# Supervised methods: Introduction and evaluation

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# Outline

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# Supervised Learning definition

## Definition

**Given:** A dataset $D$ of observations, usually represented as a table where each row is an observation and each column a descriptor.

**Goal**: Learn to predict one column of the dataset, named *label*, for new data.

# Dataset example

Table (5 fields, 151 records) #2

File Edit Generate

Table Annotations

| | Sepal_len_cm | Sepal_wid_cm | Petal_len_cm | Petal_wid_cm | Class |
|---|---|---|---|---|---|
| 1 | 5.100 | 3.500 | 1.400 | 0.200 | Iris-setosa |
| 2 | 4.900 | 3.000 | 1.400 | 0.200 | Iris-setosa |
| 3 | 4.700 | 3.200 | 1.300 | 0.200 | Iris-setosa |
| 4 | 4.600 | 3.100 | 1.500 | 0.200 | Iris-setosa |
| 5 | 5.000 | 3.600 | 1.400 | 0.200 | Iris-setosa |
| 6 | 5.400 | 3.900 | 1.700 | 0.400 | Iris-setosa |
| 7 | 4.600 | 3.400 | 1.400 | 0.300 | Iris-setosa |
| 8 | 5.000 | 3.400 | 1.500 | 0.200 | Iris-setosa |
| 9 | 4.400 | 2.900 | 1.400 | 0.200 | Iris-setosa |
| 10 | 4.900 | 3.100 | 1.500 | 0.100 | Iris-setosa |
| 11 | 5.400 | 3.700 | 1.500 | 0.200 | Iris-setosa |
| 12 | 4.800 | 3.400 | 1.600 | 0.200 | Iris-setosa |
| 13 | 4.800 | 3.000 | 1.400 | 0.100 | Iris-setosa |
| 14 | 4.300 | 3.000 | 1.100 | 0.100 | Iris-setosa |
| 15 | 5.800 | 4.000 | 1.200 | 0.200 | Iris-setosa |

# Supervised Learning examples

## Some examples

- From a dataset of bank costumers, *predict* whether a new costumer will return a loan or not.
- From a dataset of images of digits, learn to *identify* the digit represented by a new image.
- From a dataset of emails, learn to *distinguish* between SPAM and not SPAM.
- From a dataset of Magnetoencephalography recordings of patients, *diagnose* whether a new individual is schizophrenic or not.

# Supervised Learning as Classification

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- All the previous tasks were examples of *learning* (why?) to *classify* (a lot of tasks can be expressed as classification tasks)
- Notice that labels are discrete values (in other case we are talking about *regression*)
- In order to classify an object in a right class, we need to build a *classifier*

# Supervised Learning constraints

Usual considerations:

- Dataset contains **positive** and **negative** examples for each labels.
- Examples are randomly sampled (i.i.d.).
- ... Other assumptions later on.

# Outline

# Generalization

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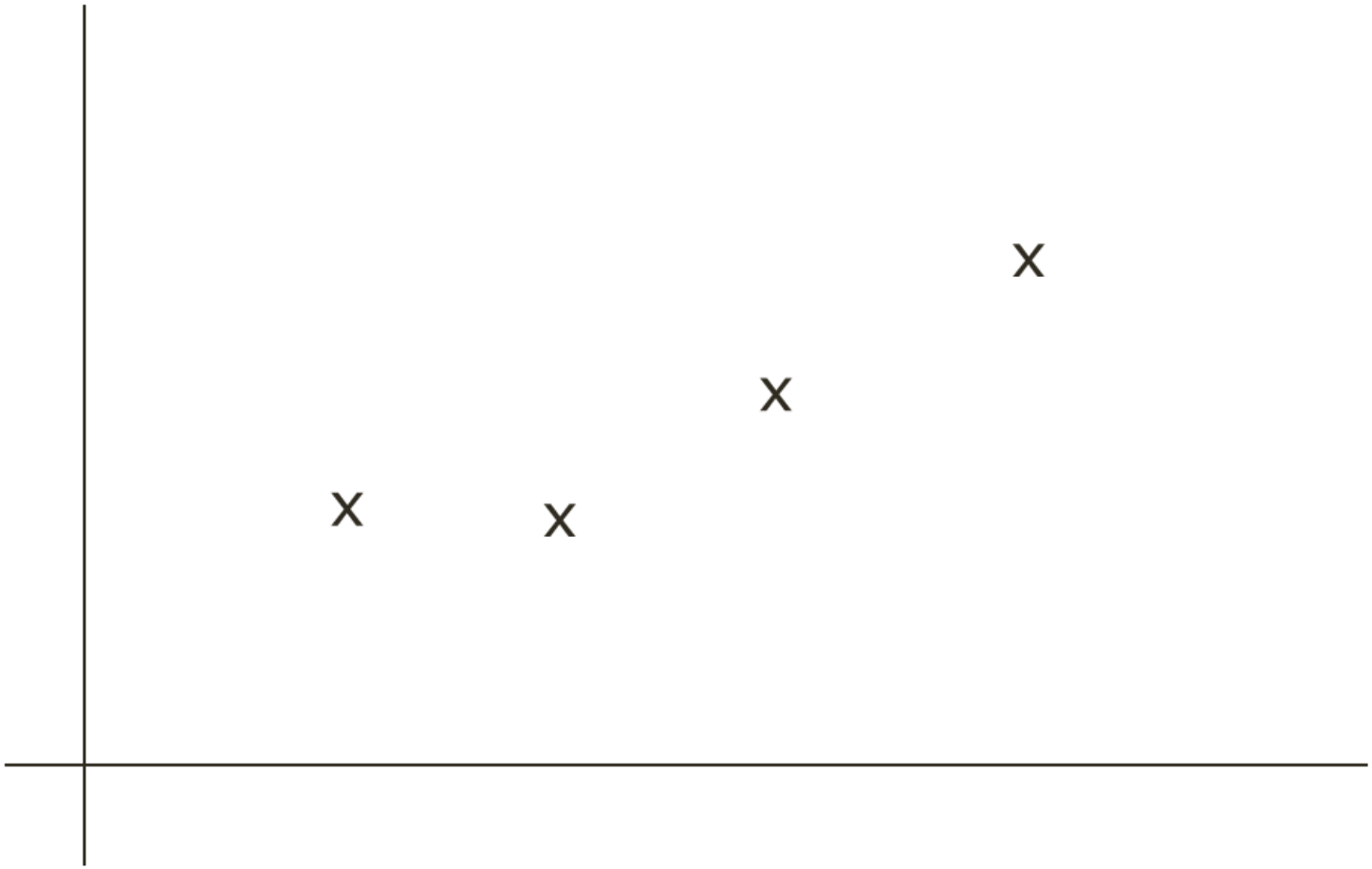
- But which is the source of the magic of generalization?

