Statistical Learning

Some Machine Learning Terminology

- Two forms of learning:
    - *supervised learning*: *features* and responses are available for a *training set*, and a way of predicting response from features of new data is to be *learned*.
    - *unsupervised learning*: no distinguished responses are available; the goal is to discover patterns and associations among features.
- Classification and regression are supervised learning methods.
- Clustering, multi-dimensional scaling, and principal curves are unsupervised learning methods.
- *Data mining* involves extracting information from large (many cases and/or many variables), messy (many missing values, many different kinds of variables and measurement scales) data bases.
- Machine learning often emphasizes methods that are sufficiently fast and automated for use in data mining.
- Machine learning is now often considered a branch of *Artificial Intelligence (AI)*.

- Tree models are popular in machine learning
  - supervised: as predictors in classification and regression settings
  - unsupervised: for describing clustering results.
- Some other methods often associated with machine learning:
  - Bagging
  - Boosting
  - Random Forests
  - Support Vector Machines
  - Neural Networks
- References:
  - T. Hastie, R. Tibshirani, and J. Friedman (2009). *The Elements of Statistical Learning, 2nd Ed.*.
  - G. James, D. Witten, T. Hastie, and R. Tibshirani (2013). *An Introduction to Statistical Learning, with Applications in R*.
  - D. Hand, H, Mannila, and P. Smyth (2001). *Principles of Data Mining*.
  - C. M. Bishop (2006). *Pattern Recognition and Machine Learning*.
  - M. Shu (2008). Kernels and ensembles: perspectives on statistical learning, *The American Statistician* 62(2), 97–109.

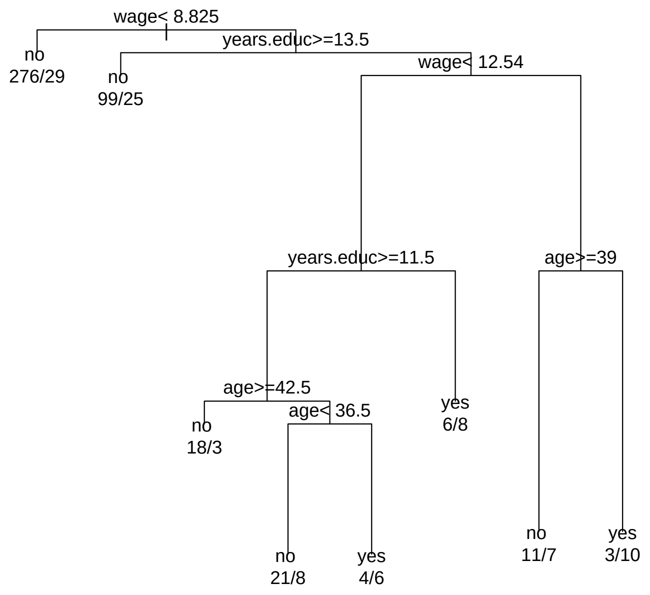
Some examples are available in

`http://www.stat.uiowa.edu/~luke/classes/STAT7400/examples/learning.Rmd`

Tree Models

- Tree models were popularized by a book and software named CART, for *Classification and Regression Trees*.
- The name CART was trademarked and could not be used by other implementations.
- Tree models partition the predictor space based on a series of binary splits.
- Leaf nodes predict a response
  - a category for *classification trees*
  - a numerical value for *regression trees*
- Regression trees may also use a simple linear model within leaf nodes of the partition.
- Using `rpart` a tree model for predicting union membership can be constructed by

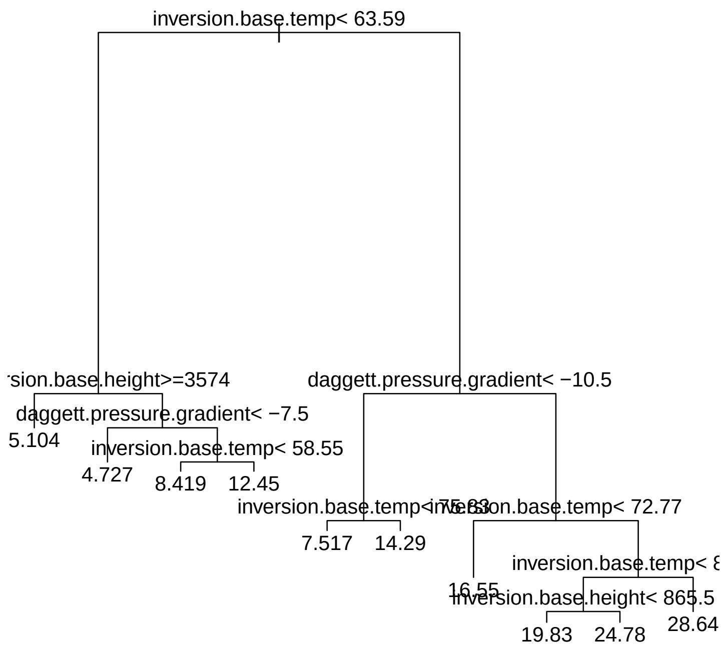
```
library(SemiPar) # for trade union data
library(rpart)
trade.union$member.fac <-
    as.factor(ifelse(trade.union$union.member, "yes", "no"))
fit <- rpart(member.fac ~ wage + age + years.educ,
             data = trade.union)
plot(fit)
text(fit, use.n = TRUE)
```



Left branch is TRUE, right branch is FALSE.

