Announcements, 30 Jun 2016

- Upload your assignment to Canvas
  You need to submit all 5 Assignments

- Capstone project is mandatory (2-3 per team), *Start week 4*

Data Science

Deriving Knowledge from Data at Scale

Wee Hyong Tok

Jun 30, 2016

Overview

- Doing Data Science
- Bias and Variance
- Supervised and Unsupervised
- Classification

“The goal of machine learning is to build computer systems that can adapt and learn from their experience.”

– Tom Dietterich

Doing Data Science

The Data Science Workflow

Review

Stay in the **immediate zone** during exploratory modeling, to extent possible:

- 5 to 10 minutes per experiment, results in 100's per day;
- Small, statistically sound/relevant samples;
- Linear modelling during feature exploration;
- Don't write ML algorithms, use packages, do learn to write data manipulation code;

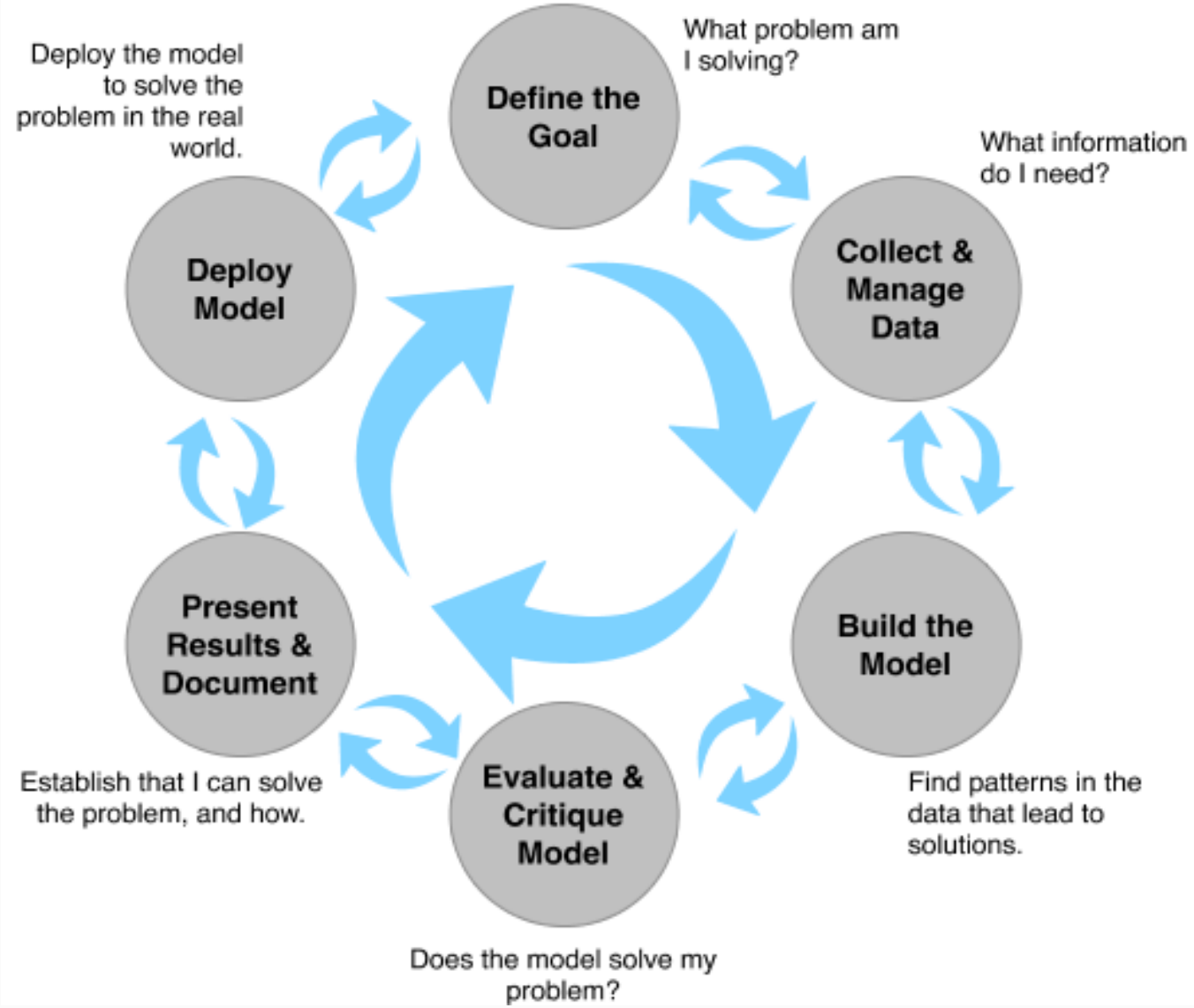
Start with a sample of data, *as soon as you can get it…*

- You will learn a considerable amount from that first data sample
- Quality of the data, what fields are being collected, possible missing values and/or missing fields, and the questions will begin to flow (dialogue with customer will be at a much more meaningful level).

If your customer can't quantify it, you can't change/improve it…

The Data Science Workflow

Loops within loops…



The Data Science Workflow
Define the Goal

The first task in a data science project is to define a **measurable** & **quantifiable** goal. At this stage, *learn all that you can about the context of your project*.

- Why do the project sponsors want the project in the first place? What do they lack, and what do they need?
- What are they doing to solve the problem now, and why isn't that good enough?
- What resources will you need: what kind of data, how much staff, will you have domain experts to collaborate with, what are the computational resources?
- How do the project sponsors plan to deploy your results? What are the constraints that have to be met for successful deployment?

Not We want to get better at finding bad loans.

But We want to reduce our rate of **loan charge-offs by at least 10%**, using a model that predicts which loan applicants are likely to default.

A concrete goal begets concrete ***stopping conditions*** *and concrete* ***acceptance criteria****. The less specific the goal, the likelier that the project will go unbounded, because no result will be "good enough." If you don't know what you want to achieve, you don't know when to stop trying – or even what to try. When the project eventually terminates – because either time or resources run out –* ***no one will be happy with the outcome…***

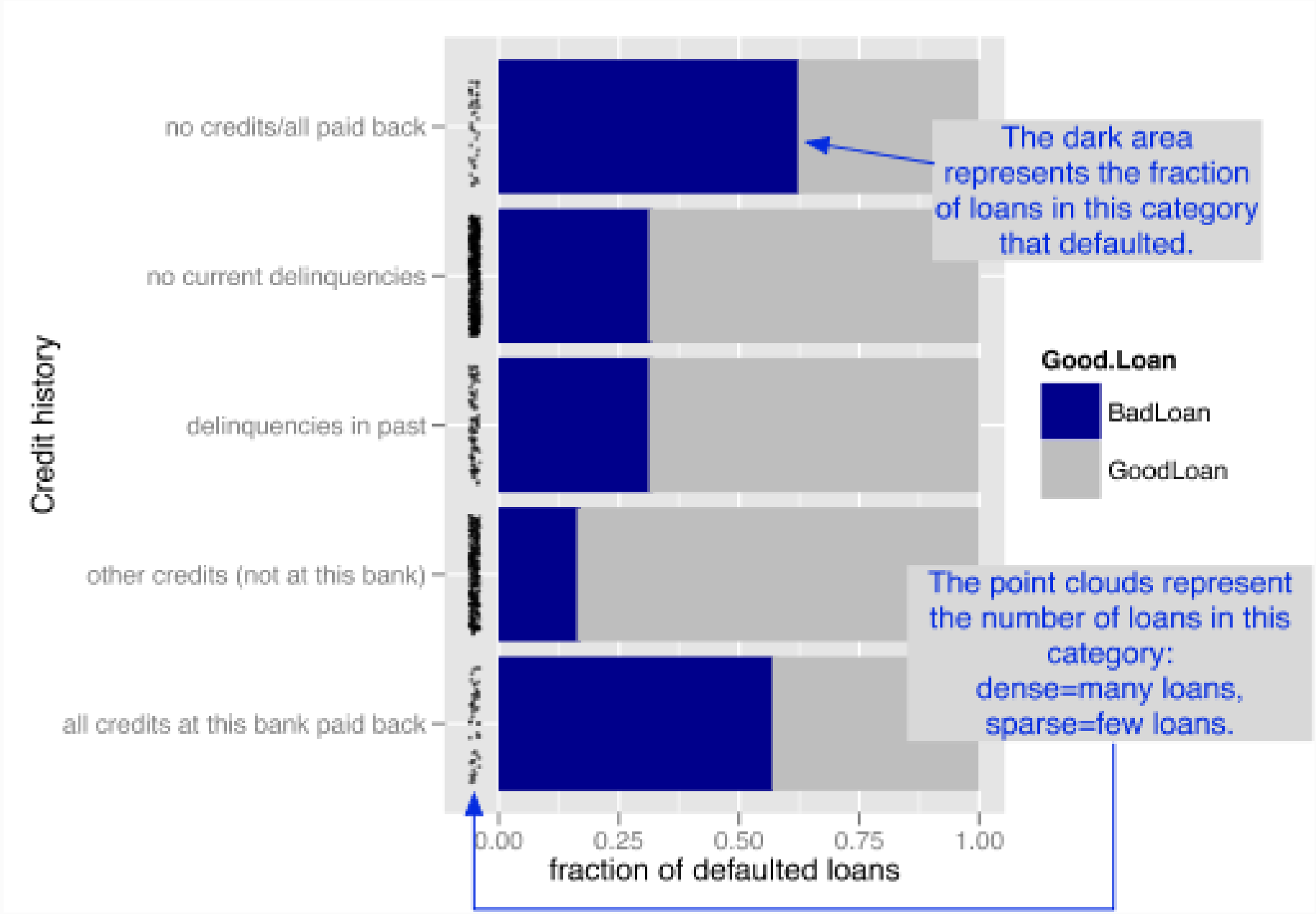
The Data Science Workflow

Data Collection and Management

This step encompasses identifying the data you need, exploring it, and conditioning it to be suitable for analysis. This stage is often the most time-consuming step in the process. It's also one of the most important.

- What data is available to me?
- Will it help me solve the problem?
- Is it enough?
- Is it of good enough quality?

Rule First piece of data is *very informative*, data set utility is roughly logarithmic in size.
Prefer Direct measurements, but if they are not available identify proxy variables.

