# Regularization Techniques in Neural Networks

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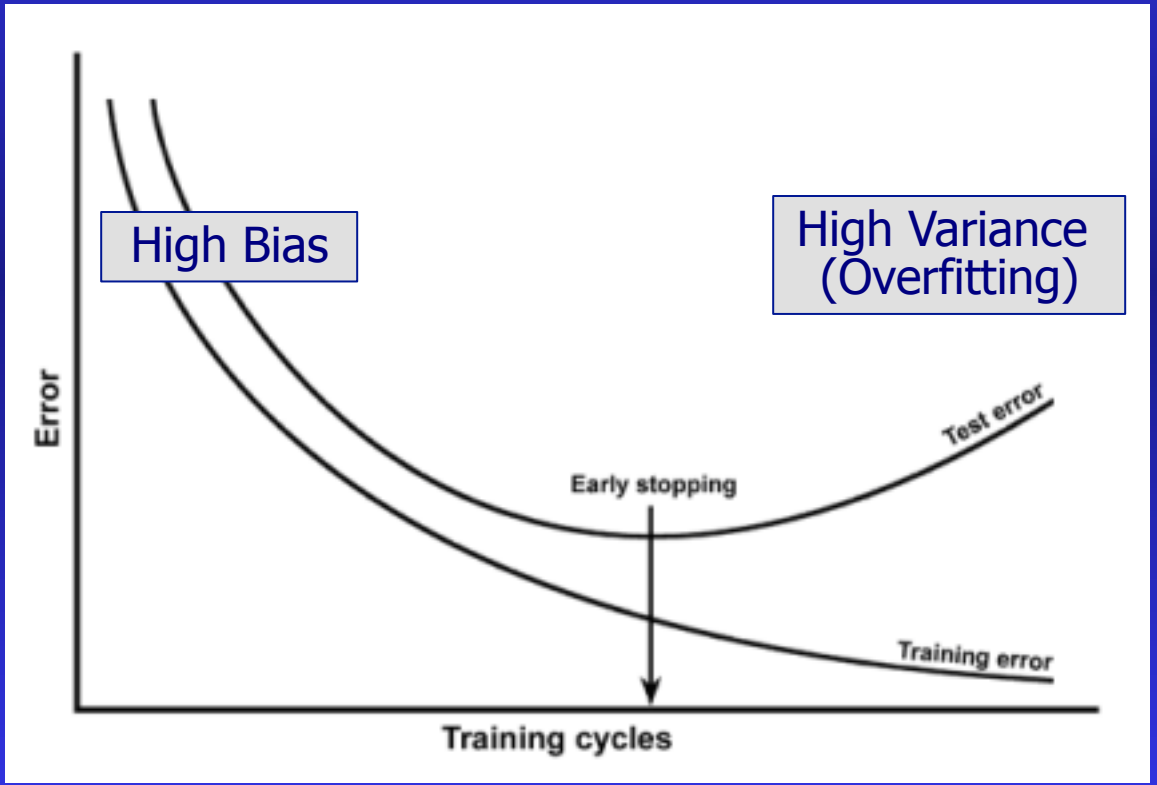
# What is Overfitting

- The training data contains information about the regularities in the mapping from input to output. But it also **contains sampling error.**
  - There will be accidental regularities just because of the particular training cases that were chosen.
- When we fit the model, it cannot tell which regularities are real and which are caused by sampling error.
  - So it fits both kinds of regularity. If the model is very flexible it can model the sampling error really well.
- This means the model will **not generalize well** to unseen data

# Diagnosing Overfitting

- Consider Training vs. Test Error as a function of training iterations



# Preventing Overfitting

- **Approach 1:** Get more data!
  - Almost always the best bet if you have enough compute power to train on more data.
- **Approach 2:** Use a model that has the right capacity:
  - enough to fit the true regularities.
  - not enough to also fit spurious regularities (if they are weaker).
- **Approach 3:** Average many different models.
  - Use models with different forms.
  - Or train the model on different subsets of the training data (this is called “bagging”).