**... Simplicity**

# Generalization



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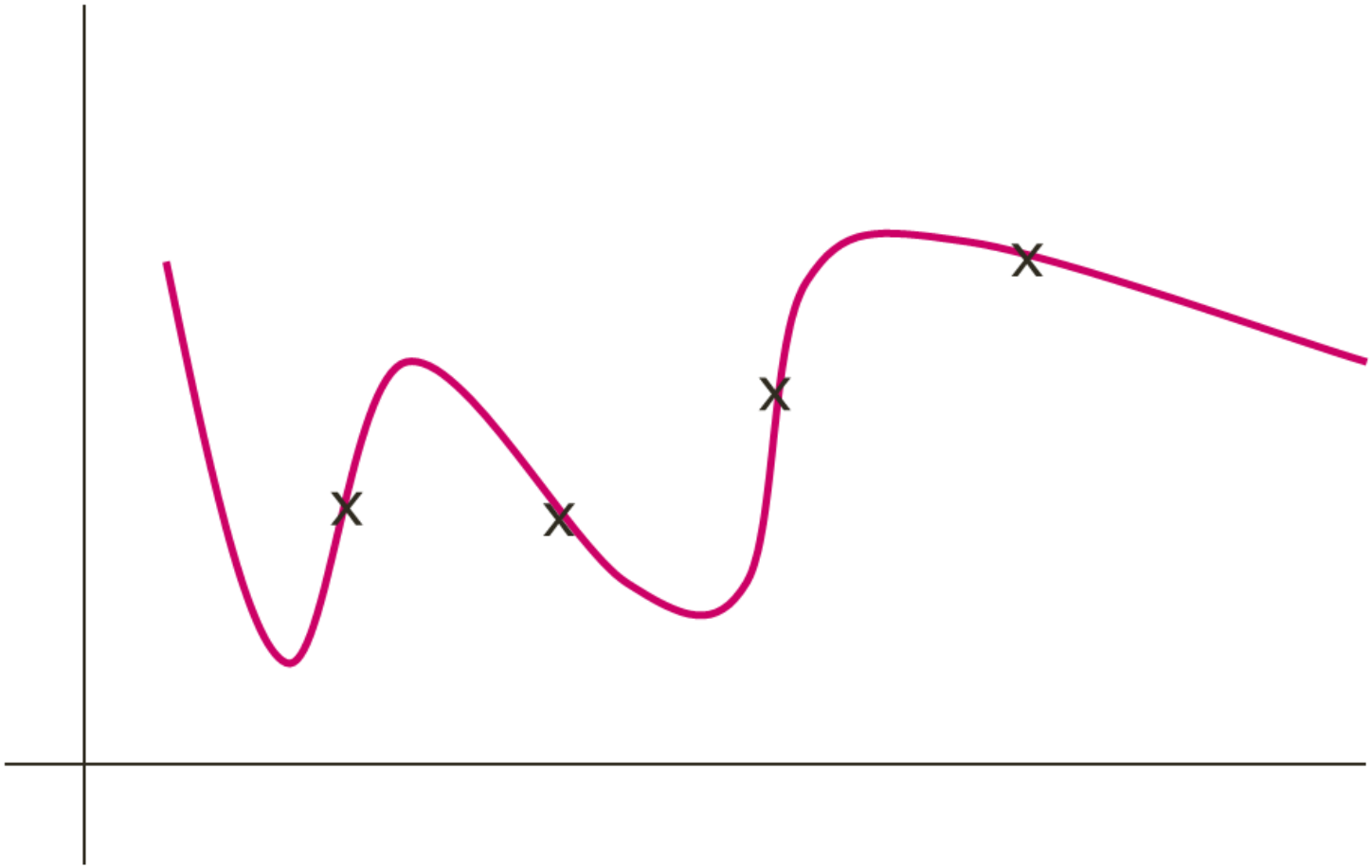

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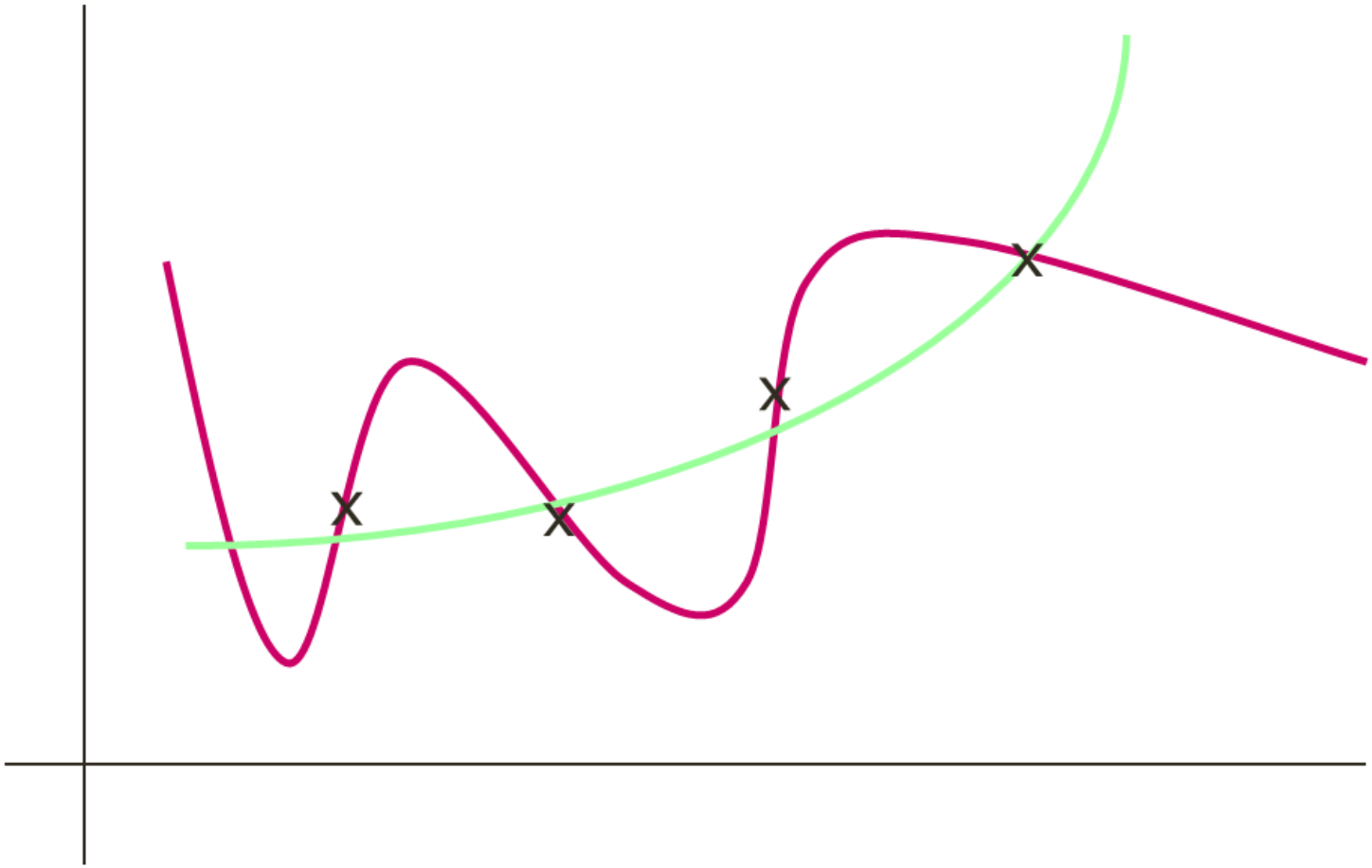

