Lecture 10: Tools for your deep learning toolbox – Part III

Machine Learning and Imaging

BME 548L
Roarke Horstmeyer

Thanks to Kevin Zhou for helping with material preparation

Class project details

- Full details are here: https://deepimaging.github.io/proj-info/
- Can work alone or in a group (up to 4 people), required effort will scale with # of people
- Select a “base” dataset (online, or from a list I’ll make)
- Simulate parameters of a physical (imaging) system with base dataset
- Train deep neural net with simulated dataset
- Report results

What you’ll need to submit:

1) The project’s source code

2) A short research-style paper (3 pages minimum, 5 pages maximum) that includes an introduction, results, a discussion section, references and at least 2 figures

3) A completed web template containing the main results from the research paper

4) A 7-10 minute presentation that each student will deliver to the class

Project requirements

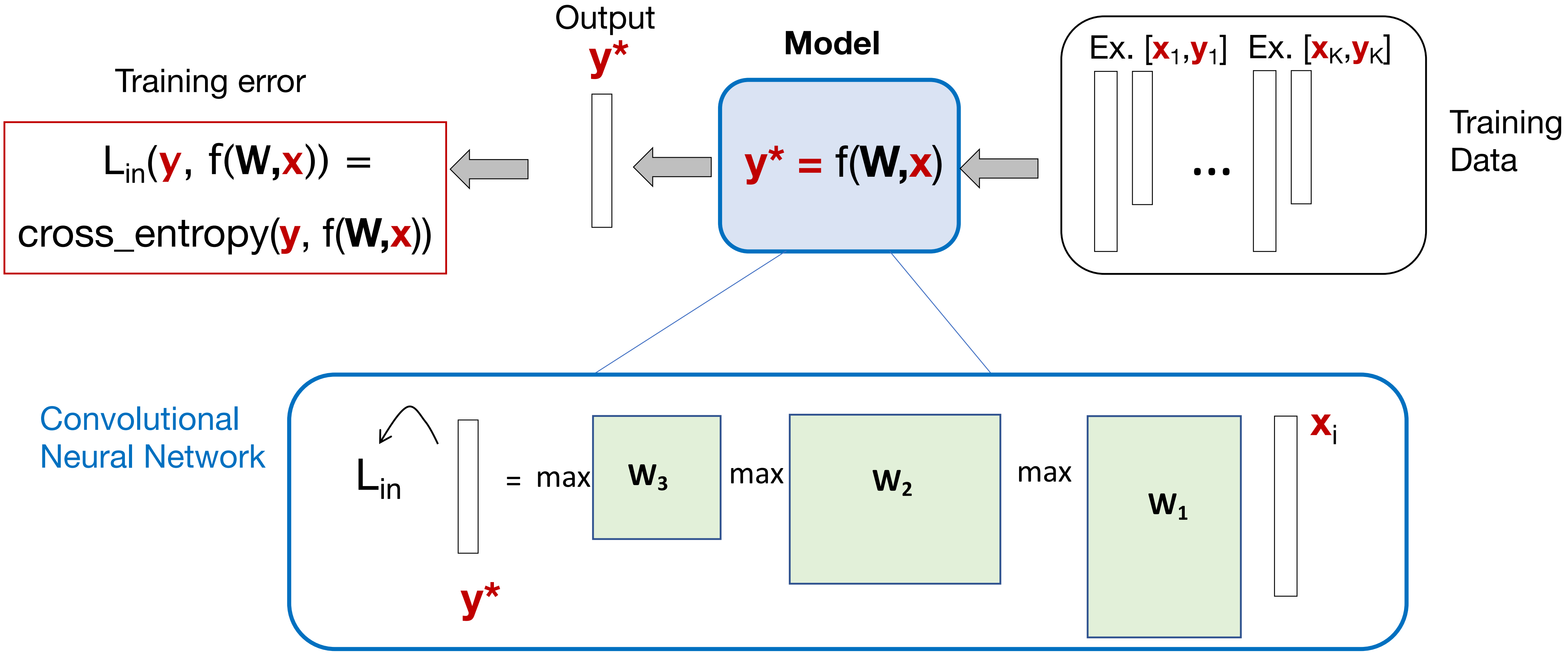
- Select a “base” dataset (from online, lab, or colleagues)
- Examine how physical (imaging) system impacts base dataset
  - What are key parameters that impact data quality?
  - What are key parameters that impact overall system performance?
  - What parameters can be optimized? How might you optimize them?
    - Noise, resolution, speed, size, weight, power, data, safety, specimen type, etc.
- Train deep neural while jointly exploring or optimizing key parameters
- Report results in context of current/future use of imaging system

Class project – what are the first steps?

1. Think about it!
2. Discuss with your friends/others in the class (feel free to use Slack!) to form group
3. Look at previous projects: https://deepimaging.github.io/proj-past/
4. Schedule a short 15 meeting with myself or TA's
   - **Meetings will occur the week after spring break, will send out details soon**
5. Start to write-up a proposal
   - General aim: 1 paragraph, specifying physical layer or hardware analysis component
   - Discussion: (a) data source(s), (b) expected simulations, (c) expected CNN, (d) quantitative analysis of physical layer/physical component (comparison, plot, etc).

