Chapters 1 & 2. Introduction & Overview

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Big Data

- *Big Data is on the rise, bringing big questions* (WSJ, 11-29-2012)
  just try a Google search on "Big Data"
- *Big data: the next frontier for innovation, competition, and productivity* (McKinsey report 05-2011)
  from a business perspective, that an enterprise mine all the data it collects right across its operations to unlock golden nuggets of business intelligence (WSJ, 04-29-2012).
- *Big Data's big problem: little talent* (WSJ, 04-29-2012)
  "though bits of it do exist in various university departments and businesses, as an integrated discipline it is only just starting to emerge".
- Recent NSF, NIH Big Data initiatives; NIH PMI.
  2014 NIH Big Data RFA: needs CS, Stat/Math, bio.
- Projects/platforms: CancerLinQ; IBM Watson (Health) ...

- How is this related to statistics?
- Change and expand the subjects
  Many unhappy with the current culture (Breiman, Hand, ...);
  "Data Science" (Cleveland 2001/2014; Yu 2014);
  Computing: Hadoop (or RHadoop), MapReduce, Spark, ...
- You do not need to do everything ...
  DeltaRho (formerly, Tessera): interface b/w R and Hadoop...
  `http://deltarho.org/`
  R packages `datadr`, `trelliscope`
  Based on "Divide and Recombine" (D&R) (Guha et al 2012).
- So ...still need to go back to the basics of ...!

Introduction

- Focus: prediction or discovery.
  Approach: build a model $\hat{f}(x)$.
- Types: supervised vs unsupervised vs semi-supervised learning.
  Training data: with vs without known response values vs a mixture of both.
- Supervised learning: classification vs regression.
  Training data: (Y_i, X_i)'s; Y_i is categorical (e.g. binary) vs quantitative.
  X_i: typically multivariate and mixed types.
  Tuning and test data: (Y_i, X_i)'s;
  Future use: only X_i's.

Examples

- Example 1. X_i^0: an email; $Y_i = 0$ or 1, indicating whether it is a junk email; $i = 1, ..., 4601$.
- Feature extraction: e.g. use some key words in emails as X_i.
- A classification problem: use a 0-1 loss, build a model $\hat{f}(x) \in \{0, 1\}$, calculate misclassification rate,...
- Loss function: here a false positive is much more costly than a false negative.

- Example 2. Predict prostate specific antigen (PSA) using some lab measurements.
- A regression problem.
- Example 3. Handwritten digit recognition.
- X_i^0: a 16 by 16 black/white image ($=$ a 16 by 16 binary matrix); $Y_i \in \{1, 2, ..., 9\}$.
- X_i: maybe (vectorized) X_i^0, or better its summary stat's, e.g. marginal histograms or numbers of "crossing changes" ...

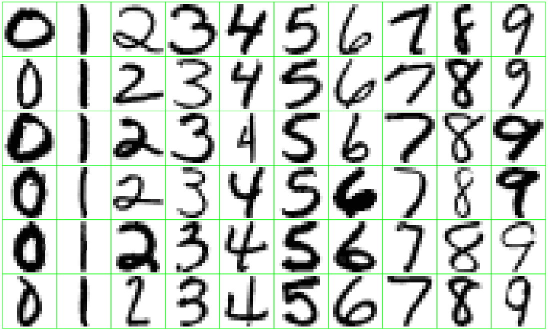
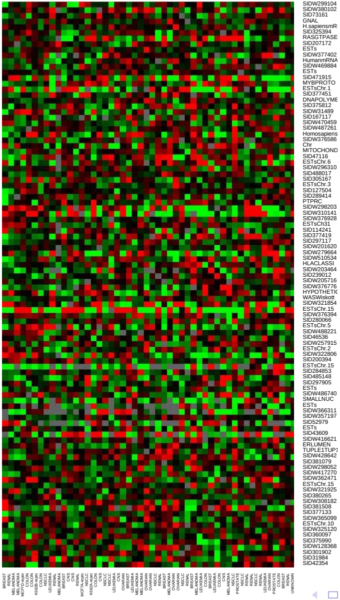


FIGURE 1.2. *Examples of handwritten digits from U.S. postal envelopes.*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SIDW376586
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MITOCHOND
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ESTsChr.6
SIDW296310
SID488017
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ESTsChr.3
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ESTsChr.5
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ESTsChr.2
SIDW322806
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ESTsChr.15
SID284853
SID485148
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SIDW486740
SMALLNUC
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SID381079
SIDW298052
SIDW417270
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- Example 4. Microarray gene expression data.
- X_i: 6830 genes' expression levels; quantitative;
  Y_i: tumor types.
- A typical "smalll n, large p" problem: $n = 64$ vs $p = 6830$.
- A classification problem.
- Can be an unsupervised learning problem: finding subtypes of cancer.
  only use X_i's to find new class labels Y_i^*; clustering analysis.
- Can be a semi-supervised learning problem: some known and possibly novel subtypes of cancer.

