16 *Adaptive basis function models*

16.1 Introduction

In Chapters 14 and 15, we discussed kernel methods, which provide a powerful way to create nonlinear models for regression and classification. The prediction takes the form $f(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$, where we define

$$\boldsymbol{\phi}(\mathbf{x}) = [\kappa(\mathbf{x}, \boldsymbol{\mu}_1), \ldots, \kappa(\mathbf{x}, \boldsymbol{\mu}_N)] \tag{16.1}$$

and where $\boldsymbol{\mu}_k$ are either all the training data or some subset. Models of this form essentially perform a form of **template matching**, whereby they compare the input $\mathbf{x}$ to the stored prototypes $\boldsymbol{\mu}_k$.

Although this can work well, it relies on having a good kernel function to measure the similarity between data vectors. Often coming up with a good kernel function is quite difficult. For example, how do we define the similarity between two images? Pixel-wise comparison of intensities (which is what a Gaussian kernel corresponds to) does not work well. Although it is possible (and indeed common) to hand-engineer kernels for specific tasks (see e.g., the pyramid match kernel in Section 14.2.7), it would be more interesting if we could learn the kernel.

In Section 15.2.4, we discussed a way to learn the parameters of a kernel function, by maximizing the marginal likelihood. For example, if we use the ARD kernel,

$$\kappa(\mathbf{x}, \mathbf{x}') = \theta_0 \exp\left(-\frac{1}{2}\sum_{j=1}^{D} \theta_j (x_j - x'_j)^2\right) \tag{16.2}$$

we can can estimate the θ_j, and thus perform a form of nonlinear feature selection. However, such methods can be computationally expensive. Another approach, known as multiple kernel learning (see e.g., (Rakotomamonjy et al. 2008)) uses a convex combination of base kernels, $\kappa(\mathbf{x}, \mathbf{x}') = \sum_j w_j \kappa_j(\mathbf{x}, \mathbf{x}')$, and then estimates the mixing weights w_j. But this relies on having good base kernels (and is also computationally expensive).

An alternative approach is to dispense with kernels altogether, and try to learn useful features $\boldsymbol{\phi}(\mathbf{x})$ directly from the input data. That is, we will create what we call an **adaptive basis-function model** (ABM), which is a model of the form

$$f(\mathbf{x}) = w_0 + \sum_{m=1}^{M} w_m \phi_m(\mathbf{x}) \tag{16.3}$$

where $\phi_m(\mathbf{x})$ is the m'th basis function, which is learned from data. This framework covers all of the models we will discuss in this chapter.

Typically the basis functions are parametric, so we can write $\phi_m(\mathbf{x}) = \phi(\mathbf{x}; \mathbf{v}_m)$, where $\mathbf{v}_m$ are the parameters of the basis function itself. We will use $\boldsymbol{\theta} = (w_0, \mathbf{w}_{1:M}, \{\mathbf{v}_m\}_{m=1}^M)$ to denote the entire parameter set. The resulting model is not linear-in-the-parameters anymore, so we will only be able to compute a locally optimal MLE or MAP estimate of $\boldsymbol{\theta}$. Nevertheless, such models often significantly outperform linear models, as we will see.

16.2 Classification and regression trees (CART)

Classification and regression trees or **CART** models, also called **decision trees** (not to be confused with the decision trees used in decision theory) are defined by recursively partitioning the input space, and defining a local model in each resulting region of input space. This can be represented by a tree, with one leaf per region, as we explain below.

16.2.1 Basics

To explain the CART approach, consider the tree in Figure 16.1(a). The first node asks if x_1 is less than some threshold t_1. If yes, we then ask if x_2 is less than some other threshold t_2. If yes, we are in the bottom left quadrant of space, R_1. If no, we ask if x_1 is less than t_3. And so on. The result of these **axis parallel splits** is to partition 2d space into 5 regions, as shown in Figure 16.1(b). We can now associate a mean response with each of these regions, resulting in the piecewise constant surface shown in Figure 16.1(c).

We can write the model in the following form

$$f(\mathbf{x}) = \mathbb{E}[y|\mathbf{x}] = \sum_{m=1}^M w_m \mathbb{I}(\mathbf{x} \in R_m) = \sum_{m=1}^M w_m \phi(\mathbf{x}; \mathbf{v}_m) \tag{16.4}$$

where R_m is the m'th region, w_m is the mean response in this region, and $\mathbf{v}_m$ encodes the choice of variable to split on, and the threshold value, on the path from the root to the m'th leaf. This makes it clear that a CART model is just a an adaptive basis-function model, where the basis functions define the regions, and the weights specify the response value in each region. We discuss how to find these basis functions below.

We can generalize this to the classification setting by storing the distribution over class labels in each leaf, instead of the mean response. This is illustrated in Figure 16.2. This model can be used to classify the data in Figure 1.1. For example, we first check the color of the object. If it is blue, we follow the left branch and end up in a leaf labeled "4,0", which means we have 4 positive examples and 0 negative examples which match this criterion. Hence we predict $p(y = 1|\mathbf{x}) = 4/4$ if $\mathbf{x}$ is blue. If it is red, we then check the shape: if it is an ellipse, we end up in a leaf labeled "1,1", so we predict $p(y = 1|\mathbf{x}) = 1/2$. If it is red but not an ellipse, we predict $p(y = 1|\mathbf{x}) = 0/2$; If it is some other colour, we check the size: if less than 10, we predict $p(y = 1|\mathbf{x}) = 4/4$, otherwise $p(y = 1|\mathbf{x}) = 0/5$. These probabilities are just the empirical fraction of positive examples that satisfy each conjunction of feature values, which defines a path from the root to a leaf.

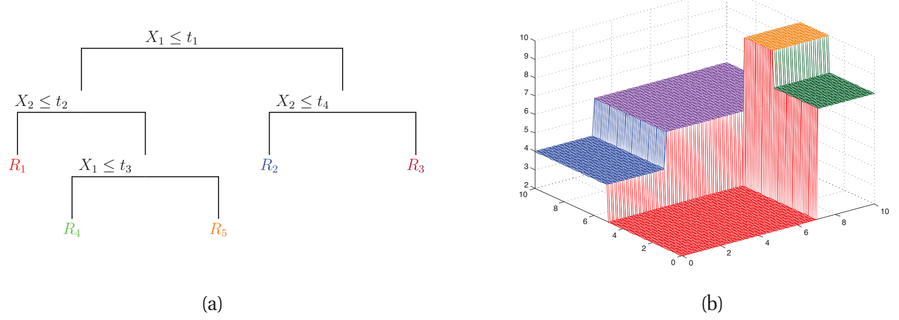


Figure 16.1 A simple regression tree on two inputs. Based on Figure 9.2 of (Hastie et al. 2009). Figure generated by `regtreeSurfaceDemo`.

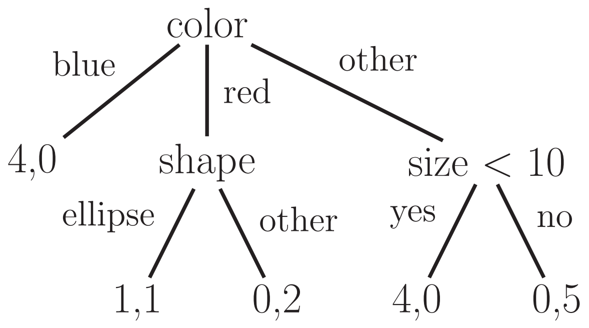


Figure 16.2 A simple decision tree for the data in Figure 1.1. A leaf labeled as (n_1, n_0) means that there are n_1 positive examples that match this path, and n_0 negative examples. In this tree, most of the leaves are "pure", meaning they only have examples of one class or the other; the only exception is leaf representing red ellipses, which has a label distribution of $(1, 1)$. We could distinguish positive from negative red ellipses by adding a further test based on size. However, it is not always desirable to construct trees that perfectly model the training data, due to overfitting.

16.2.2 Growing a tree

Finding the optimal partitioning of the data is NP-complete (Hyafil and Rivest 1976), so it is common to use the greedy procedure shown in Algorithm 6 to compute a locally optimal MLE. This method is used by CART, (Breiman et al. 1984) **C4.5**(Quinlan 1993), and **ID3** (Quinlan 1986), which are three popular implementations of the method. (See `dtfit` for a simple Matlab implementation.)

The split function chooses the best feature, and the best value for that feature, as follows:

$$(j^*, t^*) = \arg \min_{j \in \{1,\ldots,D\}} \min_{t \in \mathcal{T}_j} \text{cost}(\{\mathbf{x}_i, y_i : x_{ij} \leq t\}) + \text{cost}(\{\mathbf{x}_i, y_i : x_{ij} > t\}) \quad (16.5)$$

Algorithm 16.1: Recursive procedure to grow a classification/ regression tree

```
function fitTree(node, $\mathcal{D}$, depth) ;
node.prediction = mean($y_i : i \in \mathcal{D}$) // or class label distribution ;
$(j^*, t^*, \mathcal{D}_L, \mathcal{D}_R) = \text{split}(\mathcal{D})$;
if not worthSplitting(depth, cost, $\mathcal{D}_L$, $\mathcal{D}_R$) then
    return node
else
    node.test = $\lambda \mathbf{x}.x_{j^*} < t^*$ // anonymous function;
    node.left = fitTree(node, $\mathcal{D}_L$, depth+1);
    node.right = fitTree(node, $\mathcal{D}_R$, depth+1);
    return node;
```

where the cost function for a given dataset will be defined below. For notational simplicity, we have assumed all inputs are real-valued or ordinal, so it makes sense to compare a feature x_{ij} to a numeric value t. The set of possible thresholds $\mathcal{T}_j$ for feature j can be obtained by sorting the unique values of x_{ij}. For example, if feature 1 has the values $\{4.5, -12, 72, -12\}$, then we set $\mathcal{T}_1 = \{-12, 4.5, 72\}$. In the case of categorical inputs, the most common approach is to consider splits of the form $x_{ij} = c_k$ and $x_{ij} \neq c_k$, for each possible class label c_k. Although we could allow for multi-way splits (resulting in non-binary trees), this would result in **data fragmentation**, meaning too little data might "fall" into each subtree, resulting in overfitting.

The function that checks if a node is worth splitting can use several stopping heuristics, such as the following:

- is the reduction in cost too small? Typically we define the gain of using a feature to be a normalized measure of the reduction in cost:

$$\Delta \triangleq \text{cost}(\mathcal{D}) - \left(\frac{|\mathcal{D}_L|}{|\mathcal{D}|}\text{cost}(\mathcal{D}_L) + \frac{|\mathcal{D}_R|}{|\mathcal{D}|}\text{cost}(\mathcal{D}_R) \right) \tag{16.6}$$

- has the tree exceeded the maximum desired depth?
- is the distribution of the response in either $\mathcal{D}_L$ or $\mathcal{D}_R$ sufficiently homogeneous (e.g., all labels are the same, so the distribution is **pure**)?
- is the number of examples in either $\mathcal{D}_L$ or $\mathcal{D}_R$ too small?

All that remains is to specify the cost measure used to evaluate the quality of a proposed split. This depends on whether our goal is regression or classification. We discuss both cases below.

16.2.2.1 Regression cost

In the regression setting, we define the cost as follows:

$$\text{cost}(\mathcal{D}) = \sum_{i \in \mathcal{D}} (y_i - \overline{y})^2 \tag{16.7}$$

where $\overline{y} = \frac{1}{|\mathcal{D}|}\sum_{i\in\mathcal{D}} y_i$ is the mean of the response variable in the specified set of data. Alternatively, we can fit a linear regression model for each leaf, using as inputs the features that were chosen on the path from the root, and then measure the residual error.

16.2.2.2 Classification cost

In the classification setting, there are several ways to measure the quality of a split. First, we fit a multinoulli model to the data in the leaf satisfying the test $X_j < t$ by estimating the class-conditional probabilities as follows:

$$\hat{\pi}_c = \frac{1}{|\mathcal{D}|}\sum_{i\in\mathcal{D}} \mathbb{I}(y_i = c) \tag{16.8}$$

where $\mathcal{D}$ is the data in the leaf. Given this, there are several common error measures for evaluating a proposed partition:

- **Misclassification rate**. We define the most probable class label as $\hat{y}_c = \operatorname{argmax}_c \hat{\pi}_c$. The corresponding error rate is then

$$\frac{1}{|\mathcal{D}|}\sum_{i\in\mathcal{D}} \mathbb{I}(y_i \neq \hat{y}) = 1 - \hat{\pi}_{\hat{y}} \tag{16.9}$$

- **Entropy**, or **deviance**:

$$\mathbb{H}(\hat{\boldsymbol{\pi}}) = -\sum_{c=1}^{C} \hat{\pi}_c \log \hat{\pi}_c \tag{16.10}$$

  Note that minimizing the entropy is equivalent to maximizing the **information gain** (Quinlan 1986) between test $X_j < t$ and the class label Y, defined by

$$\begin{aligned} \text{infoGain}(X_j < t, Y) &\triangleq \mathbb{H}(Y) - \mathbb{H}(Y|X_j < t) & (16.11)\\ &= \left(-\sum_c p(y=c)\log p(y=c)\right) & (16.12)\\ &\quad + \left(\sum_c p(y=c|X_j<t)\log p(c|X_j<t)\right) & (16.13)\end{aligned}$$

  since $\hat{\pi}_c$ is an MLE for the distribution $p(c|X_j < t)$.[1]

1. If X_j is categorical, and we use tests of the form $X_j = k$, then taking expectations over values of X_j gives the mutual information between X_j and Y: $\mathbb{E}[\text{infoGain}(X_j, Y)] = \sum_k p(X_j = k)\text{infoGain}(X_j = k, Y) = \mathbb{H}(Y) - \mathbb{H}(Y|X_j) = \mathbb{I}(Y; X_j)$.

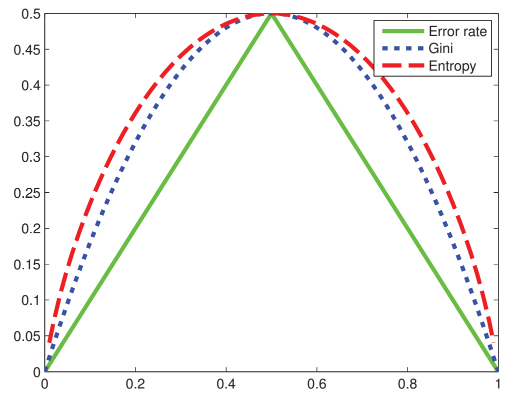


Figure 16.3 Node impurity measures for binary classification. The horizontal axis corresponds to p, the probability of class 1. The entropy measure has been rescaled to pass through (0.5,0.5). Based on Figure 9.3 of (Hastie et al. 2009). Figure generated by `giniDemo`.

- **Gini index**

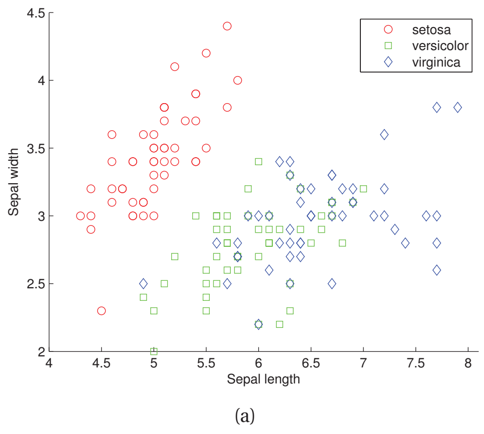
$$\sum_{c=1}^{C} \hat{\pi}_c(1-\hat{\pi}_c) = \sum_c \hat{\pi}_c - \sum_c \hat{\pi}_c^2 = 1 - \sum_c \hat{\pi}_c^2 \tag{16.14}$$

  This is the expected error rate. To see this, note that $\hat{\pi}_c$ is the probability a random entry in the leaf belongs to class c, and $(1-\hat{\pi}_c$ is the probability it would be misclassified.

In the two-class case, where $p = \pi_m(1)$, the misclassification rate is $1 - \max(p, 1-p)$, the entropy is $\mathbb{H}_2(p)$, and the Gini index is $2p(1-p)$. These are plotted in Figure 16.3. We see that the cross-entropy and Gini measures are very similar, and are more sensitive to changes in class probability than is the misclassification rate. For example, consider a two-class problem with 400 cases in each class. Suppose one split created the nodes (300,100) and (100,300), while the other created the nodes (200,400) and (200,0). Both splits produce a misclassification rate of 0.25. However, the latter seems preferable, since one of the nodes is **pure**, i.e., it only contains one class. The cross-entropy and Gini measures will favor this latter choice.

16.2.2.3 Example

As an example, consider two of the four features from the 3-class iris dataset, shown in Figure 16.4(a). The resulting tree is shown in Figure 16.5(a), and the decision boundaries are shown in Figure 16.4(b). We see that the tree is quite complex, as are the resulting decision boundaries. In Figure 16.5(b), we show that the CV estimate of the error is much higher than the training set error, indicating overfitting. Below we discuss how to perform a tree-pruning stage to simplify the tree.



