STA 414/2104

Statistical Methods for Machine Learning and Data Mining

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Week 6

Neural Networks

“Curse of Dimensionality” for Linear Basis Function Models

Modeling a general non-linear relationship of y to x with a linear basis function model seems attractive when x is of low dimension, but when there are many inputs, we would seem to need a huge number of local basis functions to “cover” the high dimensional input space.

This is at least a computational problem — part of the “curse of dimensionality”.

One possibility is to use a relatively small number of basis functions, that cover only the actual area where x values are found, which may be the vicinity of a manifold of much lower dimension. We might:

- pick a subset of data points as centres for basis functions
- make the basis functions depend on parameters that adapt to the data.

We’ll look now at one class of models of the second type.

“Neural Networks” with One “Hidden Layer”

The term “neural network” can refer to many models that were originally inspired by thoughts on how the brain might work. We’ll look here at the most common one — a “multilayer perceptron” network (MLP) with one “hidden layer”.

This can be seen as a linear basis function model extended to make the basis functions depend on some additional parameters. (So the model is no longer linear with respect to these additional parameters.)

As before, we model the response y for a case with inputs x as

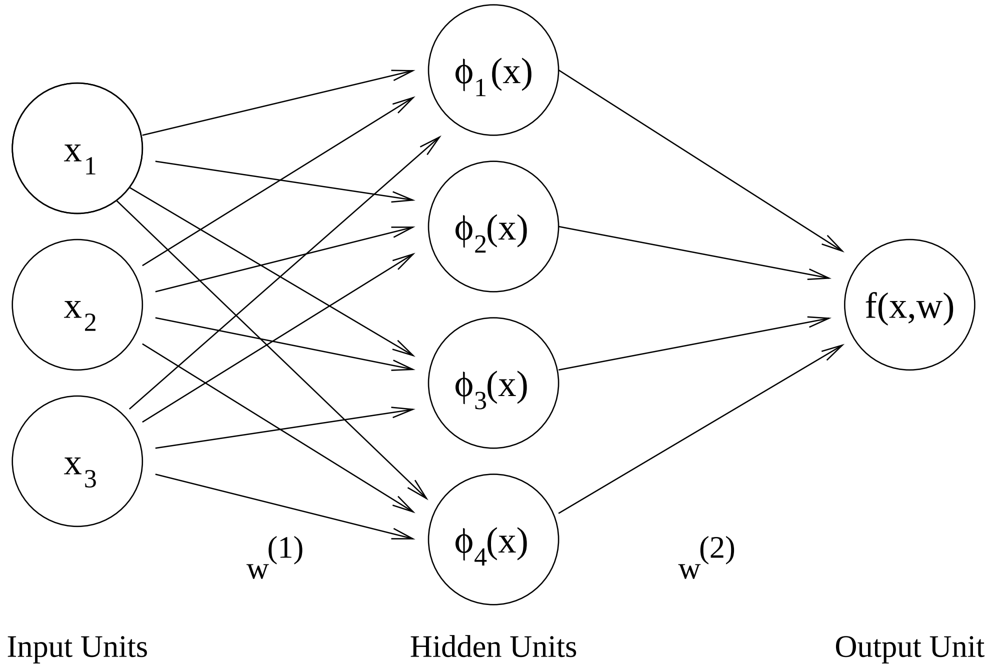
$$y \;=\; f(x,w) \;+\; \text{noise}$$

but now the parameters w — called “weights” — come in two groups:

- A matrix $w^{(1)}$ defines the basis functions.
- A vector $w^{(2)}$ defines a linear combination of these basis functions.

The Architecture of a Multilayer Perceptron Network

A multilayer perceptron with one layer of four "hidden" units looks like this:



Each element of $w^{(1)}$ and $w^{(2)}$ is associated with one of the arrows (connections) above. Each hidden unit computes a value that is a function of a linear combination of the values of units that point into it, with weights given by $w^{(1)}$.

More layers of hidden units can be added — the hidden unit values in one layer are computed from linear combinations of hidden unit values in the previous layer. There could be more than one response variable, in which case $w^{(2)}$ will be a matrix.

