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.

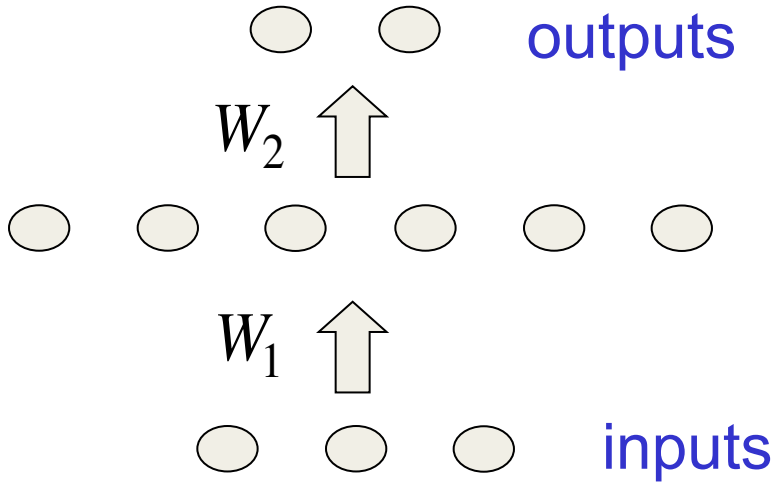
Method:
- start with very small weights
- let them grow until the performance on validation set starts getting worse

Model capacity:
refers to the complexity of the underlying pattern that the model (referring neural network here) is able to learn. Usually going deep increases the capacity of the neural network by increasing the number of model parameters which means it can fit more complex functions.

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.

When the weights are small, the whole network is the same as a linear network that maps the inputs straight to the outputs.



Neural Networks for Machine Learning

Lecture 9b
Limiting the size of the weights

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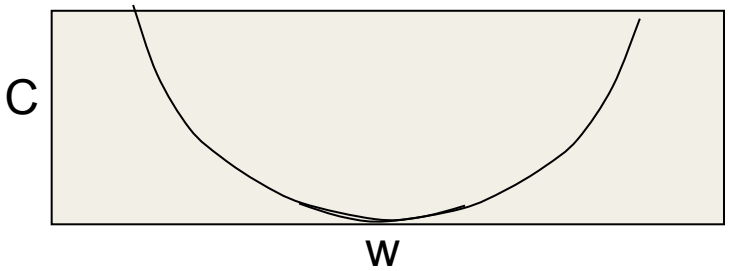
Limiting the size of the weights

- 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.

λ is some times called the weight cost. It determines how strong the penalty is.

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

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

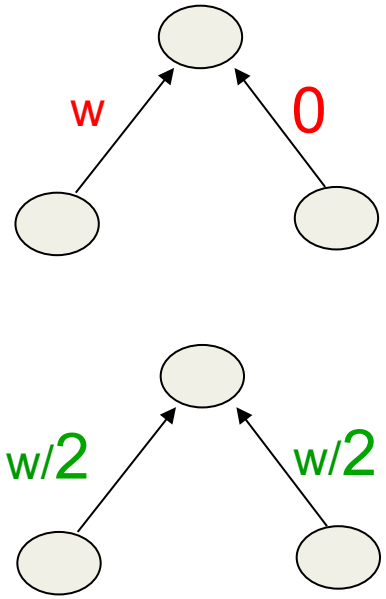


$$when \quad \frac{\partial C}{\partial w_i} = 0, \qquad w_i = -\frac{1}{\lambda}\frac{\partial E}{\partial w_i}$$

Note: The only way you can have big weights when you want to attain the minimum of the cost function is that they also have big error derivatives.

The effect of L2 weight cost

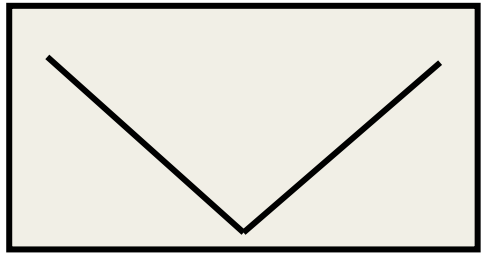
- It prevents the network from using weights that it does not need.
  - This can often improve generalization a lot because it helps to stop the network from fitting the sampling error.
  - It makes a smoother model in which the output changes more slowly as the input changes.
- If the network has two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