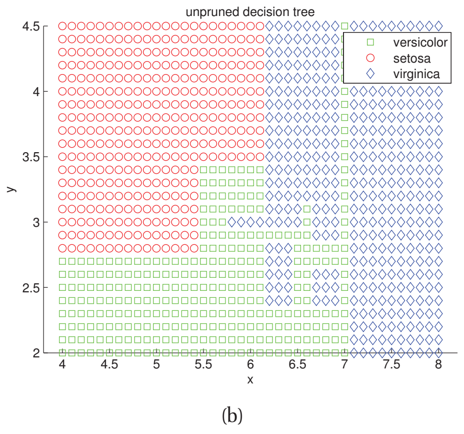
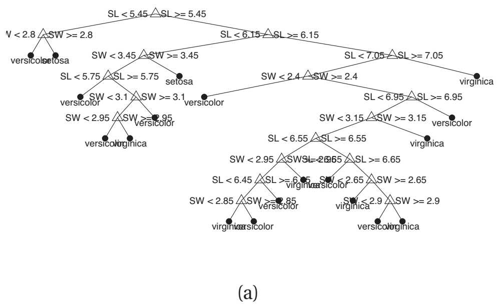


Figure 16.4 (a) Iris data. We only show the first two features, sepal length and sepal width, and ignore petal length and petal width. (b) Decision boundaries induced by the decision tree in Figure 16.5(a).



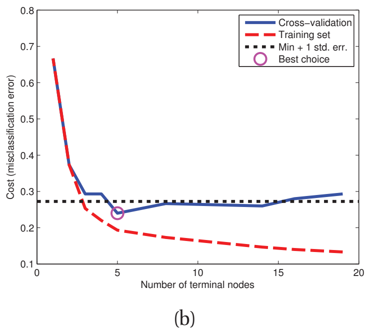


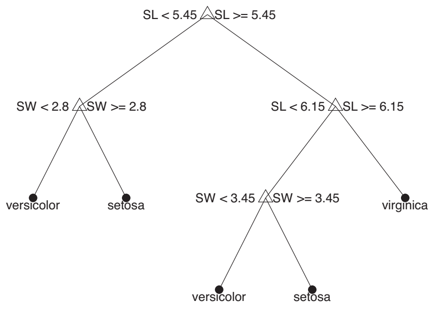
Figure 16.5 (a) Unpruned decision tree for Iris data. (b) Plot of misclassification error rate vs depth of tree. Figure generated by `dtreeDemoIris`.

16.2.3 Pruning a tree

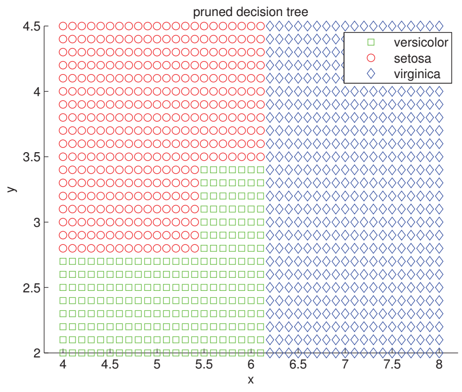
To prevent overfitting, we can stop growing the tree if the decrease in the error is not sufficient to justify the extra complexity of adding an extra subtree. However, this tends to be too myopic. For example, on the xor data in Figure 14.2(c), it would might never make any splits, since each feature on its own has little predictive power.

The standard approach is therefore to grow a "full" tree, and then to perform **pruning**. This can be done using a scheme that prunes the branches giving the least increase in the error. See (Breiman et al. 1984) for details.

To determine how far to prune back, we can evaluate the cross-validated error on each such subtree, and then pick the tree whose CV error is within 1 standard error of the minimum. This is illustrated in Figure 16.4(b). The point with the minimum CV error corresponds to the simple tree in Figure 16.6(a).



(a)



(b)

Figure 16.6 Pruned decision tree for Iris data. Figure generated by `dtreeDemoIris`.

16.2.4 Pros and cons of trees

CART models are popular for several reasons: they are easy to interpret[2], they can easily handle mixed discrete and continuous inputs, they are insensitive to monotone transformations of the inputs (because the split points are based on ranking the data points), they perform automatic variable selection, they are relatively robust to outliers, they scale well to large data sets, and they can be modified to handle missing inputs.[3]

However, CART models also have some disadvantages. The primary one is that they do not predict very accurately compared to other kinds of model. This is in part due to the greedy nature of the tree construction algorithm. A related problem is that trees are **unstable**: small changes to the input data can have large effects on the structure of the tree, due to the hierarchical nature of the tree-growing process, causing errors at the top to affect the rest of the tree. In frequentist terminology, we say that trees are high variance estimators. We discuss a solution to this below.

16.2.5 Random forests

One way to reduce the variance of an estimate is to average together many estimates. For example, we can train M different trees on different subsets of the data, chosen randomly with

2. We can postprocess the tree to derive a series of logical **rules** such as "If $x_1 < 5.45$ then ..." (Quinlan 1990).

3. The standard heuristic for handling missing inputs in decision trees is to look for a series of "backup" variables, which can induce a similar partition to the chosen variable at any given split; these can be used in case the chosen variable is unobserved at test time. These are called **surrogate splits**. This method finds highly correlated features, and can be thought of as learning a local joint model of the input. This has the advantage over a generative model of not modeling the entire joint distribution of inputs, but it has the disadvantage of being entirely ad hoc. A simpler approach, applicable to categorical variables, is to code "missing" as a new value, and then to treat the data as fully observed.

replacement, and then compute the ensemble

$$f(\mathbf{x}) = \sum_{m=1}^{M} \frac{1}{M} f_m(\mathbf{x}) \tag{16.15}$$

where f_m is the m'th tree. This technique is called **bagging** (Breiman 1996), which stands for "bootstrap aggregating".

Unfortunately, simply re-running the same learning algorithm on different subsets of the data can result in highly correlated predictors, which limits the amount of variance reduction that is possible. The technique known as **random forests** (Breiman 2001a) tries to decorrelate the base learners by learning trees based on a randomly chosen subset of input variables, as well as a randomly chosen subset of data cases. Such models often have very good predictive accuracy (Caruana and Niculescu-Mizil 2006), and have been widely used in many applications (e.g., for body pose recognition using Microsoft's popular kinect sensor (Shotton et al. 2011)).

Bagging is a frequentist concept. It is also possible to adopt a Bayesian approach to learning trees. In particular, (Chipman et al. 1998; Denison et al. 1998; Wu et al. 2007) perform approximate inference over the space of trees (structure and parameters) using MCMC. This reduces the variance of the predictions. We can also perform Bayesian inference over the space of ensembles of trees, which tends to work much better. This is known as **Bayesian adaptive regression trees** or **BART** (Chipman et al. 2010). Note that the cost of these sampling-based Bayesian methods is comparable to the sampling-based random forest method. That is, both approaches are farily slow to train, but produce high quality classifiers.

Unfortunately, methods that use multiple trees (whether derived from a Bayesian or frequentist standpoint) lose their nice interpretability properties. Fortunately, various post-processing measures can be applied, as discussed in Section 16.8.

16.2.6 CART compared to hierarchical mixture of experts *

An interesting alternative to a decision tree is known as the hierarchical mixture of experts. Figure 11.7(b) gives an illustration where we have two levels of experts. This can be thought of as a probabilistic decision tree of depth 2, since we recursively partition the space, and apply a different expert to each partition. Hastie et al. (Hastie et al. 2009, p331) write that "The HME approach is a promising competitor to CART trees". Some of the advantages include the following:

- The model can partition the input space using any set of nested linear decision boundaries. By contrast, standard decision trees are constrained to use axis-parallel splits.
- The model makes predictions by averaging over all experts. By contrast, in a standard decision tree, predictions are made only based on the model in the corresponding leaf. Since leaves often contain few training examples, this can result in overfitting.
- Fitting an HME involves solving a smooth continuous optimization problem (usually using EM), which is likely to be less prone to local optima than the standard greedy discrete optimization methods used to fit decision trees. For similar reasons, it is computationally easier to "be Bayesian" about the parameters of an HME (see e.g., (Peng et al. 1996; Bishop

and Svensén 2003)) than about the structure and parameters of a decision tree (see e.g., (Wu et al. 2007)).

16.3 Generalized additive models

A simple way to create a nonlinear model with multiple inputs is to use a **generalized additive model** (Hastie and Tibshirani 1990), which is a model of the form

$$f(\mathbf{x}) = \alpha + f_1(x_1) + \cdots + f_D(x_D) \tag{16.16}$$

Here each f_j can be modeled by some scatterplot smoother, and $f(\mathbf{x})$ can be mapped to $p(y|\mathbf{x})$ using a link function, as in a GLM (hence the term *generalized* additive model).

If we use regression splines (or some other fixed basis function expansion approach) for the f_j, then each $f_j(x_j)$ can be written as $\boldsymbol{\beta}_j^T \boldsymbol{\phi}_j(x_j)$, so the whole model can be written as $f(\mathbf{x}) = \boldsymbol{\beta}^T \boldsymbol{\phi}(\mathbf{x})$, where $\boldsymbol{\phi}(\mathbf{x}) = [1, \boldsymbol{\phi}_1(x_1), \ldots, \boldsymbol{\phi}_D(x_D)]$. However, it is more common to use smoothing splines (Section 15.4.6) for the f_j. In this case, the objective (in the regression setting) becomes

$$J(\alpha, f_1, \ldots, f_D) = \sum_{i=1}^{N} \left(y_i - \alpha - \sum_{j=1}^{D} f_j(x_{ij}) \right)^2 + \sum_{j=1}^{D} \lambda_j \int f_j''(t_j)^2 dt_j \tag{16.17}$$

where λ_j is the strength of the regularizer for f_j.

16.3.1 Backfitting

We now discuss how to fit the model using MLE. The constant α is not uniquely identifiable, since we can always add or subtract constants to any of the f_j functions. The convention is to assume $\sum_{i=1}^N f_j(x_{ij}) = 0$ for all j. In this case, the MLE for α is just $\hat{\alpha} = \frac{1}{N}\sum_{i=1}^N y_i$.

To fit the rest of the model, we can center the responses (by subtracting $\hat{\alpha}$), and then iteratively update each f_j in turn, using as a target vector the residuals obtained by omitting term f_j:

$$\hat{f}_j := \text{smoother}(\{y_i - \sum_{k \neq j} \hat{f}_k(x_{ik})\}_{i=1}^N) \tag{16.18}$$

We should then ensure the output is zero mean using

$$\hat{f}_j := \hat{f}_j - \frac{1}{N}\sum_{i=1}^{N} \hat{f}_j(x_{ij}) \tag{16.19}$$

This is called the **backfitting** algorithm (Hastie and Tibshirani 1990). If $\mathbf{X}$ has full column rank, then the above objective is convex (since each smoothing spline is a linear operator, as shown in Section 15.4.2), so this procedure is guaranteed to converge to the global optimum.

In the GLM case, we need to modify the method somewhat. The basic idea is to replace the weighted least squares step of IRLS (see Section 8.3.4) with a weighted backfitting algorithm. In the logistic regression case, each response has weight $s_i = \mu_i(1 - \mu_i)$ associated with it, where $\mu_i = \text{sigm}(\hat{\alpha} + \sum_{j=1}^D \hat{f}_j(x_{ij}))$.)

16.3.2 Computational efficiency

Each call to the smoother takes $O(N)$ time, so the total cost is $O(NDT)$, where T is the number of iterations. If we have high-dimensional inputs, fitting a GAM is expensive. One approach is to combine it with a sparsity penalty, see e.g., the **SpAM** (sparse additive model) approach of (Ravikumar et al. 2009). Alternatively, we can use a greedy approach, such as boosting (see Section 16.4.6)

16.3.3 Multivariate adaptive regression splines (MARS)

We can extend GAMs by allowing for interaction effects. In general, we can create an ANOVA decomposition:

$$f(\mathbf{x}) = \beta_0 + \sum_{j=1}^{D} f_j(x_j) + \sum_{j,k} f_{jk}(x_j, x_k) + \sum_{j,k,l} f_{jkl}(x_j, x_k, x_l) + \cdots \tag{16.20}$$

Of course, we cannot allow for too many higher-order interactions, because there will be too many parameters to fit.

It is common to use greedy search to decide which variables to add. The **multivariate adaptive regression splines** or **MARS** algorithm is one example of this (Hastie et al. 2009, Sec9.4). It fits models of the form in Equation 16.20, where it uses a tensor product basis of regression splines to represent the multidimensional regression functions. For example, for 2d input, we might use

$$\begin{aligned} f(x_1, x_2) &= \beta_0 + \sum_m \beta_{1m}(x_1 - t_{1m})_+ \\ &\quad + \sum_m \beta_{2m}(t_{2m} - x_2)_+ + \sum_m \beta_{12m}(x_1 - t_{1m})_+(t_{2m} - x_2)_+ \end{aligned} \tag{16.21}$$

To create such a function, we start with a set of candidate basis functions of the form

$$\mathcal{C} = \{(x_j - t)_+, (t - x_j)_+ : t \in \{x_{1j}, \ldots, x_{Nj}\}, j = 1, \ldots, D\} \tag{16.22}$$

These are 1d linear splines where the knots are at all the observed values for that variable. We consider splines sloping up in both directions; this is called a **reflecting pair**. See Figure 16.7(a).

Let $\mathcal{M}$ represent the current set of basis functions. We initialize by using $\mathcal{M} = \{1\}$. We consider creating a new basis function pair by multplying an $h_m \in \mathcal{M}$ with one of the reflecting pairs in $\mathcal{C}$. For example, we might initially get

$$f(\mathbf{x}) = 25 - 4(x_1 - 5)_+ + 20(5 - x_1)_+ \tag{16.23}$$

obtained by multiplying $h_0(\mathbf{x}) = 1$ with a reflecting pair involving x_1 with knot $t = 5$. This pair is added to $\mathcal{M}$. See Figure 16.7(b). At the next step, we might create a model such as

$$\begin{aligned} f(\mathbf{x}) &= \; = 2 - 2(x_1 - 5)_+ + 3(5 - x_1)_+ \\ &\quad -(x_2 - 10)_+ \times (5 - x_1) + -1.2(10 - x_2)_+ \times (5 - x_1)_+ \end{aligned} \tag{16.24}$$

obtained by multiplying $(5-x_1)+$ from $\mathcal{M}$ by the new reflecting pair $(x_2-10)_+$ and $(10-x_2)_+$. This new function is shown in Figure 16.7(c).

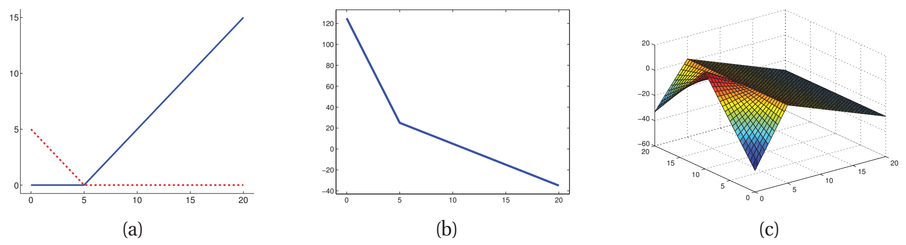


Figure 16.7 (a) Linear spline function with a knot at 5. Solid blue: $(x-5)_+$. Dotted red: $(5-x)_+$. (b) A MARS model in 1d given by Equation 16.23. (c) A simple MARS model in 2d given by Equation 16.24. Figure generated by `marsDemo`.

We proceed in this way until the model becomes very large. (We may impose an upper bound on the order of interactions.) Then we prune backwards, at each step eliminating the basis function that causes the smallest increase in the residual error, until the CV error stops improving.

The whole procedure is closely related to CART. To see this, suppose we replace the piecewise linear basis functions by step functions $\mathbb{I}(x_j > t)$ and $\mathbb{I}(x_j < t)$. Multiplying by a pair of reflected step functions is equivalent to splitting a node. Now suppose we impose the constraint that once a variable is involved in a multiplication by a candidate term, that variable gets replaced by the interaction, so the original variable is no longer available. This ensures that a variable can not be split more than once, thus guaranteeing that the resulting model can be represented as a tree. In this case, the MARS growing strategy is the same as the CART growing strategy.

16.4 Boosting

Boosting (Schapire and Freund 2012) is a greedy algorithm for fitting adaptive basis-function models of the form in Equation 16.3, where the ϕ_m are generated by an algorithm called a **weak learner** or a **base learner**. The algorithm works by applying the weak learner sequentially to weighted versions of the data, where more weight is given to examples that were misclassified by earlier rounds.

This weak learner can be any classification or regression algorithm, but it is common to use a CART model. In 1998, the late Leo Breiman called boosting, where the weak learner is a shallow decision tree, the "best off-the-shelf classifier in the world" (Hastie et al. 2009, p340). This is supported by an extensive empirical comparison of 10 different classifiers in (Caruana and Niculescu-Mizil 2006), who showed that boosted decision trees were the best both in terms of misclassification error and in terms of producing well-calibrated probabilities, as judged by ROC curves. (The second best method was random forests, invented by Breiman; see Section 16.2.5.) By contrast, single decision trees performed very poorly.

