Training Neural Networks
Regularization

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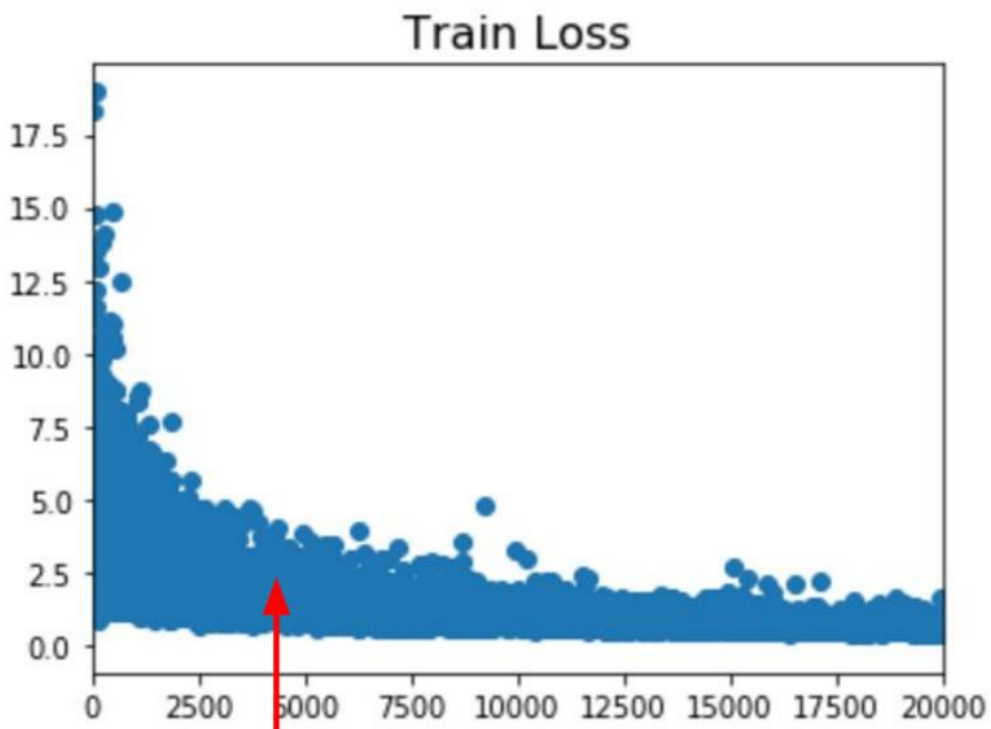
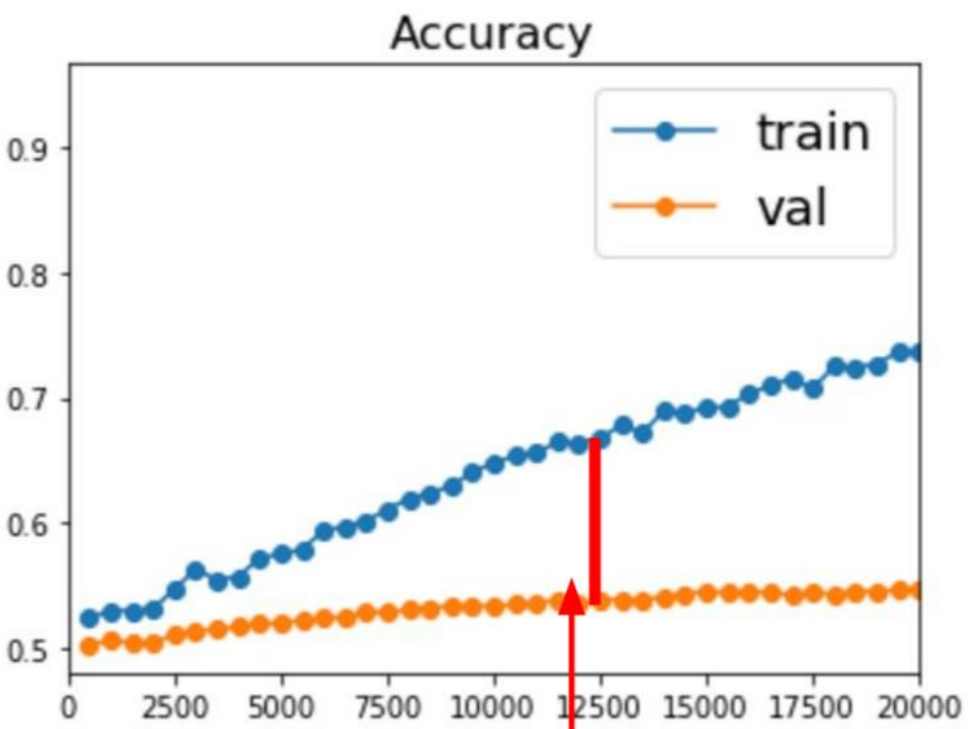
Most slides have been adapted from Fei Fei Li and colleagues lectures, cs231n, Stanford 2017, some from Andrew Ng lectures, “Deep Learning Specialization”, coursera, 2017,

Outline

- Regularization
- Drop-out
- Data Augmentation
- Early stopping
- Model ensembles
- Hyper-parameter selection

Beyond Training Error

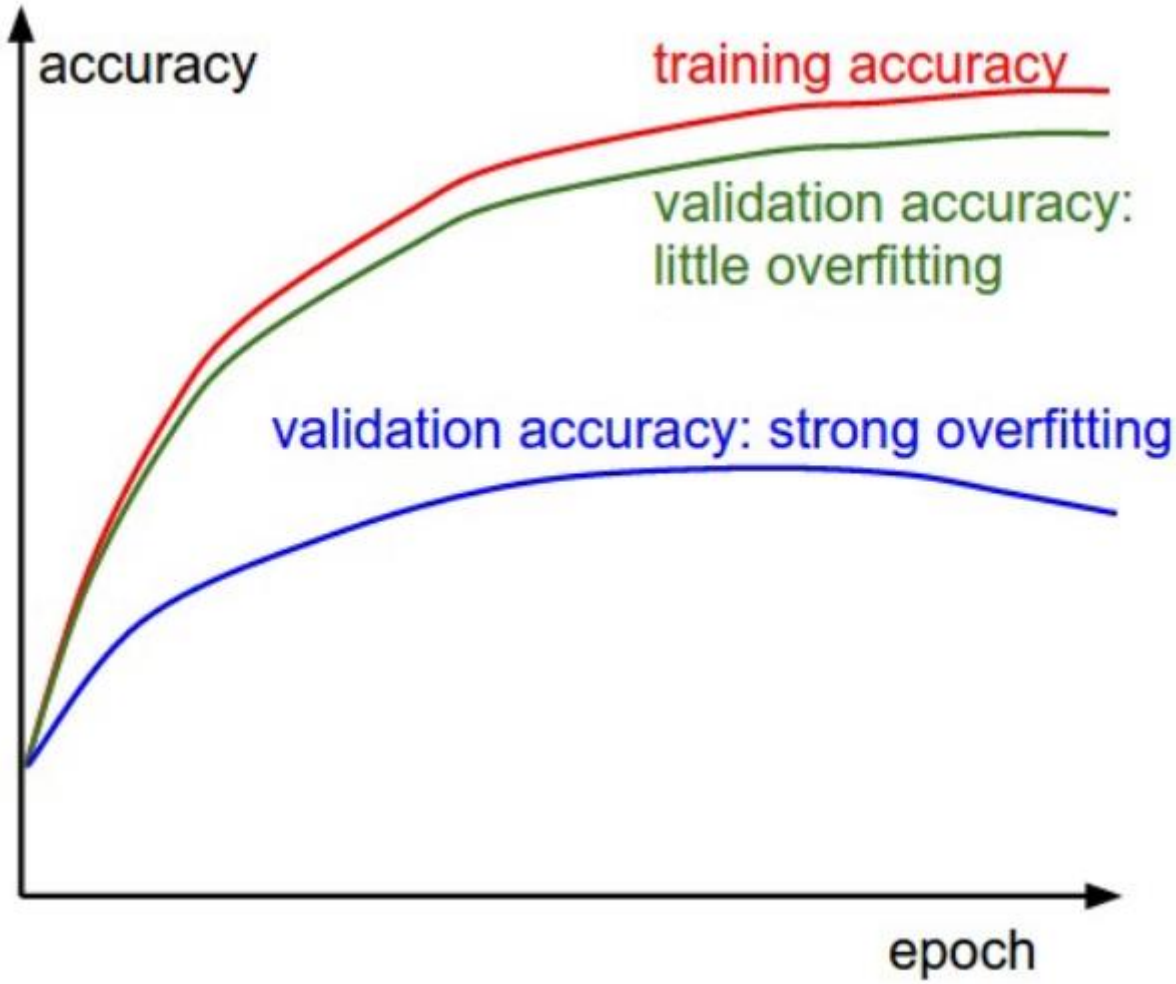




Better optimization algorithms help reduce training loss

But we really care about error on new data - how to reduce the gap?

