1 Introduction

1.1 Syllabus

Course goals: Understand the models, intuition, statistical underpinnings, strengths and weaknesses, assumptions and trade-offs of various machine learning approaches. Can run R/Python to analyze data. Technical details such as optimization algorithms and theoretical properties are not of primary interest.

Books, participation, homework, exams, etc.

ISLR	http://www-bcf.usc.edu/~gareth/ISL/
DLwR	https://www.safaribooksonline.com/library/view/deep-learning-with/9781617295546/
HOML	http://proquest.safaribooksonline.com/9781491962282?uicode=ohlink
NNDL	http://neuralnetworksanddeeplearning.com/
ESL	http://www.stanford.edu/~hastie/ElemStatLearn/
CASI	https://web.stanford.edu/~hastie/CASI/
DL	http://www.deeplearningbook.org/
MMDS	http://www.mmds.org/
R4DS	http://r4ds.had.co.nz

Prerequisites: Calculus, linear algebra, and some exposure to statistics (minimum EPBI/PQHS 431). Familiarity with matrices (such as explained in ISLR Chapter 1; DL Chapter 2).

Languages/environments: R, Python, git/GitHub (highly recommended), Linux (recommended)

IDEs: RStudio (https://www.rstudio.com/) (recommended), spyder (comes with Anaconda)

Useful websites: https://www.r-bloggers.com/, https://www.kaggle.com/

1.2 Overview of Data Science

Overlapping fields:

- Statistics: Supposedly synonymous to "data science". It covers all aspects of data-oriented activities: data collection, analysis, and interpretation. Historically it has focused on inference, including parameter estimation, hypothesis testing, and decision making. It studies function estimation (aka prediction) from the perspective of smoothing instead of prediction accuracy. Historically the field was confined to small datasets and limited by lack of computing power, and has thus developed certain tastes in its approaches: It prefers interpretable models and probabilistic thinking. These have made the field shy away from prediction-oriented tasks, algorithmic approaches, and analyses of large messy data.
- Computer Science:
  - Machine learning: Similar to Statistics, often using more colorful language. Supervised learning heavily focuses on prediction. ML methods are often algorithmic rather than probabilistic.
  - Data mining: Detection of unknown relationships in large data, sometimes with the help of visualization. In Statistics, it is called exploratory data analysis (EDA), a notion introduced in the era of small data. DM problems are often less well defined than those in ML.
  - Artificial intelligence: Has much broader goals than data-oriented tasks. Modern "AI" successes are due to large training datasets and advances in computation. But the successes are task-specific and the algorithms learn in a cumbersome way, unlike humans.
- Other names: Biostatistics, Statistical learning, Pattern recognition, Predictive/data analytics, Business intelligence, etc.

$$\text{Data science} = \text{Statistics/ML/DM} + \text{algorithms on big data}$$

Related fields:

- Mathematical optimization
- Informatics: Focused on data capture/retrieval, feature retrieval
- Natural language processing

Big data: Volume, Velocity and Variety. (data vs. information vs. knowledge)

1.3 R Packages and Datasets

Package installation: One can install R packges from CRAN using the R function `install.packages()`. For example, to install the ISLR package, use `install.packages("ISLR")`. The default directory for package installation is the first element of `.libPaths()`.

If a package had been installed in the past, you may want to check its version to see if it is up to date.

```
packageVersion("ISLR")  ## installed version for package "ISLR"; v1.2 (01/03/2018)
available.packages()["ISLR", "Version"]  ## latest version of "ISLR" on CRAN
packageDescription("ISLR")  ## description of package "ISLR"
```

`sessionInfo()` and `devtools::session_info()` give information about the current R session and loaded libraries.

```
library(ISLR)
sessionInfo()  ## check all relevant version information
devtools::session_info()  ## another version
```

The following libraries are used in the R Labs of ISLR. A simple way to install/update all these packages is:

```
install.packages(c("ISLR", "MASS", "ROCR", "akima", "boot", "car",
                   "class", "e1071" , "gam", "gbm", "glmnet", "leaps",
                   "pls", "randomForest", "tree"))
```

Note that the `tree` package is not as useful as the `rpart` package. A few other packages (e.g., `caret`, `xgboost`) will be used in class demonstration. You can install them when you need them.