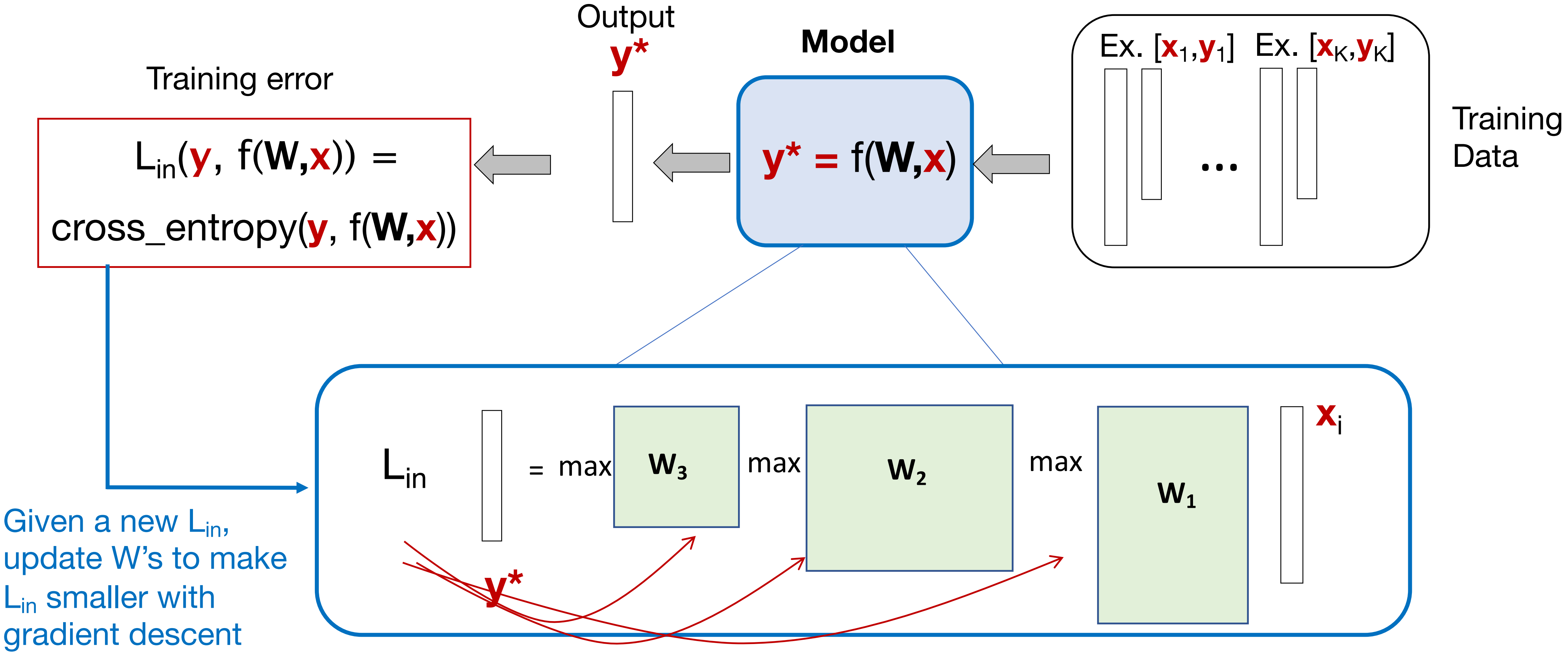
- Project proposal due date: **Wed March 6 at 11:59pm**, revisions after if needed
- Final project will be presented during final exam slot
- (note: due to large class size, this may go a bit over 3 hours, can maybe split in 2 sessions)

Our very basic convolutional neural network



Forward pass: from $\mathbf{x}_i$ and current $\mathbf{W}$'s, find L_{in}

Our very basic convolutional neural network



Next Class: Effectively achieve this with automatic differentiation (backprop)

Important components of a CNN

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CNN Architecture

- CONV size, stride, pad, depth
- ReLU & other nonlinearities
- POOL methods
- # of layers, dimensions per layer
- Fully connected layers

Loss function & optimization

- Type of loss function
- Regularization
- Gradient descent method
- SGD batch and step size

Other specifics: Pre-processing**,** initialization**,** dropout, batch normalization, augmentation

Common loss functions used for CNN optimization

- Cross-entropy loss function
  - Softmax cross-entropy – use with single-entry labels
  - Weighted cross-entropy – use to bias towards true pos./false neg.
  - Sigmoid cross-entropy
  - KL Divergence
- Pseudo-Huber loss function
- L1 loss loss function
- MSE (Euclidean error, L2 loss function)
- Mixtures of the above functions

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Regularization – the basics

λ = regularization strength (hyperparameter)

$$L(W) = \underbrace{\frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i)} + \underbrace{\lambda R(W)}$$

