Feature Selection, Projection and Extraction

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Slides from Introduction to Machine Learning and Data Mining by Carla Brodley

What is the concept?

- banana
+ grapefruit
- firetruck
+ airplane
- duck
- fire

+ graduation
+ yellow
- basket
+ garden
- class

What is Similarity?

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Classifier Construction

Objective: Construct a classifier for the data such that predictive accuracy is maximized

1. Prepare/collect training instances
   - Generate/select descriptive features
   - Collect and label instances
2. Construct a classifier

Creating Features

- **"Good" features are the key to accurate generalization**

- Domain knowledge can be used to generate a feature set
  - Medical Example: results of blood tests, age, smoking history
  - Game Playing example: number of pieces on the board, control of the center of the board

- Data might not be in vector form
  - Example: spam classification
    - "Bag of words": throw out order, keep count of how many times each word appears.
    - Sequence: one feature for first letter in the email, one for second letter, etc.
    - Ngrams: one feature for every unique string of n features

What is feature selection?

- Reducing the feature space by throwing out some of the features

Reasons for Feature Selection

- Want to find **which** features are relevant
  - Domain specialist not sure which factors are predictive of disease
  - Common practice: throw in every feature you can think of, let feature selection get rid of useless ones
- Want to **maximize accuracy**, by removing irrelevant and noisy features
  - For Spam, create a feature for each of ~10^5 English words
  - Training with all features computationally expensive
  - Irrelevant features hurt generalization
- Features have associated costs, want to **optimize accuracy with least expensive features**
  - Embedded systems with limited resources
    - Voice recognition on a cell phone
    - Branch prediction in a CPU (4K code limit)

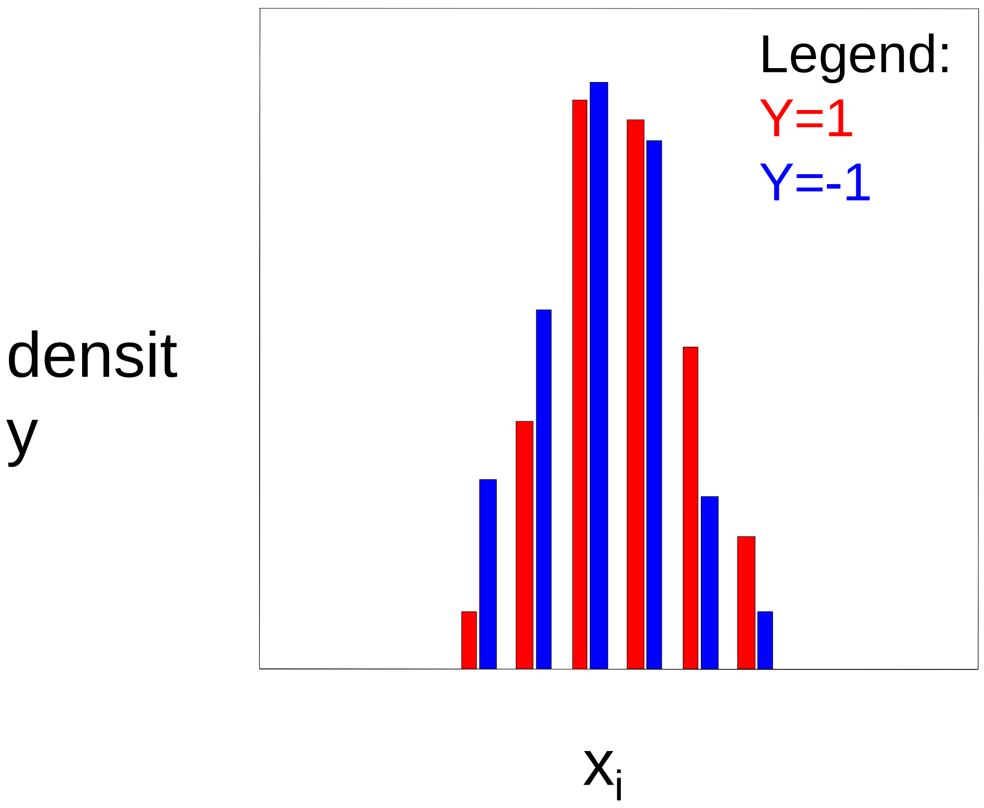
Terminology

- **Univariate method**: considers one variable (feature) at a time
- **Multivariate method:** considers subsets of variables (features) together
- **Filter method:** ranks features or feature subsets independently of the predictor (classifier)
- **Wrapper method:** uses a classifier to assess features or feature subsets