Beyond Training Error



Regularization: Add term to loss

$$J(W) = \frac{1}{N}\sum_{n=1}^{N} L^{(n)}(W) + \lambda R(W)$$

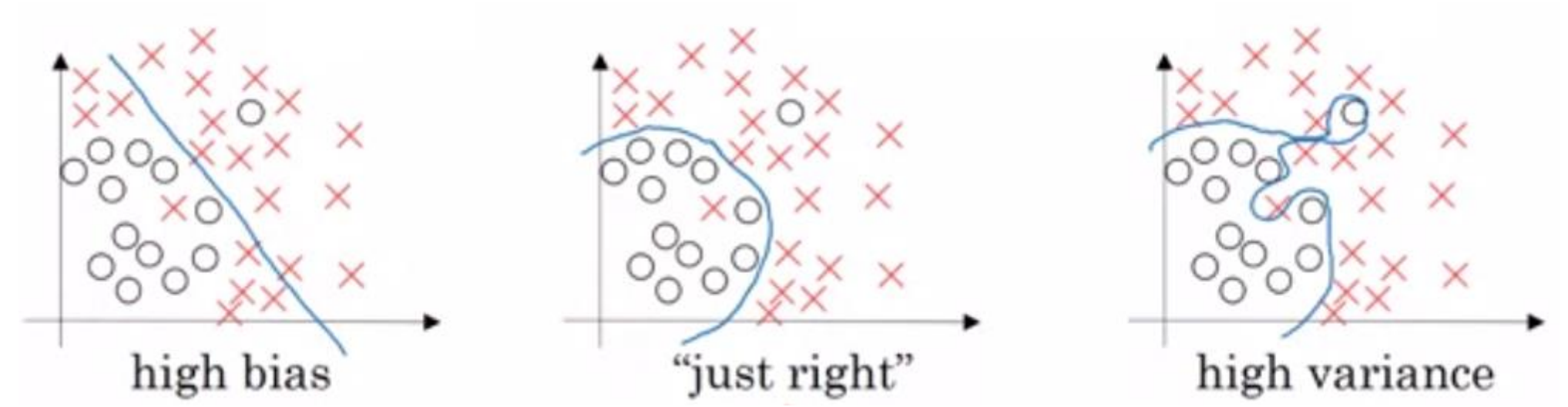
In common use:

L2 regularization $R(W) = \sum_k \sum_l W_{k,l}^2$ (Weight decay)

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 help to reduce overfitting



[Andrew Ng, Deep Learning Specialization, 2017]

Why L2 regularization called weight decay

$$J(W) = L(W) + \lambda R(W)$$

$$J(W) = L(W) + \lambda \sum_{l=1}^{L} W^{[l]^T} W^{[l]}$$

$$W^{[l]} \leftarrow W^{[l]} - \alpha \nabla_{W^{[l]}} L(W) - 2\lambda W^{[l]}$$

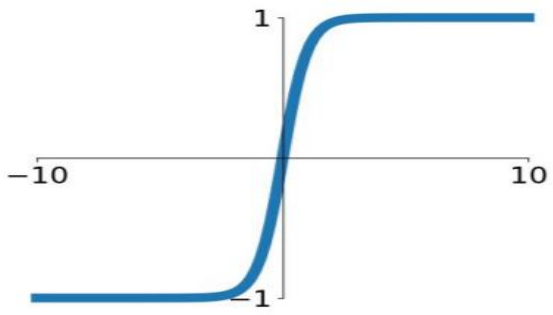
$$W^{[l]} \leftarrow W^{[l]}(1 - 2\lambda) - \alpha \nabla_{W^{[l]}} L(W)$$

Weight decay

With regularization, smoother cost vs. #epoch curve is obtained.

Regularization can prevent overfitting

- Small W linear regime of tanh
- A deep network with small W can also act as a near linear function

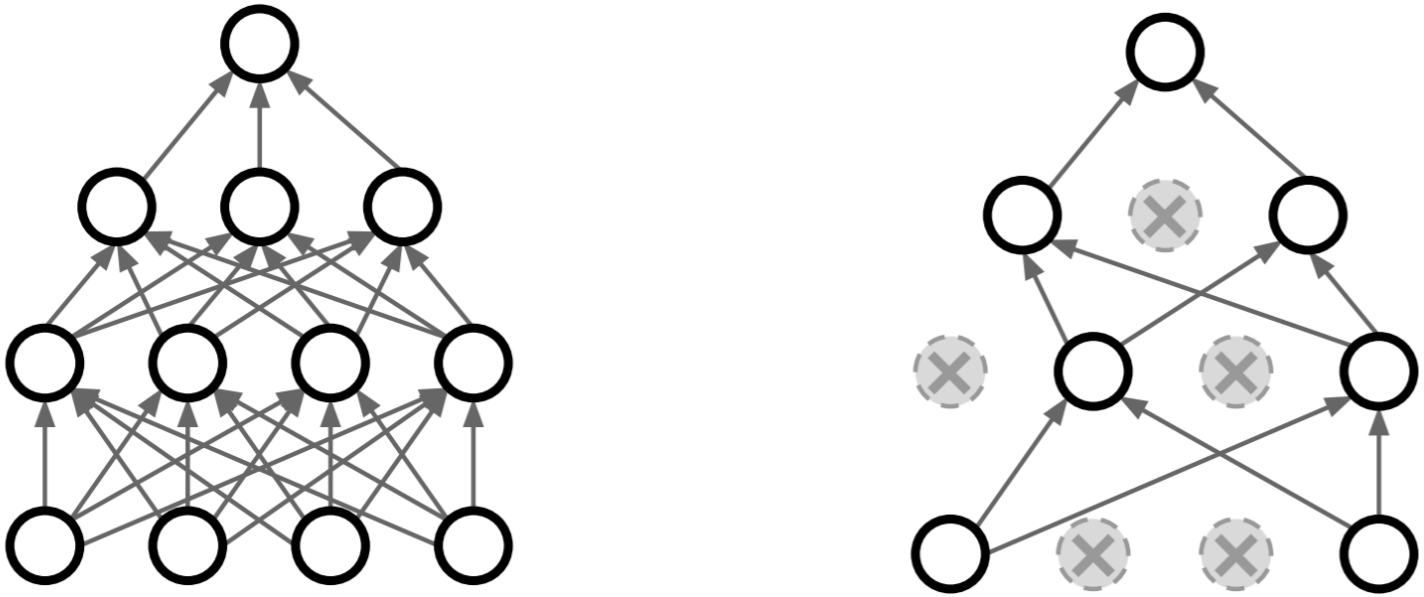


tanh(x)

Regularization: Dropout

Srivastava et al, “Dropout: A simple way to prevent neural networks from overfitting”, JMLR 2014

- In each forward pass, randomly set some neurons to zero
  - Probability of dropping is a hyperparameter; 0.5 is common



- Thus, a smaller network is trained for each sample
  - Smaller network provides a regularization effect

Implementing dropout (Inverted dropout)

- for l=1,...L
  - $d^{[l]} \leftarrow I\left(rand(\#neurons^{[l]}, 1) < keep\_prob\right)$
  - $a^{[l]} \leftarrow a^{[l]} .* d^{[l]}$

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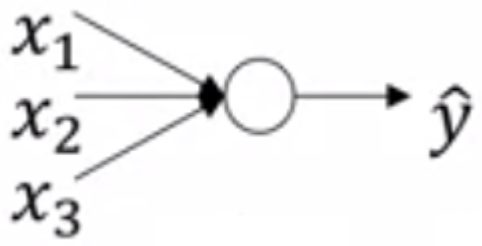
  - $a^{[l]} \leftarrow a^{[l]} / keep\_prob$

Why does drop-out work?