Data loss: Model predictions should match training data

Regularization: Prevent the model from doing *too* well on training data

Simple examples

<u>L2 regularization:</u> $R(W) = \sum_k \sum_l W_{k,l}^2$

L1 regularization: $R(W) = \sum_k \sum_l |W_{k,l}|$

Elastic net (L1 + L2): $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$

Regularization prefers less complex models & help avoids overfitting

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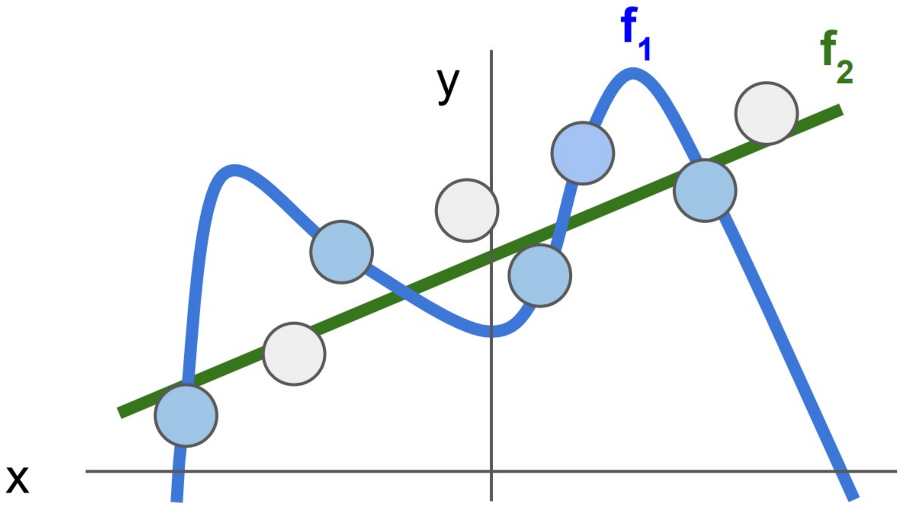
$$x = [1,1,1,1]$$
$$w_1 = [1,0,0,0]$$
$$w_2 = [0.25, 0.25, 0.25, 0.25]$$

$$w_1^T x = w_2^T x = 1$$

L2 Regularization

$$R(W) = \sum_k \sum_l W_{k,l}^2$$



Regularization pushes against fitting the data *too* well so we don't fit noise in the data

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Very quick outline

Other specifics: Pre-processing**,** initialization**,** dropout, batch normalization, augmentation

A variety of gradient descent solvers available in Tensorflow

- Stochastic Gradient Descent (bread-and-butter, when in doubt…)
- Adam Optimizer (update learning rates with mean and variance)
- Nesterov / Momentum (add a velocity term)
- AdaGrad (Adaptive Subgradients, change learning rates)
- Proximal AdaGrad (Proximal = solve second problem to stay close)
- Ftrl Proximal (Follow-the-regularized-leader)
- AdaDelta (Adaptive learning rate)

Implementation detail #1 – method for gradient descent

```
# Vanilla Gradient Descent

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

Stochastic Gradient Descent (SGD)

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

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

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Full sum expensive when N is large!

Approximate sum using a **minibatch** of examples
32 / 64 / 128 common

Implementation detail #1 – method for gradient descent

