# Neural Networks for Machine Learning

## Lecture 9a
## Overview of ways to improve generalization

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# Reminder: 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.

# 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”).
- Approach 4: (Bayesian) Use a single neural network architecture, but average the predictions made by many different weight vectors.

# Some ways to limit the 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.

# How to choose meta parameters that control capacity
## (like the number of hidden units or the size of the weight penalty)

- 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: A better way to choose meta parameters

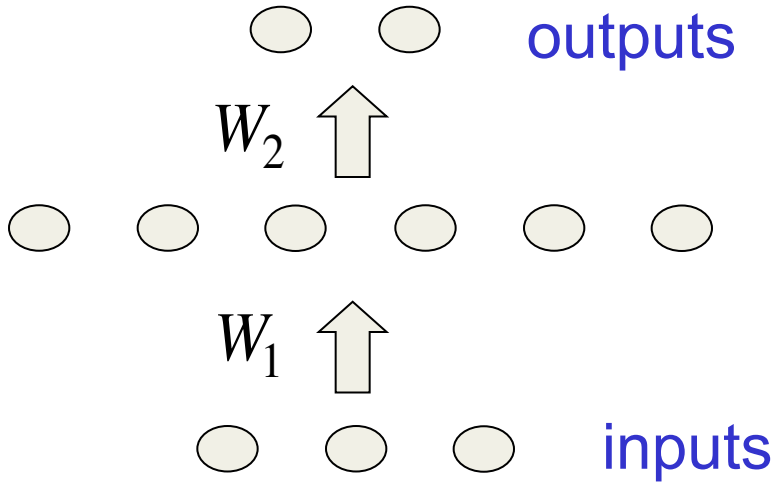
- Divide the total dataset into three subsets:
  - Training data is used for learning the parameters of the model.
  - Validation data is not used for learning but is used for deciding what settings of the meta parameters work best.
  - Test data is used to get a final, unbiased estimate of how well 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.

# Preventing overfitting by 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

- 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.



# Neural Networks for Machine Learning

## Lecture 9b
## Limiting the size of the weights

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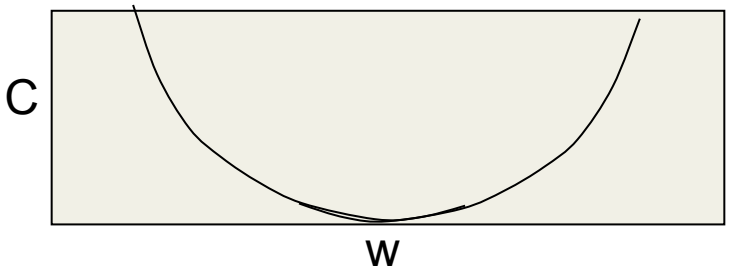
# Limiting the size of the weights

- 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.

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

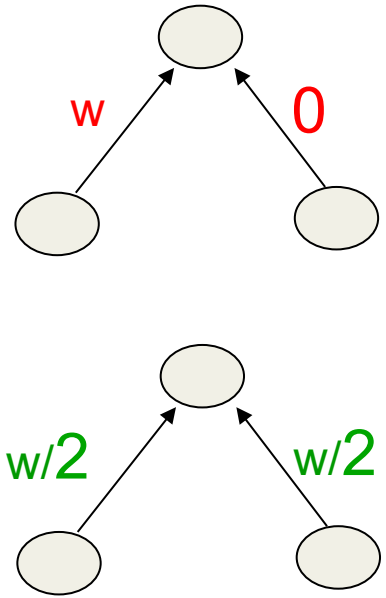
$$\frac{\partial C}{\partial w_i} = \frac{\partial E}{\partial w_i} + \lambda w_i$$




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

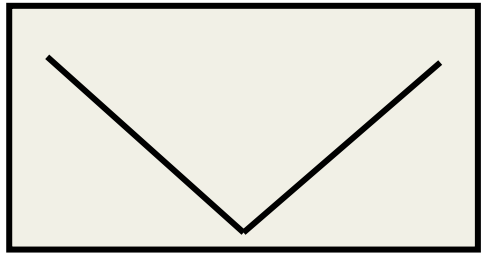
# The effect of L2 weight cost

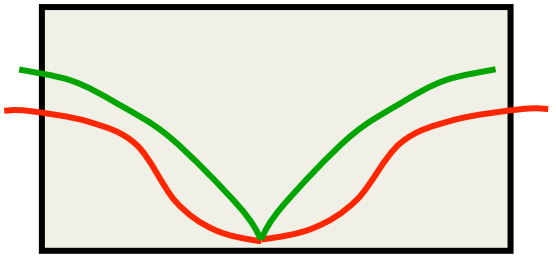
- It prevents the network from using weights that it does not need.
  - This can often improve generalization a lot because it helps to stop the network from fitting the sampling error.
  - It makes a smoother model in which the output changes more slowly as the input changes.
- If the network has two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



# Other kinds of weight penalty

- 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.