- Intuition: cannot rely on any one feature, so have to spread out weights

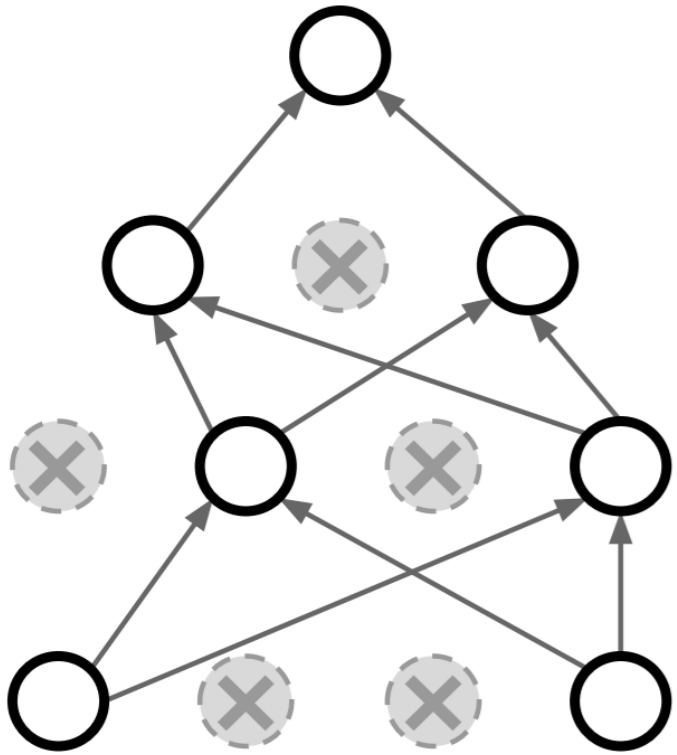


- Thus, shrinking the weights ($W^T W$) and shows similar effect to the L_2 regularization

[Andrew Ng, Deep Learning Specialization, 2017]

Regularization: Dropout

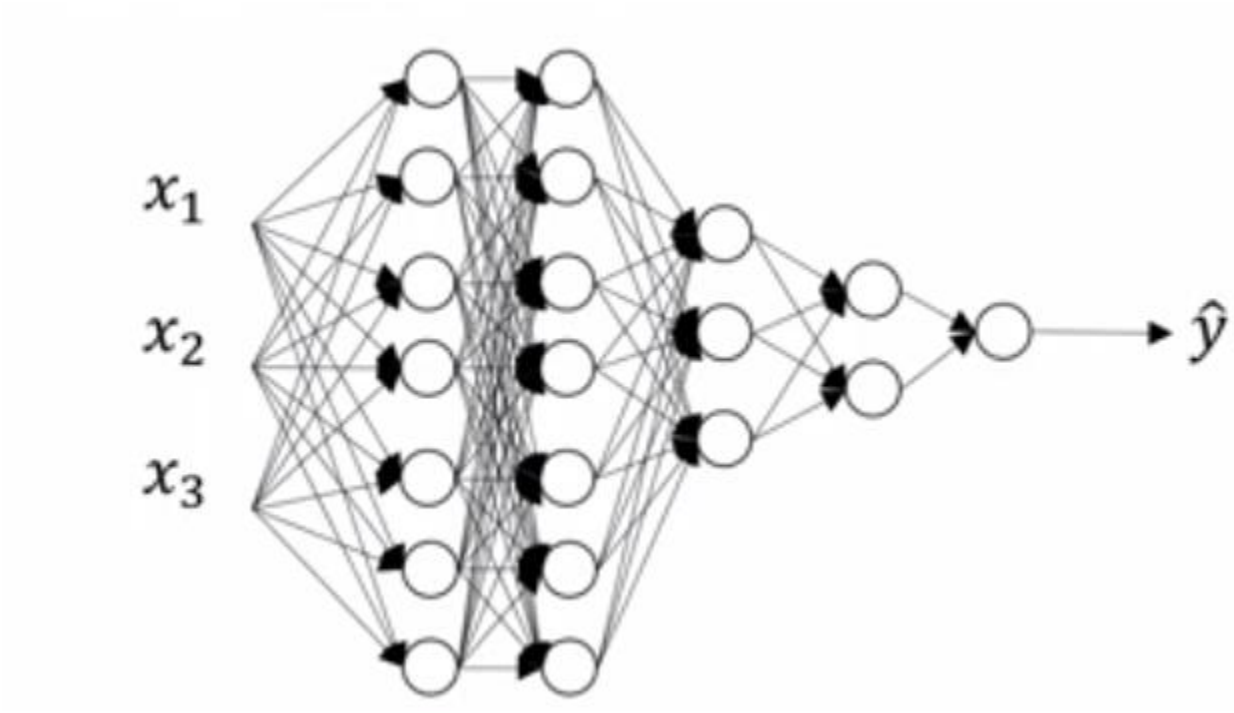
- How can dropout be a good idea?



Forces the network to have a redundant representation;
Prevents co-adaptation of features

Dropout on layers

- Different keep-prob can be used for different layers
  - However, more hyper-parameters are required



Regularization: Dropout

- How can this possibly be a good idea? (Another interpretation)
  - Dropout is training a large ensemble of models (that share parameters).
  - Each binary mask is one model
    - An FC layer with 4096 units has $2^{4096} \sim 10^{1233}$ possible masks!
    - Only $\sim 10^{82}$ atoms in the universe...

Dropout: test time

- Dropout makes our output random!

Output (label) Input (image)

$$\boxed{y} = f_W(\boxed{x}, \boxed{z})$$

Random mask

- Want to "average out" the randomness at test-time

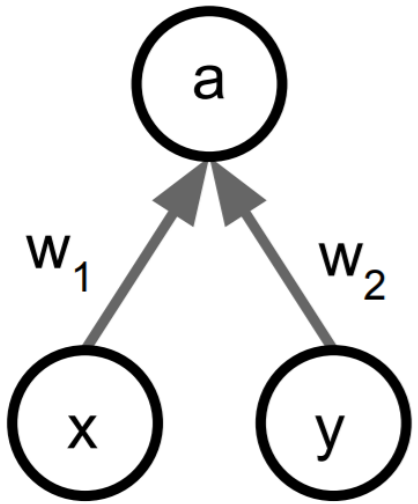
$$y = f(x) = E_z\left[f(x,z)\right] = \int p(z) f(x,z) dz$$

- But this integral seems hard …

Dropout: test time

Want to approximate the integral

$$y = f(x) = E_z\left[f(x,z)\right] = \int p(z) f(x,z) dz$$



Consider a single neuron.

At test time we have: $E\left[a\right] = w_1 x + w_2 y$

Dropout: test time

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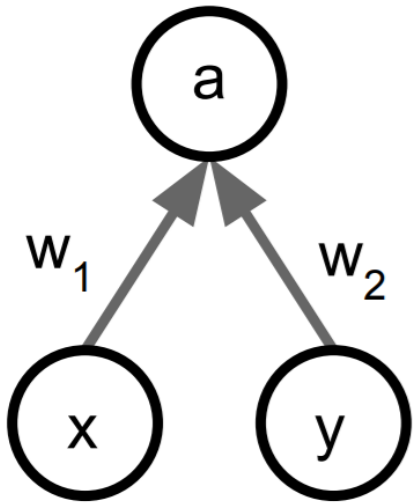

Consider a single neuron.

