Algorithmics for Data Mining

Master in Innovation and Research in Informatics
FIB, UPC

Department of Computer Science

Spring 2020

0. Course Presentation

Personnel

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Additionally, we plan for Prof. Josep Carmona to cover Business Process Mining.

Logistics

Schedule in the Racó with the initial plans.

- Quite low registration this year (about half the usual).
- The two half groups seem overkill, but the timing is not compatible.
- Could we reach an agreement on a more sensible decision?

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Additional personal conversations as needed:

- Usually available after each of our sessions;
- recommended (but not enforced) to warn me in advance by email;
- many alternative slots for appointments, again by email.

Written Support

Link to the evolving slides:
`www.cs.upc.edu/~balqui/slidesADM2020.pdf`

Link will be made available also from the Racó.

Several books available in the Main Library BRGF

(please take initiative, look for them, browse through them...)

and also freely online (like `this one`, or also `that one`...).

Mainly, individually agreed research papers for state-or-the-art advances on each topic.

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  - the second one, just before the Easter break;

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  - the second one, just before the Easter break;
  - the deadlines for third and fourth will depend on whether you give a presentation.

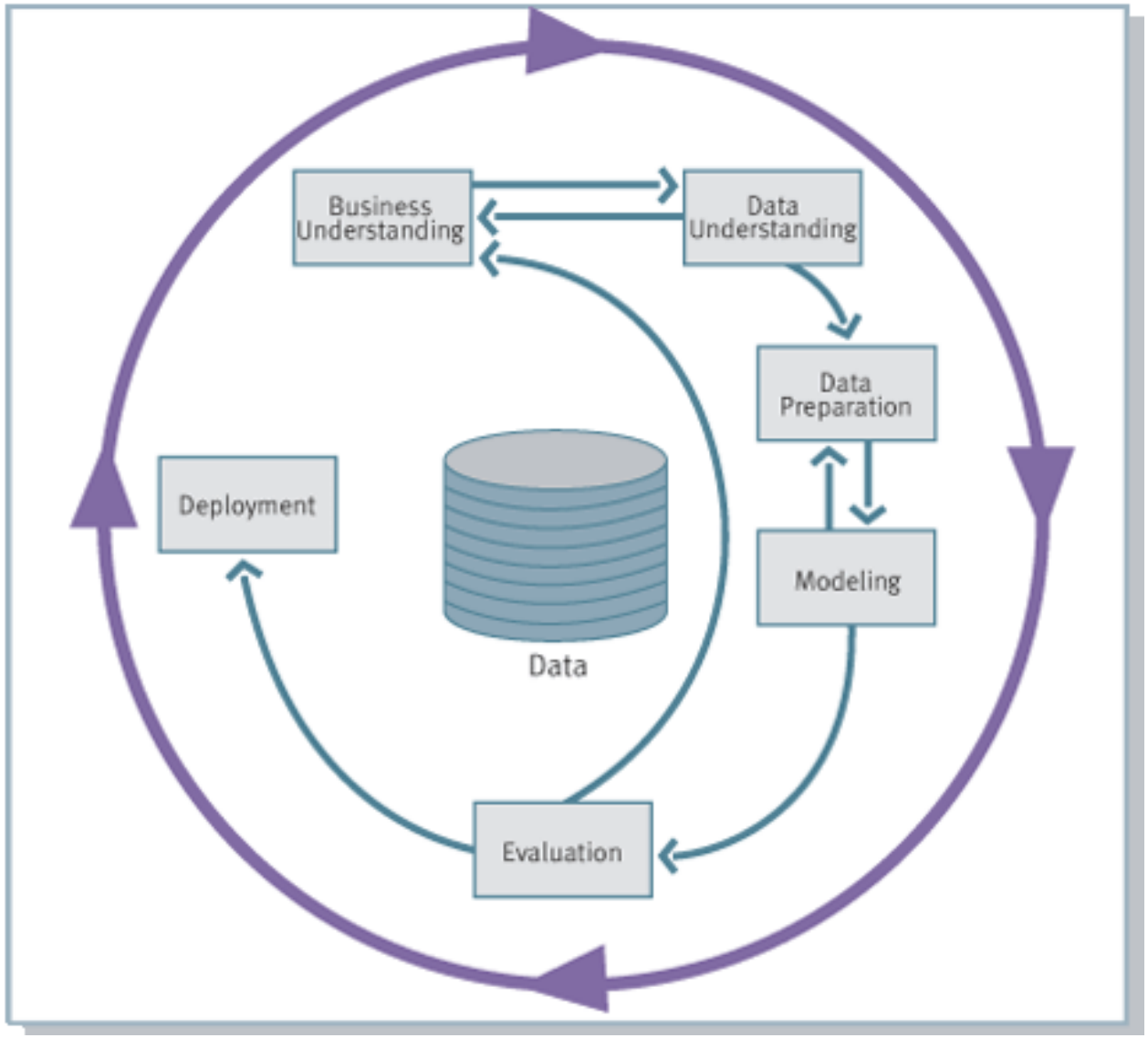
Evaluation, II

Expected characteristics

- "Your papers" must have a substantial content related to the topic of the course.
- Teamwork allowed, but:
  - Not for a paper that acts as basis of an oral presentation, and
  - your sets of coworkers on different papers must be disjoint.
- At least one of them (recommended: the first one) is to be on usage of a Data Mining tool for some Data Mining task.
- Under the previous conditions, the more your papers resemble original research papers, the better.
- Ask me if in need of clarification or if you want to propose some justified variant (I am likely to accept it).

CRISP-DM

Industry-designed diagram (1996)



Course Contents

Difficulty

Some of you may be attending, or have already listened to, courses similar to this one.

- We all must accept that there will be duplicities.
- Want most of these to still turn out to be useful!
  - By refreshing known but forgotten content,
  - By expanding the understanding,
  - By deepening the understanding.

Approximate topic guidance

- Book: The "Top Ten" Algorithms in Data Mining, `http://crcpress.com/product/isbn/9781420089646`,
- Preceding survey paper with same title, `http://link.springer.com/article/10.1007/s10115-007-0114-2`,
- plus a few variations and deeper considerations.

Taxonomy of Modeling Tools in Data Mining

Careful: not universal

- Predictive Models (always "supervised"):
  - Classification (Discrimination): non-numeric, unstructured prediction space
  - Categorization and Multiclassification: non-numeric, structured prediction space
  - Ranking: non-numeric prediction on a total ordering
  - Regression (Interpolation): numeric prediction space
    - Linear,
    - Polynomial,
    - ...
- Descriptive Models (possibly "unsupervised"):
  - Humanly interpretable predictors,
  - Clustering,
  - Pattern mining:
    - Frequent sets, frequent closures,
    - Association rule mining,
    - Pattern set mining...

Relational Data

Most common for starters

Relational data:

- Structured in tuples of attribute/value pairs.
- Akin to a SQL table.
- Often reformulated as a cloud of points in R^n.
- To predict: the value of one chosen "class" attribute.

Toy Relational Data

A simple and somewhat famous example that probably you have seen before

outlook	temperature	humidity	windy	play
sunny	hot	high	false	no
sunny	hot	high	true	no
overcast	hot	high	false	yes
rainy	mild	high	false	yes
rainy	cool	normal	false	yes
rainy	cool	normal	true	no
overcast	cool	normal	true	yes
sunny	mild	high	false	no
sunny	cool	normal	false	yes
rainy	mild	normal	false	yes
sunny	mild	normal	true	yes
overcast	mild	high	true	yes
overcast	hot	normal	false	yes
rainy	mild	high	true	no

(Source today: Witten & Frank "Data Mining".)

Transactional Data, I

Alternative context, usual for pattern mining

Each observation is seen as a data structure on itself.

On the basis of a set of atomic items:

- Simplest (and most common) case: each observation is a set. (Analogy: documents as sets of terms.)
- Slight sophistication: multiplicity is relevant (but is likely to need adjustements; analogy: tfidf-like weights. . .).
- Further sophistications!

We will return to transactional data every now and then; but, for the time being, we work mostly with relational data.

Missing Topics

(Some of) The most important notions we are not discussing

- Time Series (very important in practice);
- Visual Analytics;
- OLAP;
- Data Streams;
- Neural Models (hint at connection at the approprate time);
- ...

Practical Data Analysis, I

Tools: Programming, GUIs, and workflows

Approaches

- Programming or CLI's: mostly "verbal", visualization basically reduced to graphics of the results of analysis;

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- Programming or CLI's: mostly "verbal", visualization basically reduced to graphics of the results of analysis;
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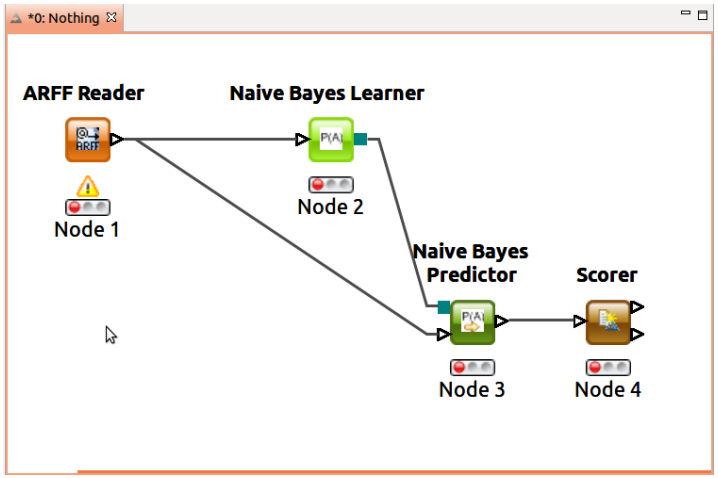
- Workflows: very much visual; everything (or almost) is handled graphically: movable icons, contextual menus to configure... — may be successful with managers.



Practical Data Analysis, II

Tools: Specific proposals

Who's who

`Recent poll` from `http://www.kdnuggets.com` (or navigate `http://www.kdnuggets.com` → `Polls`...)

- Tools with a different originary purpose:
  - Python, R, EXCEL, SQL...
- More or less traditional GUI:
  - Weka Explorer, FRIDA...
- Workflow-based:
  - KNIME, RapidMiner, Weka Knowledge Flows, Orange...
  - Cloud-supported `clowdflows`, not very mature yet but you are welcome to give it a try.
- Omitted from this course: Visual Analytics tools (Tableau, Spotfire, Qlik...)

Practical Data Analysis, III

About most datasets

To keep in mind:

Blindly feeding the data into your data analysis tools is unlikely to work well!

A substantial amount of reading and thinking must be spent in preprocessing and transformation.

`https://www.kdnuggets.com/2015/05/data-science-inconvenient-truth.html`

Practical Data Analysis, IV

Where to explore for datasets

Main dataset sources:

- `mldata.org`,
- `https://www.kaggle.com/competitions`,
- the classical `archive.ics.uci.edu/ml/`:
  - Car evaluation (synthetic),
  - Mushroom (semi-synthetic),
  - Adult (a.k.a. "census income"),
  - Congressional Voting Records,
  - Contraceptive Method Choice,
  - Covertype,
  - (Statlog) German Credit Scoring,
  - (Statlog) Shuttle...

Additional data sources for the politically motivated:
`http://databank.worldbank.org`

(and plenty of others out there!)

1. Intro to KNIME

Lab Session 1, I

http://KNIME.org

Get KNIME working on your machine!

- On Linux, only installation necessary is uncompressing the tarball.
- Self-installer on Windows: run it, keep going...
- Folder for your workflows: maybe on cloud?

Lab Session 1, IV

KNIME Nodes

Learn to:

- read in data;
- transform data matrices:
  - handle sorting criteria for visualizing tables,
  - identify and change the types of columns,
  - perform other data manipulation operations:
    column/row filters, group-by, join, sampling...
  - handle collection columns;
- get a glimpse of the basic statistics of your data;
- visualize and plot data;
  - create interactive tables, hilite instances, and propagate the highlighter marks,
  - create and manipulate scatter plots,
  - handle colors, sizes, and shapes,
  - create histograms, line plots, box plots...

Count on a bit of help from the instructor when necessary.

2. Brief Probability Review

Probabilistic Tools

Recap

1. Probability space, events, random variables;

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$$conf(A \to B) = Pr(B \mid A) = \frac{supp(AB)}{supp(A)};$$

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$$Pr(A \wedge B) = Pr(A) * Pr(B),$$
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$$Pr(B \mid A) = Pr(B);$$

5. Bayes Rule: $Pr(A|B) = Pr(B|A) * Pr(A)/Pr(B)$.

Numerical Spaces and Expectation

Main property: Linearity

If random outcomes allow for the operations of addition and of multiplication by a real number (for instance, real vectors), we can use probabilities to compute expectations, that is, weighted averages:

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Properties:

- Linearity of expectation: $E[\sum_i \alpha_i * A_i] = \sum_i (\alpha_i * E[A_i])$.
- For independent events, commuting with product: $E[A * B] = E[A] * E[B]$ provided $Pr(A \wedge B) = Pr(A) * Pr(B)$.