Boosting was originally derived in the computational learning theory literature (Schapire 1990; Freund and Schapire 1996), where the focus is binary classification. In these papers, it was proved that one could boost the performance (on the training set) of any weak learner arbitrarily

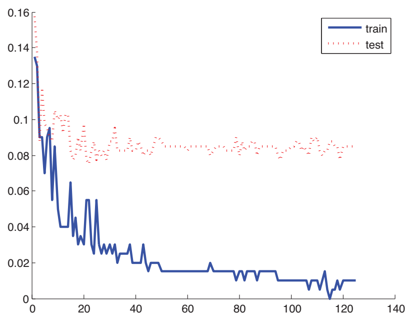


Figure 16.8 Performance of adaboost using a decision stump as a weak learner on the data in Figure 16.10. Training (solid blue) and test (dotted red) error vs number of iterations. Figure generated by `boostingDemo`, written by Richard Stapenhurst.

high, provided the weak learner could always perform slightly better than chance. For example, in Figure 16.8, we plot the training and test error for boosted decision stumps on a 2d dataset shown in Figure 16.10. We see that the training set error rapidly goes to near zero. What is more surprising is that the test set error continues to decline even after the training set error has reached zero (although the test set error will eventually go up). Thus boosting is very resistant to overfitting. (Boosted decision stumps form the basis of a very successful face detector (Viola and Jones 2001), which was used to generate the results in Figure 1.6, and which is used in many digital cameras.)

In view of its stunning empirical success, statisticians started to become interested in this method. Breiman (Breiman 1998) showed that boosting can be interpreted as a form of *gradient descent in function space*. This view was then extended in (Friedman et al. 2000), who showed how boosting could be extended to handle a variety of loss functions, including for regression, robust regression, Poisson regression, etc. In this section, we shall present this statistical interpretation of boosting, drawing on the reviews in (Buhlmann and Hothorn 2007) and (Hastie et al. 2009, ch10), which should be consulted for further details.

16.4.1 Forward stagewise additive modeling

The goal of boosting is to solve the following optimization problem:

$$\min_f \sum_{i=1}^{N} L(y_i, f(\mathbf{x}_i)) \tag{16.25}$$

and $L(y, \hat{y})$ is some loss function, and f is assumed to be an ABM model as in Equation 16.3. Common choices for the loss function are listed in Table 16.1.

If we use squared error loss, the optimal estimate is given by

$$f^*(\mathbf{x}) = \underset{f(\mathbf{x})}{\operatorname{argmin}} = \mathbb{E}_{y|\mathbf{x}}\left[(Y - f(\mathbf{x}))^2\right] = \mathbb{E}\left[Y|\mathbf{x}\right] \tag{16.26}$$

Name	Loss	Derivative	f^*	Algorithm
Squared error	$\frac{1}{2}(y_i - f(\mathbf{x}_i))^2$	$y_i - f(\mathbf{x}_i)$	$\mathbb{E}[y\|\mathbf{x}_i]$	L2Boosting
Absolute error	$\|y_i - f(\mathbf{x}_i)\|$	$\text{sgn}(y_i - f(\mathbf{x}_i))$	$\text{median}(y\|\mathbf{x}_i)$	Gradient boosting
Exponential loss	$\exp(-\tilde{y}_i f(\mathbf{x}_i))$	$-\tilde{y}_i \exp(-\tilde{y}_i f(\mathbf{x}_i))$	$\frac{1}{2}\log\frac{\pi_i}{1-\pi_i}$	AdaBoost
Logloss	$\log(1 + e^{-\tilde{y}_i f_i})$	$y_i - \pi_i$	$\frac{1}{2}\log\frac{\pi_i}{1-\pi_i}$	LogitBoost

Table 16.1 Some commonly used loss functions, their gradients, their population minimizers f^*, and some algorithms to minimize the loss. For binary classification problems, we assume $\tilde{y}_i \in \{-1, +1\}$, $y_i \in \{0, 1\}$ and $\pi_i = \text{sigm}(2f(\mathbf{x}_i))$. For regression problems, we assume $y_i \in \mathbb{R}$. Adapted from (Hastie et al. 2009, p360) and (Buhlmann and Hothorn 2007, p483).

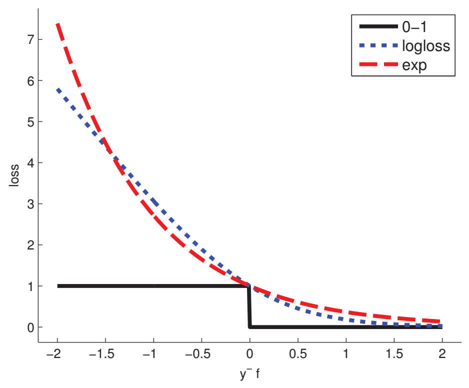


Figure 16.9 Illustration of various loss functions for binary classification. The horizontal axis is the margin $y\eta$, the vertical axis is the loss. The log loss uses log base 2. Figure generated by `hingeLossPlot`.

as we showed in Section 5.7.1.3. Of course, this cannot be computed in practice since it requires knowing the true conditional distribution $p(y|\mathbf{x})$. Hence this is sometimes called the **population minimizer**, where the expectation is interpreted in a frequentist sense. Below we will see that boosting will try to approximate this conditional expectation.

For binary classification, the obvious loss is 0-1 loss, but this is not differentiable. Instead it is common to use logloss, which is a convex upper bound on 0-1 loss, as we showed in Section 6.5.5. In this case, one can show that the optimal estimate is given by

$$f^*(\mathbf{x}) = \frac{1}{2}\log\frac{p(\tilde{y} = 1|\mathbf{x})}{p(\tilde{y} = -1|\mathbf{x})} \tag{16.27}$$

where $\tilde{y} \in \{-1, +1\}$. One can generalize this framework to the multiclass case, but we will not discuss that here.

An alternative convex upper bound is **exponential loss**, defined by

$$L(\tilde{y}, f) = \exp(-\tilde{y}f) \tag{16.28}$$

See Figure 16.9 for a plot. This will have some computational advantages over the logloss, to be discussed below. It turns out that the optimal estimate for this loss is also $f^*(\mathbf{x}) =$

$\frac{1}{2}\log\frac{p(\tilde{y}=1|\mathbf{x})}{p(\tilde{y}=-1|\mathbf{x})}$. To see this, we can just set the derivative of the expected loss (for each $\mathbf{x}$) to zero:

$$\frac{\partial}{\partial f(\mathbf{x})}\mathbb{E}\left[e^{-\tilde{y}f(\mathbf{x})}|\mathbf{x}\right] = \frac{\partial}{\partial f(\mathbf{x})}[p(\tilde{y}=1|\mathbf{x})e^{-f(\mathbf{x})} + p(\tilde{y}=-1|\mathbf{x})e^{f(\mathbf{x})}] \tag{16.29}$$

$$= -p(\tilde{y}=1|\mathbf{x})e^{-f(\mathbf{x})} + p(\tilde{y}=-1|\mathbf{x})e^{f(\mathbf{x})} \tag{16.30}$$

$$= 0 \Rightarrow \frac{p(\tilde{y}=1|\mathbf{x})}{p(\tilde{y}=1-|\mathbf{x})} = e^{2f(\mathbf{x})} \tag{16.31}$$

So in both cases, we can see that boosting should try to approximate (half) the log-odds ratio.

Since finding the optimal f is hard, we shall tackle it sequentially. We initialise by defining

$$f_0(\mathbf{x}) = \arg\min_{\boldsymbol{\gamma}} \sum_{i=1}^{N} L(y_i, f(\mathbf{x}_i;\boldsymbol{\gamma})) \tag{16.32}$$

For example, if we use squared error, we can set $f_0(\mathbf{x}) = \overline{y}$, and if we use log-loss or exponential loss , we can set $f_0(\mathbf{x}) = \frac{1}{2}\log\frac{\hat{\pi}}{1-\hat{\pi}}$, where $\hat{\pi} = \frac{1}{N}\sum_{i=1}^{N}\mathbb{I}(y_i = 1)$. We could also use a more powerful model for our baseline, such as a GLM.

Then at iteration m, we compute

$$(\beta_m, \boldsymbol{\gamma}_m) = \underset{\beta,\boldsymbol{\gamma}}{\text{argmin}} \sum_{i=1}^{N} L(y_i, f_{m-1}(\mathbf{x}_i) + \beta\phi(\mathbf{x}_i;\boldsymbol{\gamma})) \tag{16.33}$$

and then we set

$$f_m(\mathbf{x}) = f_{m-1}(\mathbf{x}) + \beta_m\phi(\mathbf{x};\boldsymbol{\gamma}_m) \tag{16.34}$$

The key point is that we do not go back and adjust earlier parameters. This is why the method is called **forward stagewise additive modeling**.

We continue this for a fixed number of iterations M. In fact M is the main tuning parameter of the method. Often we pick it by monitoring the performance on a separate validation set, and then stopping once performance starts to decrease; this is called **early stopping**. Alternatively, we can use model selection criteria such as AIC or BIC (see e.g., (Buhlmann and Hothorn 2007) for details).

In practice, better (test set) performance can be obtained by performing "partial updates" of the form

$$f_m(\mathbf{x}) = f_{m-1}(\mathbf{x}) + \nu\beta_m\phi(\mathbf{x};\boldsymbol{\gamma}_m) \tag{16.35}$$

Here $0 < \nu \leq 1$ is a step-size parameter. In practice it is common to use a small value such as $\nu = 0.1$. This is called **shrinkage**.

Below we discuss how to solve the suproblem in Equation 16.33. This will depend on the form of loss function. However, it is independent of the form of weak learner.

16.4.2 L2boosting

Suppose we used squared error loss. Then at step m the loss has the form

$$L(y_i, f_{m-1}(\mathbf{x}_i) + \beta\phi(\mathbf{x}_i;\boldsymbol{\gamma})) = (r_{im} - \phi(\mathbf{x}_i;\boldsymbol{\gamma}))^2 \tag{16.36}$$

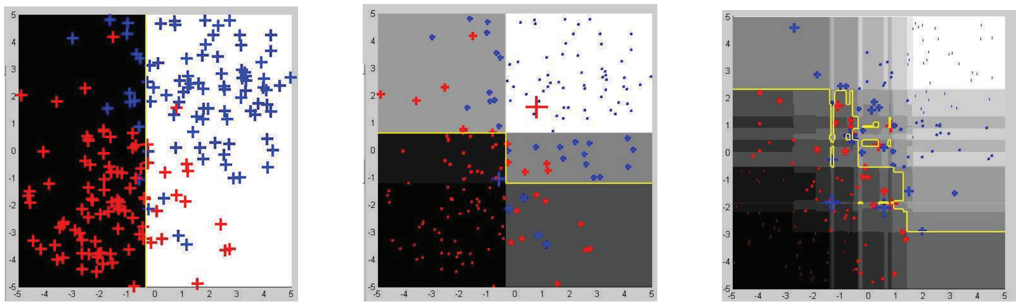

(a) (b) (c)

Figure 16.10 Example of adaboost using a decision stump as a weak learner. The degree of blackness represents the confidence in the red class. The degree of whiteness represents the confidence in the blue class. The size of the datapoints represents their weight. Decision boundary is in yellow. (a) After 1 round. (b) After 3 rounds. (c) After 120 rounds. Figure generated by `boostingDemo`, written by Richard Stapenhurst.

where $r_{im} \triangleq y_i - f_{m-1}(\mathbf{x}_i)$ is the current residual, and we have set $\beta = 1$ without loss of generality. Hence we can find the new basis function by using the weak learner to predict $\mathbf{r}_m$. This is called **L2boosting**, or **least squares boosting** (Buhlmann and Yu 2003). In Section 16.4.6, we will see that this method, with a suitable choice of weak learner, can be made to give the same results as LARS, which can be used to perform variable selection (see Section 13.4.2).

16.4.3 AdaBoost

Consider a binary classification problem with exponential loss. At step m we have to minimize

$$L_m(\phi) = \sum_{i=1}^N \exp[-\tilde{y}_i(f_{m-1}(\mathbf{x}_i) + \beta\phi(\mathbf{x}_i))] = \sum_{i=1}^N w_{i,m} \exp(-\beta\tilde{y}_i\phi(\mathbf{x}_i)) \tag{16.37}$$

where $w_{i,m} \triangleq \exp(-\tilde{y}_i f_{m-1}(\mathbf{x}_i))$ is a weight applied to datacase i, and $\tilde{y}_i \in \{-1, +1\}$. We can rewrite this objective as follows:

$$L_m = e^{-\beta} \sum_{\tilde{y}_i = \phi(\mathbf{x}_i)} w_{i,m} + e^{\beta} \sum_{\tilde{y}_i \neq \phi(\mathbf{x}_i)} w_{i,m} \tag{16.38}$$

$$= (e^{\beta} - e^{-\beta}) \sum_{i=1}^N w_{i,m}\mathbb{I}(\tilde{y}_i \neq \phi(\mathbf{x}_i)) + e^{-\beta} \sum_{i=1}^N w_{i,m} \tag{16.39}$$

Consequently the optimal function to add is

$$\phi_m = \underset{\phi}{\operatorname{argmin}}\, w_{i,m}\mathbb{I}(\tilde{y}_i \neq \phi(\mathbf{x}_i)) \tag{16.40}$$

This can be found by applying the weak learner to a weighted version of the dataset, with weights $w_{i,m}$. Subsituting ϕ_m into L_m and solving for β we find

$$\beta_m = \frac{1}{2} \log \frac{1 - \mathrm{err}_m}{\mathrm{err}_m} \tag{16.41}$$

where

$$\text{err}_m = \frac{\sum_{i=1}^N w_i \mathbb{I}(\tilde{y}_i \neq \phi_m(\mathbf{x}_i))}{\sum_{i=1}^N w_{i,m}} \tag{16.42}$$

The overall update becomes

$$f_m(\mathbf{x}) = f_{m-1}(\mathbf{x}) + \beta_m \phi_m(\mathbf{x}) \tag{16.43}$$

With this, the weights at the next iteration become

$$\begin{aligned} w_{i,m+1} &= w_{i,m} e^{-\beta_m \tilde{y}_i \phi_m(\mathbf{x}_i)} & (16.44)\\ &= w_{i,m} e^{\beta_m (2\mathbb{I}(\tilde{y}_i \neq \phi_m(\mathbf{x}_i)) - 1)} & (16.45)\\ &= w_{i,m} e^{2\beta_m \mathbb{I}(\tilde{y}_i \neq \phi_m(\mathbf{x}_i))} e^{-\beta_m} & (16.46) \end{aligned}$$

where we exploited the fact that $-\tilde{y}_i \phi_m(\mathbf{x}_i) = -1$ if $\tilde{y}_i = \phi_m(\mathbf{x}_i)$ and $-\tilde{y}_i \phi_m(\mathbf{x}_i) = +1$ otherwise. Since $e^{-\beta_m}$ will cancel out in the normalization step, we can drop it. The result is the algorithm shown in Algorithm 7, known **Adaboost.M1**.[4]

An example of this algorithm in action, using decision stumps as the weak learner, is given in Figure 16.10. We see that after many iterations, we can "carve out" a complex decision boundary. What is rather surprising is that AdaBoost is very slow to overfit, as is apparent in Figure 16.8. See Section 16.4.8 for a discussion of this point.

Algorithm 16.2: Adaboost.M1, for binary classification with exponential loss

```
1 $w_i = 1/N$;
2 for $m = 1 : M$ do
3     Fit a classifier $\phi_m(\mathbf{x})$ to the training set using weights $\mathbf{w}$;
4     Compute $\text{err}_m = \frac{\sum_{i=1}^N w_{i,m} \mathbb{I}(\tilde{y}_i \neq \phi_m(\mathbf{x}_i))}{\sum_{i=1}^N w_{i,m})}$ ;
5     Compute $\alpha_m = \log[(1 - \text{err}_m)/\text{err}_m]$;
6     Set $w_i \leftarrow w_i \exp[\alpha_m \mathbb{I}(\tilde{y}_i \neq \phi_m(\mathbf{x}_i))]$;
7 Return $f(\mathbf{x}) = \text{sgn}\left[\sum_{m=1}^M \alpha_m \phi_m(\mathbf{x})\right]$;
```

16.4.4 LogitBoost

The trouble with exponential loss is that it puts a lot of weight on misclassified examples, as is apparent from the exponential blowup on the left hand side of Figure 16.9. This makes the method very sensitive to outliers (mislabeled examples). In addition, $e^{-\tilde{y}f}$ is not the logarithm of any pmf for binary variables $\tilde{y} \in \{-1, +1\}$; consequently we cannot recover probability estimates from $f(\mathbf{x})$.

4. In (Friedman et al. 2000), this is called **discrete AdaBoost**, since it assumes that the base classifier ϕ_m returns a binary class label. If ϕ_m returns a probability instead, a modified algorithm, known as **real AdaBoost**, can be used. See (Friedman et al. 2000) for details.