At test time we have: $E\left[a\right] = w_1 x + w_2 y$

During training we have:

$$\begin{aligned} E\left[a\right] =& \frac{1}{4}(w_1 x + w_2 y) + \frac{1}{4}(w_1 x + 0y) \\ &+ \frac{1}{4}(0x + 0y) + \frac{1}{4}(0x + w_2 y) \\ =& \frac{1}{2}(w_1 x + w_2 y) \end{aligned}$$

Dropout: test time

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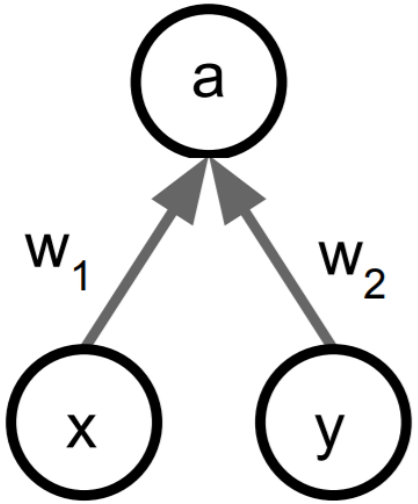

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At test time, **multiply** by dropout probability

Making prediction at test time

- No dropout is used during test time

- With dropout, the expected output of neuron will become $p \times a + (1$

Dropout summary

```python
""" Vanilla Dropout: Not recommended implementation (see notes below) """

p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
  """ X contains the data """

  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = np.random.rand(*H1.shape) < p # first dropout mask
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = np.random.rand(*H2.shape) < p # second dropout mask
  H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3

  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)

def predict(X):
  # ensembled forward pass
  H1 = np.maximum(0, np.dot(W1, X) + b1) * p # NOTE: scale the activations
  H2 = np.maximum(0, np.dot(W2, H1) + b2) * p # NOTE: scale the activations
  out = np.dot(W3, H2) + b3
```

Dropout Summary

drop in forward pass

scale at test time

Inverted dropout

- Since test-time performance is so critical, it is always preferable to use inverted dropout,
  - which performs the scaling at train time, leaving the forward pass at test time untouched.
  - Just divide the activation of each layer by keep-prob

Inverted dropout

```
p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = (np.random.rand(*H1.shape) < p) / p # first dropout mask. Notice /p!
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = (np.random.rand(*H2.shape) < p) / p # second dropout mask. Notice /p!
  H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3

  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)

def predict(X):
  # ensembled forward pass
  H1 = np.maximum(0, np.dot(W1, X) + b1) # no scaling necessary
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  out = np.dot(W3, H2) + b3
```

test time is unchanged!

Dropout issues

- If your NN is significantly overfitting, dropout usually help must to prevent overfitting
- Training takes longer time but provides better generalization
  - If your NN is not overfitting, bigger NN with dropout can help

- The cost function is no longer well defined.
- Gradcheck by turning off the dropout

Regularization: A common pattern

- Training: Add some kind of randomness Testing:

$$\hat{y} = f(x, z; W)$$

- Average out randomness (sometimes approximate)

$$\hat{y} = E_z[f(x, z; W)] = \int p(z) f(x, z; W) dz$$

Regularization: A common pattern

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$$\hat{y} = f(x, z; W)$$

- Average out randomness (sometimes approximate)

$$\hat{y} = E_z[f(x, z; W)] = \int p(z) f(x, z; W) dz$$

Example: Batch Normalization

Training: Normalize using stats from random mini-batches

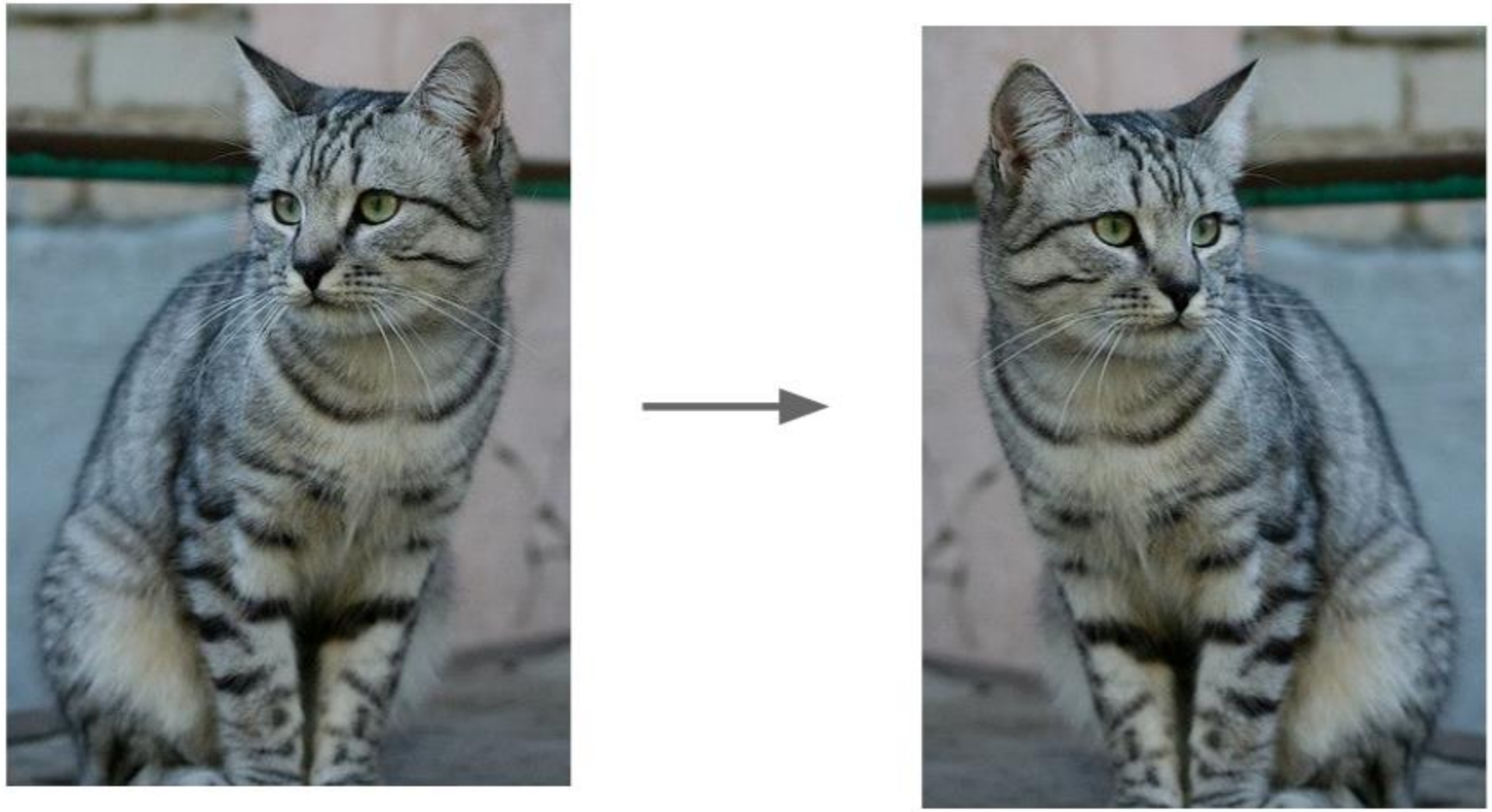
Testing: Use fixed stats to normalize

Data augmentation

- Getting more training data can be expensive
- But, sometimes we can generate more training examples from the datasets

