CQS Summer Institute: Machine Learning in Data Science

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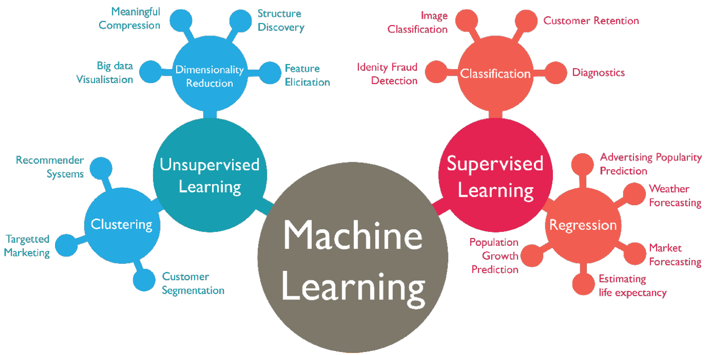
August 5, 2019

Course Overview

- Syllabus and R code:
- https://github.com/biostatmatt/cqs-ml-stat-r
- Monday: Intro and Data Management
- Tuesday: Supervised Learning Part 1
- Wednesday: Supervised Learning Part 2
- Thursday: Supervised Learning Part 3
- Friday: Unsupervised Learning

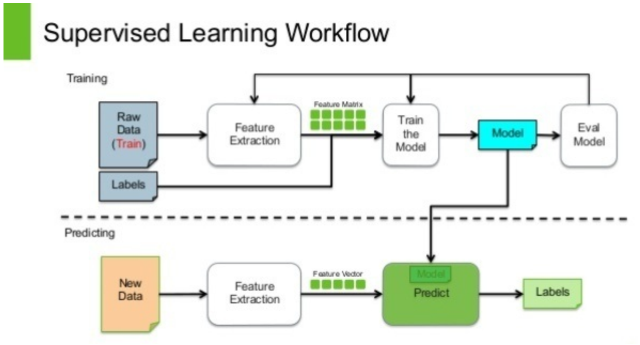
Machine learning



source: https://www.wordstream.com/blog/ws/2017/07/28/machine-learning-applications

Supervised learning

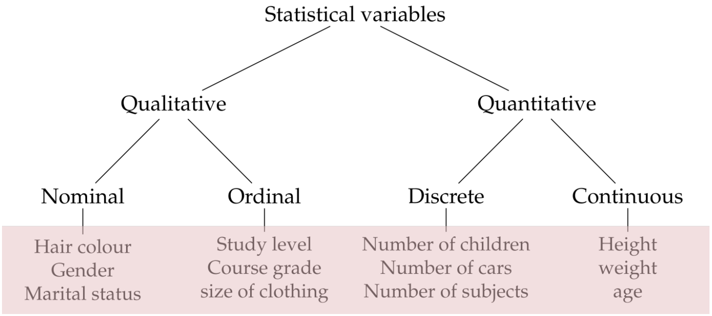
- Have input ('features') AND output ('target')
- Create a model ('learner') using observed inputs and outputs
- Goal is to predict outputs from new inputs
- "Supervised" because both inputs *and outputs* to guide model



source: https://www.quora.com/What-is-pattern-recognition

Definitions: variable types

- quantitative - e.g. blood pressure
- qualitative - e.g. gender, a.k.a. categorical, discrete, factor, numeric codes for qualitative variables called 'targets'
- ordered - e.g. numerical pain scale (0-10)



source: http://aprendeconalf.es/statistics/manual/introduction.html

Definitions: supervised learning tasks

- regression - model to predict quantitative output
- classification - model to predict qualitative output
- regression or classification - ordered output