Loading a library: use `library()` or `require()`. To unload a package, use `detach()`. By default, `library()` and `require()` search the `.libPaths()` to find the named package to load. Note that `library()` without any argument will list all installed R packages.

```
library(ISLR)
search()  ## show search path
ls("package:ISLR")  ## list all objects in package ISLR (see Table 1.1 of the ISLR book)
```

Although objects in a library can be accessed without loading the library (by using `::`; e.g., `ISLR::Wage`), loading a library makes it a lot more convenient.

In addition to the datasets in the ISLR package, the book ISLR also uses these datasets: `Boston` in the `MASS` library, `USArrests` in base R, and `Advertising`, `Heart`, `Income1`, and `Income2` in .csv format from the book website. Some datasets are simulated: `Carseats`, `Credit`, `Default`, `Portfolio`, `Income1`, and `Income2`.

Exploring and using a dataset: Most datasets should have class `data.frame`. A data frame may look like a `matrix`, but it is a `list` in which an element is a vector for a variable. Using the `Wage` dataset as an example:

```
?Wage  ## same as help(Wage); show its documentation
names(Wage); dim(Wage)  ## variable names and dataset dimensions
str(Wage)   ## show variable structures
head(Wage)  ## show the first few observations
```

To access variables in a data frame, use `$` or `with()` for a single command, and `attach()` for multiple commands.

```
levels(Wage$education)
plot(Wage$age, Wage$wage)
with(Wage, plot(age, wage))  ## same plot; ensures all variables are from the same dataset
```

Below is an example of using `attach()` when drawing Figure 1.1. Using `attach()` can lead to confusion and unexpected consequences. **Remember to `detach()`** at the end to avoid problems.

```
attach(Wage)  ## use search() to check

par(mfrow=c(1,3))  ## (also see ISLR Section 7.8)
plot(age, wage, xlab='Age', ylab='Wage', col='grey')  ## first panel
agegrid = seq(10,80,1)
lines(agegrid, predict(loess(wage ~ age), agegrid), col="blue", lwd=3)

plot(year, wage, xlab='Year', ylab='Wage', col='grey')  ## second panel
abline(lm(wage ~ year), col = "blue", lwd=3)

plot(education, wage, xlab='Education Level', ylab='Wage', col=2:6, xaxt='n')  ## third panel
axis(1, at=1:5, labels=1:5)

detach()  ## use search() to check
```

Functions: To learn the syntax and arguments of a function, use `?` (e.g., `?plot`). `?` is a shortcut for `help()`.

1.4 Python Installation, .ipynb/.py Files, Modules, and DataFrame

Anaconda: HOML requires python, various packages (e.g., numpy, scipy, pandas, scikit-learn), matplotlib, and Jupyter notebook (for running the book's code). The easiest way to install all these packages is to install Anaconda. I recommend installing Anaconda version 3.x (not 2.x).

HOML python code: Can be downloaded with `git clone https://github.com/ageron/handson-ml`.

.ipynb files are in the JSON format. Jupyter can open them.

On Linux, to open a .ipynb file, use `jupyter notebook [file.ipynb]`; to close it, use Ctrl-C in the same terminal. Jupyter's autosave feature can be annoying. To turn it off, edit file `~/.jupyter/custom/custom.js` to contain:

```
require(['base/js/namespace', 'base/js/events'], function (IPython, events) {
  events.on("notebook_loaded.Notebook", function () {
    IPython.notebook.minimum_autosave_interval = 0; // disable autosave
  });
});
```

Loading modules: `<from [module1]> import [module2] <as [alias]>`. A package can contain many modules, which are organized as a tree. For example,

```
import sklearn
import numpy.random
import pandas as pd
from sklearn import pipeline
from sklearn import linear_model as linmod
from sklearn.base import BaseEstimator, TransformerMixin
```

Packages we often use: **numpy** and **scipy** for basic data manipulation; **pandas** for DataFrame; **sklearn** for machine learning methods; **matplotlib** for graphics. Datasets in Scikit-Learn are NumPy arrays or SciPy sparse matrices.