- Regression trees use a constant fit by default.
- A regression tree for the California air pollution data:

```
library(SemiPar) # for air pollution data
library(rpart)
fit2 <- rpart(ozone.level ~ daggett.pressure.gradient +
                            inversion.base.height +
                            inversion.base.temp,
              data = calif.air.poll)
plot(fit2)
text(fit2)
```


inversion.base.temp< 63.59
sion.base.height>=3574
daggett.pressure.gradient< −7.5
5.104
inversion.base.temp< 58.55
4.727
8.419
12.45
daggett.pressure.gradient< −10.5
inversion.base.temp< 75.83
inversion.base.temp< 72.77
7.517
14.29
16.55
inversion.base.height< 865.5
19.83
24.78
28.64

- Tree models are flexible but simple
  - results are easy to explain to non-specialists
- Small changes in data
  - can change tree structure substantially
  - usually do not change predictive performance much
- Fitting procedures usually consist of two phases:
  - growing a large tree
  - pruning back the tree to reduce over-fitting
- Tree growing usually uses a greedy approach.
- Pruning usually minimizes a penalized goodness of fit measure
$$R(\mathscr{T}) + \lambda \text{size}(\mathscr{T})$$
with R a raw measure of goodness of fit.
- The parameter λ can be chosen by some form of cross-validation.
- For regression trees, mean square prediction error is usually used for both growing and pruning.
- For classification trees
  - growing usually uses a loss function that rewards class purity, e.g. a Gini index
$$G_m = \sum_{k=1}^{K} \widehat{p}_{mk}(1 - \widehat{p}_{mk})$$
or a cross-entropy
$$D_m = -\sum_{k=1}^{K} \widehat{p}_{mk} \log \widehat{p}_{mk}$$
with $\widehat{p}_{mk}$ the proportion of training observations in region m that are in class k.
  - Pruning usually focuses on minimizing classification error rates.
- The `rpart` package provides one implementation; the `tree` and `party` packages are also available, among others.

Bagging, Boosting, and Random Forests

- All three are *ensemble methods*: They combine weaker predictors, or *learners*, to form a stronger one.
- A related idea is *Bayesian Model Averaging (BMA)*

Bagging: Bootstrap AGGregation

- Bootstrapping in prediction models produces a sample of predictors
$$T_1^*(x), \ldots, T_R^*(x).$$
- Usually bootstrapping is viewed as a way of assessing the variability of the predictor $T(x)$ based on the original sample.
- For predictors that are not linear in the data an aggregated estimator such as
$$T_{\text{BAG}}(x) = \frac{1}{R}\sum_{i=1}^{R} T_i^*(x)$$
may be an improvement.
- Other aggregations are possible; for classification trees two options are
  - averaging probabilities
  - majority vote
- Bagging can be particularly effective for tree models.
  - Less pruning, or even no pruning, is needed since variance is reduced by averaging.
- Each bootstrap sample will use about 2/3 of the observations; about 1/3 will be *out of bag*, or OOB. The OOB observations can be used to construct an error estimate.
- For tree methods:

  - The resulting predictors are more accurate than simple trees, but lose the simple interpretability.
  - The total reduction in RSS or the Gini index due to splits on a particular variable can be used as a measure of variable importance.

- *Bumping* (Bootstrap umbrella of model parameters) is another approach:
  - Given a bootstrap sample of predictors $T_1^*(x), \ldots, T_R^*(x)$ choose the one that best fits the original data.
  - The original sample is included in the bootstrap sample so the original predictor can be chosen if it is best.

Random Forests

- Introduced by Breiman (2001).
- Also covered by a trademark.
- Similar to bagging for regression or classification trees.
- Draws n_{tree} bootstrap samples.
- For each sample a tree is grown *without* pruning.
  - At each node m_{try} out of p available predictors are sampled at random.
  - A common choice is $m_{\text{try}} \approx \sqrt{p}$.
  - The best split among the sampled predictors is used.
- Form an ensemble predictor by aggregating the trees.
- Error rates are measured by
  - at each bootstrap iteration predicting data not in the sample (out-of-bag, OOB, data).
  - Combine the OOB error measures across samples.
- Bagging without pruning for tree models is equivalent to a random forest with $m_{\text{try}} = p$.
- A motivation is to reduce correlation among the bootstrap trees and so increase the benefit of averaging.
- The R package `randomForest` provides an interface to FORTRAN code of Breiman and Cutler.
- The software provides measures of
  - "importance" of each predictor variable
  - similarity of observations
- Some details are available in A. Liaw and M. Wiener (2002). "Classification and Regression by randomForest," *R News*.

- Other packages implementing random forests are a available as well.
- A recent addition is the `ranger` package.