Filtering

- Basic idea: assign score to each feature x indicating how "related" x and the class y are
  - Intuition: if $x=y$ for all instances, then x is great no matter what our model is; x contains all information needed to predict y
- Pick the $\boldsymbol{n}$ highest scoring features to keep

Individual Feature Irrelevance



$P(X_i, Y) = P(X_i)\, P(Y)$

$P(X_i | Y) = P(X_i)$

$P(X_i | Y=1) = P(X_i | Y=-1)$

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Slide from I. Guyon, PASCAL Bootcamp in ML

Individual Feature Relevance

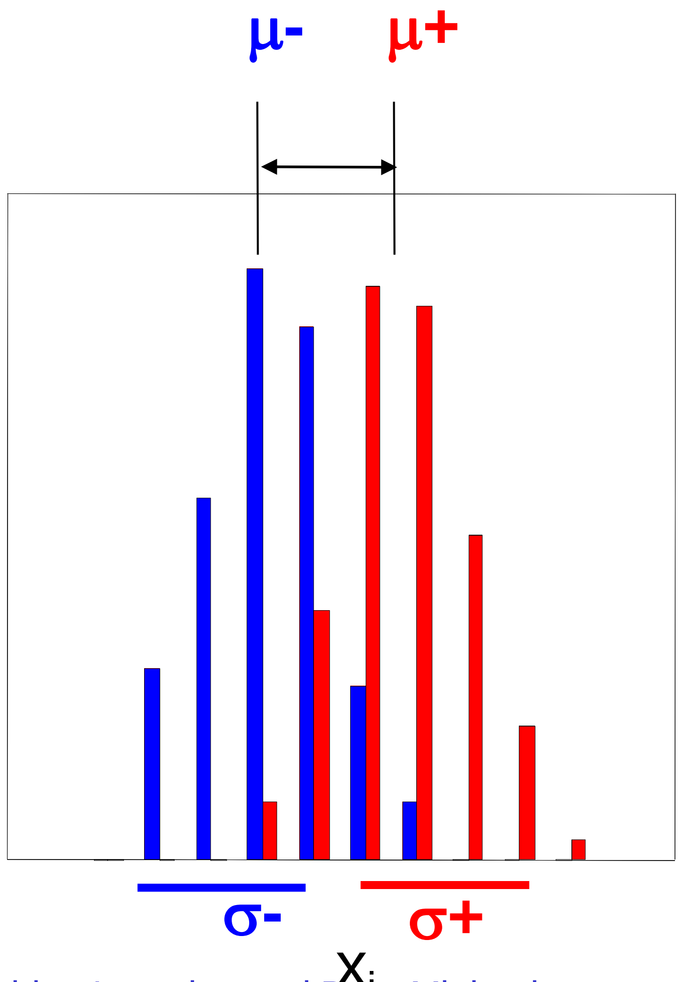

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Figure from I. Guyon, PASCAL Bootcamp in ML

Univariate Dependence

- Independence:

