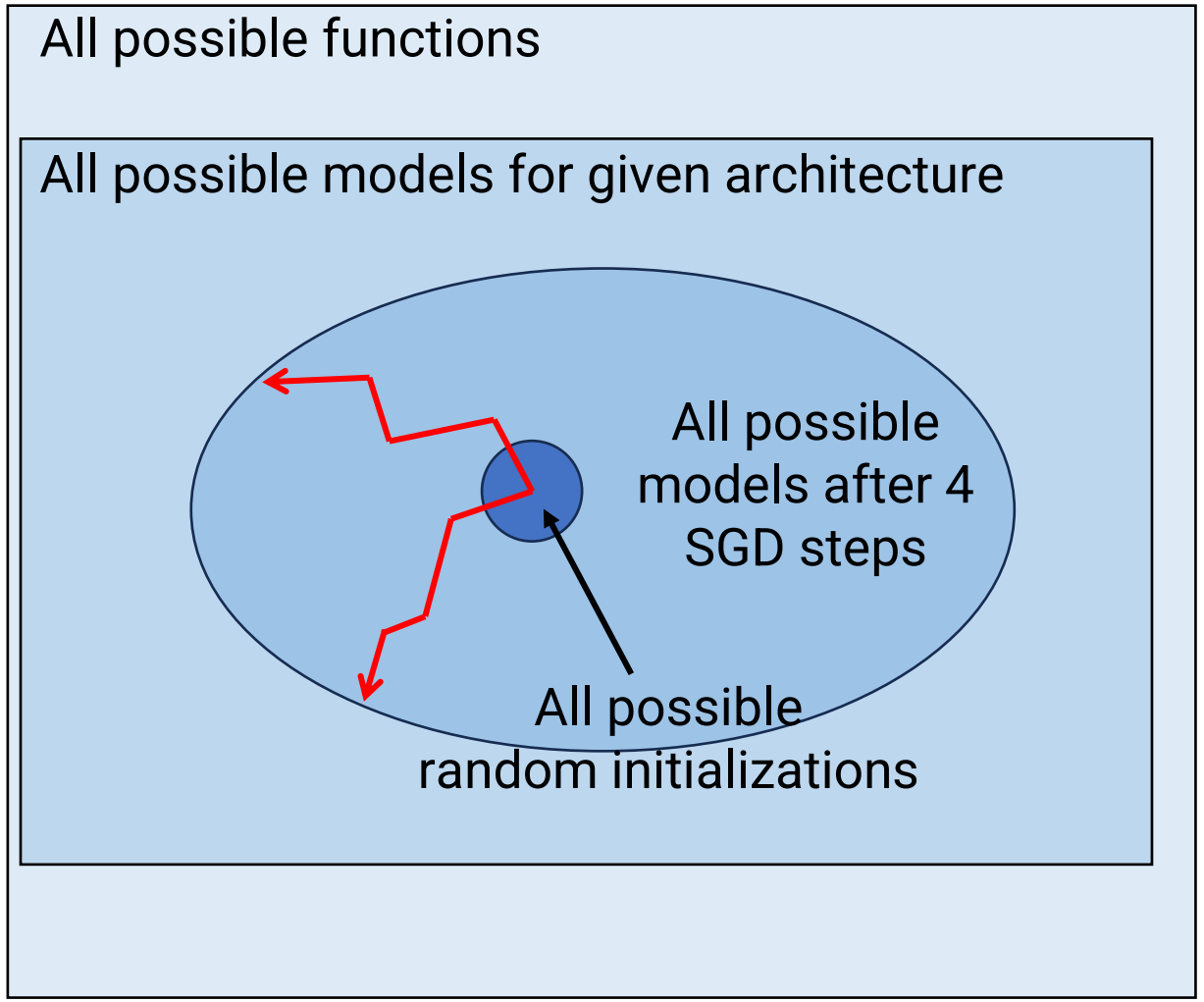
Early stopping

- Prevent overfitting by stopping training before you overfit too much
  - Every so often during training, save “checkpoint” of model parameters and evaluate development loss
  - Remember which checkpoint had best development loss
  - If development loss keeps going up, stop training
- Can be used for any model, but especially common for neural networks
  - For linear models, also common to train all the way to convergence