Data augmentation

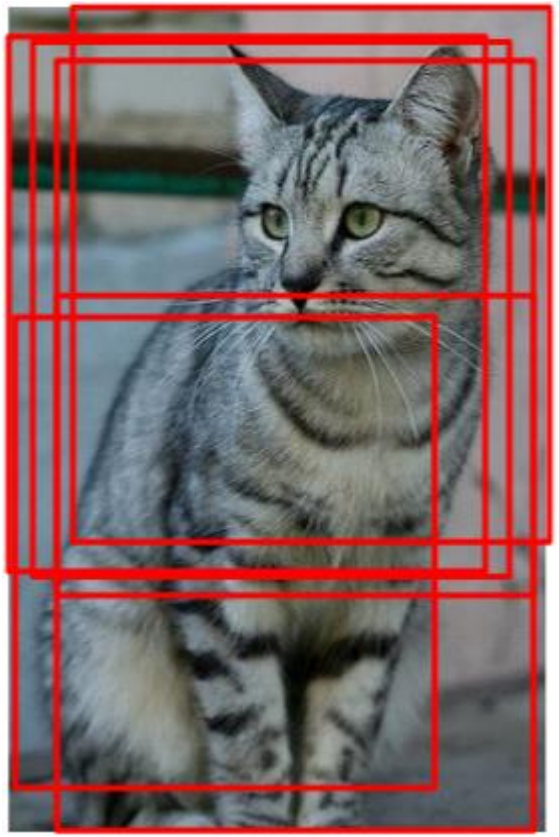
- Horizontal flip



Data augmentation

- Random crops and scales

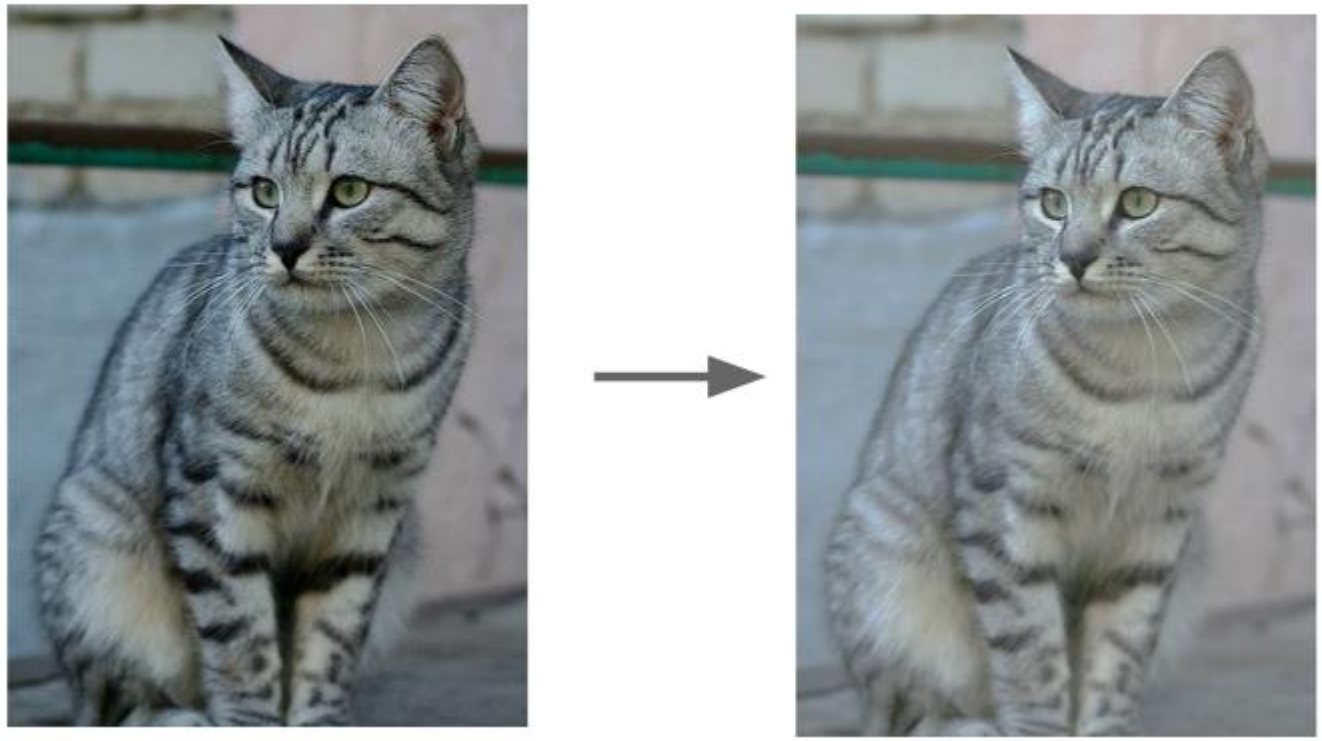
- Training: sample random crops / scales
  - ResNet:
    - 1. Pick random L in range [256, 480]
    - 2. Resize training image, short side = L
    - 3. Sample random 224 x 224 patch
- Testing: average a fixed set of crops
  - ResNet:
    - 1. Resize image at 5 scales: {224, 256, 384, 480, 640}
    - 2. For each size, use 10 224 x 224 crops: 4 corners + center, + flips



Data augmentation

- Color Jitter

Simple: Randomize contrast and brightness



Data augmentation

- Random mix/combinations of :
  - Translation
  - Rotation
  - Stretching
  - Shearing
  - …

Regularization: A common pattern

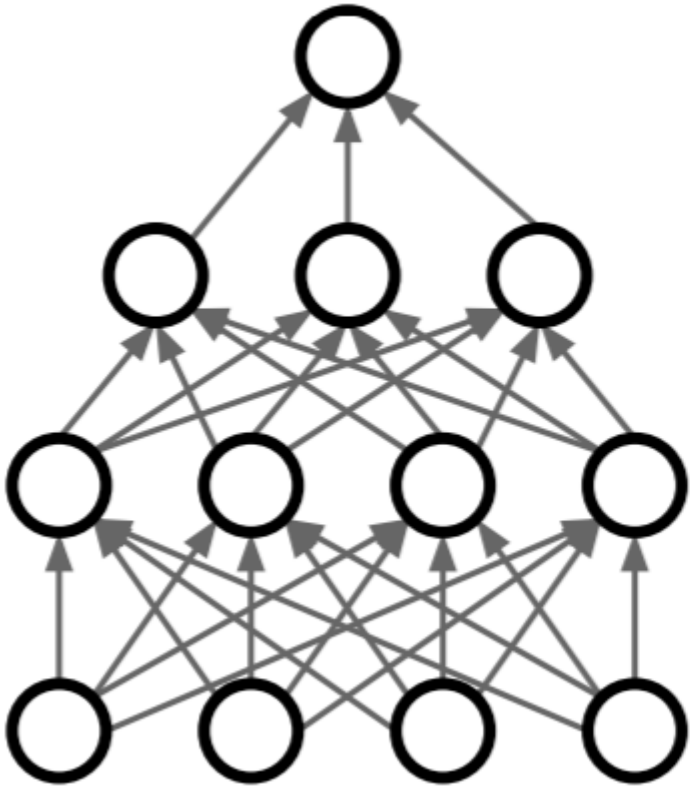
- Training: Add random noise
- Testing: Marginalize over the noise

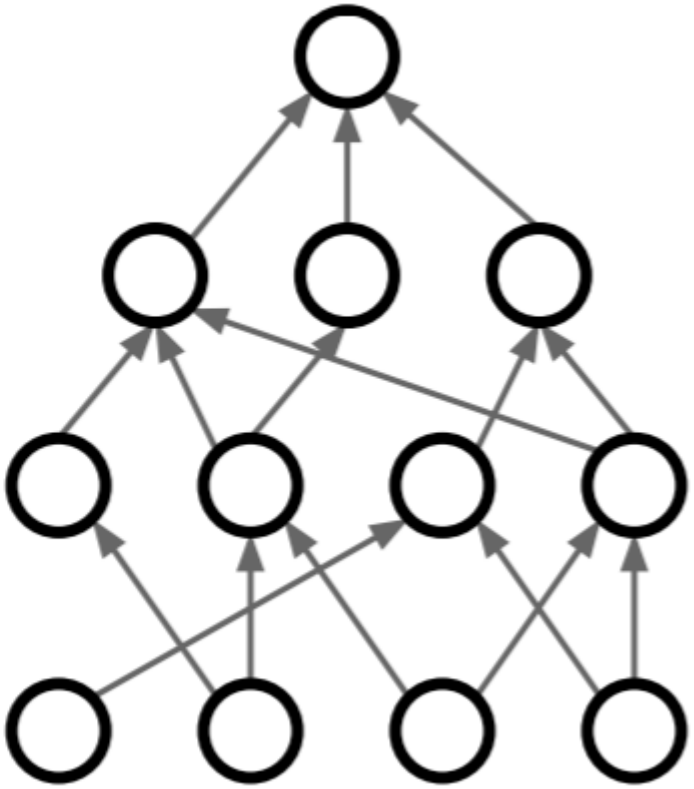
- Examples:
  - Dropout
  - Batch Normalization
  - Data Augmentation

Regularization: A common pattern

- Training: Add random noise
- Testing: Marginalize over the noise

- Examples:
  - Dropout
  - Batch Normalization
  - Data Augmentation
  - Dropconnect