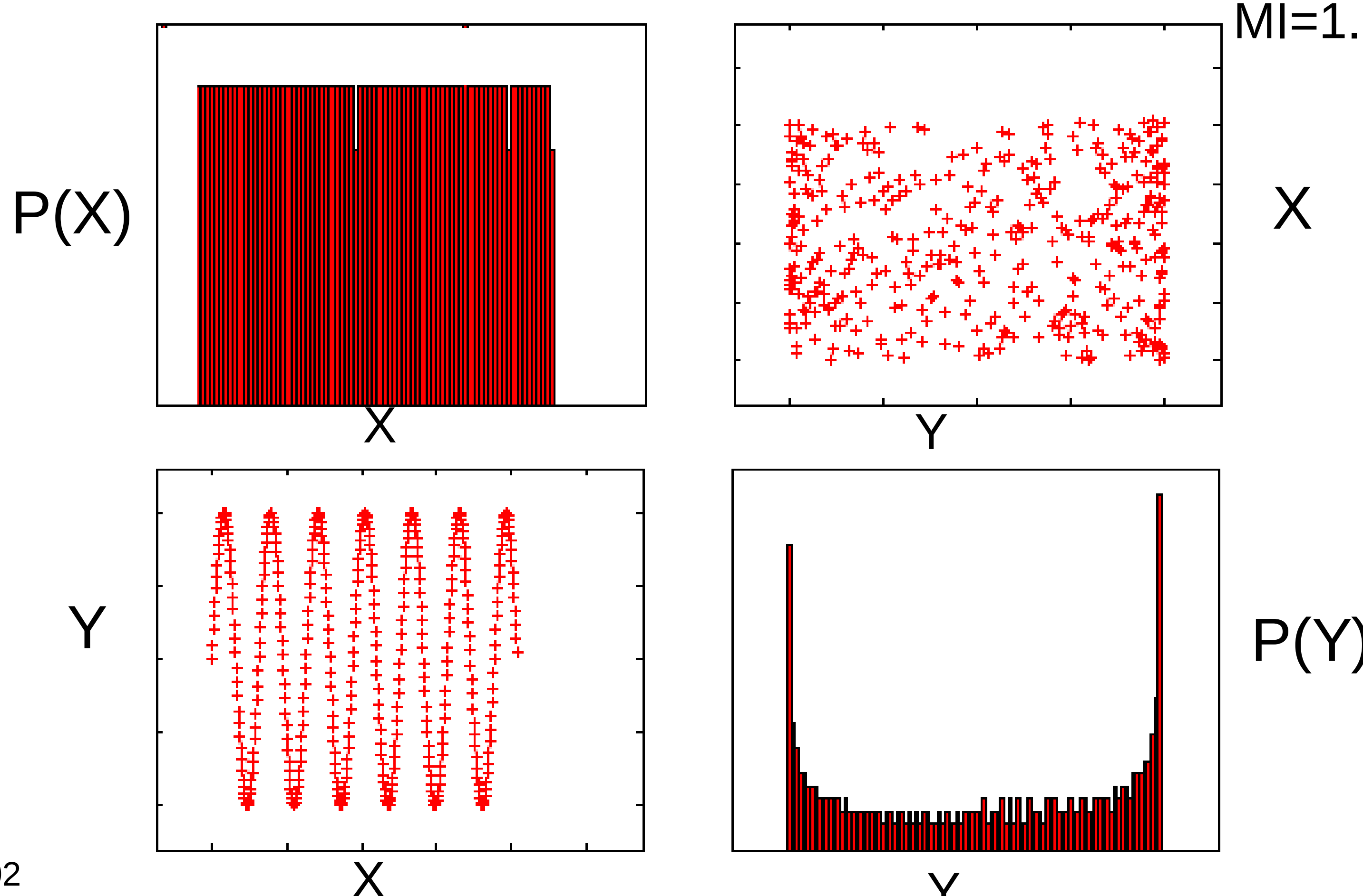
$$P(X, Y) = P(X)\,P(Y)$$

- Measures of dependence:
  - Mutual Information (see notes from board)
  - Correlation (see notes from board)

