Training Neural Networks Generalization

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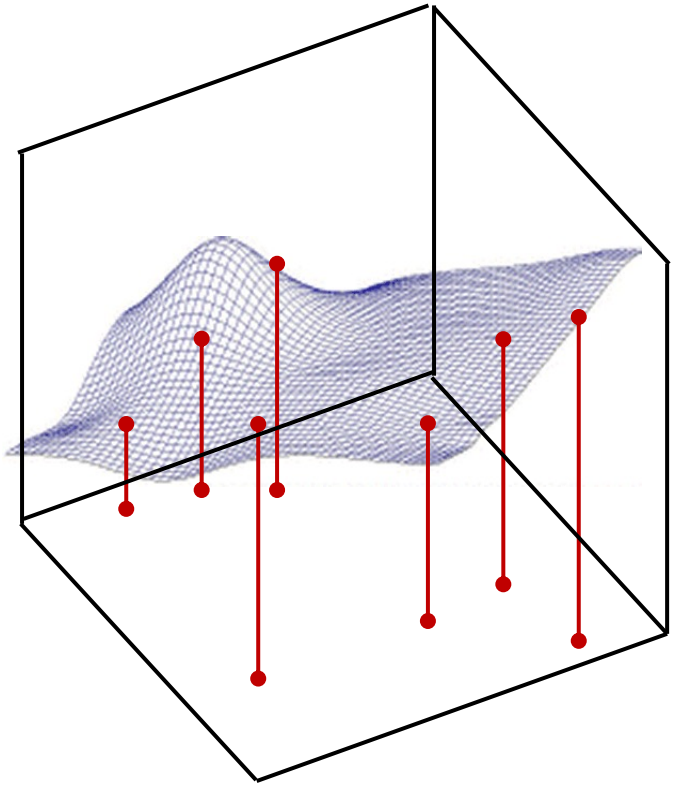
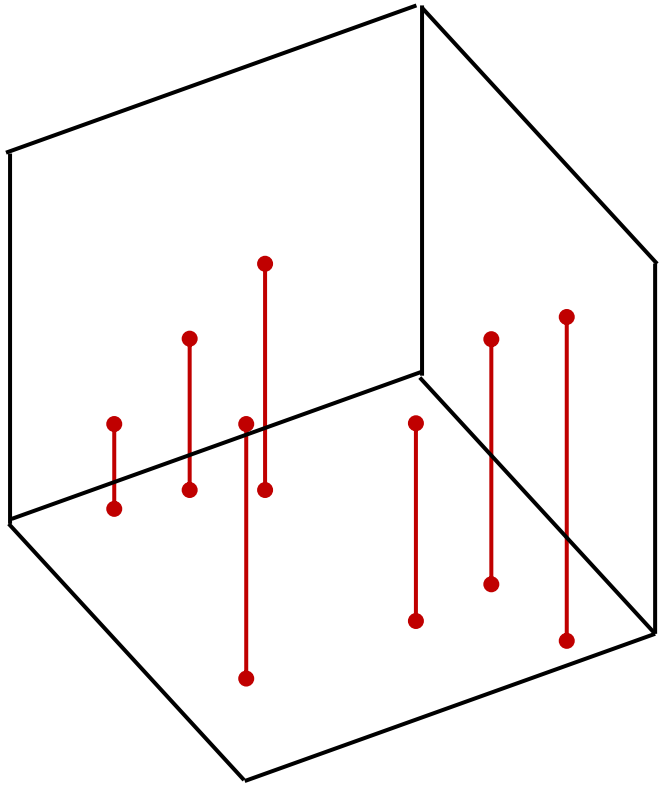
Most slides have been adapted from Bhiksha Raj, 11-785, CMU
and some from Fei Fei Li et. al, cs231n, Stanford

Outline

- Generalization
- Regularization
- Early stopping
- Model ensembles
- Drop-out
- Data Augmentation
- Common regularization pattern

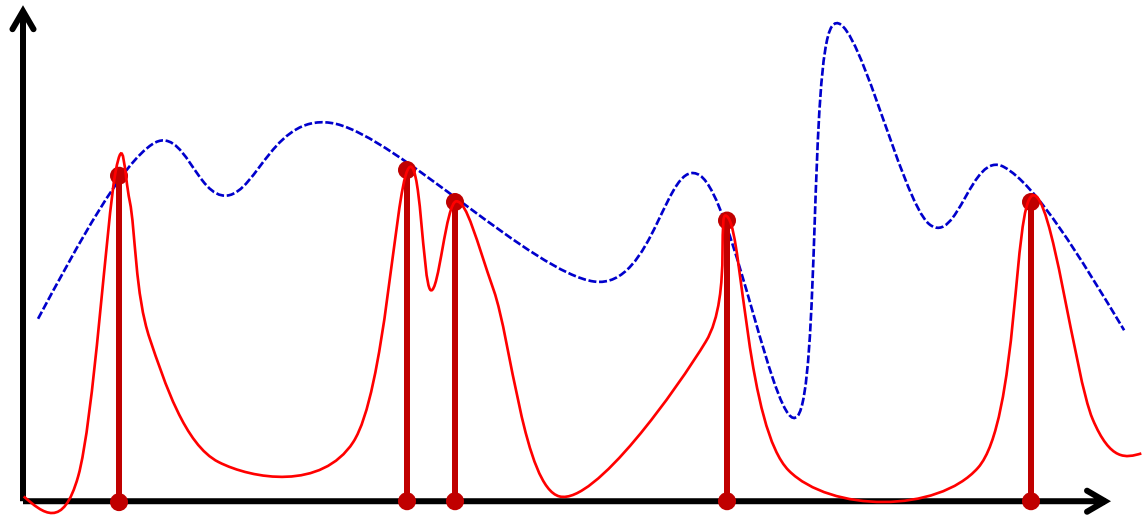
Learning the network





- We attempt to learn an entire function from just a few *snapshots* of the target function

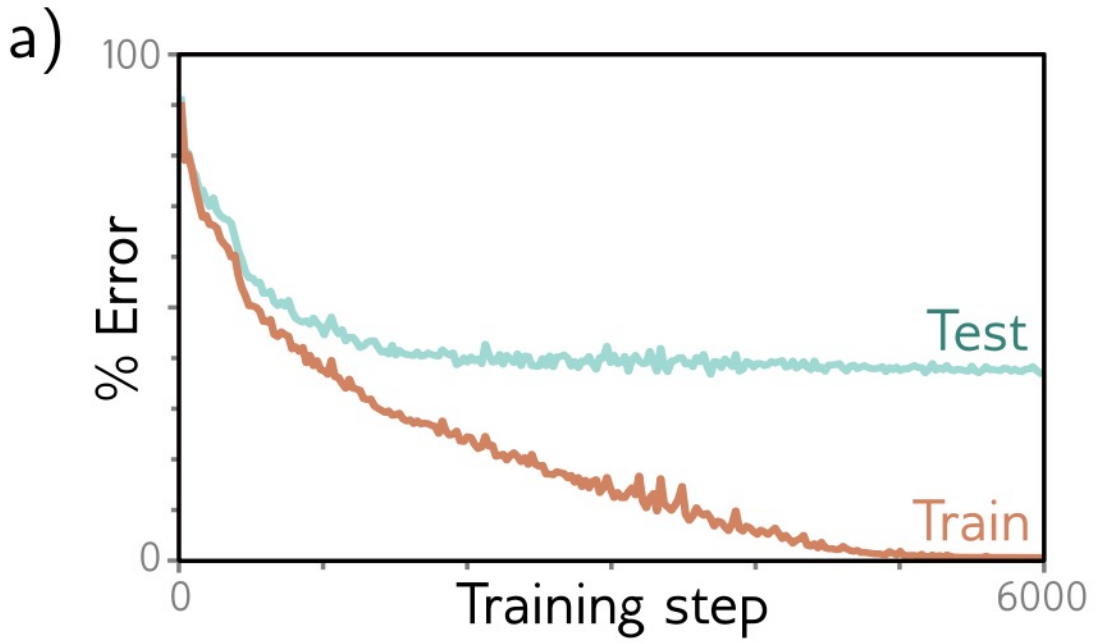
Overfitting

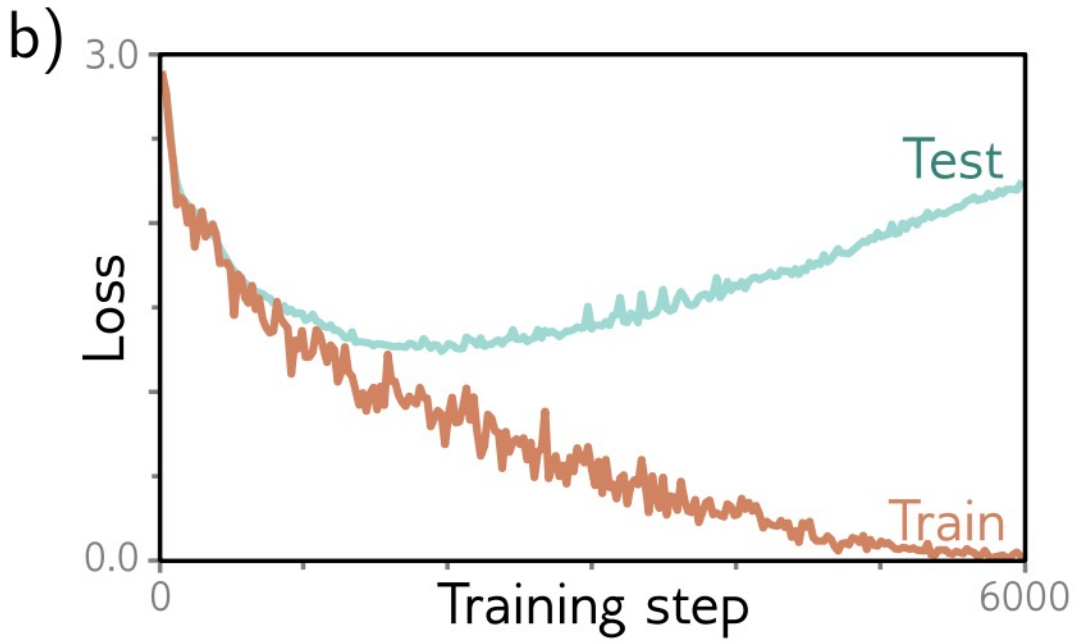


- Problem: Network may just learn the values at the inputs
  - Learn the red curve instead of the dotted blue one
    - Given only the red vertical bars as inputs

Beyond training error

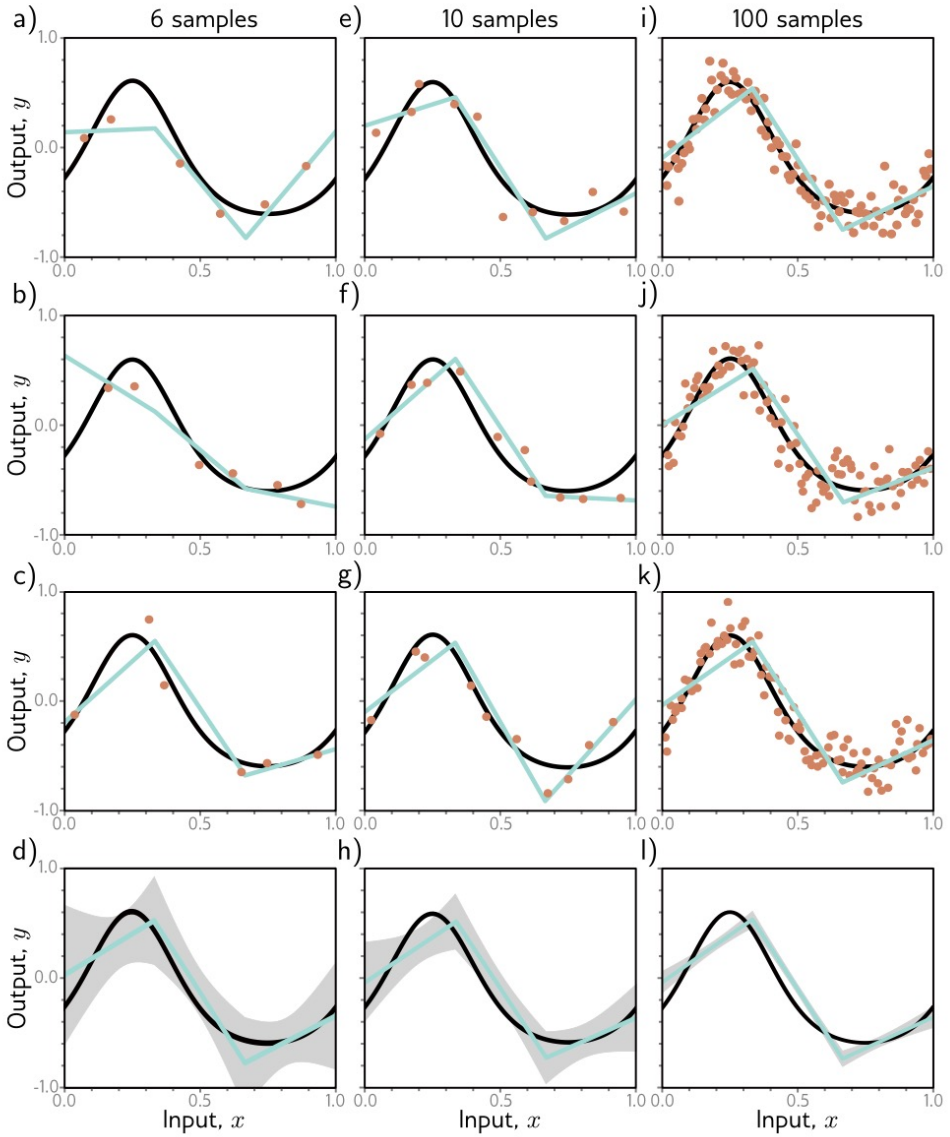
- Better optimization techniques help to reduce training loss
- Generalization gap: How to reduce generalization gap?