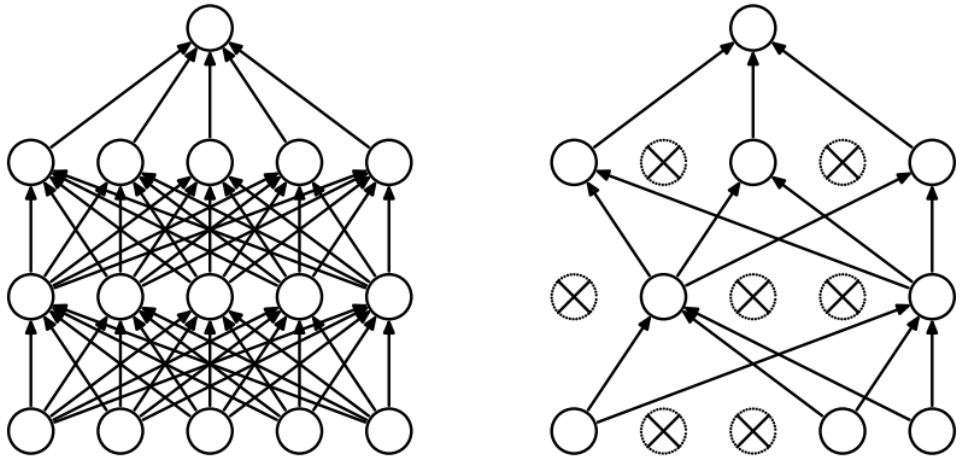


Why Does Early Stopping Apply Regularization?

- Set of “Models that can be learned after T steps” is smaller than all possible models
  - Parameters start as small random numbers
  - Early stopping prevents parameters from changing too much from this initialization
- Thus, model family is restricted!
  - Similar to L2 regularization