# Limiting Capacity of a Neural Net

- The capacity can be controlled in many ways:
  - **Architecture:** Limit the number of hidden layers and the number of units per layer.
  - **Early stopping:** Start with small weights and stop the learning before it overfits.
  - **Weight-decay:** Penalize large weights using penalties or constraints on their squared values (L2 penalty) or absolute values (L1 penalty).
  - **Noise:** Add noise to the weights or the activities.
- Typically, a combination of several of these methods is used.

# Choosing Hyperparameters

- The wrong method is to try lots of alternatives and see which gives the best performance on the test set.
  - This is easy to do, but it gives a false impression of how well the method works.
  - The settings that work best on the test set are unlikely to work as well on a new test set drawn from the same distribution.
- **An extreme example:** Suppose the test set has **random** answers that do not depend on the input.
  - The best architecture will do better than chance on the test set.
  - But it cannot be expected to do better than chance on a new test set.

# Cross-Validation for Hyperparameters

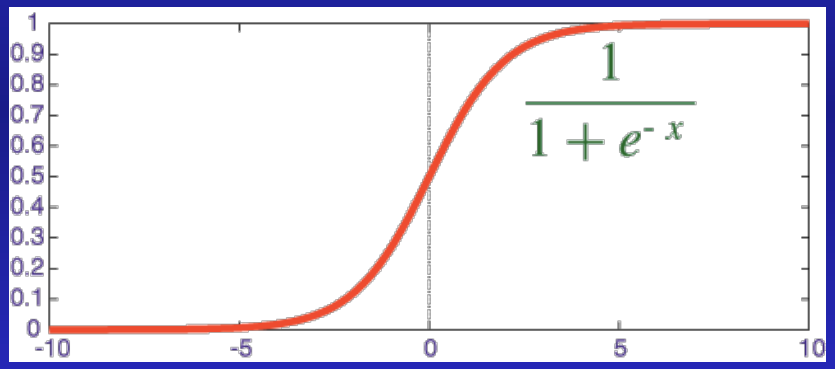
- Divide the total dataset into three subsets:
  - **Training data:** is used for learning the parameters of the model.
  - **Validation data:** is not used for learning but is used for deciding what settings of the meta parameters work best.
  - **Test data:** is used to get a final, unbiased estimate of how well the network works. We expect this estimate to be worse than on the validation data.
- We could divide the total dataset into one final test set and N other subsets and train on all but one of those subsets to get N different estimates of the validation error rate.
  - This is called N-fold cross-validation.
  - The N estimates are not independent.

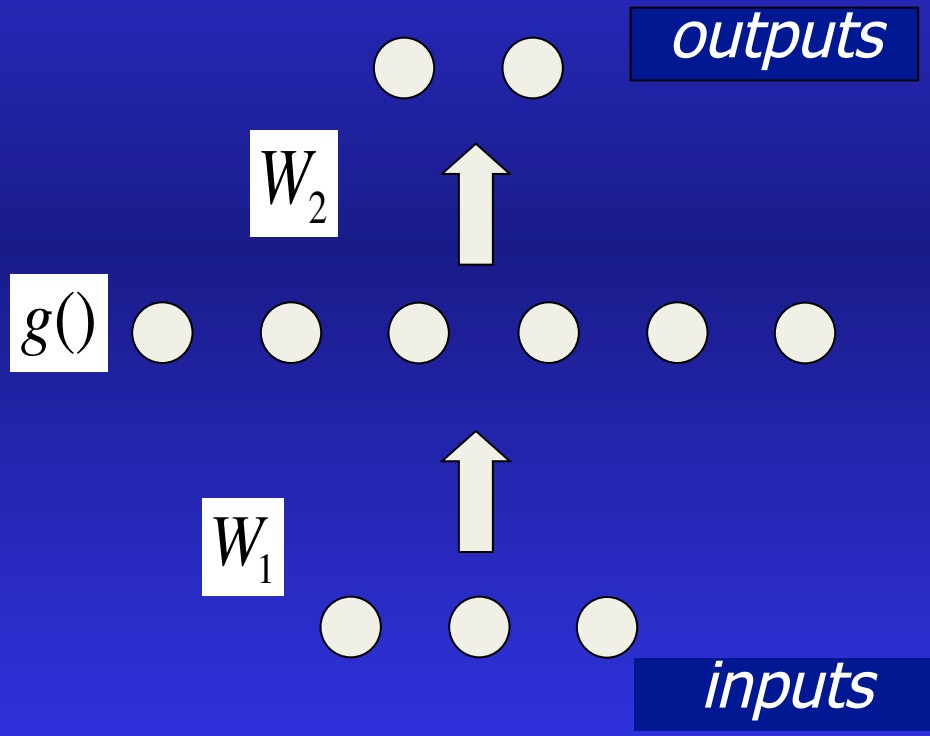
# Prevent Overfitting with Early Stopping