Definitions: notation

- inputs - X

$$X = \begin{bmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{bmatrix}$$

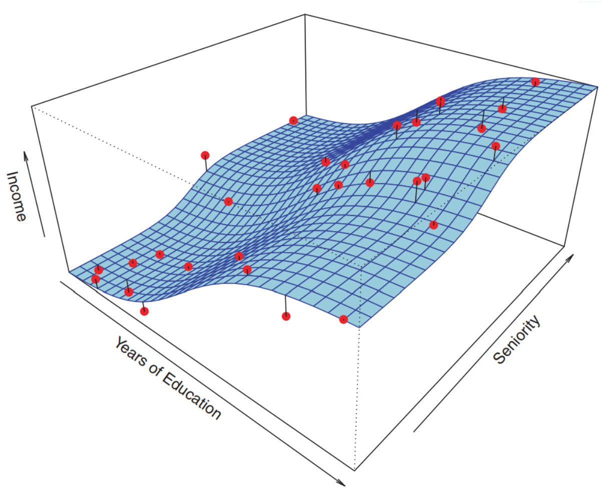
- quantitative outputs - Y

$$Y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

- qualitative outputs - G
- transpose - X^T
- prediction - $\hat{Y}$

Regression

- Find function f to predict Y: $\hat{Y} = \hat{f}(X)$



source: ISLR Fig. 2.3

Loss functions

- What makes a good predictor function f?
- To find f in $\hat{Y} = \hat{f}(X)$, need to specify a **loss function**. For regressoin we might use one of the following (different for classification):
- squared error loss: $(Y - f(X))^2$
- absolute error loss: $|Y - f(X)|$
- Then find f to minimize average loss in the training data:
- Least squared errors: minimize $1/n \sum_{i=1}^{n} (y_i - f(x_i))^2$
- Least absolute errors: minimize $1/n \sum_{i=1}^{n} |y_i - f(x_i)|$
- Also need to select a class of models $f(X)$:
- linear models:
$$f(X) = X\beta$$
- k-nearest neighbor:
$$f(X) = \sum_r I(X \in H_r^k) c_r$$
predictor is constant within each k-NN neighboorgood H_r^k

Model classes

- Once we have specified a loss function, we also need to select a class of models $f(X)$, e.g.:
- linear models:

$$f(X) = X\beta$$

- k-nearest neighbor:

$$f(X) = \sum_r I(X \in H_r^k) c_r$$

predictor is constant within each k-NN neighboorgood H_r^k

Linear least squared error regression (LS)

- LS uses linear models with squared error loss
- predict Y given X (possibly multiple dimensions of input) as follows:
$$\hat{Y} = \hat{f}(X) = X\hat{\beta}$$
where $\hat{\beta}$ (vector of same dimension as X) is the value that minimizes the sum of squared errors in the training data:
$$1/n\sum_{i=1}^{n}(y_i - x_i\beta)^2$$
- The R function 'lm' will estimate β in this way

k-nearest neighbor regression (kNN)

- kNN predictor is constant for each NN region and uses squared error loss
- Can show that average loss is minimized with we predict $\hat{Y}$ by averaging the Y values of the k nearest neighbors to X:

$$\hat{Y}(X) = \frac{1}{k} \sum_{x_i \in N_k(X)} y_i$$

- $N_k(X)$ is set of k points nearest X, as determined by a distance metric, e.g., the Euclidean distance:

$$d(X, X') = \sqrt{(X - X')^T (X - X')}$$

- k parameter is a 'smoothing parameter' or 'tuning parameter'
- 'caret::knnreg' implements kNN regression with Euclidean dist.

LS vs. NN method: flexibility, bias-variance

- LS is a parametric method; limited flexibility
- NN is a semiparametric method; very flexible, tunable using k
- LS cannot automatically discover complex associations
- NN can automatically discover complex associations (given enough data)
- However, LS can be made more flexible by making the linear predictor more flexible (i.e., doing "model selection", using 1) more predictors, 2) predictor interactions, and 3) nonlinear transformations of predictors (e.g., splines)
- more flexibility results in less bias, more variance in estimator

R Code for LS and kNN
`ls-and-knn.R`

Binary classification example

- G - qualitative (binary) outcome (orange, blue)
- Y - "target" encoding of G (orange - 1, blue - 0)
- X_1 - quantitative predictor
- X_2 - quantitative predictor
- can do LS or kNN with Y as outcome
- Think of $\hat{Y}$ as the probability of a '1' outcome