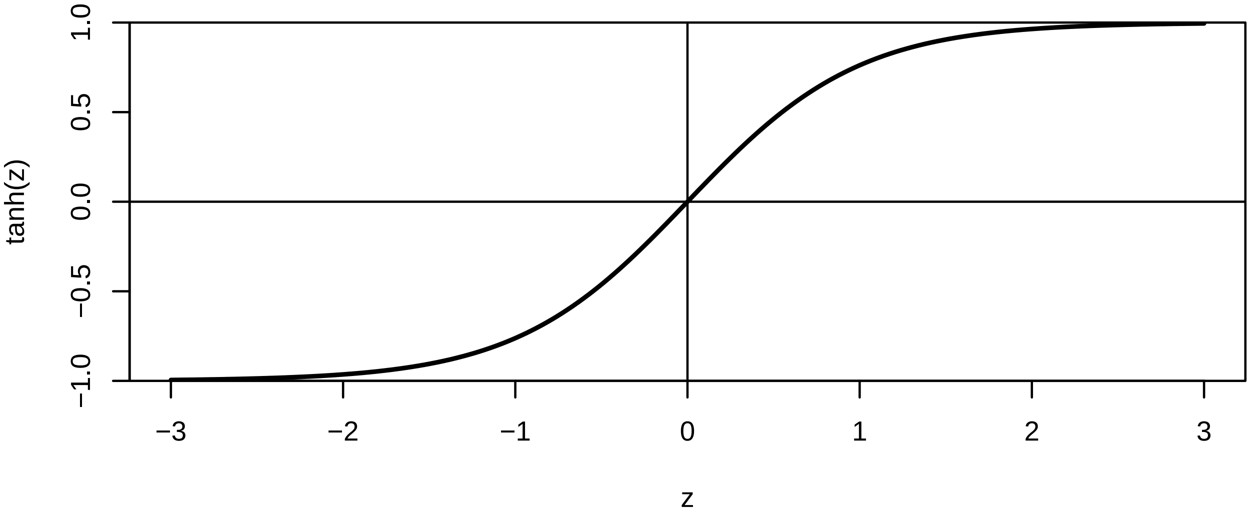
The Function Computed by the Network

The function, $f(x,w)$, computed by a multilayer perceptron network with one hidden layer of m units and one output unit can be written as follows:

$$f(x,w) \;=\; w_0^{(2)} \;+\; \sum_{j=1}^{m} w_j^{(2)} \phi_j(x,w), \qquad \phi_j(x,w) \;=\; h\Big(w_{0j}^{(1)} \;+\; \sum_{k=1}^{p} w_{kj}^{(1)} x_k\Big)$$

The network can approximate any function (better as m increases) if the *activation function*, $h(a)$, is any non-polynomial function.

A traditional choice of activation function (which I'll assume in later slides) is $\tanh(a) = (e^a - e^{-a}) \,/\, (e^a + e^{-a})$. It looks like this:



Training the Network by Maximum Likelihood

The simplest training procedure for an MLP network is to simply adjust the parameters (w) to maximize some measure of fit to the training data. The most obvious measure of fit is likelihood.

For a regresson problem, we may model the target values in training cases, $y_1, \ldots, y_n$, as being independent (given $x_1, \ldots, x_n$ and w), with responses distributed as $y_i \sim N(f(x_i, w), \sigma^2)$, for some noise variance σ^2.

The log of the likelihood (ignoring terms not involving w) is then

$$-\frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - f(x_i, w))^2$$

So maximum likelihood estimation for w just minimizes total squared error. But this is a complicated function of w, with no analytical way to find the maximum.

In real problems, the dimension of w, which is $m(p{+}2) + 1$, may be in the hundreds, thousands, tens of thousands, ...

There usually are many local maxima, and finding a global maximum is hopeless. Fortunately, good results are often obtained from fairly good local maxima.

Multiple Ways of Fitting the Data with an MLP

We may not need to find the global maximum of the likelihood because an MLP can fit the data in multiple ways — some producing identical results, others producing nearly identical results.

First, there are exact symmetries:

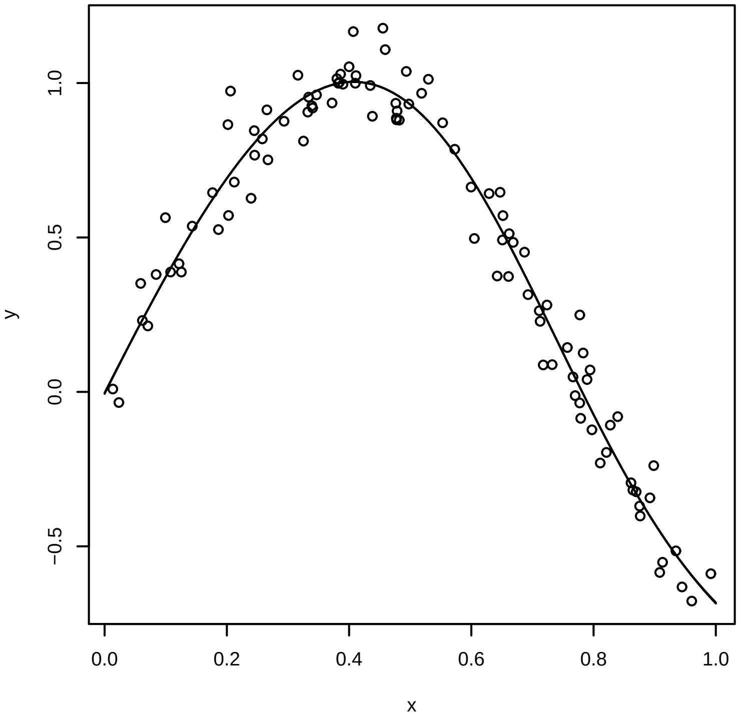
- Permuting the order of hidden units.
- For any hidden unit, j, negating $w_j^{(2)}$ and $w_{kj}^{(1)}$ for all k (including 0).

There are also similar, but different, ways to fit the data.

Suppose we have 10 hidden units, but 3 hidden units are enough to roughly fit the data. The other 7 hidden units could fit various different slight wiggles, with any of these overall fits being fairly good.

Example of Fitting a Network

Here are 100 training points (circles) that I artificially generated as $y = \sin(4x) + \text{noise}$, and the functions computed by three MLP networks with three hidden units found by fitting this data, with different starting points of the optimization procedure. The three fits are indistinguishable. The biggest difference in predicted value over the range $(0, 1)$ is about 0.003.