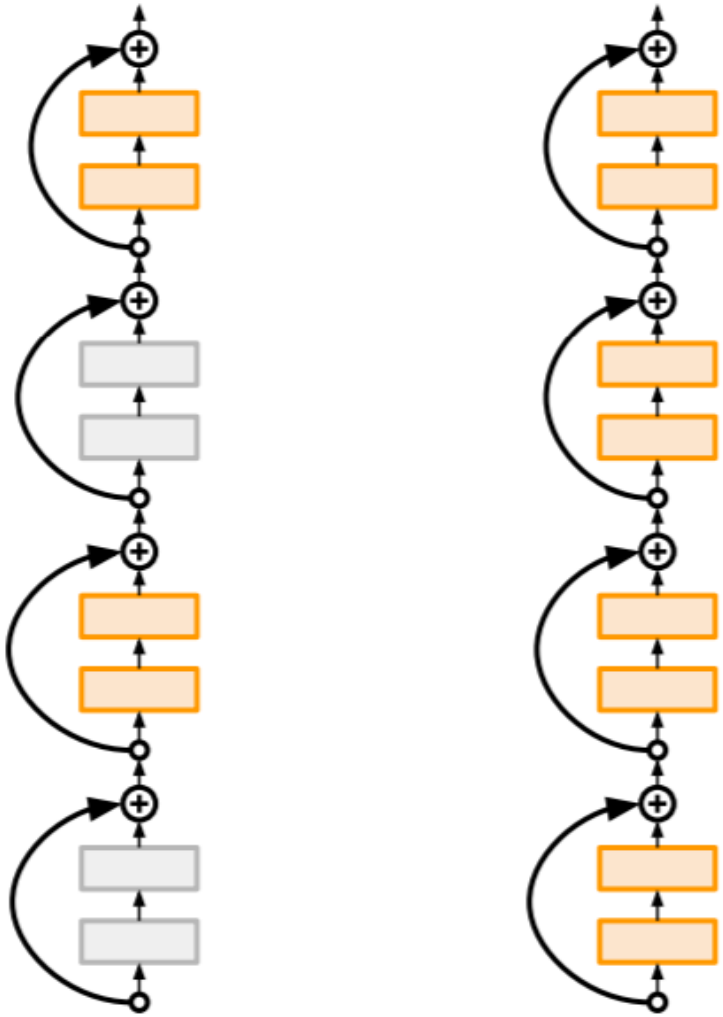




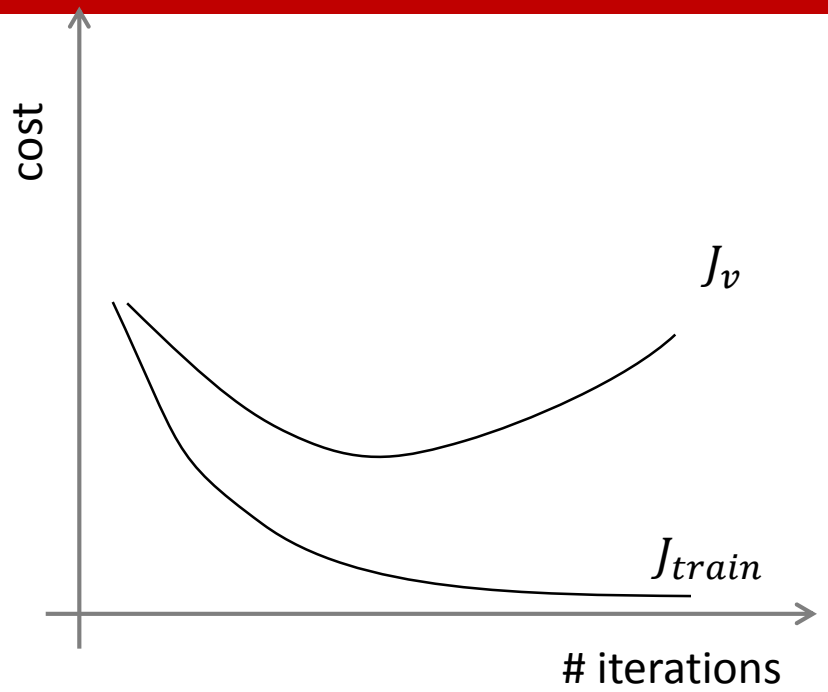
Regularization: A common pattern

- Training: Add random noise
- Testing: Marginalize over the noise

- Examples:
  - Dropout
  - Batch Normalization
  - Data Augmentation
  - Dropconnect
  - Stochastic depth



Early stopping



- Similar to L2 regularization

☹ Thinks about approximation and generalization tasks separately

- By stopping gradient descent early breaks whatever you are doing to optimize cost function