Boosting

- Boosting is a way of improving on a weak supervised learner.
- The basic learner needs to be able to work with weighted data
- The simplest version applies to binary classification with responses $y_i = \pm 1$.
- A binary classifier produced from a set of weighted training data is a function
$$G(x) : \mathscr{X} \to \{-1, +1\}$$
- The *AdaBoost.M1* (adaptive boosting) algorithm:

  1. Initialize observation weights $w_i = 1/n, i = 1, \dots, n$.
  2. For $m = 1, \dots, M$ do
     (a) Fit a classifier $G_m(x)$ to the training data with weights w_i.
     (b) Compute the weighted error rate
     $$\text{err}_m = \frac{\sum_{i=1}^n w_i 1_{\{y_i \neq G_m(x_i)\}}}{\sum_{i=1}^n w_i}$$
     (c) Compute $\alpha_m = \log((1 - \text{err}_m)/\text{err}_m)$
     (d) Set $w_i \leftarrow w_i \exp(\alpha_m 1_{\{y_i \neq G_m(x_i)\}})$
  3. Output $G(x) = \text{sign}\left(\sum_{i=1}^M \alpha_m G_m(x)\right)$

- The weights are adjusted to put more weight on points that were classified incorrectly.
- These ideas extend to multiple categories and to continuous responses.
- Empirical evidence suggests boosting is successful in a range of problems.
- Theoretical investigations support this.
- The resulting classifiers are closely related to additive models constructed from a set of elementary basis functions.

- The number of steps M plays the role of a model selection parameter
  - too small a value produces a poor fit
  - too large a value fits the training data too well

  Some form of regularization, e.g. based on a validation sample, is needed.
- Other forms of regularization, e.g. variants of shrinkage, are possible as well.

- A variant for boosting regression trees:

  1. Set $\widehat{f}(x) = 0$ and $r_i = y_i$ for all i in the training set.
  2. For $m = 1, \ldots, M$:
     (a) Fit a tree $\widehat{f}^m(x)$ with d splits to the training data X, r.
     (b) Update $\widehat{f}$ by adding a shrunken version of $\widehat{f}^m(x)$,
     $$\widehat{f}(x) \leftarrow \widehat{f}(x) + \lambda \widehat{f}^m(x).$$
     (c) Update the residuals
     $$r_i \leftarrow r_i - \lambda \widehat{f}^m(x)$$
  3. Return the boosted model
  $$\widehat{f}(x) = \sum_{m=1}^{M} \lambda \widehat{f}^m(x)$$

- Using a fairly small d often works well.
- With $d = 1$ this fits an additive model.
- Small values of λ, e.g. 0.01 or 0.001, often work well.
- M is generally chosen by cross-validation.

References on Boosting

P. Bühlmann and T. Hothorn (2007). "Boosting algorithms: regularization, prediction and model fitting (with discussion)," *Statistical Science*, 22(4),477–522.

Andreas Mayr, Harald Binder, Olaf Gefeller, Matthias Schmid (2014). "The evolution of boosting algorithms - from machine learning to statistical modelling," *Methods of Information in Medicine* 53(6), arXiv:1403.1452.

California Air Pollution Data

- Load data and split out a training sample:

```
library(SemiPar)
data(calif.air.poll)
library(mgcv)
train <- sample(nrow(calif.air.poll), nrow(calif.air.poll) / 2)
```

- Fit the additive linear model to the training data and compute the mean square prediction error for the test data:

```
fit <- gam(ozone.level ~ s(daggett.pressure.gradient)
                       + s(inversion.base.height)
                       + s(inversion.base.temp),
           data=calif.air.poll[train,])
mean((calif.air.poll$ozone.level[-train] -
      predict(fit, calif.air.poll[-train,]))^2)
```

- Fit a tree to the training data using all pedictors:

```
library(rpart)
tree.ca <- rpart(ozone.level ~ ., data = calif.air.poll[train,])
mean((calif.air.poll$ozone.level[-train] -
      predict(tree.ca, calif.air.poll[-train,]))^2)
```

- Use bagging on the training set:

```
library(randomForest)
bag.ca <- randomForest(ozone.level ~ .,
                       data = calif.air.poll[train,],
                       mtry = ncol(calif.air.poll) - 1)
mean((calif.air.poll$ozone.level[-train] -
      predict(bag.ca, calif.air.poll[-train,]))^2)
```

- Fit a random forest:

```
rf.ca <- randomForest(ozone.level ~ .,
                      data = calif.air.poll[train,])
mean((calif.air.poll$ozone.level[-train] -
      predict(rf.ca, calif.air.poll[-train,]))^2)
```

- Use `gbm` from the `gbm` package to fit booted regression trees:

```
library(gbm)
boost.ca <- gbm(ozone.level ~ ., data = calif.air.poll[train,],
                n.trees = 5000)
mean((calif.air.poll$ozone.level[-train] -
      predict(boost.ca, calif.air.poll[-train,],
              n.trees = 5000))^2)
boost.ca2 <- gbm(ozone.level ~ ., data = calif.air.poll[train,],
                 n.trees = 10000, interaction.depth=2)
mean((calif.air.poll$ozone.level[-train] -
      predict(boost.ca2, calif.air.poll[-train,],
              n.trees = 5000))^2)
```

- Results:

gam	18.34667	
tree	26.94041	
bagged	21.35568	
randomForest	19.13683	
boosted	19.90317	$M = 5000$
	19.04439	$M = 5000, d = 2$

These results were obtained without first re-scaling the predictors.