DataFrame: A pandas dataset is called a DataFrame. Pandas focuses on tabular data structures, and when doing the operations (e.g., addition, subtraction, etc.) it looks at the indices (row names), not positions. For example,

```
df = pd.DataFrame(np.random.randn(5, 3), index=list('abcde'), columns=list('xyz'))
df[1:]/df[:-1]  ## a little unexpected results
df[1:]/df[:-1].values  ## .values makes it a numpy array, and the results are like in R
```

Below is a cross reference of some basic operations between Python and R:

pandas DF	R DF	pandas DF	R DF	pandas Series	R vector
df.head()	head(df)	len(df)	nrow(df)	s.value_counts()	table(s)
df.info	str(df)	list(df)	names(df)		
df.describe()	summary(df)				
df.shape	dim(df)				
df.index	rownames(df)				
df.columns	names(df)				
df.sort()	df[order()]				

1.5 Keras installation

Keras provides an easy front-end for multiple DL libraries including TensorFlow, Theano, CNTK, and PlaidML. It is available in both python and R (https://keras.rstudio.com/). The installation of the R version has two steps:

```
install.packages("keras")  ## install a few necessary R packages first
keras::install_keras("conda")  ## install necessary conda/tensorflow packages outside R
```

In Windows, Anaconda 3.x is required for keras installation (see 1.1.5 above). `install_keras("conda")` first installs a few necessary conda packages, then creates a conda environment, and then installs TF packages into the new environment.

When Keras is loaded with `library(keras)`, by default the backend is “tensorflow” and the implementation is “keras”. Use `use_backend()` and `use_implementation()` to change them if needed. All backend API functions have a `k_` prefix.

1.6 Introduction of Git

This introduction is for CLI (command-line interface). **RStudio can act as a GUI front-end of git.**

An easy tutorial: http://product.hubspot.com/blog/git-and-github-tutorial-for-beginners
Broman’s tutorial: http://kbroman.org/github_tutorial/
Book *Pro Git*: https://git-scm.com/book/en/v2

Once a repository is set up, the most commonly used git commands are: `add`, `rm`, `status`, `commit`, `push`.

Create a local repository (repo), a working directory.

```
mkdir TestGit
cd TestGit
git init  ## initialize the repo (creating .git/ directory)
git status  ## check file status (of current branch)
## Now create some files under TestGit/
git status
```

Staging environment: Files can be tracked and untracked. To stage a file (i.e., add a file to the staging environment/index), use `git add`. To untrack a file, use `git rm`.

```
git add file1 file2
git status
```

Commit: A commit is a snapshot of a branch. Commits make up the essence of a project and allow you to go back to the state of a project at any commit. To create a commit, use `git commit`. The first commit creates a branch called `master`.

```
git commit -m "my 1st commit!"
git config --global user.name "Joe Smith"  ## info added to global configuration file ~/.gitconfig
rm -f ~/.gitconfig
git config user.name "Joe Smith"  ## info added to a local configuration file .git/config
```

```
git config user.email "me@abc.com"
git commit -m "my 1st commit!"
```

To check the history of all the commits, use

```
git log --oneline --decorate --graph --all
```

Branch: A good work habit is to create a branch to work on; once the work is done, merge the changes in the branch to the master. To create a branch, use `git branch [branchname]`. To switch to a branch, use `git checkout [branchname]`. To create a branch and switch to it, one can use a single command `git checkout -b [branchname]`. When a new branch is created without specifying a start point, its hash tag is the same as the current branch (info in `.git/HEAD`). Branch hash tags are in `.git/refs/heads/`.

```
git branch  ## check branch status; the current branch is starred
git checkout -b branch1  ##
git branch  ## check again
```