# Neural Networks for Machine Learning

## Lecture 9c
## Using noise as a regularizer

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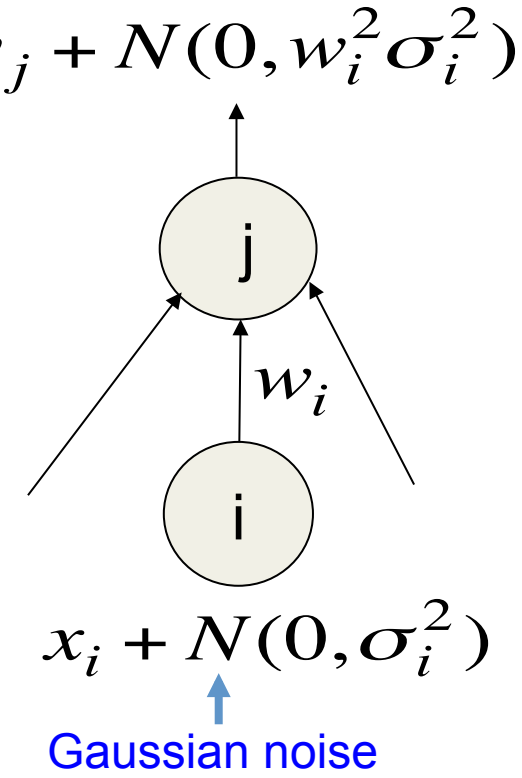
# L2 weight-decay via noisy inputs

- 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.



output on one case → $y^{noisy} = \sum_i w_i x_i + \sum_i w_i \varepsilon_i$ *where* $\varepsilon_i$ *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* $(y - t)$

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

So $\sigma_i^2$ is equivalent to an L2 penalty

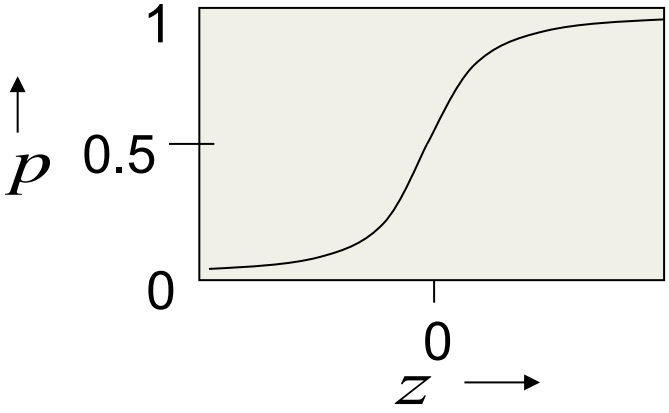
# Noisy weights in more complex nets

- Adding Gaussian noise to the weights of a multilayer non-linear neural net is not exactly equivalent to using an L2 weight penalty.
  - It may work better, especially in recurrent networks.
  - Alex Graves' recurrent net that recognizes handwriting, works significantly better if noise is added to the weights.

# Using noise in the activities as a regularizer

- Suppose we use backpropagation to train a multilayer neural net composed of logistic units.
  - What happens if we make the units binary and stochastic on the forward pass, but do the backward pass as if we had done the forward pass "properly"?
- It does worse on the training set and trains considerably slower.
  - But it does significantly better on the test set! (unpublished result).

$$p(s=1) = \frac{1}{1+e^{-z}}$$



# Neural Networks for Machine Learning

## Lecture 9d
## Introduction to the Bayesian Approach

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# The Bayesian framework

- The Bayesian framework assumes that we always have a prior distribution for everything.
  - The prior may be very vague.
  - When we see some data, we combine our prior distribution with a likelihood term to get a posterior distribution.
  - The likelihood term takes into account how probable the observed data is given the parameters of the model.
    - It favors parameter settings that make the data likely.
    - It fights the prior
    - With enough data the likelihood terms always wins.

# A coin tossing example

- Suppose we know nothing about coins except that each tossing event produces a head with some unknown probability p and a tail with probability 1-p.
  - Our model of a coin has one parameter, p.

- Suppose we observe 100 tosses and there are 53 heads. What is p?