Other kinds of weight penalty

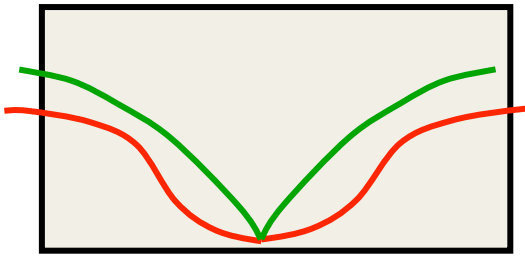
- Sometimes it works better to penalize the absolute values of the weights.
  - This can make many weights exactly equal to zero which helps interpretation a lot.
- Sometimes it works better to use a weight penalty that has negligible effect on large weights.
  - This allows a few large weights.

Weight penalty allows large weights without being pulled towards zero. Only small weights get pulled towards zero.



L1 penalty

0



weight penalties

0

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. (1)
  - They prevent hidden units getting stuck near zero. (2)
  - 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.

(1) Logistic unit has a natural scale to them. we know a weight of 1 means.
(2) When the weights are tiny, there's nothing preventing them from growing.

Neural Networks for Machine Learning

Lecture 9c
Using noise as a regularizer

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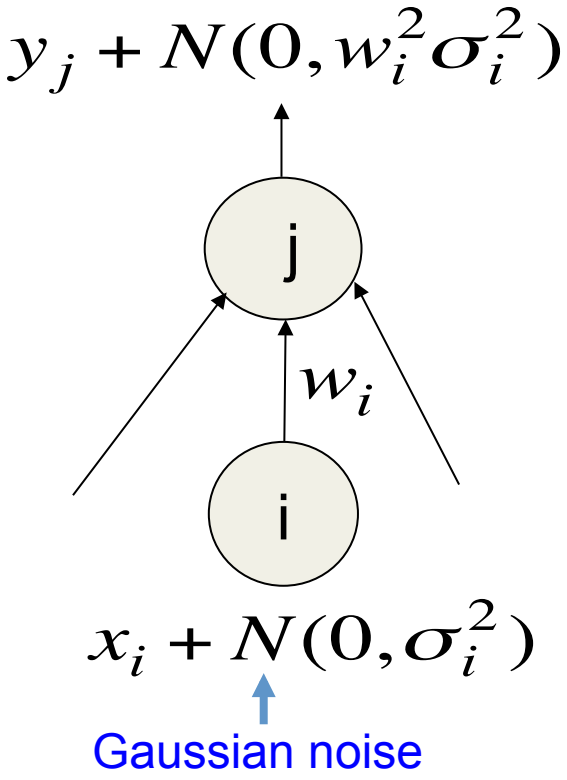
L2 weight-decay via noisy inputs

- 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* ε_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 ε_i *is independent of* ε_j

and ε_i *is independent of* $(y - t)$

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

So σ_i^2 is equivalent to an L2 penalty

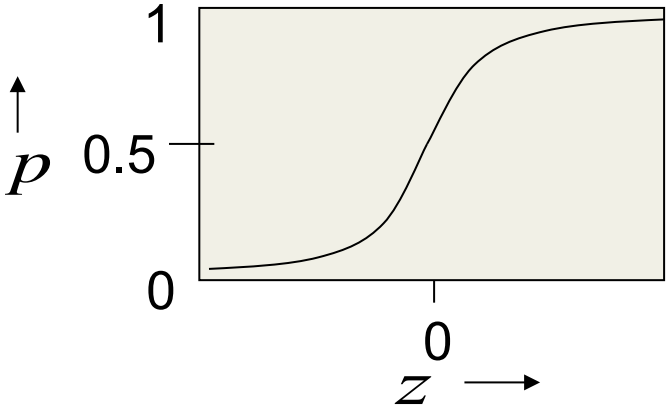
Noisy weights in more complex nets

- 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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Basic idea of Bayesian models:

Instead of looking for the most likely settings of the parameters of the model, we should consider all possible settings of the parameters.

And try to figure out, for each of these possible settings, how possible it is given the data we observed.

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.

Even if your prior is wrong, you end up with the right hypothesis. But that may take an awful lot of data.

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.