Now change some files. `git diff` is to go through the list of files in the current branch, compare the version in the working directory with the last staged version, not with the version in the last commit.

```
git add file2  ## create another file and then stage it
git diff
git status
git commit -m "my 2nd commit"  ## create a commit for the current branch
```

To merge the content from a branch to the current branch:

```
git checkout master
git status
git merge branch1  ## merge the content of branch1 into current branch, master
```

Note that switching to a branch triggers copying branch files to the working directory. To delete a local branch, use `git branch -d <branchname>`. To delete a remote branch, use `git push <remotename> --delete <branchname>`.

Github repository: Create a new, empty repository on github.com. Mine is called "FirstTest.git". Then on local machine, add a remote repo named `origin`. Information is added to `.git/config`. Version 1 below requires entering password for every push; Version 2 uses ssh key authentication to avoid this. To copy a branch to a remote repo, use `git push`. The hash tag for a branch of a remote repo is saved under `.git/refs/remotes/`. To copy a branch from a remote repo, use `git pull`, which is a `git fetch` followed by a `git merge`.

```
git remote add origin https://github.com/cxl791/FirstTest.git  ## ver 1
git remote remove origin
git remote add origin git@github.com:cxl791/FirstTest.git  ## ver 2
git remote -v  ## check remote repos
git push -u origin master
git push origin branch1

git pull origin master  ## copy the master branch from github.com to local repo
git log
git status
git checkout master
git pull
```

To clone a remote repository to your computer, use `git clone`. Make sure you are not in any repository when doing this. For example, to clone github user cxl791's repository PQHS471 (which is my repository for this course):

```
git clone https://github.com/cxl791/PQHS471
cd PQHS471
ls -a
```

`git clone` names the remote repo `origin` by default. All files in a cloned repository are staged and packed (info in `.git/objects/pack/`). One can also fork a repository first on github.com, and then clone it to your computer. For example, after I have forked user umutisik's repository Eigentechno on github.com, I can do

```
git clone git@github.com:cxl791/Eigentechno
cd Eigentechno
git remote add origin2 git://github.com/umutisik/Eigentechno
git pull origin2 master  ## Get the latest from the original source
git push origin master  ## Push changes to my repo on github.com
```

What not to commit: (1) No derived files. For a LaTeX manuscript, no .log, .dvi, .aux, etc. For R code to generate a figure, no figure file. (2) No binary files (.docx, .xlsx, etc). Git works best with text files (source code, text, markdown files) when there are merge conflicts. (3) Avoid very big files. Once a big file is committed, it take space and is hard to remove cleanly, even if you use `git rm` to remove it later. So, use `git commit -a` with caution.

Ignore file: Files you're not tracking can be indicated in an ignore file to avoid seeing them in the output of `git status`. A global ignore file can be created under home directory and set with command:

```
git config --global core.excludesfile ~/.gitignoreglobal
```

A repository can have its own ignore file `.git/info/exclude`. Every subdirectory can also have its own ignore file named `.gitignore`; the `.gitignore` file should be tracked. An example ignore file contains:

```
*~
.*~
.DS_Store
.Rhistory
.RData
```

SSH key authentication on github.com: Copy your key in `~/.ssh/id_rsa.pub`. Go to github.com, choose 'Settings', 'SSH keys', and then paste the key. To check if the key is added successfully, use `ssh -T git@github.com`. Details in http://kbroman.org/github_tutorial/pages/first_time.html