```
# Vanilla Minibatch Gradient Descent

while True:
  data_batch = sample_training_data(data, 256) # sample 256 examples
  weights_grad = evaluate_gradient(loss_fun, data_batch, weights)
  weights += - step_size * weights_grad # perform parameter update
```

Stochastic Gradient Descent (SGD)

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

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Question: Why does gradient descent still work with mini-batches?

Answer: With stochastic gradient descent, random sub-set averaging of gradients still allows one to find their way down the hill to global minimum, at least with convex and quasi-convex functions [1].

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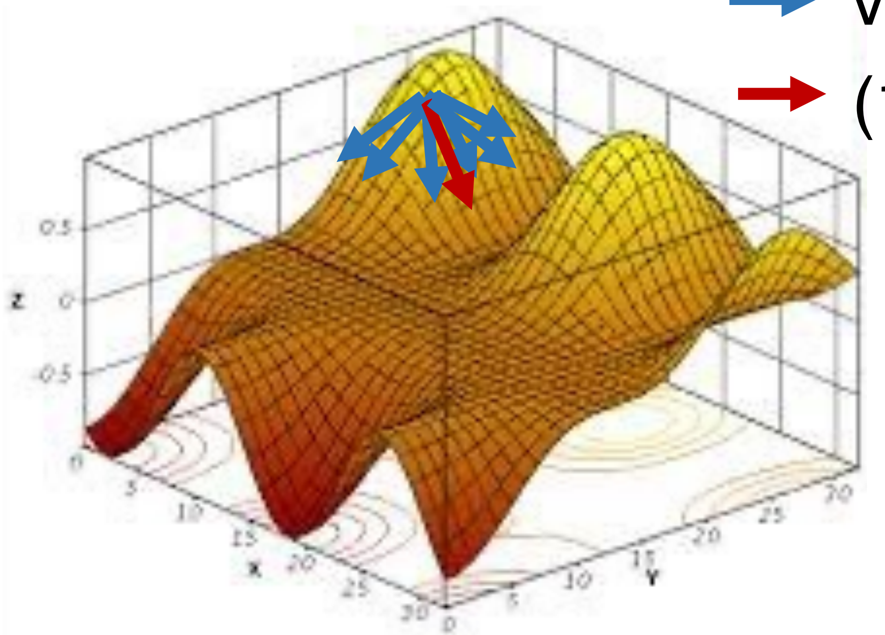

→ ∇L_i

→ $(1/N)\Sigma_N \nabla L_i$

[1] Bottou, Léon (1998). "Online Algorithms and Stochastic Approximations": https://leon.bottou.org/publications/pdf/online-1998.pdf

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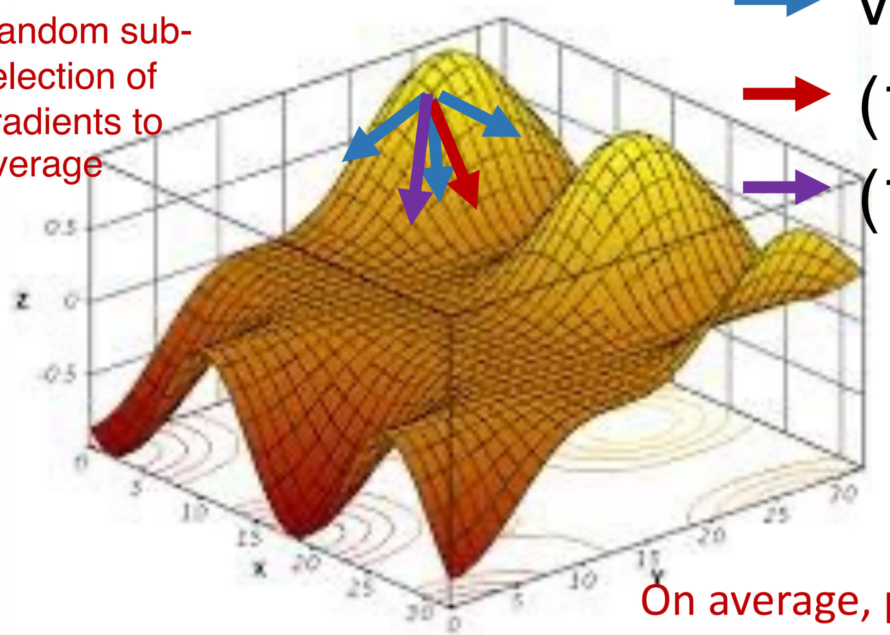
Random sub-selection of gradients to average



∇L_i

$(1/N)\Sigma_N \nabla L_i$

$(1/M)\Sigma_M \nabla L_i$

On average, purple arrow points in same direction as red arrow

[1] Bottou, Léon (1998). "Online Algorithms and Stochastic Approximations": https://leon.bottou.org/publications/pdf/online-1998.pdf

A variety of gradient descent solvers available in Tensorflow

- Stochastic Gradient Descent (bread-and-butter, when in doubt…)
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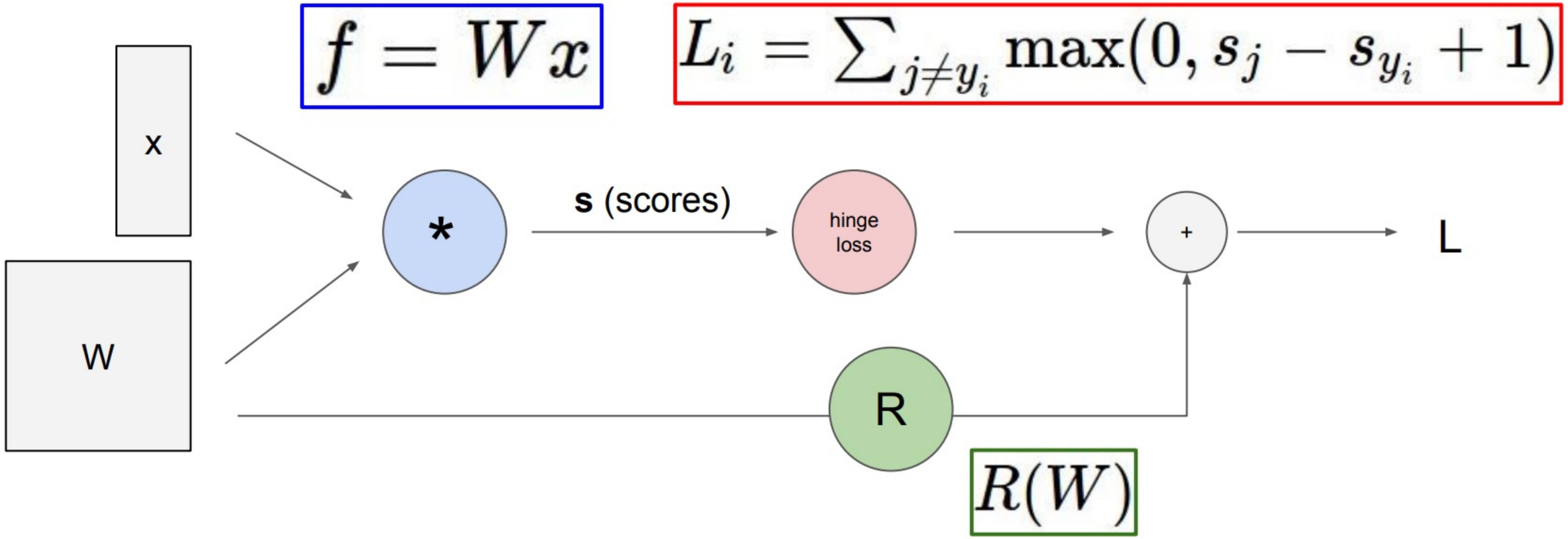