Support Vector Machines

- Support vector machines are a method of classification.
- The simplest form is for binary classification with training data $(x_1, y_1), \ldots, (x_n, y_n)$ with

$$\begin{aligned} x_i &\in \mathbb{R}^p \\ y_i &\in \{-1, +1\} \end{aligned}$$

- Various extensions to multiple classes are available; one uses a form of majority vote among all pairwise classifiers.
- Extensions to continuous resposes are also available.
- An R implementation is `svm` in package `e1071`.

Support Vector Classifiers

- A linear binary classifier is of the form

$$G(x) = \text{sign}(x^T\beta + \beta_0)$$

- One way to choose a classifier is to minimize a penalized measure of misclassification

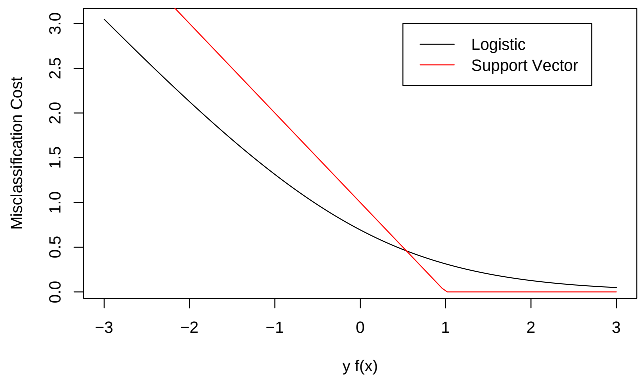
$$\min_{\beta,\beta_0} \sum_{i=1}^{n} (1 - y_i f(x))_+ + \lambda \|\beta\|^2$$

  with $f(x) = x^T\beta + \beta_0$.

  - The misclassification cost is zero for correctly classified points far from the bundary
  - The cost increases for misclassified points farther from the boundary.

- The misclassification cost is qualitatively similar to the negative log-likelihood for a logistic regression model,

$$\rho(y_i, f(x)) = -y_i f(x) + \log\left(1 + e^{y_i f(x)}\right) = \log\left(1 + e^{-y_i f(x)}\right)$$



- The support vector classifier loss function is sometimes called *hinge loss*.
- Via rewriting in terms of equivalent convex optimization problems it can be shown that the minimizer $\widehat{\beta}$ has the form.

$$\widehat{\beta} = \sum_{i=1}^{n} \widehat{\alpha}_i y_i x_i$$

for some values $\widehat{\alpha}_i \in [0, 1/(2\lambda)]$, and therefore

$$\widehat{f}(x) = x^T\widehat{\beta} + \widehat{\beta}_0 = \widehat{\beta}_0 + \sum_{i=1}^{n} \widehat{\alpha}_i y_i x^T x_i = \widehat{\beta}_0 + \sum_{i=1}^{n} \widehat{\alpha}_i y_i \langle x, x_i \rangle$$

- The values of $\widehat{\alpha}_i$ are only non-zero for x_i close to the plane $f(x) = 0$. These x_i are called *support vectors*.

- To allow for non-linear decision boundaries, we can use an extended feature set
$$h(x_i) = (h_1(x_i), \ldots, h_M(x_i))$$
- A linear boundary in $\mathbb{R}^M$ maps down to a nonlinear boundary in $\mathbb{R}^p$.
- For example, for $p = 2$ and
$$h(x) = (x_1, x_2, x_1 x_2, x_1^2, x_2^2)$$
then $M = 5$ and a linear boundary in $\mathbb{R}^5$ maps down to a quadratic boundary in $\mathbb{R}^2$.
- The estimated classification function will be of the form
$$\widehat{f}(x) = \widehat{\beta}_0 + \sum_{i=1}^{n} \widehat{\alpha}_i y_i \langle h(x), h(x_i) \rangle = \widehat{\beta}_0 + \sum_{i=1}^{n} \widehat{\alpha}_i y_i K(x, x_i)$$
where the *kernel function K* is
$$K(x, x') = \langle h(x), h(x') \rangle$$
- The kernel function is symmetric and positive semi-definite.
- We don't need to specify h explicitly, only K is needed.
- Any symmetric, positive semi-definite function can be used.
- Some common choices:
$$\begin{aligned} d\text{th degree polynimial:} K(x,x') &= (1 + \langle x, x' \rangle)^d \\ \text{radial basis:} K(x,x') &= \exp(-\|x - x'\|^2/c) \\ \text{neural network:} K(x,x') &= \tanh(a\langle x, x' \rangle + b) \end{aligned}$$
- The parameter λ in the optimization criterion is a regularization parameter. It can be chosen by cross-validation.
- Particular kernels and their parameters also need to be chosen.
  - This is analogous/equivalent to choosing sets of basis functions.
- Smoothing splines can be expressed in terms of kernels as well
  - this leads to *reproducing kernel Hilbert spaces*
  - this does not lead to the sparseness of the SVM approach