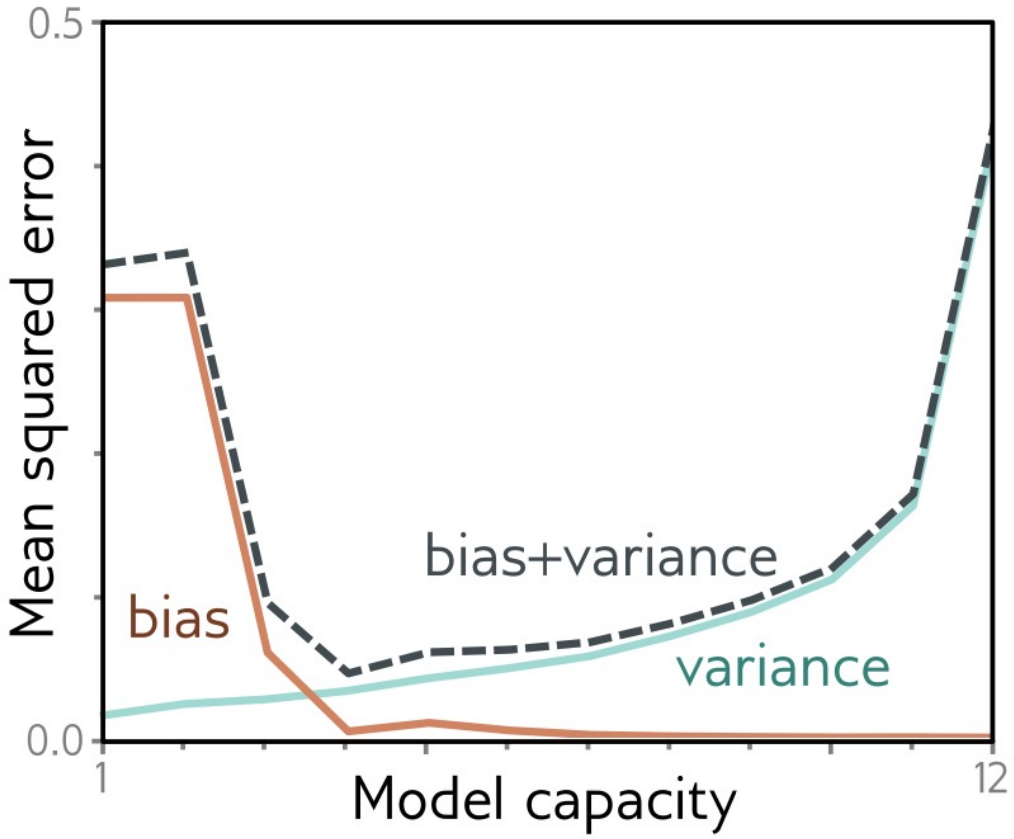
Understanding Deep Learning, 2023

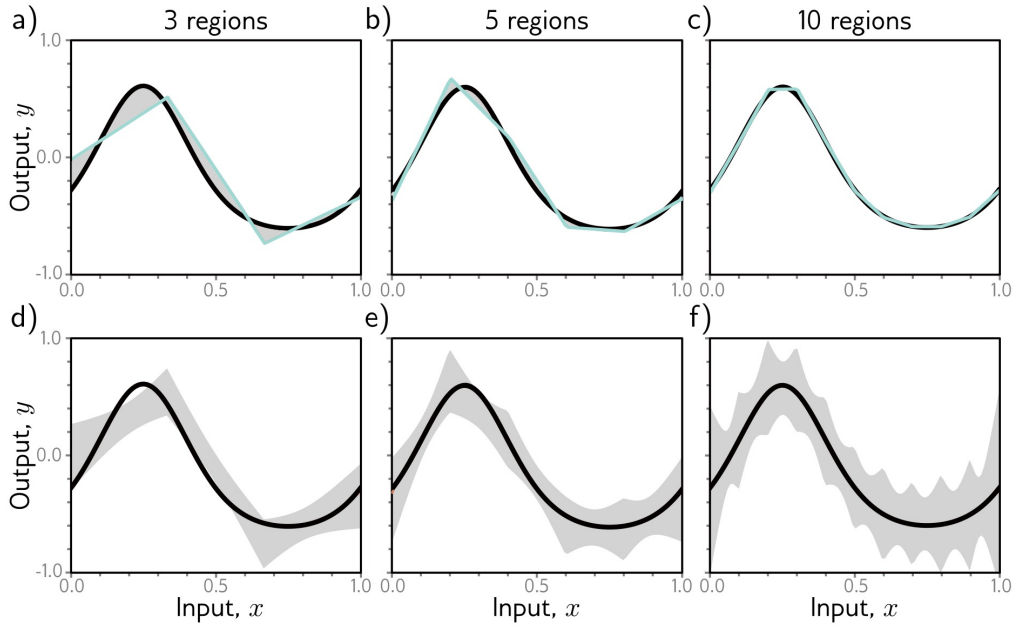
Variance of trained models on different sample sets



Understanding Deep Learning, 2023

Bias-variance trade-off





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Regularization

$$J(W) = \sum_{n=1}^{N} loss\left(y^{(n)}, f(y^{(n)}, W)\right) + \lambda R(W)$$

- How to reduce the generalization gap between training and test performance?

- Adding explicit terms to the loss function that inject our inductive biases

L2 regularization: Weight decay

$$L(W) = \sum_{n=1}^{N} loss\left(y^{(n)}, f(y^{(n)}, W)\right)$$

$$J(W) = L(W) + \lambda \|W\|^2$$

$$W \leftarrow W - \alpha \nabla_W L(W) - 2\lambda W$$

$$W \leftarrow W(1 - 2\lambda) - \alpha \nabla_W L(W)$$

Weight decay

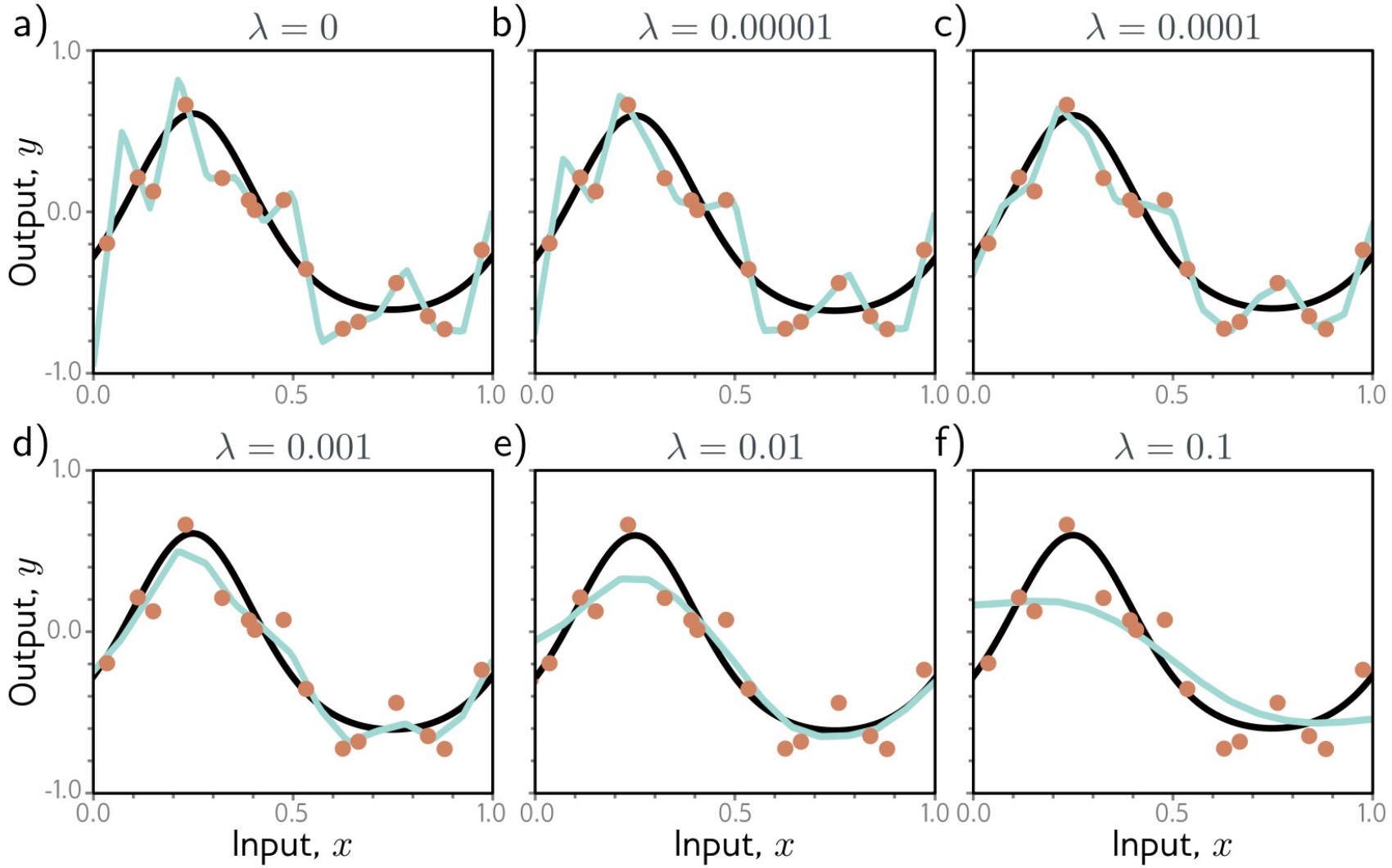
It is usually applied to the weights but not the biases

Regularization parameter

- λ is the regularization parameter whose value depends on how important it is for us to want to impose the regularizer

- Increasing λ assigns greater importance to shrinking the weights
  - Make greater error on training data, to obtain a more acceptable network

Regularization parameter



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Why L2 regularization?