- If we have **lots of data and a big model**, its very expensive to keep re-training it with different sized penalties on the weights.
- It is much cheaper to start with very small weights and let them grow until the performance on the validation set starts getting worse.
  - But it can be hard to decide when performance is getting worse.
- The capacity of the model is limited because the weights have not had time to grow big

# Why Early Stopping Works (1)

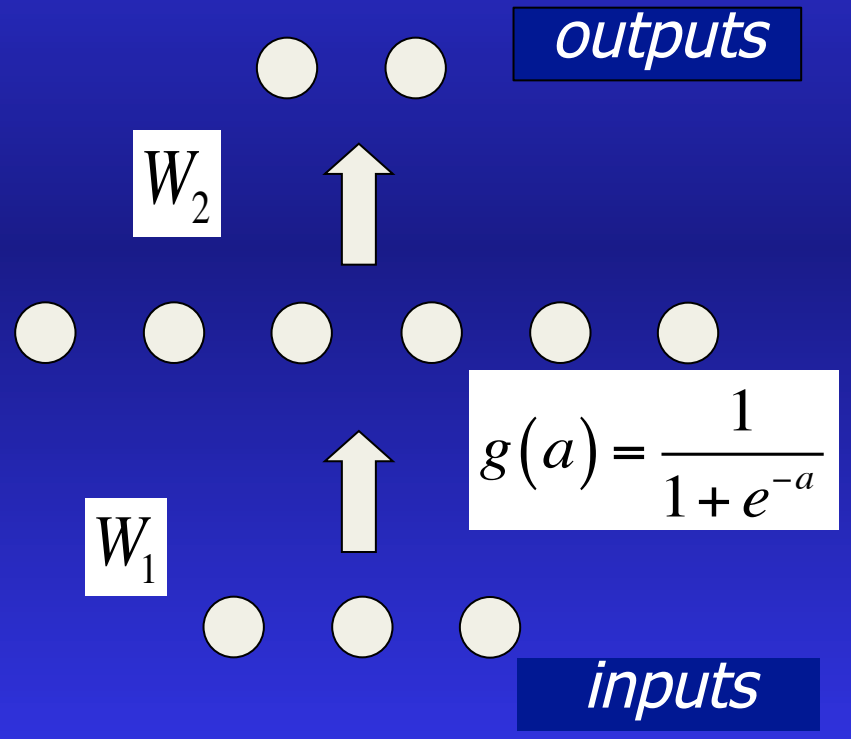
- So if we consider small weights on Sigmoidal hidden units



# Why Early Stopping Works (2)

- When the weights are very small, every hidden unit is in its linear range.
  - So a net with a large layer of hidden units is linear.
  - It has no more capacity than a linear net in which the inputs are directly connected to the outputs!
- As the weights grow, the hidden units start using their non-linear ranges so the capacity grows.