Overview

- Consider two popular, yet simple and extreme methods: LR vs NN;
  parametric vs non-parametric.
- Q: Is a non-parametric method better than a parametric one? or reverse?
- Consider simulated data: (Y_i, X_i), $Y_i = 0$ or 1 and X_i bivariate; 100 obs's in each class (as training data).
- LR: $E(Y_i|X_i) = Pr(Y_i = 1|X_i) = \beta_0 + X_i'\beta$;
  Use LS to estimate β's $\Longrightarrow \hat{Y}_i = \widehat{Pr}(Y_i = 1|X_i)$;
  $\tilde{Y}_i = I(\hat{Y}_i \geq 0.5)$.
- Decision boundary: $\hat{Y}(x) = \hat{\beta}_0 + x'\hat{\beta} = 0.5$, linear.

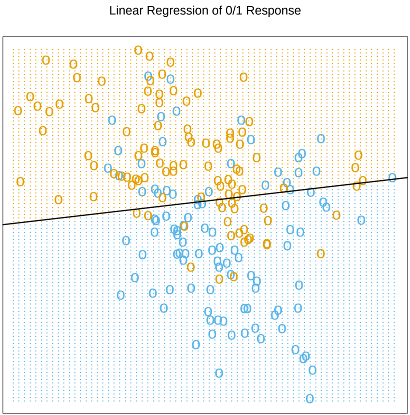

FIGURE 2.1. *A classification example in two dimensions. The classes are coded as a binary variable (BLUE = 0, ORANGE = 1), and then fit by linear regression. The line is the decision boundary defined by* $x^T\hat{\beta} = 0.5$. *The ...*

- kNN: $N_{k(x)}$ is the k nearest training data points that are closest to x,

$$\hat{Y}(x) = \frac{1}{k} \sum_{X_i \in N_k(x)} Y_i = \widehat{Pr}(Y_i = 1 | X_i).$$

- Idea: using local "smoothness" to estimate the population mean by ...
- Key: choice of k, or how much "smoothness" is to be assumed; do not know!
  Modeling assumption: larger k, higher or lower model complexity?
- Try a few values of k, then ...

15-Nearest Neighbor Classifier

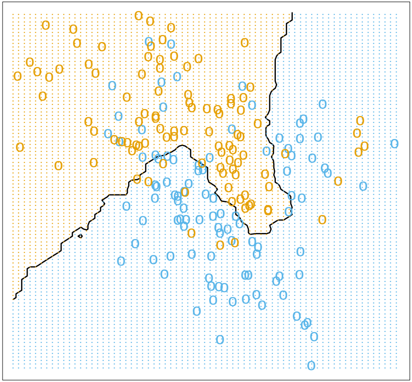

FIGURE 2.2. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable* (BLUE $= 0$, ORANGE $= 1$) *and then fit by 15-nearest-neighbor averaging as in (2.8). The pre-*

1-Nearest Neighbor Classifier

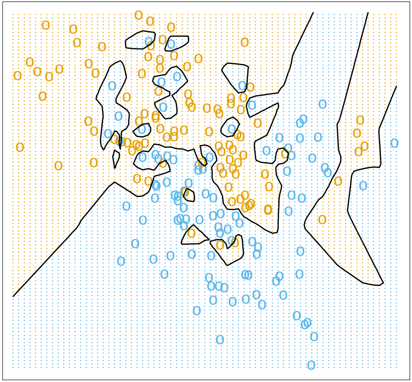

FIGURE 2.3. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable (*BLUE *= 0,* ORANGE *= 1), and then*

- Key Q: which kNN (and LR) to use?
- Key: cannot use the training data to compare models!
  Why not? too optimistic, favoring ...
  Recall: how to estimate the noise variance in linear regression?
- How? use a separate test dataset, or CV, or some model selection criterion (if any).
  Key: test data should **not** be used in model building!
  Q: how about AIC, BIC ,...
- Previous example: *generate a new test dataset* with $n = 10,000$.