Next lecture: how Tensorflow actually solves gradient descent for you

Computational Graphs and the Chain Rule!



Important components of a CNN

CNN Architecture

- CONV size, stride, pad, depth
- ReLU & other nonlinearities
- POOL methods
- # of layers, dimensions per layer
- Fully connected layers

Let's view some code!

Loss function & optimization

- Type of loss function
- Regularization
- Gradient descent method
- SGD batch and step size

Other specifics: Pre-processing**,** initialization**,** dropout, batch normalization, augmentation

Important components of a CNN

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CNN Architecture

Architecture choices

- CONV size, stride, pad, depth
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Loss function & optimization

- Type of loss function
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Optimization choices

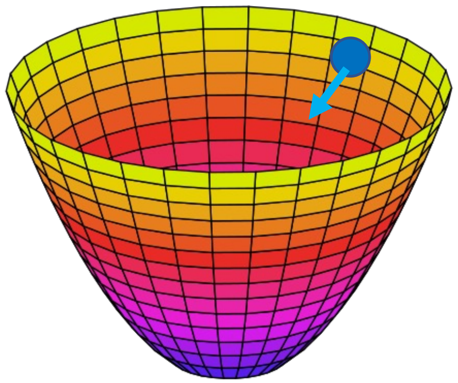
Other specifics: Variable Initialization**,** augmentation, batch normalization, dropout, gradient descent params.

The rest of this lecture: final details about deep CNN implementation

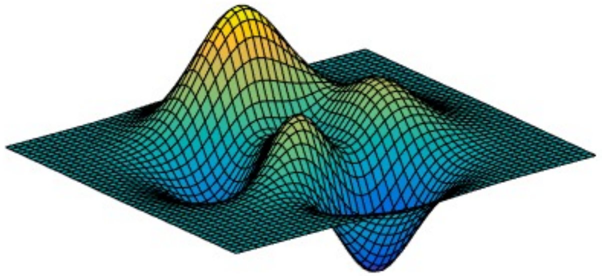
Weights initialization

- Need to start somewhere – typically best to use an appropriate random guess

Convex problem: doesn't really matter where you start



Non-convex problem: certainly matters, but you don't know where is best...



- Need to start somewhere – typically best to use an appropriate random guess sampled from a Gaussian distribution:

```
layer1_weight = tf.Variable(tf.truncated_normal([5,5, 1, 32], stddev = 0.1)
```

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Weights initialization

- Often it is helpful to take variance of weights into account
  - Having very large and very small weights leads to instabilities

- Desire: variance of inputs (x) remain unchanged as they transfer through network

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$$\mathbf{y} = \mathbf{w}^T\mathbf{x}$$

$$\mathrm{var}(\mathbf{y}) = \mathrm{var}(\mathbf{w}^T\mathbf{x}) = \mathrm{var}(w_1x_1 + \ldots w_Nx_N) = N\,\mathrm{var}(w_1x_1) \quad \text{(IID)}$$

$$\mathrm{var}(wx) = E(w)^2\mathrm{var}(x) + E(x)^2\mathrm{var}(w) + \mathrm{var}(w)\mathrm{var}(x) = \mathrm{var}(w)\mathrm{var}(x)$$

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$$\mathrm{var}(y) = N\,\mathrm{var}(w)\mathrm{var}(x)$$

$$\mathrm{var}(y) = \mathrm{var}(x) \text{ when } \mathrm{var}(w) = 1/N$$

```
layer1_weight = tf.Variable(tf.truncated_normal([5,5, 1, 32], stddev = 1/N)
```

Xavier Initialization

Data augmentation

- Machine learning is data-driven – the more data, the better!
- Nothing beats collecting more data, but that can be expensive and/or time consuming
- Data augmentation is the next best thing, and it's free!

Data augmentation one image at a time

Still a cat?

Flip left/right

Random rotation

Still a cat?

Flip up/down

Random affine transformation

Still a cat?

Change color scheme

Add random noise

Data augmentation

- Basic idea: to simulate variation that you might actually see in real life
- It’s a form of regularization
- Not an exact science, but try it out – it’s free!

Normalization: data preprocessing

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- If you use sigmoid activations, inputs that are too large could saturate them at early layers (vanishing gradient problem)
- Good practice to normalize your inputs
  - e.g. normalize to 0 mean, 1 variance; normalize to between 0 and 1 or -1 and 1
  - $X_i \leftarrow \frac{X_i - \mu}{\sigma}$
- Depending on the dataset, normalization can be done per instance or across entire dataset