# Regularization: L2 Weight Penalty

- The standard L2 weight penalty involves adding an extra term to the cost function that **penalizes the squared weights.**
  - This keeps the weights small unless they have big error derivatives.

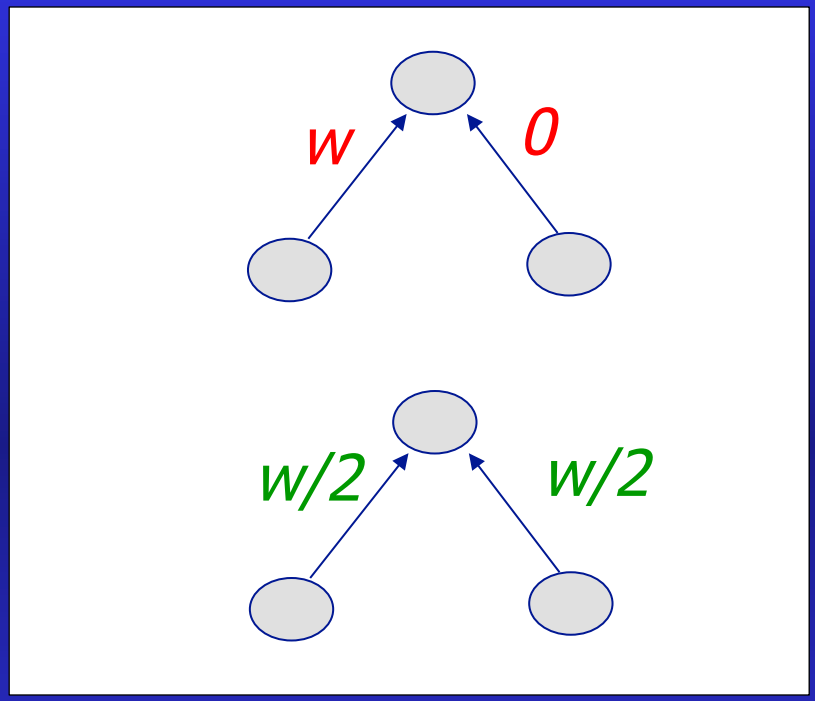
$$C = E + \frac{\lambda}{2}\sum_i w_i^2$$

$$\frac{\partial C}{\partial w_i} = \frac{\partial E}{\partial w_i} + \lambda w_i$$

$$when \quad \frac{\partial C}{\partial w_i} = 0, \quad w_i = -\frac{1}{\lambda}\frac{\partial E}{\partial w_i}$$