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

- Encouraging smaller weights, so the output function is smoother

Regularization: Add term to loss

$$J(W) = \frac{1}{N}\sum_{n=1}^{N} loss(y^{(n)}, f(x^{(n)}, W)) + \lambda R(W)$$

In common use:

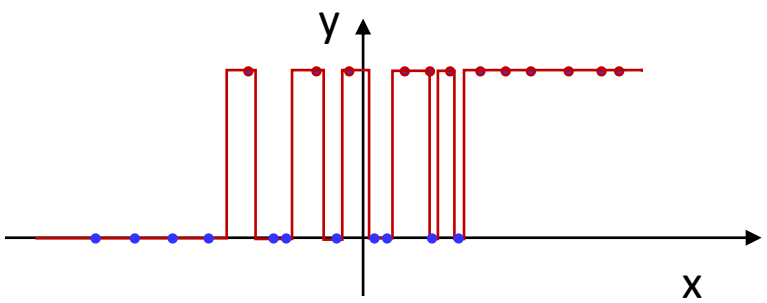
L2 regularization $R(W) = \sum_k \sum_l W_{k,l}^2$ (Weight decay)

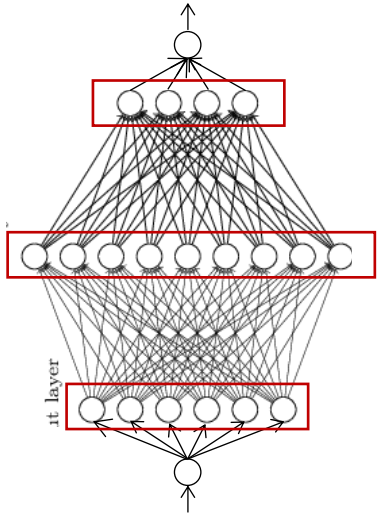
L1 regularization $R(W) = \sum_k \sum_l |W_{k,l}|$

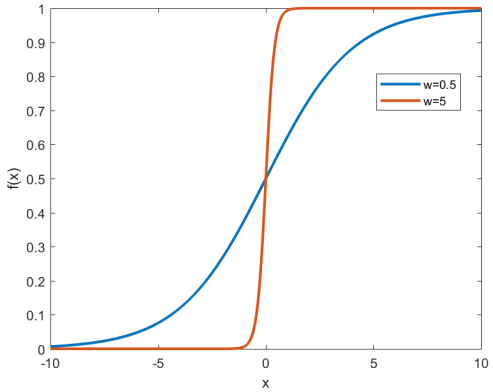
Elastic net (L1 + L2) $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$

Regularization and different activation functions

- ReLU: Lower slope for piecewise linear functions
- Sigmoid or tanh: Small W linear regime
  - A deep network with small W can also act as a near linear function
  - Steep changes facilitate overfitted responses by neurons with large w







As $|w|$ increases, the response becomes steeper

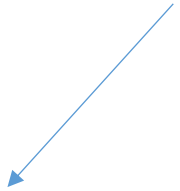
Probabilistic perspective of regularization

- MAP estimation instead of ML estimation

$$\underset{W}{\operatorname{argmax}}\, p(W|D) = \underset{W}{\operatorname{argmax}}\, p(D|W)P(W)$$

$$\underset{W}{\operatorname{argmax}}\ \log p(W) \prod_{n=1}^{N} p\left(y^{(n)}|f(x^{(n)};W)\right)$$

$$\underset{\phi}{\operatorname{argmax}} \log p(W)\ + \sum_{n=1}^{N} \log p\left(y^{(n)}\middle|f\left(x^{(n)};\phi\right)\right)$$



$$p(W) = N(0, \alpha^2 I)$$

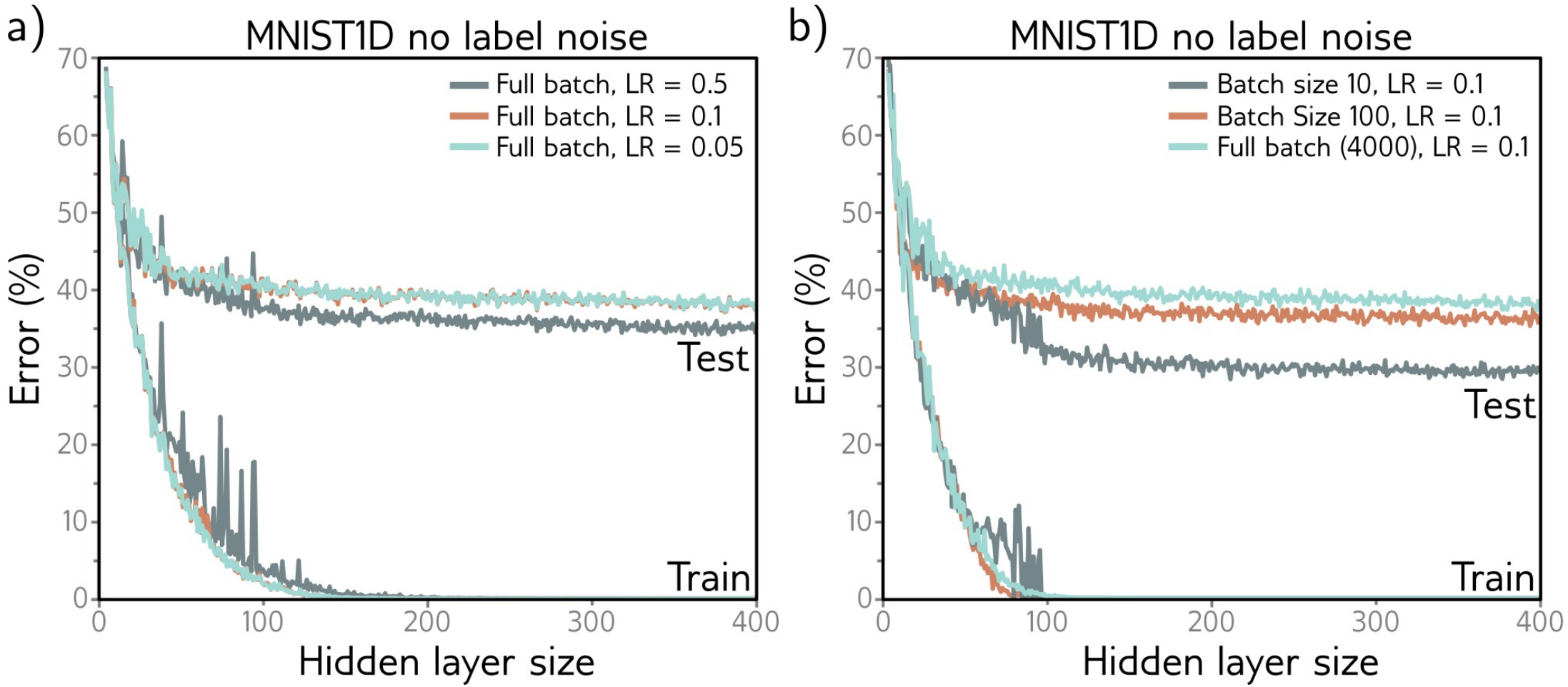
Implicit regularization

- SGD generalizes better than gradient descent
  - smaller batch sizes may perform better than larger ones
  - The inherent randomness allows to reach different parts of the loss function.

- Implicit regularization: a preference for some solutions over others
  - encourages solutions where all the data fits well (so the batch variance is small)
  - rather than solutions where some of data fit extremely well and other data less well

- SGD implicitly favors places where the gradients are stable (where all the batches agree on the slope)

SGD: Generalization



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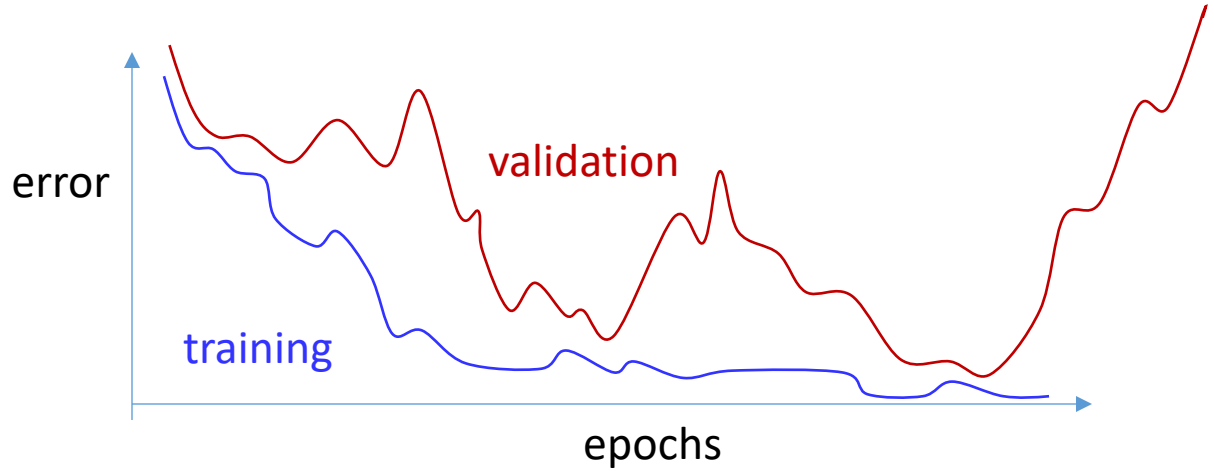
Early stopping

- Stopping the training procedure before it has fully converged

- One way of thinking about this is L2 regularization since the weights are initialized to small values
  - they simply don't have time to become large

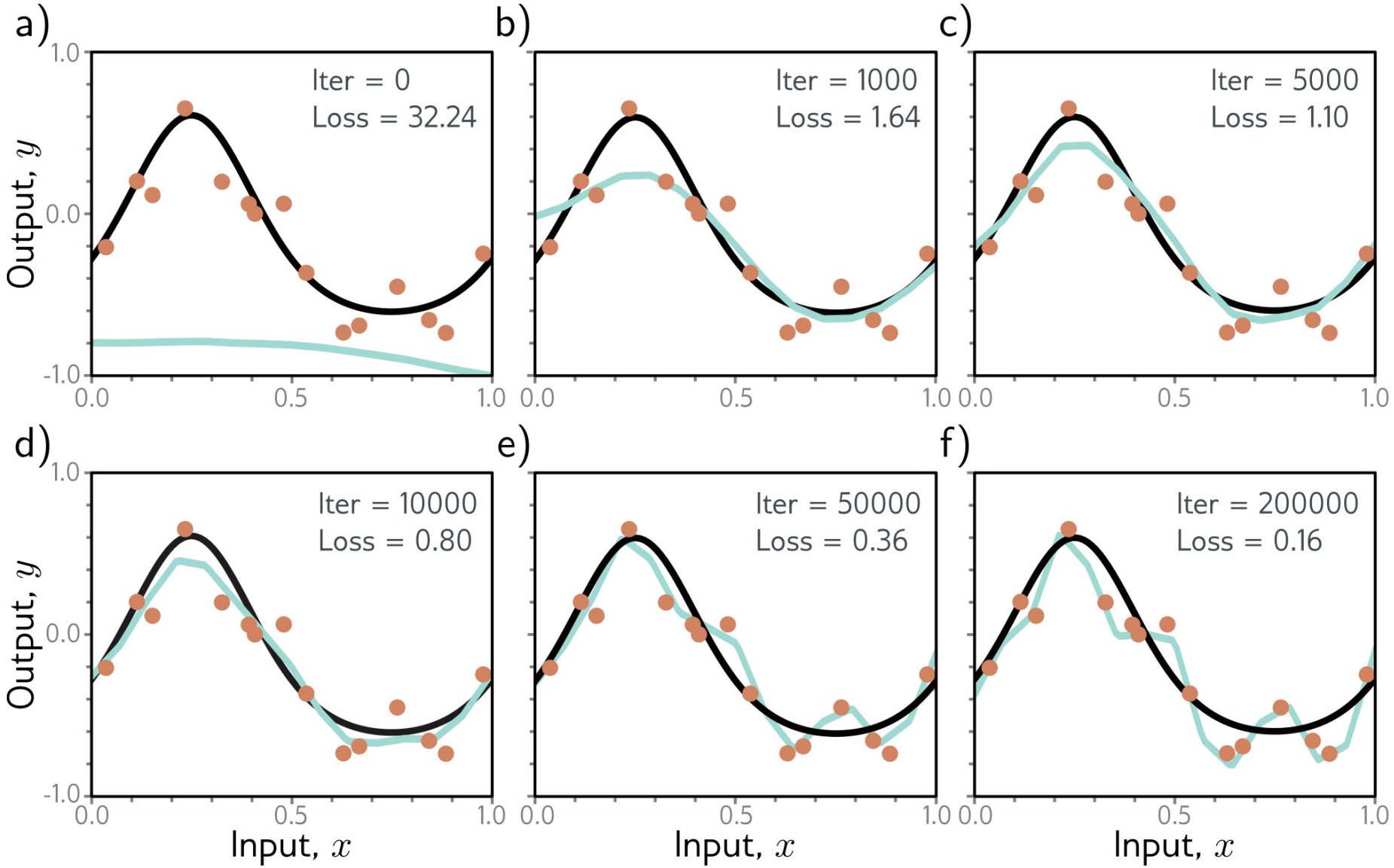
- Early stopping has a single hyperparameter
  - the number of steps after which learning is terminated

Early stopping



- Continued training can result in over fitting to training data
  - Track performance on a held-out validation set
  - Apply one of several early-stopping criterion to terminate training when performance on validation set degrades significantly

Early stopping: Example



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Model ensembles

1. Train multiple models

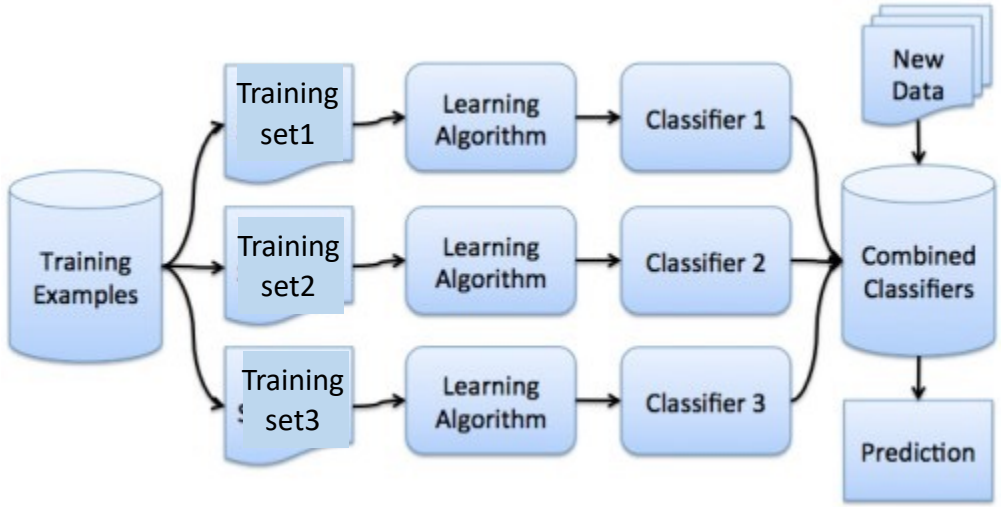
2. At test time average their results

Model ensembles

- Train multiple models, and at test time average their predictions.
  - Mean or median of the outputs (for regression problems)
  - the most frequent predicted class or mean of the pre-softmax activations (for classification problems)

- Candidates
  - **Training multiple models**
  - **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.