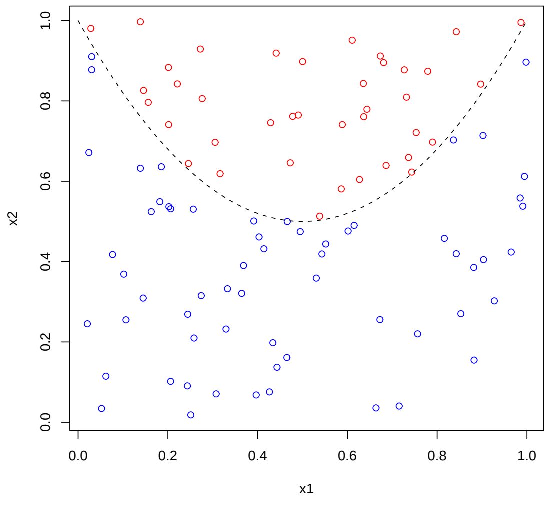
An Artificial Example

Classify random data as above or below a parabola:

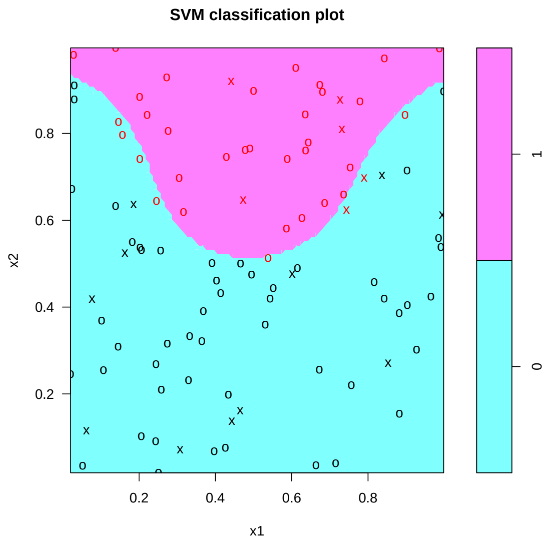
```
x1 <- runif(100)
x2 <- runif(100)
z <- ifelse(x2 > 2 * (x1 - .5)^2 + .5, 1, 0)
plot(x1,x2,col=ifelse(z, "red", "blue"))
x <- seq(0,1,len=101)
lines(x, 2* (x - .5)^2 + .5, lty = 2)
```

Fit a support vector classifier using $\lambda = \frac{1}{2\texttt{cost}}$:

```
> library(e1071)
> fit <- svm(factor(z) ~ x1 + x2, cost = 10)
> fit

Call:
svm(formula = factor(z) ~ x1 + x2, cost = 10)

Parameters:
   SVM-Type:  C-classification
 SVM-Kernel:  radial
       cost:  10
      gamma:  0.5

Number of Support Vectors:  17

plot(fit, data.frame(z=z,x1=x1,x2=x2), formula = x2 ~ x1, grid=100)
```



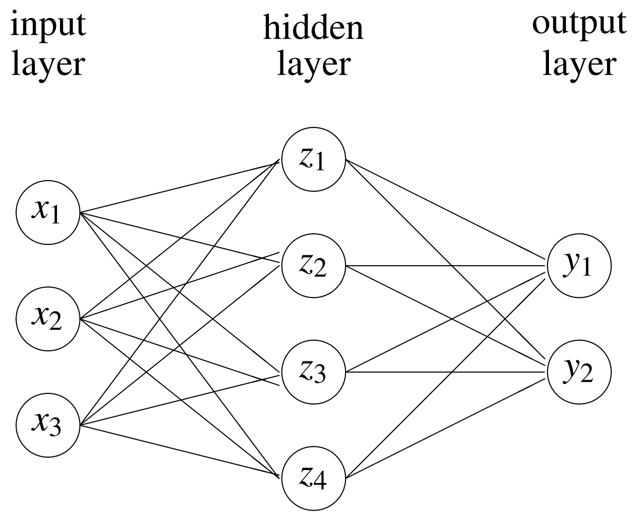
x1
x2
0.0
0.2
0.4
0.6
0.8
1.0



SVM classification plot
x1
x2
0.2
0.4
0.6
0.8
1
0

Neural Networks

- Neural networks are flexible nonlinear models.
- They are motivated by simple models for the working of neurons.
- They connect *input nodes* to *output nodes* through one or more layers of *hidden nodes*
- The simplest form is the feed-forward network with one hidden layer, inputs $x_1, \ldots, x_p$ and outputs $y_1, \ldots, y_k$
  - a graphical representation:



  - mathematical form:

$$\begin{aligned} z_m &= h(\alpha_{0m} + x^T \alpha_m) \\ t_k &= \beta_{0k} + z^T \beta_k \\ f_k(x) &= g_k(T) \end{aligned}$$