1.7 ISLR Chapter 1

Some R code examples:

```
#### Figure 1.2, Smarket data (also see ISLR Section 4.6)
?Smarket
str(Smarket)
head(Smarket)

## Fig 1.2 first panel
with(Smarket, plot(Direction, Lag1,
                   xlab="Today's Direction", ylab="Percentage change in S&P",
                   main='Yesterday', col=2:3))
```

```
#### Figure 1.4, NCI60 data (also see ISLR Section 10.6)
str(NCI60)
names(NCI60)
class(NCI60$data)
dim(NCI60$data)
NCI60$labs

## Fig 1.4 right panel (with different colors)
tmp = prcomp(NCI60$data, scale=T)
str(tmp)
pchcode = as.numeric(as.factor(NCI60$labs)) %% 4 + 20
pchcode[pchcode==22] = 24
pchcode[pchcode==20] = 22
```

```
colcode = as.numeric(as.factor(NCI60$labs)) %% 7+2
plot(tmp$x[,1], tmp$x[,2], pch=pchcode, col=colcode, bg=colcode)
```

1.8 Assignment

1. Matrix warm-up: ISLR Chapter 1; DL Chapter 2.
2. Install course relevant R packages; get familiar with RStudio.
3. R warm-up: ISLR Chapter 2 R Lab. (It shows 3 ways of plotting a function f(x,y): `contour()`, `image()`, `persp()`)
4. Warm-up reading: ISLR Chapter 1.
5. Reading for next lecture: ISLR Chapter 2; HOML Chapter 1.
6. Get familiar with git and python (not urgent).

2 Statistical learning in general

ISLR Chapter 2 provides an overview of some basic issues in data analysis methods, including the trade-off between flexibility and interpretability among existing methods, and the trade-off between bias and variance in both regression and classification problems.

2.1 ISLR 2.1

A general form of a supervised model is

$$Y = f(X) + \epsilon, \tag{2.1}$$

where ϵ is independent of X and has expectation zero. This formulation reflects probabilistic thinking. "Statistical learning refers to a set of approaches for estimating f." — ISLR

Figure 2.1 displays sales (in thousands of units) for a product vs. advertising budgets (in thousands of dollars) for TV, radio, and newspaper media.

```
Advertising = read.table("Advertising.csv", header=T, sep=',', row.names=1)
str(Advertising)
## Fig 2.1 left panel
with(Advertising, plot(TV, sales))
abline(lm(sales ~ TV, data=Advertising))
```

- 2.1.1: Prediction vs. inference. Reducible vs. irreducible errors.

Reducible vs. irreducible errors. Consider the squared error loss $L(y, \hat{y}) = (y - \hat{y})^2$. Suppose we have a fitted model $\hat{f}$. For a future record with a feature set x_0, we can make a prediction of its outcome as $\hat{f}(x_0)$. Let y_0 be the outcome value for a future record with feature set x_0. Note that y_0 may vary from one record to another because $y_0 = f(x_0) + \epsilon$. The expected loss (e.g., the expectation of loss in the long run) for our prediction is

$$E(y_0 - \hat{f}(x_0))^2 = [f(x_0) - \hat{f}(x_0)]^2 + Var(\epsilon) = [Bias(\hat{f}(x_0))]^2 + Var(\epsilon), \tag{2.3}$$

When the variation for estimating $\hat{f}$ is taken into account, the expected loss for our prediction at x_0 is

$$E(y_0 - \hat{f}(x_0))^2 = Var[\hat{f}(x_0)] + [Bias(\hat{f}(x_0))]^2 + Var(\epsilon). \tag{2.7}$$

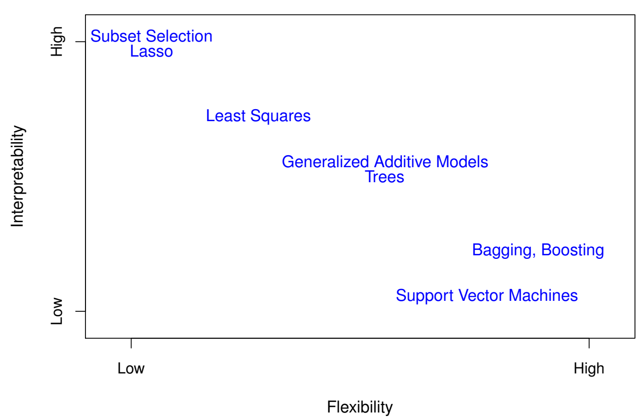
These are the three sources of variability in prediction: (1) sampling variation, (2) choices during modeling, and (3) irreducible error. Irreducible error provides a bound on the accuracy of our prediction. The bound is almost always unknown in practice.