A brief detour.. Bagging

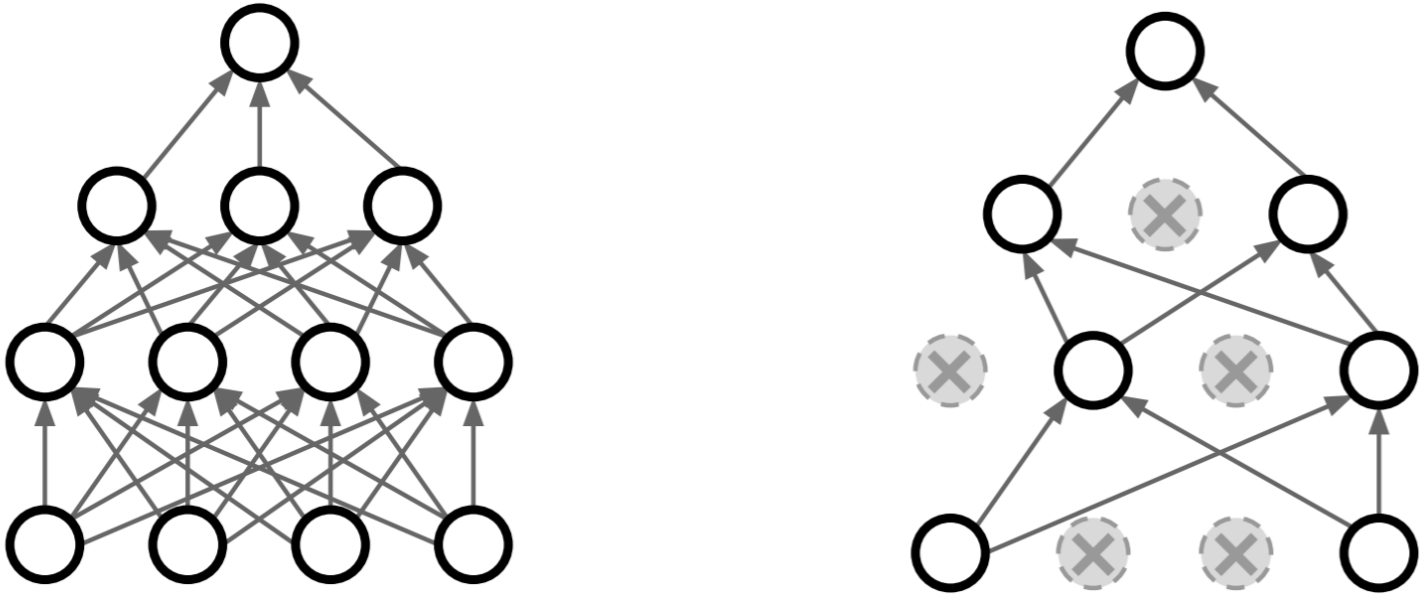


- Popular method proposed by Leo Breiman:
  - Sample training data and train several different classifiers
  - Classify test instance with entire ensemble of classifiers
  - Vote across classifiers for final decision
  - Empirically shown to improve significantly over training a single classifier from combined data

Regularization: Dropout

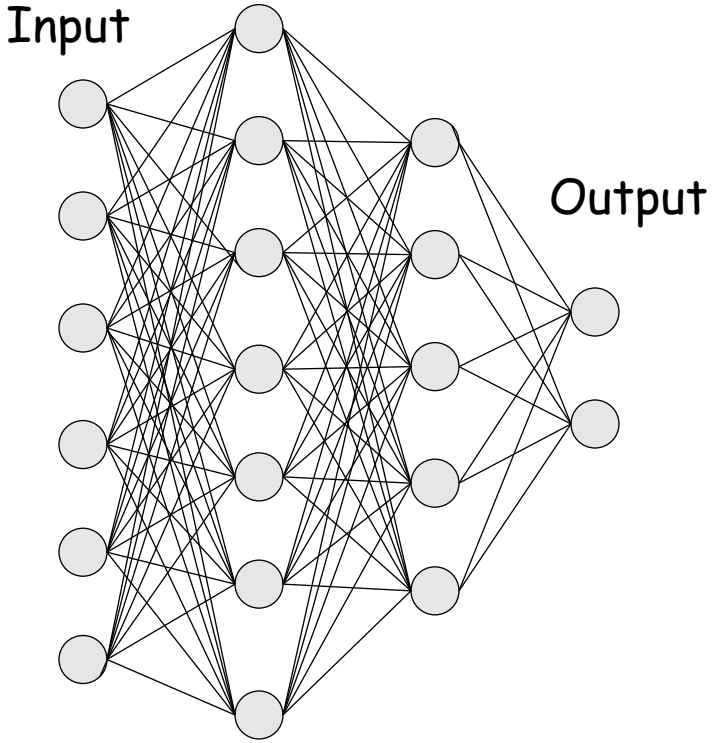
Srivastava et al, “Dropout: A simple way to prevent neural networks from overfitting”, JMLR 2014

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



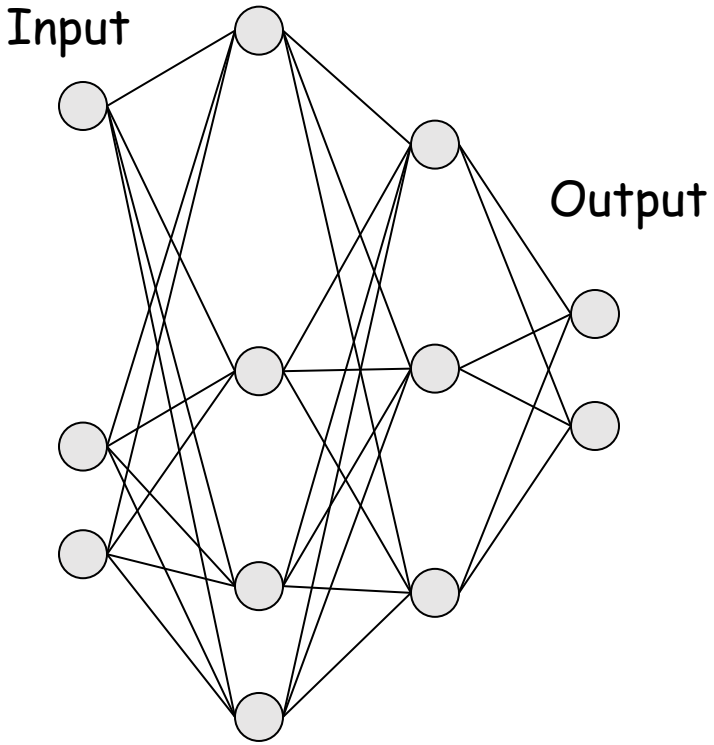
- Thus, a smaller network is trained for each sample
  - Smaller network provides a regularization effect

Dropout



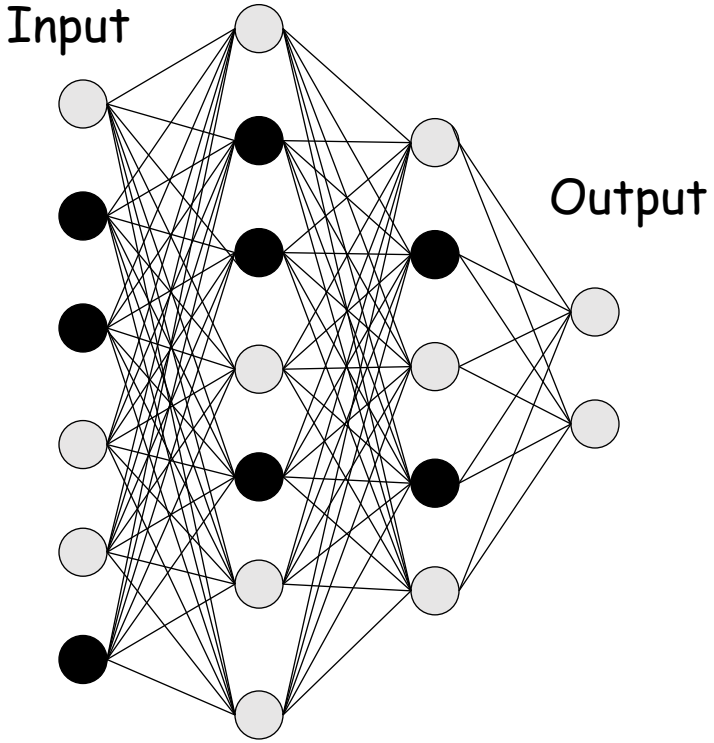
- **During training:** For each input, at each iteration, “turn off” each neuron with a probability 1-α
  - α shows keep probability

Dropout



- **During training:** For each input, at each iteration, "turn off" each neuron with a probability 1-α
  - Also turn off inputs similarly

Dropout



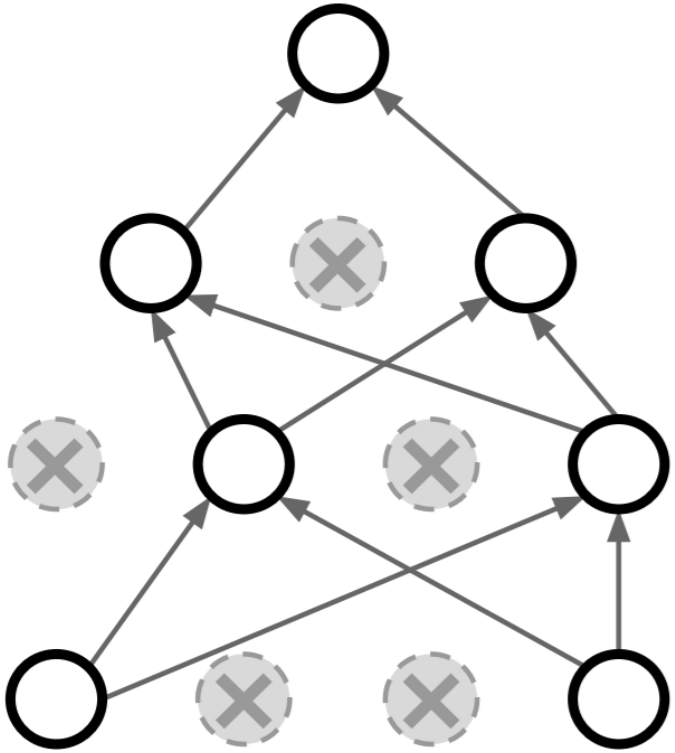
- **During training:** For each input, at each iteration, "turn off" each neuron (including inputs) with a probability 1-α
  - In practice, set them to 0 according to the success of a Bernoulli random number generator with success probability 1-α