Here are the parameter values for the three fits:

$w_{11}^{(1)}$	$w_{12}^{(1)}$	$w_{13}^{(1)}$	$w_{01}^{(1)}$	$w_{02}^{(1)}$	$w_{03}^{(1)}$	$w_{1}^{(2)}$	$w_{2}^{(2)}$	$w_{3}^{(2)}$	$w_{0}^{(2)}$
-1.807	1.422	-2.923	-0.159	-0.224	2.052	-1.565	1.162	1.894	-1.829
-1.906	3.018	-0.218	0.005	-2.132	0.436	-2.140	-1.690	-0.530	-1.418
2.924	0.621	1.906	-2.078	-0.435	0.004	-1.867	0.885	1.987	-1.459

Iteratively Finding the MLP Parameters that Maximize the Likelihood

There is no analytical way of finding the parameters, w, of a multilayer perceptron network that maximize the likelihood, so iterative methods are used.

To start, we set all the network parameters to small random values — eg, values drawn uniformly from $[-0.1, +0.1]$. (Except we might set $w_0^{(2)}$ to the mean of y in the training cases, so it won't be far off if this mean is large.)

Setting all the $w_j^{(2)}$ and $w_{kj}^{(1)}$ to zero would not work, since the hidden units are then all identical, and an iterative method that treats them symmetrically could never make them non-identical.

We stop trying to increase the likelihood when either (a) the likelihood seems to be at a local maximum, or (b) it seems that trying to increase the likelihood further would actually make performance on test cases worse, or (c) our patience runs out. For (b), we need to use a held-out set of "validation" cases.

Optimizing neural network parameters may be quick for simple problems, but for the most difficult problems, network training can take days (or even weeks).

Three Approaches to Optimization

We'll see that it's easy to compute the partial derivatives of the log likelihood. Second derivatives can also be computed.

Using these derivatives, several iterative approaches to maximizing the log likelihood are possible:

- Newton and quasi-Newton methods — use the matrix of second derivatives (or estimates) to approximate the log likelihood as a quadratic function of the parameters. Move to the maximum of this approximation at each iteration. *Infeasible if there are many parameters (matrix too big); may not work well anyway, if the likelihood is very non-quadratic.*

- Conjugate gradient methods — cleverly choose good directions to look for the maximum, moving to the maximum along that direction at each iteration.

- Gradient descent — always move in the direction of the gradient (vector of partial derivatives). In the simplest scheme, we change w by some constant times the gradient of the log likelihood. *The original, and crudest, method, but sometimes the best — it doesn't need a big matrix of second derivatives, and can be used "on-line", without looking at all training cases at once.*

Computing Derivatives of the Log Likelihood

Partial derivatives of the log likelihood with respect to the network parameters are found by applying the chain rule backwards from the network output. Since training cases are assumed to be independent, we calculate derivates separately for each training case, then just sum them. I'll denote **minus** the log likelihood for just one training case by E, so that smaller E is better.

We first do "forward propagation", computing the summed input to each hidden unit, a_j, then the values of the hidden units, z_j, and finally the value of the output unit, f:

$$\begin{aligned} a_j &= w_{0j}^{(1)} + \sum_{k=1}^{p} w_{kj}^{(1)} x_k \\ z_j &= \tanh(a_j) \\ f &= w_0^{(2)} + \sum_{j=1}^{m} w_j^{(2)} z_j \end{aligned}$$

We then use "backpropagation" to find the derivatives of E with respect to f, with respect to z_j, and with respect to a_j. From these, we can find the derivatives with respect all the components of w.

Derivatives of E With Respect to f, z_j, and a_j

To start, we find the derivative of E with respect to the network output, f. If the response, y, is modeled as Gaussian with mean f and variance σ^2, then minus the log likelihood for just one case is $E = (y - f(x, w))^2/2\sigma^2$, and its derivative with respect to f is

$$\frac{\partial E}{\partial f} \;=\; (f - y) \,/\, \sigma^2$$

Once we have computed $\partial E/\partial f$, we work backward to (for all j) compute $\partial E/\partial z_j$, found assuming that $w_j^{(2)}$ and the $z_{j'}$ for $j' \neq j$ are fixed:

$$\frac{\partial E}{\partial z_j} \;=\; \frac{\partial E}{\partial f}\,\frac{\partial f}{\partial z_j} \;=\; w_j^{(2)}\,\frac{\partial E}{\partial f}$$

Next, we use the fact that $\tanh'(a) \;=\; 1 - \tanh(a)^2$ to work back to the derivative of E with respect to a_j, the summed input to hidden unit j:

$$\frac{\partial E}{\partial a_j} \;=\; \frac{\partial E}{\partial z_j}\,\frac{\partial z_j}{\partial a_j} \;=\; (1 - z_j^2)\,\frac{\partial E}{\partial z_j}$$

If we had more than one hidden layer, we would continue working backwards, finding the derivatives of E with respect to the values of all hidden units, and with respect to the summed inputs for these hidden units.

Derivatives of E With Respect to w

We can find the derivative of E w.r.t. a parameter on a connection from unit A to unit B by multiplying the value of A by the derivative of E w.r.t. the summed input to B.

For $w_1^{(2)}, \ldots, w_m^{(2)}$:

$$\frac{\partial E}{\partial w_j^{(2)}} \;=\; \frac{\partial E}{\partial f} \frac{\partial f}{\partial w_j^{(2)}} \;=\; z_j \frac{\partial E}{\partial f}$$

Also, $\partial E \,/\, \partial w_0^{(2)} \;=\; \partial E \,/\, \partial f$.