A natural alternative is to use logloss instead. This only punishes mistakes linearly, as is clear from Figure 16.9. Furthermore, it means that we will be able to extract probabilities from the final learned function, using

$$p(y=1|\mathbf{x}) = \frac{e^{f(\mathbf{x})}}{e^{-f(\mathbf{x})}+e^{f(\mathbf{x})}} = \frac{1}{1+e^{-2f(\mathbf{x})}} \tag{16.47}$$

The goal is to minimze the expected log-loss, given by

$$L_m(\phi) = \sum_{i=1}^{N} \log\left[1+\exp\left(-2\tilde{y}_i(f_{m-1}(\mathbf{x})+\phi(\mathbf{x}_i))\right)\right] \tag{16.48}$$

By performing a Newton upate on this objective (similar to IRLS), one can derive the algorithm shown in Algorithm 8. This is known as **logitBoost** (Friedman et al. 2000). It can be generalized to the multi-class setting, as explained in (Friedman et al. 2000).

Algorithm 16.3: LogitBoost, for binary classification with log-loss

```
1 $w_i = 1/N$, $\pi_i = 1/2$;
2 for $m = 1 : M$ do
3     Compute the working response $z_i = \frac{y_i^* - \pi_i}{\pi_i(1-\pi_i)}$;
4     Compute the weights $w_i = \pi_i(1-\pi_i)$;
5     $\phi_m = \operatorname{argmin}_\phi \sum_{i=1}^N w_i(z_i - \phi(\mathbf{x}_i))^2$;
6     Update $f(\mathbf{x}) \leftarrow f(\mathbf{x}) + \frac{1}{2}\phi_m(\mathbf{x})$;
7     Compute $\pi_i = 1/(1+\exp(-2f(\mathbf{x}_i)))$;
8 Return $f(\mathbf{x}) = \operatorname{sgn}\left[\sum_{m=1}^M \phi_m(\mathbf{x})\right]$;
```

16.4.5 Boosting as functional gradient descent

Rather than deriving new versions of boosting for every different loss function, it is possible to derive a generic version, known as **gradient boosting** (Friedman 2001; Mason et al. 2000). To explain this, imagine minimizing

$$\hat{\mathbf{f}} = \operatorname*{argmin}_{\mathbf{f}} L(\mathbf{f}) \tag{16.49}$$

where $\mathbf{f} = (f(\mathbf{x}_1), \ldots, f(\mathbf{x}_N))$ are the "parameters". We will solve this stagewise, using gradient descent. At step m, let $\mathbf{g}_m$ be the gradient of $L(\mathbf{f})$ evaluated at $\mathbf{f} = \mathbf{f}_{m-1}$:

$$g_{im} = \left[\frac{\partial L(y_i, f(\mathbf{x}_i))}{\partial f(\mathbf{x}_i)}\right]_{f=f_{m-1}} \tag{16.50}$$

Gradients of some common loss functions are given in Table 16.1. We then make the update

$$\mathbf{f}_m = \mathbf{f}_{m-1} - \rho_m \mathbf{g}_m \tag{16.51}$$

where ρ_m is the step length, chosen by

$$\rho_m = \underset{\rho}{\operatorname{argmin}}\, L(\mathbf{f}_{m-1} - \rho \mathbf{g}_m) \tag{16.52}$$

This is called **functional gradient descent**.

In its current form, this is not much use, since it only optimizes f at a fixed set of N points, so we do not learn a function that can generalize. However, we can modify the algorithm by fitting a weak learner to approximate the negative gradient signal. That is, we use this update

$$\boldsymbol{\gamma}_m = \underset{\boldsymbol{\gamma}}{\operatorname{argmin}} \sum_{i=1}^{N} (-g_{im} - \phi(\mathbf{x}_i; \boldsymbol{\gamma}))^2 \tag{16.53}$$

The overall algorithm is summarized in Algorithm 6. (We have omitted the line search step, which is not strictly necessary, as argued in (Buhlmann and Hothorn 2007).)

Algorithm 16.4: Gradient boosting

```
1 Initialize $f_0(\mathbf{x}) = \operatorname{argmin}_{\boldsymbol{\gamma}} \sum_{i=1}^N L(y_i, \phi(\mathbf{x}_i; \boldsymbol{\gamma}))$;
2 for $m = 1 : M$ do
3     Compute the gradient residual using $r_{im} = -\left[\frac{\partial L(y_i, f(\mathbf{x}_i))}{\partial f(\mathbf{x}_i)}\right]_{f(\mathbf{x}_i) = f_{m-1}(\mathbf{x}_i)}$;
4     Use the weak learner to compute $\boldsymbol{\gamma}_m$ which minimizes $\sum_{i=1}^N (r_{im} - \phi(\mathbf{x}_i; \boldsymbol{\gamma}_m))^2$;
5     Update $f_m(\mathbf{x}) = f_{m-1}(\mathbf{x}) + \nu \phi(\mathbf{x}; \boldsymbol{\gamma}_m)$;
6 Return $f(\mathbf{x}) = f_M(\mathbf{x})$
```

If we apply this algorithm using squared loss, we recover L2Boosting. If we apply this algorithm to log-loss, we get an algorithm known as **BinomialBoost** (Buhlmann and Hothorn 2007). The advantage of this over LogitBoost is that it does not need to be able to do weighted fitting: it just applies any black-box regression model to the gradient vector. Also, it is relatively easy to extend to the multi-class case (see (Hastie et al. 2009, p387)). We can also apply this algorithm to other loss functions, such as the Huber loss (Section 7.4), which is more robust to outliers than squared error loss.

16.4.6 Sparse boosting

Suppose we use as our weak learner the following algorithm: search over all possible variables $j = 1 : D$, and pick the one $j(m)$ that best predicts the residual vector:

$$\begin{aligned}
j(m) &= \underset{j}{\operatorname{argmin}} \sum_{i=1}^{N} (r_{im} - \hat{\beta}_{jm} x_{ij})^2 && (16.54) \\
\hat{\beta}_{jm} &= \frac{\sum_{i=1}^N x_{ij} r_{im}}{\sum_{i=1}^N x_{ij}^2} && (16.55) \\
\phi_m(\mathbf{x}) &= \hat{\beta}_{j(m),m}\, x_{j(m)} && (16.56)
\end{aligned}$$

This method, which is known as **sparse boosting** (Buhlmann and Yu 2006), is identical to the matching pursuit algorithm discussed in Section 13.2.3.1.

It is clear that this will result in a sparse estimate, at least if M is small. To see this, let us rewrite the update as follows:

$$\boldsymbol{\beta}_m := \boldsymbol{\beta}_{m-1} + \nu(0, \ldots, 0, \hat{\beta}_{j(m),m}, 0, \ldots, 0) \tag{16.57}$$

where the non-zero entry occurs in location $j(m)$. This is known as **forward stagewise linear regression** (Hastie et al. 2009, p608), which becomes equivalent to the LAR algorithm discussed in Section 13.4.2 as $\nu \to 0$. Increasing the number of steps m in boosting is analogous to decreasing the regularization penalty λ. If we modify boosting to allow some variable deletion steps (Zhao and Yu 2007), we can make it equivalent to the LARS algorithm, which computes the full regularization path for the lasso problem. The same algorithm can be used for sparse logistic regression, by simply modifying the residual to be the appropriate negative gradient.

Now consider a weak learner that is similar to the above, except it uses a smoothing spline instead of linear regression when mapping from x_j to the residual. The result is a sparse generalized additive model (see Section 16.3). It can obviously be extended to pick pairs of variables at a time. The resulting method often works much better than MARS (Buhlmann and Yu 2006).

16.4.7 Multivariate adaptive regression trees (MART)

It is quite common to use CART models as weak learners. It is usually advisable to use a shallow tree, so that the variance is low. Even though the bias will be high (since a shallow tree is likely to be far from the "truth"), this will compensated for in subsequent rounds of boosting.

The height of the tree is an additional tuning parameter (in addition to M, the number of rounds of boosting, and ν, the shrinkage factor). Suppose we restrict to trees with J leaves. If $J = 2$, we get a stump, which can only split on a single variable. If $J = 3$, we allow for two-variable interactions, etc. In general, it is recommended (e.g., in (Hastie et al. 2009, p363) and (Caruana and Niculescu-Mizil 2006)) to use $J \approx 6$.

If we combine the gradient boosting algorithm with (shallow) regression trees, we get a model known as **MART**, which stands for "multivariate adaptive regression trees". This actually includes a slight refinement to the basic gradient boosting algorithm: after fitting a regression tree to the residual (negative gradient), we re-estimate the parameters at the leaves of the tree to minimize the loss:

$$\gamma_{jm} = \underset{\gamma}{\operatorname{argmin}} \sum_{x_i \in R_{jm}} L(y_i, f_{m-1}(\mathbf{x}_i) + \gamma) \tag{16.58}$$

where R_{jm} is the region for leaf j in the m'th tree, and γ_{jm} is the corresponding parameter (the mean response of y for regression problems, or the most probable class label for classification problems).

16.4.8 Why does boosting work so well?

We have seen that boosting works very well, especially for classifiers. There are two main reasons for this. First, it can be seen as a form of ℓ_1 regularization, which is known to help prevent overfitting by eliminating "irrelevant" features. To see this, imagine pre-computing all possible weak-learners, and defining a feature vector of the form $\boldsymbol{\phi}(\mathbf{x}) = [\phi_1(\mathbf{x}), \ldots, \phi_K(\mathbf{x})]$. We could use ℓ_1 regularization to select a subset of these. Alternatively we can use boosting, where at each step, the weak learner creates a new ϕ_k on the fly. It is possible to combine boosting and ℓ_1 regularization, to get an algorithm known as **L1-Adaboost** (Duchi and Singer 2009). Essentially this method greedily adds the best features (weak learners) using boosting, and then prunes off irrelevant ones using ℓ_1 regularization.

Another explanation has to do with the concept of margin, which we introduced in Section 14.5.2.2. (Schapire et al. 1998; Ratsch et al. 2001) proved that AdaBoost maximizes the margin on the training data. (Rosset et al. 2004) generalized this to other loss functions, such as log-loss.

16.4.9 A Bayesian view

So far, our presentation of boosting has been very frequentist, since it has focussed on greedily minimizing loss functions. A likelihood interpretation of the algorithm was given in (Neal and MacKay 1998; Meek et al. 2002). The idea is to consider a mixture of experts model of the form

$$p(y|\mathbf{x}, \boldsymbol{\theta}) = \sum_{m=1}^{M} \pi_m p(y|\mathbf{x}, \boldsymbol{\gamma}_m) \tag{16.59}$$

where each expert $p(y|\mathbf{x}, \boldsymbol{\gamma}_m)$ is like a weak learner. We usually fit all M experts at once using EM, but we can imagine a sequential scheme, whereby we only update the parameters for one expert at a time. In the E step, the posterior responsibilities will reflect how well the existing experts explain a given data point; if this is a poor fit, these data points will have more influence on the next expert that is fitted. (This view naturally suggest a way to use a boosting-like algorithm for unsupervised learning: we simply sequentially fit mixture models, instead of mixtures of experts.)

Notice that this is a rather "broken" MLE procedure, since it never goes back to update the parameters of an old expert. Similarly, if boosting ever wants to change the weight assigned to a weak learner, the only way to do this is to add the weak learner again with a new weight. This can result in unnecessarily large models. By contrast, the BART model (Chipman et al. 2006, 2010) uses a Bayesian version of backfitting to fit a small sum of weak learners (typically trees).

16.5 Feedforward neural networks (multilayer perceptrons)

A **feedforward neural network**, aka **multi-layer perceptron** (**MLP**), is a series of logistic regression models stacked on top of each other, with the final layer being either another logistic regression or a linear regression model, depending on whether we are solving a classification or regression problem. For example, if we have two layers, and we are solving a regression problem, the model has the form

$$p(y|\mathbf{x}, \boldsymbol{\theta}) = \mathcal{N}(y|\mathbf{w}^T\mathbf{z}(\mathbf{x}), \sigma^2) \tag{16.60}$$

$$\mathbf{z}(\mathbf{x}) = g(\mathbf{V}\mathbf{x}) = [g(\mathbf{v}_1^T\mathbf{x}), \ldots, g(\mathbf{v}_H^T\mathbf{x})] \tag{16.61}$$

where g is a non-linear **activation** or **transfer function** (commonly the logistic function), $\mathbf{z}(\mathbf{x}) = \boldsymbol{\phi}(\mathbf{x}, \mathbf{V})$ is called the **hidden layer** (a deterministic function of the input), H is the

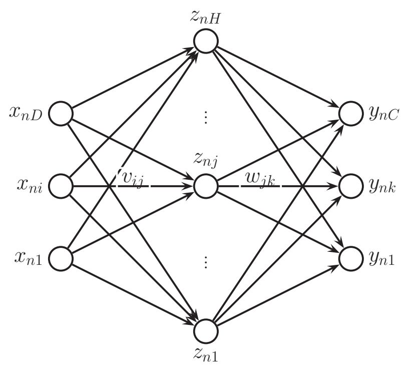


Figure 16.11 A neural network with one hidden layer.

number of **hidden units**, $\mathbf{V}$ is the weight matrix from the inputs to the hidden nodes, and $\mathbf{w}$ is the weight vector from the hidden nodes to the output. It is important that g be non-linear, otherwise the whole model collapses into a large linear regression model of the form $y = \mathbf{w}^T(\mathbf{V}\mathbf{x})$. One can show that an MLP is a **universal approximator**, meaning it can model any suitably smooth function, given enough hidden units, to any desired level of accuracy (Hornik 1991).

To handle binary classification, we pass the output through a sigmoid, as in a GLM:

$$p(y|\mathbf{x}, \boldsymbol{\theta}) = \text{Ber}(y|\text{sigm}(\mathbf{w}^T\mathbf{z}(\mathbf{x}))) \tag{16.62}$$

We can easily extend the MLP to predict multiple outputs. For example, in the regression case, we have

$$p(\mathbf{y}|\mathbf{x}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{y}|\mathbf{W}\ \boldsymbol{\phi}(\mathbf{x}, \mathbf{V}), \sigma^2\mathbf{I}) \tag{16.63}$$

See Figure 16.11 for an illustration. If we add **mutual inhibition** arcs between the output units, ensuring that only one of them turns on, we can enforce a sum-to-one constraint, which can be used for multi-class classification. The resulting model has the form

$$p(y|\mathbf{x}, \boldsymbol{\theta}) \quad = \quad \text{Cat}(y|\mathcal{S}(\mathbf{W}\mathbf{z}(\mathbf{x})) \tag{16.64}$$

16.5.1 Convolutional neural networks

The purpose of the hidden units is to learn non-linear combinations of the original inputs; this is called **feature extraction** or **feature construction**. These hidden features are then passed as input to the final GLM. This approach is particularly useful for problems where the original input features are not very individually informative. For example, each pixel in an image is not very informative; it is the combination of pixels that tells us what objects are present. Conversely, for a task such as document classification using a bag of words representation, each feature (word count) *is* informative on its own, so extracting "higher order" features is less important. Not suprisingly, then, much of the work in neural networks has been motivated by visual pattern

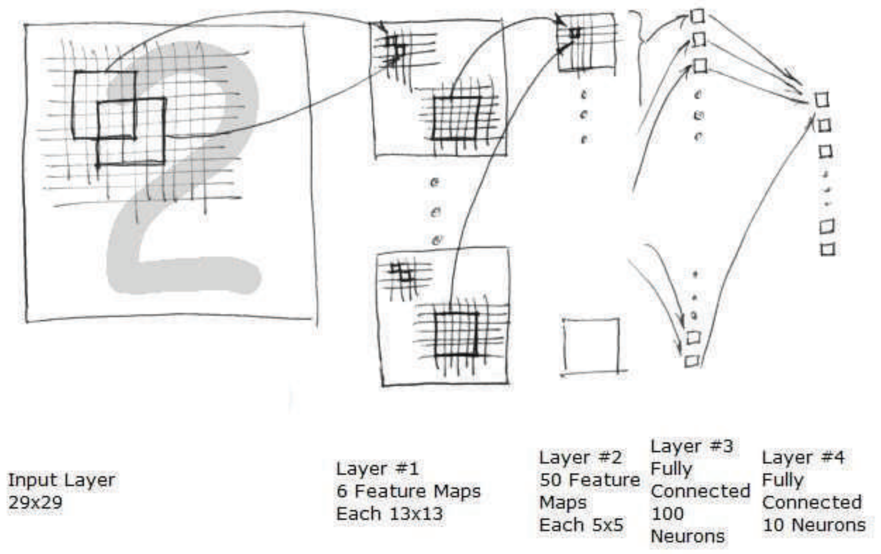


Figure 16.12 The convolutional neural network from (Simard et al. 2003). Source: `http://www.codeproject.com/KB/library/NeuralNetRecognition.aspx` . Used with kind permission of Mike O'Neill.

recognition (e.g., (LeCun et al. 1989)), although they have also been applied to other types of data, including text (e.g., (Collobert and Weston 2008)).