- The frequentist answer (also called maximum likelihood): Pick the value of p that makes the observation of 53 heads and 47 tails most probable.
  - This value is p=0.53

# A coin tossing example: the math

probability of a particular sequence containing 53 heads and 47 tails.

$$P(D) = p^{53}(1-p)^{47}$$

$$\frac{dP(D)}{dp} = 53p^{52}(1-p)^{47} - 47p^{53}(1-p)^{46}$$

$$= \left(\frac{53}{p} - \frac{47}{1-p}\right)\left[p^{53}(1-p)^{47}\right]$$

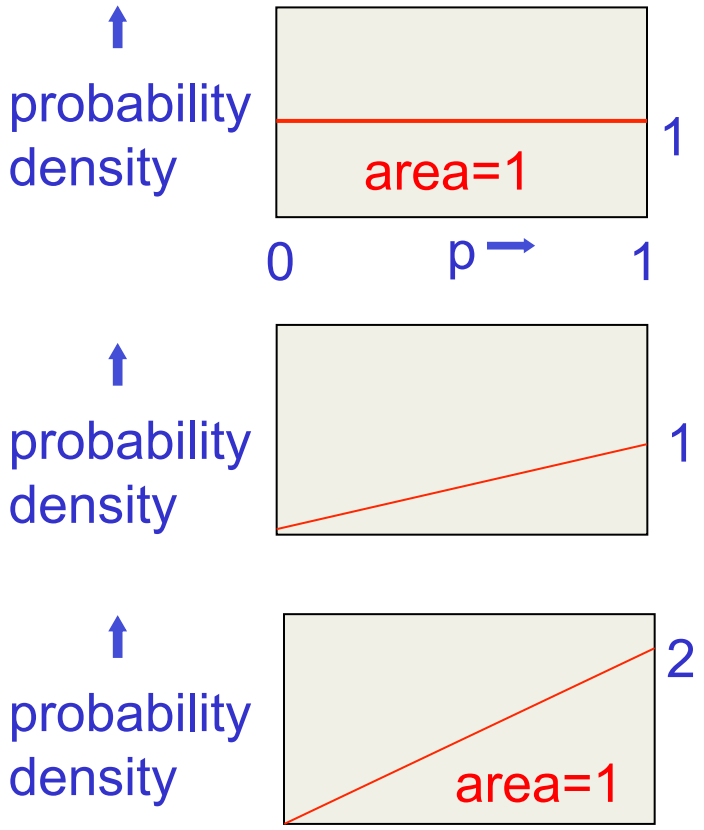
$$= 0 \quad if \quad p = .53$$

# Some problems with picking the parameters that are most likely to generate the data

- What if we only tossed the coin once and we got 1 head?
  - Is p=1 a sensible answer?
  - Surely p=0.5 is a much better answer.
- Is it reasonable to give a single answer?
  - If we don't have much data, we are unsure about p.
  - Our computations of probabilities will work much better if we take this uncertainty into account.

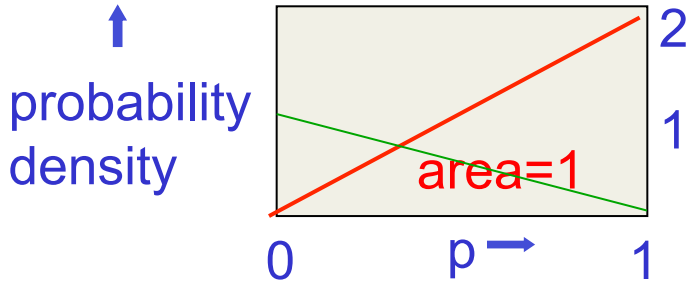
# Using a distribution over parameter values

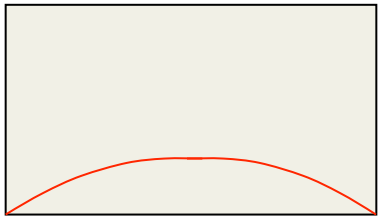
- Start with a prior distribution over p. In this case we used a uniform distribution.
- Multiply the prior probability of each parameter value by the probability of observing a head given that value.
- Then scale up all of the probability densities so that their integral comes to 1. This gives the posterior distribution.

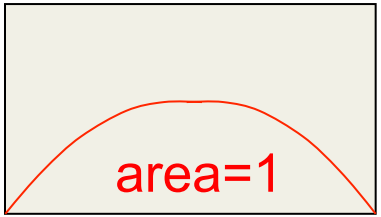


# Lets do it again: Suppose we get a tail

- Start with a prior distribution over p.
- Multiply the prior probability of each parameter value by the probability of observing a tail given that value.
- Then renormalize to get the posterior distribution. Look how sensible it is!