Similarly, for $w_{1j}^{(1)}, \ldots, w_{pj}^{(1)}$:

$$\frac{\partial E}{\partial w_{kj}^{(1)}} \;=\; \frac{\partial E}{\partial a_j} \frac{\partial a_j}{\partial w_{kj}^{(1)}} \;=\; x_k \frac{\partial E}{\partial a_j}$$

Also, $\partial E \,/\, \partial w_{0j}^{(1)} \;=\; \partial E \,/\, \partial a_j$.

Maximizing the Likelihood by Simple Gradient Ascent

After randomly initializing the parameters, w, to small values, we maximize the log likelihood repeatedly doing the following, using some suitably chosen "learning rate" or "stepsize", η:

1. For each training case:

   – Compute the values of the units by forward propagation.
   – Compute the derivatives of E w.r.t. the unit values by backpropagation.
   – Compute the derivatives of E w.r.t. the parameters from these results.

2. Sum these derivatives over all training cases, to get the gradient vector, g, of minus the total log likelihood.

3. Change w by moving in the direction of (minus) this gradient, replacing w by $w - \eta g$.

If η is too big, the changes will "overshoot", and end up decreasing the likelihood rather than increasing it. We have to set η by trial-and-error.

On-line Learning

The procedure in the previous slide is sometimes called “batch” gradient ascent learning, since the derivatives from the training cases are handled as one batch.

It’s also possible to do “on-line” learning, in which we update the parameters based on each training case in turn. This may work better if the training cases are redundant — many cases provide the same information. Batch learning then wastes time looking at them all before doing anything.

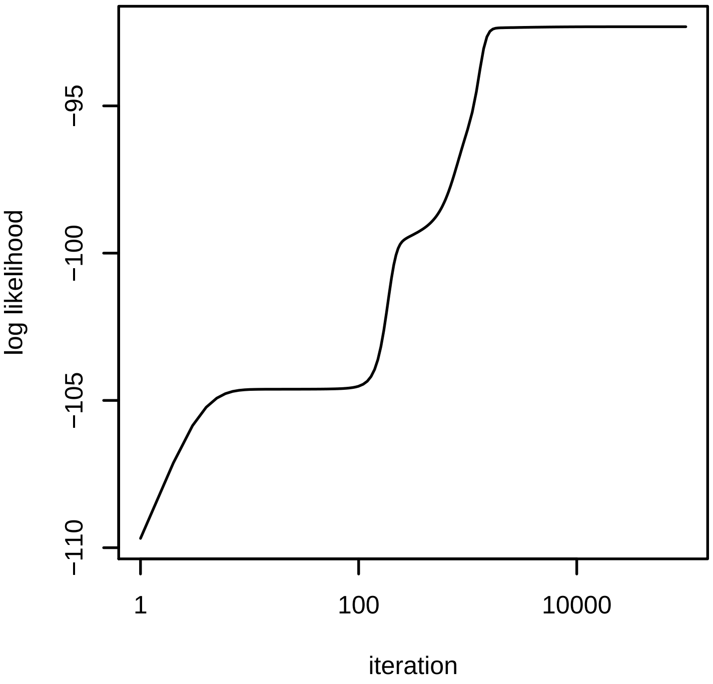
However, for on-line learning to converge to a (local) maximum, we will have to decrease η with time (or switch to batch learning once we’re near the maximum).

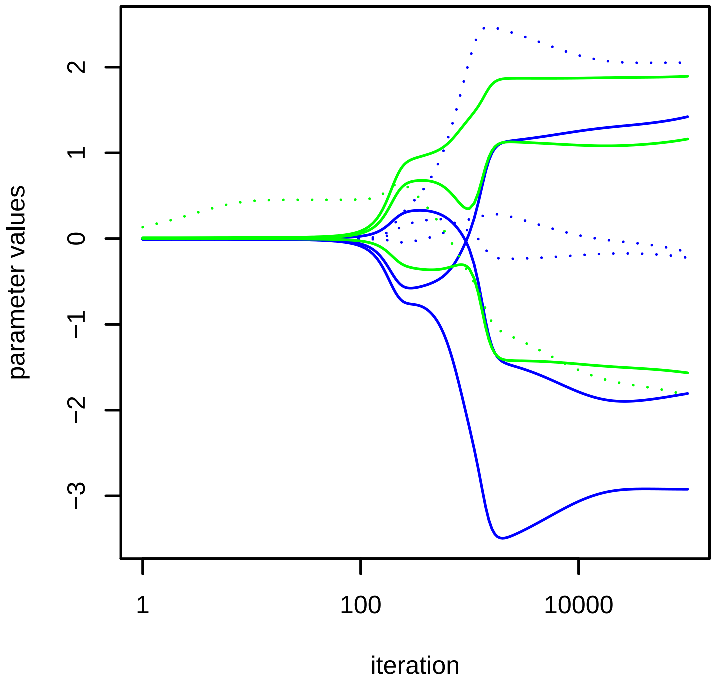
Actually, *true* on-line learning uses a new training case for each update — there is no finite training set, but rather a continuous stream of training cases. This is the situation for perceptual learning in humans.

Example of Simple Gradient Ascent Learning

Recall the previous example, with one input (ranging over $(0,1)$), one real target (equal to $\sin(4x) + \text{noise}$), and 100 training cases.