- 2.1.2: Estimation of f: Parametric vs. nonparametric vs. semiparametric models. Data are split into training set and test set. Model fitting criterion (e.g., least squares, minimum cost, maximum likelihood, etc.). Overfitting.

Thin-plate spline using the `fields` package. Datasets `Income1` and `Income2` are simulated and they are different datasets!

```
library(fields)
library(rgl)  ## for #3D plots

Income2 = read.table("Income2.csv", header=T, sep=',', row.names=1)
names(Income2); dim(Income2); summary(Income2)

fit = with(Income2, Tps(cbind(Education, Seniority), Income, m=3, scale.type="range"))

ngrid = 100
gridedu = seq(10, 22, length.out=ngrid)
gridsen = seq(20, 188, length.out=ngrid)
grid2 = expand.grid(gridedu, gridsen)
grid2$pred = predict(fit, x=as.matrix(grid2))
names(grid2)

with(Income2, plot3d(Education, Seniority, Income, col=2, size=5))
plot3d(grid2$Var1, grid2$Var2, grid2$pred, add=T, alpha=.5)
```

- 2.1.3: Model flexibility vs. interpretability. Figure 2.7. With big data, traditional interpretable models tend to underfit, which derail their "interpretability". Artificial neural networks (ANNs) would be at the lower right corner (high flexibility but low interpretability).



- 2.1.4: supervised vs. unsupervised vs. semi-supervised learning (also see HOML Chapter 1)
- 2.1.5: regression vs. classification models

2.2 Demonstration of variation in a fitted model, $Var(\hat{f})$

We use `horsepower` vs `mpg` (in `Auto` dataset) as an example of joint distribution of (X, Y), and subsample the data. Suppose we could only afford to collect data for $n = 50$ cars, and we fitted quantile regression to our data ($n = 50$). The fitted model varies from one dataset to another. The smaller n, the higher variation in $\hat{f}$ across datasets.

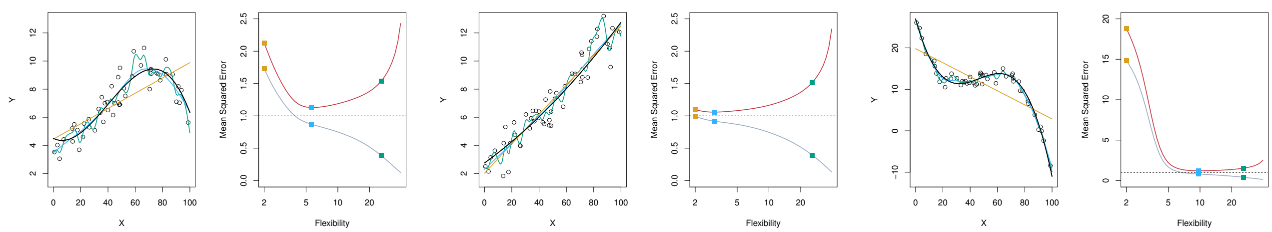
```
library(quantreg)  ## quantile regression package
library(ISLR)
str(Auto)
with(Auto, plot(horsepower, mpg))

## Repeat this 100 times (i.e., 100 replicates)
with(Auto, plot(horsepower, mpg))
for(ii in 1:10) {
```

```
  subidx = sample.int(392, 50)
  Autosub = Auto[subidx,]
  mod = rq(mpg ~ horsepower + I(horsepower^2), data=Autosub, tau=.5)
  idx = order(Autosub$horsepower)
  points(Autosub$horsepower[idx], fitted(mod)[idx], type='l')
}

mod = rq(mpg ~ horsepower + I(horsepower^2), data=Auto, tau=.5)
idx = order(Auto$horsepower)
points(Auto$horsepower[idx], fitted(mod)[idx], type='l', lwd=3, col=2)
```

2.3 ISLR 2.2

- 2.2.1: Continuous outcomes: MSE as a measure of the quality of fit; it effectively uses squared error as the measure of loss.