Classification loss function

- Loss functions look different for classification, e.g.,
- zero-one loss: loss is zero if prediction is correct, 1 otherwise
- by minimizing the average zero-one loss, we arrive at the following classification rule
- classification rule: $\hat{G} =$ the class with highest $\hat{Y}$

Linear classification

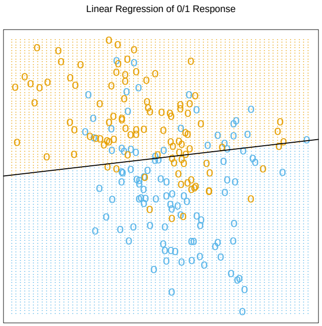


FIGURE 2.1. *A classification example in two dimensions. The classes are coded as a binary variable (*BLUE $= 0$, ORANGE $= 1$*), and then fit by linear regression. The line is the decision boundary defined by* $x^T\hat{\beta} = 0.5$*. The orange shaded region denotes that part of input space classified as* ORANGE*, while the blue region is classified as* BLUE.

k-nearest neighbor classification

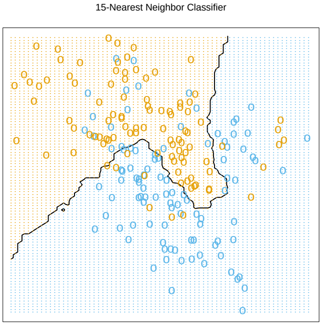


FIGURE 2.2. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable* (BLUE $= 0$, ORANGE $= 1$) *and then fit by* 15*-nearest-neighbor averaging as in (2.8). The predicted class is hence chosen by majority vote amongst the* 15*-nearest neighbors.*

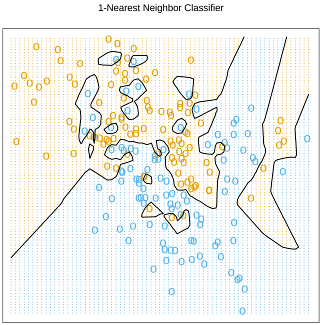


FIGURE 2.3. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable* (`BLUE` $= 0$, `ORANGE` $= 1$)*, and then predicted by* 1*-nearest-neighbor classification.*

Evaluating the model and ‘optimism’

- Need a mechanism to evaluate predictive quality of model and thus tune the model.
- The **prediction error** of a model is evaluated using the same average loss function used for estimation (e.g., mean of squared errors: $1/n \sum_{i=1}^{n}(y_i - x_i\beta)^2$). However, this can be an *optimistic* estimate if computed using the training data.
- The **training prediction error** is computed on the training data
- The **test prediction error** is computed on new data
- The **optimism** is the difference in training and test error
- Training error is optimistic, especially when the model is overfitted. It should not be used to select tuning parameters: for k-NN, $k = 1$ results in zero training error; the model is “overfitted”
- Need an estimate of test error to select tuning parameters

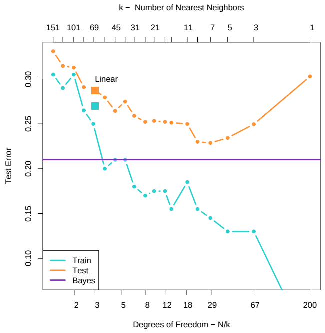


FIGURE 2.4. *Misclassification curves for the simulation example used in Figures 2.1, 2.2 and 2.3. A single training sample of size* 200 *was used, and a test sample of size* 10, 000*. The orange curves are test and the blue are training error for k-nearest-neighbor classification. The results for linear regression are the bigger orange and blue squares at three degrees of freedom. The purple line is the optimal Bayes error rate.*

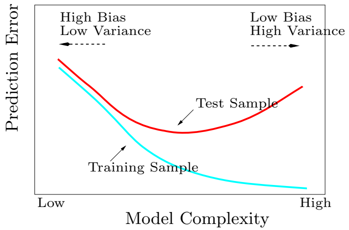


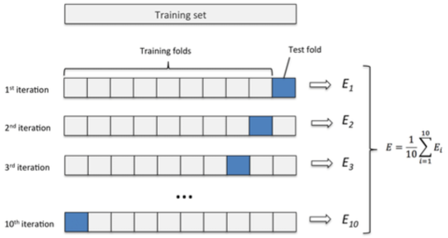
FIGURE 2.11. *Test and training error as a function of model complexity.*