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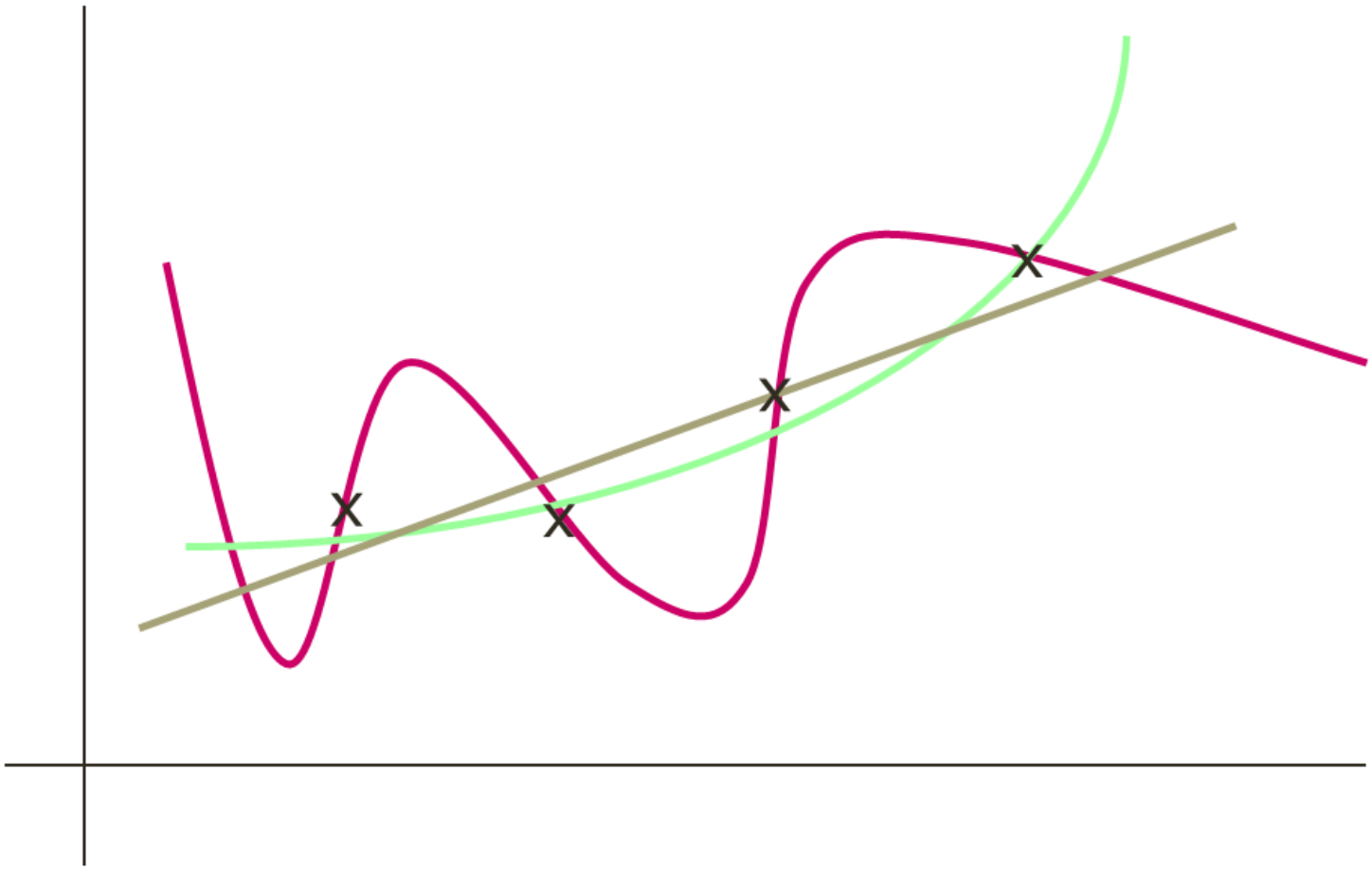

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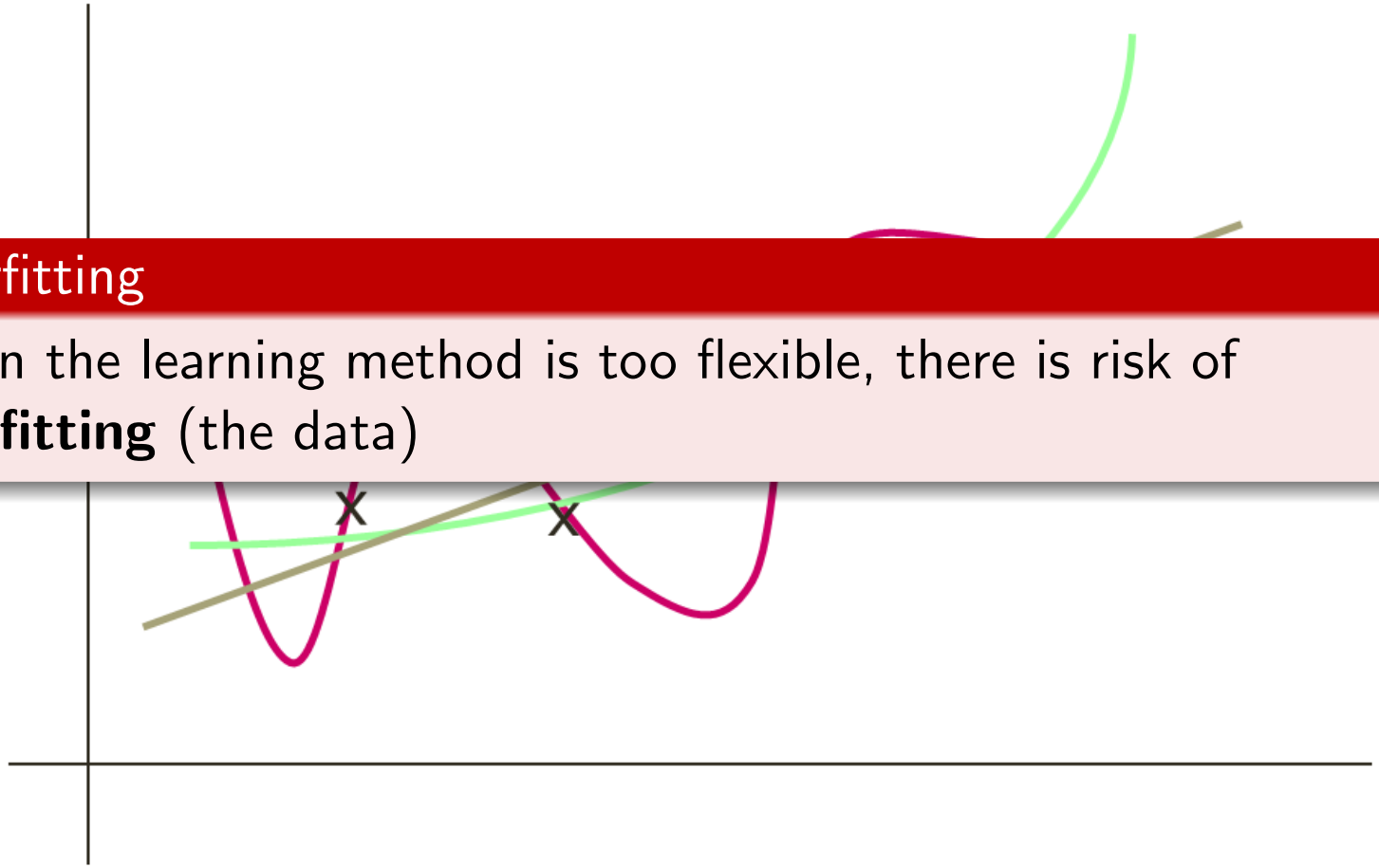

**Overfitting**

When the learning method is too flexible, there is risk of **overfitting** (the data)

# Generalization

Any learning method will show a tendency to *simple explanations* for data:

- Shortest description:
  - Minimum description length
  - Shortest tree size
  - Fewest parameters model
  - Independence of columns
- Regularization about complexity of the classifier:
  - Values of parameters (f.i. limited weight in neural networks)
  - Trade-off on capacity of classifier and error

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- Data mining in supervised mode has a target column.
- Differently than in the case of clustering, now we have an objective way to measure the success of classifiers: Test new cases with the classifier and check predicted labels with reality.