Implementing dropout

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

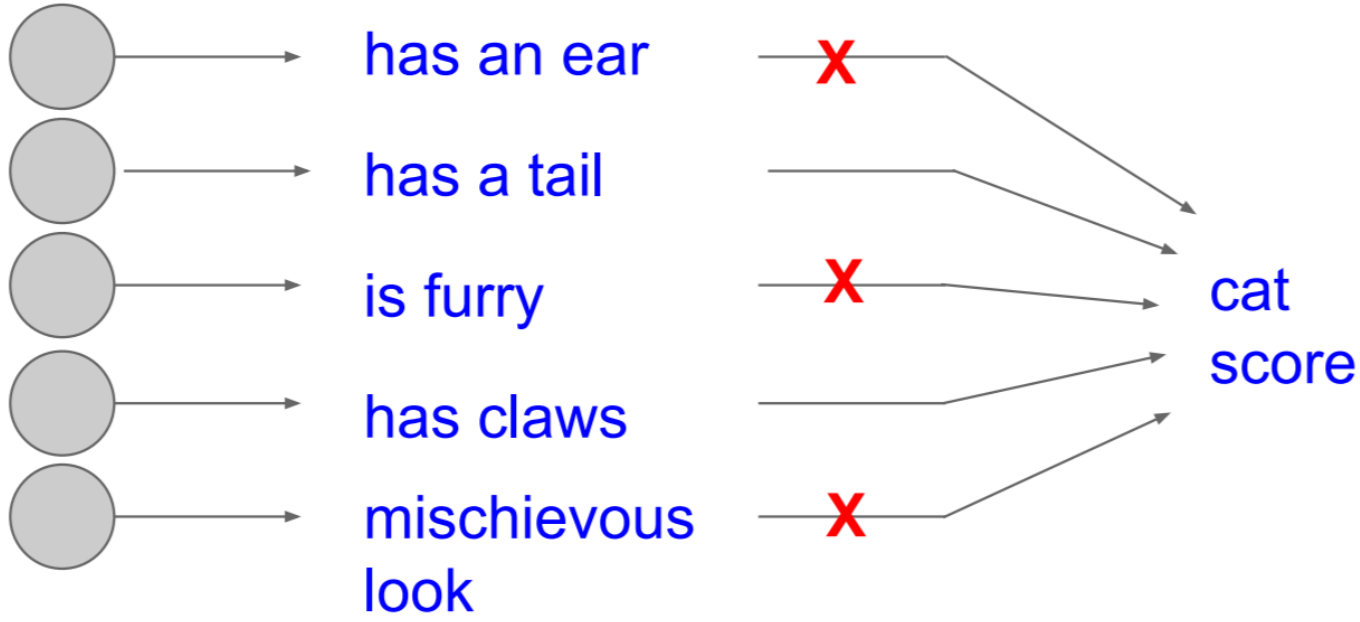
Regularization: Dropout

- How can dropout be a good idea?



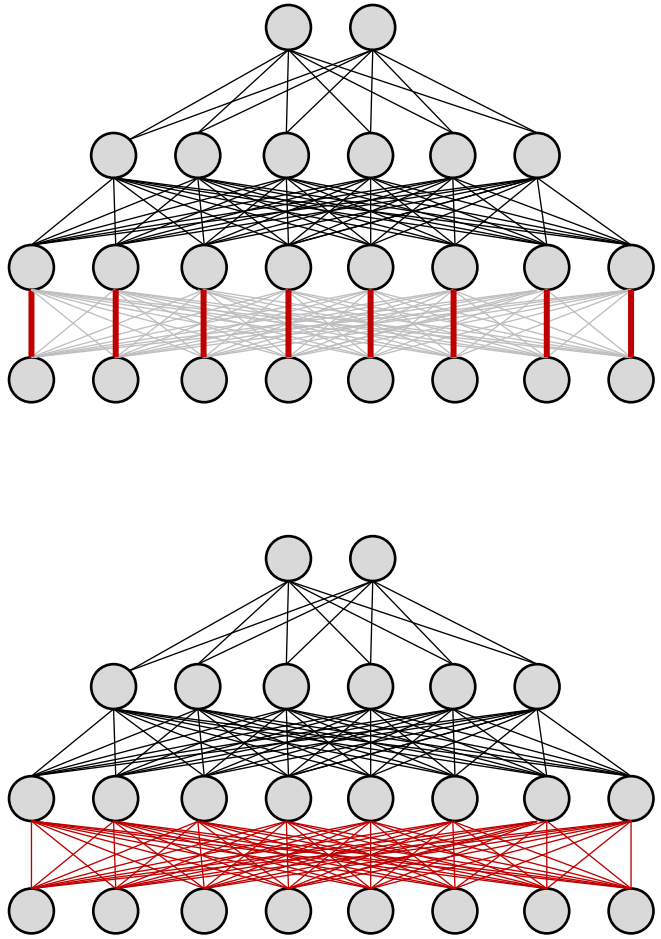
Forces the network to have a redundant representation;
Prevents co-adaptation of features

[Hinton et al., 2012]

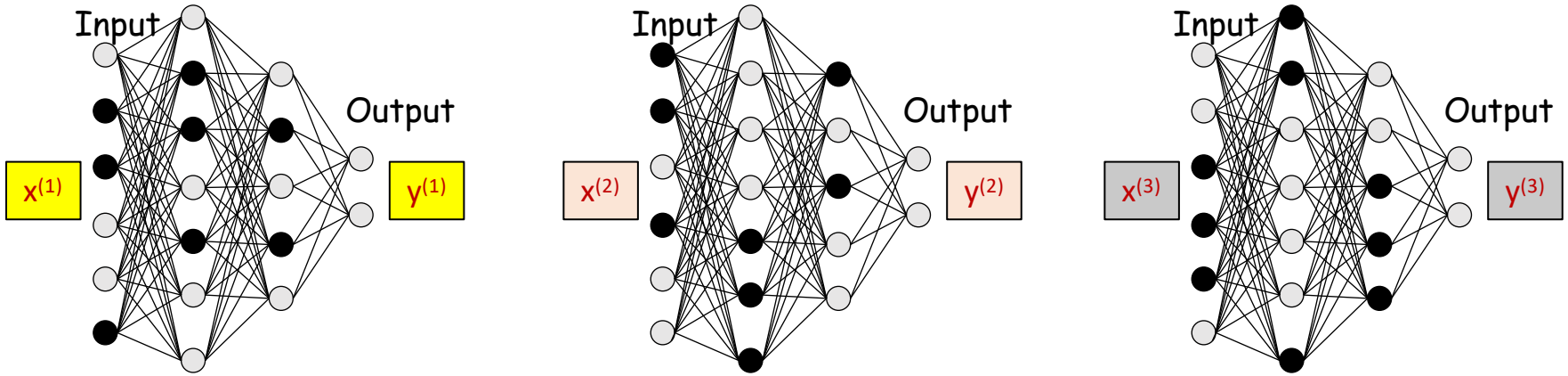


Dropout as a mechanism to increase pattern density

- Dropout forces the neurons to learn “rich” and redundant patterns
- E.g. without dropout, a non-compressive layer may just “clone” its input to its output
  - Transferring the task of learning to the rest of the network
- Dropout forces the neurons to learn denser patterns
  - With redundancy



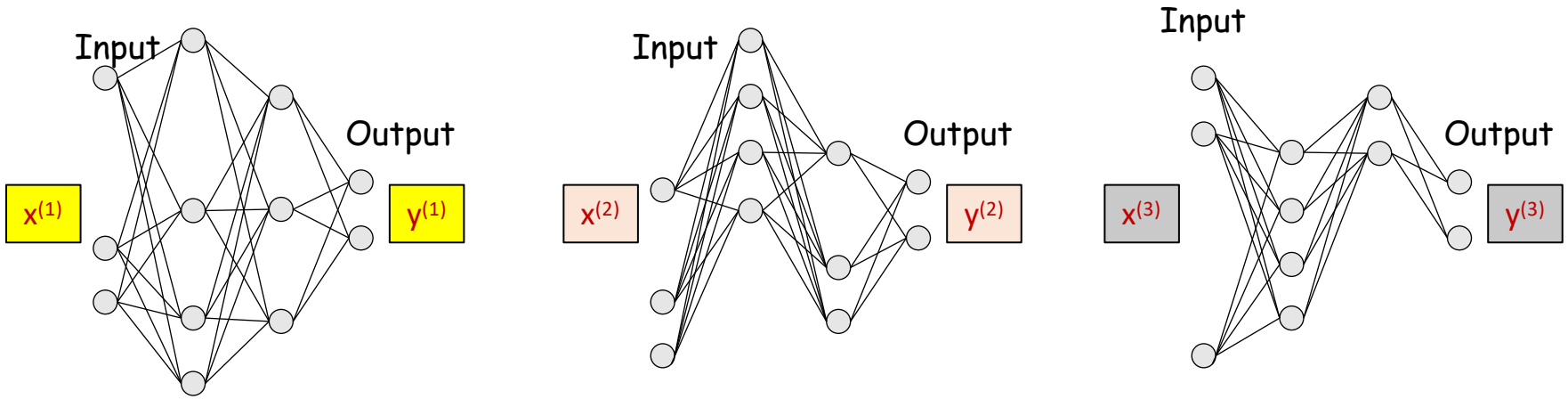
Dropout



The pattern of dropped nodes changes for *each input*
i.e. in every pass through the net

- **During training:** For each input, at each iteration, "turn off" each neuron (including inputs) with a probability 1-α

Dropout



The pattern of dropped nodes changes for *each input*
i.e. in every pass through the net

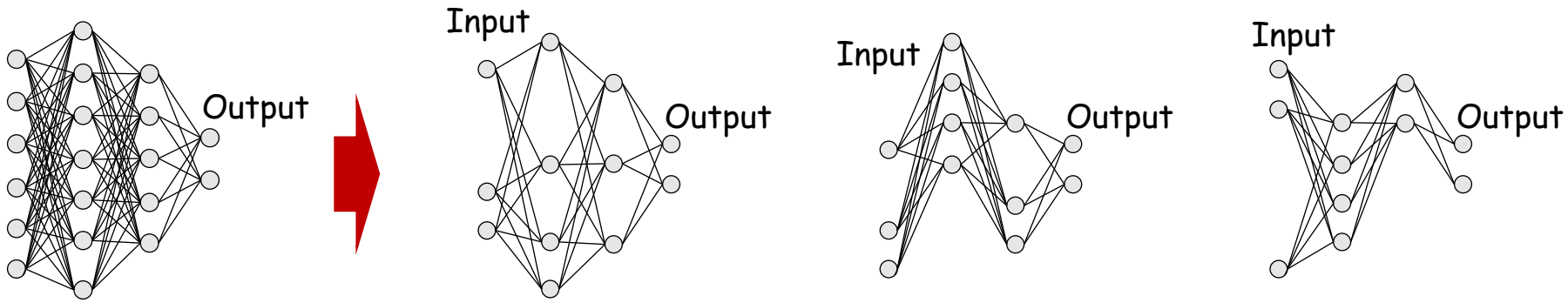
- **During training:** Backpropagation is effectively performed only over the remaining network
  - The effective network is different for different inputs
  - Gradients are obtained only for the weights and biases *from* "On" nodes *to* "On" nodes
    - For the remaining, the gradient is just 0

Why does drop-out work?

- **Intuition I**: It cannot rely on any one feature

- This makes the network less dependent on any unit and thus encourages the weights to have smaller magnitudes
  - similar effect to the L_2 regularization

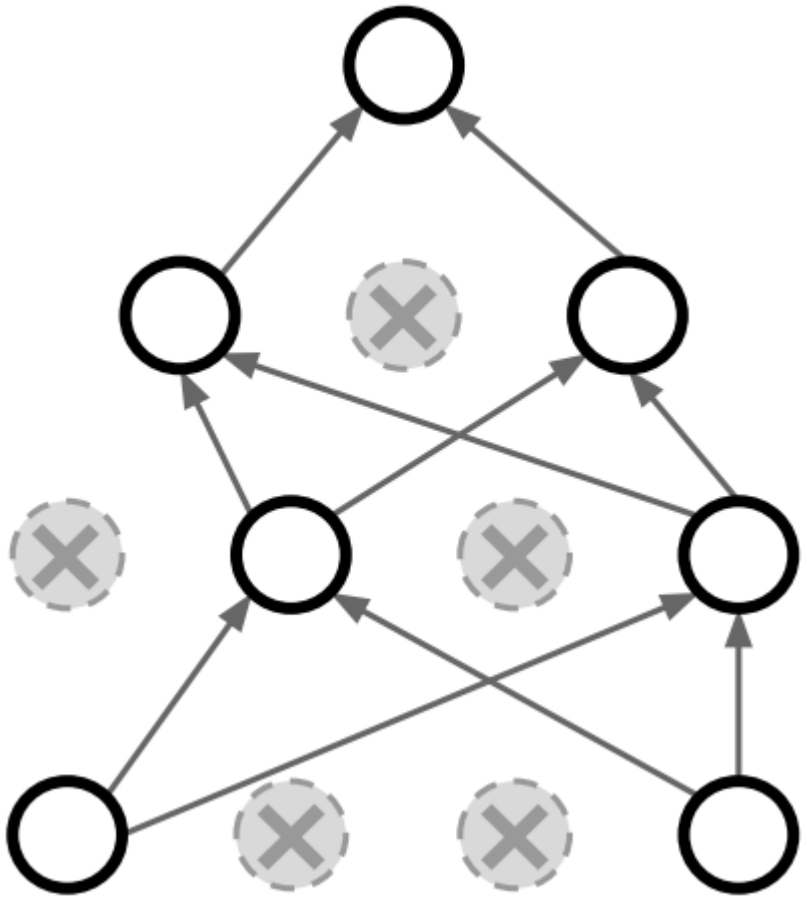
Why does drop-out work?