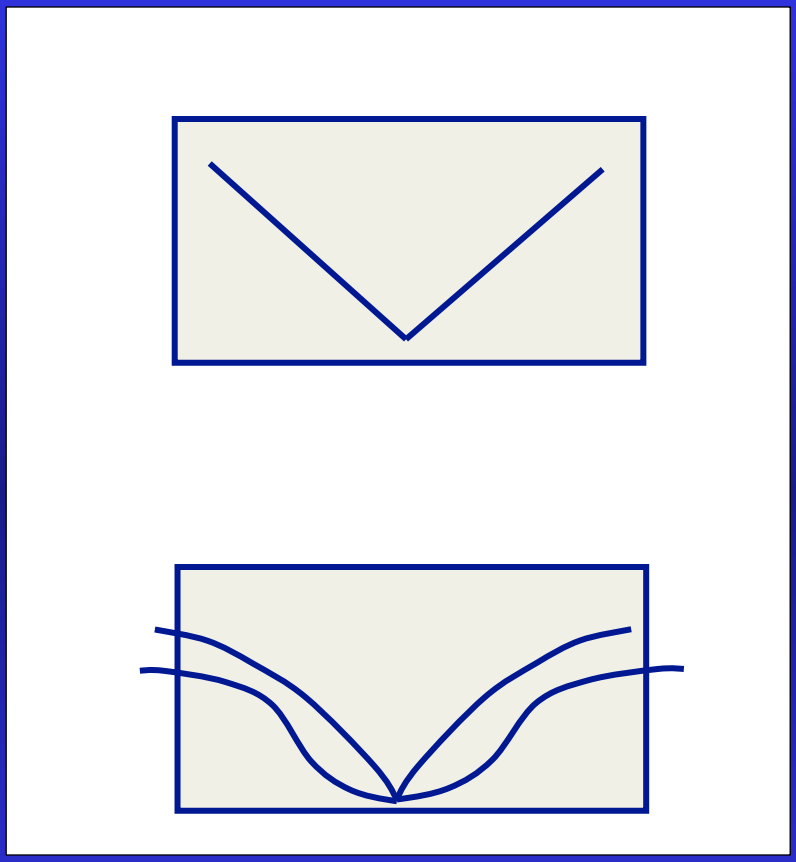
# Regularization: Effect of L2 Penalty

- It prevents the network from using weights that it does not need.
  - This can often improve generalization a lot because it helps to stop the network from fitting the sampling error.
  - It makes a smoother model in which the output changes more slowly as the input changes.
- If the network has two very similar inputs it prefers to put **half the weight on each rather than all the weight on one.**



# Regularization: Other Penalties

- Sometimes it works better to penalize the absolute values of the weights.
  - This can make many weights exactly equal to zero which helps interpretation a lot.
- Sometimes it works better to use a weight penalty that has negligible effect on large weights.
  - This allows a few large weights.

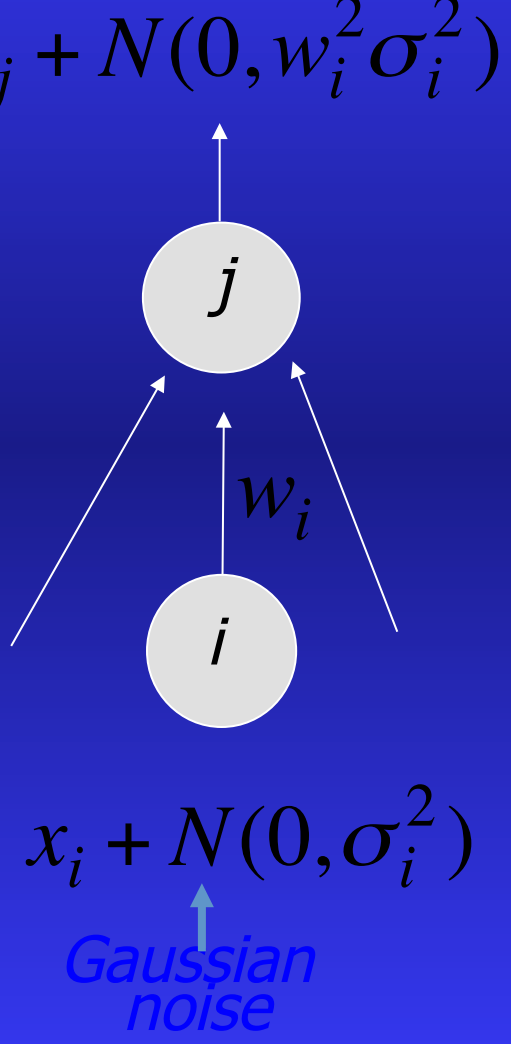


# Weight Penalties vs Weight Constraints

- We usually penalize the squared value of each weight separately.
- Instead, we can put a constraint on the maximum squared length of the incoming weight vector of each unit.
  - If an update violates this constraint, we scale down the vector of incoming weights to the allowed length.
- Weight constraints have **several advantages** over weight penalties.
  - Its easier to set a sensible value.
  - They prevent hidden units getting stuck near zero.
  - They prevent weights exploding.
- When a unit hits it's limit, the effective weight penalty on all of it's weights is determined by the big gradients.
  - This is more effective than a fixed penalty at pushing irrelevant weights towards zero.