Figures 2.9–2.11 show 3 simulated scenarios, all with a single predictor, $n = 50$ in training data. The true curve is in black, and there are 3 fitted curves (from a linear model and 2 smoothing splines). Training MSE and test MSE are shown as functions of model flexibility (or model DF). Here model DF is a hyperparameter.

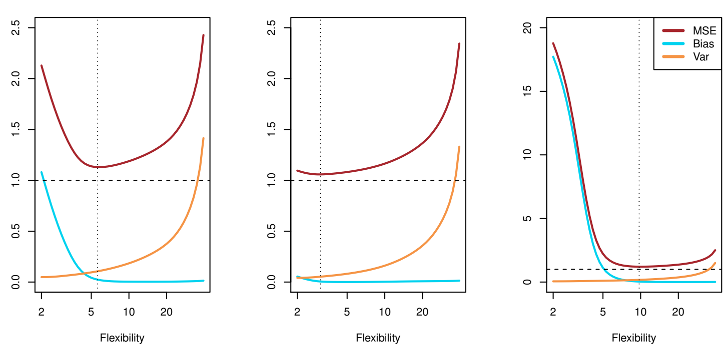


In practice, we can use cross-validation on the training data (or a separate validation set) to estimate test MSE to help determine model complexity. With a single predictor, linear models often underfit. When there are many predictors but the sample size is not very large, even a linear model may overfit (due to curse of dimensionality; ISLR 3.5) and require regularization.

- 2.2.2: Bias–variance trade-off in test MSE.

$$E(y_0 - \hat{f}(x_0))^2 = Var[\hat{f}(x_0)] + [Bias(\hat{f}(x_0))]^2 + Var(\epsilon). \tag{2.7}$$

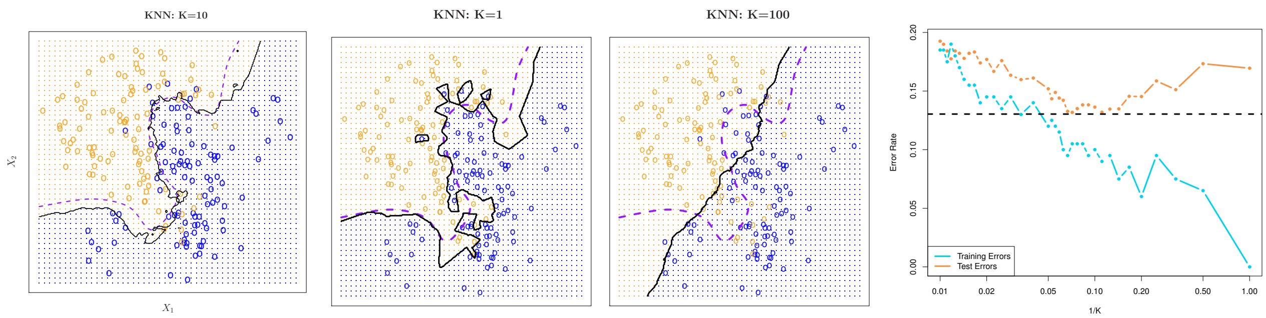
The three sources of variability are due to (1) sampling variation, (2) choice during modeling, and (3) irreducible error. Given a fixed dataset, a more complex/flexible model tends to reduce bias but increase variation. Figure 2.12 shows all three components for the simulation scenarios in Figures 2.9–2.11.



- 2.2.3: Discrete outcomes: Classification error rate (effectively using 0-1 loss as the measure of loss). Similar decomposition of the sources of variation as in (2.7).