Slide from I. Guyon, PASCAL Bootcamp in ML

Correlation and MI

R=0.02
MI=1.03 nat



R=0.00$_{02}$
MI=1.65 nat

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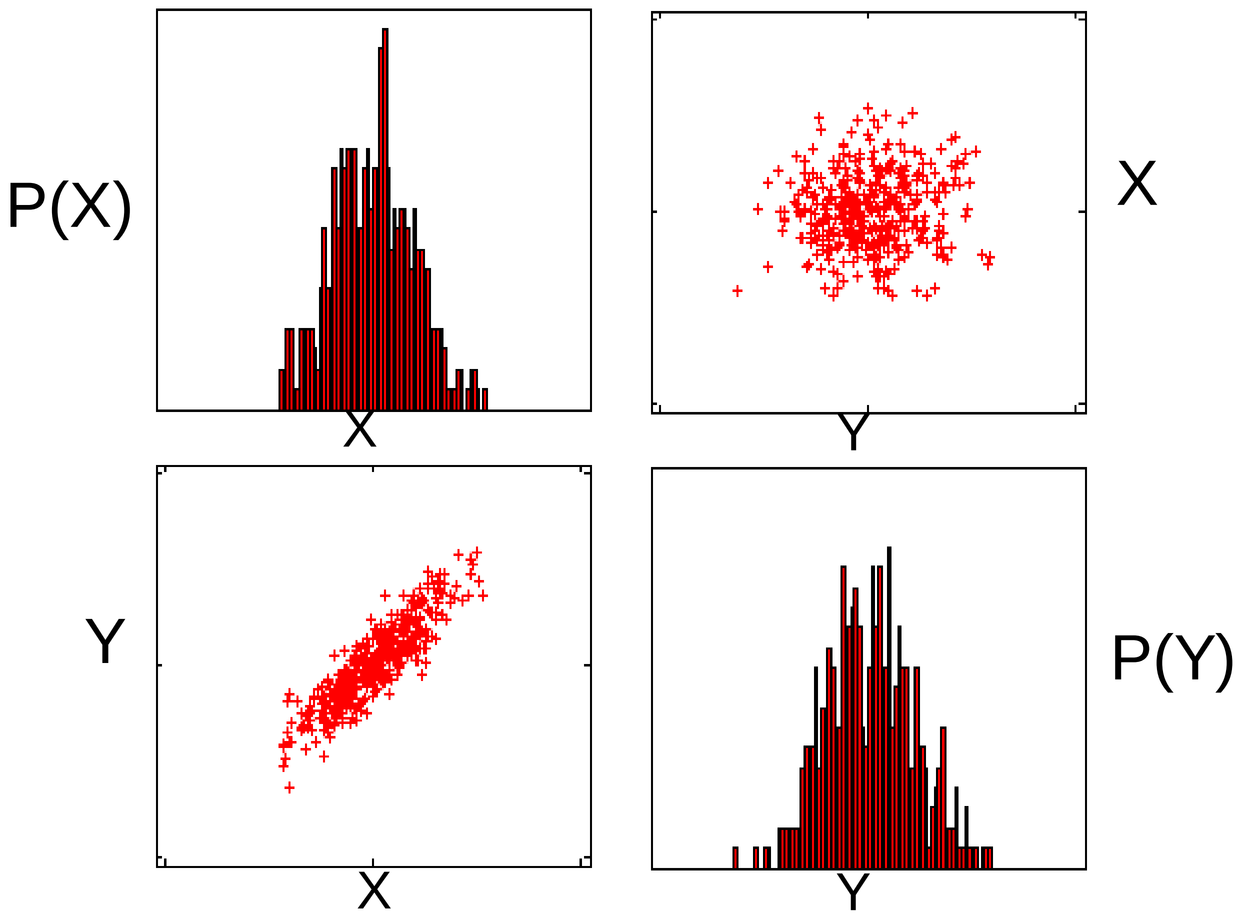
Gaussian Distribution



$$MI(X, Y) = -(1/2)\log(1-R^2)$$

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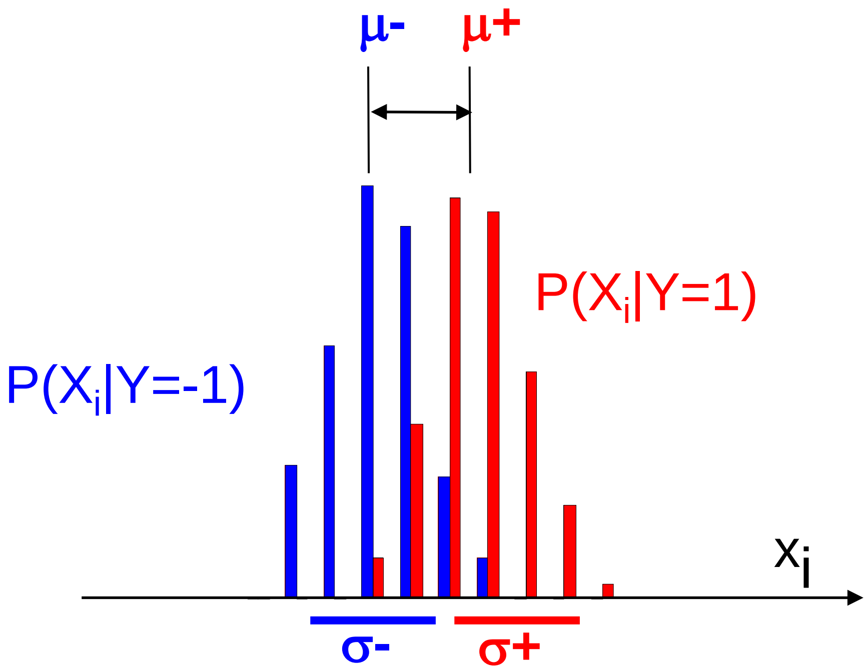
T-test