☺ Advantage is that it needs running gradient descent process just once

Model ensembles

1. Train multiple independent models

2. At test time average their results

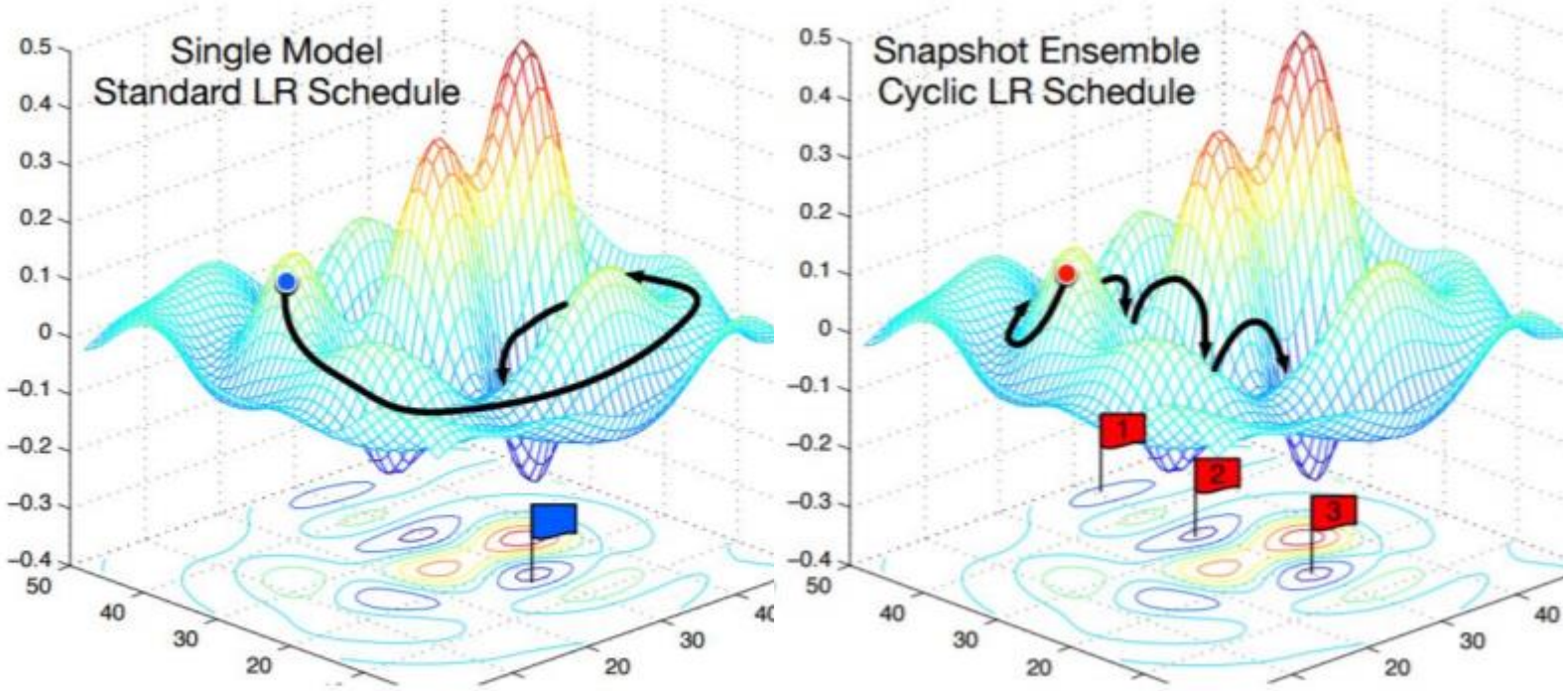
Model ensembles

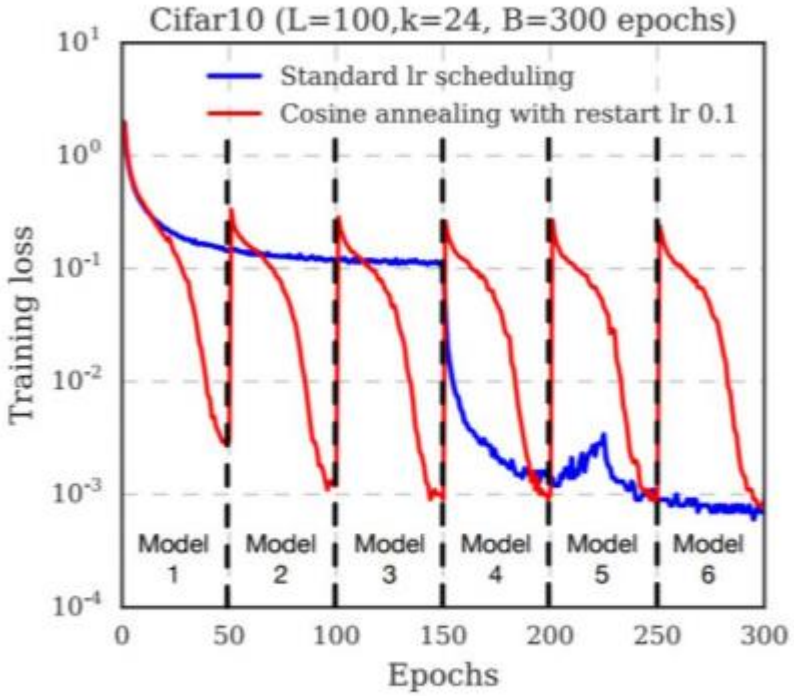
- Train multiple independent models, and at test time average their predictions.
  - improving the performance by a few percent

- Candidates
  - **Same model, different initializations** (after selecting the best hyperparameters**)**
  - **Top models discovered during cross-validation**
  - **Different checkpoints of a single model** (If training is very expensive)
    - maybe limited success to form an ensemble.
  - **Running average of parameters during training**
    - maintains an exponentially decaying sum of previous weights during training.

Model ensembles: Tips and tricks

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





Cyclic learning rate schedules can make this work even better!

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

Model ensembles: Tips and tricks

- Instead of using actual parameter vector, keep a moving average of the parameter vector and use that at test time (Polyak averaging)

```
while True:
  data_batch = dataset.sample_data_batch()
  loss = network.forward(data_batch)
  dw = network.backward()
  w += - learning_rate * dw
  w_test = 0.995*w_test + 0.005*w # use for test set
```

Hyperparameter selection

- Finding a good set of hyperparameters to provide better convergence
  - initial learning rate α
  - regularization strength (L2 penalty, dropout strength)
  - # of hidden units and # of layers
  - mini-batch size
  - decay schedule (such as the decay constant), update type

  - parameters of optimization algorithms (momentum, adam, …)
    - These are usually fixed to $\beta_1 = 0.9$, $\beta_2 = 0.999$, and $\epsilon = 10^{-8}$ or 10^{-7}

Hyperparameter search

- Larger Neural Networks typically require a long time to train
  - so performing hyperparameter search can take many days/weeks

- A single validation set of respectable size substantially simplifies the code base, without the need for cross-validation with multiple folds

Cross-validation strategy

- **coarse -> fine** cross-validation in stages
  - Zoom in to smaller region of hyperparameters and sample very densely in them

- **First stage**: only a few epochs to get rough idea of what params work
- **Second stage**: longer running time, finer search … (repeat as necessary)

For example: run coarse search for 5 epochs

```
max_count = 100
for count in xrange(max_count):
      reg = 10**uniform(-5, 5)
      lr = 10**uniform(-3, -6)

      trainer = ClassifierTrainer()
      model = init_two_layer_model(32*32*3, 50, 10) # input size, hidden size, number of classes
      trainer = ClassifierTrainer()
      best_model_local, stats = trainer.train(X_train, y_train, X_val, y_val,
                                              model, two_layer_net,
                                              num_epochs=5, reg=reg,
                                              update='momentum', learning_rate_decay=0.9,
                                              sample_batches = True, batch_size = 100,
                                              learning_rate=lr, verbose=False)
```

note it's best to optimize in log space!

```
val_acc: 0.412000, lr: 1.405206e-04, reg: 4.793564e-01, (1 / 100)
val_acc: 0.214000, lr: 7.231888e-06, reg: 2.321281e-04, (2 / 100)
val_acc: 0.208000, lr: 2.119571e-06, reg: 8.011857e+01, (3 / 100)
val_acc: 0.196000, lr: 1.551131e-05, reg: 4.374936e-05, (4 / 100)
val_acc: 0.079000, lr: 1.753300e-05, reg: 1.200424e+03, (5 / 100)
val_acc: 0.223000, lr: 4.215128e-05, reg: 4.196174e+01, (6 / 100)
val_acc: 0.441000, lr: 1.750259e-04, reg: 2.110807e-04, (7 / 100)
val_acc: 0.241000, lr: 6.749231e-05, reg: 4.226413e+01, (8 / 100)
val_acc: 0.482000, lr: 4.296863e-04, reg: 6.642555e-01, (9 / 100)
val_acc: 0.079000, lr: 5.401602e-06, reg: 1.599828e+04, (10 / 100)
val_acc: 0.154000, lr: 1.618508e-06, reg: 4.925252e-01, (11 / 100)
```

nice

Now run finer search

```
max_count = 100
for count in xrange(max_count):
      reg = 10**uniform(-5, 5)
      lr = 10**uniform(-3, -6)
```

adjust range →

```
max_count = 100
for count in xrange(max_count):
      reg = 10**uniform(-4, 0)
      lr = 10**uniform(-3, -4)
```

```
val_acc: 0.527000, lr: 5.340517e-04, reg: 4.097824e-01, (0 / 100)
val_acc: 0.492000, lr: 2.279484e-04, reg: 9.991345e-04, (1 / 100)
val_acc: 0.512000, lr: 8.680827e-04, reg: 1.349727e-02, (2 / 100)
val_acc: 0.461000, lr: 1.028377e-04, reg: 1.220193e-02, (3 / 100)
val_acc: 0.460000, lr: 1.113730e-04, reg: 5.244309e-02, (4 / 100)
val_acc: 0.498000, lr: 9.477776e-04, reg: 2.001293e-03, (5 / 100)
val_acc: 0.469000, lr: 1.484369e-04, reg: 4.328313e-01, (6 / 100)
val_acc: 0.522000, lr: 5.586261e-04, reg: 2.312685e-04, (7 / 100)
val_acc: 0.530000, lr: 5.808183e-04, reg: 8.259964e-02, (8 / 100)
val_acc: 0.489000, lr: 1.979168e-04, reg: 1.010889e-04, (9 / 100)
val_acc: 0.490000, lr: 2.036031e-04, reg: 2.406271e-03, (10 / 100)
val_acc: 0.475000, lr: 2.021162e-04, reg: 2.287807e-01, (11 / 100)
val_acc: 0.460000, lr: 1.135527e-04, reg: 3.905040e-02, (12 / 100)
val_acc: 0.515000, lr: 6.947668e-04, reg: 1.562808e-02, (13 / 100)
val_acc: 0.531000, lr: 9.471549e-04, reg: 1.433895e-03, (14 / 100)
val_acc: 0.509000, lr: 3.140888e-04, reg: 2.857518e-01, (15 / 100)
val_acc: 0.514000, lr: 6.438349e-04, reg: 3.033781e-01, (16 / 100)
val_acc: 0.502000, lr: 3.921784e-04, reg: 2.707126e-04, (17 / 100)
val_acc: 0.509000, lr: 9.752279e-04, reg: 2.850865e-03, (18 / 100)
val_acc: 0.500000, lr: 2.412048e-04, reg: 4.997821e-04, (19 / 100)
val_acc: 0.466000, lr: 1.319314e-04, reg: 1.189915e-02, (20 / 100)
val_acc: 0.516000, lr: 8.039527e-04, reg: 1.528291e-02, (21 / 100)
```

But this best cross-validation result is worrying. Why?