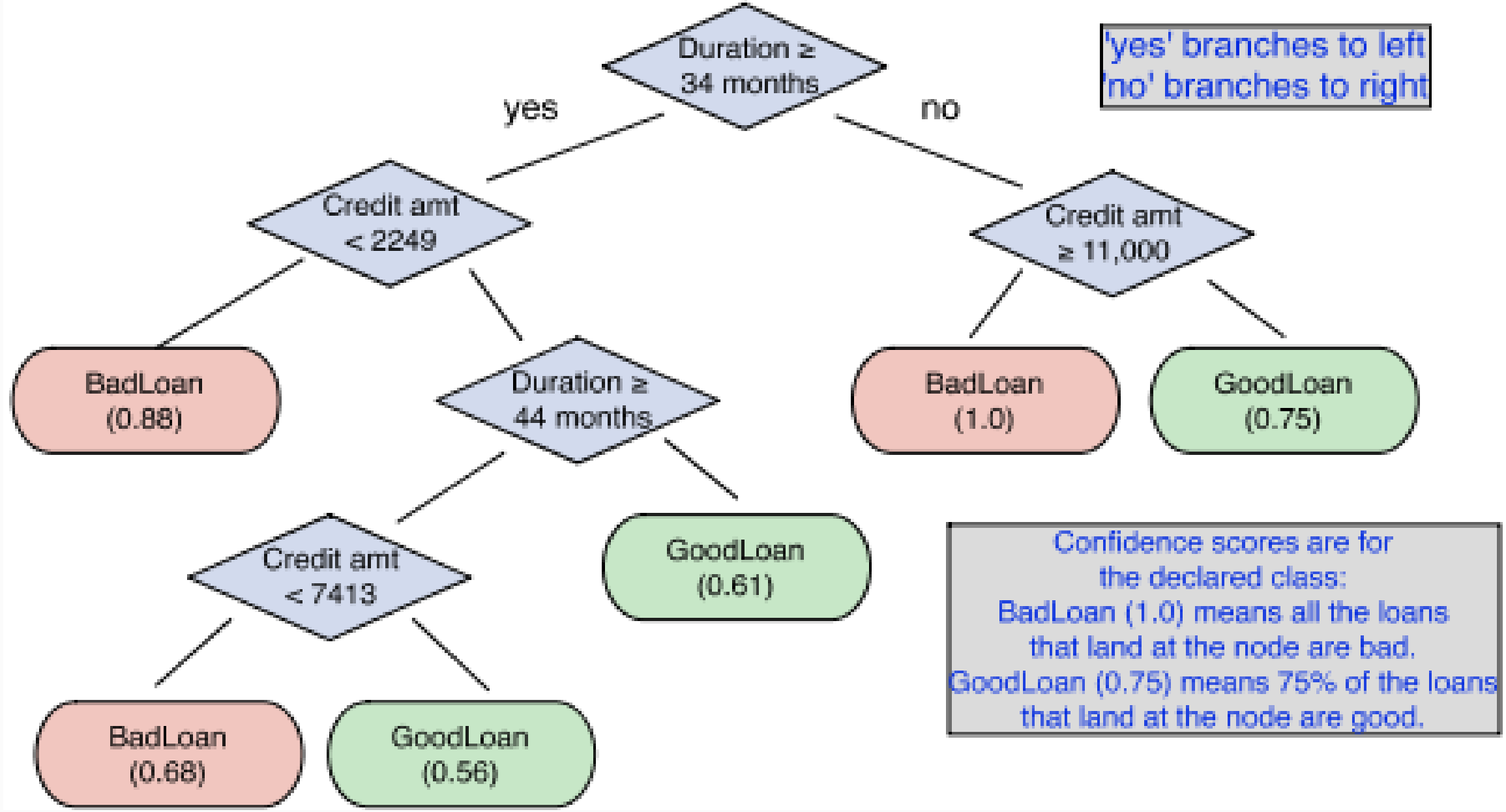

Credit history
no credits/all paid back
no current delinquencies
delinquencies in past
other credits (not at this bank)
all credits at this bank paid back
0.00
0.25
0.50
0.75
1.00
fraction of defaulted loans
The dark area represents the fraction of loans in this category that defaulted.
Good.Loan
BadLoan
GoodLoan
The point clouds represent the number of loans in this category: dense=many loans, sparse=few loans.

The Data Science Workflow

Modeling

We get to statistics and machine learning during the modeling stage. Here is where you try to extract useful insights from the data. Many modeling procedures make specific assumptions about data distribution and relationships, *there will be back-and-forth between the modeling and data cleaning stages as you try to find the best way to represent and model the data*. The most common data science modeling tasks are:

- **Classification**: deciding if something belongs to one category or another.
- **Scoring**: predicting or estimating a numeric value such as a price or probability.
- **Ranking**: learning to order items by preferences.
- **Clustering**: grouping items into most similar groups.
- **Finding Relations**: finding correlations or potential causes of effects seen in the data.
- **Characterization**: very general plotting and report generation from data.


Duration ≥ 34 months
yes
no
'yes' branches to left
'no' branches to right
Credit amt < 2249
Credit amt ≥ 11,000
BadLoan (0.88)
Duration ≥ 44 months
BadLoan (1.0)
GoodLoan (0.75)
Credit amt < 7413
GoodLoan (0.61)
BadLoan (0.68)
GoodLoan (0.56)
Confidence scores are for the declared class:
BadLoan (1.0) means all the loans that land at the node are bad.
GoodLoan (0.75) means 75% of the loans that land at the node are good.

The Data Science Workflow

Model Evaluation and Critique

Once you have a model, you need to determine if it meets your goals.

- Is it accurate enough for your needs?
- Does it generalize well?
- Does it perform better than "the obvious guess"? Better than whatever estimate you currently use?
- Do the results of the model (coefficients, clusters, rules) make sense in the context of the problem domain?

If you've answered "no" to any of the above questions, it's time to loop back to the modeling step — or decide that the data doesn't support the goal you are trying to achieve.

The Data Science Workflow

Model Deployment and Maintenance

Finally, the model is put into operation.

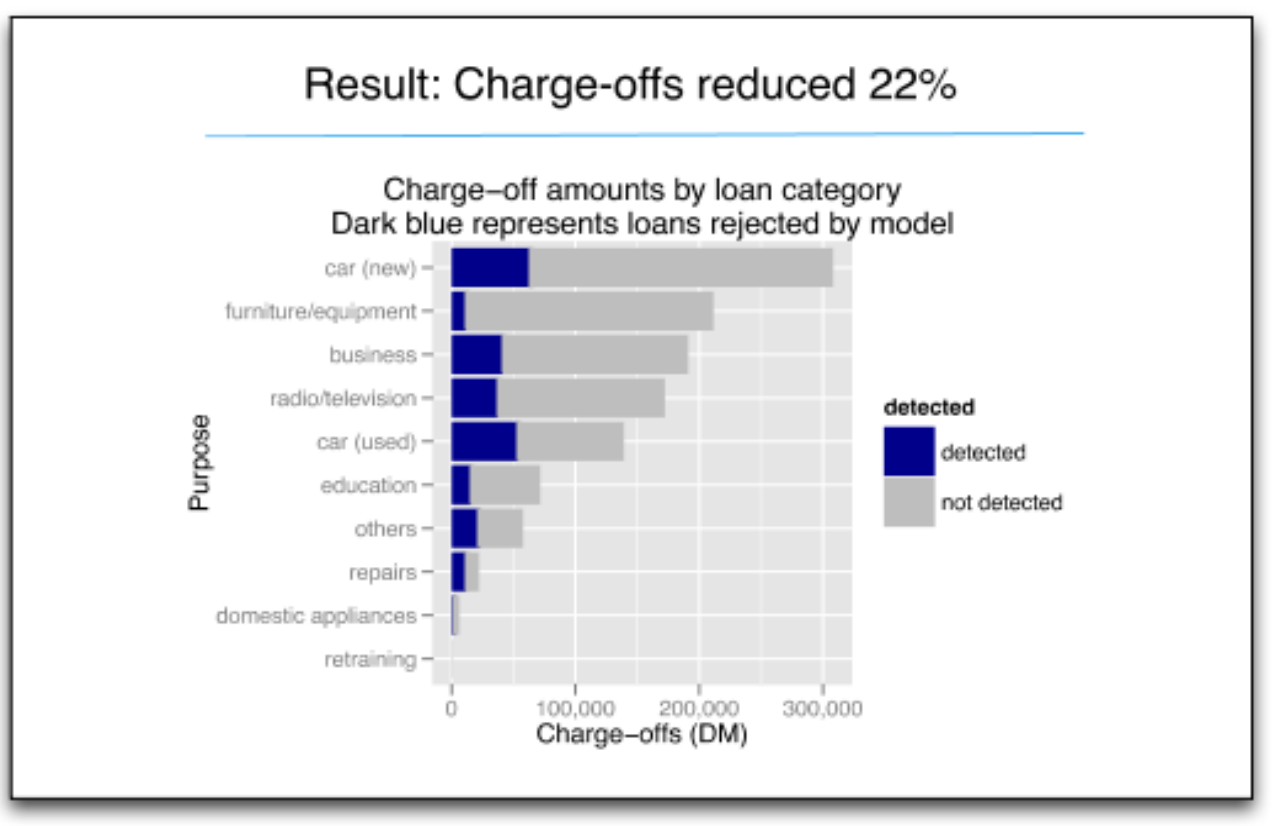
In many organizations this means the data scientist no longer has primary responsibility for the day-to-day operation of the model. However, you still should ***ensure that the model will run smoothly*** and will not make disastrous unsupervised decisions. You also want to make sure that the ***model can be updated*** as its environment changes. And in many situations, the model will initially be ***deployed in a small pilot program***.

The test might bring out issues that you didn't anticipate, and you will have to adjust the model appropriately.

The Data Science Workflow

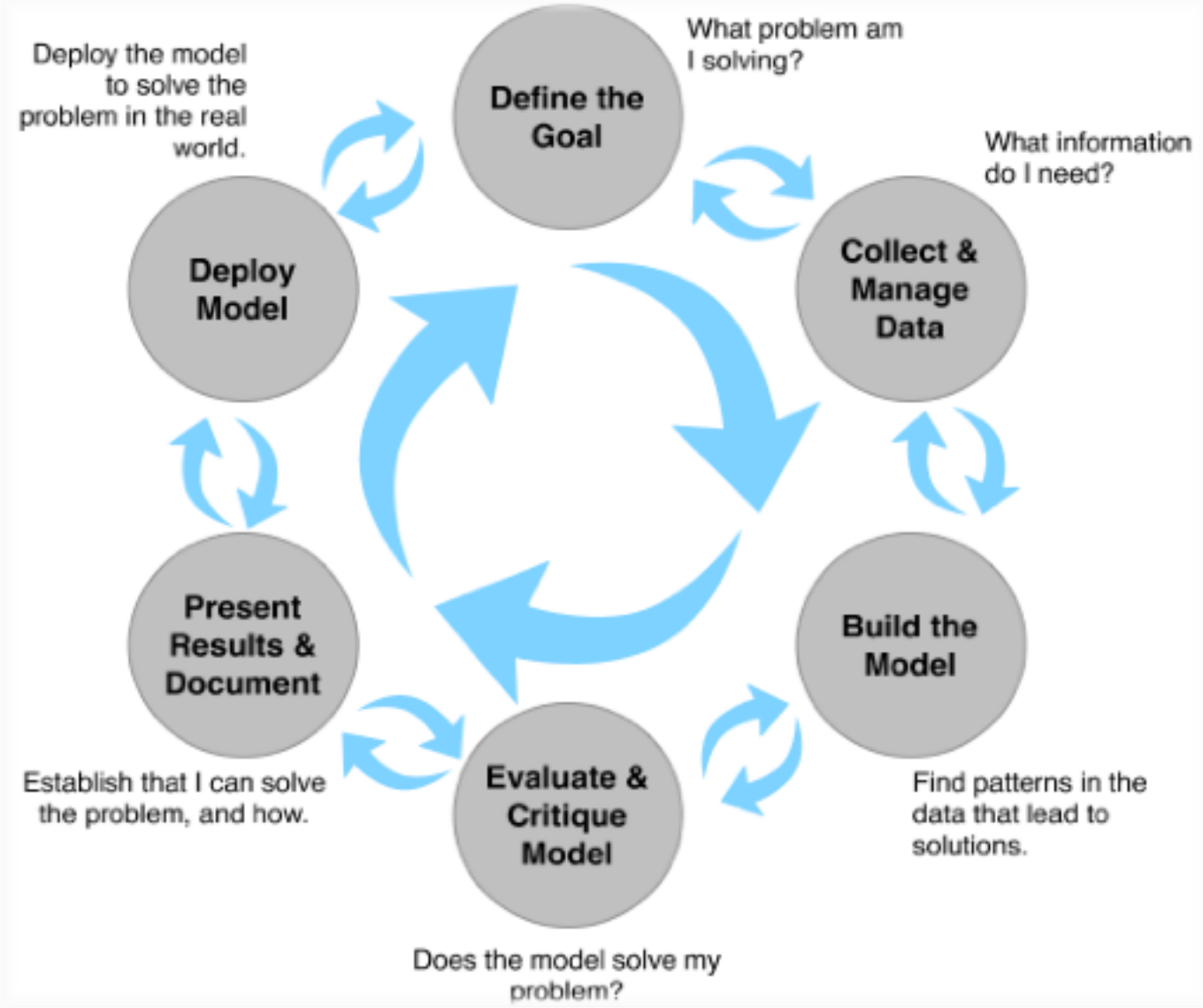
Presentation and Documentation

Once you have a model that meets your success criteria, you will present your results to your project sponsor and other stakeholders. You must also document the model for those in the organization who are responsible for using, running, and maintaining the model once it has been deployed. ***Model interpretability may be an issue***…