- Normally distributed classes, equal variance σ^2 unknown; estimated from data as σ^2_{within}.
- Null hypothesis H_0: $\mu+ = \mu-$
- T statistic: If H_0 is true,

$$t = (\mu+ - \mu-)/(\sigma_{within}\sqrt{1/m^+ + 1/m^-}) \sim \text{Student}(m^+ + m^- - 2 \text{ d.f.})$$

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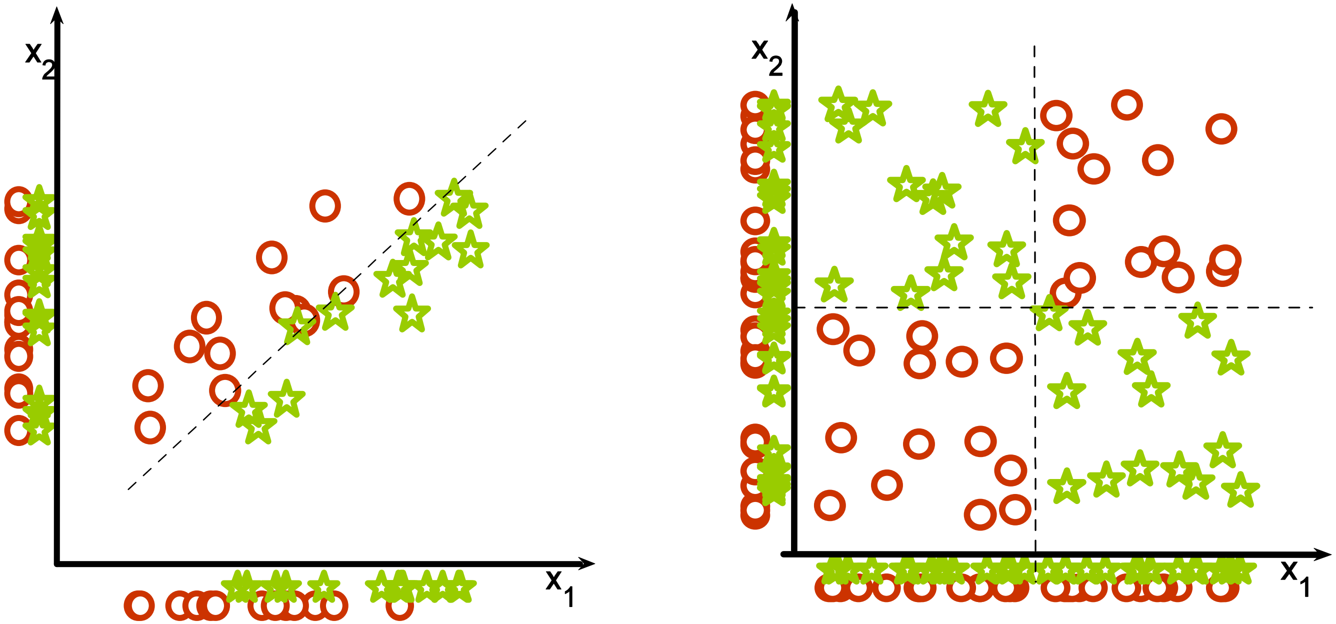
Other ideas for Univariate Feature Selection?

Considering each feature alone may fail



Guyon-Elisseeff, JMLR 2004; Springer 2006

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Multivariate Filter Methods?