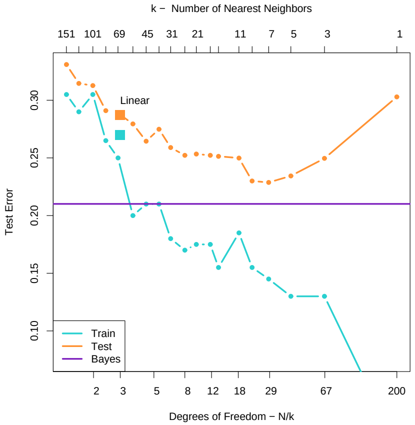

FIGURE 2.4. *Misclassification curves for the simulation example used in Figures 2.1, 2.2 and 2.3. A single training sample of size* 200 *was used, and a test sample of size* 10,000*. The orange curves are test and the blue*

- Q: is there a best classifier?
- Ideal situation: if we know the data distribution, then use the Bayes rule:

$$k_0 = \arg\max_k Pr(k|x).$$

- An example: 1) prior $\pi_k = Pr(k)$; 2) PDF of class k, $f_k(x) = f(x|k)$, then

$$Pr(k|x) = \frac{\pi_k f_k(x)}{\sum_i \pi_i f_i(x)}.$$

  If f_k is assumed to be Normal, then LDA or QDA.
  LR and kNN are also estimating $Pr(k|x)$.
- Bayes rule: offering a theoretical lower bound of the test error rate; often unknown.
- Previous example: R code example 2.1.

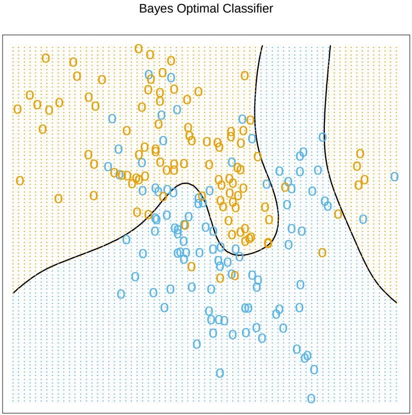

FIGURE 2.5. *The optimal Bayes decision boundary for the simulation example of Figures 2.1, 2.2 and 2.3. Since the generating density is known for each class, this boundary can be calculated exactly (Exercise 2.2).*

- Q: for real data, often cannot generate new data; how to evaluate models?
- Use sample splitting: divide the original whole dataset into two parts, (e.g. 1/2 or 2/3) for training and (the remaining) for test.
  efficient?
- Use cross-validation (CV); read §7.10
- K-fold CV: Divide the data D into almost equally sized and none-overlapping $D_1,...,D_K$, then

$$\text{CVerr} = \sum_{j=1}^{K} \sum_{(Y_i,X_i)\in D_j} L[Y_i, \hat{f}(X_i|D - D_j)]/n.$$

- Leave-One-Out-CV (LOOCV): $K = n$.
- Remarks: 1) not necessarily larger K, the better; CV related to AIC/BIC; 2) maybe better to use bootstrap (§7.11).
- Previous example: R code example 2.1.

- Key: celebrated bias-variance trade-off!
- Suppose $\hat{f}$ is any estimate of f,

$$\begin{aligned} MSE &= E[(\hat{f} - f)^2] = E[(\hat{f} - E(\hat{f}) + E(\hat{f}) - f)^2] \\ &= E[(\hat{f} - E(\hat{f})^2] + E[E(\hat{f}) - f)^2] \\ &= \text{Var} + \text{Bias}^2. \end{aligned}$$

- Very very useful: helps explain
  i) Complex models vs simple models;
  ii) Nonparametrics vs parametrics; ...
- Perhaps the most important plot in the course:

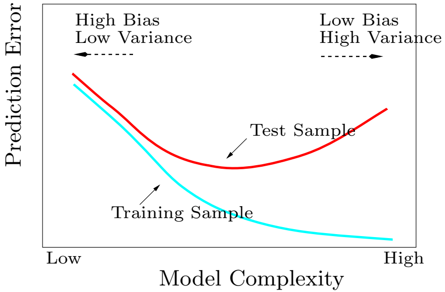

FIGURE 2.11. *Test and training error as a function of model complexity.*