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

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

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

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

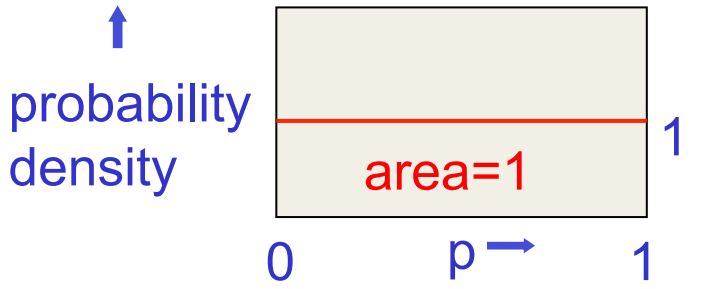
Some problems with picking the parameters that are most likely to generate the data

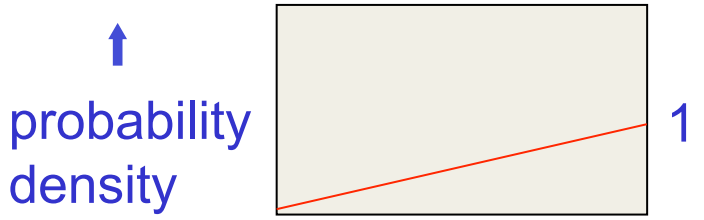
- What if we only tossed the coin once and we got 1 head?
  - Is p=1 a sensible answer?
  - Surely p=0.5 is a much better answer.
- Is it reasonable to give a single answer?
  - If we don't have much data, we are unsure about p.
  - Our computations of probabilities will work much better if we take this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

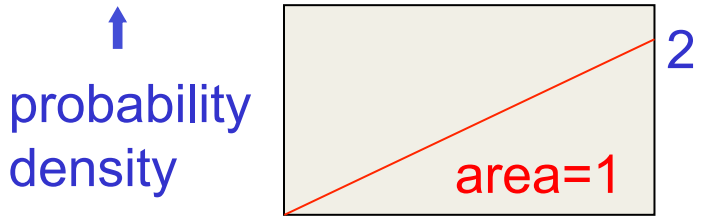
IMPORTANT!

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.



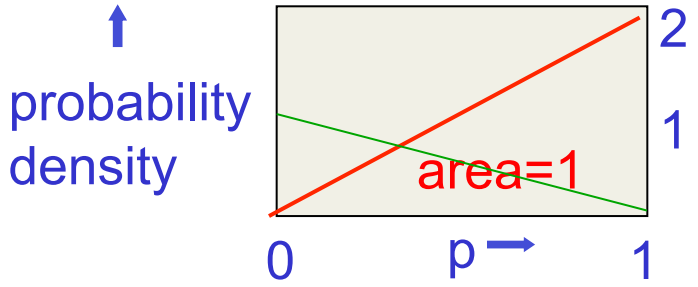


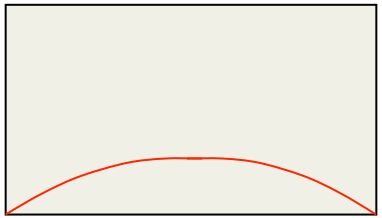


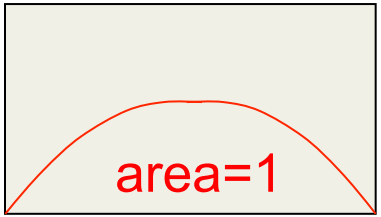
rescale it up to 1 to make it a probability distribution

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!