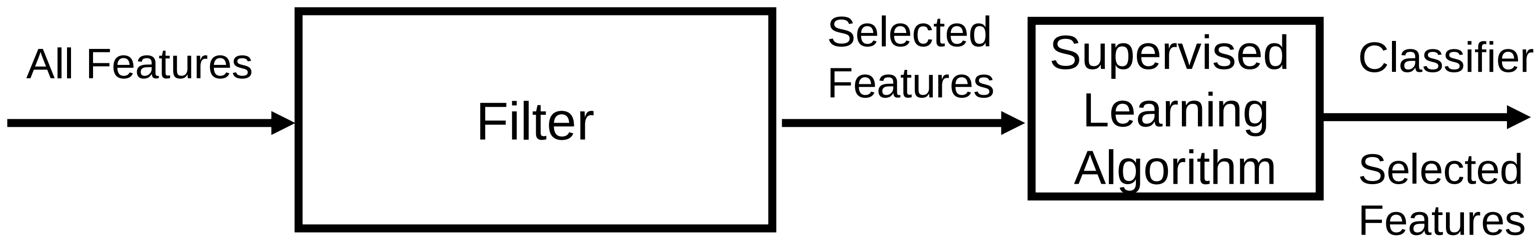
Filtering

- Advantages:
  - Fast, simple to apply

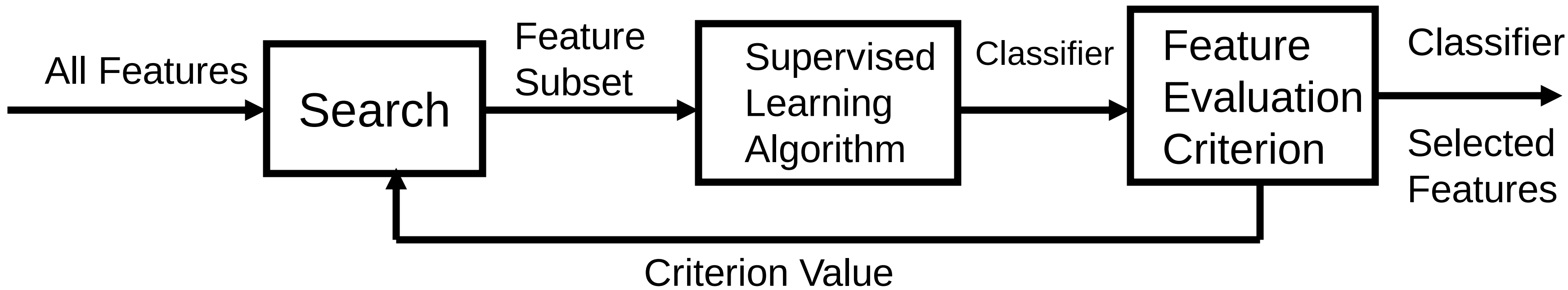
- Disadvantages:
  - Doesn’t take into account which learning algorithm will be used
  - Doesn’t take into account correlations between features, just correlation of each feature to the class label

Feature Selection Methods

Filter:



Wrapper:



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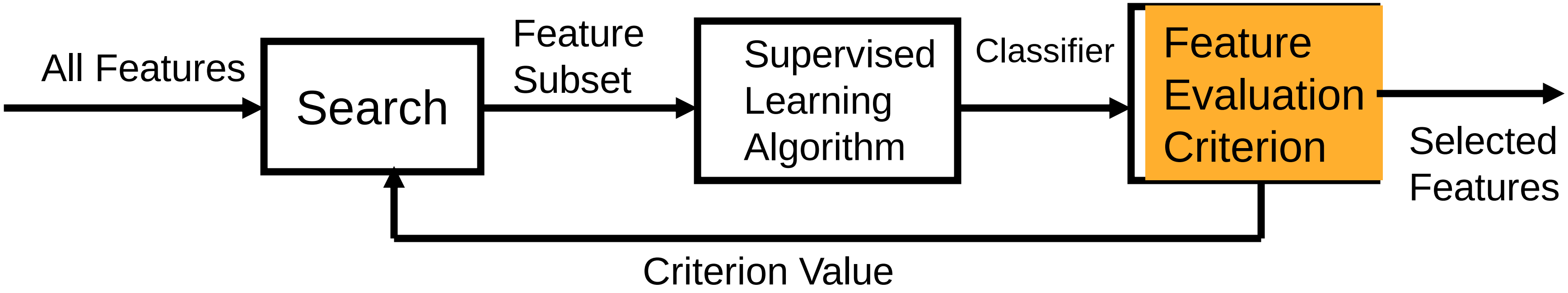
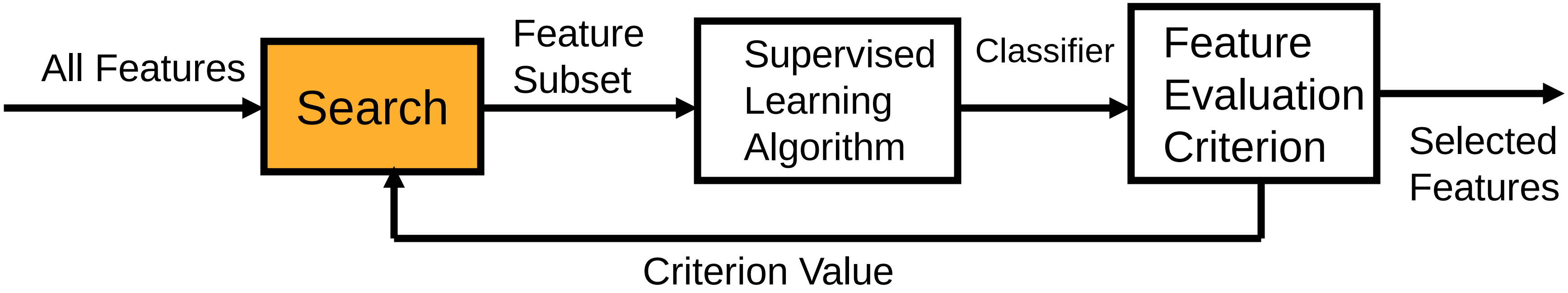
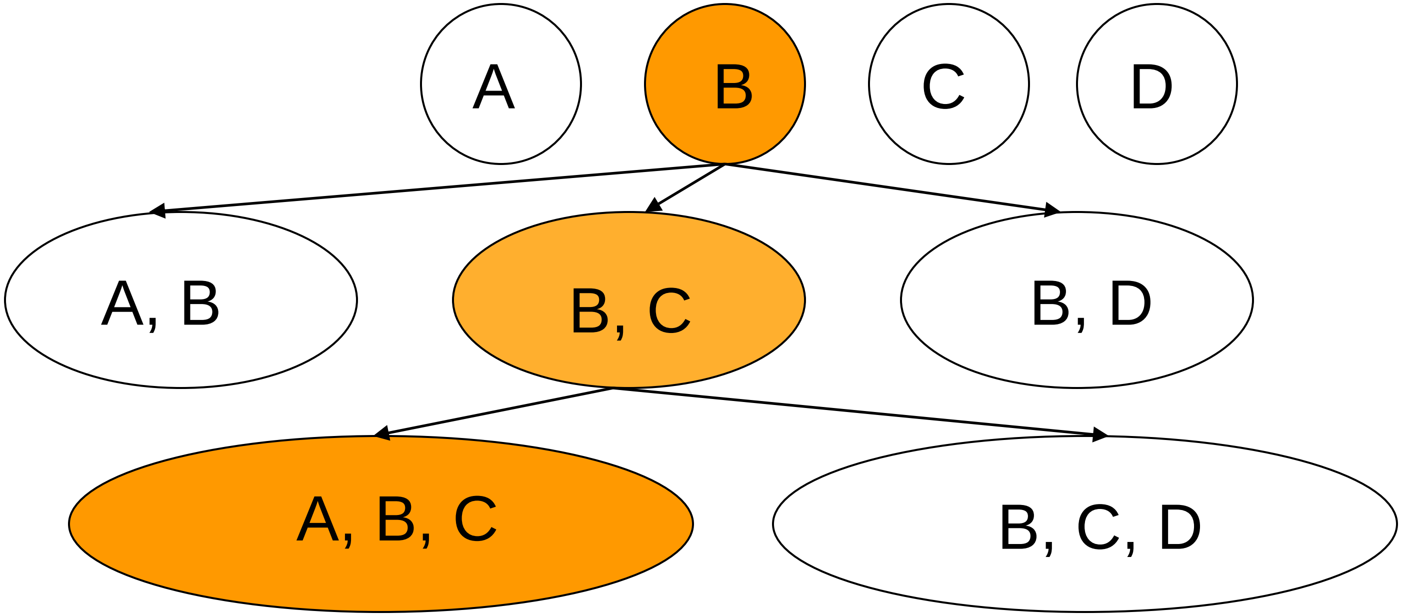

All Features
Search
Feature
Subset
Supervised
Learning
Algorithm
Classifier
Feature
Evaluation
Criterion
Selected
Features
Criterion Value