The Data Science Workflow

Loops within loops…



Supervised vs Un-supervised

Machine learning and our focus

- Like human learning from past experiences.
- A computer does not have "experiences".
- A computer system learns from data, which represent some "past experiences" of an application domain.
- Our focus: learn a target function that can be used to predict the values of a discrete class attribute, e.g., approve or not-approved, and high-risk or low risk.
- The task is commonly called: Supervised learning, classification, or inductive learning.

Example Application 1 - Healthcare

- An emergency room in a hospital measures 17 variables (e.g., blood pressure, age, etc) of newly admitted patients.
- A decision is needed: whether to put a new patient in an intensive-care unit.
- Due to the high cost of ICU, those patients who may survive less than a month are given higher priority.
- Problem: to predict high-risk patients and discriminate them from low-risk patients.

Example Application 2 – Financial Institution

- A credit card company receives thousands of applications for new cards. Each application contains information about an applicant,
  - age
  - Marital status
  - annual salary
  - outstanding debts
  - credit rating
  - etc.
- Problem: to decide whether an application should be approved, or to classify applications into two categories, approved and not approved.

The data and the goal

- Data: A set of data records (also called examples, instances or cases) described by
  - *k* attributes: A_1, A_2, … A_k.
  - a class: Each example is labelled with a pre-defined class.

- Goal: To learn a classification model from the data that can be used to predict the classes of new (future, or test) cases/instances.

An example: data (loan application)

Approved or not

ID	Age	Has_Job	Own_House	Credit_Rating	Class
1	young	false	false	fair	**No**
2	young	false	false	good	**No**
3	young	true	false	good	**Yes**
4	young	true	true	fair	**Yes**
5	young	false	false	fair	**No**
6	middle	false	false	fair	**No**
7	middle	false	false	good	**No**
8	middle	true	true	good	**Yes**
9	middle	false	true	excellent	**Yes**
10	middle	false	true	excellent	**Yes**
11	old	false	true	excellent	**Yes**
12	old	false	true	good	**Yes**
13	old	true	false	good	**Yes**
14	old	true	false	excellent	**Yes**
15	old	false	false	fair	**No**

An example: the learning task

- Learn a classification model from the data
- Use the model to classify future loan applications into
  - Yes (approved) and
  - No (not approved)
- What is the class for following case/instance?

Age	Has_Job	Own_house	Credit-Rating	Class
young	false	false	good	?

Supervised vs. Unsupervised Learning

- Supervised learning: classification is seen as supervised learning from examples.
  - Supervision: The data (observations, measurements, etc.) are labeled with pre-defined classes. It is like that a "teacher" gives the classes (supervision).
  - Test data are classified into these classes too.

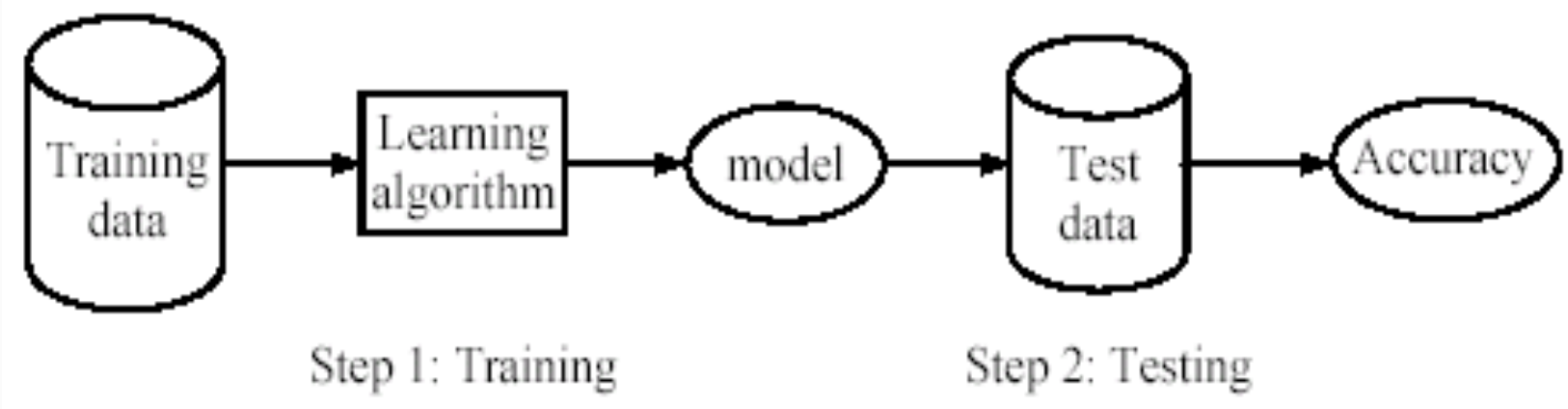
- Unsupervised learning (clustering)
  - Class labels of the data are unknown
  - Given a set of data, the task is to establish the existence of classes or clusters in the data

Supervised learning process: two steps

Learning (training): Learn a model using the training data

Testing: Test the model using unseen test data to assess the model accuracy

$$Accuracy = \frac{\text{Number of correct classifications}}{\text{Total number of test cases}},$$



What do we mean by learning?

- Given
  - a data set *D*,
  - a task *T*, and
  - a performance measure *M*,

  a computer system is said to **learn** from *D* to perform the task *T* if after learning the system's performance on *T* improves as measured by *M*.
- In other words, the learned model helps the system to perform *T* better as compared to no learning.

An example

- Data: Loan application data
- Task: Predict whether a loan should be approved or not.
- Performance measure: accuracy.

No learning: classify all future applications (test data) to the majority class (i.e., Yes):

Accuracy = 9/15 = 60%.

- We can do better than 60% with learning.

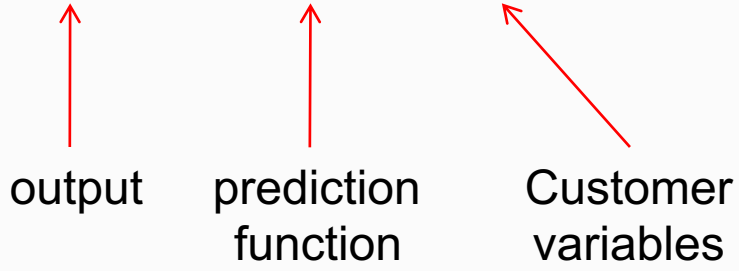
Fundamental assumption of learning

Assumption: The distribution of training examples is identical to the distribution of test examples (including future unseen examples).

- In practice, this assumption is often violated to certain degree.
- Strong violations will clearly result in poor classification accuracy.
- To achieve good accuracy on the test data, training examples must be sufficiently representative of the test data.