  - Datasets with instances that have inconsistent ranges, although theoretically not a problem, in practice could speed up learning

Generalizing normalization to hidden layers

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- Batch normalization
- Layer normalization
- Instance normalization
- Group normalization

- All of these normalize hidden layers to 0 mean and 1 variance, but these means and variances are computed across different dimensions
  - $X_i \leftarrow \frac{X_i - \mu}{\sigma}$

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Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift

Sergey Ioffe
Google Inc., *sioffe@google.com*

Christian Szegedy
Google Inc., *szegedy@google.com*

Cited ~21,000 times! (as of 2020)

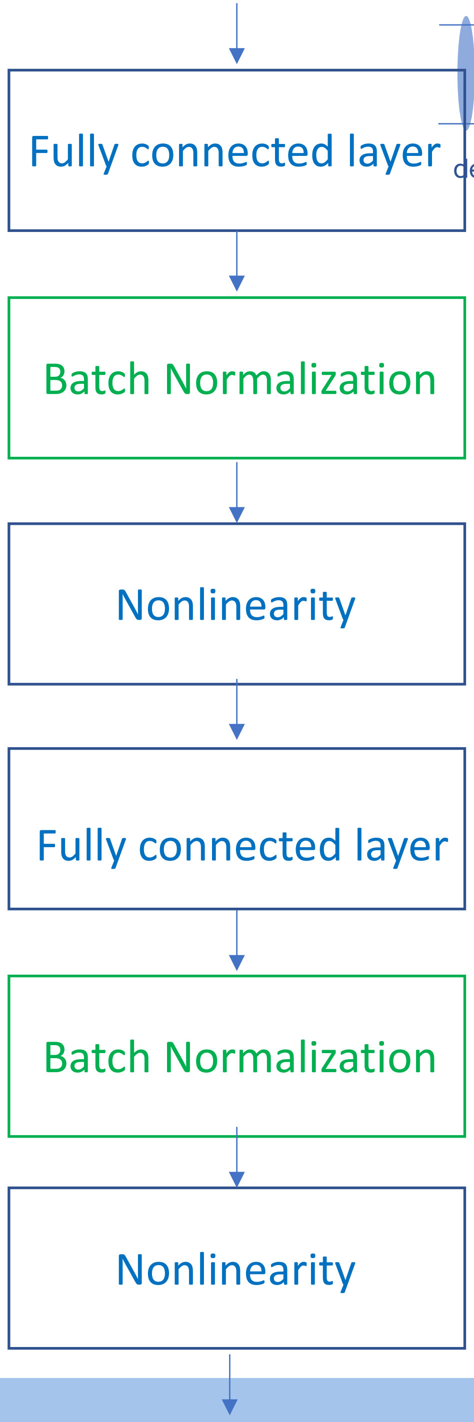
Batch normalization (BN)

- Before BN, training very deep networks was hard
  - If using sigmoid activations, large weights could result in saturation
  - Updating earlier layers' weights causes the distribution of weights in later layers to shift – the *internal covariate shift*
- To address this covariate shift, BN "resets" the layer it is applied to by normalizing to 0 mean, 1 variance
  - Mean and variance are computed over the batch at the current iteration

Batch normalization update for inputs x:

$$\boxed{x'(i) = (x(i) - E[x(i)]) \,/\, STD[x(i)]}$$

- Mean subtract
- Normalize by standard deviation



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Problems

- Normalizing to 0 mean 1 variance reduces the expressivity of the layer
  - E.g., if using a sigmoid activation, you're stuck in the linear regime
- Solution: reintroduce mean (β) and standard deviation (γ) parameters:
  - $X_i \leftarrow \frac{X_i - \mu}{\sigma}$ #normalize
  - $X_i \leftarrow \gamma X_i + \beta$ #new mean and standard deviations
  - γ and β are trainable parameters

- Accuracy of μ and σ depends on the batch size being large

Other hidden layer normalizations (for CNNs)

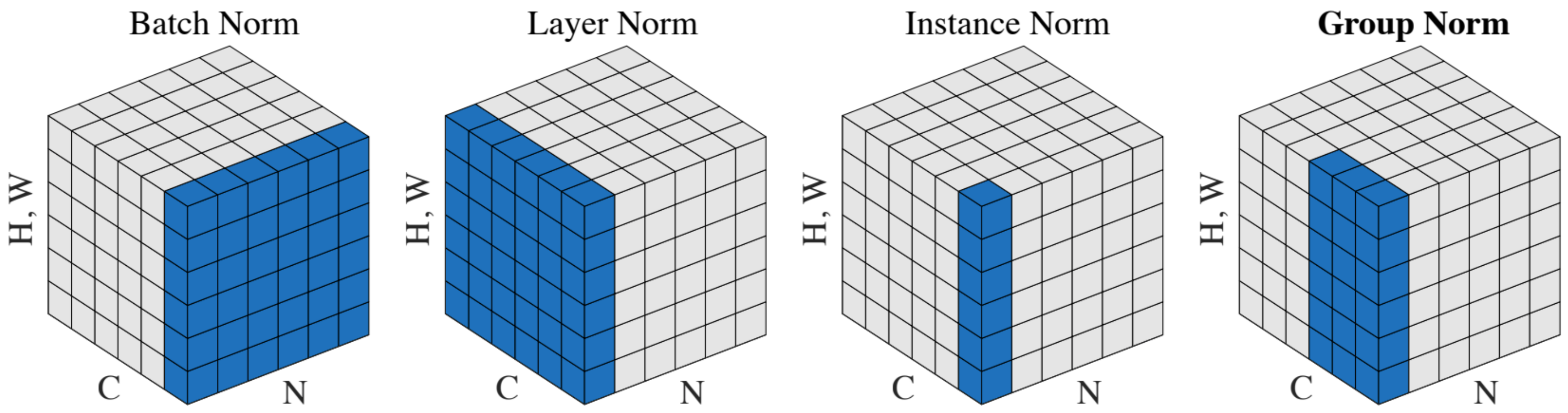

Figure 2. **Normalization methods**. Each subplot shows a feature map tensor, with N as the batch axis, C as the channel axis, and (H, W) as the spatial axes. The pixels in blue are normalized by the same mean and variance, computed by aggregating the values of these pixels.