Counterintuitive Facts About Probability, I

"Rosencrantz and Guildenstern are dead" (Link)

Some context: http://en.wikisource.org/wiki/The_Tragedy_of_Hamlet,_Prince_of_Denmark/Act_5

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  Actually, no.

  They are independent events!
- Related:
  - http://en.wikipedia.org/wiki/Ludic_fallacy.
  - "Bayesian" point of view: infer that the coins are not fair.

Counterintuitive Facts About Probability, II

Three doors in TV

Monty Hall paradox:

There are three doors. All participants know the rules:

- Behind one door there is a prize ("the car"). Behind the others, less desirable items ("big pumpkins", "goats").
- You choose one door.
- Monty Hall opens one door, different from the one you have chosen: the prize is not there.
- Then he asks you: do you want to switch?

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The first correct answer right away is actually another question: What do we mean by "better"?

But, for a sensible notion of "better", it is better to switch.

Counterintuitive Facts About Probability (III)

Expectation of linearity

Simpson's Paradox:

Somebody has performed a survey.

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No! We cannot make that inference. It is possible that the comparison of the ratios gets reversed upon considering the whole population.

Counterintuitive Facts About Probability (IV)

Don't place too much confidence on confidence

Dataset CMC (Contraceptive Method Choice)

A "partial implication" of over 10% support and 90% confidence:

`near-low-wife-education` `no-contraception-method`

$\longrightarrow$

`good-media-exposure`

Seems like a reliable "partial implication".

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But the support of "`good-media-exposure`" is over 92%.

The "correlation" is actually negative!

3. Predictors and their Evaluation

Probabilistic Prediction

Probability-based predictive models

Probabilistic prediction

In a merely frequentist sense: counting;

- when is the prediction to be issued?
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- when is the prediction to be issued?
  - before seeing anything?
    "a priori" predictor: the most common value for the class
    (*ZeroR* predictor);
  - after seeing all values for all non-class attributes?
    "a posteriori" predictor: the most common value for the class, conditioned to the values seen
    (*MAP* predictor, for "maximum a posteriori").

$$\arg\max_C \{Pr(C|A_1 \ldots A_n)\}$$

MAP Prediction

Unfortunately infeasible

A small case:

Task of binary classification:

- Assume ten attributes with four values each;
- Then we need to store 2^{20} conditional probabilities;
- and we need to estimate 2^{20} conditional probabilities.

Rule of thumb:

Ten or more observations per parameter to estimate might be still far from sufficient, but are necessary anyway; with less, don't even dream.

Conditional Independence Assumption

One way out

Bayes rule

Applied to arg $\max_C \{Pr(C|A_1 \ldots A_n)\}$:

$$Pr(C|A_1 \ldots A_n) =$$
$$Pr(A_1 \ldots A_n|C) * Pr(C)/Pr(A_1 \ldots A_n)$$

We can forget about the divisor, as it is the same for all values of C and does not modify the max.

Now we assume independence conditioned to the class value:

$$Pr(A_1 \ldots A_n|C) * Pr(C) =$$
$$Pr(A_1|C) * \ldots * Pr(A_n|C) * Pr(C)$$

Naïve Bayes

Rather good for such a simple approach

Precompute $Pr(A_i|C)$ for each value of each attribute conditioned to the class value; do it through the empirical frequency.

Instead of predicting

$$\arg\max_C\{Pr(C|A_1 \ldots A_n)\},$$

we predict

$$\arg\max_C\{Pr(A_1|C) * \ldots * Pr(A_n|C) * Pr(C)\}$$

Variant: the "Laplace correction" makes up for cases that might be potentially missing; some tools (like Weka) apply it (without warning).

Autonomous Learning Topics, I

Proposals to explore on yourself

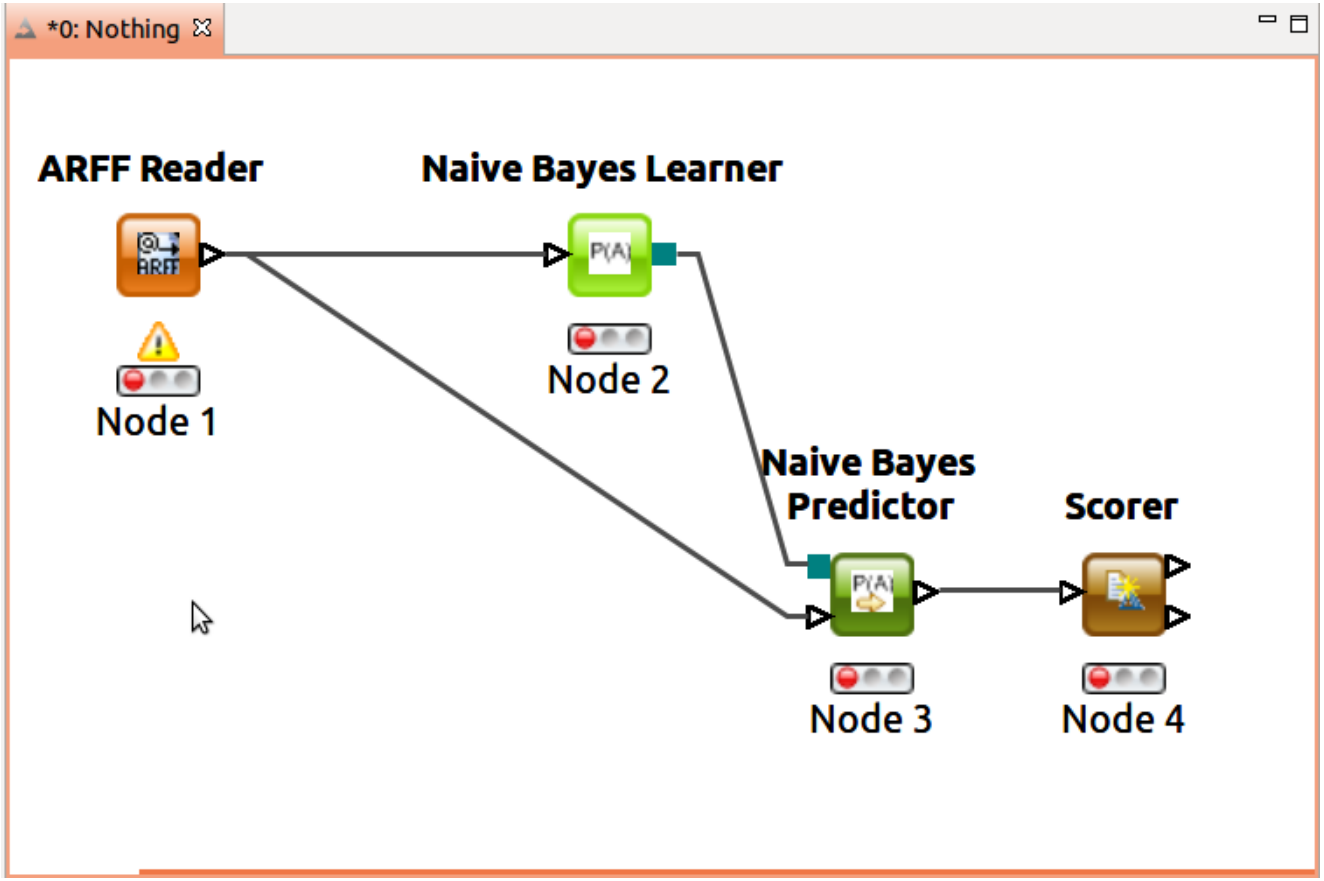
Some of these, if worked out in sufficient depth, may provide us with one of your four papers for the evaluation of the course.

1. Learn all details of the usage of Naïve Bayes predictors in various systems like R, KNIME, scikit-learn... (including the notion and usage of the Laplace correction).
2. Write your own implementation of MAP and Naïve Bayes in your favorite programming language (or, even better, in a programming language you don't master yet but want to practice further with).

How to Test a Predictor, I

On the original data?

Resubstitution error



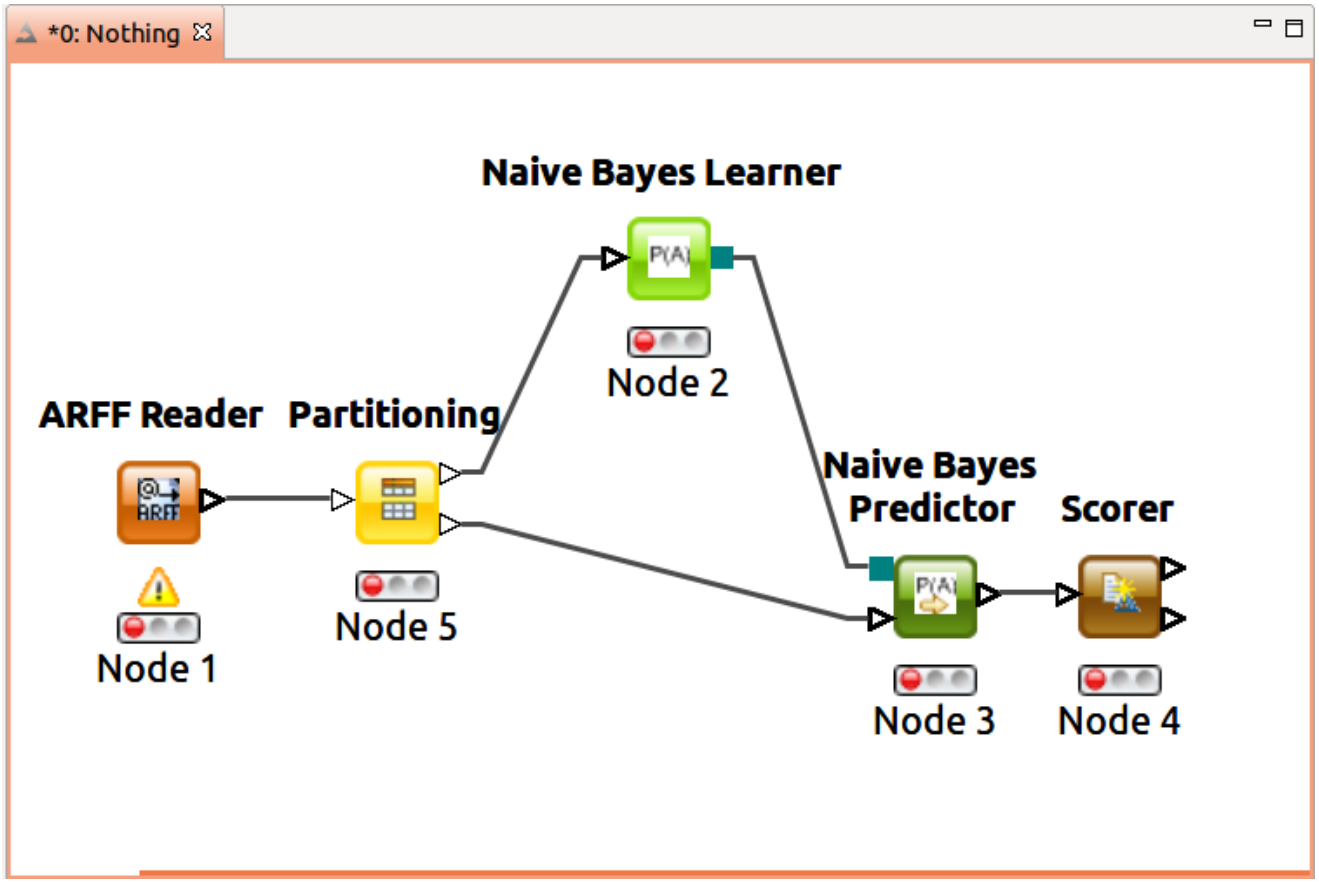
Far too optimistic!

How to Test a Predictor, II

On holdout data?

Test error

after training on a different subset.



How to Test a Predictor, III

Advantages and disadvantages

Resubstitution error

- Employs data to the maximum.

How to Test a Predictor, III

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Resubstitution error

- Employs data to the maximum.
- However, it cannot detect overfitting:
  - A predictor overfits when it adjusts very closely to peculiarities of the specific instances used for training.
  - Overfitting may hinder predictions on unseen instances.

How to Test a Predictor, III

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Holdout data

- Requires us to balance scarce instances into two tasks: training and test.
- Usual: train with 2/3 of the instances — but, which ones?
- It does not sound fully right that some available data instances are never seen for training.

How to Test a Predictor, III

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Holdout data

- Requires us to balance scarce instances into two tasks: training and test.
- Usual: train with 2/3 of the instances — but, which ones?
- It does not sound fully right that some available data instances are never seen for training.
- It sounds even worse that some are never used for testing.

How to Test a Predictor, IV

The idea of x-val

Cross-validation

The key intuitions to get the maximum information from scoring the predictor:

- To run a scorer on a maximum of data instances, we wish exactly one prediction per training instance.
- Let's make sure that each instance is used exactly once for testing.
- Let's run several prediction rounds: each instance will be used for testing in exactly one round.
- The instances used for testing in one round are used for training in all the other rounds.

Cross-validation, I

Basic description

Partition the available data

into N disjoint subsets called folds. (Often, $N = 10$.)