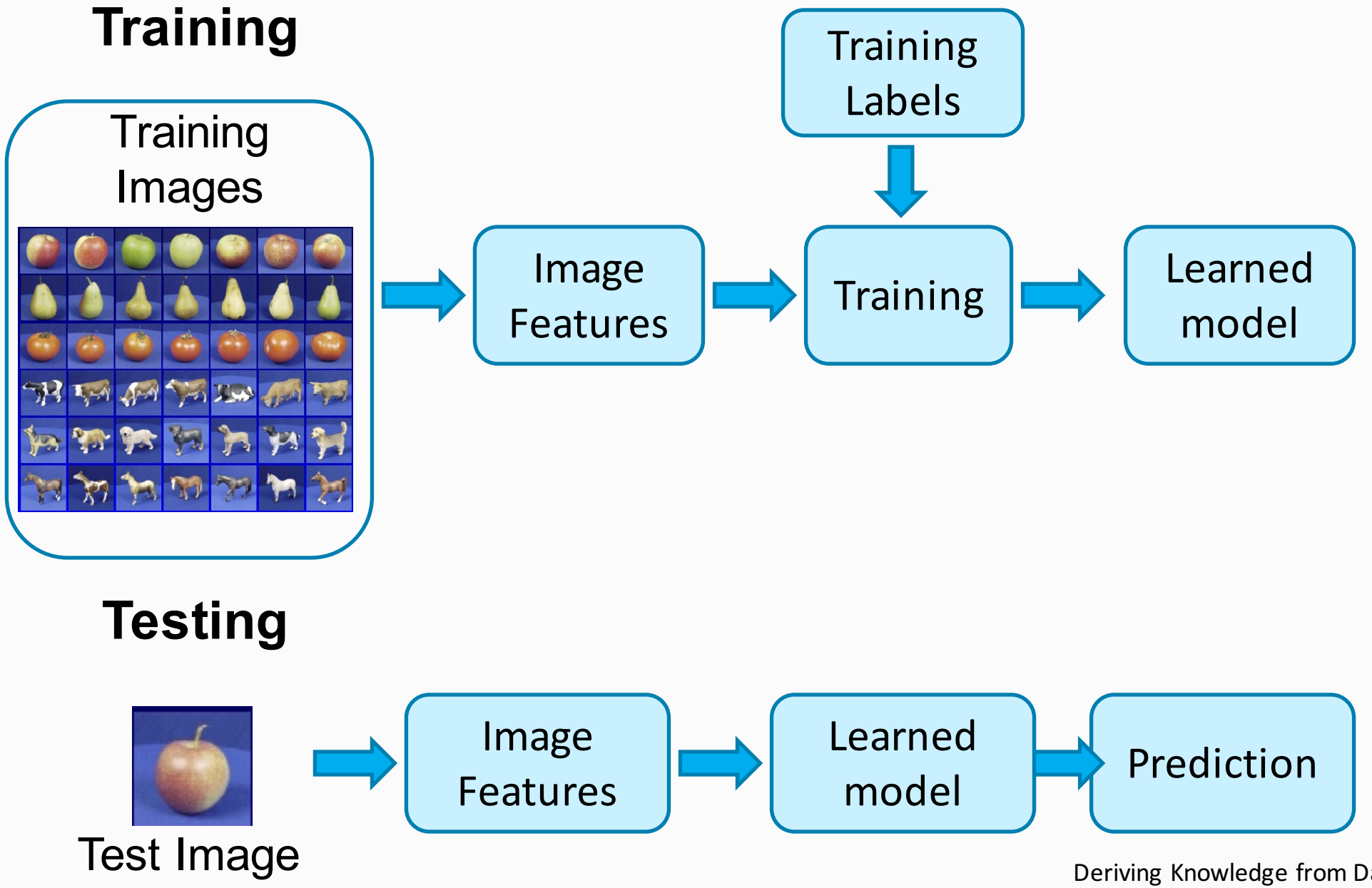
The machine learning framework

$$y = f(\mathbf{x})$$

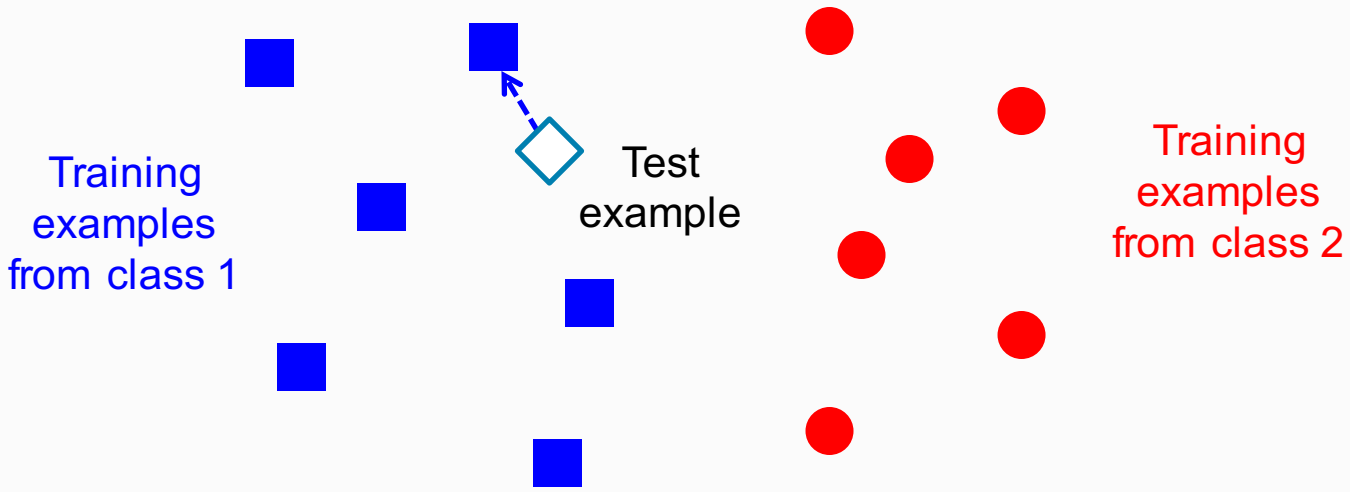


- Training: given a *training set* of labeled examples $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$, estimate the prediction function f by minimizing the prediction error on the training set
- Testing: apply f to a never before seen *test example* $\mathbf{x}$ and output the predicted value $y = f(\mathbf{x})$

Steps


Training
Training Images
Training Labels
Image Features
Training
Learned model
Testing
Test Image
Image Features
Learned model
Prediction

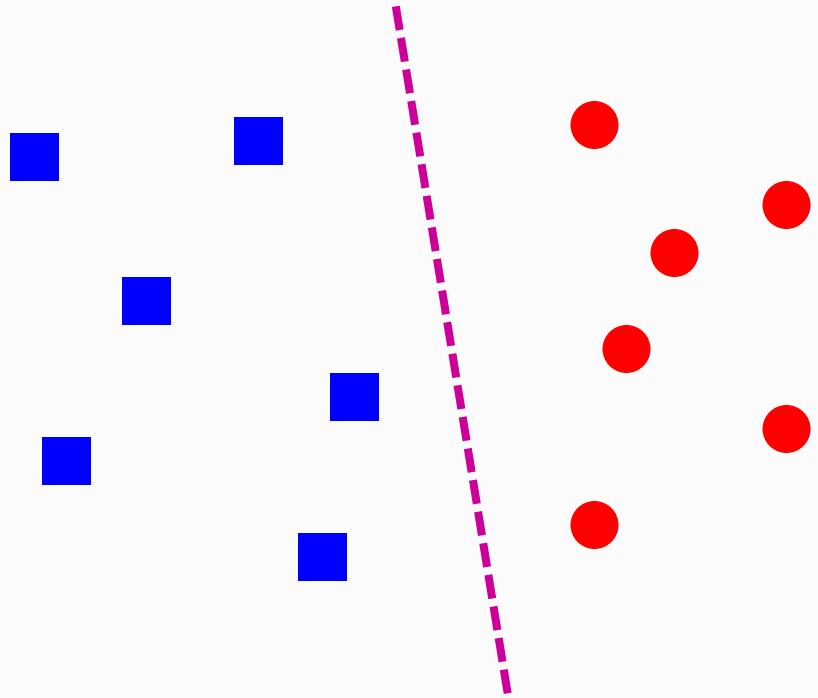
Classifiers: Nearest neighbor



f(**x**) = label of the training example nearest to **x**

- All we need is a distance function for our inputs
- No training required!

Classifiers: Linear



- Find a *linear function* to separate the classes:

$$f(\mathbf{x}) = \text{sgn}(\mathbf{w} \cdot \mathbf{x} + b)$$

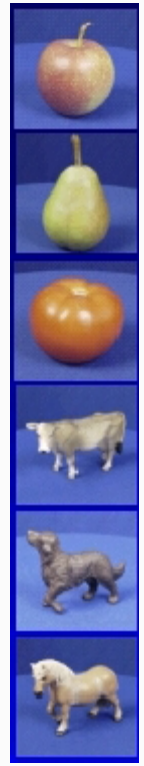
Many classifiers to choose from

- SVM
- Neural networks
- Naïve Bayes
- Bayesian network
- Logistic regression
- Randomized Forests
- Boosted Decision Trees
- K-nearest neighbor
- Etc.

Which is the best one?

Generalization

Training set (labels known)



Test set (labels unknown)

How well does a learned model generalize from the data it was trained on to a new test set?

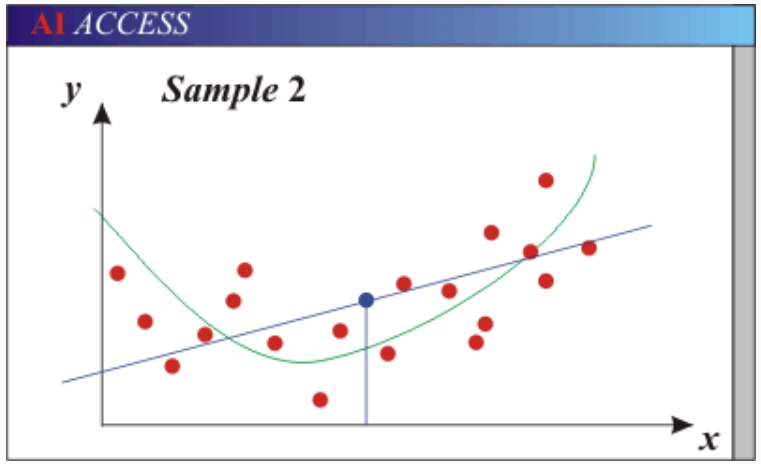
Generalization

- Components of generalization error
  - Bias: how much the average model over all training sets differ from the true model?
    - Error due to inaccurate assumptions/simplifications made by the model
  - Variance: how much models estimated from different training sets differ from each other
- Underfitting: model is too “simple” to represent all the relevant class characteristics
  - High bias and low variance
  - High training error and high test error
- Overfitting: model is too “complex” and fits irrelevant characteristics (noise) in the data
  - Low bias and high variance
  - Low training error and high test error

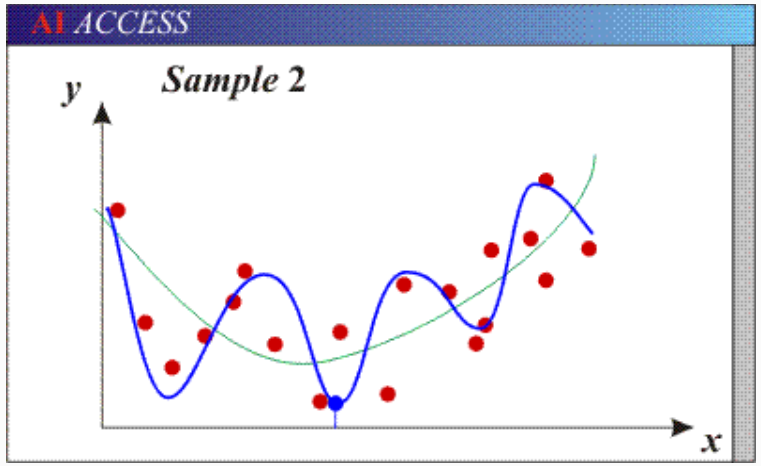
No Free Lunch Theorem

Bias Variance Tradeoff

Bias-Variance Trade-off



- Models with too few parameters are inaccurate because of a large bias (not enough flexibility).



- Models with too many parameters are inaccurate because of a large variance (too much sensitivity to the sample).