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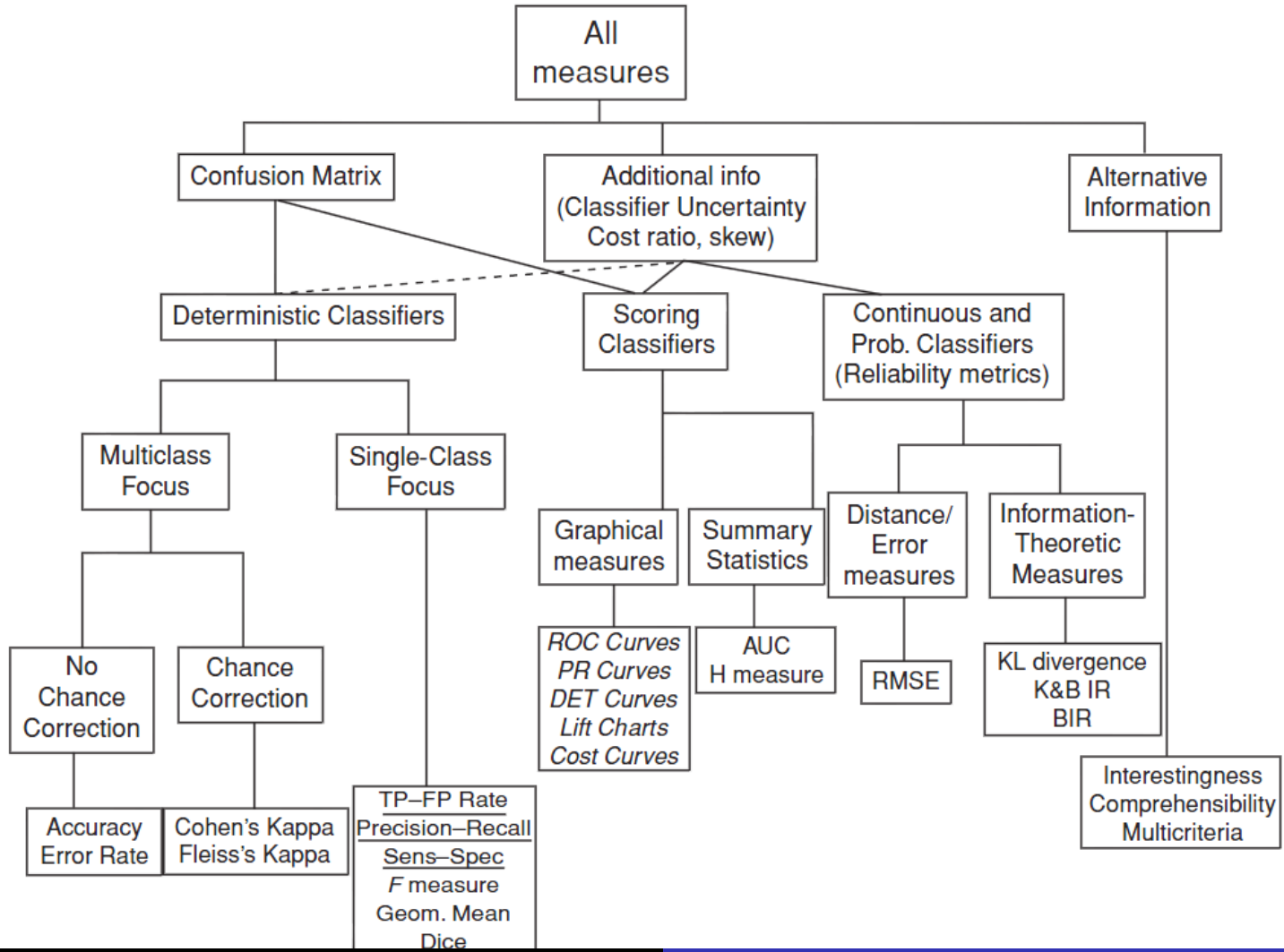
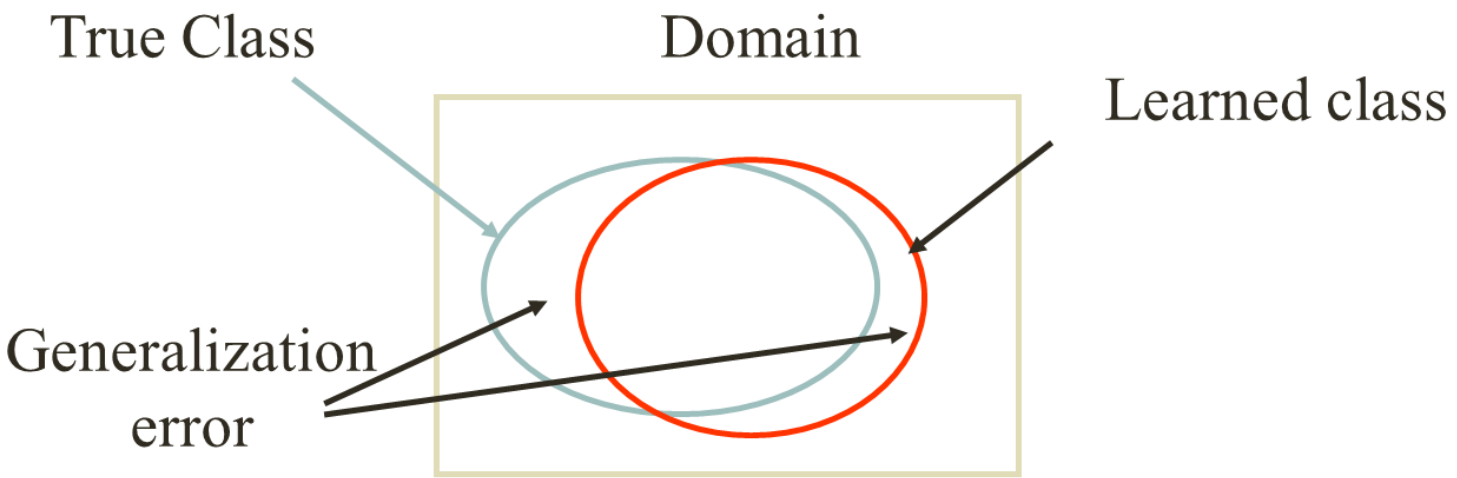
- Data mining in supervised mode has a target column.
- Differently than in the case of clustering, now we have an objective way to measure the success of classifiers: Test new cases with the classifier and check predicted labels with reality.
- But not so easy. There are a lot of different measures to qualify success of a classifier.

# Measures


All measures
Confusion Matrix
Additional info (Classifier Uncertainty Cost ratio, skew)
Alternative Information
Deterministic Classifiers
Scoring Classifiers
Continuous and Prob. Classifiers (Reliability metrics)
Multiclass Focus
Single-Class Focus
Graphical measures
Summary Statistics
Distance/ Error measures
Information-Theoretic Measures
No Chance Correction
Chance Correction
ROC Curves
PR Curves
DET Curves
Lift Charts
Cost Curves
AUC
H measure
RMSE
KL divergence
K&B IR
BIR
Accuracy
Error Rate
Cohen's Kappa
Fleiss's Kappa
TP–FP Rate
Precision–Recall
Sens–Spec
F measure
Geom. Mean
Dice
Interestingness
Comprehensibility
Multicriteria

# Measures




$$E_{empiric} = \frac{1}{n}\sum_{i}^{n} \left\| \{ i \mid H(x_i) \neq C(x_i) \} \right\|$$

# Confussion matrix

Given a classifier, asses the error it produces on a set of instances from the **confusion matrix**:

| | *Actually Positive* | *Actually Negative* |
|---|---|---|
| *Predicted Positive* | True Positive cases (TP) | False Positive cases (FP) |
| *Predicted Negative* | False Negative cases(FN) | True Negative cases (TN) |

Each entry is the number of instances.