- Each instance goes exactly into one fold.
- Run the learner and predictor N times.
- For each fold i ($1 \leq i \leq N$), the learned is trained on the union of all folds except fold i, and is then used to obtain predictions on all the instances of fold i as test.

Cross-validation, II

Options

Further precisions:

- How many folds?
  - Leave-One-Out X-validation:
    - one fold per instance;
    - most often unacceptably slow;
    - exhibits often too large variance to be reliable.
  - Very standard approach: 10 folds.
- Construct folds as instances come in? Randomize instead?
  - Keep present reproducibility!
- Potential problems if some values of the class attribute are infrequent. How to solve this?

Cross-validation, III

Stratification

Stratified X-validation

means that the folds are constructed in such a way that all the values of the class attribute are as evenly split as possible.

- Ensures even presence of all labels in all folds.
- Turns out to reduce the variance of the computed approximate accuracy.

Predictor Evaluation, I

Simplest case first: binary accuracy

Confusion matrix

(also known as Contingency matrix):

- True positives (positive prediction, hit)
- False positives (positive prediction, fail: false alarm)
- True negatives (negative prediction, hit)
- False negatives (negative prediction, fail)

Accuracy, hit ratio:

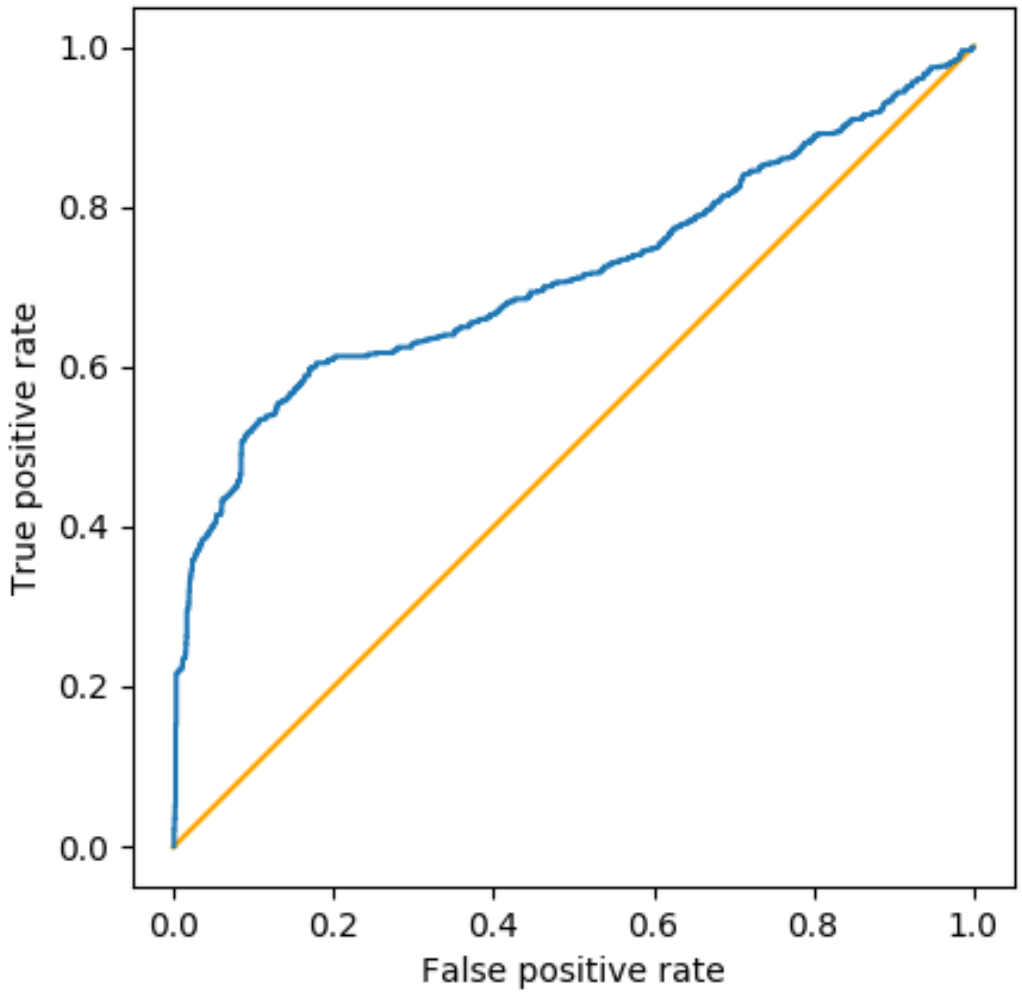
Number of hits divided by total number of predictions.

Warnings:

- Note that our reference to the true label is only indirect.
- Simple generalization to an $n \times n$ confusion matrix if the problem at hand consists of n class values.
- Some problems may suggest (or require) to weight differently the false positives and the false negatives.

ROC space and ROC curves

The curve is formalized subsequently



ROC Space

Predictors lead to points in ROC space

Consider the unit square:

Top left will mean performing quite well.

- The x coordinate is the false positive rate: the ratio of false positives to negative labels.
- The y coordinate is the true positive rate: ratio of true positives to positive labels.

The various regions of ROC space

Each has an intuitive meaning:

- Half-square below the main diagonal,
- around the center,
- near the corners...

The ROC Curve, I

Some predictors provide further information

Ranked predictions:

Predictors that may "bet" on pairs of observations, effectively sorting them.

- For instance, MAP and Naïve Bayes have several options:
  - Higher probability for the "positive" class value;
  - Larger difference of probabilities with respect to other class values...
- Regression-based predictors inherit the real line ordering;
- *Information Retrieval* algorithms are often able to order observations according to the expected relevance.

The ROC Curve, II

For predictors that are able to rank their observations

Tweak the predictor (usually by thresholding or by sorting all the n observations), so as to classify as negative exactly k points.

ROC curve:
(Receiver/Relative Operating Characteristics).

for each k from 0 to n,

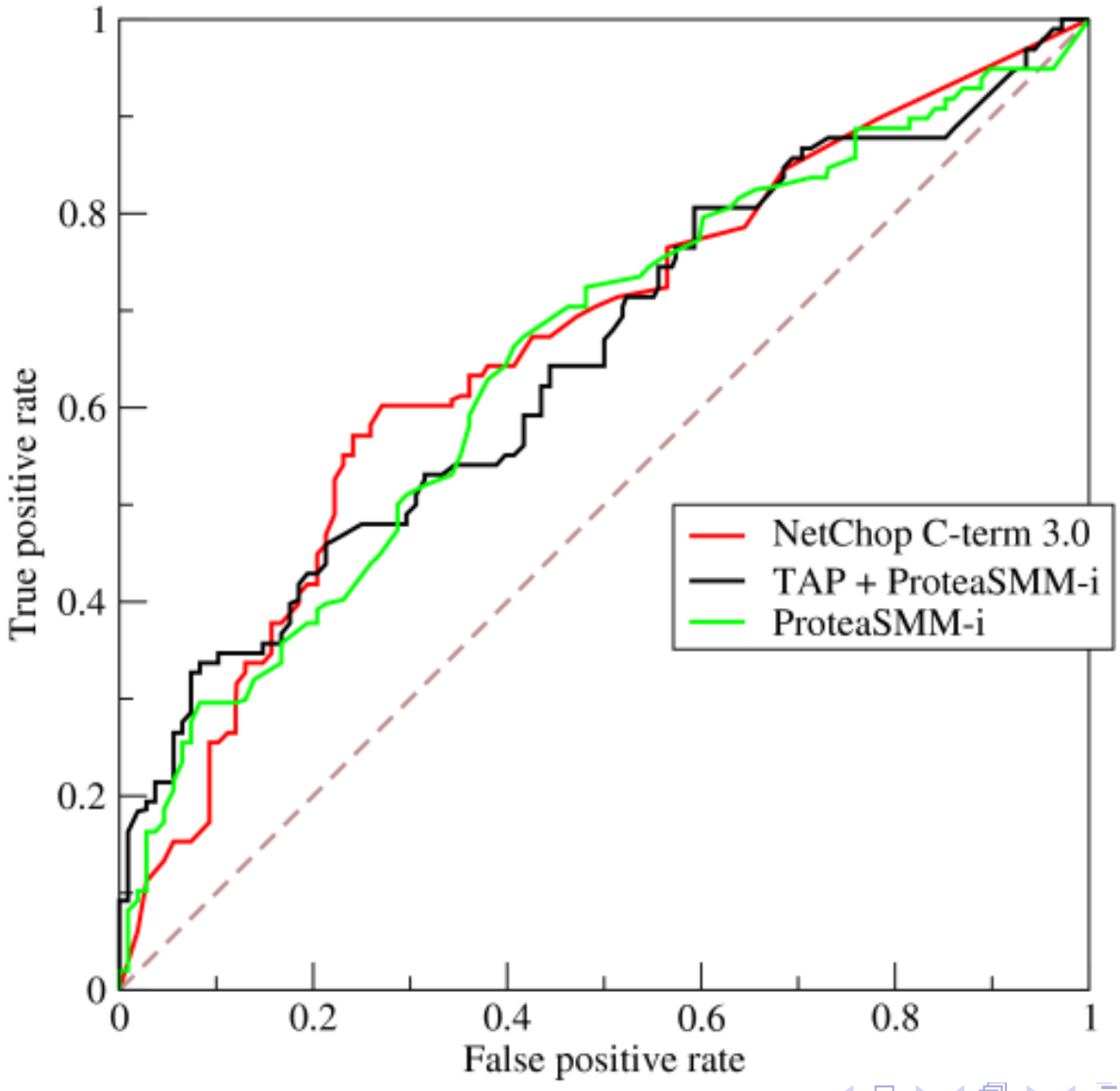
plot the ROC space point corresponding to predicting negatively to k cases (e.g. the k lowest-ranked observations).

We get a curve from (0,0), where we reject everything and there are no false positives, all the way to (1,1) where we accept everything and there are no false negatives.

The ROC Curve, III

Source: Wikipedia, 2009

Further Examples of ROC curves:



The Area Under the ROC Curve, AUC

Fashionable but dangerous

Motivation:

ROC Curves often do not lead to a clear winner among several choices of a classifier.

- AUC reduces each classifier's performance on a dataset to a single number.
- Thus allowing us to compare classifiers.
- However, it corresponds to weighting differently the false positive errors than the false negative errors,

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- AUC reduces each classifier's performance on a dataset to a single number.
- Thus allowing us to compare classifiers.
- However, it corresponds to weighting differently the false positive errors than the false negative errors,
- and the weights depend on the classifier.
- Thus, we should avoid that usage.
- See Hand (Machine Learning Journal, 2009) for further explanations and alternatives.

Predictor Evaluation, II

Sometimes accuracy is insufficient

Alternative quantities:

- Confidence of "positive label" $\Longrightarrow$ "positive prediction":

  Sensitivity (recall in *IR*): ratio of true positives to all positively labeled cases;

- Confidence of "positive prediction" $\Longrightarrow$ "positive label":

  Precision: ratio of true positives to all positively predicted cases;

- Confidence of "negative label" $\Longrightarrow$ "negative prediction":

  Specificity: ratio of true negatives to all negatively labeled cases.

For you to think about:

- How do these notions connect with the axes in ROC space?
- Express accuracy as a linear combination of sensitivity and specificity, and interpret the weights.

Predictor Evaluation, III

Train set, test set, and validation set

Even if we evaluate just accuracy, we may have two frequent reasons for the evaluation.

- We may just want to know (an approximate assessment of) the accuracy of our predictor.
  - A hold-out train/test approach will do,
  - but cross-validation will do better.
- Or, we may want to have (approximate assessments of) the accuracies of several predictors, in order to choose the one with best accuracy.
- But: what if we want both?
  - Then the cross-validation accuracy is unreliable!
  - We chose the best among several possibilities, hence it is "biased towards optimism".
  - We should combine both: hold out a subset for final validation, and run cross-validation on the rest.

Autonomous Learning Topics, II

Proposals to explore on yourself

3. Find out `why` people tend to use 10-fold X-validation schemes (link to a research paper of 1995; also the `presentation slides` are available and quite interesting).
4. Write your own implementation of a ROC curve visualizer.
5. There are several possibilities to handle ties in the construction of a ROC curve. Find bibliography on ROC curves and investigate whether these references mention this issue.
6. Ask the instructor for the link to the paper by David Hand which critizices the AUC measure and offers an alternative, and try to construct your own summary and intuitive explanation of the research findings reported there.

Prediction on Transactional Data

Still on simple predictors

Our discussion of predictors has assumed relational data.

(Often, real-valued vectors.)

What if we are to predict on transactional data?

A very common application: classification on texts.

Like:

- Spam detection,
- sentiment analysis

  (movie reviews, tweets. . .),
- news classification. . .

From Texts to Transactional Data

A wide set of issues

Preprocessing:

Very important! However, not covered in this course.

- Stemming: mapping each word to its stem.
- Feature selection: only keep things that matter
  (remove stop words, maybe punctuation...).
- ...

Terms as attributes:

With values *true* or *false*: binary representation.