https://nealjean.com/ml/neural-network-normalization/

Journal of Machine Learning Research 15 (2014) 1929-1958 Submitted 11/13; Published 6/14

Dropout: A Simple Way to Prevent Neural Networks from Overfitting

Nitish Srivastava NITISH@CS.TORONTO.EDU
Geoffrey Hinton HINTON@CS.TORONTO.EDU
Alex Krizhevsky KRIZ@CS.TORONTO.EDU
Ilya Sutskever ILYA@CS.TORONTO.EDU
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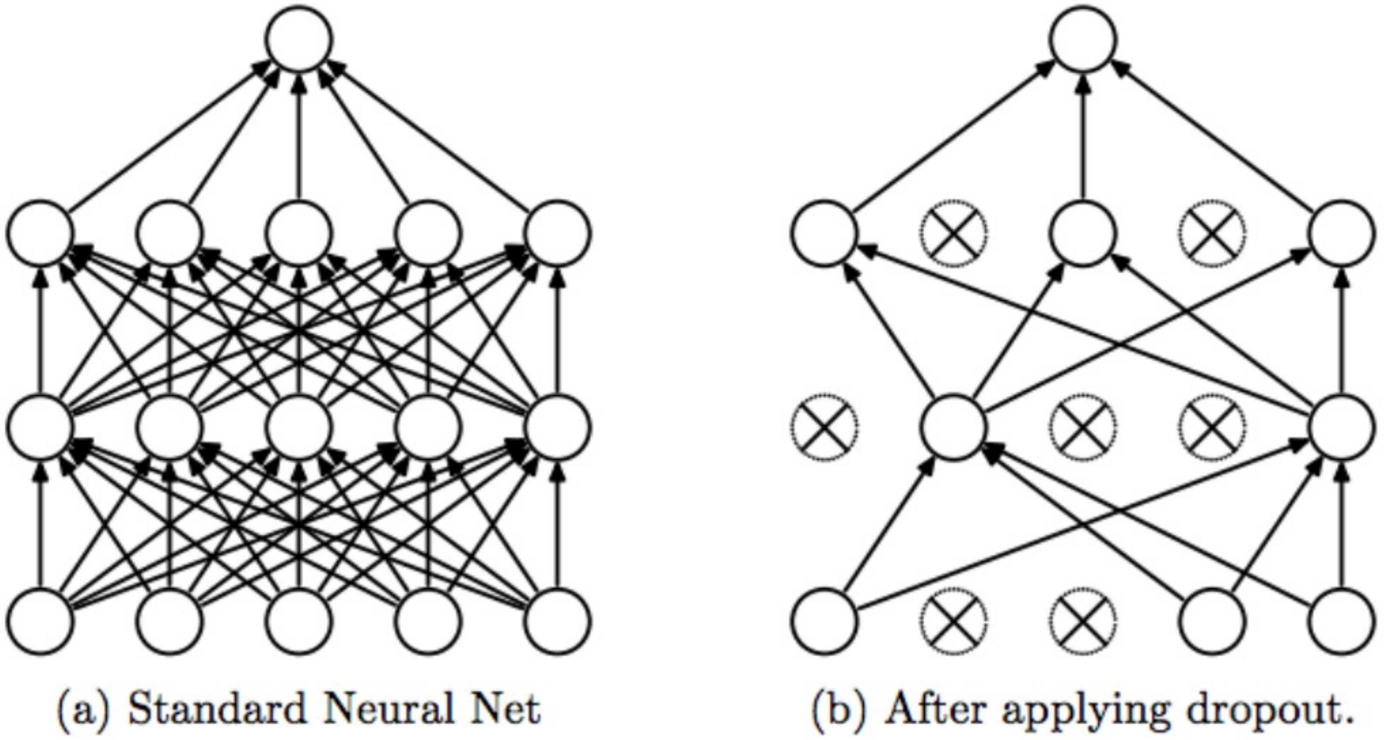
Editor: Yoshua Bengio

Cited over 22,000 times!
(as of 2020)

Dropout

- At each train iteration, randomly delete a fraction p of the nodes
- Prevents neurons from being lazy
- A form of model averaging
- (related: DropConnect – drop the connections instead of nodes)



https://medium.com/@amarbudhiraja/https-medium-com-amarbudhiraja-learning-less-to-learn-better-dropout-in-deep-machine-learning-74334da4bfc5

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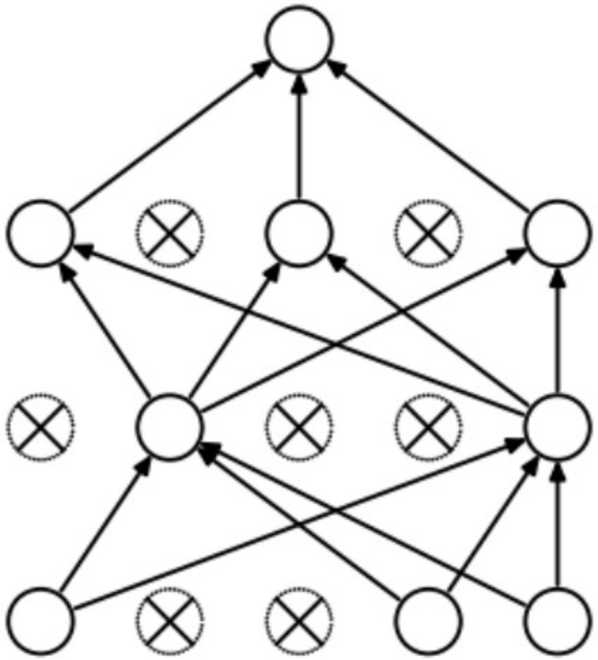
Dropout

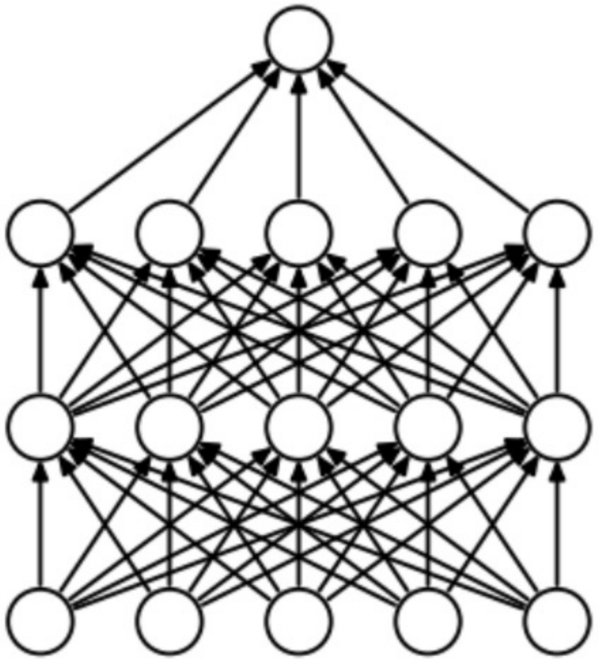
- Only one hyperparameter “rate” = p, the expected fraction of neurons to drop in a given layer
- In TensorFlow:
  - next_layer = tf.layers.dropout(previous_layer, rate=0.5)
- Common practices:
  - Set p=0.5
  - Make the layer wider (more units/neurons)
  - Apply to fully connected layers, not convolutional layers (already sparse)

Dropout training vs testing

- Training: at a given layer, each node is dropped with probability p
- Testing: multiply the outgoing weights by 1-p (*weight scaling inference rule*)
- As a model averaging technique, other possibilities exist



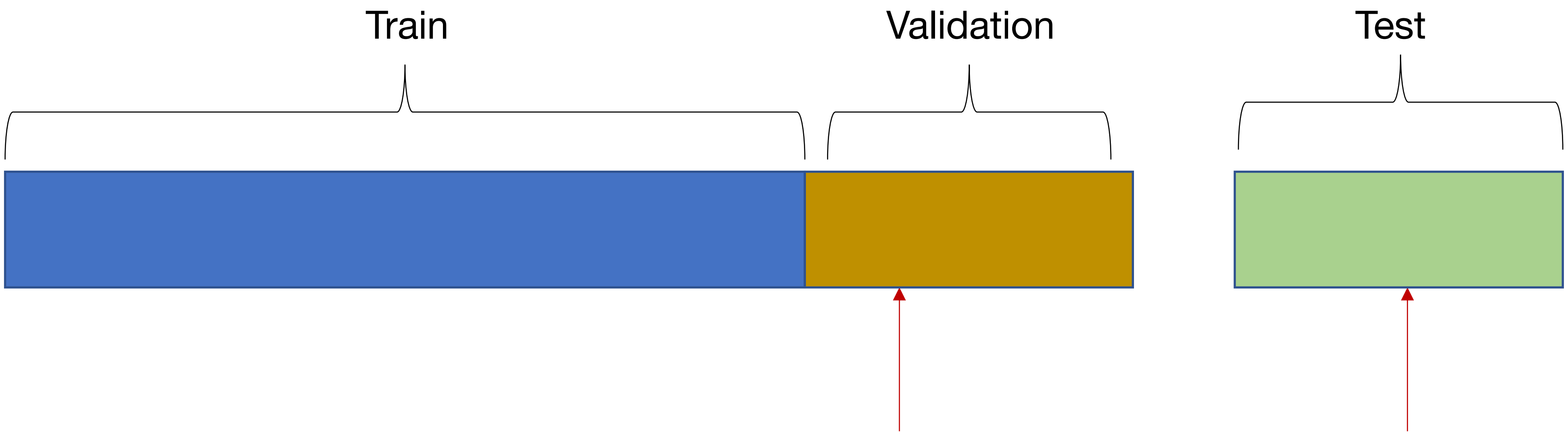
Training
(each node dropped with probability)



Testing
(all weights multiplied by 1-p)

https://medium.com/@amarbudhiraja/https-medium-com-amarbudhiraja-learning-less-to-learn-better-dropout-in-deep-machine-learning-74334da4bfc5

Training dataset, test dataset and validation dataset



Use to evaluate while tuning hyperparameters

- effect will creep into model as you continue to use it

Final test set is always separate!
Don’t touch until the end!