Careful with best values on border

Random search vs. grid search

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

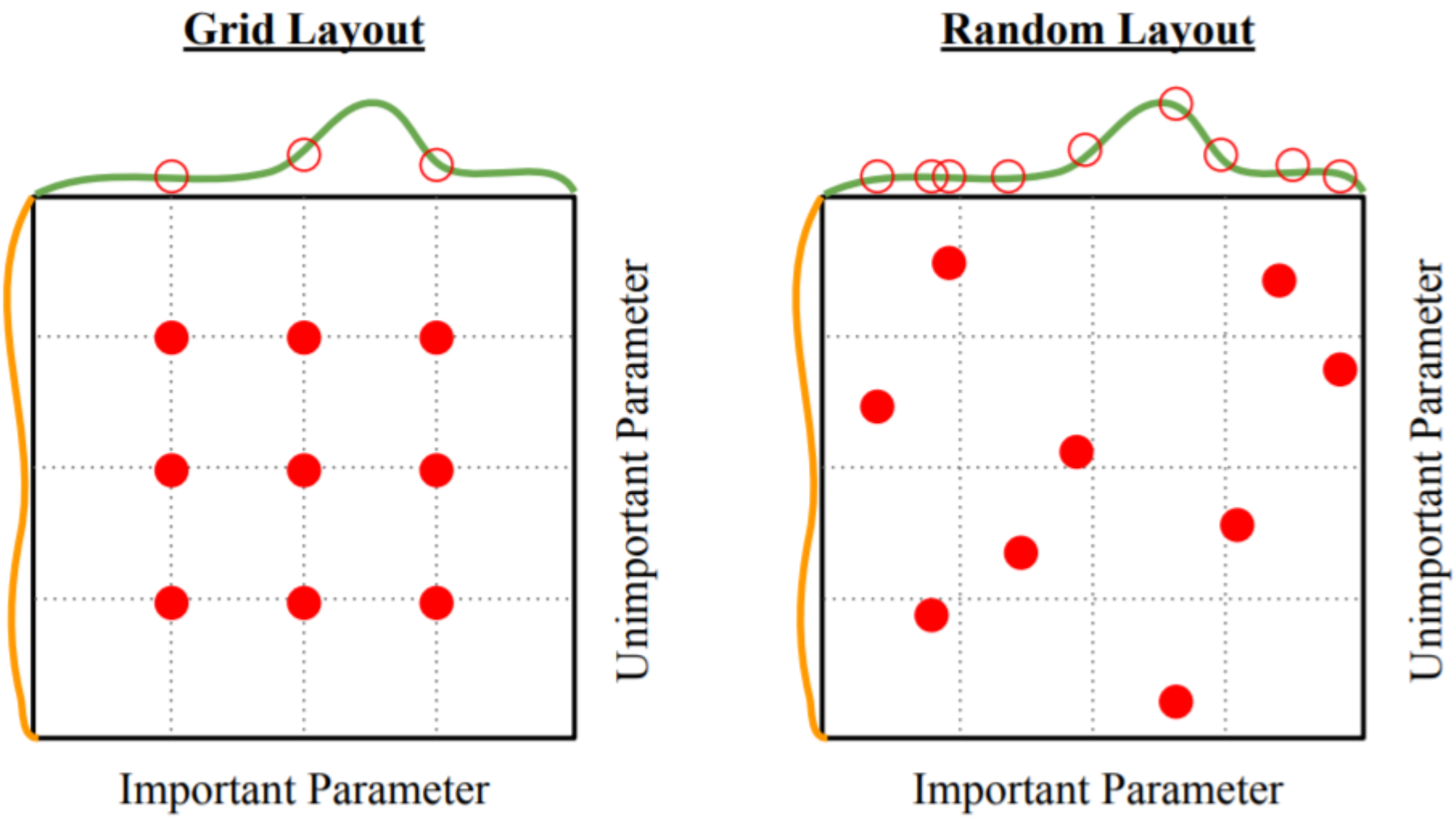


Illustration of Bergstra et al., 2012 by Shayne Longpre, copyright CS231n 2017

Random search

- Random search is more effective and richly exploring when:
  - The performance may not be such sensitive to the value of all hyperparameters (some parameters are actually much more important)
    - We don’t know it in advance
    - More distinct values of the more important hyperparameter are tried.
    - Especially when the number of hyperparameters becomes larger

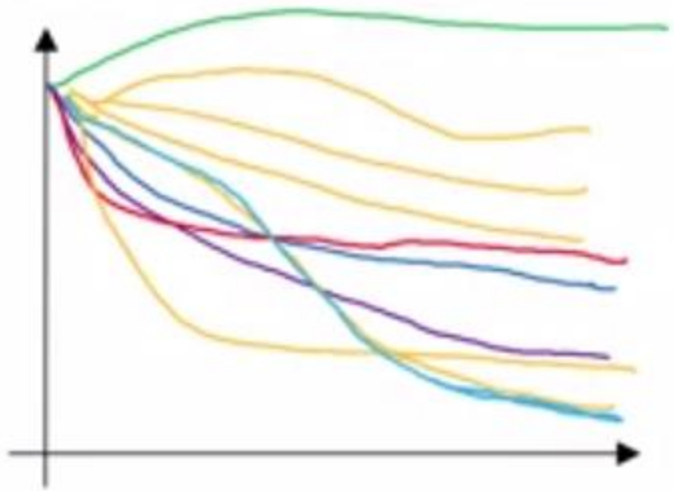
Babysitting one model vs. training models in parallel

- When we do not have sufficient computational resources to train a lot of models
  - Watching performance of one model during the time and tune its parameters by nudging them up and down

- Train many different models in parallel (with different hyperparameetrs) and just pick the one that works best

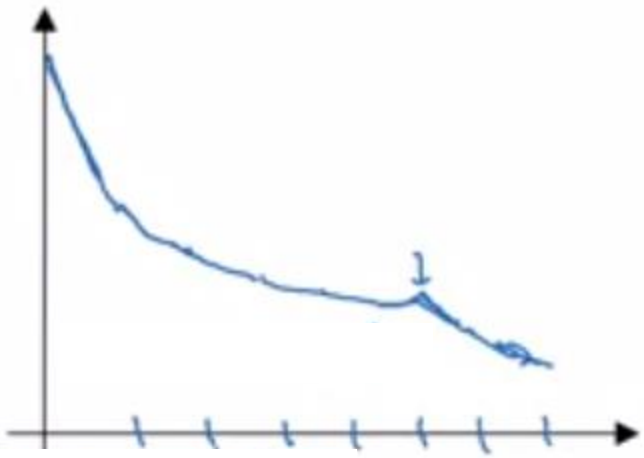
- Babysitting one model called Panda while training many models in parallel called Cavier approach for selecting hyperparameters

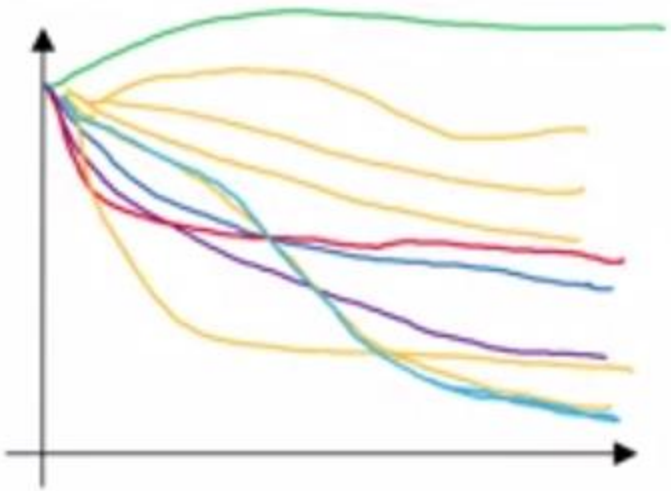
Babysitting one model vs. training models in parallel



[Andrew Ng, Deep Learning Specialization, 2017]

Babysitting one model vs. training models in parallel





Panda

Caviar

[Andrew Ng, Deep Learning Specialization, 2017]

Resources

- Deep Learning Book, Chapter 8.
- Please see the following note:
  - http://cs231n.github.io/neural-networks-3/