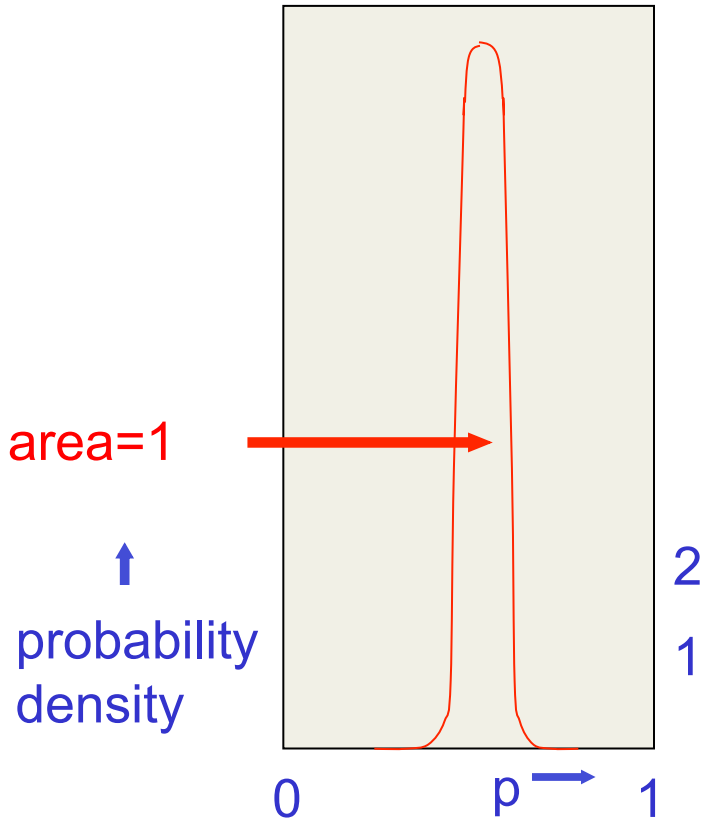




# Lets do it another 98 times

- After 53 heads and 47 tails we get a very sensible posterior distribution that has its peak at 0.53 (assuming a uniform prior).



# Bayes Theorem

joint probability

conditional probability

$$p(D)p(W \mid D) = p(D,W) = p(W)p(D \mid W)$$

prior probability of weight vector W

probability of observed data given W

$$p(W \mid D) = \frac{p(W)\quad p(D \mid W)}{p(D)}$$

posterior probability of weight vector W given training data D

$$\int_W p(W)p(D \mid W)$$

# Neural Networks for Machine Learning

## Lecture 9e
## The Bayesian interpretation of weight decay

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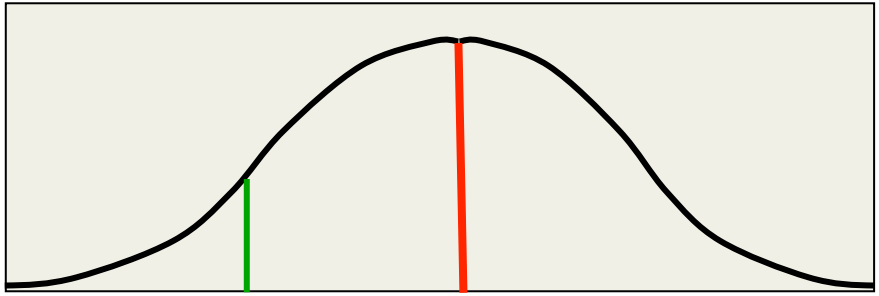
# Supervised Maximum Likelihood Learning

- Finding a weight vector that minimizes the squared residuals is equivalent to finding a weight vector that maximizes the log probability density of the correct answer.

- We assume the answer is generated by adding Gaussian noise to the output of the neural network.



t
correct answer

y
model's estimate of most probable value

# Supervised Maximum Likelihood Learning

output of the net → $y_c = f(input_c, W)$

probability density of the target value given the net's output plus Gaussian noise →

$$p(t_c \mid y_c) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(t_c - y_c)^2}{2\sigma^2}}$$

← Gaussian distribution centered at the net's output

Cost →

$$-\log p(t_c \mid y_c) = k + \frac{(t_c - y_c)^2}{2\sigma^2}$$

Minimizing squared error is the same as maximizing log prob under a Gaussian.