- For a network with a total of M neurons, there are 2^{M} possible sub-networks
  - Obtained by choosing different subsets of nodes
  - Dropout *samples* over all 2^{M} possible networks
  - Effectively learns a network that *averages* over all possible networks
    - Bagging

Regularization: Dropout

- **Intuition II:** Ensemble approach



Dropout is training a **large ensemble** of models (that share parameters).

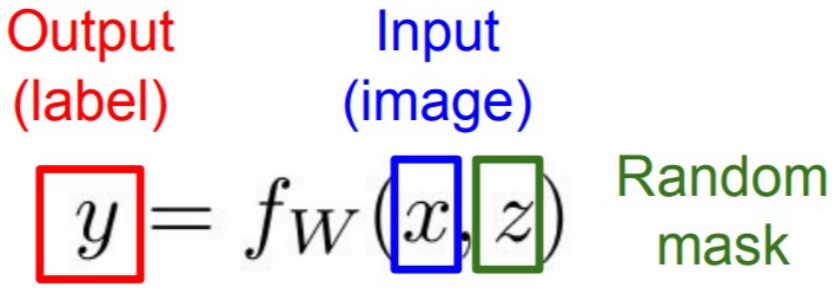
Each binary mask is one model

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!



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

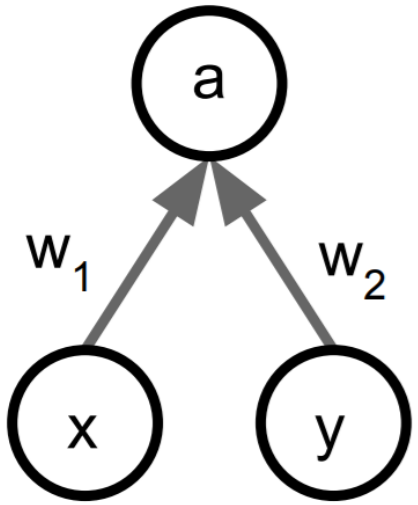
$$y = f(x) = E_z\big[f(x,z)\big] = \int p(z) f(x,z) dz$$

- But this integral seems hard …

Dropout: Test time

Want to approximate the integral

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



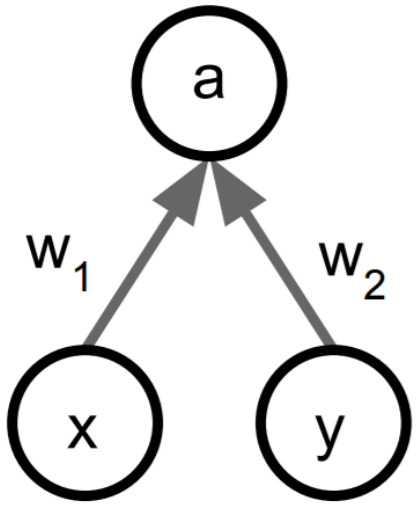
Consider a single neuron.

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

Dropout: Test time

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: $E\left[a\right] = w_1 x + w_2 y$

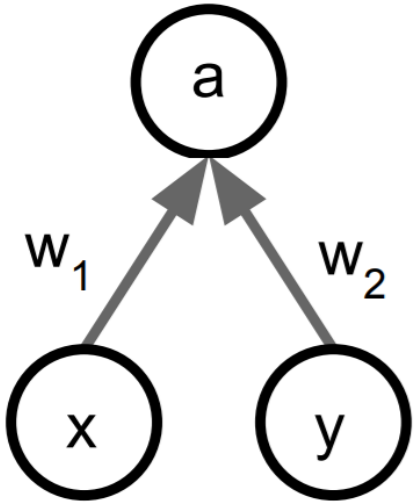
During training we have:

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

Dropout: Test time

Want to approximate the integral

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



Consider a single neuron.

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

During training we have:

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

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

What each neuron computes

- Each neuron actually has the following activation:

$$a_i^{[l]} = D\phi\left(\sum_j w_{ji}^{[l]} a_j^{[l-1]} + b_i^{[l]}\right)$$

  - Where D is a Bernoulli variable that takes a value 1 with probability α

- D may be switched on or off for individual sub networks, but over the ensemble, the *expected output* of the neuron is

$$a_i^{[l]} = \alpha\phi\left(\sum_j w_{ji}^{[l]} a_j^{[l-1]} + b_i^{[l]}\right)$$

- During *test* time, we will use the *expected* output of the neuron
  - Which corresponds to the bagged average output
  - Consists of simply scaling the output of each neuron by α

Dropout: Test time

```
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
```

At test time all neurons are active always

=> We must scale the activations so that for each neuron:

output at test time = expected output at training time

Dropout summary

```
""" 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 critical, it is 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

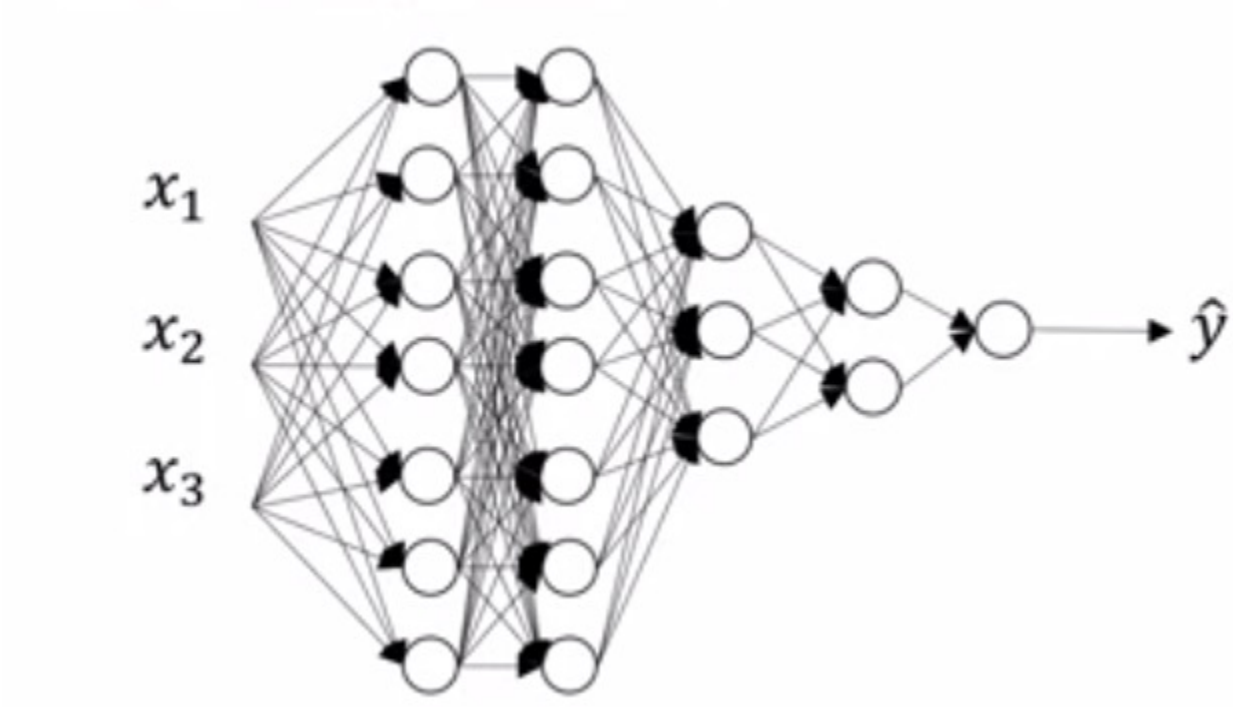
```
p = 0.5 # probability of keeping a unit active. higher = less dropout