Bayes classifier: $f(x) = \arg\max_g P(Y = g|X = x)$, is the best classifier because it minimizes the expected classification error rate. It is often used as a reference in simulation studies; Figure 2.13 is an example. A Bayes classifier has a corresponding Bayes decision boundary and a Bayes error rate. (Note that this is not Bayesian statistics.) The Bayes classifier is often **unknown in practice.**

k-nearest neighbors (KNN) is a local estimation method, with k being a hyperparameter. KNN requires a measure of similarity (for defining neighborhoods). It is similar to moving-window approaches; in KNN k is fixed, while in a moving-window approach, window size is fixed. The smaller k the higher model flexibility; an example is in Figures 2.15–2.17 ($n = 200$, $p = 2$). With high dimensional predictors, all local estimation methods suffer from the curse of dimensionality (ISLR 3.5). KNN is also applicable to continuous outcomes (ISLR 3.5).



2.4 HOML Chapter 1

Types of ML systems:

- From the problem perspective: Supervised vs. unsupervised vs. semisupervised learning. “Labels” are called outcomes in Statistics.
- From the algorithm perspective: Batch vs. online learning. Out-of-core learning.
- From the method perspective: Instant-based vs. model-based learning. In Statistics, “instant-based learning” is local estimation.

Reinforcement learning describes learning in a scenario where new observations (x, y) can be generated automatically by randomly trying a condition x and obtaining a result y. This can be very effective because the sample size n can be very large and the data can be truly random. Applications include games and robotics studies. A famous example is AlphaGo (and AlphaGo Zero) for the Go game.

Main challenges in ML/Statistics:

- Algorithm development vs. corpus development. “Unreasonable Effectiveness of Data” in language learning
- Sampling bias: when data are not representative (not randomly drawn from the target population). “Sampling noise” in this book is called sampling variation in Statistics.
- Data quality: Outliers, missing data, missing features.
- Too many (irrelevant) features. Feature engineering (selection, extraction, collection).
- Overfitting. Signs of overfitting. Regularization prevents overfitting.
- Underfitting.

The example behind Figure 1-23 is misleading: Regularization is known to push slope estimates closer to zero. Random missing of observations does not lead to an elevated slope (it leads to a higher variation in slope). The fact that the slope obtained from the full data is closer to zero than the slope for that specific subset is because the missing observations probably were not randomly chosen (as shown in the figure). With a single predictor, there is no guarantee that regularization gives results closer to the truth; this is because a linear model with a single predictor is much more likely to underfit than to overfit. With many predictors or a very complex model (e.g., ANN), the model may overfit and regularization often gives better results.

Hyperparameters and validation:

- Hyperparameters fall in three categories:
  1. Those defining the model structure, e.g., number of included features, neighbor size.

   2. Those in model fitting criteria, e.g., cost function, amount of regularization.
   3. Those used in model fitting process, e.g., parameter initialization, learning rate, mini-batch size, epochs.
- Some hyperparameters are also called *tuning parameters*.
- Hyperparameters can be selected using validation. Data can be split into training/validation/test sets, or training/test sets with cross-validation on the training set. Cross-validation is preferred to a standalone validation set unless the sample size is very large.

Training set vs. validation set vs. test set

The test set is for evaluation of the final fitted model. If we do not know the structure of the final model, we will have to do model selection (e.g., by tuning hyperparameters), and we need to make sure the test set is not used during this process. Validation set(s) are needed to validate our choices. We need to carve out a portion of data from the training set, either in a single training-validation split or using cross-validation. In summary,

1. Training set is for estimation of parameters;
2. Validation set or cross-validation is for selection of hyperparameters (selection criteria often less formalized);
3. Test set is for evaluation of the final fitted model, which has all parameters and hyperparameters determined.

2.5 Assignment

1. **Homework**: ISLR Chapter 2 Exercises 1, 3, 8 (`College` dataset in ISLR)
2. Reading for next lecture: ISLR 3.1–3.2
3. ISLR Chapter 3 R Labs
4. Try out the python code for HOML Chapter 1