Estimating test error: testing/training split

- Split data into training and testing data
- Use training data to build models
- Use testing data to evaluate models
- Simple, but not most efficient use of data

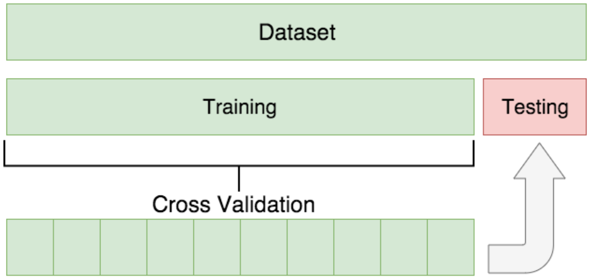
Estimating test error: k-fold cross validation

- Split training data into k subsets or ‘folds’
- Use k-1 subsets to build model
- Use holdout subset to evaluate model
- Repeat for all k permutations
- Results in k estimates of test error; use mean and sd
- More complicated, but also more efficient use of data



Estimating test error: combined CV and train/test

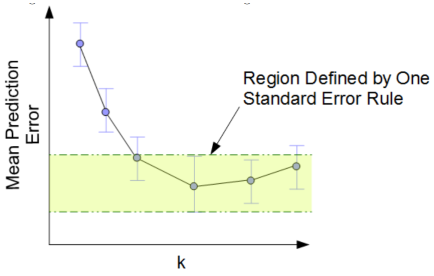
Supervised learning workflow can involves both train/test and CV:



Many model-building functions do cross-validation automatically.

Estimating test error: k-fold CV one-SD rule

- k-fold CV generates k estimates
- Can use their SD to gauge uncertainty
- When tuning a model, use the one-SD rule for parsimony
- Select least complex model whose CV error is within one SD of the best model



source: https://www.cs.cmu.edu/~psarkar/sds383c_16/lecture9_scribe.pdf

R Code for kNN 5-fold CV: `ls-and-knn.R`

Classification and regression trees (CART)

- trees partition feature space into a set of rectangles
- fit simple model in each partition (e.g., constant)
- for regression, mean within each partition
- for binary classification, compute probability within each partition
- trees are flexible like kNN, can automatically discover complexity

- top-left: partitions can't be described by tree
- top-right: partitions are recursive, can be described by tree
- bottom-left: tree describing top-right partitions
- bottom-right: regression surface for top-right partitions
- trees have (root, internal, and terminal) nodes and branches
- terminal nodes also called leaf node

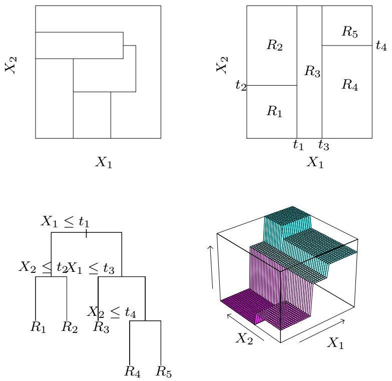


FIGURE 9.2. *Partitions and CART. Top right panel shows a partition of a two-dimensional feature space by recursive binary splitting, as used in CART, applied to some fake data. Top left panel shows a general partition that cannot be obtained from recursive binary splitting. Bottom left panel shows the tree corresponding to the partition in the top right panel, and a perspective plot of the prediction surface appears in the bottom right panel.*

Tree-growing and tuning parameter

- step 1. find optimal split (consider all possible splits on all variables)
- step 2. within each resulting partition find next optimal split
- repeat steps 1 and 2 until stopping criterion met (e.g., maximum complexity)
- tree complexity (e.g., number of branches) is a tuning parameter
- one approach: grow a large tree, stopping only when minimum node size (i.e., minimum number of $x_i \in R_m$) is reached, then "prune" tree back using a "cost-complexity" criterion