    The *activation function h* is usually a *sigmoidal* function, like the logistic CDF

$$h(x) = 1/(1+e^{-x})$$

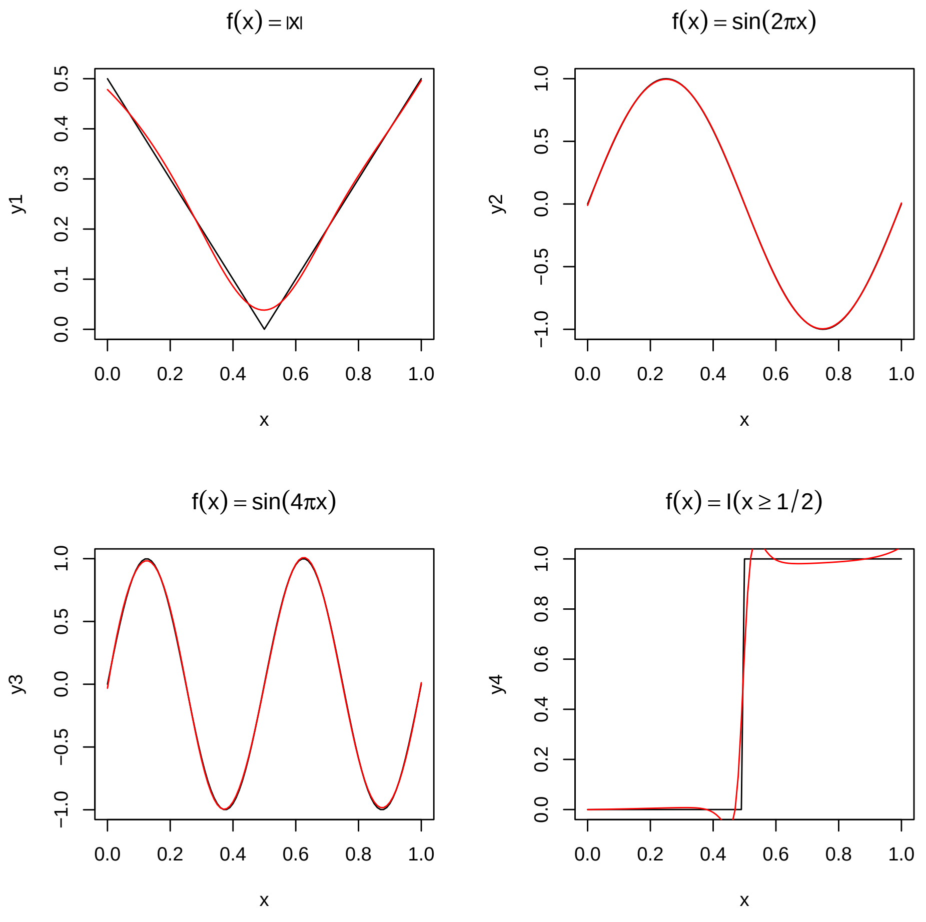
  - For regression there is usually one output with $g_1(t)$ the identity function.

- For binary classification there is usually one output with $g_1(t) = 1/(1+e^{-t})$
- For k-class classification with $k > 2$ usually there are k outputs, corresponding to binary class indicator data, with

$$g_k(t) = \frac{e^{t_k}}{\sum_j e^{t_j}}$$

  This is often called a *softmax* criterion.

- By increasing the size of the hidden layer M a neural network can uniformly approximate any continuous function on a compact set arbitrarily well.
- Some examples, fit to $n = 101$ data points using function `nnet` from package `nnet` with a hidden layer with $M = 5$ nodes:



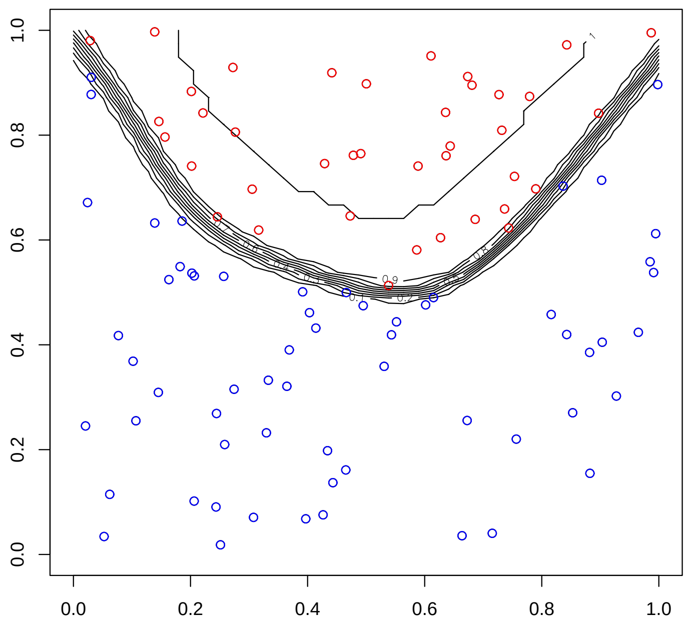
- Fitting is done by maximizing a log likelihood $L(\alpha, \beta)$ assuming
  - normal errors for regression
  - a logistic model for classification
- The likelihood is highly multimodal and the parameters are not identified
  - relabeling hidden nodes does not change the model, for example
  - random starting values are usually used
  - parameters are not interpretable
- If M is large enough to allow flexible fitting then over-fitting is a risk.
- Regularization is used to control overfitting: a penalized log likelihood of the form

  $$L(\alpha,\beta)-\lambda(\sum_m \|\alpha_m\|^2+\sum_k \|\beta_k\|^2)$$

  is maximized.
  - For this to make sense it is important to center and scale the features to have comparable units.
  - This approach is referred to as *weight decay* and λ is the decay parameter.
- As long as M is large enough and regularization is used, the specific value of M seems to matter little.
- The weight decay parameter is often determined by N-fold cross validation, often with $N = 10$
- Because of the random starting points, results in repeated runs can differ.
  - one option is to make several runs and pick the best fit
  - another is to combine results from several runs by averaging or majority voting.