A form of MLP which is particularly well suited to 1d signals like speech or text, or 2d signals like images, is the **convolutional neural network**. This is an MLP in which the hidden units have local **receptive fields** (as in the primary visual cortex), and in which the weights are **tied** or shared across the image, in order to reduce the number of parameters. Intuitively, the effect of such spatial parameter tying is that any useful features that are "discovered" in some portion of the image can be re-used everywhere else without having to be independently learned. The resulting network then exhibits **translation invariance**, meaning it can classify patterns no matter where they occur inside the input image.

Figure 16.12 gives an example of a convolutional network, designed by Simard and colleagues (Simard et al. 2003), with 5 layers (4 layers of adjustable parameters) designed to classify 29×29 gray-scale images of handwritten digits from the MNIST dataset (see Section 1.2.1.3). In layer 1, we have 6 **feature maps** each of which has size 13×13. Each hidden node in one of these feature maps is computed by convolving the image with a 5×5 weight matrix (sometimes called a kernel), adding a bias, and then passing the result through some form of nonlinearity. There are therefore $13 \times 13 \times 6 = 1014$ neurons in Layer 1, and $(5 \times 5 + 1) \times 6 = 156$ weights. (The "+1" is for the bias.) If we did not share these parameters, there would be $1014 \times 26 = 26,364$ weights at the first layer. In layer 2, we have 50 feature maps, each of which is obtained by convolving each feature map in layer 1 with a 5×5 weight matrix, adding them up, adding a bias, and passing through a nonlinearity. There are therefore $5 \times 5 \times 50 = 1250$ neurons in Layer 2, $(5 \times 5 + 1) \times 6 \times 50 = 7800$ adjustable weights (one kernel for each pair of feature maps in layers 1 and 2), and $1250 \times 26 = 32,500$ connections. Layer 3 is fully connected to layer 2, and has 100 neurons and $100 \times (1250 + 1) = 125,100$ weights. Finally, layer 4 is also fully connected, and has 10 neurons, and $10 \times (100 + 1) = 1010$ weights. Adding the above numbers, there are a total of 3,215 neurons, 134,066 adjustable weights, and 184,974 connections.

This model is usually trained using stochastic gradient descent (see Section 16.5.4 for details). A single pass over the data set is called an epoch. When Mike O'Neill did these experiments in 2006, he found that a single epoch took about 40 minutes (recall that there are 60,000 training examples in MNIST). Since it took about 30 epochs for the error rate to converge, the total training time was about 20 hours.[5] Using this technique, he obtained a misclassification rate on the 10,000 test cases of about 1.40%.

To further reduce the error rate, a standard trick is to expand the training set by including **distorted** versions of the original data, to encourage the network to be invariant to small changes that don't affect the identity of the digit. These can be created by applying a random flow field to shift pixels around. See Figure 16.13 for some examples. (If we use online training, such as stochastic gradient descent, we can create these distortions on the fly, rather than having to store them.) Using this technique, Mike O'Neill obtained a misclassification rate on the 10,000 test cases of about 0.74%, which is close to the current state of the art.[6]

Yann Le Cun and colleagues (LeCun et al. 1998) obtained similar performance using a slightly more complicated architecture shown in Figure 16.14. This model is known as **LeNet5**, and historically it came before the model in Figure 16.12. There are two main differences. First, LeNet5 has a **subsampling** layer between each convolutional layer, which either averages or computes the max over each small window in the previous layer, in order to reduce the size, and to obtain a small amount of shift invariance. The convolution and sub-sampling combination was inspired by Hubel and Wiesel's model of simple and complex cells in the visual cortex (Hubel and Wiesel 1962), and it continues to be popular in neurally-inspired models of visual object recognition (Riesenhuber and Poggio 1999). A similar idea first appeared in Fukushima's **neocognitron** (Fukushima 1975), though no globally supervised training algorithm was available at that time.

The second difference between LeNet5 and the Simard architecture is that the final layer is actually an RBF network rather than a more standard sigmoidal or softmax layer. This model gets a test error rate of about 0.95% when trained with no distortions, and 0.8% when trained with distortions. Figure 16.15 shows all 82 errors made by the system. Some are genuinely ambiguous, but several are errors that a person would never make. A web-based demo of the LeNet5 can be found at `http://yann.lecun.com/exdb/lenet/index.html`.

Of course, classifying isolated digits is of limited applicability: in the real world, people usually write strings of digits or other letters. This requires both segmentation and classification. Le Cun and colleagues devised a way to combine convolutional neural networks with a model similar to a conditional random field (described in Section 19.6) to solve this problem. The system was eventually deployed by the US postal service. (See (LeCun et al. 1998) for a more detailed account of the system, which remains one of the best performing systems for this task.)

5. Implementation details: Mike used C++ code and a variety of speedup tricks. He was using standard 2006 era hardware (an Intel Pentium 4 hyperthreaded processor running at 2.8GHz). See `http://www.codeproject.com/KB/library/NeuralNetRecognition.aspx` for details.

6. A list of various methods, along with their misclassification rates on the MNIST test set, is available from `http://yann.lecun.com/exdb/mnist/`. Error rates within 0.1–0.2% of each other are not statistically significantly different.

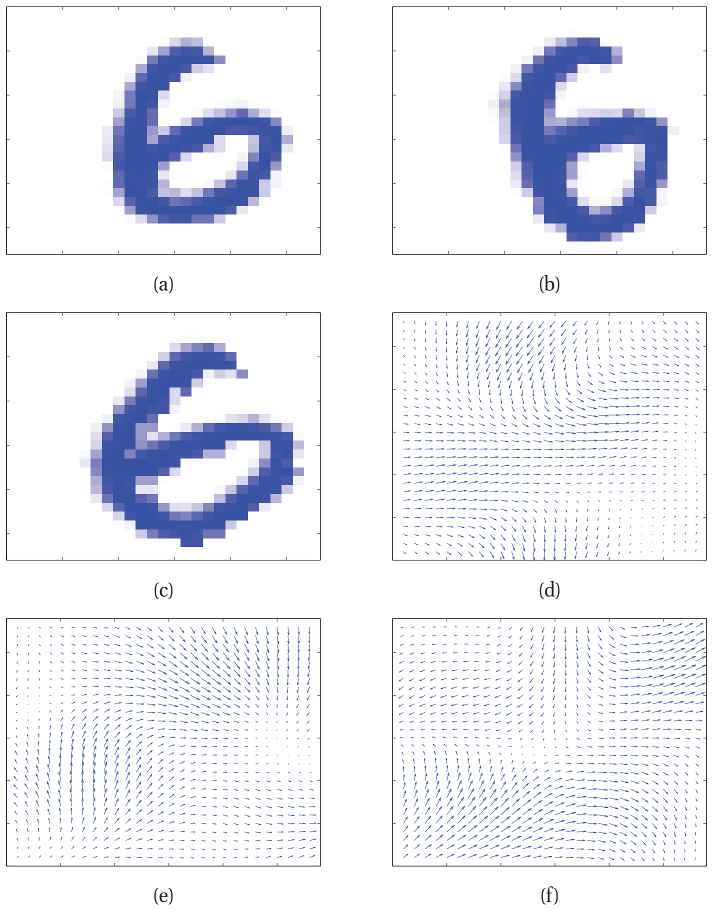


Figure 16.13 Several synthetic warpings of a handwritten digit. Based on Figure 5.14 of (Bishop 2006a). Figure generated by `elasticDistortionsDemo`, written by Kevin Swersky.

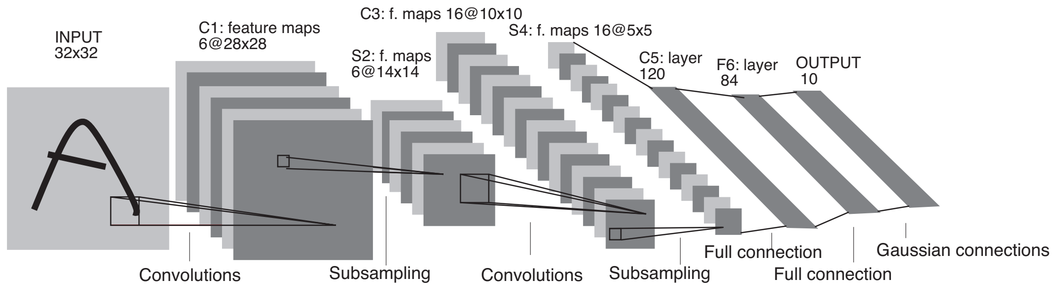


Figure 16.14 LeNet5, a convolutional neural net for classifying handwritten digits. Source: Figure 2 from (LeCun et al. 1998) . Used with kind permission of Yann LeCun.

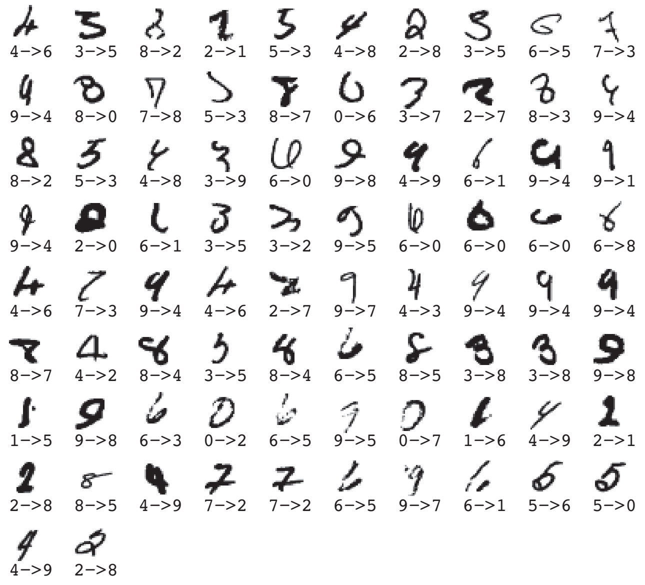


Figure 16.15 These are the 82 errors made by LeNet5 on the 10,000 test cases of MNIST. Below each image is a label of the form correct-label $\rightarrow$ estimated-label. Source: Figure 8 of (LeCun et al. 1998). Used with kind permission of Yann LeCun. (Compare to Figure 28.4(b) which shows the results of a deep generative model.)

16.5.2 Other kinds of neural networks

Other network topologies are possible besides the ones discussed above. For example, we can have **skip arcs** that go directly from the input to the output, skipping the hidden layer; we can have sparse connections between the layers; etc. However, the MLP always requires that the weights form a directed acyclic graph. If we allow feedback connections, the model is known as a **recurrent neural network**; this defines a nonlinear dynamical system, but does not have a simple probabilistic interpretation. Such RNN models are currently the best approach for language modeling (i.e., performing word prediction in natural language) (Tomas et al. 2011), significantly outperforming the standard n-gram-based methods discussed in Section 17.2.2.

If we allow symmetric connections between the hidden units, the model is known as a **Hopfield network** or **associative memory**; its probabilistic counterpart is known as a Boltzmann machine (see Section 27.7) and can be used for unsupervised learning.

16.5.3 A brief history of the field

Neural networks have been the subject of great interest for many decades, due to the desire to understand the brain, and to build learning machines. It is not possible to review the entire history here. Instead, we just give a few “edited highlights”.

The field is generally viewed as starting with McCulloch and Pitts (McCullich and Pitts 1943), who devised a simple mathematical model of the neuron in 1943, in which they approximated the output as a weighted sum of inputs passed through a threshold function, $y = \mathbb{I}(\sum_i w_i x_i > \theta)$, for some threshold θ. This is similar to a sigmoidal activation function. Frank Rosenblatt invented the perceptron learning algorithm in 1957, which is a way to estimate the parameters of a McCulloch-Pitts neuron (see Section 8.5.4 for details). A very similar model called the **adaline** (for adaptive linear element) was invented in 1960 by Widrow and Hoff.

In 1969, Minsky and Papert (Minsky and Papert 1969) published a famous book called "Perceptrons" in which they showed that such linear models, with no hidden layers, were very limited in their power, since they cannot classify data that is not linearly separable. This considerably reduced interest in the field.

In 1986, Rumelhart, Hinton and Williams (Rumelhart et al. 1986) discovered the backpropagation algorithm (see Section 16.5.4), which allows one to fit models with hidden layers. (The backpropagation algorithm was originally discovered in (Bryson and Ho 1969), and independently in (Werbos 1974); however, it was (Rumelhart et al. 1986) that brought the algorithm to people's attention.) This spawned a decade of intense interest in these models.

In 1987, Sejnowski and Rosenberg (Sejnowski and Rosenberg 1987) created the famous **NETtalk** system, that learned a mapping from English words to phonetic symbols which could be fed into a speech synthesizer. An audio demo of the system as it learns over time can be found at `http://www.cnl.salk.edu/ParallelNetsPronounce/nettalk.mp3`. The systems starts by "babbling" and then gradually learns to pronounce English words. NETtalk learned a **distributed representation** (via its hidden layer) of various sounds, and its success spawned a big debate in psychology between **connectionism**, based on neural networks, and **computationalism**, based on syntactic rules. This debate lives on to some extent in the machine learning community, where there are still arguments about whether learning is best performed using low-level, "neural-like" representations, or using more structured models.

In 1989, Yann Le Cun and others (LeCun et al. 1989) created the famous LeNet system described in Section 16.5.1.

In 1992, the support vector machine (see Section 14.5) was invented (Boser et al. 1992). SVMs provide similar prediction accuracy to neural networks while being considerably easier to train (since they use a convex objective function). This spawned a decade of interest in kernel methods in general.[7] Note, however, that SVMs do not use adaptive basis functions, so they require a fair amount of human expertise to design the right kernel function.

In 2002, Geoff Hinton invented the contrastive divergence training procedure (Hinton 2002), which provided a way, for the first time, to learn deep networks, by training one layer at a time in an unsupervised fashion (see Section 27.7.2.4 for details). This in turn has spawned renewed interest in neural networks over the last few years (see Chapter 28).

16.5.4 The backpropagation algorithm

Unlike a GLM, the NLL of an MLP is a non-convex function of its parameters. Nevertheless, we can find a locally optimal ML or MAP estimate using standard gradient-based optimization methods. Since MLPs have lots of parameters, they are often trained on very large data sets.

7. It became part of the folklore during the 1990s that to get published in the top machine learning conference known as NIPS, which stands for "neural information processing systems", it was important to ensure your paper did not contain the word "neural network"!

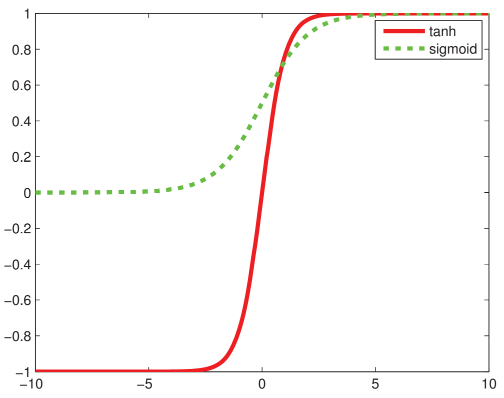


Figure 16.16 Two possible activation functions. $\tanh$ maps $\mathbb{R}$ to $[-1, +1]$ and is the preferred nonlinearity for the hidden nodes. sigm maps $\mathbb{R}$ to $[0, 1]$ and is the preferred nonlinearity for binary nodes at the output layer. Figure generated by `tanhPlot`.

Consequently it is common to use first-order online methods, such as stochastic gradient descent (Section 8.5.2), whereas GLMs are usually fit with IRLS, which is a second-order offline method.

We now discuss how to compute the gradient vector of the NLL by applying the chain rule of calculus. The resulting algorithm is known as **backpropagation**, for reasons that will become apparent.

For notational simplicity, we shall assume a model with just one hidden layer. It is helpful to distinguish the pre- and post-synaptic values of a neuron, that is, before and after we apply the nonlinearity. Let $\mathbf{x}_n$ be the n'th input, $\mathbf{a}_n = \mathbf{V}\mathbf{x}_n$ be the pre-synaptic hidden layer, and $\mathbf{z}_n = g(\mathbf{a}_n)$ be the post-synaptic hidden layer, where g is some **transfer function**. We typically use $g(a) = \text{sigm}(a)$, but we may also use $g(a) = \tanh(a)$: see Figure 16.16 for a comparison. (When the input to sigm or $\tanh$ is a vector, we assume it is applied component-wise.)

We now convert this hidden layer to the output layer as follows. Let $\mathbf{b}_n = \mathbf{W}\mathbf{z}_n$ be the pre-synaptic output layer, and $\hat{\mathbf{y}}_n = h(\mathbf{b}_n)$ be the post-synaptic output layer, where h is another nonlinearity, corresponding to the canonical link for the GLM. (We reserve the notation $\mathbf{y}_n$, without the hat, for the output corresponding to the n'th training case.) For a regression model, we use $h(\mathbf{b}) = \mathbf{b}$; for binary classifcation, we use $h(\mathbf{b}) = [\text{sigm}(b_1), \ldots, \text{sigm}(b_c)]$; for multi-class classification, we use $h(\mathbf{b}) = \mathcal{S}(\mathbf{b})$.