Pros and cons of (single) trees

Pros:

- interpretable (nice tree structure)
- flexible
- easily handle quant. and qual. data
- simple to implement

Cons:

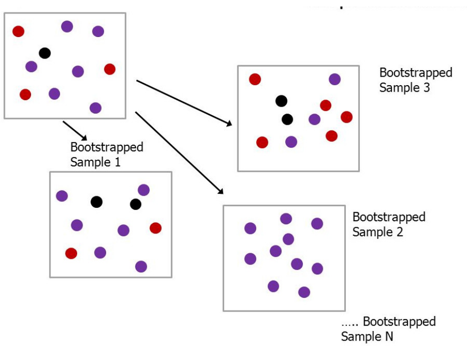
- instability; sample variability in tree structure
- lack of smoothness of prediction surface in feature space
- categorical features difficult to split

R Code for CART: ‘rpart’: `rpart-randomForest.R`

Random Forests

- Random forests fits many trees to the same dataset and aggregates predictions across trees. Each tree is fit to a slightly modified version of the dataset, which is generated by resampling (bootstrap). This is generically called ‘bagging’ or ‘bootstrap aggregation’.
- regression: average predictions across trees
- classification: avarage probs. or “committee vote”
- reduces variance of estimated predictor

Resampling (bootstrap)



source: https://slideplayer.com/slide/8340508/

Random Forests

- resamples share some information
- predictions from trees are correlated
- weakens the “wisdom of crowds”
- random forests uses a special technique to *de-correlate* trees

Random Forests

- in bagging, trees are identically distributed (i.d.)
- $\rightarrow$ bias of bagged trees is same as individual tree
- $\rightarrow$ can only hope to improve variance

Random Forests

- variance of the average of B i.d. random variables with variance σ^2 and pairwise correlation ρ:

$$\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2$$

- as B grows, second term vanishes
- can only reduce first term by reducing ρ
- random forests: reduce ρ without increasing σ^2 too much

Random Forests

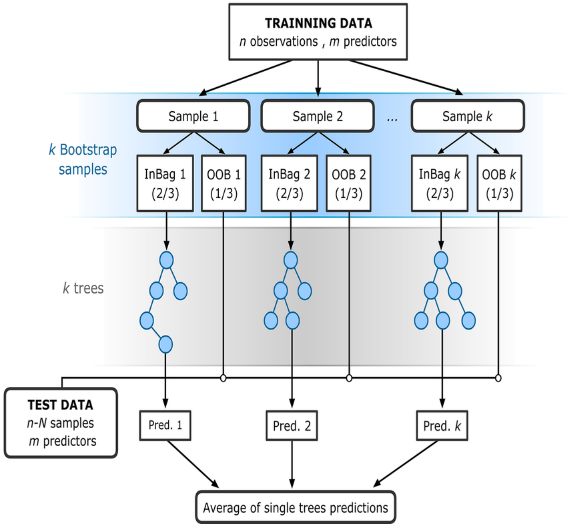
- random forests modifies the tree-growing procedure
- before each split, select $m \leq p$ input variables at random as candidates for splitting
- typically $m = \lfloor \sqrt{p} \rfloor$ for regression
- typically $m = \lfloor p/3 \rfloor$ for classification
- random forest predictor after B trees grown is

$$\hat{f}_{\mathrm{rf}}^{B}(x) = \frac{1}{B} \sum_{b=1}^{B} T(x; \Theta_b)$$

Random Forests: built-in model evaluation

- before each tree grown, resample is split into training (in bag) and testing (out of bag; OOB); built-in CV

Random forest



source: Rodriguez-Galiano et al. (2016). Biogeosciences. 13. 3305-3317

Pros and cons of random forest

Pros:

- more stable (less variance) than single trees
- better predictive performance
- flexible
- easily handle quant. and qual. data

Cons:

- more complex to implement
- less interpretable (cannot represent as tree)
- lack of smoothness of prediction surface in feature space
- categorical features difficult to split

R Code for random forest: ‘randomForest’