# Regularization: L2 weight-decay via noisy inputs

- Suppose we add Gaussian noise to the inputs.
  - The variance of the noise is amplified by the squared weight before going into the next layer.
- In a simple net with a linear output unit directly connected to the inputs, the amplified noise gets added to the output.
- This makes an additive contribution to the squared error.
  - So minimizing the squared error tends to minimize the squared weights when the inputs are noisy.



# Derivation

$$y^{noisy} = \sum_i w_i x_i + \sum_i w_i \varepsilon_i \quad \text{where } \varepsilon_i \text{ is sampled from } N(0,\sigma_i^2)$$

$$E\left[(y^{noisy} - t)^2\right] = E\left[\left(y + \sum_i w_i \varepsilon_i - t\right)^2\right] = E\left[\left((y-t) + \sum_i w_i \varepsilon_i\right)^2\right]$$

$$= (y-t)^2 + E\left[2(y-t)\sum_i w_i \varepsilon_i\right] + E\left[\left(\sum_i w_i \varepsilon_i\right)^2\right]$$

$$= (y-t)^2 + E\left[\sum_i w_i^2 \varepsilon_i^2\right]$$

*because* $\varepsilon_i$ *is independent of* $\varepsilon_j$ *and* $\varepsilon_i$ *is independent of* $(y-t)$

$$= (y-t)^2 + \sum_i w_i^2 \sigma_i^2$$

# Regularization: Dropout

- An efficient way to **combine neural nets models**, without training many different models!
- Two classical ways to average models:

  MIXTURE: We can combine models by averaging their output probabilities.

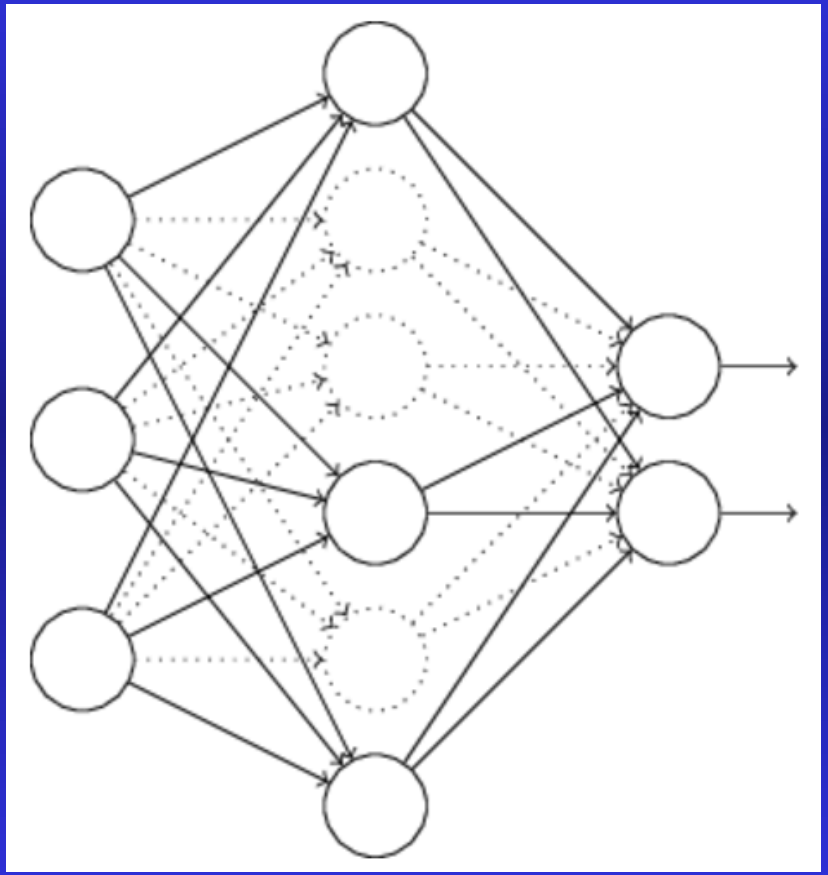
| | | | |
|---|---|---|---|
| Model A: | .3 | .2 | .5 |
| Model B: | .1 | .8 | .1 |
| Combined | .2 | .5 | .3 |