Terms as items:

Texts as transactions: but,

- do repetitions matter?
- does order matter? (Sequence mining!, not covered either.)

Bernouilli Naïve Bayes

The direct transformation for binary representation

Terms as attributes with boolean values:

- $N =$ total number of terms,
- x_i is boolean (presence or absence of term),
- $P(x_i|y)$ is the probability of finding term i in a training observation labeled y, if $x_i =$ True,
- $P(x_i|y)$ is the probability of not finding term i in a training observation labeled y, if $x_i =$ False.

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That is:
if the ratio of observations labeled y that have term i, among the total of observations labeled y, is p, then $P(x_i|y)$ is either

- p, for x_i = True, or
- $1 - p$, for x_i = False.

Multinomial Naïve Bayes

Appropriate for bag-of-words representation

Count only occurrences:

- Ignore absence of the items/terms,
- ignore also their order, but
- take into account repetitions:
  - $N =$ size of the observation (transaction) on which we predict,
  - x_i are the actual items in that observation,
  - some of them may be the same,
  - $P(x_i|y)$ is the proportion of item x_i among all items in all transactions of class y.

$$P(x_i|y) = \frac{\text{frequency of item } x_i \text{ in transactions of class } y}{\text{total of items in transactions of class } y}$$

Additional Considerations, I

Must be taken into account!

Upon implementation

A couple of relevant ideas:

- Multiplying together probabilities: very small numbers, high risk of underflow!

  Work instead with their logarithms (often negative!):

  addition instead of multiplication.

- Always apply a Laplace correction, unless you are pretty sure that all counts are positive

  (it is like adding implicitly to the training observations new, artificial ones that make sure that no counts remain at zero).

Additional Considerations, II

Numerical attributes?

Naive Bayes Learner View - 0:4 - Naive Bayes Learner

File

Class counts for Score

Class:	bad	good
Count:	300	700

Total count: 1000

Threshold to used for zero probabilities: 1.0E-4

P(Foreign worker | class=?)

Class/Foreign worker	No	Yes
bad	4	296
good	33	667
Rate:	4%	96%

P(Personal status and sex | class=?)

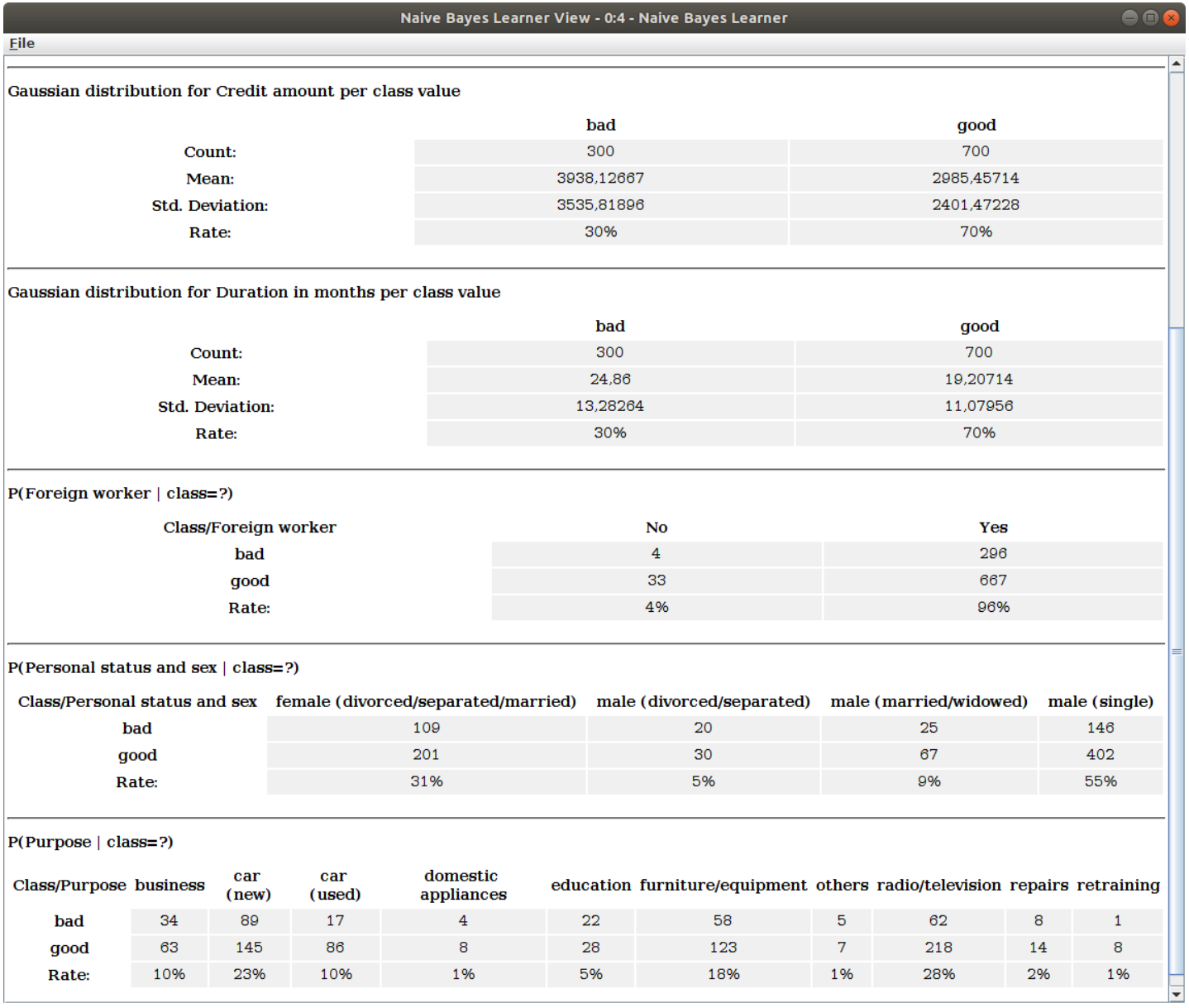
Class/Personal status and sex	female (divorced/separated/married)	male (divorced/separated)	male (married/widowed)	male (single)
bad	109	20	25	146
good	201	30	67	402
Rate:	31%	5%	9%	55%

P(Purpose | class=?)

Class/Purpose	business	car (new)	car (used)	domestic appliances	education	furniture/equipment	others	radio/television	repairs	retraining
bad	34	89	17	4	22	58	5	62	8	1
good	63	145	86	8	28	123	7	218	14	8
Rate:	10%	23%	10%	1%	5%	18%	1%	28%	2%	1%

Additional Considerations, II

Numerical attributes, standard approach: parametric view assuming Gaussians



Naive Bayes Learner View - 0:4 - Naive Bayes Learner

File

Gaussian distribution for Credit amount per class value

	bad	good
Count:	300	700
Mean:	3938,12667	2985,45714
Std. Deviation:	3535,81896	2401,47228
Rate:	30%	70%

Gaussian distribution for Duration in months per class value

	bad	good
Count:	300	700
Mean:	24,86	19,20714
Std. Deviation:	13,28264	11,07956
Rate:	30%	70%

P(Foreign worker | class=?)

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P(Personal status and sex | class=?)

Class/Personal status and sex	female (divorced/separated/married)	male (divorced/separated)	male (married/widowed)	male (single)
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Additional Considerations, III

Alternative approaches related to Naïve Bayes

Good candidates for your papers!

- A proposal to discretize numerical attributes into "bins" instead of fitting a Gaussian (and how to do that smart);
- trying to find out explicitly dependencies among the attributes: Bayesian networks;
- trying to account for dependencies among the attributes "implicitly": Hidden Naïve Bayes.

4. Regression, Bias, and Variance

Approximating a Real Value

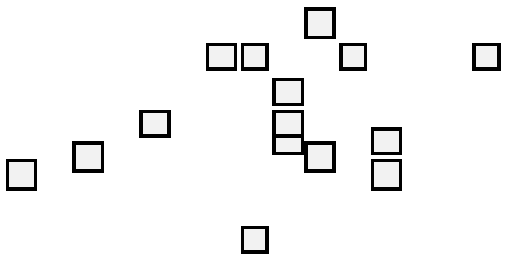
Analyzing sources of error

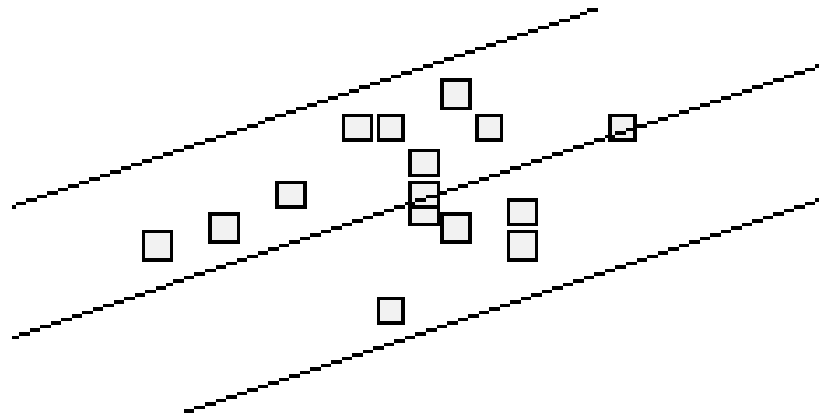
A rather common need:

- Regression tasks: predicting $f(x)$ given x and a sample of points $(x_i, f(x_i))$;
- Estimating the expected accuracy of a given classifier on unseen data, given how well it performs on sample data.
- Estimating other quantities related to properties of predictors.
- Common difficulty: the value to estimate depends on a number of explicit or implicit variables.

Regression: Prediction of Real Values

Rather: floats





Linear regression using minimum square error

The most classical and venerable predictor

A linear predictor is a line in 2D space
or a hyperplane in higher dimensions.

Absolute error is the difference between the value given by the hyperplane and the actual value.

By differentiating the expression that sums all the squares of the absolute errors and equating to zero, we can solve for the "best" hyperplane.

(Other options exist: minimum margin for one.)

The Intuition Of Variance

One source of prediction error

Why may the result be incorrect?

Variance:

Risk arising from the data.

- Data is seen as a sample;
- one cannot rule out the risk that the sample is a particularly bad one, just due to sheer bad luck;
- different samples may lead to different predictions — how different? Can the answer vary very much?
- This question is modeled by variance in the good old statistics sense: expected squared difference between the obtained values and their own mean.
- If the outcome is very concentrated around the mean outcome, there is little risk of being misled due to hitting a bad sample.

The Intuition Of Bias

Another source of prediction error

Why may the result be incorrect?

Bias:

Risk arising from your family of hypotheses.

- In a poor family of hypothesis,

  even the best one might not be very good;
- besides, the reference hypothesis is not the best one: it is the expected one with respect to the sample data; how good is it?

The Intuition Of Bias

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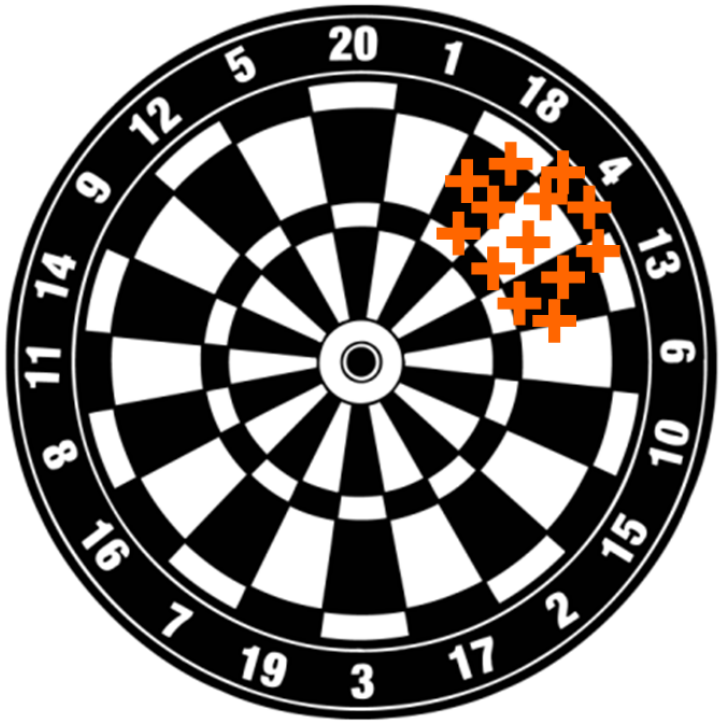
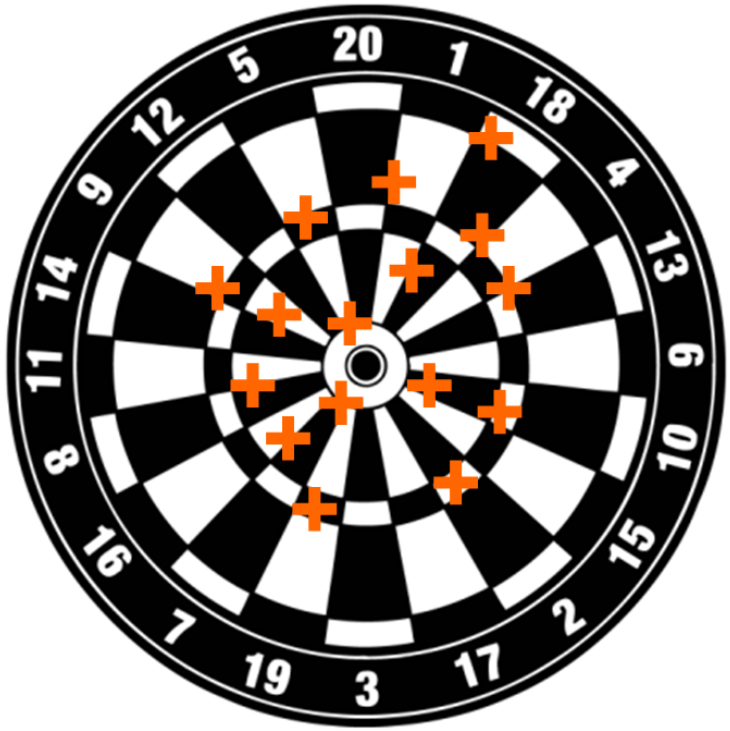
  even the best one might not be very good;
- besides, the reference hypothesis is not the best one: it is the expected one with respect to the sample data; how good is it?