We can write the overall model as follows:

$$\mathbf{x}_n \xrightarrow{\mathbf{V}} \mathbf{a}_n \xrightarrow{g} \mathbf{z}_n \xrightarrow{\mathbf{W}} \mathbf{b}_n \xrightarrow{h} \hat{\mathbf{y}}_n \tag{16.65}$$

The parameters of the model are $\boldsymbol{\theta} = (\mathbf{V}, \mathbf{W})$, the first and second layer weight matrices. Offset or bias terms can be accomodated by clamping an element of $\mathbf{x}_n$ and $\mathbf{z}_n$ to 1.[8]

8. In the regression setting, we can easily estimate the variance of the output noise using the empirical variance of the residual errors, $\hat{\sigma}^2 = \frac{1}{N}||\hat{\mathbf{y}}(\hat{\boldsymbol{\theta}}) - \mathbf{y}||^2$, after training is complete. There will be one value of σ^2 for each output node, if we are performing multi-target regression, as we usually assume.

In the regression case, with K outputs, the NLL is given by the squared error:

$$J(\boldsymbol{\theta}) = -\sum_n \sum_k (\hat{y}_{nk}(\boldsymbol{\theta}) - y_{nk})^2 \tag{16.66}$$

In the classification case, with K classes, the NLL is given by the cross entropy

$$J(\boldsymbol{\theta}) = -\sum_n \sum_k y_{nk} \log \hat{y}_{nk}(\boldsymbol{\theta}) \tag{16.67}$$

Our task is to compute $\nabla_{\boldsymbol{\theta}} J$. We will derive this for each n separately; the overall gradient is obtained by summing over n, although often we just use a mini-batch (see Section 8.5.2).

Let us start by considering the output layer weights. We have

$$\nabla_{\mathbf{w}_k} J_n = \frac{\partial J_n}{\partial b_{nk}} \nabla_{\mathbf{w}_k} b_{nk} = \frac{\partial J_n}{\partial b_{nk}} \mathbf{z}_n \tag{16.68}$$

since $b_{nk} = \mathbf{w}_k^T \mathbf{z}_n$. Assuming h is the canonical link function for the output GLM, then Equation 9.91 tells us that

$$\frac{\partial J_n}{\partial b_{nk}} \triangleq \delta^w_{nk} = (\hat{y}_{nk} - y_{nk}) \tag{16.69}$$

which is the error signal. So the overall gradient is

$$\nabla_{\mathbf{w}_k} J_n = \delta^w_{nk} \mathbf{z}_n \tag{16.70}$$

which is the pre-synaptic input to the output layer, namely $\mathbf{z}_n$, times the error signal, namely δ^w_{nk}.

For the input layer weights, we have

$$\nabla_{\mathbf{v}_j} J_n = \frac{\partial J_n}{\partial a_{nj}} \nabla_{\mathbf{v}_j} a_{nj} \triangleq \delta^v_{nj} \mathbf{x}_n \tag{16.71}$$

where we exploited the fact that $a_{nj} = \mathbf{v}_j^T \mathbf{x}_n$. All that remains is to compute the first level error signal δ^v_{nj}. We have

$$\delta^v_{nj} = \frac{\partial J_n}{\partial a_{nj}} = \sum_{k=1}^K \frac{\partial J_n}{\partial b_{nk}} \frac{\partial b_{nk}}{\partial a_{nj}} = \sum_{k=1}^K \delta^w_{nk} \frac{\partial b_{nk}}{\partial a_{nj}} \tag{16.72}$$

Now

$$b_{nk} = \sum_j w_{kj} g(a_{nj}) \tag{16.73}$$

so

$$\frac{\partial b_{nk}}{\partial a_{nj}} = w_{kj} g'(a_{nj}) \tag{16.74}$$

where $g'(a) = \frac{d}{da} g(a)$. For tanh units, $g'(a) = \frac{d}{da} \tanh(a) = 1 - \tanh^2(a) = \operatorname{sech}^2(a)$, and for sigmoid units, $g'(a) = \frac{d}{da}\sigma(a) = \sigma(a)(1-\sigma(a))$. Hence

$$\delta^v_{nj} = \sum_{k=1}^K \delta^w_{nk} w_{kj} g'(a_{nj}) \tag{16.75}$$

Thus the layer 1 errors can be computed by passing the layer 2 errors back through the $\mathbf{W}$ matrix; hence the term "backpropagation". The key property is that we can compute the gradients locally: each node only needs to know about its immediate neighbors. This is supposed to make the algorithm "neurally plausible", although this interpretation is somewhat controversial.

Putting it all together, we can compute all the gradients as follows: we first perform a forwards pass to compute $\mathbf{a}_n$, $\mathbf{z}_n$, $\mathbf{b}_n$ and $\hat{\mathbf{y}}_n$. We then compute the error for the output layer, $\boldsymbol{\delta}_n^{(2)} = \hat{\mathbf{y}}_n - \mathbf{y}_n$, which we pass backwards through $\mathbf{W}$ using Equation 16.75 to compute the error for the hidden layer, $\boldsymbol{\delta}_n^{(1)}$. We then compute the overall gradient as follows:

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \sum_n [\boldsymbol{\delta}_n^v \mathbf{x}_n,\ \boldsymbol{\delta}_n^w \mathbf{z}_n] \tag{16.76}$$

16.5.5 Identifiability

It is easy to see that the parameters of a neural network are not identifiable. For example, we can change the sign of the weights going into one of the hidden units, so long as we change the sign of all the weights going out of it; these effects cancel, since tanh is an odd function, so $\tanh(-a) = -\tanh(a)$. There will be H such sign flip symmetries, leading to 2^H equivalent settings of the parameters. Similarly, we can change the identity of the hidden units without affecting the likelihood. There are $H!$ such permutations. The total number of equivalent parameter settings (with the same likelihood) is therefore $H!2^H$.

In addition, there may be local minima due to the non-convexity of the NLL. This can be a more serious problem, although with enough data, these local optima are often quite "shallow", and simple stochastic optimization methods can avoid them. In addition, it is common to perform multiple restarts, and to pick the best solution, or to average over the resulting predictions. (It does not make sense to average the parameters themselves, since they are not identifiable.)

16.5.6 Regularization

As usual, the MLE can overfit, especially if the number of nodes is large. A simple way to prevent this is called **early stopping**, which means stopping the training procedure when the error on the validation set first starts to increase. This method works because we usually initialize from small random weights, so the model is initially simple (since the $\tanh$ and sigm functions are nearly linear near the origin). As training progresses, the weights become larger, and the model becomes nonlinear. Eventually it will overfit.

Another way to prevent overfitting, that is more in keeping with the approaches used elsewhere in this book, is to impose a prior on the parameters, and then use MAP estimation. It is standard to use a $\mathcal{N}(0, \alpha^{-1}\mathbf{I})$ prior (equivalent to ℓ_2 regularization), where α is the precision (strength) of the prior. In the neural networks literature, this is called **weight decay**, since it encourages small weights, and hence simpler models. The penalized NLL objective becomes

$$J(\boldsymbol{\theta}) = -\sum_{n=1}^{N} \log p(y_n|\mathbf{x}_n, \boldsymbol{\theta}) + \frac{\alpha}{2}[\sum_{ij} v_{ij}^2 + \sum_{jk} w_{jk}^2] \tag{16.77}$$

(Note that we don't penalize the bias terms.) The gradient of the modified objective becomes

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = [\sum_n \boldsymbol{\delta}_n^v \mathbf{x}_n + \alpha \mathbf{v},\ \sum_n \boldsymbol{\delta}_n^w \mathbf{z}_n + \alpha \mathbf{w}] \tag{16.78}$$

as in Section 8.3.6.

If the regularization is sufficiently strong, it does not matter if we have too many hidden units (apart from wasted computation). Hence it is advisable to set H to be as large as you can afford (say 10–100), and then to choose an appropriate regularizer. We can set the α parameter by cross validation or empirical Bayes (see Section 16.5.7.5).

As with ridge regression, it is good practice to standardize the inputs to zero mean and unit variance, so that the spherical Gaussian prior makes sense.

16.5.6.1 Consistent Gaussian priors *

One can show (MacKay 1992) that using the same regularization parameter for both the first and second layer weights results in the lack of a certain desirable invariance property. In particular, suppose we linearly scale and shift the inputs and/or outputs to a neural network regression model. Then we would like the model to learn to predict the same function, by suitably scaling its internal weights and bias terms. However, the amount of scaling needed by the first and second layer weights to compensate for a change in the inputs and/or outputs is not the same. Therefore we need to use a different regularization strength for the first and second layer. Fortunately, this is easy to do — we just use the following prior:

$$p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{W}|\mathbf{0}, \frac{1}{\alpha_w}\mathbf{I})\mathcal{N}(\mathbf{V}|\mathbf{0}, \frac{1}{\alpha_v}\mathbf{I})\mathcal{N}(\mathbf{b}|\mathbf{0}, \frac{1}{\alpha_b}\mathbf{I})\mathcal{N}(\mathbf{c}|\mathbf{0}, \frac{1}{\alpha_c}\mathbf{I}) \tag{16.79}$$

where $\mathbf{b}$ and $\mathbf{c}$ are the bias terms.[9]

To get a feeling for the effect of these hyper-parameters, we can sample MLP parameters from this prior and plot the resulting random functions. Figure 16.17 shows some examples. Decreasing α_v allows the first layer weights to get bigger, making the sigmoid-like shape of the functions steeper. Decreasing α_b allows the first layer biases to get bigger, which allows the center of the sigmoid to shift left and right more. Decreasing α_w allows the second layer weights to get bigger, making the functions more "wiggly" (greater sensitivity to change in the input, and hence larger dynamic range). And decreasing α_c allows the second layer biases to get bigger, allowing the mean level of the function to move up and down more. (In Chapter 15, we will see an easier way to define priors over functions.)

16.5.6.2 Weight pruning

Since there are many weights in a neural network, it is often helpful to encourage sparsity. Various ad-hoc methods for doing this, with names such as "optimal brain damage", were devised in the 1990s; see e.g., (Bishop 1995) for details.

9. Since we are regularizing the output bias terms, it is helpful, in the case of regression, to normalize the target responses in the training set to zero mean, to be consistent with the fact that the prior on the output bias has zero mean.

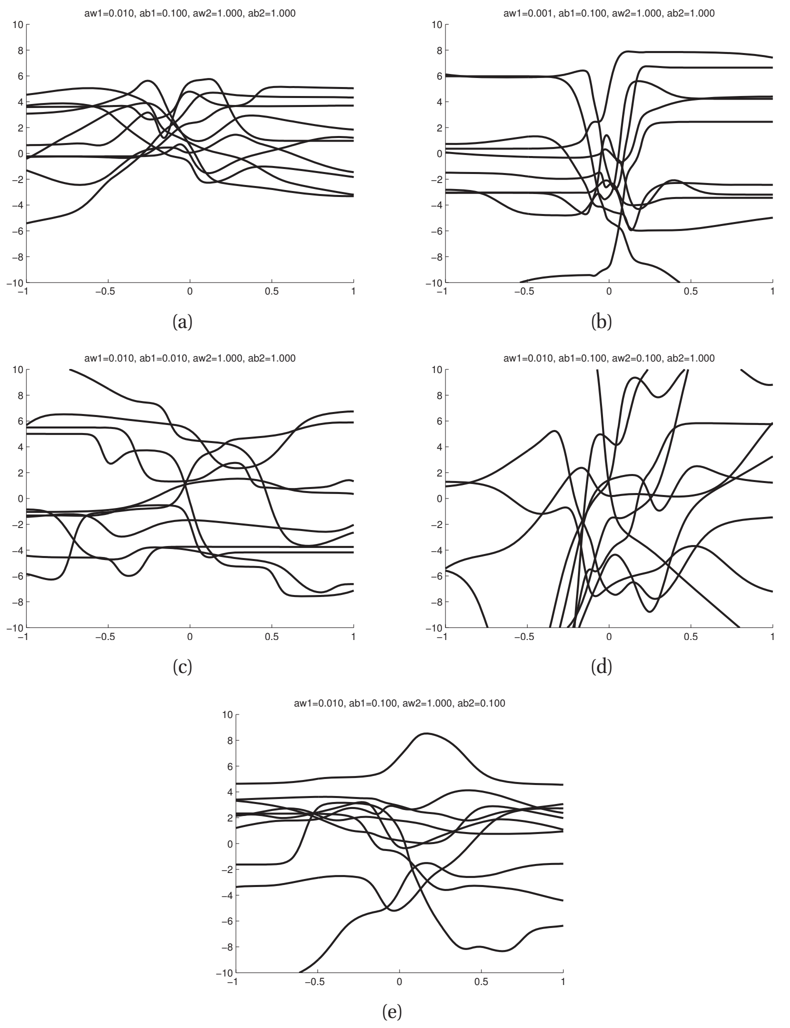
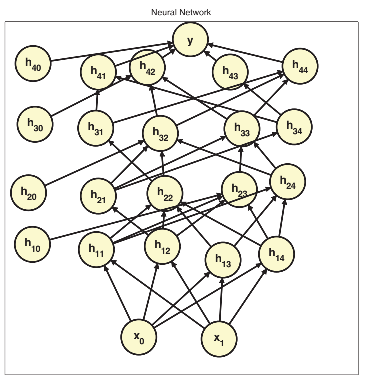
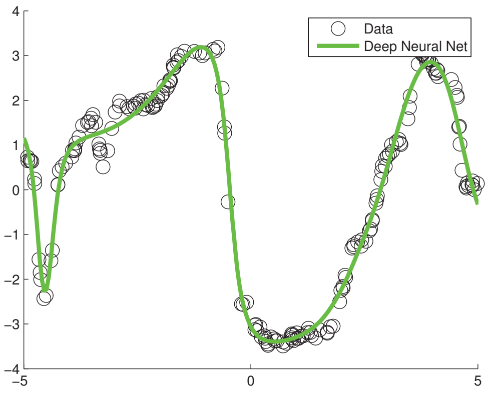


Figure 16.17 The effects of changing the hyper-parameters on an MLP. (a) Default parameter values $\alpha_v = 0.01$, $\alpha_b = 0.1$, $\alpha_w = 1$, $\alpha_c = 1$. (b) Decreasing α_v by factor of 10. (c) Decreasing α_b by factor of 10. (d) Decreasing α_w by factor of 10. (e) Decreasing α_c by factor of 10. Figure generated by `mlpPriorsDemo`.



(a)



(b)

Figure 16.18 (a) A deep but sparse neural network. The connections are pruned using ℓ_1 regularization. At each level, nodes numbered 0 are clamped to 1, so their outgoing weights correspond to the offset/bias terms. (b) Predictions made by the model on the training set. Figure generated by `sparseNnetDemo`, written by Mark Schmidt.

However, we can also use the more principled sparsity-promoting techniques we discussed in Chapter 13. One approach is to use an ℓ_1 regularizer. See Figure 16.18 for an example. Another approach is to use ARD; this is discussed in more detail in Section 16.5.7.5.

16.5.6.3 Soft weight sharing*

Another way to regularize the parameters is to encourage similar weights to share statistical strength. But how do we know which parameters to group together? We can learn this, by using a mixture model. That is, we model $p(\boldsymbol{\theta})$ as a mixture of (diagonal) Gaussians. Parameters that are assigned to the same cluster will share the same mean and variance and thus will have similar values (assuming the variance for that cluster is low). This is called **soft weight sharing** (Nowlan and Hinton 1992). In practice, this technique is not widely used. See e.g., (Bishop 2006a, p271) if you want to know the details.

16.5.6.4 Semi-supervised embedding *

An interesting way to regularize "deep" feedforward neural networks is to encourage the hidden layers to assign similar objects to similar representations. This is useful because it is often easy to obtain "side" information consisting of sets of pairs of similar and dissimilar objects. For example, in a video classification task, neighboring frames can be deemed similar, but frames that are distant in time can be deemed dis-similar (Mobahi et al. 2009). Note that this can be done without collecting any labels.

Let $S_{ij} = 1$ if examples i and j are similar, and $S_{ij} = 0$ otherwise. Let $f(\mathbf{x}_i)$ be some embedding of item $\mathbf{x}_i$, e.g., $f(\mathbf{x}_i) = \mathbf{z}(\mathbf{x}_i, \boldsymbol{\theta})$, where $\mathbf{z}$ is the hidden layer of a neural network. Now define a loss function $L(f(\mathbf{x}_i), f(\mathbf{x}_j), S_{ij})$ that depends on the embedding of two objects, and the observed similarity measure. For example, we might want to force similar objects to have similar embeddings, and to force the embeddings of dissimilar objects to be a minimal distance apart:

$$L(\mathbf{f}_i, \mathbf{f}_j, S_{ij}) = \begin{cases} ||\mathbf{f}_i - \mathbf{f}_j||^2 & \text{if } S_{ij} = 1 \\ \max(0, m - ||\mathbf{f}_i - \mathbf{f}_j||^2) & \text{if } S_{ij} = 0 \end{cases} \tag{16.80}$$

where m is some minimal margin. We can now define an augmented loss function for training the neural network:

$$\sum_{i \in \mathcal{L}} \text{NLL}(f(\mathbf{x}_i), y_i) + \lambda \sum_{i,j \in \mathcal{U}} L(f(\mathbf{x}_i), f(\mathbf{x}_j), S_{ij}) \tag{16.81}$$

where $\mathcal{L}$ is the labeled training set, $\mathcal{U}$ is the unlabeled training set, and $\lambda \geq 0$ is some tradeoff parameter. This is called **semi-supervised embedding** (Weston et al. 2008).