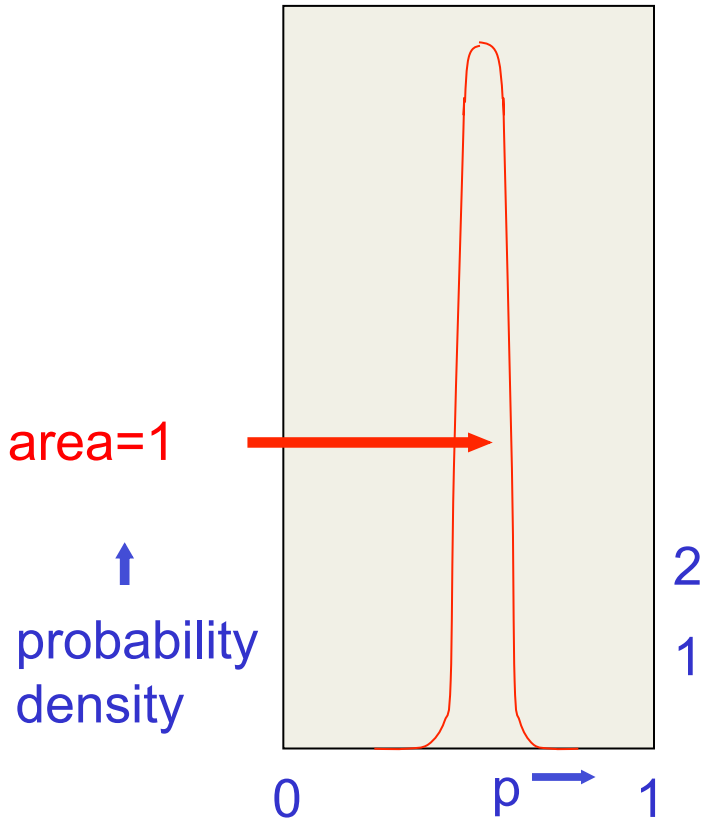






Lets do it another 98 times

- 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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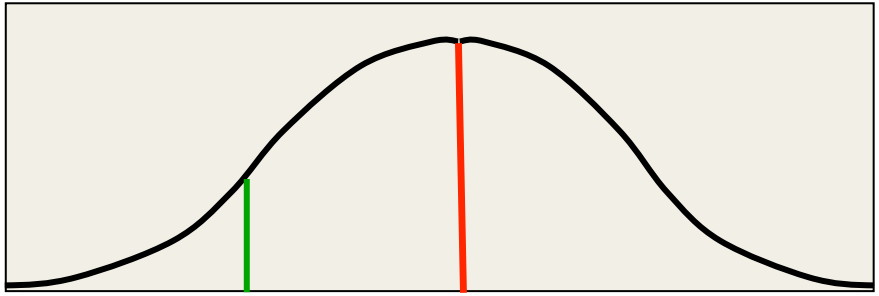
Goal:
Use weight decay to control the capacity of a neural network model.

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

Assume: t ~ Normal(y, σ^2)

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.

limitation

- 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.

solution

- 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

next slide

log prob of target values given W

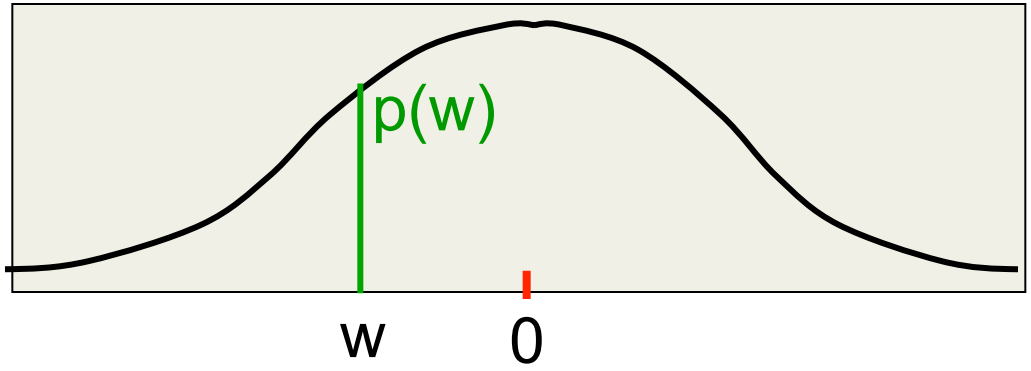
figured out previously

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

constant

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

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

E = squared error

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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- developed in the 1990s
- Goal: determine the weight penalties in the neural networks without using a validation set.
- It's based on the idea that we can interpret weight penalties as doing map estimation so that the magnitude of the weight penalty is related to the tightness of the prior distribution of the weights.
- This allows us to have different weight penalties for different subsets of connections in the NN, something would be very expensive to do using validation set.

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.

Algorithm:

- Start with guesses for both the noise variance and the weight prior variance. *Just guess the ratio.*
- While not yet bored
  - Do some learning using the ratio of the variances as the weight penalty coefficient. *use gradient descent*
  - 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.