- Fitting a neural net to the artificial data example:

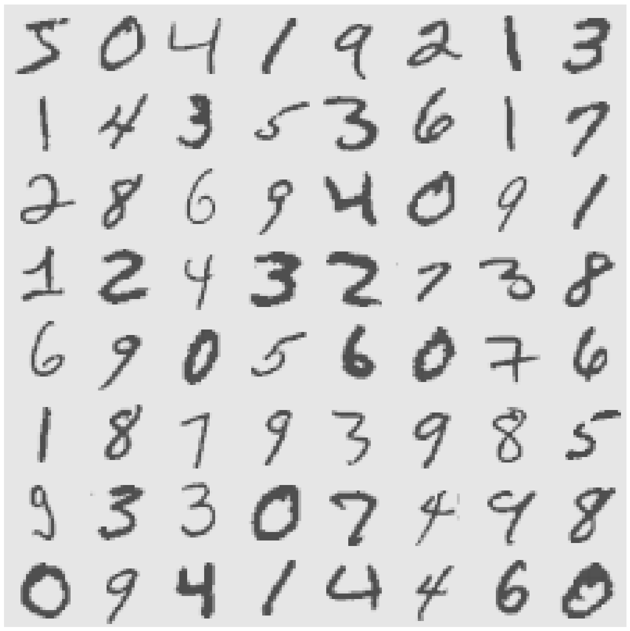
```
nnet(z ~ x1 + x2, size=10, entropy = TRUE, decay = .001,
     maxit = 300)
```



Example: Recognizing Handwritten Digits

- Data consists of scanned ZIP code digist from the U.S. postal service. Available at `http://yann.lecun.com/exdb/mnist/` as a binary file.

  Training data consist of a small number of original images, around 300, and additional images generated by random shifts. Data are 28×28 grayscale images, along with labels.

  This has become a standard machine learning test example.

- Data can be read into R using `readBin`.
- The fit, using 6000 observations and $M = 100$ nodes in the hidden layer took 11.5 hours on `r-lnx400`:

```
fit <- nnet(X, class.ind(lab), size = 100,
            MaxNWts = 100000, softmax = TRUE)
```

  and produced a training misclassification rate of about 8% and a test misclassification rate of about 12%.

- Other implementations are faster and better for large problems.

Deep Learning

- Deep learning models are multi-level non-linear models
- A supervised model with observed responses Y and features X with M layers would be

  $$Y \sim f_1(y|Z_1), Z_1 \sim f_2(z_1|Z_2), \ldots, Z_M \sim f_M(z_M|X)$$

  with $Z_1, \ldots, Z_M$ unobserved latent values.
- An unsupervised model with observed features X would be

  $$X \sim f_1(x|Z_1), Z_1 \sim f_2(z_1|Z_2), \ldots, Z_M \sim f_M(z_M)$$

- These need to be nonlinear so they don't collapse into one big linear model.
- The layers are often viewed as capturing features at different levels of granularity.
- For image classification these might be
  - X: pixel intensities
  - Z_1: edges
  - Z_2: object parts (e.g. eyes, noses)
  - Z_3: whole objects (e.g. faces)
- Multi-layer, or deep, neural networks are one approach, that has become very successful.

- Deep learning methods have become very successful in recent years due to a combination of increased computing power and algorithm improvements.
- Some key algorithm developments include:
  - Use of *stochastic gradient descent* for optimization.
  - Backpropagation for efficient gradient evaluation.
  - Using the piece-wise linear *Rectified Linear Unit (ReLU)* activation function
$$\mathrm{ReLU}(x) = \begin{cases} x & \text{if } x \geq 0 \\ 0 & \text{otherwise.} \end{cases}$$
  - Specialized structures, such as convolutional and recurrent neural networks.
  - Use of dropout, regularization, and early stopping to avoid over-fitting.

Stochastic Gradient Descent

- *Gradient descent* for minimizing a function f tries to improve a current guess by taking a step in the direction of the negative gradient:

$$x' = x - \eta \nabla f(x)$$

- The step size η is sometimes called the *learning rate*.
- In one dimension the best step size near the minimum is $1/f''(x)$.
- A step size that is too small converges to slowly; a step size too large may not converge at all.
- Line search is possible but may be expensive.
- Using a fixed step size, with monitoring to avoid divergence, or using a slowly decreasing step size are common choices.
- For a DNN the function to be minimized with respect to parameters A is typically of the form

$$\sum_{i=1}^{n} L_i(y_i, x_i, A)$$

  for large n.
- Computing function and gradient values for all n training cases can be very costly.
- *Stochastic gradient descent* at each step chooses a random *minibatch* of B of the training cases and computes a new step based on the loss function for the minibatch.
- The minibatch size can be as small as $B = 1$.
- Stochastic gradient descent optimizations are usually divided into *epochs*, with each epoch expected to use each training case once.