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
```

Backward Pass

- Output layer (L) :
  - $\frac{\partial loss(a_i^{[L]}, y)}{\partial a_i^{[L]}}$
  - $\frac{\partial loss}{\partial z_i^{[L]}} = f_L'\left(z_i^{[L\}}\right)\frac{\partial loss}{\partial a_i^{[L\}}}$
- For layer $l = L - 1\ downto\ 0$
  - For $i = 1 \ldots d^{[l]}$
    - if (not dropout layer OR $mask(l, i)$)
      - $\frac{\partial loss}{\partial a_i^{[l]}} = \sum_j w_{ij}^{[l+1]} \frac{\partial loss}{\partial z_j^{[l+1]}} mask(l+1, j)$
      - $\frac{\partial loss}{\partial z_i^{[l]}} = f_l'\left(z_i^{[l]}\right)\frac{\partial loss}{\partial a_i^{[l]}}$
      - $\frac{\partial loss}{\partial w_{ij}^{[l+1]}} = a_i^{[l]} \frac{\partial loss}{\partial z_j^{[l+1]}} mask(l+1, j)$ for $j = 1 \ldots d^{[l+1]}$
    - else
      - $\frac{\partial loss}{\partial z_i^{[l]}} = 0$

Dropout on layers

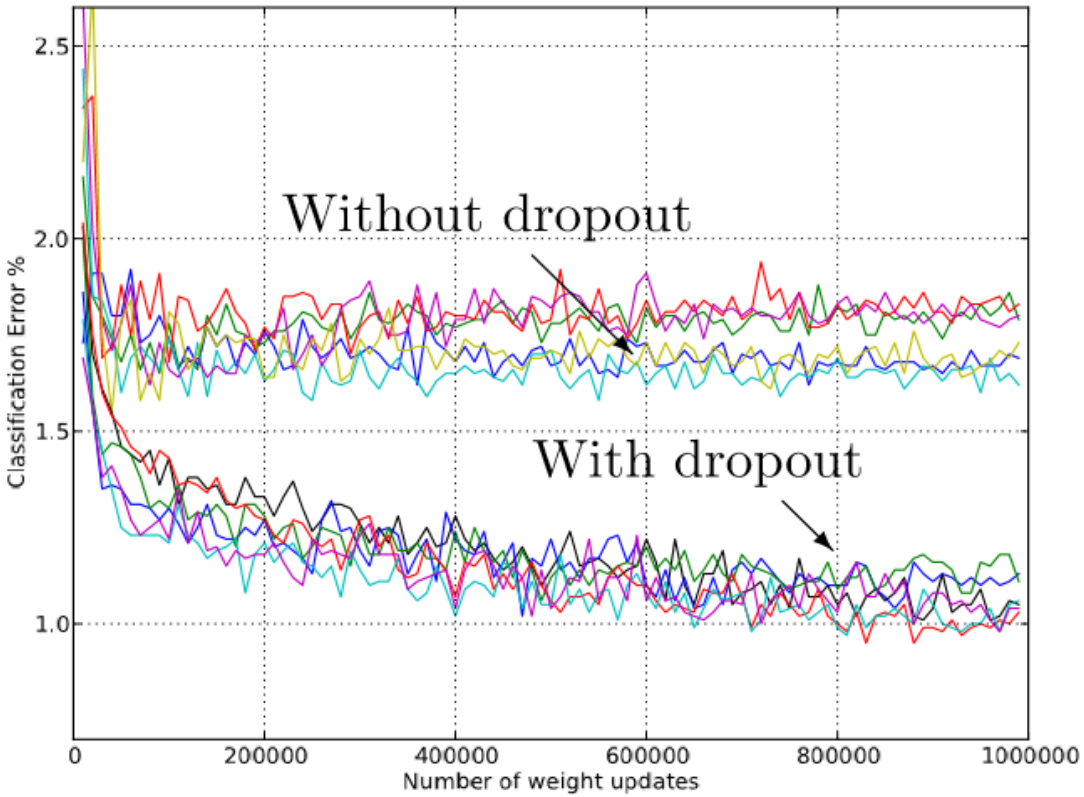
- Different keep-prob can be used for different layers
  - However, more hyper-parameters are required



Dropout issues

- If your NN is significantly overfitting, dropout usually help to prevent overfitting
- Training takes longer time but provides better generalization
  - Since in each iteration of weight update, only a subset of weights are updated.
- If your NN is not overfitting, bigger NN with dropout may help
- The cost function is no longer well defined.

Dropout: Typical results



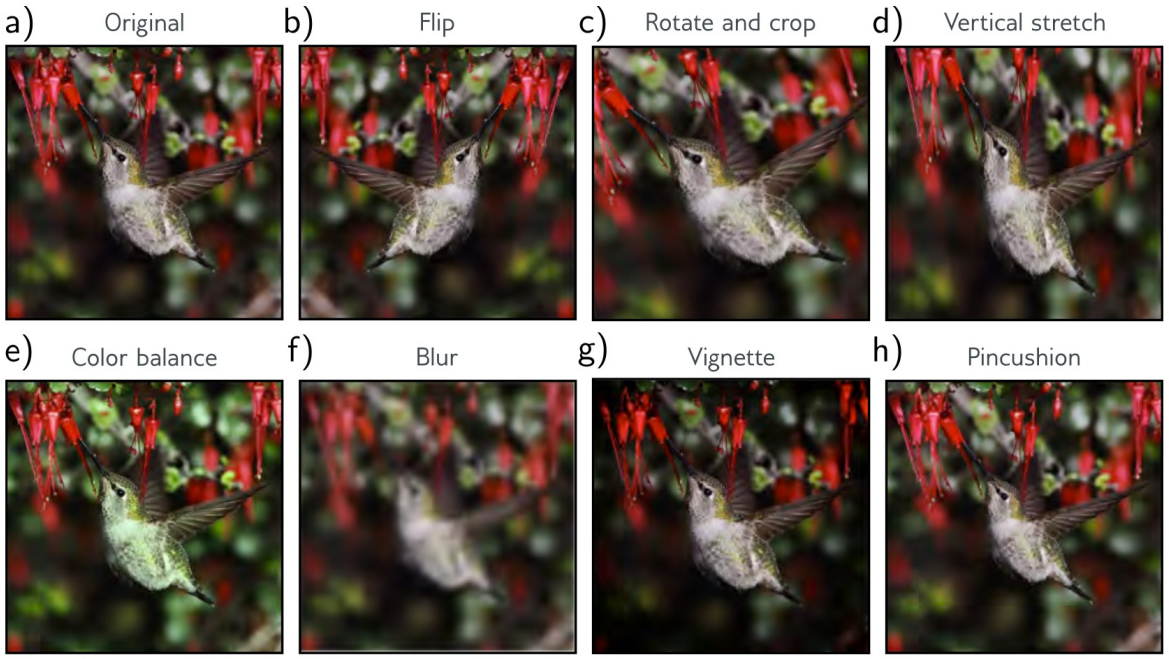
- Test error for different architectures on MNIST with and without dropout
  - 2-4 hidden layers with 1024-2048 units

Srivastava et al., 2013

Data augmentation

- Getting more training data can be expensive
- But, sometimes we can generate more training examples from the datasets
- transform each input data example in such a way that the label stays the same

Additional heuristics: Data augmentation



Understanding Deep Learning, 2023

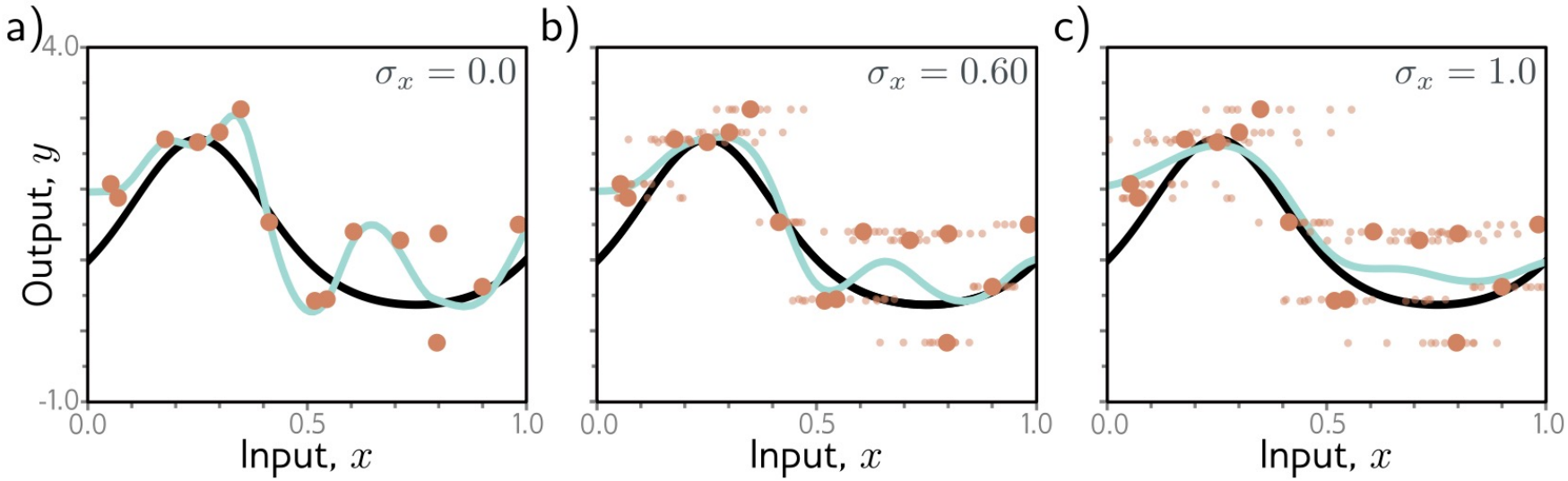