Such an objective can be easily optimized by stochastic gradient descent. At each iteration, pick a random labeled training example, $(\mathbf{x}_n, y_n)$, and take a gradient step to optimize $\text{NLL}(f(\mathbf{x}_i), y_i)$. Then pick a random pair of similar unlabeled examples $\mathbf{x}_i$, $\mathbf{x}_j$ (these can sometimes be generated on the fly rather than stored in advance), and make a gradient step to optimize $\lambda L(f(\mathbf{x}_i), f(\mathbf{x}_j), 1)$, Finally, pick a random unlabeled example $\mathbf{x}_k$, which with high probability is dissimilar to $\mathbf{x}_i$, and make a gradient step to optimize $\lambda L(f(\mathbf{x}_i), f(\mathbf{x}_k), 0)$.

Note that this technique is effective because it can leverage massive amounts of data. In a related approach, (Collobert and Weston 2008) trained a neural network to distinguish valid English sentences from invalid ones. This was done by taking all 631 million words from English Wikipedia (`en.wikipedia.org`), and then creating windows of length 11 containing neighboring words. This constitutes the positive examples. To create negative examples, the middle word of each window was replaced by a random English word (this is likely to be an "invalid" sentence — either grammatically and/or semantically — with high probability). This neural network was then trained over the course of 1 week, and its latent representation was then used as the input to a supervised semantic role labeling task, for which very little labeled training data is available. (See also (Ando and Zhang 2005) for related work.)

16.5.7 Bayesian inference *

Although MAP estimation is a succesful way to reduce overfitting, there are still some good reasons to want to adopt a fully Bayesian approach to "fitting" neural networks:

- Integrating out the parameters instead of optimizing them is a much stronger form of regularization than MAP estimation.
- We can use Bayesian model selection to determine things like the hyper-parameter settings and the number of hidden units. This is likely to be much faster than cross validation, especially if we have many hyper-parameters (e.g., as in ARD).
- Modelling uncertainty in the parameters will induce uncertainty in our predictive distributions, which is important for certain problems such as active learning and risk-averse decision making.

- We can use online inference methods, such as the extended Kalman filter, to do online learning (Haykin 2001).

One can adopt a variety of approximate Bayesian inference techniques in this context. In this section, we discuss the Laplace approximation, first suggested in (MacKay 1992, 1995b). One can also use hybrid Monte Carlo (Neal 1996), or variational Bayes (Hinton and Camp 1993; Barber and Bishop 1998).

16.5.7.1 Parameter posterior for regression

We start by considering regression, following the presentation of (Bishop 2006a, sec 5.7), which summarizes the work of (MacKay 1992, 1995b). We will use a prior of the form $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, (1/\alpha)\mathbf{I})$, where $\mathbf{w}$ represents all the weights combined. We will denote the precision of the noise by $\beta = 1/\sigma^2$.

The posterior can be approximated as follows:

$$p(\mathbf{w}|\mathcal{D}, \alpha, \beta) \propto \exp(-E(\mathbf{w})) \tag{16.82}$$

$$E(\mathbf{w}) \triangleq \beta E_D(\mathbf{w}) + \alpha E_W(\mathbf{w}) \tag{16.83}$$

$$E_D(\mathbf{w}) \triangleq \frac{1}{2}\sum_{n=1}^{N}(y_n - f(\mathbf{x}_n, \mathbf{w}))^2 \tag{16.84}$$

$$E_W(\mathbf{w}) \triangleq \frac{1}{2}\mathbf{w}^T\mathbf{w} \tag{16.85}$$

where E_D is the data error, E_W is the prior error, and E is the overall error (negative log prior plus log likelihood). Now let us make a second-order Taylor series approximation of $E(\mathbf{w})$ around its minimum (the MAP estimate)

$$E(\mathbf{w}) \approx E(\mathbf{w}_{MP}) + \frac{1}{2}(\mathbf{w} - \mathbf{w}_{MP})^T\mathbf{A}(\mathbf{w} - \mathbf{w}_{MP}) \tag{16.86}$$

where $\mathbf{A}$ is the Hessian of E:

$$\mathbf{A} = \nabla\nabla E(\mathbf{w}_{MP}) = \beta\mathbf{H} + \alpha\mathbf{I} \tag{16.87}$$

where $\mathbf{H} = \nabla\nabla E_D(\mathbf{w}_{MP})$ is the Hessian of the data error. This can be computed exactly in $O(d^2)$ time, where d is the number of parameters, using a variant of backpropagation (see (Bishop 2006a, sec 5.4) for details). Alternatively, if we use a quasi-Newton method to find the mode, we can use its internally computed (low-rank) approximation to $\mathbf{H}$. (Note that diagonal approximations of $\mathbf{H}$ are usually very inaccurate.) In either case, using this quadratic approximation, the posterior becomes Gaussian:

$$p(\mathbf{w}|\alpha, \beta, \mathcal{D}) \approx \mathcal{N}(\mathbf{w}|\mathbf{w}_{MP}, \mathbf{A}^{-1}) \tag{16.88}$$

16.5.7.2 Parameter posterior for classification

The classification case is the same as the regression case, except $\beta = 1$ and E_D is a cross-entropy error of the form

$$E_D(\mathbf{w}) \triangleq \sum_{n=1}^{N} [y_n \ln f(\mathbf{x}_n, \mathbf{w}) + (1 - y_n) \ln f(\mathbf{x}_n, \mathbf{w})] \tag{16.89}$$

$$\tag{16.90}$$

16.5.7.3 Predictive posterior for regression

The posterior predictive density is given by

$$p(y|\mathbf{x}, \mathcal{D}, \alpha, \beta) = \int \mathcal{N}(y|f(\mathbf{x}, \mathbf{w}), 1/\beta)\mathcal{N}(\mathbf{w}|\mathbf{w}_{MP}, \mathbf{A}^{-1})d\mathbf{w} \tag{16.91}$$

This is not analytically tractable because of the nonlinearity of $f(\mathbf{x}, \mathbf{w})$. Let us therefore construct a first-order Taylor series approximation around the mode:

$$f(\mathbf{x}, \mathbf{w}) \approx f(\mathbf{x}, \mathbf{w}_{MP}) + \mathbf{g}^T(\mathbf{w} - \mathbf{w}_{MP}) \tag{16.92}$$

where

$$\mathbf{g} = \nabla_{\mathbf{w}} f(\mathbf{x}, \mathbf{w})|_{\mathbf{w}=\mathbf{w}_{MP}} \tag{16.93}$$

We now have a linear-Gaussian model with a Gaussian prior on the weights. From Equation 4.126 we have

$$p(y|\mathbf{x}, \mathcal{D}, \alpha, \beta) \approx \mathcal{N}(y|f(\mathbf{x}, \mathbf{w}_{MP}), \sigma^2(\mathbf{x})) \tag{16.94}$$

where the predictive variance depends on the input $\mathbf{x}$ as follows:

$$\sigma^2(\mathbf{x}) = \beta^{-1} + \mathbf{g}^T\mathbf{A}^{-1}\mathbf{g} \tag{16.95}$$

The error bars will be larger in regions of input space where we have little training data. See Figure 16.19 for an example.

16.5.7.4 Predictive posterior for classification

In this section, we discuss how to approximate $p(y|\mathbf{x}, \mathcal{D})$ in the case of binary classification. The situation is similar to the case of logistic regression, discussed in Section 8.4.4, except in addition the posterior predictive mean is a non-linear function of $\mathbf{w}$. Specifically, we have $\mu = \mathbb{E}[y|\mathbf{x}, \mathbf{w}] = \text{sigm}(a(\mathbf{x}, \mathbf{w}))$, where $a(\mathbf{x}, \mathbf{w})$ is the pre-synaptic output of the final layer. Let us make a linear approximation to this:

$$a(\mathbf{x}, \mathbf{w}) \approx a_{MP}(\mathbf{x}) + \mathbf{g}^T(\mathbf{w} - \mathbf{w}_{MP}) \tag{16.96}$$

where $a_{MP}(\mathbf{x}) = a(\mathbf{x}, \mathbf{w}_{MP})$ and $\mathbf{g} = \nabla_{\mathbf{x}} a(\mathbf{x}, \mathbf{w}_{MP})$ can be found by a modified version of backpropagation. Clearly

$$p(a|\mathbf{x}, \mathcal{D}) \approx \mathcal{N}(a(\mathbf{x}, \mathbf{w}_{MP}), \mathbf{g}(\mathbf{x})^T\mathbf{A}^{-1}\mathbf{g}(\mathbf{x})) \tag{16.97}$$

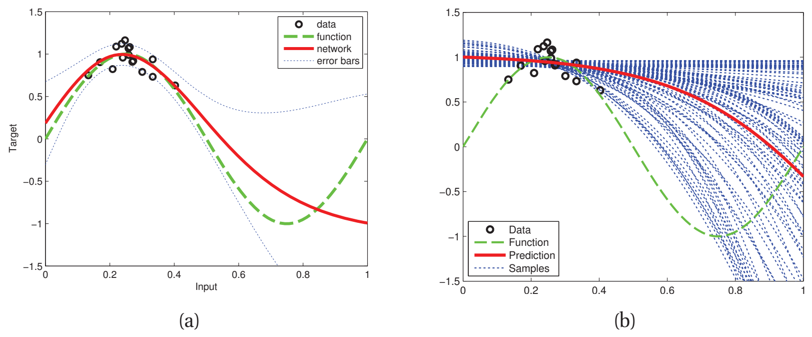


Figure 16.19 The posterior predictive density for an MLP with 3 hidden nodes, trained on 16 data points. The dashed green line is the true function. (a) Result of using a Laplace approximation, after performing empirical Bayes to optimize the hyperparameters. The solid red line is the posterior mean prediction, and the dotted blue lines are 1 standard deviation above and below the mean. Figure generated by `mlpRegEvidenceDemo`. (b) Result of using hybrid Monte Carlo, using the same trained hyperparameters as in (a). The solid red line is the posterior mean prediction, and the dotted blue lines are samples from the posterior predictive. Figure generated by `mlpRegHmcDemo`, written by Ian Nabney.

Hence the posterior predictive for the output is

$$p(y=1|\mathbf{x},\mathcal{D}) = \int \text{sigm}(a)p(a|\mathbf{x},\mathcal{D})da \approx \text{sigm}(\kappa(\sigma_a^2)\mathbf{b}^T\mathbf{w}_{MP}) \tag{16.98}$$

where κ is defined by Equation 8.70, which we repeat here for convenience:

$$\kappa(\sigma^2) \triangleq (1+\pi\sigma^2/8)^{-\frac{1}{2}} \tag{16.99}$$

Of course, a simpler (and potentially more accurate) alternative to this is to draw a few samples from the Gaussian posterior and to approximate the posterior predictive using Monte Carlo.

In either case, the effect of taking uncertainty of the parameters into account, as in Section 8.4.4, is to "moderate" the confidence of the output; the decision boundary itself is unaffected, however.

16.5.7.5 ARD for neural networks

Once we have made the Laplace approximation to the posterior, we can optimize the marginal likelihood wrt the hyper-parameters $\boldsymbol{\alpha}$ using the same fixed-point equations as in Section 13.7.4.2. Typically we use one hyper-parameter for the weight vector leaving each node, to achieve an effect similar to group lasso (Section 13.5.1). That is, the prior has the form

$$p(\boldsymbol{\theta}) = \prod_{i=1}^{D} \mathcal{N}(\mathbf{v}_{:,i}|\mathbf{0}, \frac{1}{\alpha_{v,i}}\mathbf{I}) \prod_{j=1}^{H} \mathcal{N}(\mathbf{w}_{:,j}|\mathbf{0}, \frac{1}{\alpha_{w,j}}\mathbf{I}) \tag{16.100}$$

If we find $\alpha_{v,i} = \infty$, then input feature i is irrelevant, and its weight vector $\mathbf{v}_{:,i}$ is pruned out. Similarly, if we find $\alpha_{w,j} = \infty$, then hidden feature j is irrelevant. This is known as automatic relevancy determination or ARD, which was discussed in detail in Section 13.7. Applying this to neural networks gives us an efficient means of variable selection in non-linear models.

The software package NETLAB contains a simple example of ARD applied to a neural network, called `demard`. This demo creates some data according to a nonlinear regression function $f(x_1, x_2, x_3) = \sin(2\pi x_1) + \epsilon$, where x_2 is a noisy copy of x_1. We see that x_2 and x_3 are irrelevant for predicting the target. However, x_2 is correlated with x_1, which is relevant. Using ARD, the final hyper-parameters are as follows:

$$\boldsymbol{\alpha} = [0.2, \quad 21.4, \quad 249001.8] \tag{16.101}$$

This clearly indicates that feature 3 is irrelevant, feature 2 is only weakly relevant, and feature 1 is very relevant.

16.6 Ensemble learning

Ensemble learning refers to learning a weighted combination of base models of the form

$$f(y|\mathbf{x}, \boldsymbol{\pi}) = \sum_{m \in \mathcal{M}} w_m f_m(y|\mathbf{x}) \tag{16.102}$$

where the w_m are tunable parameters. Ensemble learning is sometimes called a **committee method**, since each base model f_m gets a weighted "vote".

Clearly ensemble learning is closely related to learning adaptive-basis function models. In fact, one can argue that a neural net is an ensemble method, where f_m represents the m'th hidden unit, and w_m are the output layer weights. Also, we can think of boosting as kind of ensemble learning, where the weights on the base models are determined sequentially. Below we describe some other forms of ensemble learning.

16.6.1 Stacking

An obvious way to estimate the weights in Equation 16.102 is to use

$$\hat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{i=1}^{N} L(y_i, \sum_{m=1}^{M} w_m f_m(\mathbf{x})) \tag{16.103}$$

However, this will result in overfitting, with w_m being large for the most complex model. A simple solution to this is to use cross-validation. In particular, we can use the LOOCV estimate

$$\hat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{i=1}^{N} L(y_i, \sum_{m=1}^{M} w_m \hat{f}_m^{-i}(\mathbf{x})) \tag{16.104}$$

where $\hat{f}_m^{-i}(\mathbf{x})$ is the predictor obtained by training on data excluding $(\mathbf{x}_i, y_i)$. This is known as **stacking**, which stands for "stacked generalization" (Wolpert 1992). This technique is more robust to the case where the "true" model is not in the model class than standard BMA (Clarke 2003). This approach was used by the Netflix team known as "The Ensemble", which tied the submission of the winning team (BellKor's Pragmatic Chaos) in terms of accuracy (Sill et al. 2009). Stacking has also been used for problems such as image segmentation and labeling.

Class	C_1	C_2	C_3	C_4	C_5	C_6	$\cdots$	C_{15}
0	1	1	0	0	0	0	$\cdots$	1
1	0	0	1	1	1	1	$\cdots$	0
					$\vdots$			
9	0	1	1	1	0	0	$\cdots$	0

Table 16.2 Part of a 15-bit error-correcting output code for a 10-class problem. Each row defines a two-class problem. Based on Table 16.1 of (Hastie et al. 2009).

16.6.2 Error-correcting output codes

An interesting form of ensemble learning is known as **error-correcting output codes** or **ECOC** (Dietterich and Bakiri 1995), which can be used in the context of multi-class classification. The idea is that we are trying to decode a symbol (namely the class label) which has C possible states. We could use a bit vector of length $B = \lceil \log_2 C \rceil$ to encode the class label, and train B separate binary classifiers to predict each bit. However, by using more bits, and by designing the codewords to have maximal Hamming distance from each other, we get a method that is more resistant to individual bit-flipping errors (misclassification). For example, in Table 16.2, we use $B = 15$ bits to encode a $C = 10$ class problem. The minimum Hamming distance between any pair of rows is 7. The decoding rule is

$$\hat{c}(\mathbf{x}) = \min_c \sum_{b=1}^{B} |C_{cb} - \hat{p}_b(\mathbf{x})| \tag{16.105}$$

where C_{cb} is the b'th bit of the codeword for class c. (James and Hastie 1998) showed that a random code worked just as well as the optimal code: both methods work by averaging the results of multiple classifiers, thereby reducing variance.