# Measures based on confusion matrix

| | *Actually Positive* | *Actually Negative* |
|---|---|---|
| *Predicted Positive* | True Positive cases (TP) | False Positive cases (FP) |
| *Predicted Negative* | False Negative cases(FN) | True Negative cases (TN) |

## Accuracy

**Accuracy**: Empiric error on the set of cases given

$$Ac = \frac{TP + TN}{TP + TN + FP + FN}$$

# Measures based on confusion matrix

**Accuracy is not a good measure when:**

- Unbalanced datasets
- Different costs for each kind of error

| | *Act. Pos.* | *Act. Neg.* |
|---|---|---|
| *Pred. Pos.* | 10 | 100 |
| *Pred. Neg.* | 40 | 300 |

| | *Act. Pos.* | *Act. Neg.* |
|---|---|---|
| *Pred. Pos.* | 50 | 140 |
| *Pred. Neg.* | 0 | 260 |

**Unbalanced case:** Assume we are interested in detecting one kind of documents from a large corpus. Both tables same accuracy but show different behaviors.

# Measures based on confusion matrix

**Accuracy is not a good measure when:**

- Unbalanced datasets
- Different costs for each kind of error

| | *Act. Pos.* | *Act. Neg.* |
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**Different costs:** Assume cost of misclassifying a positive case is 10 times misclassifying a negative case. Same accuracy but different cost.

# Measures based on confusion matrix

Measures taken from document classification (imbalanced case)

- **Recall**: Proportion of positive cases that were detected

$$R = \frac{TP}{TP + FN}$$

- **Precision**: Proportion of positive cases with respect the number of cases labeled positive

$$P = \frac{TP}{TP + FP}$$

- **F-measure**: Harmonic mean of Recall and Precision

$$F = \frac{2}{\frac{1}{P} + \frac{1}{R}} = \frac{2PR}{P + R}$$

# ROC curve

When the classifier can return *belief* in prediction, then we can obtain different predicitons by changing the cut-off point that separates examples. We can plot then the ROC curve (FP *vs.* TP rate).

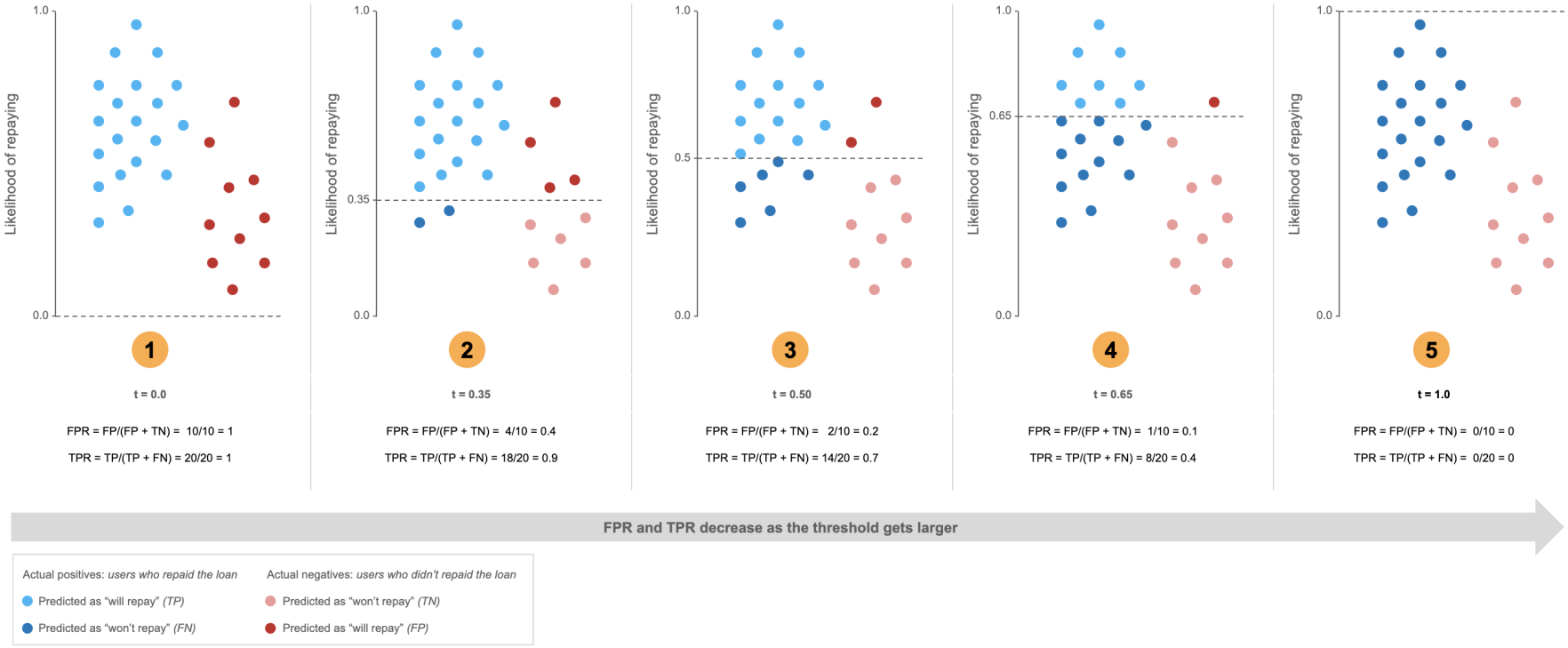
- True Positive Rate (TPR):

$$TPR = \frac{TP}{TP + FN}$$

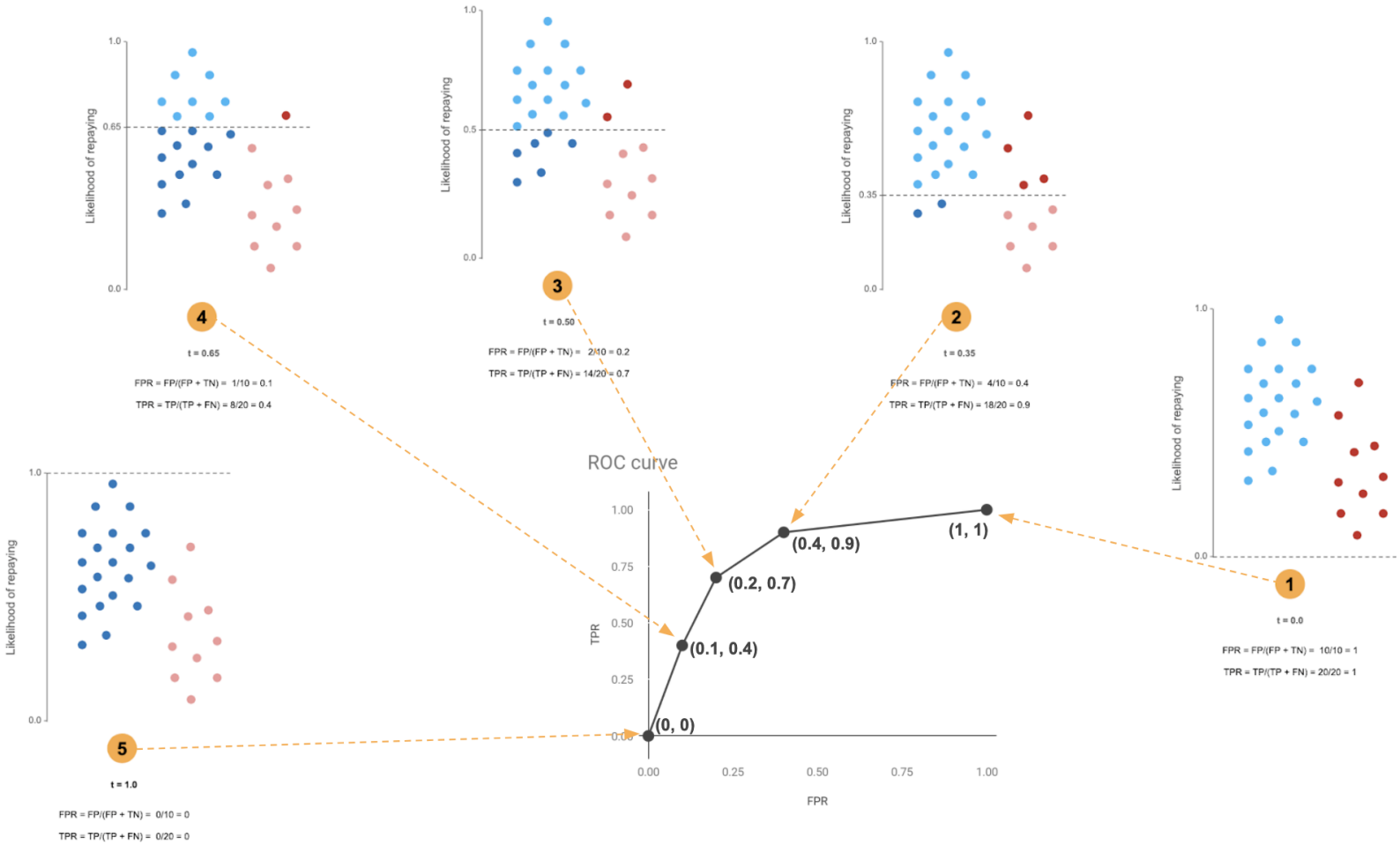
- False Positive Rate (FPR):