I trained a MLP network with three hidden units for 100000 iterations of simple gradient descent ($\eta = 0.3$). Here are plots of the log likelihood and of the 10 parameters as a function of iteration (log scale):

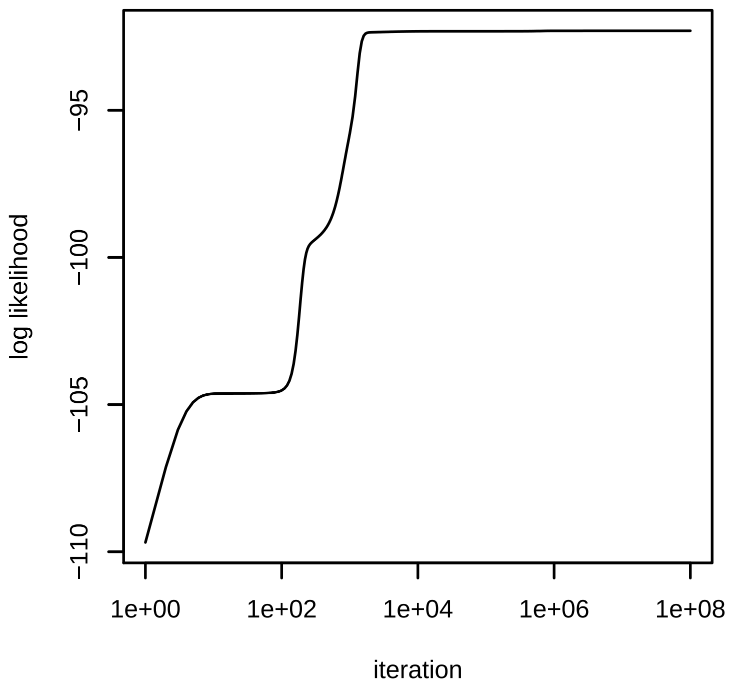


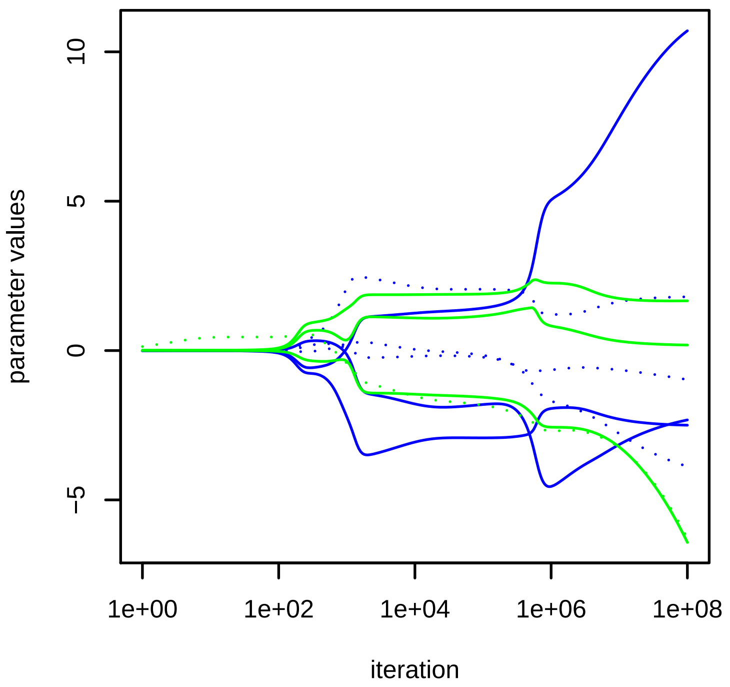


Blue lines are $w^{(1)}_{kj}$ ($k = 0$ dotted). Green lines are $w^{(2)}_{j}$ ($j = 0$ dotted).

Continuing the Example...

It may seem like the optimization has converged after 100000 iterations. But what happens if we continue training for many more iterations?