But: avoiding bias error requires using rich families of hypotheses... which leads to high variance!

Visual Intuition

Of bias versus variance





Source: R. Gavaldà

A Very Simple Example

That may help understanding bias versus variance

A case with a single additional parameter.

We wish to estimate the average of a Gaussian

from a sample from it.

- It can be proved that the best estimation is the average of the sample:

  We receive a couple dozen *floats*,

  we are told they come from our Gaussian,

  we estimate the true average by the empirical average...

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- It can be proved that the best estimation is the average of the sample:

  We receive a couple dozen *floats*,

  we are told they come from our Gaussian,

  we estimate the true average by the empirical average...

  ... using how many decimal places?

The data could be y values for very close x values if we are facing a standard regression problem with Gaussian noise.

Is it better to use very few decimal places? We use a `Python (actually web-based Brython) program` to try a few cases.

Bias and Variance: Formalization, I

Main ingredients at play

Context:

- A real value we want to predict, y;
- A sample s which reveals some information about y;
- An estimator $e(s)$ that tries to pinpoint y after seeing s.

As $e(s)$ depends on sample s, it is actually a random variable.

But note that y does not depend on s: from the point of view of the sample, y is a constant.

Bias and Variance: Formalization, II

Formalizing bias and variance

Variance:

Quadratic average error of $e(s)$ used as estimator of its own average $E[e(s)]$: $E[(e(s) - E[e(s)])^2]$.

Bias and Variance: Formalization, II

Formalizing bias and variance

Variance:

Quadratic average error of $e(s)$ used as estimator of its own average $E[e(s)]$: $E[(e(s) - E[e(s)])^2]$.

Bias:

Absolute expected error of e with respect to the true target: $|E[e(s)] - y|$. Note: $E[e(s)]$ and similar quantities, as well as the difference with y, are again independent of s.

Note the different "scale":
we will square the bias to compensate for this.

Error Descomposition

Error is made of bias and variance

Let's add up variance and bias squared:

$$
\begin{aligned}
&E[(e(s) - E[e(s)])^2] + \\
&\qquad (E[e(s)] - y)^2 = \\
&E\left[e(s)^2 - 2E[e(s)]e(s) + E[e(s)]^2\right] + \\
&\qquad E[e(s)]^2 - 2yE[e(s)] + y^2 = \\
&E[e(s)^2] - 2E[e(s)]E[e(s)] + E[e(s)]^2 + \\
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\end{aligned}
$$

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&E[(e(s) - y)^2]
\end{aligned}
$$

They add up to the average quadratic error!

Consequences

Why prediction is difficult

Mean square error, bias, and variance:

- Rigid estimators, that is, with relatively limited possibilities for the result, risk converging to a result rather far away from the truth:

  high error caused by high bias.

- Flexible estimators, with very many possibilities for the result, are likely to converge to the true value (low bias error) but even small sample perturbations will change the outcome:

  high error caused by high variance.

- How to strike the best balance in terms of rigidity or flexibility of the estimators?
- Variance can be reduced if we have large datasets, but in many practical cases available datasets are very far from large enough.

Lab Session 2, I

First couple of predictors

MAP and Naïve Bayes

- Brief recap:
  - *MAP* predictor:

    $$\arg\max_C \{Pr(C|A_1 \ldots A_n)\}$$

  - *Naïve Bayes* predictor:

    $$\arg\max_C \{Pr(A_1|C) * \ldots * Pr(A_n|C) * Pr(C)\}$$

- Today: Watch them running!
  - Check confusion matrices,
  - view the internal parameters,
  - check ROC curves,
  - run comparisons...

Lab Session 2, I

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    $$\arg\max_C \{Pr(A_1|C) * \ldots * Pr(A_n|C) * Pr(C)\}$$

- Today: Watch them running!
  - Check confusion matrices,
  - view the internal parameters,
  - check ROC curves,
  - run comparisons...
- Run them on additional datasets.
- See the MAP predictor fail.

Lab Session 2, II

Using Predictors

File: `http://www.cs.upc.edu/~balqui/LabADM20200226.zip`

Parts of the Python code depend on `matplotlib` and are not runnable if you don't have it.

Explore first `LabADM20200226.py` which loads in the dataset `weatherNominalTr.txt` (in the `datasets` folder) and calls a predictor.

- Understand the code,
- uncomment `pr.show()`,
- uncomment the `print...` line inside the `for` loop,
- swap predictors to use `NaiveBayes` instead;
- now explore `compare.py` and understand the comparison.
- Explore on your own the code for both predictors and see how it fits what we discussed so far.

Lab Session 2, III

Comparing Predictors

Move on to other datasets.

- Change the main program so as to load in the `titanicTr` dataset instead;
- Redo the whole thing with both predictors: which one seems better?
- Ask the predictors to predict on new tuples (see bottom of file `maxapost.py`):

  ```
  print pr.predict(('Class:1st','Sex:Female','Age:Child'))
  print pr.predict(('Class:Crew','Sex:Female','Age:Child'))
  ```

  Explain what happens!
- Try predicting other attributes.
- Explore the other datasets:
  - which predictor seems better for each?
  - Try to make the MAP predictor fail again like before.

Lab Session 2, IV

Evaluating Predictors

Train/test split

- In the Python `LabADM...` file, replace the declaration `Data(filename)` with `Data(filename,75)` (or a different figure in [0,100]).
- Understand what happens; then move to `compare.py` and work likewise on it.
- Explore this train/test decomposition for other datasets on yourself, using `naivebayes.py`, `maxapost.py`, `compare.py`...

ROC Curves

If you have `matplotlib`, proceed to exploring ROC curves through the source `roc.py` using both predictors and varying the dataset (and the value of the label to analyze).

Make sure to understand what happens!

Lab Session 2, V

Back to KNIME

On KNIME

redo parts of what you have done today (see Slides 35, 36):

- Manage to read in some dataset.
- Find the nodes for Naïve Bayes Learning and for Naïve Bayes Prediction (that uses the model learned).
- Find the Scorer node, that implements confusion matrices and accuracy evaluation, and compute resubstitution error.
- Add a Partitioning node to split the data into training set and test set, and compute the test set error.
- Try several partitioning strategies to check whether the test set error is stable.
- Find the ROC Curve node and show ROC curves of your predictors on your datasets.

Autonomous Learning Topics, III

Proposals to explore on yourself

7. Design and explore in practice cases of bias-variance trade-offs:
   - according to the degree, interpolating polynomials may incur high bias or high variance;
   - according to the number of units, neural networks may incur high bias or high variance...
8. The bias-variance trade-off has been shown for estimating a real value. Is there a way of analyzing in similar ways binary predictors? (Yes, of course; the problem is, there are several of them... Explore the literature!).

5. Additional Predictors

Nearest Neighbors, I

The data is the model

Assumption:

Similar observations lead to similar responses.

- Keep all the data in an appropriate data structure, and
- predict the most common response among the k nearest neighbors of a new observation to predict on.
- (Lots of demos on youtube.)

Nearest Neighbors, I

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Assumption:

Similar observations lead to similar responses.

- Keep all the data in an appropriate data structure, and
- predict the most common response among the k nearest neighbors of a new observation to predict on.
- (Lots of demos on youtube.)
- Essentially, we are assuming a "bias of continuity"!
  - Often, the continuity assumption is correct.
  - Often, it is not.

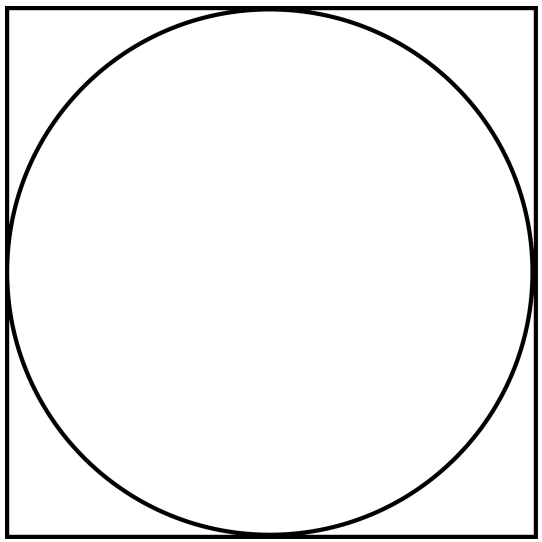
Careful!

In high dimensionality, "everything is far away".

- Is the difference between the closest neighbors and the farthest ones significative?
- `Hardly ever the case` beyond a couple dozen attributes! `(Alternative link.)`

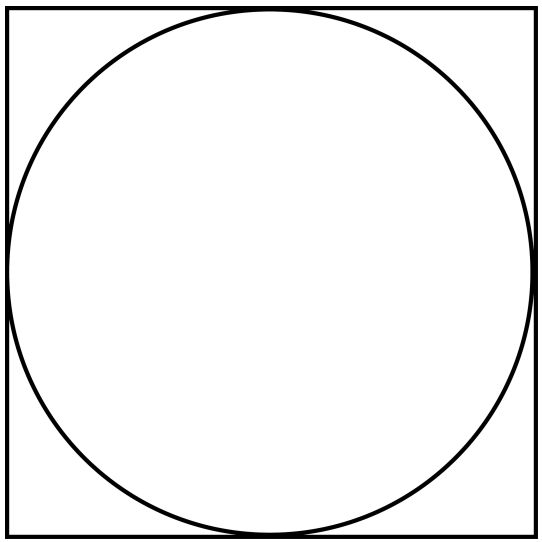
From 2 to 3 dimensions

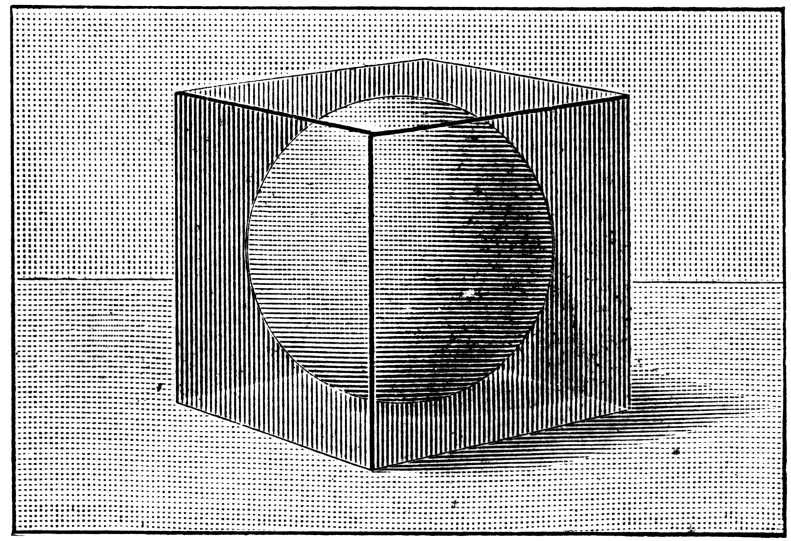
To grasp the trend



From 2 to 3 dimensions

To grasp the trend





Source: FCIT

Nearest Neighbors, II

Variations

Value of k?

(Odd for 2-class problems.)

Scale into similar intervals all the numeric attributes? Imagine:

- one attribute is age,
- another is annual salary in euros...

Options:

$$x' = \frac{x - \mu}{\sigma} \qquad x' = \frac{x - min}{max - min}$$

Weighted majority instead of plain majority?

(Then can use largish k.)

Nearest Neighbors, III

Data structures

In high dimensions, finding out the k nearest neighbors is computationally nontrivial.