# MAP: Maximum a Posteriori

- The proper Bayesian approach is to find the full posterior distribution over all possible weight vectors.
  - If we have more than a handful of weights this is hopelessly difficult for a non-linear net.
  - Bayesians have all sort of clever tricks for approximating this horrendous distribution.
- Suppose we just try to find the most probable weight vector.
  - We can find an optimum by starting with a random weight vector and then adjusting it in the direction that improves p( W | D ).
  - But it's only a local optimum.
- It is easier to work in the log domain. If we want to minimize a cost we use negative log probs

# Why we maximize sums of log probabilities

- We want to maximize the product of the probabilities of the producing the target values on all the different training cases.
  - Assume the output errors on different cases, c, are independent.

$$p(D \mid W) = \prod_c p(t_c \mid W) = \prod_c p\left(t_c \mid f(input_c, W)\right)$$

- Because the log function is monotonic, it does not change where the maxima are. So we can maximize sums of log probabilities

$$\log p(D \mid W) = \sum_c \log p(t_c \mid W)$$

# MAP: Maximum a Posteriori

$$p(W \mid D) = p(W)\, p(D \mid W) \,/\, p(D)$$

$$Cost = -\log p(W \mid D) = -\log p(W) - \log p(D \mid W) + \log p(D)$$

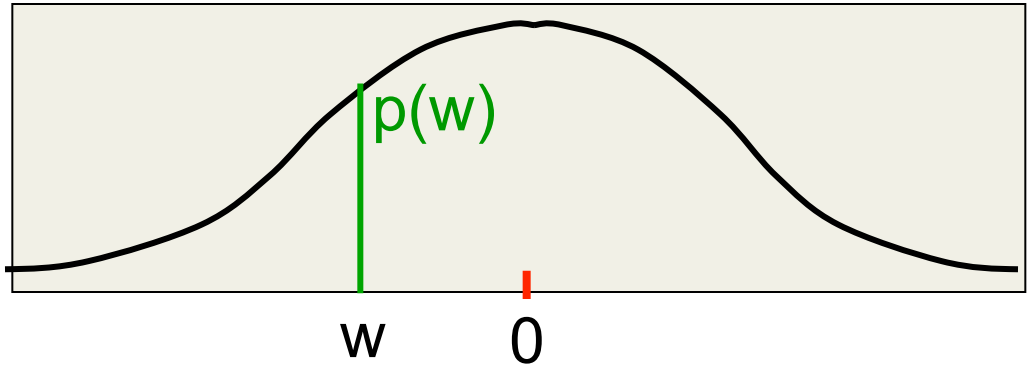
log prob of W under the prior

log prob of target values given W

This is an integral over all possible weight vectors so it does not depend on W

# The log probability of a weight under its prior

- Minimizing the squared weights is equivalent to maximizing the log probability of the weights under a zero-mean Gaussian prior.




$$p(w) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{w^2}{2\sigma_W^2}}$$

$$-\log p(w) = \frac{w^2}{2\sigma_W^2} + k$$

# The Bayesian interpretation of weight decay

$$-\log p(W \mid D) \;=\; -\log p(D \mid W) \;-\log p(W) \;+\log p(D)$$

constant

$$C^* \;=\; \frac{1}{2\sigma_D^2}\sum_c (y_c - t_c)^2 \;+\; \frac{1}{2\sigma_W^2}\sum_i w_i^2$$

assuming that the model makes a Gaussian prediction

assuming a Gaussian prior for the weights

$$C \;=\; E \;+\; \frac{\sigma_D^2}{\sigma_W^2}\sum_i w_i^2$$

So the correct value of the weight decay parameter is the ratio of two variances. It's not just an arbitrary hack.

# Neural Networks for Machine Learning

## Lecture 9f
## MacKay's quick and dirty method of fixing weight costs

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# Estimating the variance of the output noise

- After we have learned a model that minimizes the squared error, we can find the best value for the output noise.
  - The best value is the one that maximizes the probability of producing exactly the correct answers after adding Gaussian noise to the output produced by the neural net.
  - The best value is found by simply using the variance of the residual errors.

# Estimating the variance of the Gaussian prior on the weights

- After learning a model with some initial choice of variance for the weight prior, we could do a dirty trick called “empirical Bayes”.
  - Set the variance of the Gaussian prior to be whatever makes the weights that the model learned most likely.
    - i.e. use the data itself to decide what your prior is!
  - This is done by simply fitting a zero-mean Gaussian to the one-dimensional distribution of the learned weight values.
    - We could easily learn different variances for different sets of weights.
- We don’t need a validation set!

# MacKay's quick and dirty method of choosing the ratio of the noise variance to the weight prior variance.

- Start with guesses for both the noise variance and the weight prior variance.
- While not yet bored
  - Do some learning using the ratio of the variances as the weight penalty coefficient.
  - Reset the noise variance to be the variance of the residual errors.
  - Reset the weight prior variance to be the variance of the distribution of the actual learned weights.
- Go back to the start of this loop.