Bias-Variance Trade-off

$$E(MSE) = noise^2 + bias^2 + variance$$

Unavoidable error

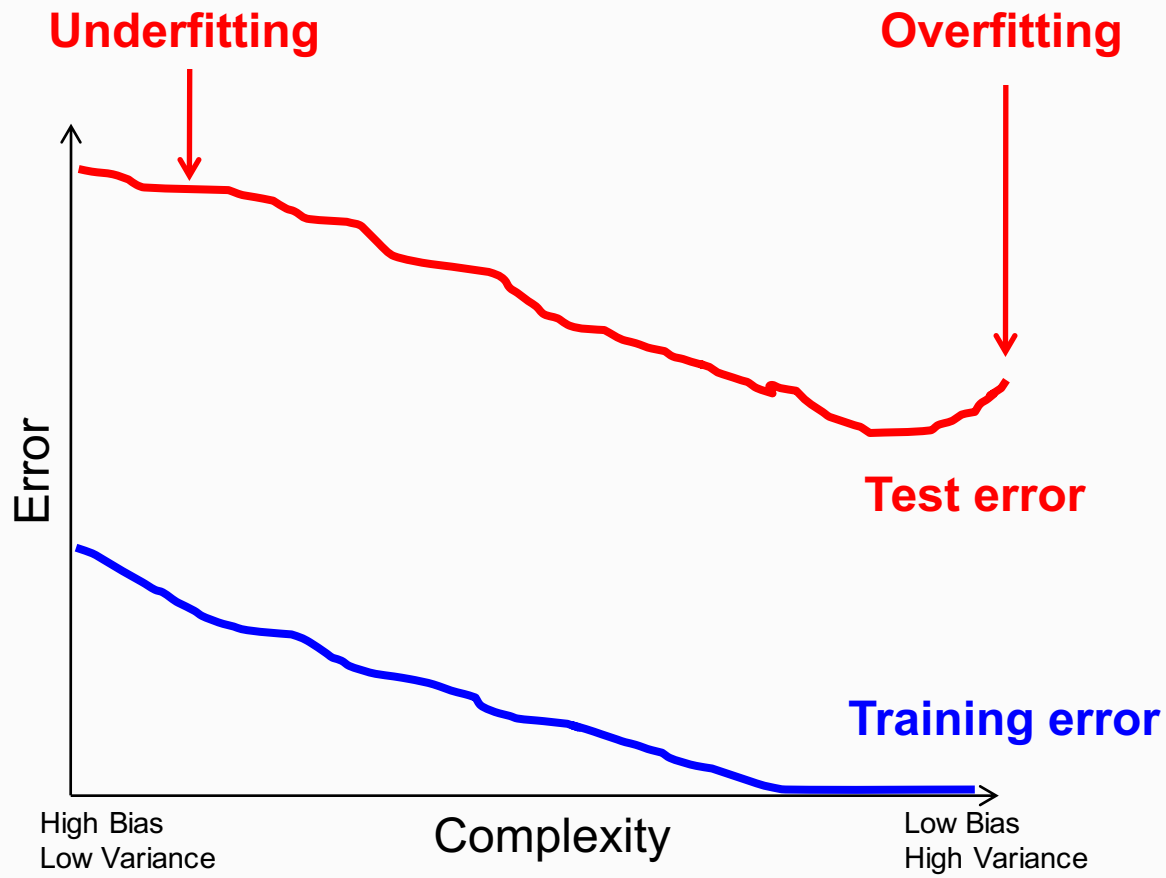
Error due to incorrect assumptions

Error due to variance of training samples

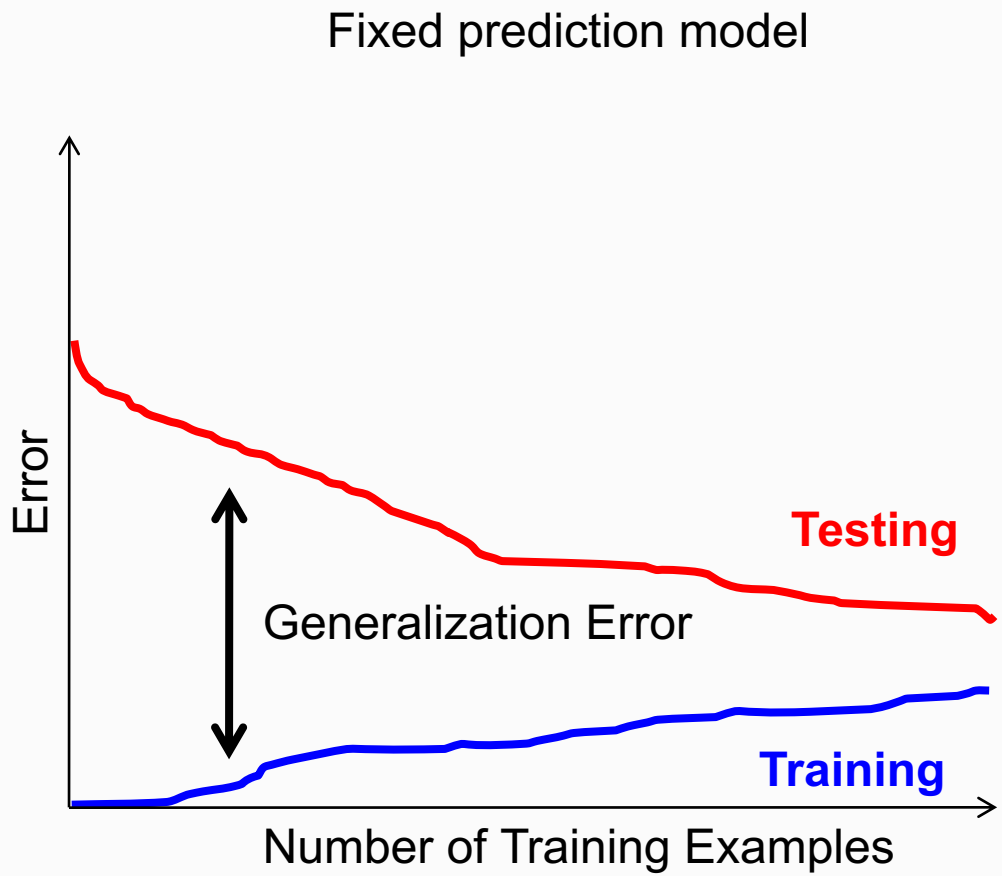
See the following for explanations of bias-variance (also Bishop's "Neural Networks" book):

- http://www.inf.ed.ac.uk/teaching/courses/mlsc/Notes/Lecture4/BiasVariance.pdf

Bias-variance tradeoff



Effect of Training Size



Classification

Remember…

- No classifier is inherently better than any other: you need to make assumptions to generalize

- Three kinds of error
  - Inherent: unavoidable
  - Bias: due to over-simplifications
  - Variance: due to inability to perfectly estimate parameters from limited data

How to reduce variance?

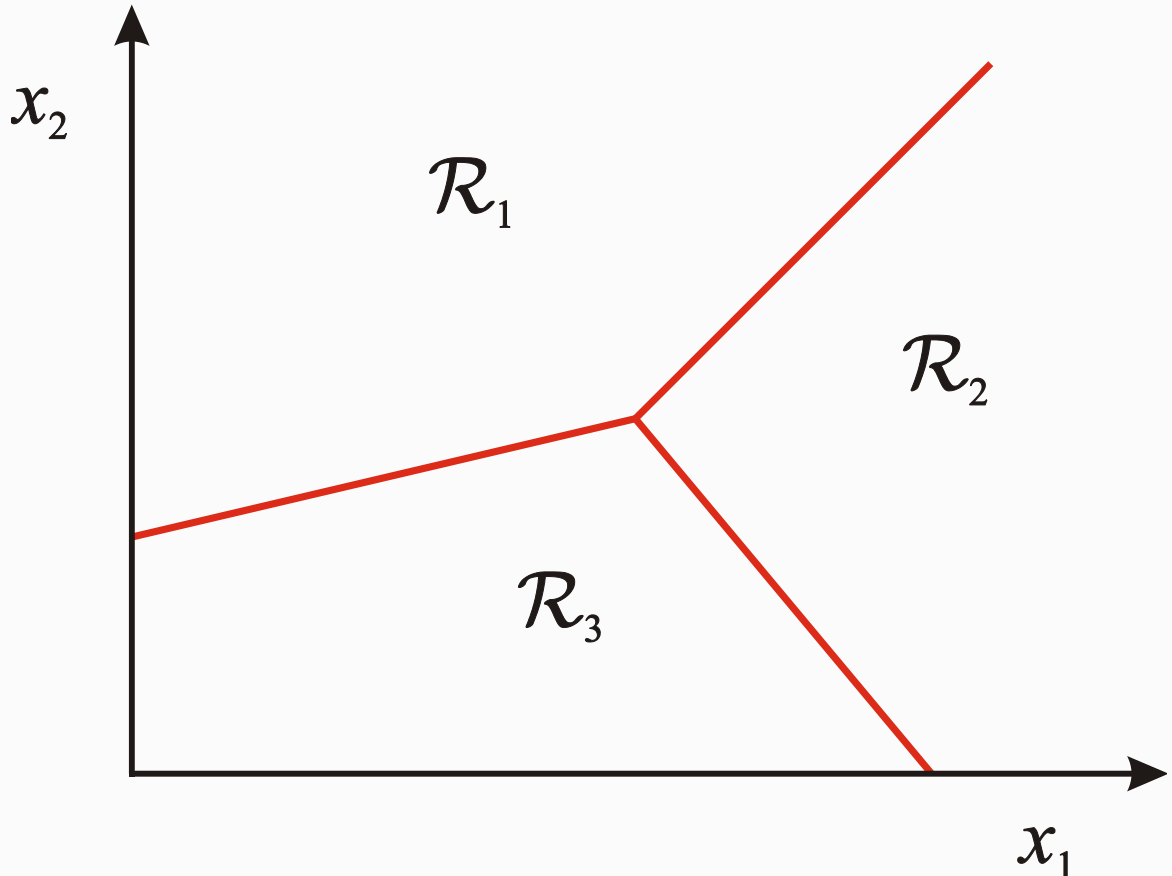
- Choose a simpler classifier
- Regularize the parameters
- Get more training data

Very brief tour of some classifiers

- **K-nearest neighbor**
- **SVM**
- **Boosted Decision Trees**
- Neural networks
- Naïve Bayes
- Bayesian network
- Logistic regression
- Randomized Forests
- Etc.

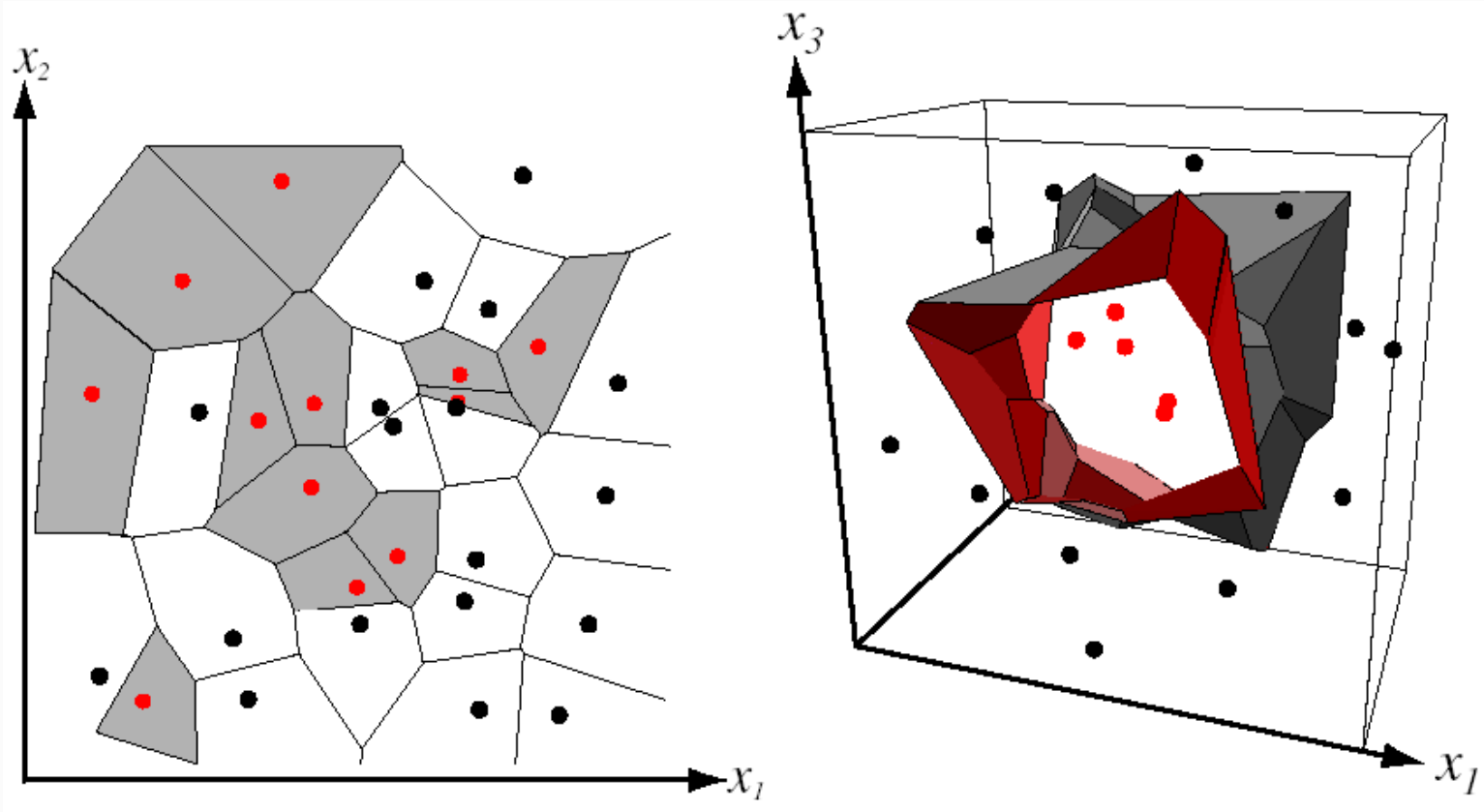
Classification

- Assign input vector to one of two or more classes
- Any decision rule divides input space into *decision regions* separated by *decision boundaries*