$$FPR = \frac{TN}{TN + FP}$$

# ROC curve


Likelihood of repaying
1.0
0.0
1
t = 0.0
FPR = FP/(FP + TN) = 10/10 = 1
TPR = TP/(TP + FN) = 20/20 = 1
0.35
2
t = 0.35
FPR = FP/(FP + TN) = 4/10 = 0.4
TPR = TP/(TP + FN) = 18/20 = 0.9
0.5
3
t = 0.50
FPR = FP/(FP + TN) = 2/10 = 0.2
TPR = TP/(TP + FN) = 14/20 = 0.7
0.65
4
t = 0.65
FPR = FP/(FP + TN) = 1/10 = 0.1
TPR = TP/(TP + FN) = 8/20 = 0.4
5
t = 1.0
FPR = FP/(FP + TN) = 0/10 = 0
TPR = TP/(TP + FN) = 0/20 = 0
FPR and TPR decrease as the threshold gets larger
Actual positives: users who repaid the loan
Predicted as "will repay" (TP)
Predicted as "won't repay" (FN)
Actual negatives: users who didn't repaid the loan
Predicted as "won't repay" (TN)
Predicted as "will repay" (FP)

# ROC curve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5
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FPR = FP/(FP + TN) = 0/10 = 0
TPR = TP/(TP + FN) = 0/20 = 0
ROC curve
TPR
FPR
0.00
0.25
0.50
0.75
1.00
(0, 0)
(0.1, 0.4)
(0.2, 0.7)
(0.4, 0.9)
(1, 1)

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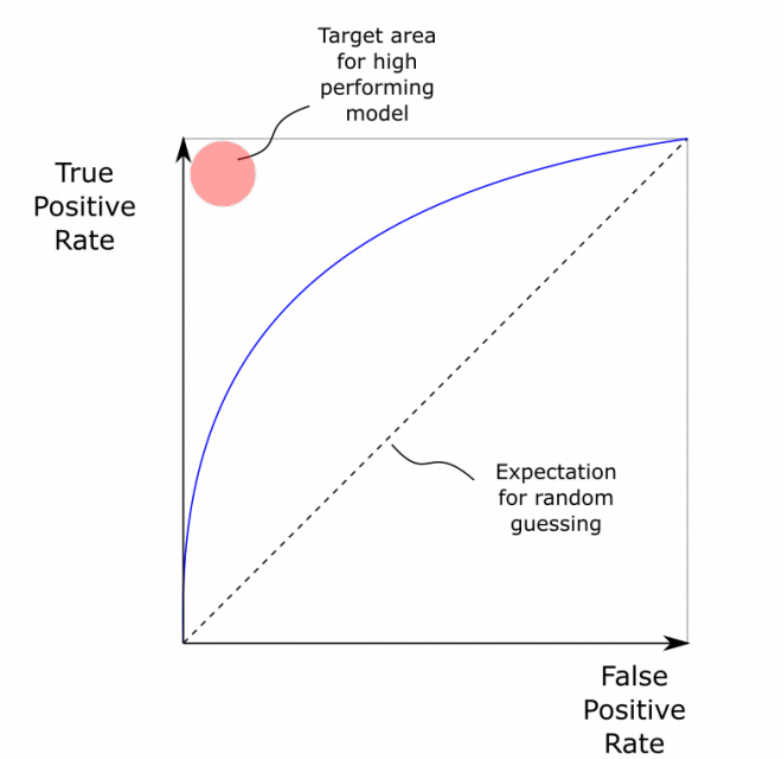
When the classifier can return *belief* in prediction, then we can obtain different predicitons by changing the cut-off point that separates examples. We can plot then the ROC curve (FP *vs.* TP rate).




- Are Under Curve (AUC) measure to compare classifiers
- Interesting to find best threshold for classifier
- ...specially good for imbalanced data sets

# Outline

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**Solution**

Do not use all your data for learning.... Keep some examples for testing!

# Cross-validation

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- Use more data for training than for testing. Usually 66% data for training - 33% of data testing

# Problems with cross-validation

- When data is scarce you "waste" your data for testing.
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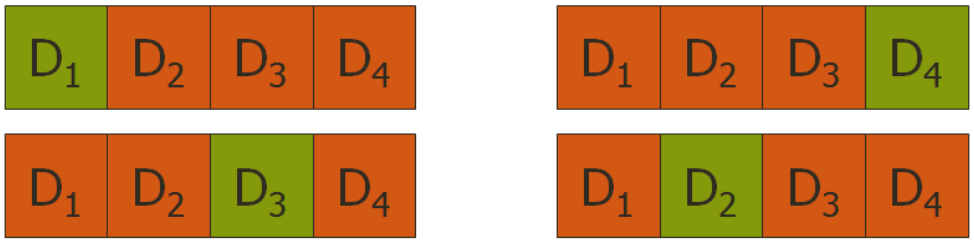
- More importantly, *results may depend on the split of data into training and testing.*
- How can we solve that?
- ... repeating the split several times and averaging results.
  - k-fold cross-validation
  - leave-one-out
  - Bootstrapping

# Outline

# k-fold cross-validation

**k-fold cross-validation:** Divide your dataset into $k$ disjoints subsets of equal length.


Repeat $k$ times the learning process, each time leaving out for testing a different subset.




Average the $k$ accuracy estimators.

# k-fold cross-validation

Advantages:

- More robust estimator (less variance)

Problems:

- We still waste 1/k of your data for testing
- We have to repeat the learning process $k$ times

How do we set $k$? Trade-off time/variance. Usually set to 5 or 10.

# Leave-one-out (LOO)

**Leave-one-out (LOO):** Extreme version of k-fold cross-validation where $k$ is set to $n$, the number of examples in your dataset.

Repeat $n$ executions of the learning algorithm with $n-1$ examples for learning and 1 for testing (every time a different one).

Average the $n$ estimators.

Obviously it takes time to compute, but takes maximum profit of examples and reduces variance of estimator.