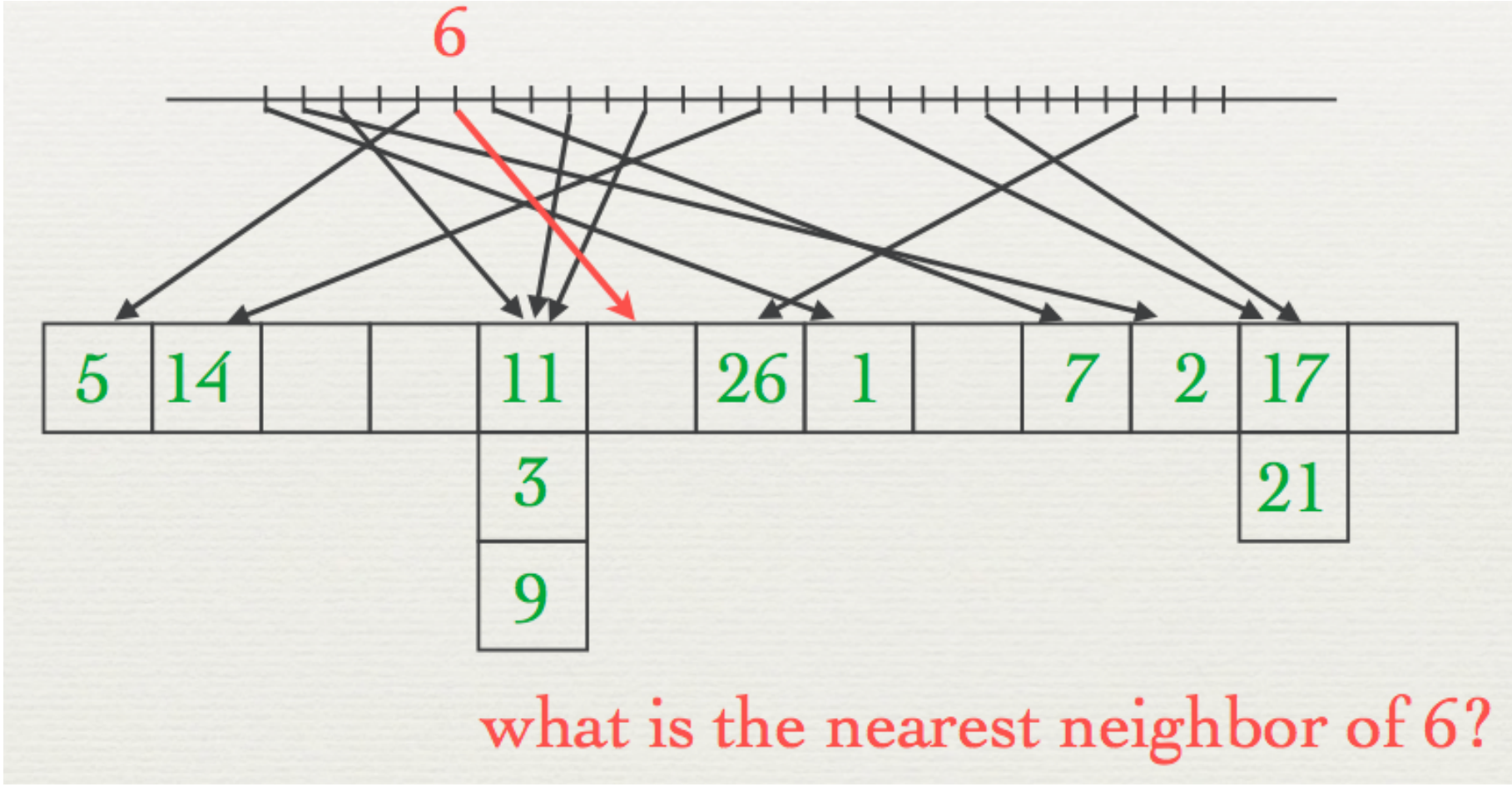
Computational options:

- Multidimensional search trees:
  - k-d-trees,
  - metric trees,
  - cover trees,
  - ball-trees;
- proximity graphs;
- locality-sensitive hashing

  (we study this one a bit more);
- ...

Usual Schemes for Hashing

Do not preserve any locality



Locality sensitive hashing functions, I

Definition

Goal:

- Collision probability for similar objects is high enough.
- Collision probability for dissimilar objects is rather low.

(Exercise: how is the algorithm, once we have this?)

Locality sensitive hashing functions, I

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Goal:

- Collision probability for similar objects is high enough.
- Collision probability for dissimilar objects is rather low.

(Exercise: how is the algorithm, once we have this?)

Let $c < 1$ and $0 \leq p_1 < p_2 \leq 1$; function $s(x, y)$ measures how similar objects x and y are in a scale $[0, 1]$.

A family $\mathcal{F}$ is called $(s, c \cdot s, p_1, p_2)$-sensitive if for any two objects x and y we have:

- if $s(x, y) \geq s$, then $P[h(x) = h(y)] \geq p_2$,
- if $s(x, y) \leq c \cdot s$, then $P[h(x) = h(y)] \leq p_1$,

where the probability is taken over chosing h from $\mathcal{F}$.

Locality sensitive hashing functions, II

An example for bit-vectors

Consider the following context and hashing family:

- Objects are vectors in $\{0,1\}^d$.
- Distances are measured using Hamming distance

$$d(x,y) = \sum_{i=1}^{d} |x_i - y_i|.$$

- Similarity is measured as

$$s(x,y) = 1 - \frac{d(x,y)}{d}.$$

(Example: if $x = 10010$ and $y = 11011$, then $d(x,y) = 2$ and $s(x,y) = 1 - 2/5 = 0.6$.)

Then: the i-th hashing function just samples the i-th bit.

Locality sensitive hashing functions, III

Playing with the probabilities

The probability of collision is

$$P[h(x) = h(y)] = s(x, y).$$

Locality sensitive hashing functions, III

Playing with the probabilities

The probability of collision is

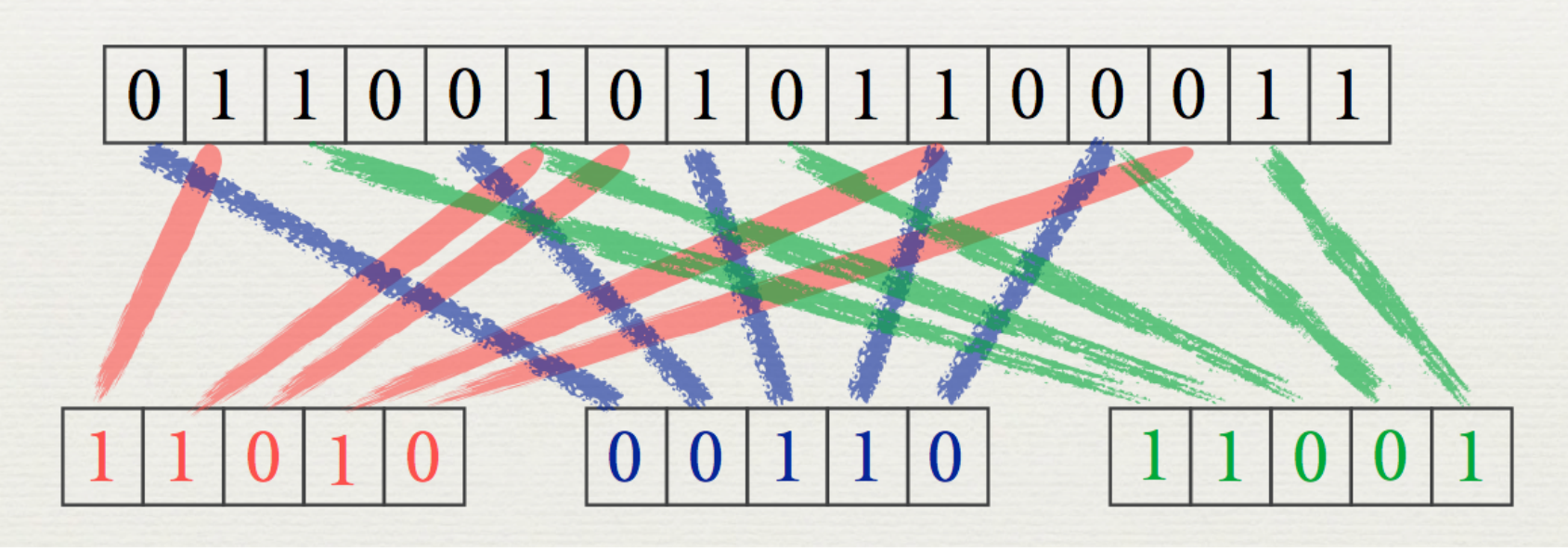
$$P[h(x) = h(y)] = s(x, y).$$

Amplifying the gap:

- By stacking together k hash functions:
  - $h(x) = (h_1(x), .., h_k(x))$ where $h_i \in \mathcal{F}$;
  - probability of collision of similar objects decreases to ${p_2}^k$;
  - probability of collision of dissimilar objects decreases even more to ${p_1}^k$.
- By repeating the process m times:
  - Probability of collision of similar objects increases to $1 - (1 - p_2)^m$.

Locality sensitive hashing functions, IV

Illustrating the bit-vector particular case



Lab Session 3

KNIME Prediction Nodes

Refresh:

- read in, transform, explore, and visualize data;
- clarify its basic statistic properties;

Today:

- Find some relational datasets,
- create workflows to run, evaluate, and compare several varied predictors on them:
  - partitioning into train/test data,
  - cross-validating. . .

  Count on a bit of help from the instructor when necessary.

Alternatively:

- Keep working hard on your first (or second!) deliverable.

Decision Trees, I

Can you imagine explaining your NB predictor to your boss?

Can we make do by checking a single attribute?

If not. . .

Decision Trees, I

Can you imagine explaining your NB predictor to your boss?

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If not... recurse!

Decision Trees, I

Can you imagine explaining your NB predictor to your boss?

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If not... recurse!

- Measure somehow the "heterogeneity" of the observations, and
- Pick one "test" of the value of an attribute so that the split reduces the "joint heterogeneity".

Decision Trees, I

Can you imagine explaining your NB predictor to your boss?

Can we make do by checking a single attribute?

If not... recurse!

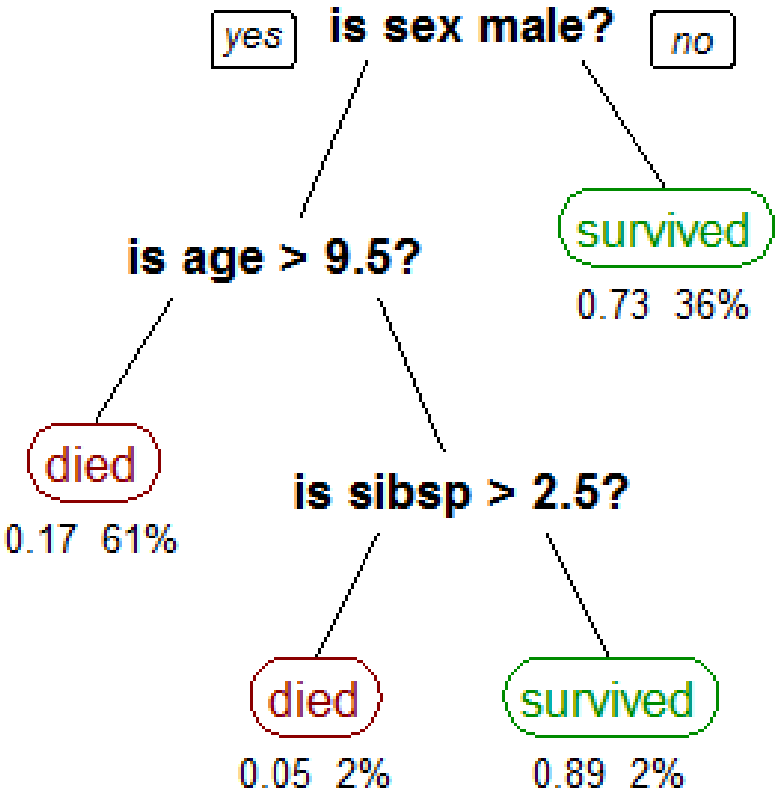
- Measure somehow the "heterogeneity" of the observations, and
- Pick one "test" of the value of an attribute so that the split reduces the "joint heterogeneity".

Several variants of this idea (ID3, C4.5, j48, C5.0, CART):

- the prediction follows a decomposition of the input space in "axis-parallel cuboids", but
- "tests" can be made in different ways, and
- there are several possible notions of "heterogeneity".

Decision Trees, II

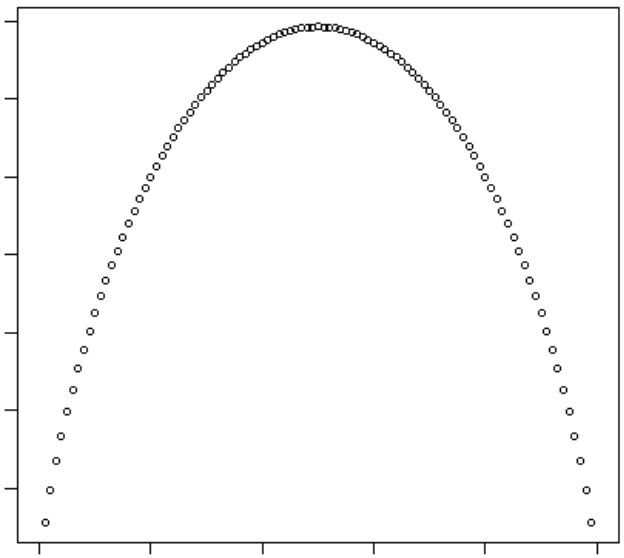
How do they look like?