Nearest Neighbor Classifier

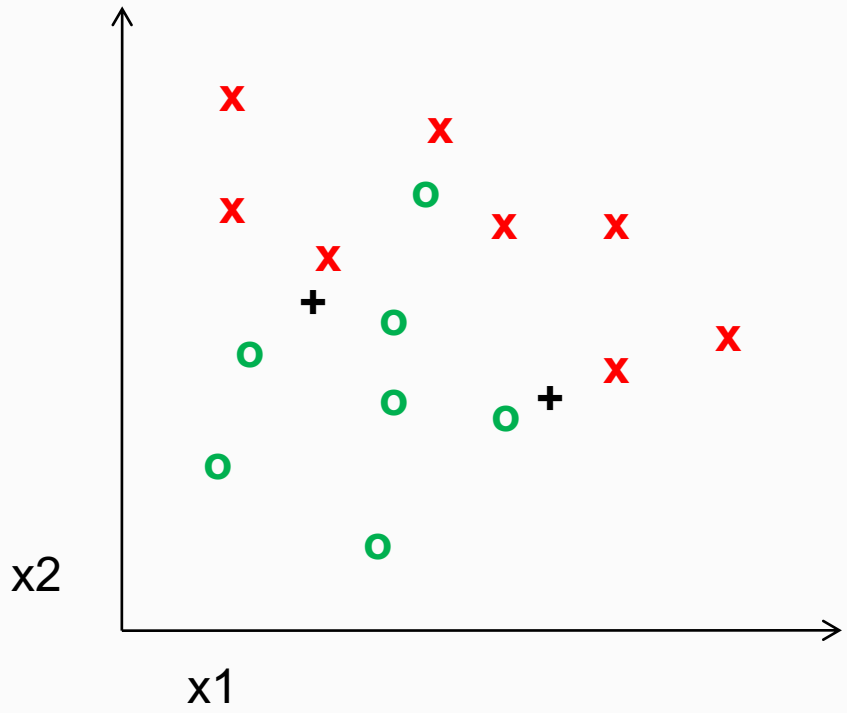
- Assign label of nearest training data point to each test data point



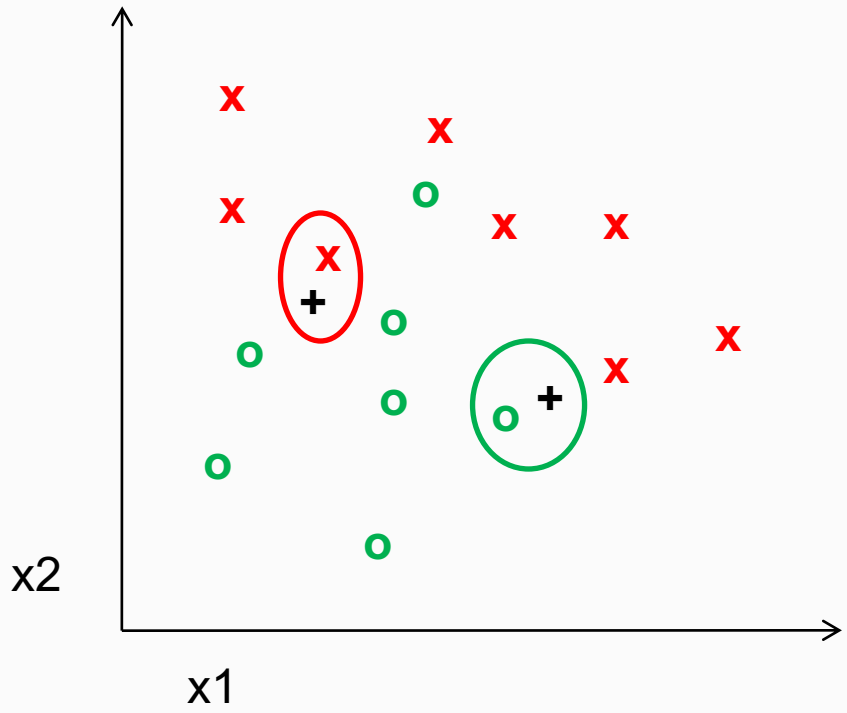
from Duda *et al.*

Voronoi partitioning of feature space
for two-category 2D and 3D data

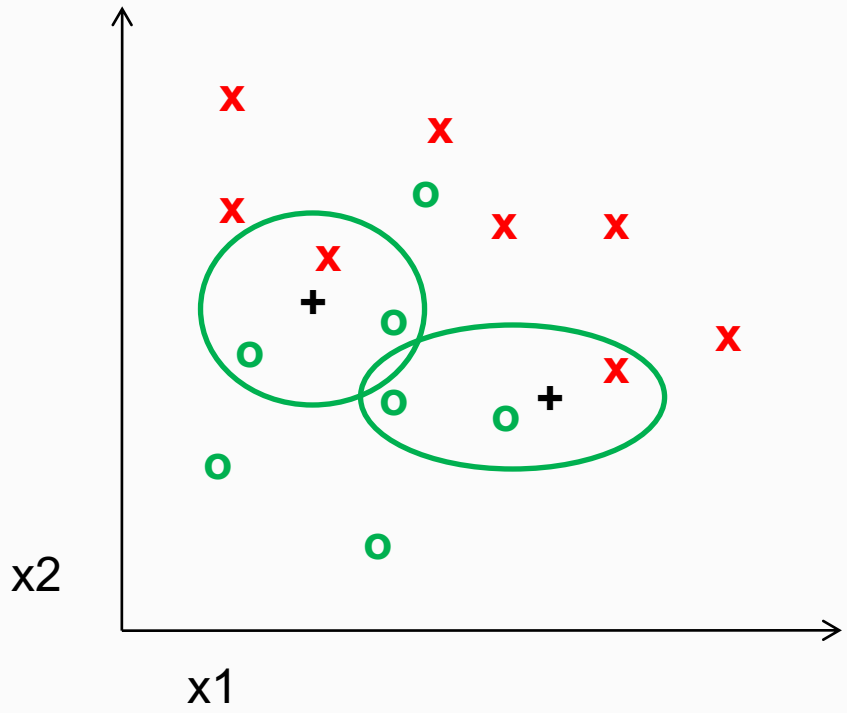
K-nearest neighbor



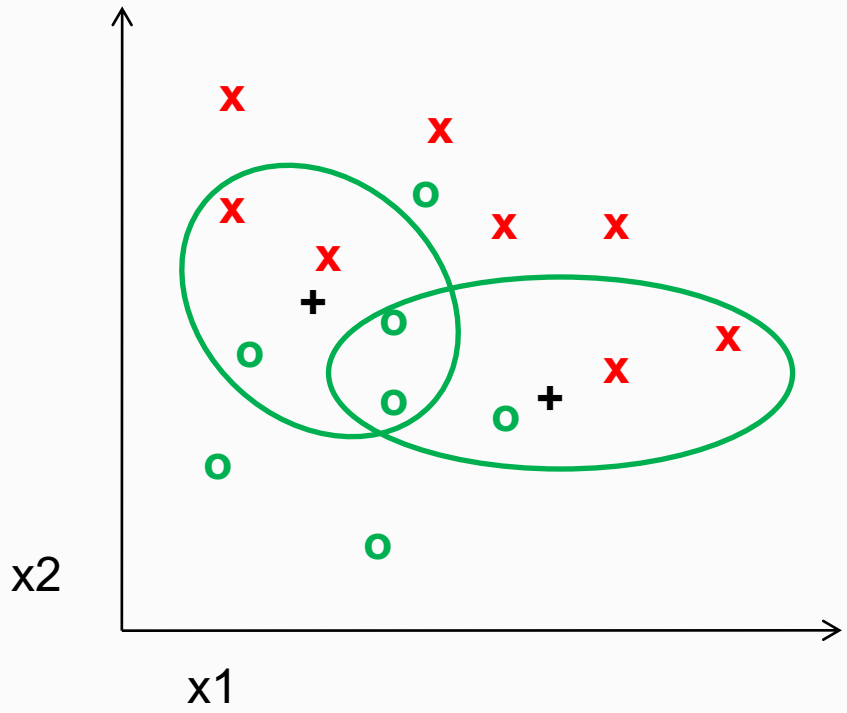
1-nearest neighbor



3-nearest neighbor



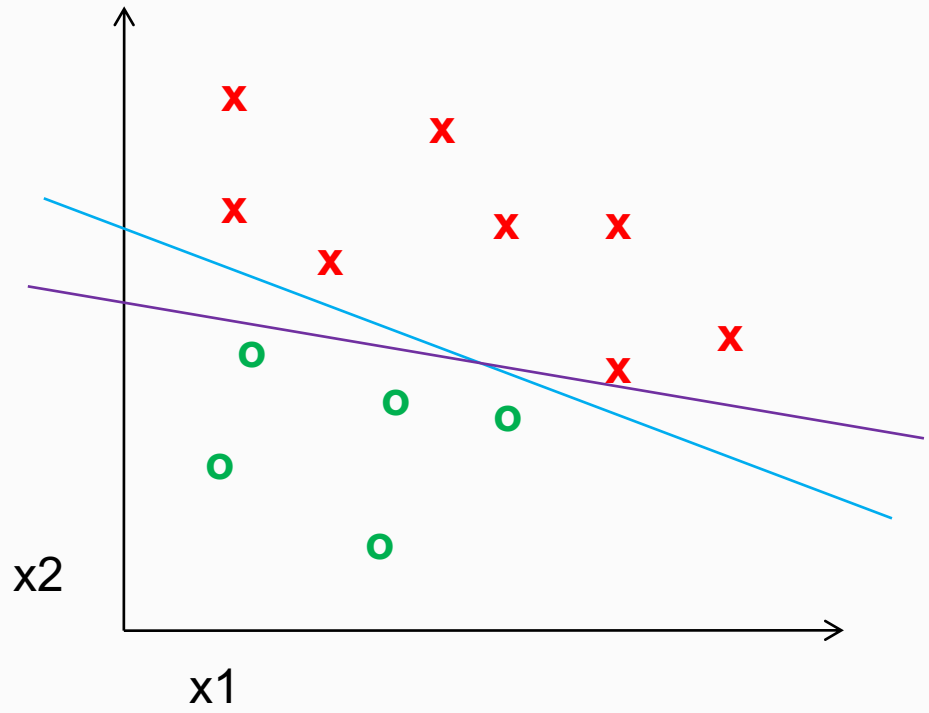
5-nearest neighbor



Using K-NN

- Simple, a good one to try first
- With infinite examples, 1-NN probably has error that is at most twice Bayes optimal error