Dropout

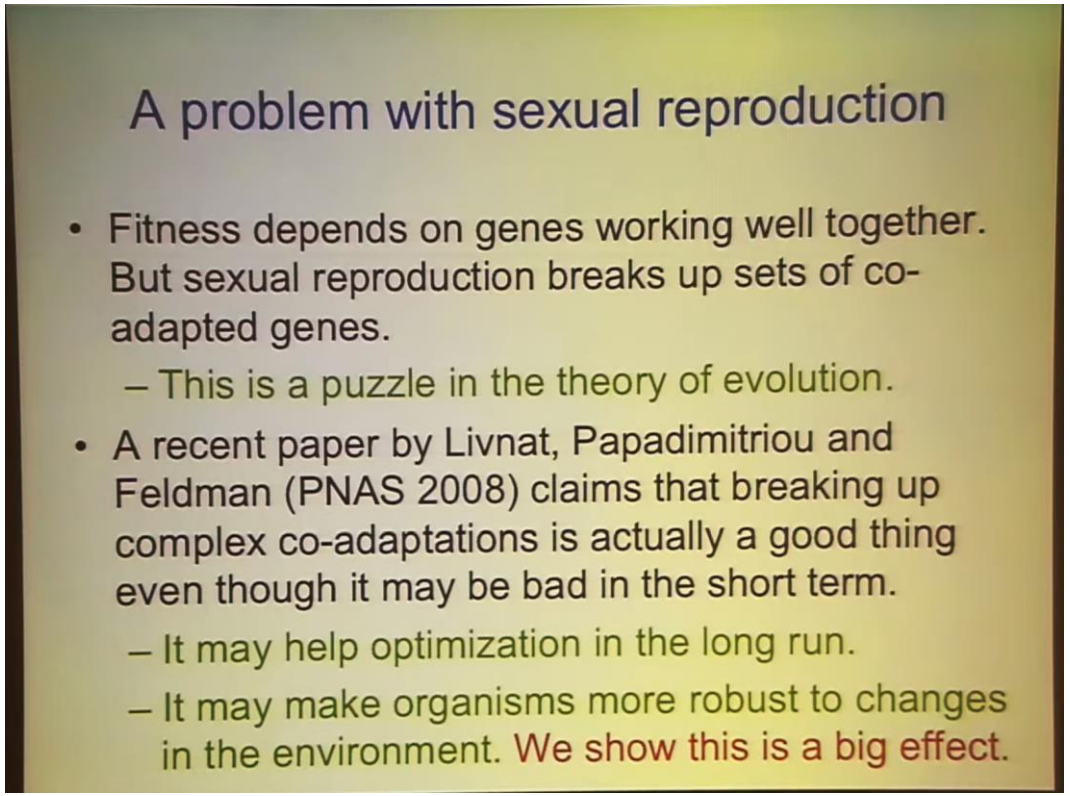


(a) Standard Neural Net

(b) After applying dropout.

- During Training: Randomly “drop out” some neurons by setting their value to 0
  - Drop each out with probability p
  - To compensate, scale the other neurons up by 1/p
- During testing, don’t do dropout

Dropout prevents "Co-adapted" features



Geoffrey Hinton
(Turing Award winner,
One of the "Godfathers" of
deep learning)

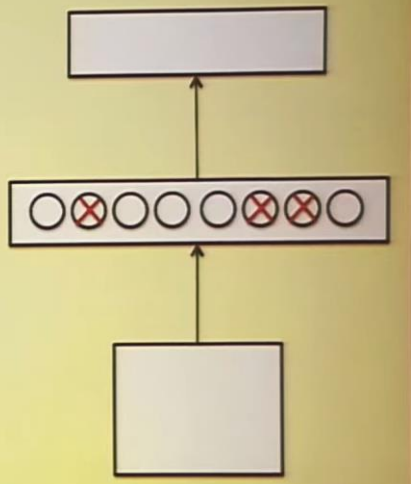
- Without dropout, two neurons could compute features that are only useful in tandem
  - E.g., A and B individually are bad predictors, but A+B is useful predictor
  - A and B are "co-adapted"
- Dropout disincentivizes this—each neuron individually should be useful

https://www.youtube.com/watch?v=05MpycrocRI

Dropout as an Ensemble

Dropout: An efficient way to average many large neural nets.

- Consider a neural net with one hidden layer.
- Each time we present a training example, we randomly omit each hidden unit with probability 0.5.
- So we are randomly sampling from 2^H different architectures.
  - All architectures share weights.



But what do we do at test time?