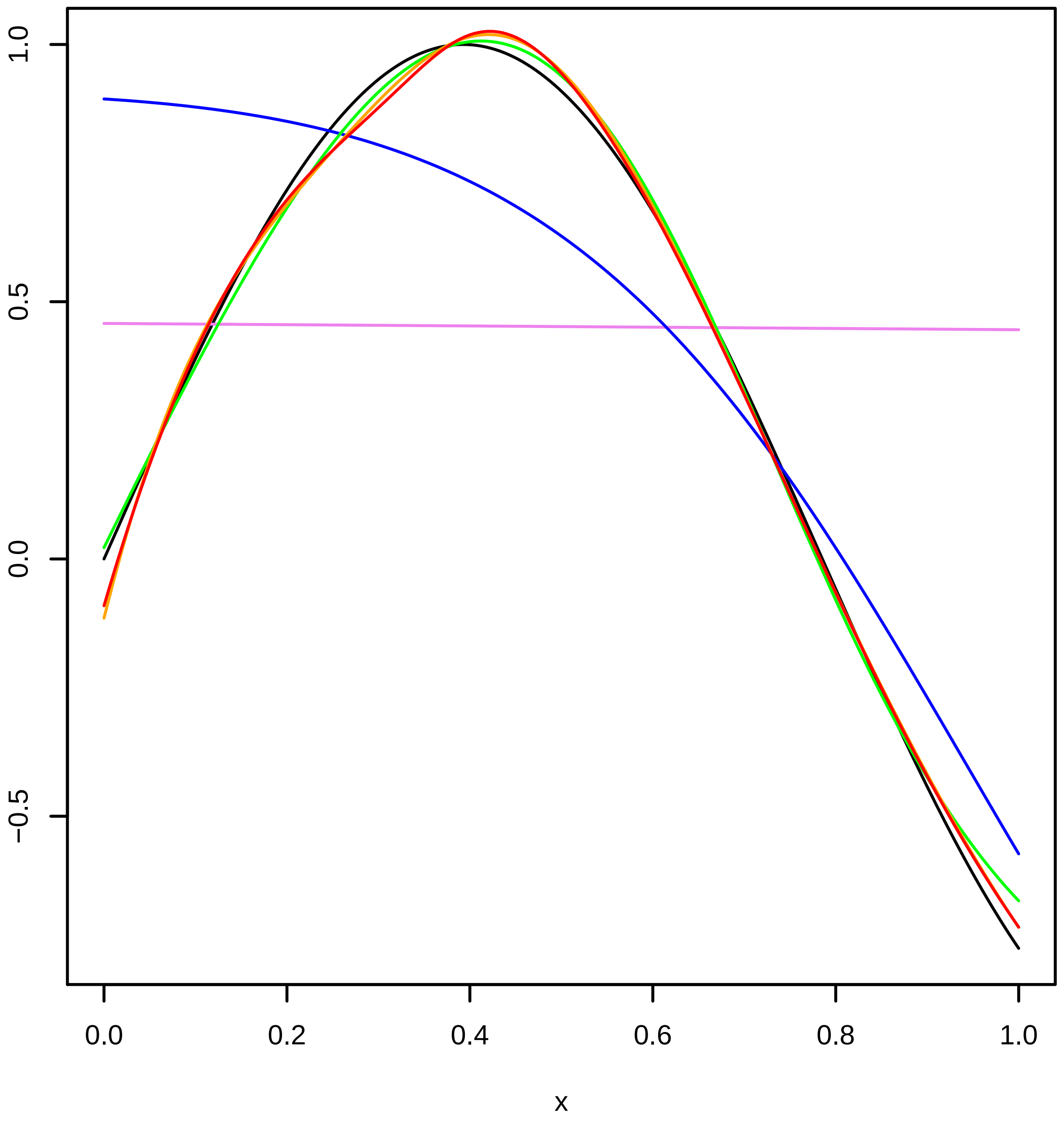


This shows how tricky the MLP likelihood function can be! In practice, we don't try to find the absolute maximum, since with complex networks it is sure to overfit the training data anyway...

Overfitting in This Example

Here is the true regression function, $\sin(4x)$, in black, and the regression functions defined by the networks after training for 10^2 (violet), 10^3 (blue), 10^4 (green), 10^6 (orange), and 10^8 (red) iterations.

The last two curves may have slightly overfit the data. Much more severe overfitting can occur when there are more inputs and/or more hidden units.



Avoiding Overfitting Using a Penalty

As for linear basis function models, we can try to avoid overfitting by maximizing the log likelihood plus a penalty function.

For an MLP with one hidden layer, a suitable penalty to add to minus the log likelihood might be

$$\lambda_1 \sum_{k=1}^{p} \sum_{j=1}^{m} \left[w_{kj}^{(1)} \right]^2 \ + \ \lambda_2 \sum_{j=1}^{m} \left[w_{j}^{(2)} \right]^2$$

We need to select two constants controlling the penalty, λ_1 and λ_2. Setting $\lambda_1 = \lambda_2$ isn't always reasonable, since a suitable value for λ_1 depends on the measurement units used for the inputs, whereas a suitable value for λ_2 depends on the measurement units for the response.

We might try S-fold cross-validation, but it may not work well, if each training run goes to a different local maximum. So we might use a single split into estimation and validation sets, with no re-training on the whole training set.

Avoiding Overfitting Using “Early Stopping”

We saw in the example that gradient descent spent a long time in a reasonable solution (not overfitted) before things went a bit crazy. Maybe we can somehow stop at this good point.

Some impressive results of MLP training that have been reported actually depended on having done this without meaning to — they just stopped when they lost patience with gradient descent, and that happened to be at a good point.

We’d like an “early stopping” method that doesn’t rely on being lucky.

Early Stopping Using a Validation Set

We can tell when to stop gradient descent optimization using a set of validation cases that's separate from the cases used to compute the gradient.

Here's the procedure:

1. Randomly divide the training set into an estimation set and a validation set — eg, 80% of cases in the estimation set and 20% n the validation set.