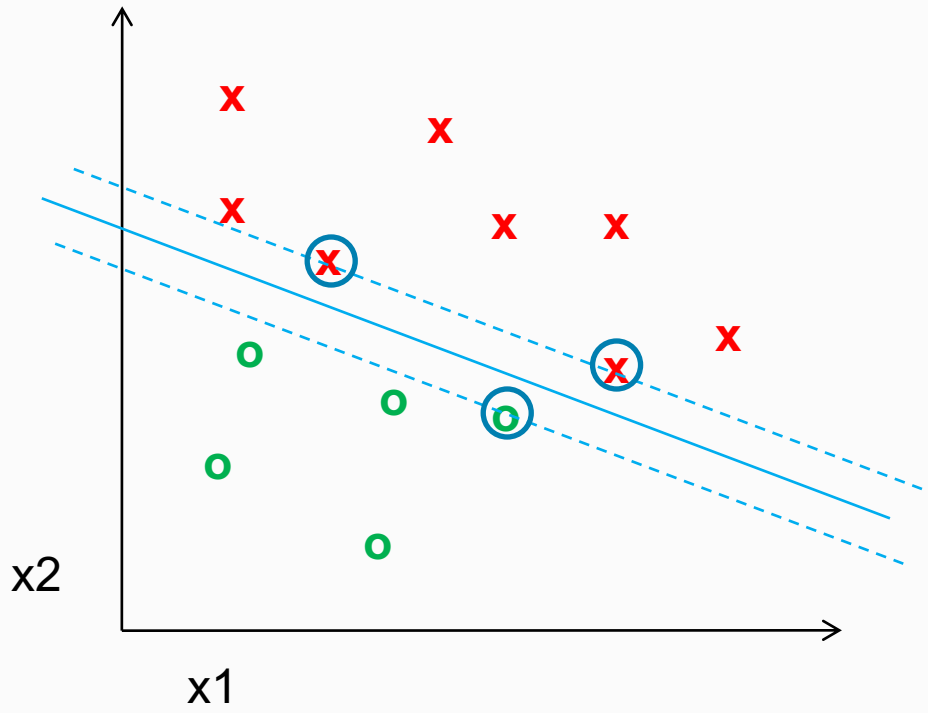
Classifiers: Linear SVM



- Find a *linear function* to separate the classes:

$$f(\mathbf{x}) = \text{sgn}(\mathbf{w} \cdot \mathbf{x} + b)$$

Classifiers: Linear SVM



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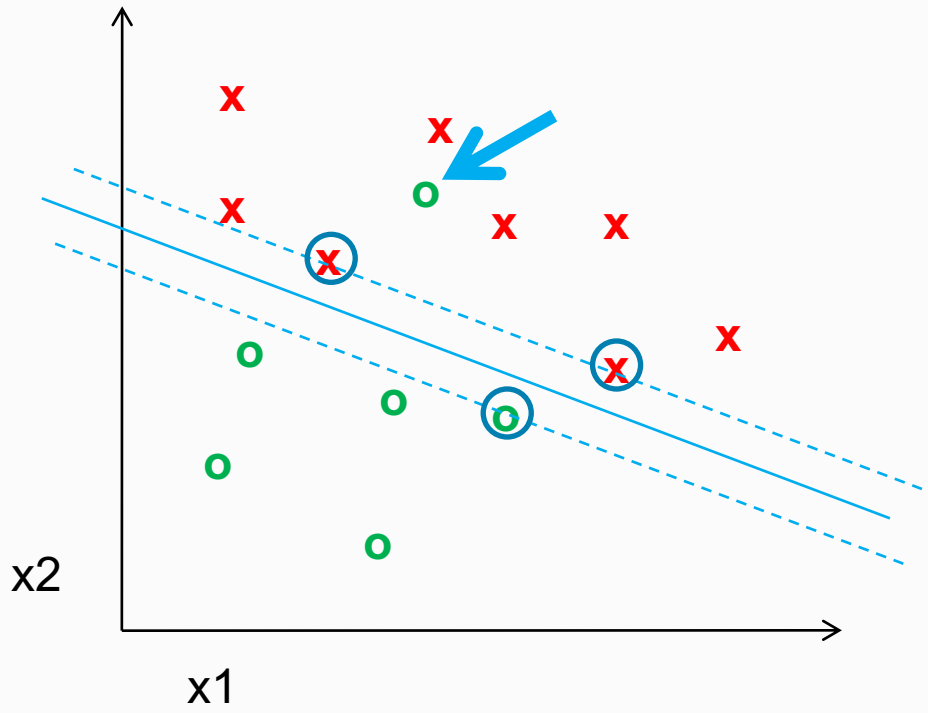
Classifiers: Linear SVM

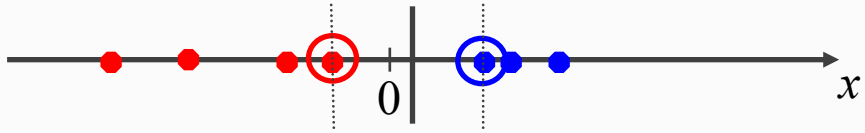


- Find a *linear function* to separate the classes:

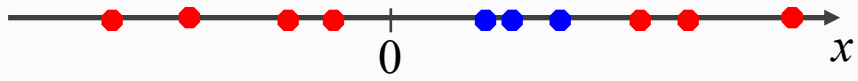
$$f(\mathbf{x}) = \text{sgn}(\mathbf{w} \cdot \mathbf{x} + b)$$

Nonlinear SVMs

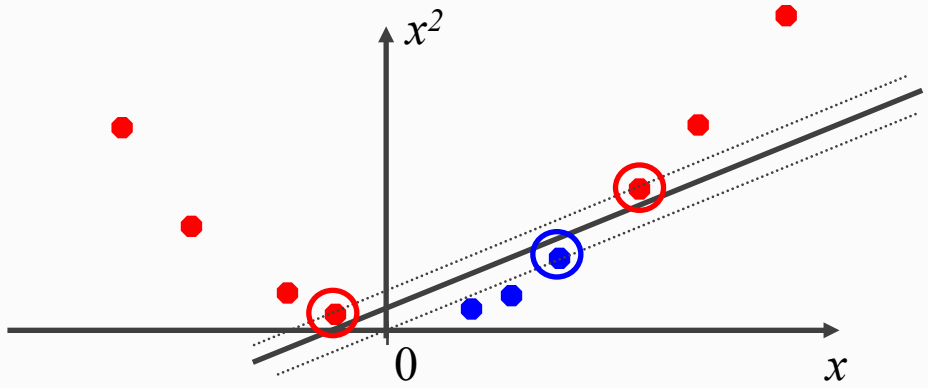
- Datasets that are linearly separable work out great:



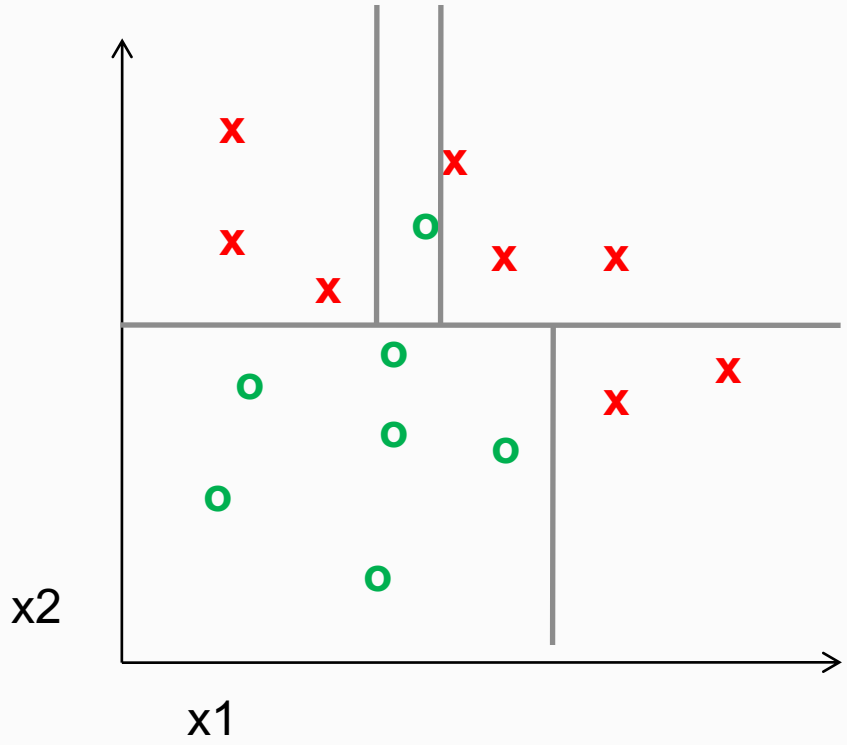
- But what if the dataset is just too hard?



- We can map it to a higher-dimensional space:



Classifiers: Decision Trees

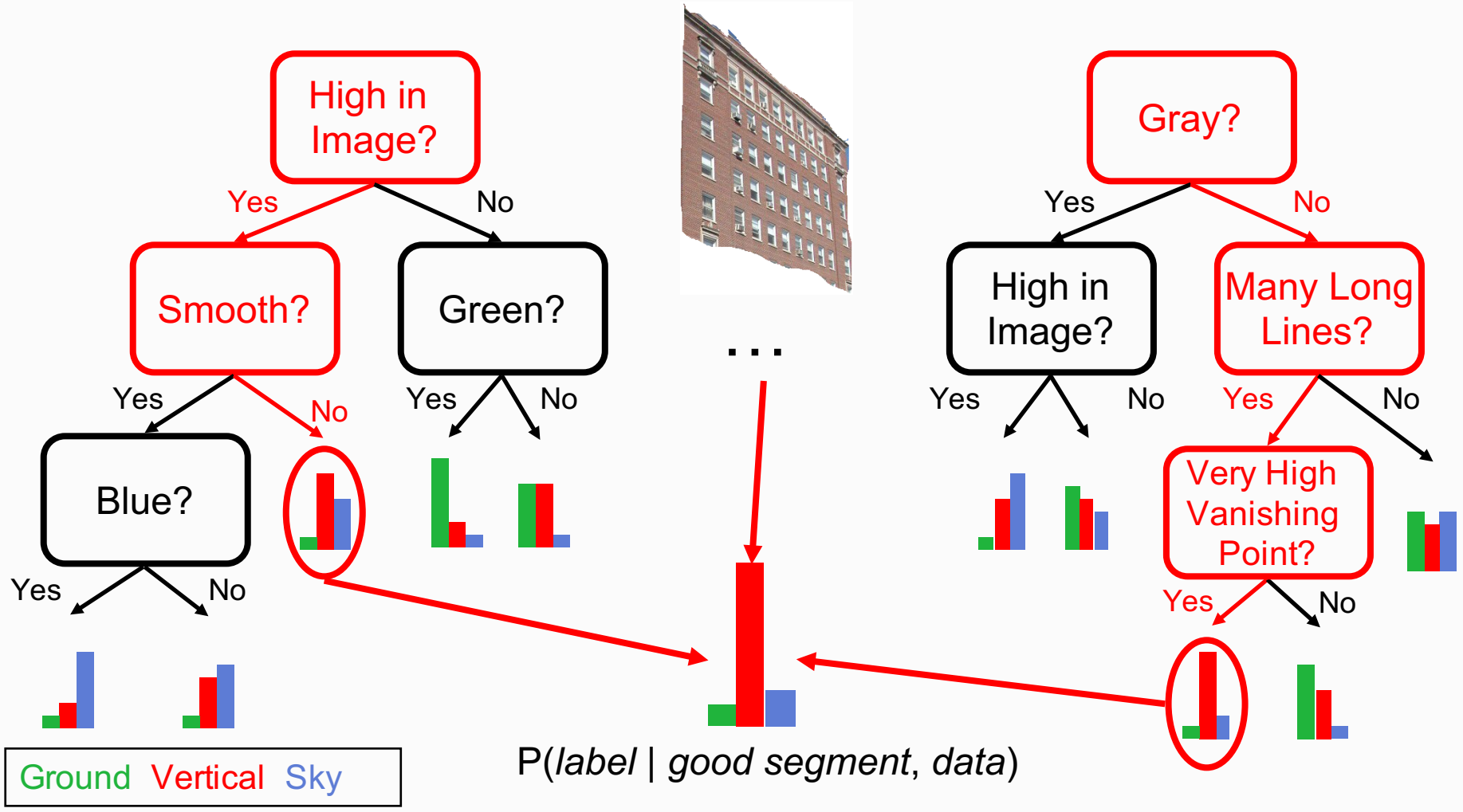


Ensemble Methods: Boosting

Discrete AdaBoost(Freund & Schapire 1996*b*)