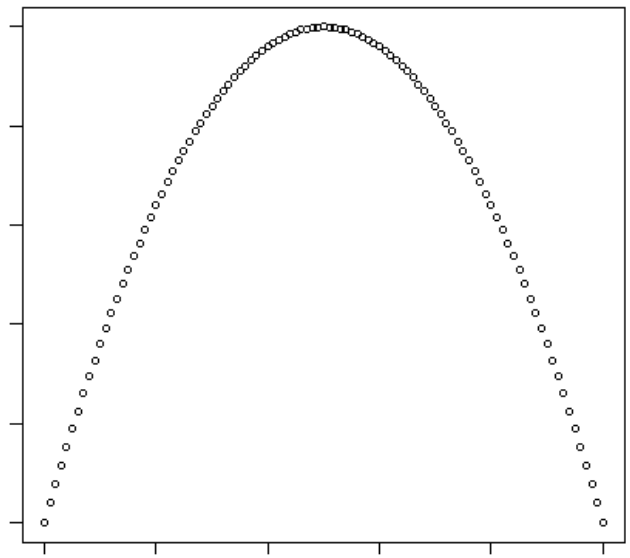


A CART example tree. Source: Wikipedia, 2014.

Heterogeneity

Shannon information versus Gini index (2-valued case)





Decision Rules, I

Related to decision trees

Decision rules: Decision trees explained verbally instead of depicted. (Horn-clause-like syntax!) `Example.`

Both:

- Are predictive and descriptive models;
- Easy to understand (as long as they are small enough).
- Low bias, but very high variance, hence low tolerance to "noise";
- Occassional slight advantage of decision rules over decision trees.
- A frequent outcome: branches or rules carve out small, very well-predictable niches but fail to get global patterns.
- Syntactic allusion to a suggested causality connection (*policy-makers* love it!)

Decision Rules, II

How to select them? How to apply them?

Several options for several choices,

hence many slightly different algorithms:
CN2, IREP, Ripper (JRip)...

- Which rules build up the predictor?
- At the time of applying the predictor,
  - what if no rule fires?
  - what if several rules fire, and lead to different predictions?
- One easy way out: rules are the branches of a decision tree.
- Other criteria:
  - coverage per rule,
  - accuracy per rule,
  - *default* rule,
  - exceptions...

Exploring and Extending KNIME

Many extra possibilities and modules

Learn to:

- Extend KNIME: suggestions of interesting imports are the Text Processing extension and the Weka extension.
- Use meta-nodes:
  - Find them in their appropriate place — do not confuse their place with the place for "nodes that are used to construct meta-nodes".
  - Practice with the cross-validation meta-node.
  - Practice with the feature elimination meta-node.
- Use variables:
  - Show variable ports,
  - inject variables defined through Java snippets,
  - use them in the corresponding tab,
  - explore further nodes handling variables...
- Program loops!
  - Explore nodes for loop programming;
  - combine them with variables such as the current iteration.

Feature Elimination

A process for reducing dimensionality

Works as follows:

- Combines a dataset with your predictor of choice.
- Repeats the following process:
  - For each attribute in turn:
    - Remove the column temporarily,
    - train with the rest,
    - test or x-validate;
  - The attribute that got worst accuracy along the loop is eliminated.
- Keep like this until reaching a fixed accuracy threshold or a given number of attributes.

KNIME Assignments

To work on your own as a means of mastering the tool

(These assignments are not compulsory. They are just proposals, expected to facilitate one or more of your coming evaluable papers.)

1. Create KNIME workflows that try several values of some parameter of some predictive model in search of good accuracies.
2. The `shuttle` dataset from the UCI Irvine repository has been reported to exhibit the following property: at some ratios of training/test split, larger training sets lead to an unexpected decrease of accuracy of the Naïve Bayes classifier. Create a KNIME workflow to try and replicate this experiment.
3. Repeat the experiment by playing with the number of folds in x-val instead of the ratio of training/test sets, and/or employing other classifiers.
4. Learn to program your own KNIME nodes!

Classifier Border Repertory

Class-separation shapes

- Decision Stumps:
  - axis-parallel hyperplanes,
- Decision Trees:
  - unions thereof,
- kNN, NB:
  - complex shapes...

Classifier Border Repertory

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- Linear predictors:
  - Separating hyperplanes

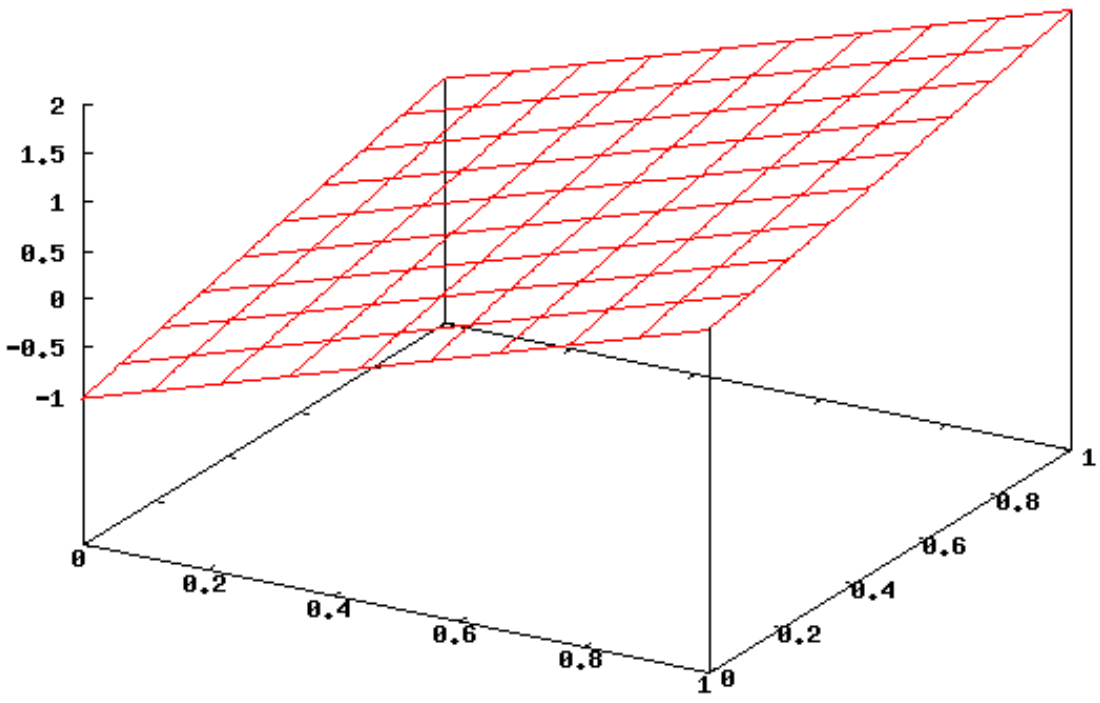
Classifier Border Repertory

Class-separation shapes

- Decision Stumps:
  - axis-parallel hyperplanes,
- Decision Trees:
  - unions thereof,
- kNN, NB:
  - complex shapes...
- Linear predictors:
  - Separating hyperplanes (not necessarily in the same space!)
    - Hard threshold,
    - Soft threshold.

A linear separator

In R^3: $2x + y - 1$



Support Vector Machines, I

SVM: the modern linear predictors

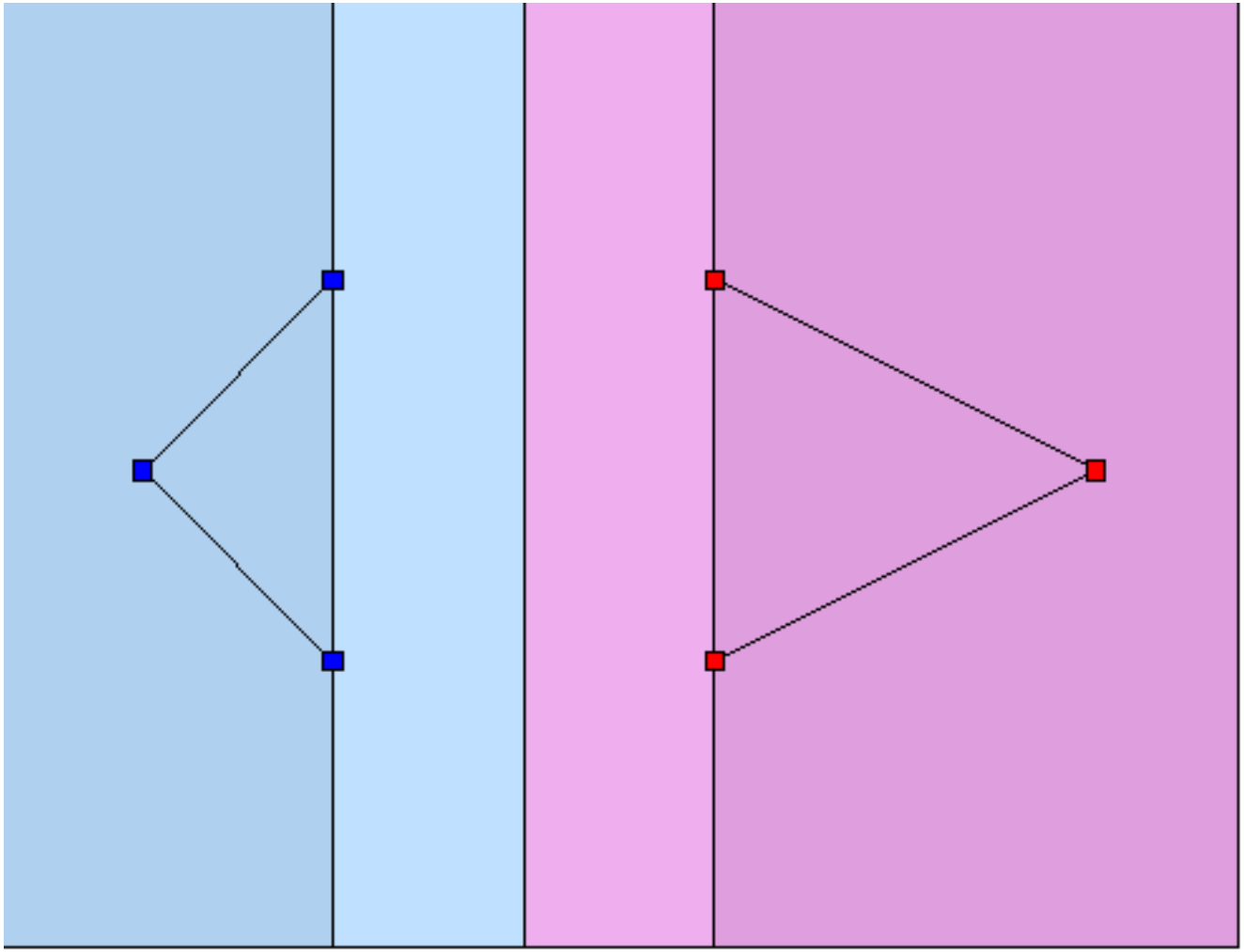
Slogan: maximal margin; don't get closer to any of the classes more than absolutely necessary.

- Hard margin: requires linear separability.
- Two alternatives for coping with nonlinearly separable data:
  - soft margin and
  - expanding the data into a feature space with a kernel.

We start with a couple of little toy implementations from `Suverat` and from `LIBSVM`.

Maximal-Margin Hyperplane, I

Linearly separable cases



Support Vector Machines, II

Some related hints

Optimization rendering:

Maximize m, under the constraints: $y_i \frac{(w^T x_i + b)}{||w||} \geq m$.

(Plus a funny trick on the scaling!)