16.6.3 Ensemble learning is not equivalent to Bayes model averaging

In Section 5.3, we discussed Bayesian model selection. An alternative to picking the best model, and then using this to make predictions, is to make a weighted average of the predictions made by each model, i.e., we compute

$$p(y|\mathbf{x}, \mathcal{D}) = \sum_{m \in \mathcal{M}} p(y|\mathbf{x}, m, \mathcal{D}) p(m|\mathcal{D}) \tag{16.106}$$

This is called **Bayes model averaging** (BMA), and can sometimes give better performance than using any single model (Hoeting et al. 1999). Of course, averaging over all models is typically computationally infeasible (analytical integration is obviously not possible in a discrete space, although one can sometimes use dynamic programming to perform the computation exactly, e.g., (Meila and Jaakkola 2006)). A simple approximation is to sample a few models from the posterior. An even simpler approximation (and the one most widely used in practice) is to just use the MAP model.

It is important to note that BMA is not equivalent to ensemble learning (Minka 2000c). This latter technique corresponds to enlarging the model space, by defining a single new model

MODEL	1ST	2ND	3RD	4TH	5TH	6TH	7TH	8TH	9TH	10TH
BST-DT	0.580	0.228	0.160	0.023	0.009	0.000	0.000	0.000	0.000	0.000
RF	0.390	0.525	0.084	0.001	0.000	0.000	0.000	0.000	0.000	0.000
BAG-DT	0.030	0.232	0.571	0.150	0.017	0.000	0.000	0.000	0.000	0.000
SVM	0.000	0.008	0.148	0.574	0.240	0.029	0.001	0.000	0.000	0.000
ANN	0.000	0.007	0.035	0.230	0.606	0.122	0.000	0.000	0.000	0.000
KNN	0.000	0.000	0.000	0.009	0.114	0.592	0.245	0.038	0.002	0.000
BST-STMP	0.000	0.000	0.002	0.013	0.014	0.257	0.710	0.004	0.000	0.000
DT	0.000	0.000	0.000	0.000	0.000	0.000	0.004	0.616	0.291	0.089
LOGREG	0.000	0.000	0.000	0.000	0.000	0.000	0.040	0.312	0.423	0.225
NB	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.030	0.284	0.686

Table 16.3 Fraction of time each method achieved a specified rank, when sorting by mean performance across 11 datasets and 8 metrics. Based on Table 4 of (Caruana and Niculescu-Mizil 2006). Used with kind permission of Alexandru Niculescu-Mizil.

which is a convex combination of base models, as follows:

$$p(y|\mathbf{x}, \boldsymbol{\pi}) = \sum_{m \in \mathcal{M}} \pi_m p(y|\mathbf{x}, m) \tag{16.107}$$

In principle, we can now perform Bayesian inference to compute $p(\boldsymbol{\pi}|\mathcal{D})$; we then make predictions using $p(y|\mathbf{x}, \mathcal{D}) = \int p(y|\mathbf{x}, \boldsymbol{\pi})p(\boldsymbol{\pi}|\mathcal{D})d\boldsymbol{\pi}$. However, it is much more common to use point estimation methods for $\boldsymbol{\pi}$, as we saw above.

16.7 Experimental comparison

We have described many different methods for classification and regression. Which one should you use? That depends on which inductive bias you think is most appropriate for your domain. Usually this is hard to assess, so it is common to just try several different methods, and see how they perform empirically. Below we summarize two such comparisons that were carefully conducted (although the data sets that were used are relatively small). See the website `mlcomp.org` for a distributed way to perform large scale comparisons of this kind. Of course, we must always remember the no free lunch theorem (Section 1.4.9), which tells us that there is no universally best learning method.

16.7.1 Low-dimensional features

In 2006, Rich Caruana and Alex Niculescu-Mizil (Caruana and Niculescu-Mizil 2006) conducted a very extensive experimental comparison of 10 different binary classification methods, on 11 different data sets. The 11 data sets all had 5000 training cases, and had test sets containing $\sim 10,000$ examples on average. The number of features ranged from 9 to 200, so this is much lower dimensional than the NIPS 2003 feature selection challenge. 5-fold cross validation was used to assess average test error. (This is separate from any internal CV a method may need to use for model selection.)

The methods they compared are as follows (listed in roughly decreasing order of performance, as assessed by Table 16.3):

- BST-DT: boosted decision trees
- RF: random forest
- BAG-DT: bagged decision trees
- SVM: support vector machine
- ANN: artificial neural network
- KNN: K-nearest neighbors
- BST-STMP: boosted stumps
- DT: decision tree
- LOGREG: logistic regression
- NB: naive Bayes

They used 8 different performance measures, which can be divided into three groups. Threshold metrics just require a point estimate as output. These include accuracy, F-score (Section 5.7.2.3), etc. Ordering/ ranking metrics measure how well positive cases are ordered before the negative cases. These include area under the ROC curve (Section 5.7.2.1), average precision, and the precision/recall break even point. Finally, the probability metrics included cross-entropy (log-loss) and squared error, $(y - \hat{p})^2$. Methods such as SVMs that do not produce calibrated probabilities were post-processed using Platt's logistic regression trick (Section 14.5.2.3), or using isotonic regression. Performance measures were standardized to a 0:1 scale so they could be compared.

Obviously the results vary by dataset and by metric. Therefore just averaging the performance does not necessarily give reliable conclusions. However, one can perform a bootstrap analysis, which shows how robust the conclusions are to such changes. The results are shown in Table 16.3. We see that most of the time, boosted decision trees are the best method, followed by random forests, bagged decision trees, SVMs and neural networks. However, the following methods all did relatively poorly: KNN, stumps, single decision trees, logistic regression and naive Bayes.

These results are generally consistent with conventional wisdom of practioners in the field. Of course, the conclusions may change if there the features are high dimensional and/ or there are lots of irrelevant features (as in Section 16.7.2), or if there is lots of noise, etc.

16.7.2 High-dimensional features

In 2003, the NIPS conference ran a competition where the goal was to solve binary classification problems with large numbers of (mostly irrelevant) features, given small training sets. (This was called a "feature selection" challenge, but performance was measured in terms of predictive accuracy, not in terms of the ability to select features.) The five datasets that were used are summarized in Table 16.4. The term **probe** refers to artifical variables that were added to the problem to make it harder. These have no predictive power, but are correlated with the original features.

Results of the competition are discussed in (Guyon et al. 2006). The overall winner was an approach based on Bayesian neural networks (Neal and Zhang 2006). In a follow-up study

Dataset	Domain	Type	D	% probes	N_{train}	N_{val}	N_{test}
Aracene	Mass spectrometry	Dense	10,000	30	100	100	700
Dexter	Text classification	Sparse	20,000	50	300	300	2000
Dorothea	Drug discovery	Sparse	100,000	50	800	350	800
Gisette	Digit recognition	Dense	5000	30	6000	1000	6500
Madelon	Artificial	Dense	500	96	2000	600	1800

Table 16.4 Summary of the data used in the NIPS 2003 "feature selection" challenge. For the Dorothea datasets, the features are binary. For the others, the features are real-valued.

	Screened features		ARD	
Method	Avg rank	Avg time	Avg rank	Avg time
HMC MLP	1.5	384 (138)	1.6	600 (186)
Boosted MLP	3.8	9.4 (8.6)	2.2	35.6 (33.5)
Bagged MLP	3.6	3.5 (1.1)	4.0	6.4 (4.4)
Boosted trees	3.4	3.03 (2.5)	4.0	34.1 (32.4)
Random forests	2.7	1.9 (1.7)	3.2	11.2 (9.3)

Table 16.5 Performance of different methods on the NIPS 2003 "feature selection" challenge. (HMC stands for hybrid Monte Carlo; see Section 24.5.4.) We report the average rank (lower is better) across the 5 datasets. We also report the average training time in minutes (standard error in brackets). The MCMC and bagged MLPs use two hidden layers of 20 and 8 units. The boosted MLPs use one hidden layer with 2 or 4 hidden units. The boosted trees used depths between 2 and 9, and shrinkage between 0.001 and 0.1. Each tree was trained on 80% of the data chosen at random at each step (so-called **stochastic gradient boosting**). From Table 11.3 of (Hastie et al. 2009).

(Johnson 2009), Bayesian neural nets (MLPs with 2 hidden layers) were compared to several other methods based on bagging and boosting. Note that all of these methods are quite similar: in each case, the prediction has the form

$$\hat{f}(\mathbf{x}_*) = \sum_{m=1}^{M} w_m \mathbb{E}\left[y|\mathbf{x}_*, \boldsymbol{\theta}_m\right] \tag{16.108}$$

The Bayesian MLP was fit by MCMC (hybrid Monte Carlo), so we set $w_m = 1/M$ and set $\boldsymbol{\theta}_m$ to a draw from the posterior. In bagging, we set $w_m = 1/M$ and $\boldsymbol{\theta}_m$ is estimated by fitting the model to a bootstrap sample from the data. In boosting, we set $w_m = 1$ and the $\boldsymbol{\theta}_m$ are estimated sequentially.

To improve computational and statistical performance, some feature selection was performed. Two methods were considered: simple uni-variate screening using T-tests, and a method based on MLP+ARD. Results of this follow-up study are shown in Table 16.5. We see that Bayesian MLPs are again the winner. In second place are either random forests or boosted MLPs, depending on the preprocessing. However, it is not clear how statistically significant these differences are, since the test sets are relatively small.

In terms of training time, we see that MCMC is much slower than the other methods. It would be interesting to see how well deterministic Bayesian inference (e.g., Laplace approximation) would perform. (Obviously it will be much faster, but the question is: how much would one lose

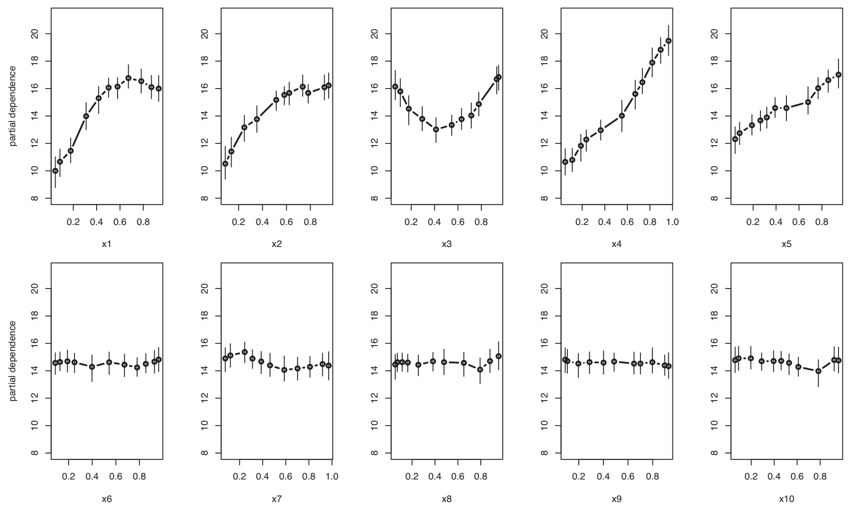


Figure 16.20 Partial dependence plots for the 10 predictors in Friedman's synthetic 5-dimensional regression problem. Source: Figure 4 of (Chipman et al. 2010) . Used with kind permission of Hugh Chipman.

in statistical performance?)

16.8 Interpreting black-box models

Linear models are popular in part because they are easy to interpet. However, they often are poor predictors, which makes them a poor proxy for "nature's mechanism". Thus any conclusions about the importance of particular variables should only be based on models that have good predictive accuracy (Breiman 2001b). (Interestingly, many standard statistical tests of "goodness of fit" do not test the predictive accuracy of a model.)

In this chapter, we studied **black-box** models, which do have good predictive accuracy. Unfortunately, they are hard to interpret directly. Fortunately, there are various heuristics we can use to "probe" such models, in order to assess which input variables are the most important.

As a simple example, consider the following non-linear function, first proposed (Friedman 1991) to illustrate the power of MARS:

$$f(\mathbf{x}) = 10\sin(\pi x_1 x_2) + 20(x_3 - 0.5)^2 + 10x_4 + 5x_5 + \epsilon \tag{16.109}$$

where $\epsilon \sim \mathcal{N}(0, 1)$. We see that the output is a complex function of the inputs. By augmenting the $\mathbf{x}$ vector with additional irrelevant random variables, all drawn uniform on $[0, 1]$, we can create a challenging feature selection problem. In the experiments below, we add 5 extra dummy variables.

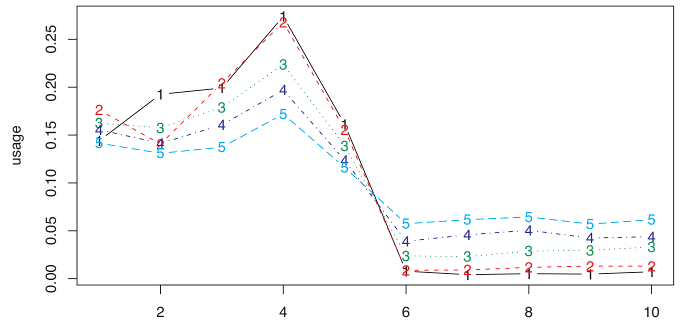


Figure 16.21 Average usage of each variable in a BART model fit to data where only the first 5 features are relevant. The different coloured lines correspond to different numbers of trees in the ensemble. Source: Figure 5 of (Chipman et al. 2010) . Used with kind permission of Hugh Chipman.

One useful way to measure the effect of a set s of variables on the output is to compute a **partial dependence plot** (Friedman 2001). This is a plot of $f(\mathbf{x}_s)$ vs $\mathbf{x}_s$, where $f(\mathbf{x}_s)$ is defined as the response to $\mathbf{x}_s$ with the other predictors averaged out:

$$f(\mathbf{x}_s) = \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_s, \mathbf{x}_{i,-s}) \tag{16.110}$$

Figure 16.20 shows an example where we use sets corresponding to each single variable. The data was generated from Equation 16.109, with 5 irrelevant variables added. We then fit a BART model (Section 16.2.5) and computed the partial dependence plots. We see that the predicted response is invariant for $s \in \{6, \ldots, 10\}$, indicating that these variables are (marginally) irrelevant. The response is roughly linear in x_4 and x_5, and roughly quadratic in x_3. (The error bars are obtained by computing empirical quantiles of $f(\mathbf{x}, \boldsymbol{\theta})$ based on posterior samples of $\boldsymbol{\theta}$; alternatively, we can use bootstrap.)

Another very useful summary computes the **relative importance of predictor variables**. This can be thought of as a nonlinear, or even "model free", way of performing variable selection, although the technique is restricted to ensembles of trees. The basic idea, originally proposed in (Breiman et al. 1984), is to count how often variable j is used as a node in any of the trees. In particular, let $v_j = \frac{1}{M}\sum_{m=1}^{M} \mathbb{I}(j \in T_m)$ be the proportion of all splitting rules that use x_j, where T_m is the m'th tree. If we can sample the posterior of trees, $p(T_{1:M}|\mathcal{D})$, we can easily compute the posterior for v_j. Alternatively, we can use bootstrap.

Figure 16.21 gives an example, using BART. We see that the five relevant variables are chosen much more than the five irrelevant variables. As we increase the number M of trees, all the variables are more likely to be chosen, reducing the sensitivity of this method, but for small M, the method is farily diagnostic.

Exercises

Exercise 16.1 Nonlinear regression for inverse dynamics

In this question, we fit a model which can predict what torques a robot needs to apply in order to make its arm reach a desired point in space. The data was collected from a SARCOS robot arm with 7 degrees of freedom. The input vector $\mathbf{x} \in \mathbb{R}^{21}$ encodes the desired position, velocity and accelaration of the 7 joints. The output vector $\mathbf{y} \in \mathbb{R}^7$ encodes the torques that should be applied to the joints to reach that point. The mapping from $\mathbf{x}$ to $\mathbf{y}$ is highly nonlinear.

We have $N = 48,933$ training points and $N_{test} = 4,449$ testing points. For simplicity, we following standard practice and focus on just predicting a scalar output, namely the torque for the first joint.

Download the data from `http://www.gaussianprocess.org/gpml`. Standardize the inputs so they have zero mean and unit variance on the training set, and center the outputs so they have zero mean on the training set. Apply the corresponding transformations to the test data. Below we will describe various models which you should fit to this transformed data. Then make predictions and compute the standardized mean squared error on the test set as follows:

$$SMSE = \frac{\frac{1}{N_{test}} \sum_{i=1}^{N_{test}} (y_i - \hat{y}_i)^2}{\sigma^2} \tag{16.111}$$

where $\sigma^2 = \frac{1}{N_{train}} \sum_{i=1}^{Ntrain} (y_i - \overline{y})^2$ is the variance of the output computed on the training set.

a. The first method you should try is standard linear regression. Turn in your numbers and code. (According to (Rasmussen and Williams 2006, p24), you should be able to achieve a SMSE of 0.075 using this method.)

b. Now try running K-means clustering (using cross validation to pick K). Then fit an RBF network to the data, using the $\boldsymbol{\mu}_k$ estimated by K-means. Use CV to estimate the RBF bandwidth. What SMSE do you get? Turn in your numbers and code. (According to (Rasmussen and Williams 2006, p24), Gaussian process regression can get an SMSE of 0.011, so the goal is to get close to that.)

c. Now try fitting a feedforward neural network. Use CV to pick the number of hidden units and the strength of the ℓ_2 regularizer. What SMSE do you get? Turn in your numbers and code.