1. Start with weights $w_i = 1/N$, $i = 1, \ldots, N$.
2. Repeat for $m = 1, 2, \ldots, M$:
   (a) Fit the classifier $f_m(x) \in \{-1, 1\}$ using weights w_i on the training data.
   (b) Compute $\text{err}_m = E_w[1_{(y \neq f_m(x))}]$, $c_m = \log((1 - \text{err}_m)/\text{err}_m)$.
   (c) Set $w_i \leftarrow w_i \exp[c_m \cdot 1_{(y_i \neq f_m(x_i))}]$, $i = 1, 2, \ldots N$, and renormalize so that $\sum_i w_i = 1$.
3. Output the classifier $\text{sign}[\sum_{m=1}^{M} c_m f_m(x)]$

Boosted Decision Trees



Model Validation

- To estimate generalization error, we need data unseen during training. We split the data as
  - Training set (50%)
  - Validation set (25%)
  - Test (publication) set (25%)

- **Resample** when there is **few data**
- **Resample** from **the minority** when there is **data skew**

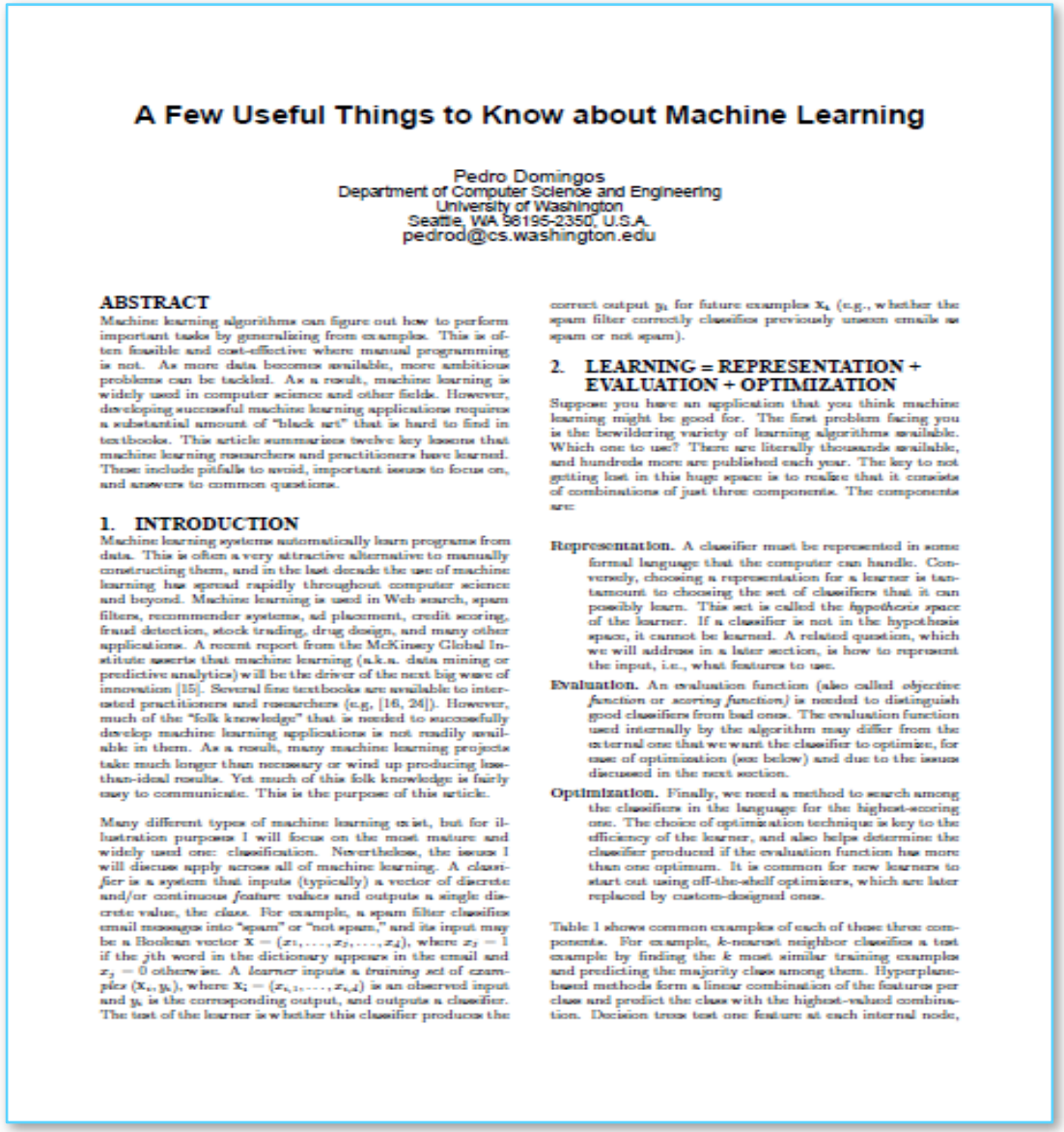
Evaluating Models

- Infinite data is best, but…
- N (**N=10**) Fold cross validation
  - Create N folds or subsets from the training data (approximately equally distributed with approximately the same number of instances).
  - Build N models, each with a different set of N-1 folds, and evaluate each model on the remaining fold
  - Error estimate is average error over all N models

What to remember about classifiers

- Try simple classifiers first
- Better to have smart features and simple classifiers than simple features and smart classifiers
- Use increasingly powerful classifiers with more training data (bias-variance tradeoff)

Reading



A Few Useful Things to Know about Machine Learning

Pedro Domingos
Department of Computer Science and Engineering
University of Washington
Seattle, WA 98195-2350, U.S.A.
pedrod@cs.washington.edu

ABSTRACT

Machine learning algorithms can figure out how to perform important tasks by generalizing from examples. This is often feasible and cost-effective where manual programming is not. As more data becomes available, more ambitious problems can be tackled. As a result, machine learning is widely used in computer science and other fields. However, developing successful machine learning applications requires a substantial amount of "black art" that is hard to find in textbooks. This article summarizes twelve key lessons that machine learning researchers and practitioners have learned. These include pitfalls to avoid, important issues to focus on, and answers to common questions.

1. INTRODUCTION

Machine learning systems automatically learn programs from data. This is often a very attractive alternative to manually constructing them, and in the last decade the use of machine learning has spread rapidly throughout computer science and beyond. Machine learning is used in Web search, spam filters, recommender systems, ad placement, credit scoring, fraud detection, stock trading, drug design, and many other applications. A recent report from the McKinsey Global Institute asserts that machine learning (a.k.a. data mining or predictive analytics) will be the driver of the next big wave of innovation [15]. Several fine textbooks are available to interested practitioners and researchers (e.g., [16, 24]). However, much of the "folk knowledge" that is needed to successfully develop machine learning applications is not readily available in them. As a result, many machine learning projects take much longer than necessary or wind up producing less-than-ideal results. Yet much of this folk knowledge is fairly easy to communicate. This is the purpose of this article.

Many different types of machine learning exist, but for illustration purposes I will focus on the most mature and widely used one: classification. Nevertheless, the issues I will discuss apply across all of machine learning. A *classifier* is a system that inputs (typically) a vector of discrete and/or continuous *feature* values and outputs a single discrete value, the *class*. For example, a spam filter classifies email messages into "spam" or "not spam," and its input may be a Boolean vector $\mathbf{x} = (x_1, \ldots, x_j, \ldots, x_d)$, where $x_j = 1$ if the jth word in the dictionary appears in the email and $x_j = 0$ otherwise. A *learner* inputs a *training set* of *examples* $(\mathbf{x}_i, y_i)$, where $\mathbf{x}_i = (x_{i,1}, \ldots, x_{i,d})$ is an observed input and y_i is the corresponding output, and outputs a classifier. The test of the learner is whether this classifier produces the correct output y_t for future examples $\mathbf{x}_t$ (e.g., whether the spam filter correctly classifies previously unseen emails as spam or not spam).

2. LEARNING = REPRESENTATION + EVALUATION + OPTIMIZATION

Suppose you have an application that you think machine learning might be good for. The first problem facing you is the bewildering variety of learning algorithms available. Which one to use? There are literally thousands available, and hundreds more are published each year. The key to not getting lost in this huge space is to realize that it consists of combinations of just three components. The components are:

Representation. A classifier must be represented in some formal language that the computer can handle. Conversely, choosing a representation for a learner is tantamount to choosing the set of classifiers that it can possibly learn. This set is called the *hypothesis space* of the learner. If a classifier is not in the hypothesis space, it cannot be learned. A related question, which we will address in a later section, is how to represent the input, i.e., what features to use.

Evaluation. An evaluation function (also called *objective function* or *scoring function*) is needed to distinguish good classifiers from bad ones. The evaluation function used internally by the algorithm may differ from the external one that we want the classifier to optimize, for ease of optimization (see below) and due to the issues discussed in the next section.

Optimization. Finally, we need a method to search among the classifiers in the language for the highest-scoring one. The choice of optimization technique is key to the efficiency of the learner, and also helps determine the classifier produced if the evaluation function has more than one optimum. It is common for new learners to start out using off-the-shelf optimizers, which are later replaced by custom-designed ones.

Table 1 shows common examples of each of these three components. For example, k-nearest neighbor classifies a test example by finding the k most similar training examples and predicting the majority class among them. Hyperplane-based methods form a linear combination of the features per class and predict the class with the highest-valued combination. Decision trees test one feature at each internal node,

Some Machine Learning References

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  - Friedman, Hastie, and Tibshirani, “Additive logistic regression: a statistical view of boosting”, Annals of Statistics, 2000
- SVMs
  - http://www.support-vector.net/icml-tutorial.pdf

Data Science

Deriving Knowledge from Data at Scale

That's all for tonight….