  PRODUCT: We can combine models by taking the geometric means of their output probabilities.

| | | | | |
|---|---|---|---|---|
| Model A: | .3 | .2 | .5 | |
| Model B: | .1 | .8 | .1 | |
| Combined | $\sqrt{.03}$ | $\sqrt{.16}$ | $\sqrt{.05}$ | /sum |

# Regularization: Dropout

- An efficient way to average many large neural nets.
- Consider a neural net with one hidden layer.
- **Procedure:**
    1. Each time we present a training example, we randomly omit each hidden unit with probability 0.5.
    2. So we are randomly sampling from 2^H different architectures.
        - All architectures share weights.

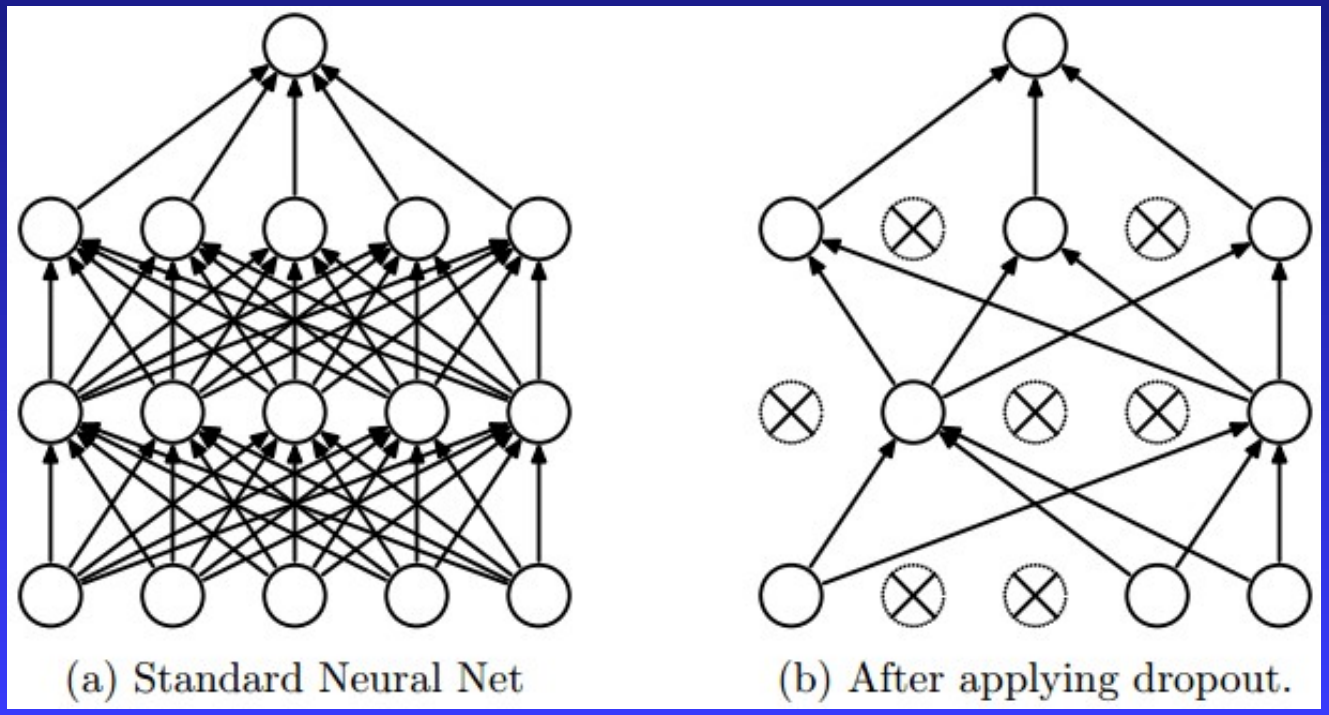


# Dropout: Form of Model Averaging

- We sample from 2^H models. So only a few of the models ever get trained, and they only get one training example.
  - This is as extreme as bagging can get.
- The sharing of the weights means that every model is very strongly regularized.
  - It's a much better regularizer than L2 or L1 penalties that pull the weights towards zero.
- In 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.

# Dropout for more hidden layers

- Use dropout of 0.5 in every layer.
- At test time, use the "mean net" that has all the outgoing weights halved.
  - This is not exactly the same as averaging all the separate dropped out models, but it's a pretty good approximation, and its fast.
- Alternatively, run the stochastic model several times on the same input.
  - This gives us an idea of the uncertainty in the answer.



(a) Standard Neural Net (b) After applying dropout.