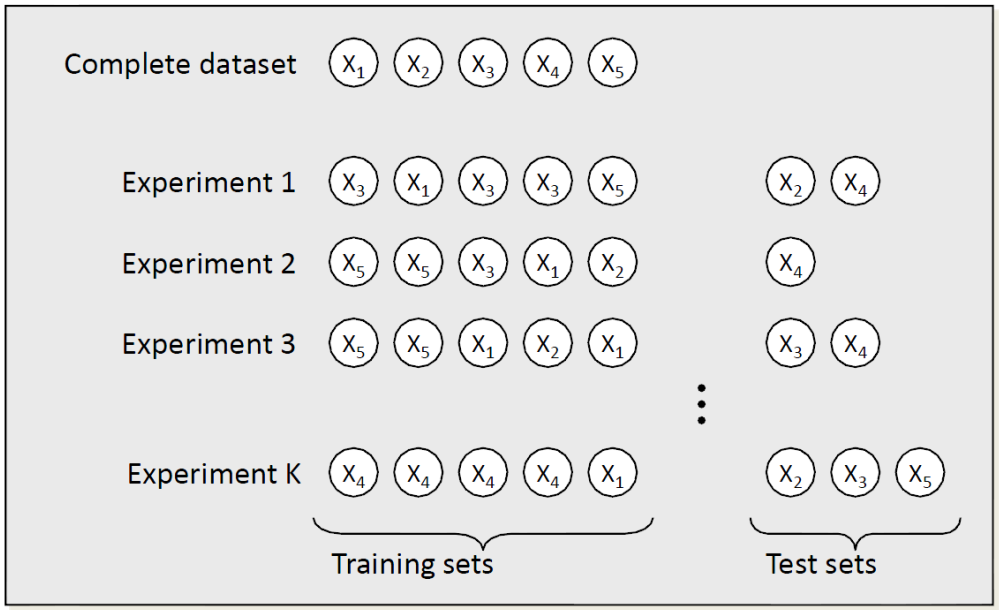
# Outline

# Bootstrapping

Repeat this process $K$ times (hundreds!):

- Randomly select (*with replacement*) $n$ examples for training
- Examples not selected for training are used for testing (number of examples is likely to change from fold to fold)

True error is estimated as the average error rate on test data



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- When $n\,\hat{\epsilon}\,(1-\hat{\epsilon}) \geq 5$ binomial can be approximated by a Normal distribution with same mean and variance. So:

$$\hat{\epsilon} - z_{\alpha/2}\,\sigma \leq \epsilon \leq \hat{\epsilon} + z_{\alpha/2}\,\sigma$$

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- When $n\,\hat{\epsilon}\,(1-\hat{\epsilon}) < 5$, apply cumulative distribution function of binomial: prob. of doing maximum $k$ errors is $\Pr\{X \leq k\} = \sum_{i=0}^{k} \binom{n}{i} \hat{\epsilon}^i (1-\hat{\epsilon})^{n-i}$.