Backpropagation

- Derivatives of the objective function are computed by the chain rule.
- This is done most efficiently by working backwards; this corresponds to the *reverse mode* of automatic differentiation.
- A DNN with two hidden layers can be represented as

$$F(x;A) = G(A_3 H_2(A_2 H_1(A_1 x)))$$

  If G is elementwise the identity, and the H_i are elementwise ReLU, then this is a piece-wise linear function of x.

- The computation of $w = F(x;A)$ can be broken down into intermediate steps as

$$\begin{aligned} t_1 &= A_1 x & z_1 &= H_1(t_1) \\ t_2 &= A_2 z_1 & z_2 &= H_2(t_2) \\ t_3 &= A_3 z_2 & w &= G(t_3) \end{aligned}$$

- The gradient components are then computed as

$$\begin{aligned} B_3 &= \nabla G(t_3) & \frac{\partial w}{\partial A_3} &= \nabla G(t_3) z_2 = B_3 z_2 \\ B_2 &= B_3 A_3 \nabla H_2(t_2) & \frac{\partial w}{\partial A_2} &= \nabla G(t_3) A_3 \nabla H_2(t_2) z_1 = B_2 z_1 \\ B_1 &= B_2 A_2 \nabla H_1 x & \frac{\partial w}{\partial A_1} &= \nabla G(t_3) A_3 \nabla H_2(t_2) A_2 \nabla H_1(t_1) x = B_1 x \end{aligned}$$

- For ReLU activations the elements of $\nabla H_i(t_i)$ will be 0 or 1.
- For n parameters the computation will typically be of order $O(n)$.
- Many of the computations can be effectively parallelized.

Convolutional and Recurrent Neural Networks

- In image processing features (pixel intensities) have a neighborhood structure.
- A convolutional neural network uses one or more hidden layers that are:
  - only locally connected;
  - use the same parameters at each location.
- A simple convolution layer might use a pixel and each of its 4 neighbors with

  $$t = (a_1 R + a_2 L + a_3 U + a_4 D) z$$

  where, e.g.

  $$R_{ij} = \begin{cases} 1 & \text{if pixel } i \text{ is immediately to the right of pixel } j \\ 0 & \text{otherwise.} \end{cases}$$

- With only a small nunber of parameters per layer it is feasible to add tens of layers.
- Similarly, a recurrent neural network can be designed to handle temporal dependencies for time series or speech recognition.

Avoiding Over-Fitting

- Both L_1 and L_2 regularization are used.
- Another strategy is *dropout*:
  - In each epoch keep a node with probability p and drop with probability $1 - p$.
  - In the final fit multiply each node's output by p.

  This simulates an ensemble method fitting many networks, but costs much less.
- Random starts are an important component of fitting networks.
- Stopping early, combined with random starts and randomness from stochastic gradient descent, is also thought to be an effective regularization.
- Cross-validation during training can be used to determine when to stop.

Notes and References

- Deep learning methods have been very successful in a number of areas, such as:
  - Image classification and face recognition. *AlexNet* is a very successful image classifier.
  - *Google Translate* is now based on a deep neural network approach.
  - Speech recognition.
  - Playing Go and chess.
- Being able to effectively handle large data sets is an important consideration in this research.
- Highly parallel GPU based and distributed architectures are often needed.
- Some issues:
  - Very large training data sets are often needed.
  - In high dimensional problems having a high signal to noise ratio seems to be needed.
  - Models can be very brittle – small data perturbations can lead to very wrong results.
  - Biases in data will lead to biases in predictions. A probably harmless example deals with evaluating selfies in social media; there are much more serious examples.
- Some R packages for deep learning include `darch`, `deepnet`, `deepr`, `domino`, `h2o`, `keras`.
- Some references:
  - A nice introduction was provided by Thomas Lumley in a 2019 Ihaka Lecture
  - deeplearning.net web site
  - Li Deng and Dong Yu (2014), *Deep Learning: Methods and Applications*
  - Charu Aggarwal (2018), *Neural Networks and Deep Learning*.

  - A Primer on Deep Learning
  - A blog post on deep learning software in R.
  - A nice simulator.

Some examples are available in

```
http://www.stat.uiowa.edu/~luke/classes/STAT7400/
                examples/keras.Rmd
```

Mixture of Experts

- Mixture models for prediction of y based on fearures x produce predictive distributions of the form

$$f(y|x) = \sum_{i=1}^{M} f_i(y|x)\pi_i$$

  with f_i depending on parameters that need to be learned from training data.

- A generalization allows the mixing probabilities to depend on the features:

$$f(y|x) = \sum_{i=1}^{M} f_i(y|x)\pi_i(x)$$

  with f_i and π_i depending on parameters that need to be learned.

- The f_i are referred to as *experts*, with different experts being better informed about different ranges of x values, and f this is called a *mixture of experts*.

- Tree models can be viewed as a special case of a mixture of experts with $\pi_i(x) \in \{0,1\}$.

- The mixtures π_i can themselves be modeled as a mixture of experts. This is the *hierarchical mixture of experts* (HME) model.