# Dropout: how and why does it work?

- The record breaking object recognition net developed by Alex Krizhevsky uses dropout and it helps a lot.

- Almost every deep network today uses dropout.

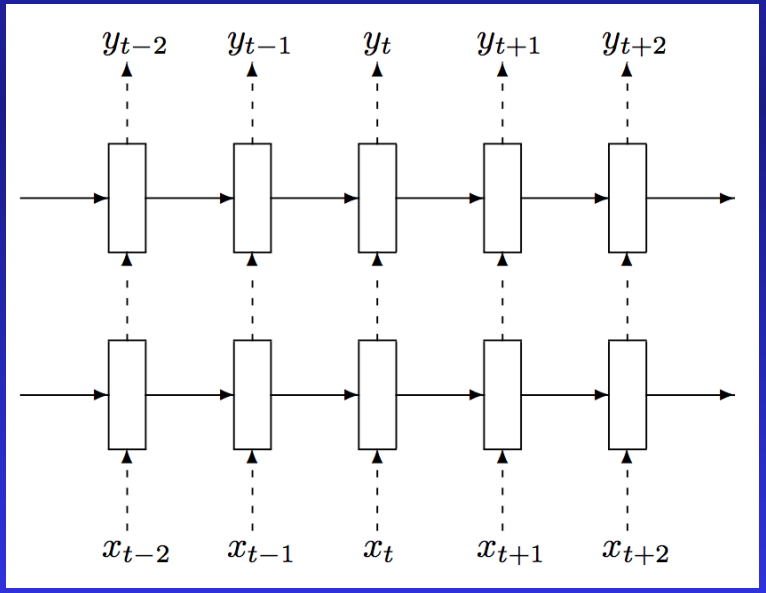
- If your deep neural net is significantly overfitting, dropout will usually reduce the number of errors by a lot.
    - Any net that uses "early stopping" can do better by using dropout (at the cost of taking quite a lot longer to train).

- If your deep neural net is not overfitting you should be using a bigger one!
- Hidden units may co-adapt when it knows what other hidden units are present
- Dropout forces the units to do something individually **useful** and **different** than what the other hidden units are doing

# Dropout: Recurrent Networks

- Deep recurrent neural networks also have high excess capacity and may overfit.
- Until recently, dropout was believed to corrupt the information carried by recurrent networks and this makes it difficult for LSTMs to learn to store information for extended periods

- Wojciech et al. 2014 determined that by applying Dropout only to non-recurrent connections, performance could be enhanced in deep recurrent neural networks
- Architecture, as shown to the right, reduced overfitting on a variety of tasks



# Regularization: Dropconnect

- Generalization of Hinton's Droput procedure, Dropconnect instead drops connections (weights), not entire activations (nodes)
- Wan et al, ICML 2014 showed that Dropconnect could lead to faster convergence than use of Dropout and that it often outperforms Dropout