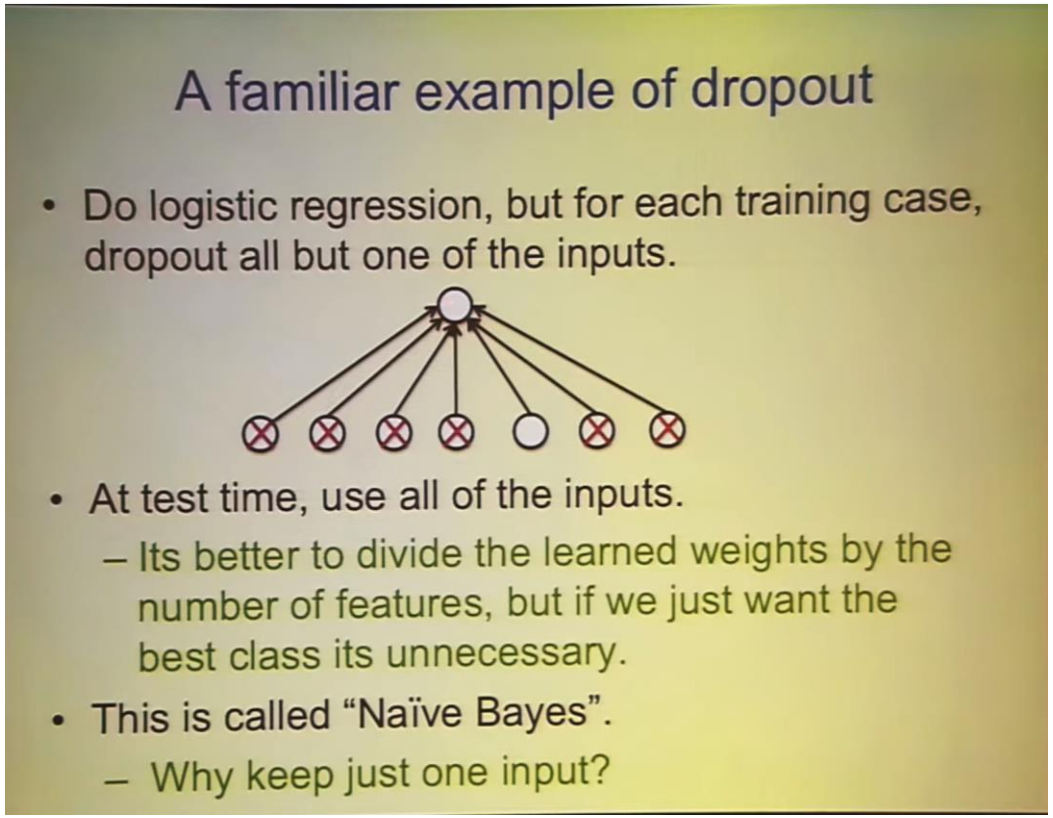
- We could sample many different architectures and take the geometric mean of their output distributions.
- It better to use all of the hidden units, but to halve their outgoing weights.
  - This exactly computes the geometric mean of the predictions of all 2^H models.

During training, each neuron is on 1/2 the time and its value is 2x, so **on average** its output is the same as during testing

- "Ensemble" = average of multiple models' predictions
- Usually better than using a single model
- Dropout ensembles over all 2^h different ways to dropout the h hidden neurons

https://www.youtube.com/watch?v=05MpycrocRI

Dropout as a Generalization of Naïve Bayes



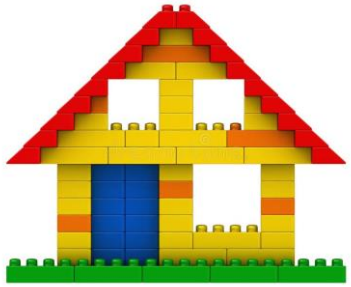
- What about dropout at the input layer?
  - If we dropout all but one feature x_j, we are just estimating $P(y|x_j)$, which is closely related to $P(x_j|y)$:

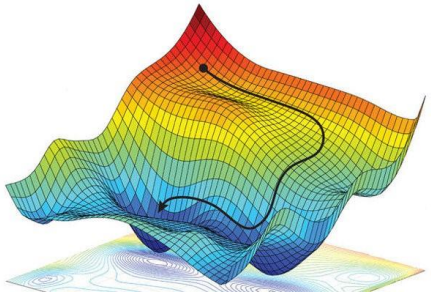
$$P(x_j \mid y) = \frac{P(x_j)P(y \mid x_j)}{P(y)}$$

  - At test time, we use all features: same as multiplying all $P(x_j|y)$'s
  - This is Naïve Bayes!
- Thus, Dropout at the input layer *generalizes* Naïve Bayes

https://www.youtube.com/watch?v=05MpycrocRI

Neural Network Hyperparameters





- Architecture
  - How many “neurons” (i.e., how big is hidden layer)?
  - How many layers?
  - Which activation function (sigmoid, tanh, ReLU)?
- Optimization
  - Learning rate (initial & decay)
  - Batch size
  - Optimizer (momentum? Adam?)
- Regularization
  - Weight decay
  - Early stopping
  - Dropout

Conclusion

- Optimization: Neural networks are non-convex, so choice of optimization strategy really matters!
- Regularization: Neural networks are very good at overfitting, need to counterbalance this
- Lots of hyperparameters!