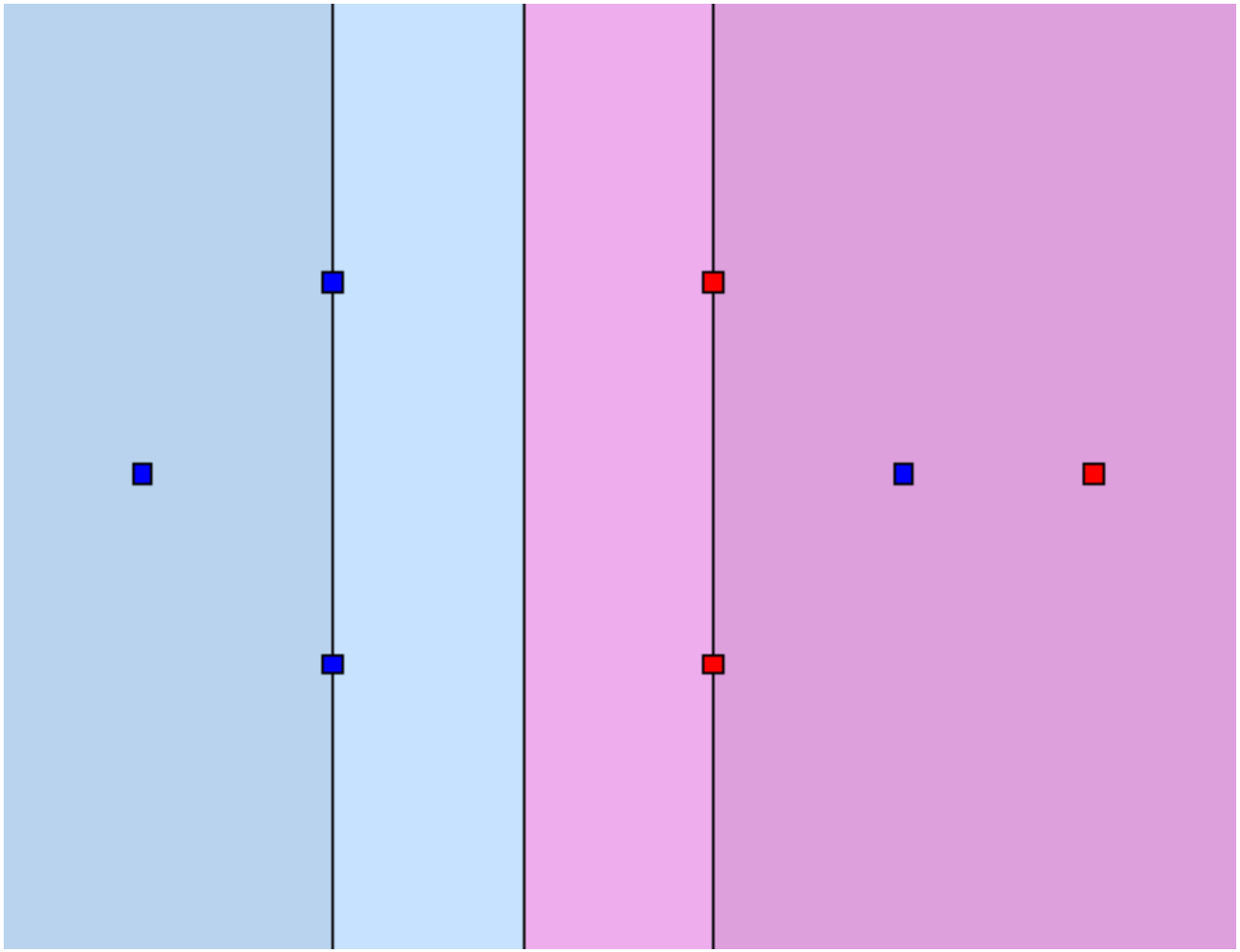
Duality and Lagrange multipliers:

The separating hyperplane is defined as linear combination of the data points.

- Coefficient is zero for many points! Nonzero coefficients only for the support vectors that lie exactly at the margin or (in the nonseparable case) within it.
- Polynomial-time semidefinite programming solution.
- Only operation required on the data points: their scalar product.

Maximal-Margin Hyperplane, II

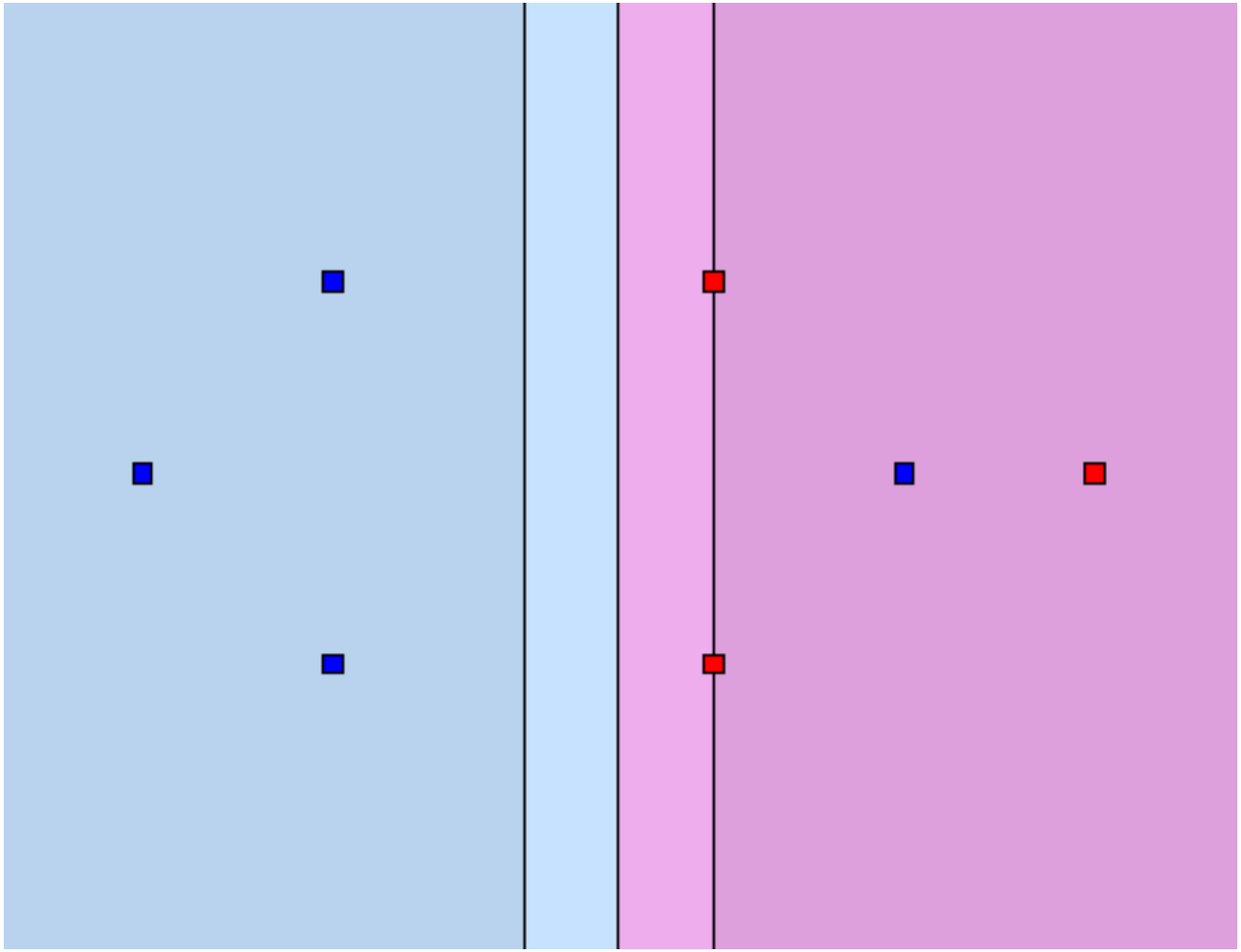
Linearly inseparable cases: not the same hyperplane due to misclassified instances



Hyperparameter to balance margin amount and mistakes made.

Maximal-Margin Hyperplane, III

Linearly inseparable cases: misclassified instances push the separator



Intuition: convex hulls! (Bennet and Bredensteiner.)

Support Vector Machines, III

Several implementations out there

Alternative algorithmics:

- Reduction to general-purpose semi-definite quadratic programming (QP) software — usual cost $O(n^2 m^2)$ for m points in n dimensions.
- Decomposition methods:

  they concentrate on just a subset of the points at each time.
  - The extreme case is Sequential Minimal Optimization: nontrivial to do it well, see `LIBSVM` (and, in particular, the paper linked there in the ACM Transactions on Intelligent Systems).
  - Reweighting scheme able to go down to $O(n^3 \log m)$, better when n much smaller than m, based on the Simple Sampling Lemma of Gärtner and Welzl
    (to demo it, we go back to our little `toy implementation` of this scheme).

Kernels

Switch to a richer space

Reproducing Kernel Hilbert Spaces:

Can be obtained through scalar products.

A two-dimensional conic:

$$w_1 x_1^2 + w_2 x_2^2 + w_s x_1 x_2 + w_4 x_1 + w_5 x_2 + w_6$$

is the scalar product of the weights $(w_1, w_2, w_3, w_4, w_5, w_6)$ with a "transformed" input point (x_1, x_2) a R^6:

$$f(x_1, x_2) = (x_1^2, x_2^2, x_1 x_2, x_1, x_2, 1)$$

(Please compute $((x_1, x_2)(y_1, y_2) + 1)^2$.)

`Search for 'svm' on youtube.`

Scheme may be made to work even on infinite-dimensional feature spaces!

Ensemble Methods

Improving weak but fast predictors

Often, getting good predictions require slow training algorithms.

Simple predictors are fast to train, but often weak — but, how weak? Would do they better than random guessing?

- Quite small decision trees,
- decision stumps (that is, minimally small decision trees),
- quite small decision rules,
- Naïve Bayes and variants...

Can we enhance the predictions of a simple predictor by combining several of them?

- Bagging (Random Forests, Random Naïve Bayes...),
- boosting (mainly Adaboost but there are many others),
- stacking...

Bagging: bootstrapping aggregates

Assume a relational dataset with n observations.

Fix some weak but fast-to-train predictive model.

- Sample $m \leq n$ observations (*bootstrap*), most often $m = n$.

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- Train a predictor on the sample.
- Repeat k times.

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Fix some weak but fast-to-train predictive model.

- Sample $m \leq n$ observations (*bootstrap*), most often $m = n$.
- With replacement!
- Train a predictor on the sample.
- Repeat k times.

Predict: according to majority.

Newly available measure of accuracy: Error OOB (*Out-Of-Bag*), predicting on each x, by majority only of those predictors that "did not see" x upon being trained.

Random Forests

Apply bagging:

- on a form of decision trees,
- where each bifurcation is on the best splitting attribute among a small sample of them,
- and applying no pruning.

Properties:

- Several "success stories".
- Fast construction as few attributes examined per split.
- Some lucky nodes that catch very discriminative attributes compensate for the rest.
- Often still overfits.
- Not very good in the presence of many irrelevant attributes.

Random Naïve Bayes

Tricky!

Bagging on Naïve Bayes... but...

Recall that each Naïve Bayes prediction is actually a number:

- Obtained as a product of probabilities.
- For standalone Naïve Bayes, we "discretize" by looking for the class value that maximizes the probability.

Trick: instead, use them as weights that quantify how reliable the prediction is, obtaining the final prediction as a weighted majority.

Boosting

Formally, "boosting" means that there is a theorem that tells you how to combine bounded-but-large-error predictors so as to obtain small-error predictors.

Many people confuse Boosting (as a general property) with the most famous boosting algorithm: AdaBoost.

AdaBoost is similar to *bagging* but more sophisticate: sampling is potentially not uniform.

AdaBoost, I

Applies to binary classification.

New ingredient D: explicitly maintained probability distribution on the n data points.
(Initially uniform: $1/n$ probability mass per point.)

Algorithm:

- Train a predictor by taking the weights $D(x)$ into account:
  - Sample by independently choosing each x according to $D(x)$.
  - Train the predictor on the sample.
- Assign a weight to that predictor for the later weighted-majority prediction.
- Recompute D: increase the weight of errors (and normalize, of course).
- Repeat as long as the predictor obtained works better than random guessing.

AdaBoost, II

Tuning the scheme to recompute weights

Each round provides us with a new predictor h:

- Compute ϵ, its weighted error
  - (replacement error on the sample used to construct it, that is, that sample is both training set and test set; and
  - weighted error is the sum of the weights $D(x)$ for those x in the sample where $h(x)$ is wrong).
  - If $\epsilon \geq \frac{1}{2}$ then discard h and finish the training process.
- Tune the weights:
  - let $d = \frac{1-\epsilon}{\epsilon}$ (note: $d > 1$);
  - let $D(x) := D(x)/d$ if h is correct on x;
  - let $D(x) := D(x) * d$ otherwise;
- and don't forget to normalize D.
- For the final weighted majority prediction, store $\log d$ as weight to be assigned to h.

AdaBoost, III

Properties guaranteed by mathematical theorems

After T rounds, let ϵ_t be the error of the weak predictor obtained at round t. (All $\epsilon_t < \frac{1}{2}$ due to the finishing condition!)
Then, the error of the weighted majority is bounded by

$$e^{-2\sum(\frac{1}{2}-\epsilon_t)^2}.$$

For example: if weak-predictor error is always under 40%, then reaching $T = 10$ gives error under 7%, and reaching $T = 20$ gives error under 0.7%.

"Difficult" data is easily spotted because AdaBoost terminates in just a few rounds on them.

Additionally, there are theorems bounding the generalization error and also the classification margin: these explain the observed phenomenon that AdaBoost often avoids overfitting.

Autonomous Learning Topics, IV

Proposals to explore on yourself

9. Study alternative data structures supporting Nearest Neighbors.
10. Deepen in your understanding of some predictor(s), such as Decision Trees or Support Vector Machines (consider doing it by building your own implementation).
11. Deepen in your understanding of some meta-predictor, such as AdaBoost or Random Forests (consider doing it by building your own implementation).
12. Learn how to program your own KNIME nodes.