2. Randomly initialize the parameters to values near zero.

3. Repeatedly do the following:

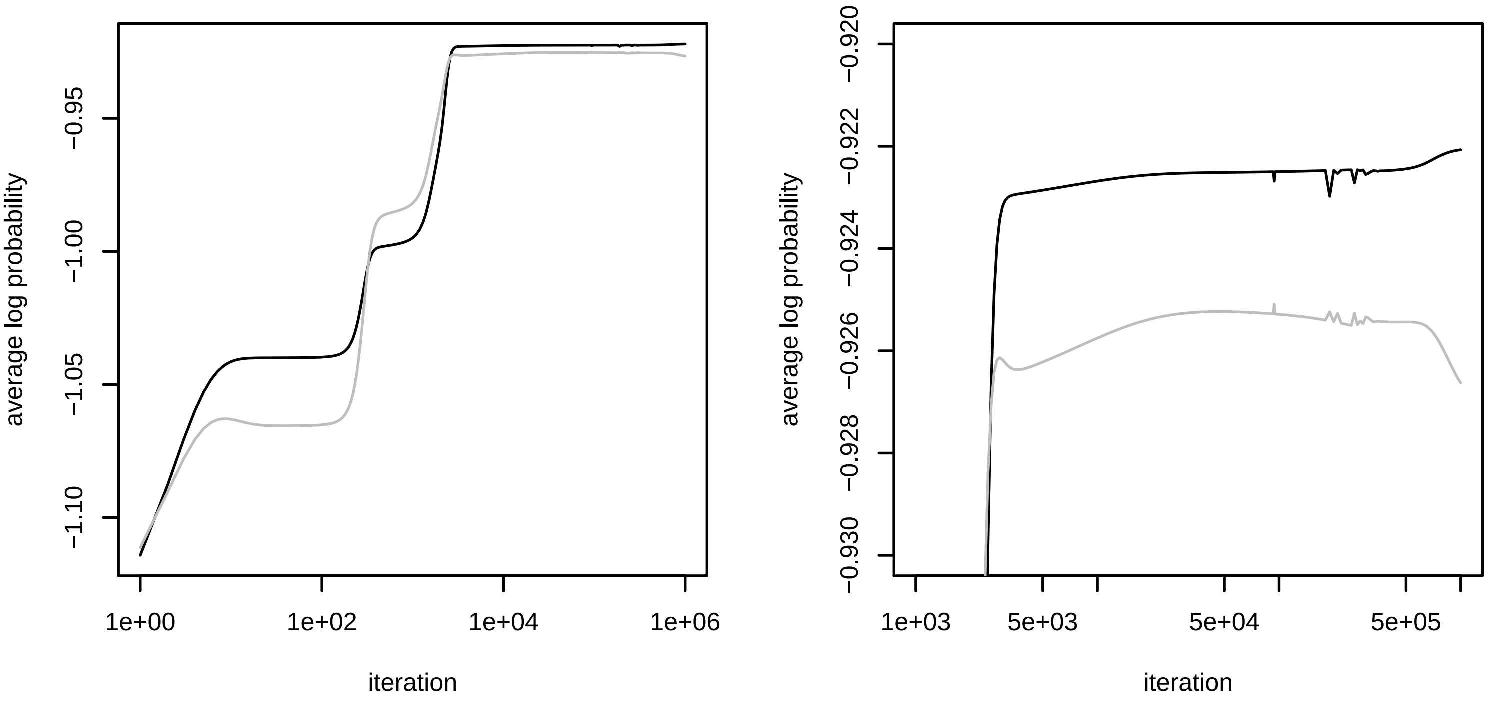
    - Compute the gradient of the log likelihood using the estimation set.
    - Update the parameters by adding η times the gradient.
    - Compute the log probability of y given x for the validation cases.

    Stop when the average log probability for validation cases is substantially less than the maximum of the values found previously (definitely getting worse).

4. Make predictions for test cases using the parameter values from the loop above that gave the highest average log probability to the validation cases.

An Example of Early Stopping Using Cross Validation

I tried same example as before, but with 75 of the 100 training cases used for estimation (computing the gradient) and 25 used for validation (deciding when to stop / which parameters to use). I used 20 hidden units this time, and set $\eta = 0.2$.