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```
binom.test(k, n, e, "less", conf.level)
```

# Confidence interval of averaging k classifiers

- Addition of Binomials can be approximated by Normal. So again:

$$\hat{\epsilon} - z_{\alpha/2}\,\sigma \leq \epsilon \leq \hat{\epsilon} + z_{\alpha/2}\,\sigma$$

But now, $\hat{\epsilon}$ is the average of all cross-validation runs and $\sigma = \sqrt{\frac{\hat{\epsilon}\,(1-\hat{\epsilon})}{n}}$ where $n$ is the numbre of examples used in all cross-validation runs

# Comparing two classifiers: McNemar's Test

- Goal: decide which of two classifiers $h_0$ and $h_1$ has lower error rate
- Run $h_0$ and $h_1$ and build the following table:

| | |
|---|---|
| $n_{00}$: number of cases both right | $n_{01}$: number of cases $h_0$ right and $h_1$ fails |
| $n_{10}$: number of cases $h_0$ fails and $h_1$ right | $n_{11}$: number of cases both fail |

# Comparing two classifiers: McNemar's Test

- Null hypothesis: $n_{01} = n_{10}$ (both same error)
- McNemar's Test:

$$M = \frac{(|n_{01} - n_{10}| - 1)^2}{n_{01} + n_{10}} > \chi^2_{1,\alpha}$$

- M is distributed approximately as $\chi^2$ with 1 degree of freedom. For a 95% confidence test, $\chi^2_{1,0.95} = 3.84$. So if M is larger than 3.84, then with 95% confidence, we can reject the null hypothesis
- Once we know they don't have the same error, which one is better?

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# Some observations:

1. Multi-class classification
2. Data preparation
3. General approaches to build classifiers

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# Multi-class problem

Some observations:

- In some classifiers labels are assumed to be binary: $+1/\text{-}1$
- We name *positive examples* to observations with label $+1$ and *negative examples* to observations with labels -1

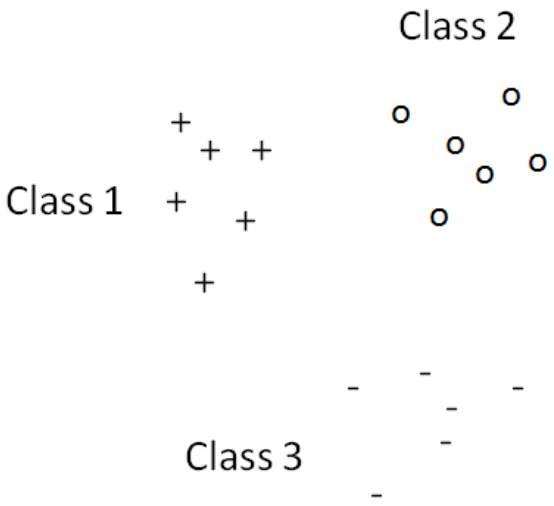
When labels are not binary we always can build a combination of classifiers

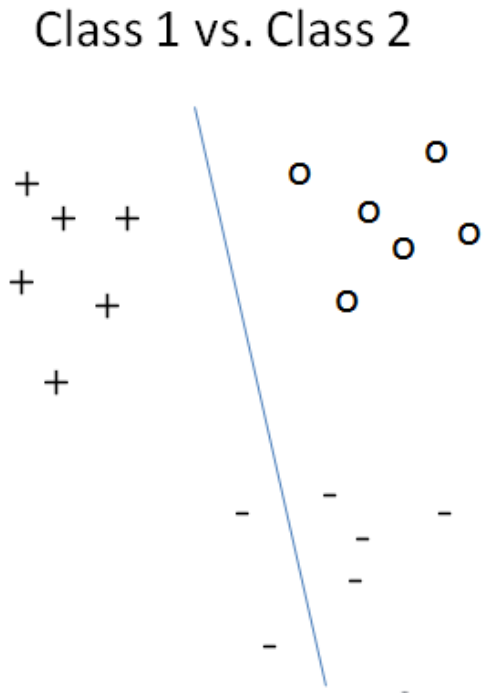
Two approximations:

- One versus One (OVO)
- One versus All (OVA)

# One Versus One

Given $k$ labels, learn to separate class 1 from 2, class 1 from 3, ... class 1 from $k$, class 2 from 3, class 2 from 4, ... class 2 from $k$, .... class $k-1$ from class $k$



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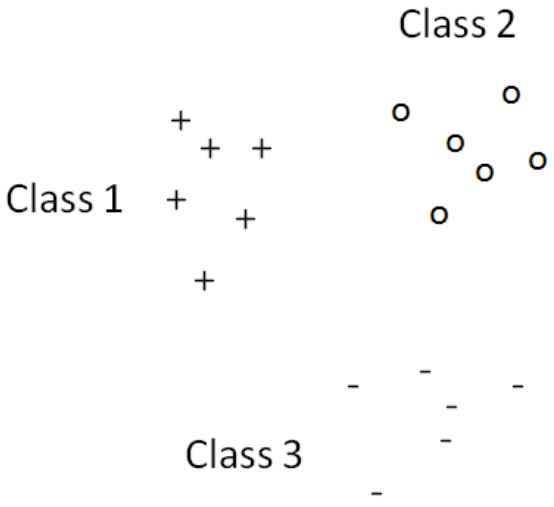


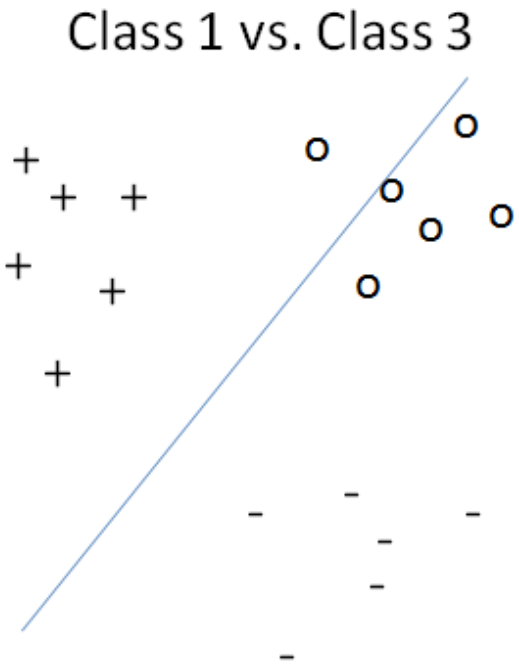

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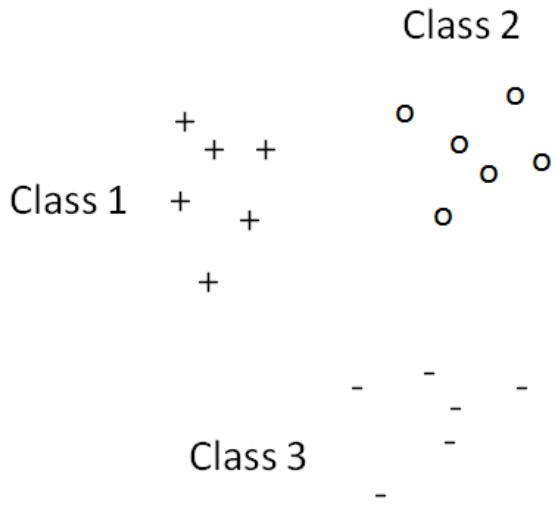


# One Versus One

After learning $\frac{k(k-1)}{2}$ classifiers, when label for a new observation is required, apply all classifiers and *vote*.

Ties are broken by randomly choosing one label.

Example:

| Classifier | Vote |
|---|---|
| 1 vs. 2 | 1 |
| 1 vs. 3 | 1 |
| 2 vs. 3 | 3 |

Final label: 1

# One Versus All

Given $k$ labels, learn to separate class 1 from all other classes, class 2 from all other classes .... class $k-1$ from all other classes.

# One Versus All

After learning $k$ classifiers, when label for a new observation is required, apply all classifiers and *vote*.

Ties are broken by randomly choosing one label.

Example:

| Classifier | Vote |
|---|---|
| 1 vs. All | 1 |
| 2 vs. All | All |
| 3 vs. All | All |

Final label: 1

# Some comments:

1. Multi-class classification
2. Data preparation
3. General approaches to build classifiers

# Dataset preparation

From now on, we assume we have a relatively clean dataset. That means:

- **No missing values**.
- Relevant features included in dataset (with not an overwhelming amount of irrelevant columns).
- Some algorithms only work with numerical data or with categorical data.
- Usually, we work with normalized or standardized data.

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# Relevant features

- Most algorithms work with a moderate amount of irrelevant columns. However, when the number of irrelevant columns is too much large, the algorithm can be fooled.
- Some methods remove irrelevant features (this is know as feature selection). For instance, sort features by some correlation measure with labels (Correlation, Information Gain, etc.) and keep the top ones.
- We'll see that in the next set of slides

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# When numerical data is needed

- Build a new column for each category.

| Object | Color |
|---|---|
| Obj1 | blue |
| Obj2 | green |
| Obj3 | green |
| Obj4 | red |

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| Object | Color |
|---|---|
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| Obj2 | green |
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$\Rightarrow$

| Object | blue | green | red |
|---|---|---|---|
| Obj1 | 1 | 0 | 0 |
| Obj2 | 0 | 1 | 0 |
| Obj3 | 0 | 1 | 0 |
| Obj4 | 0 | 0 | 1 |

# When categorical data is needed

Discretization of continuous data. Several approaches:

- Rounding (Decimation)
- Finding best cut places
  - Minimize:

$$ER = \sum_{n=1}^{k} \left( \sum_{i \in bin_k} |v_{i,n} - v_{\mathrm{moda},n}| \right)$$

    where $k$ is the number of bins (categories). For instance $\{1, 1, 2, 2, 2, 5, 6, 8, 8, 9\}$ into three bins: **A**$=\{1, 1, 2, 2, 2\}$, **B**$=\{5, 6\}$, **C**$=\{8, 8, 9\}$

  - Target oriented methods: Look for the statistically best splitting of data according to label distribution, f.i., ChiMerge method

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# Normalization and standardization

In order to give the same weight to all features we normalize the data to make them independent of units.

- Normalization 0,1:

$$v_i^n(k) = \frac{v_i(k) - min(v_i)}{max(v_i) - min(v_i)}$$

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- Standardization to mean 0, sigma 1

$$v_i^n(k) = \frac{v_i(k) - \mu(v_i)}{\sigma(v_i)}$$

# Some comments:

1. Multi-class classification
2. Data preparation
3. General approaches to build classifiers

# Supervised Learning as Classification

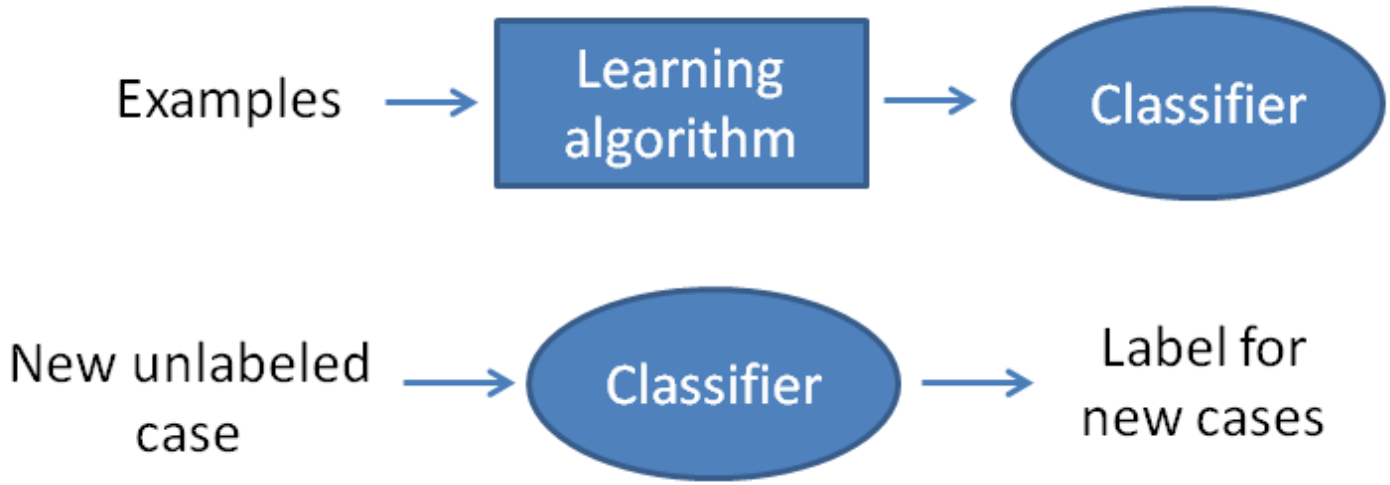
How to determine the right label for a given data? Use of learning algorithms (or data mining algorithms)

Two different approaches:

- Discriminative methods
- Generative methods

# Discriminative

Build a mechanism that allows to discriminate (separate) cases of different classes without any assumption about data



# Generative

Assume a parametric distribution of data, learn the parameters for the distribution (model the classes) and, when needed, find the most likely class for new observations.