- Available training data will often be small
- "Extend" it by distorting examples in a variety of ways to generate synthetic labelled examples

Applying noise

- Input data
- Weights
- Labels

Applying noise

- **Input data**
- Weights
- Labels



Understanding Deep Learning, 2023

Applying noise

- Input data
- **Weights**
  - encourages sensible predictions even for small perturbations of the weights
- Labels

Applying noise

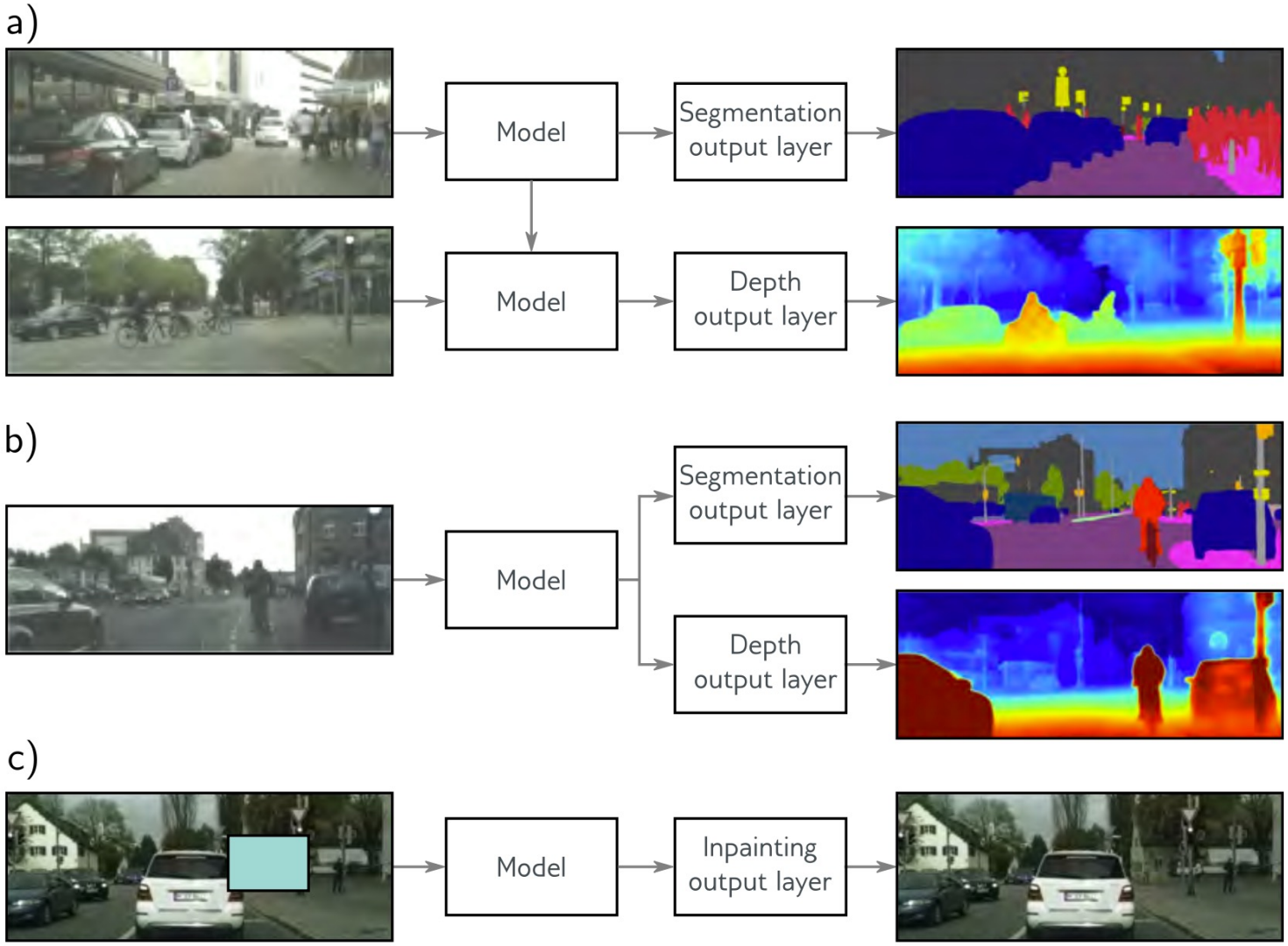
- Input data
- Weights
- **Labels**
  - MLE for multiclass classification is pushed to overconfident behavior
    - very large logit for the correct class and very small logit for the wrong classes
  - randomly changing a subset of the labels at each training iteration to avoid the above problem

Inductive bias via architecture: Weight sharing

- Inductive bias injecting into a network to express some known invariances

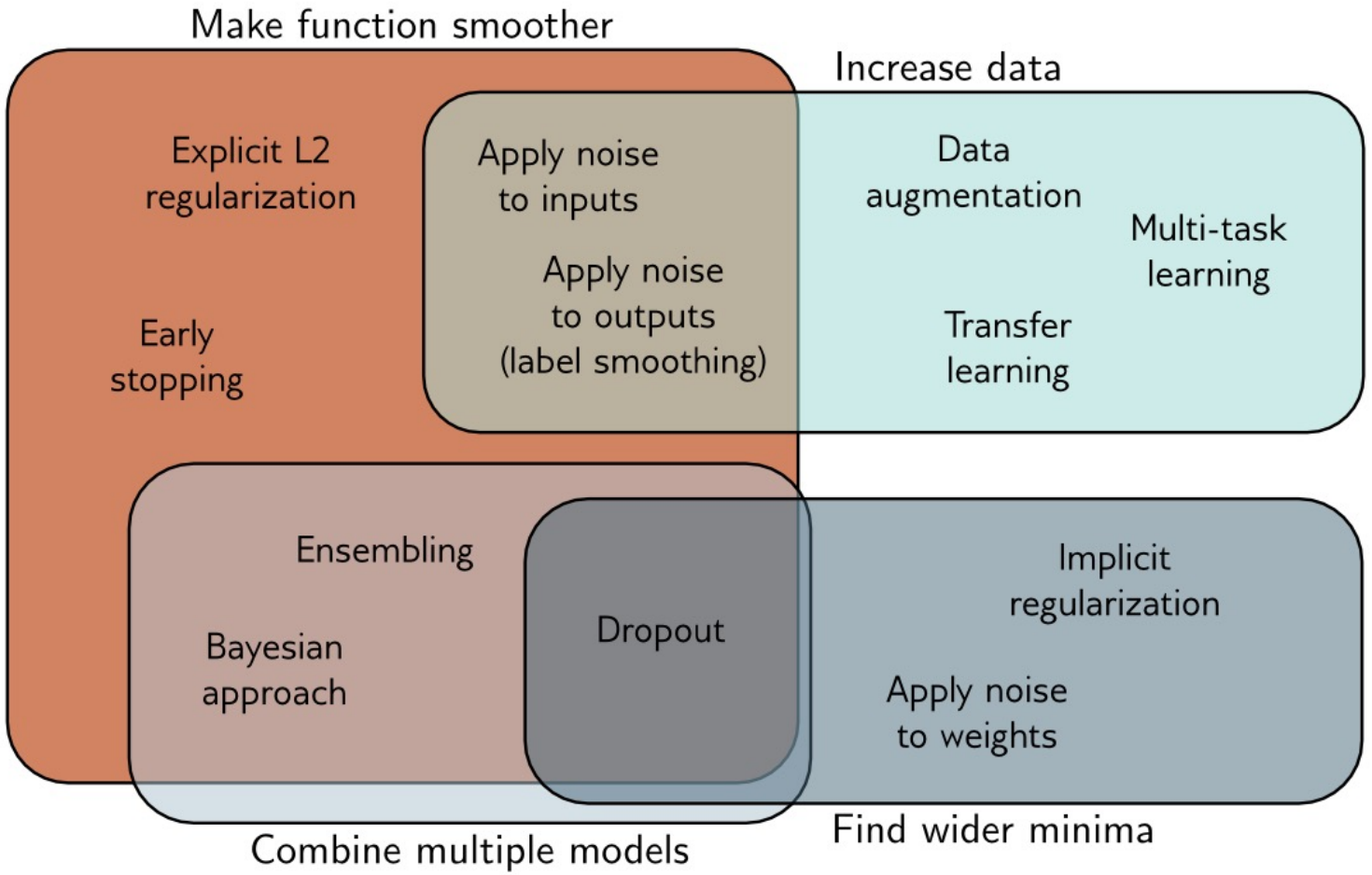
- Parameter or weight sharing
  - forming weights into groups and requiring that all weights of each group share the same value

Generalization by learning approach



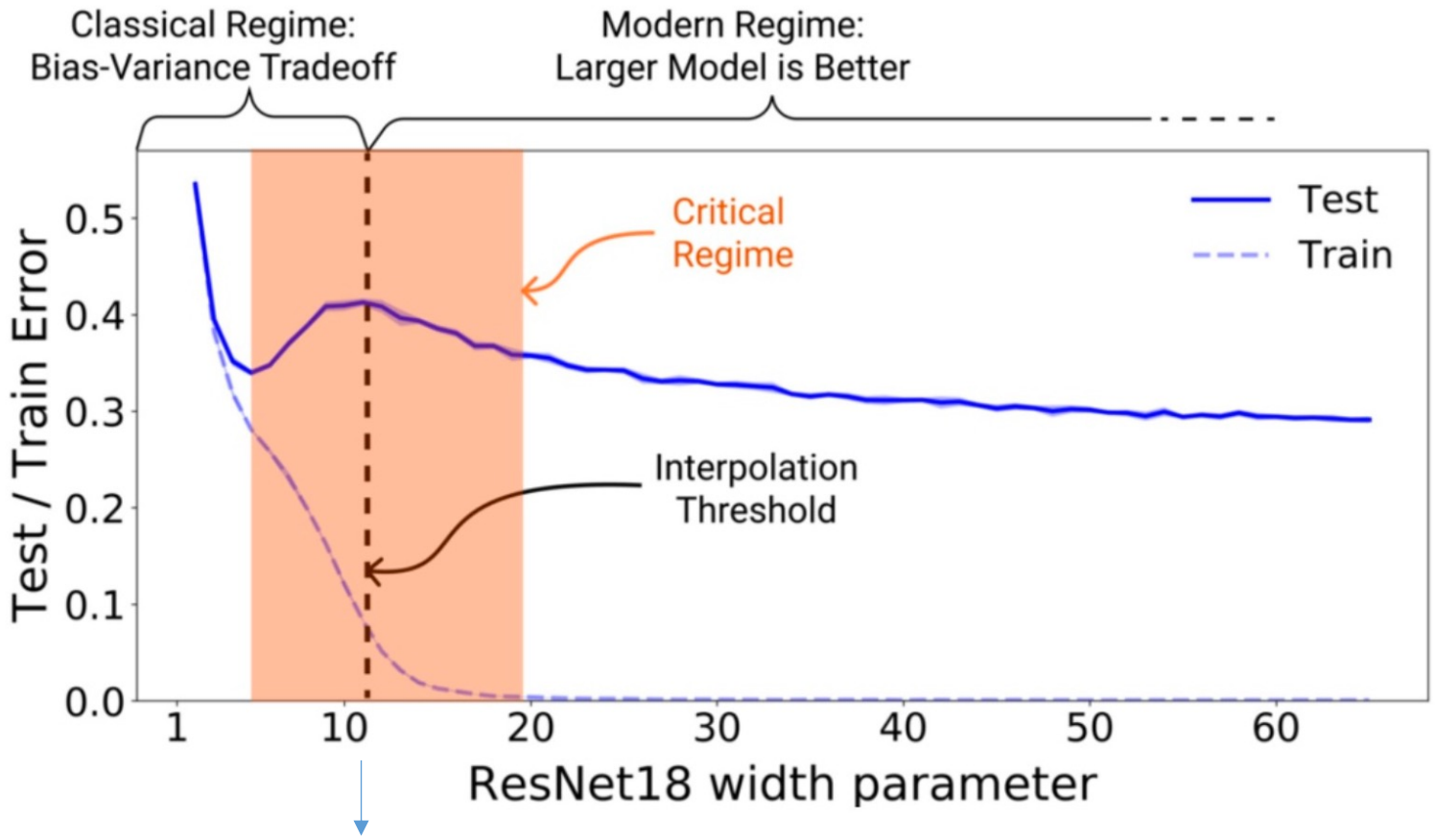
Understanding Deep Learning, 2023

Overview of regularization techniques



Understanding Deep Learning, 2023

Double descent

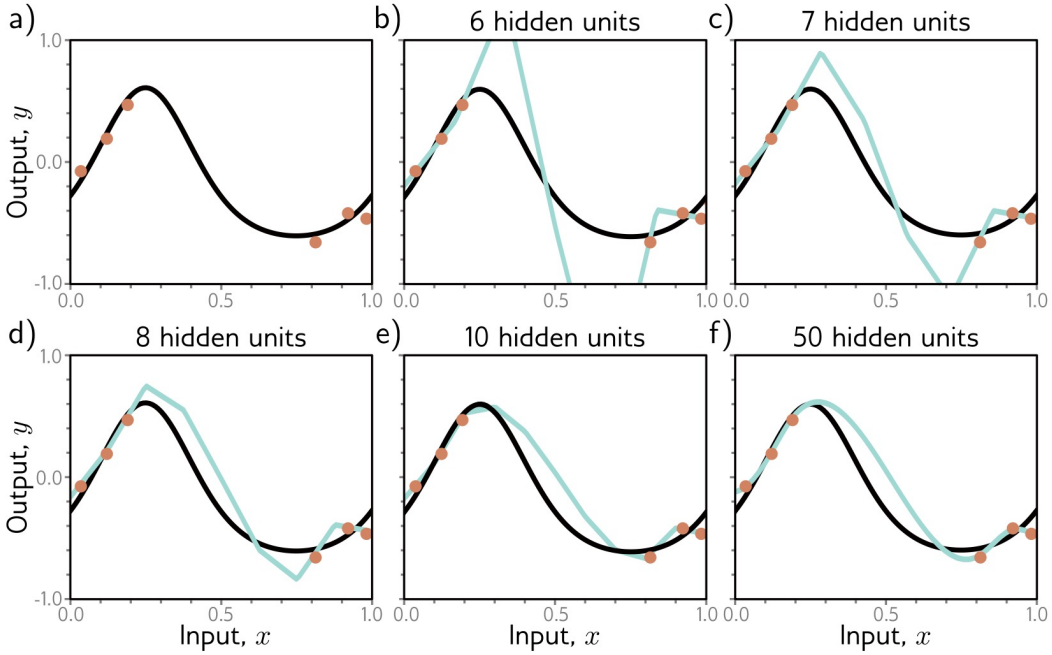


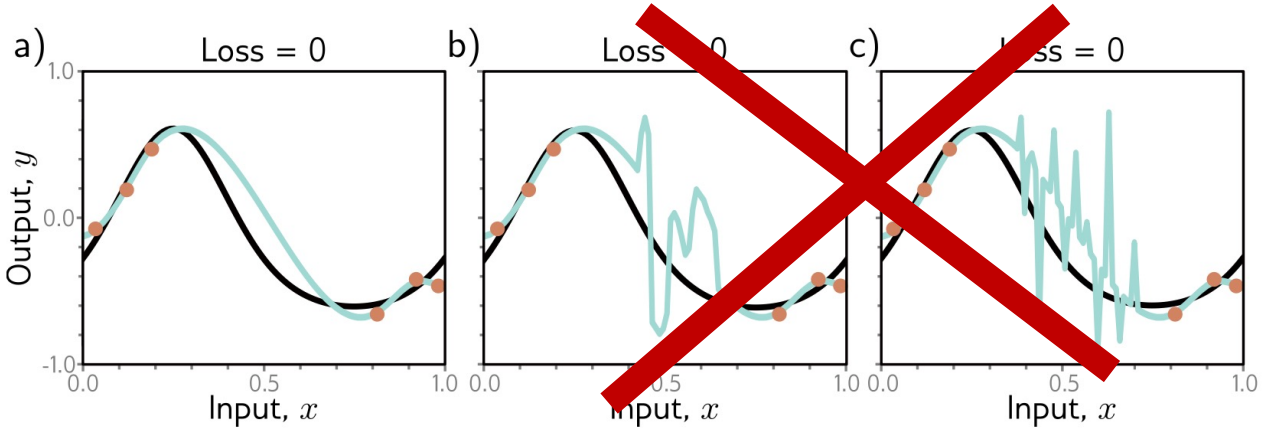
Where the effective model complexity equals the number of data points in the training set

Nakkiran *et al.,* 2019

Double Descent

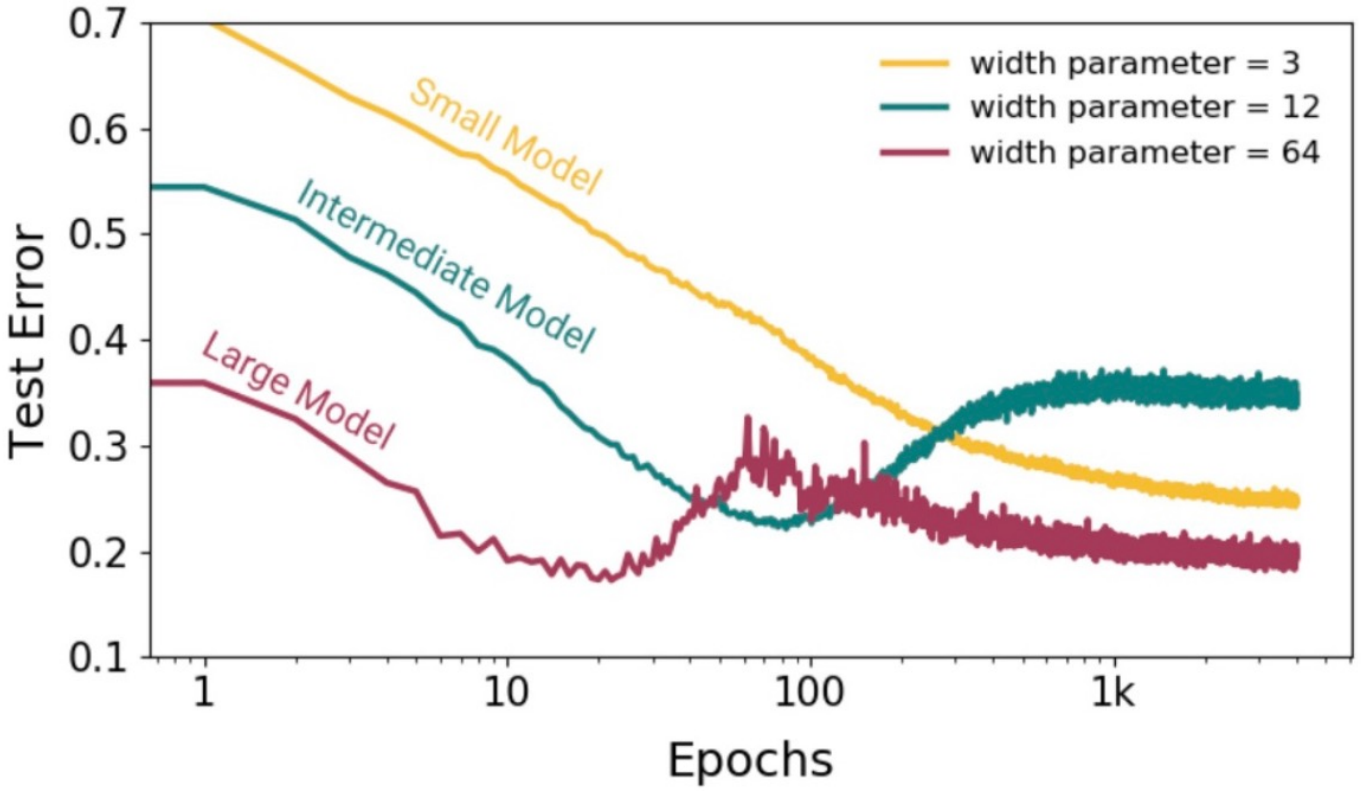
- As we add more capacity to the model will have the capability to create smoother functions.





- Why over-parameterized models should produce smooth functions? Maybe:
  - the network initialization encourage smoothness
  - the training algorithm may somehow “prefer” to converge to smooth functions

Double descent



Nakkiran *et al.,* 2019

Resources

- Understanding Deep Learning, Chapter 9.
- Deep Learning Book, Chapter 8.