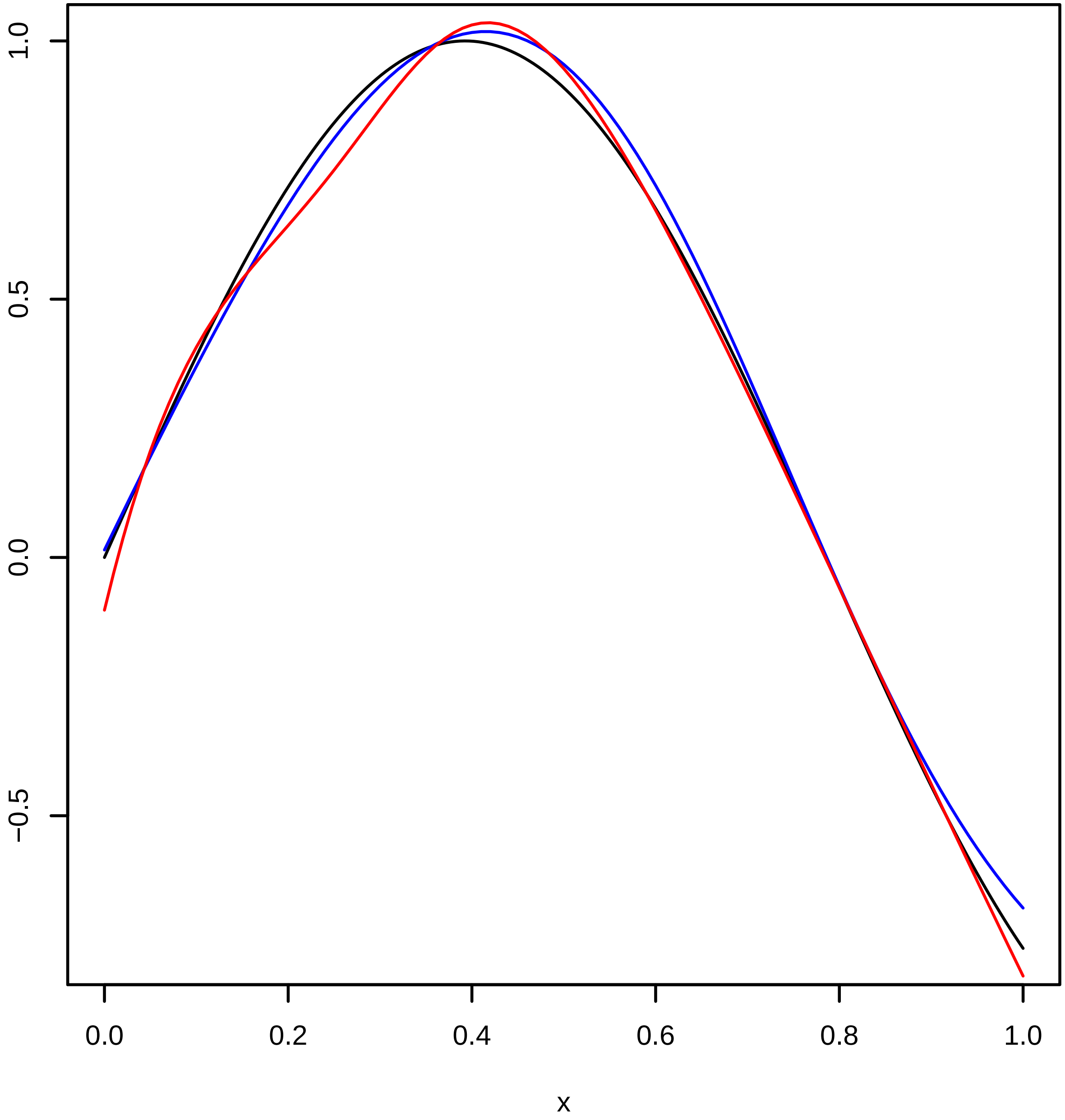


I divide total log probability by the number of cases in these plots, so that 75 vs. 25 won't matter. The average for estimation cases is shown in black, for validation cases in grey. The highest log probability for validation cases is at iteration 94000.

The Function Computed by the Network Selected

Here is the true regression function (black), the regression function defined by the network at iteration 94000 that was selected by cross validation (blue) ,and the last network at iteration 1000000 (red).

Cross validation worked this time, but 25 validation cases is really too few for reliable results.



Advantages of Early Stopping

Early stopping using a validation set has some advantages over a penalty method, in which you set λ_1 and λ_2 using S-fold cross validation, then train again on all the data with the λ_1 and λ_2 you choose.

With early stopping:

- You only have to train the network *once* — not once for each setting of λ_1 and λ_2 you consider, and then again on all the training data to get the final parameters. Important if training takes a week!
- The performance measure from cross-validation applies directly to the actual set of network parameters you will use, not to values of λ_1 and λ_2 that may not do the same thing for a different local maximum.

Disadvantages of Early Stopping

Early stopping also has some problems:

- It's very *ad hoc* — what's the justification for this procedure?
- It depends on details of the optimization method — eg, results could be different with a different η.
- In particular, we might want to use a different η for $w^{(1)}$ than for $w^{(2)}$ — sort of like using different values of λ for a penalty method.
- Some of the training data is used only to decide when to stop — this seems wasteful.

We could try to solve the third problem by doing training runs using different values of η for $w^{(1)}$ and for $w^{(2)}$, and then pick the best parameters (using the validation set) from all these runs.

The fourth problem can also be solved, by doing more training runs…

Using an Ensemble of Early-Stopped Networks

Rather than train just once, with a single split into estimation and validation sets, we can train several times, with several splits, to create an *ensemble* of networks.

It seems best to split the training set into S equal portions, and then train S times. Each training run uses $S-1$ portions of the training set for estimation, and one portion for validation (to choose which parameters from the run to use).

We get S sets of parameters this way. To make predictions for test cases, we *average* the predictions from all S networks.

This way we use the whole training set for estimation. Averaging several network outputs also reduces the effect of any single peculiar training run.

Modeling Non-Gaussian Response Variables

So far, we've used the function computed by the network to define a Gaussian distribution for the response variable, y, given the input variables, x:

$$y \,|\, x,\, w \;\;\sim\;\; N(f(x,w), \sigma^2)$$

More generally, we can use the network to define any sort of conditional distribution for y given x. Some useful examples:

- Binary classification models, where y is 0 or 1.
- Multi-class classification, where y is a value from some finite set.
- Regression with non-Gaussian residuals, where y is real, but $y|x$ is not Gaussian. Eg, we might use a heavier-tailed t-distribution if some cases have residuals that are larger than is typical of other cases.

The Logistic Model for Binary Responses

Logistic models are very common way of handling binary responses, such as when learning to classify items into two groups.

If $f(x,w)$ is the function computed by the network, we define the probability for a response of $y=1$ to be

$$P(y=1 \,|\, x,\, w) \quad = \quad \Big[1+\exp(-f(x,w))\Big]^{-1} \quad = \quad \sigma(f(x,w))$$

where $\sigma(a) = 1/(1+e^{-a})$.

One can easily show that the derivative of σ is $\sigma'(a) = \sigma(a)\,(1-\sigma(a))$. This is used when computing derivatives by backpropagation.