Search Method: sequential forward search



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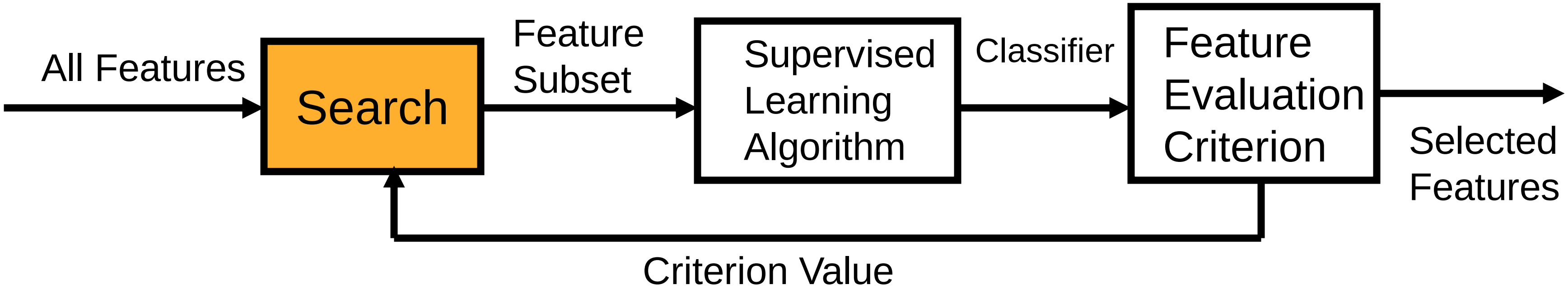
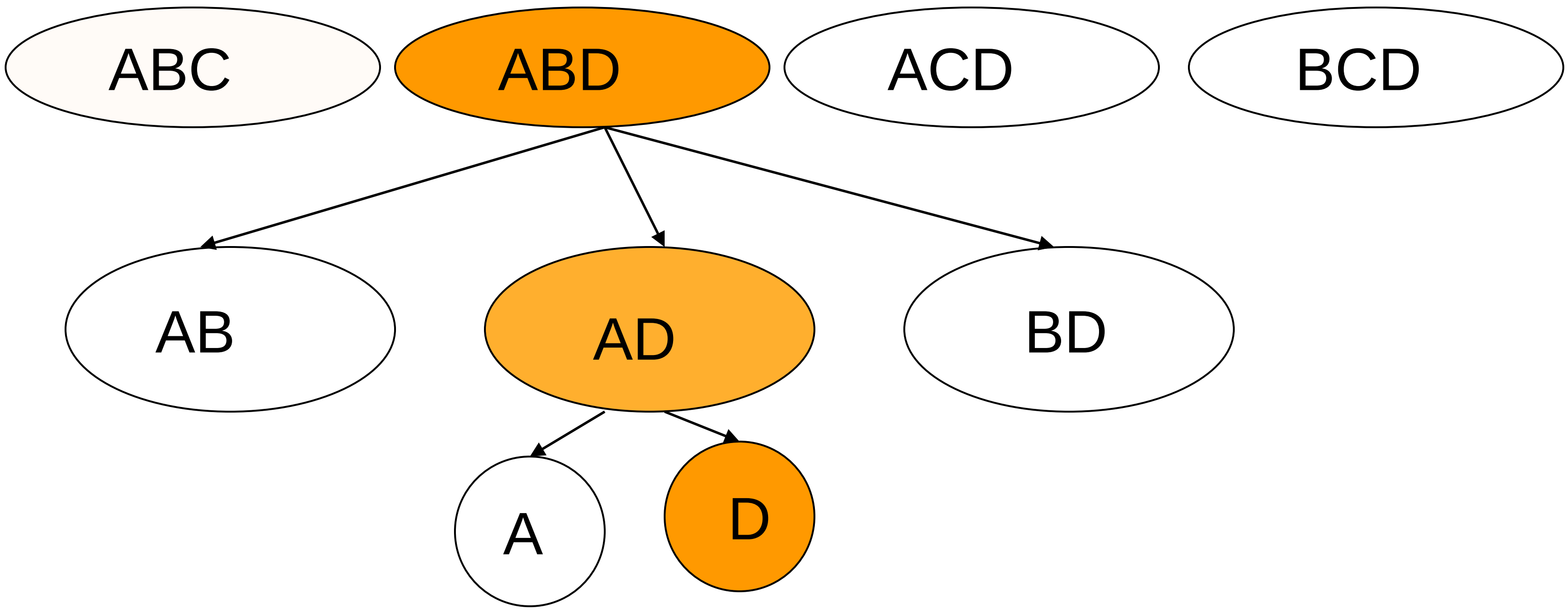
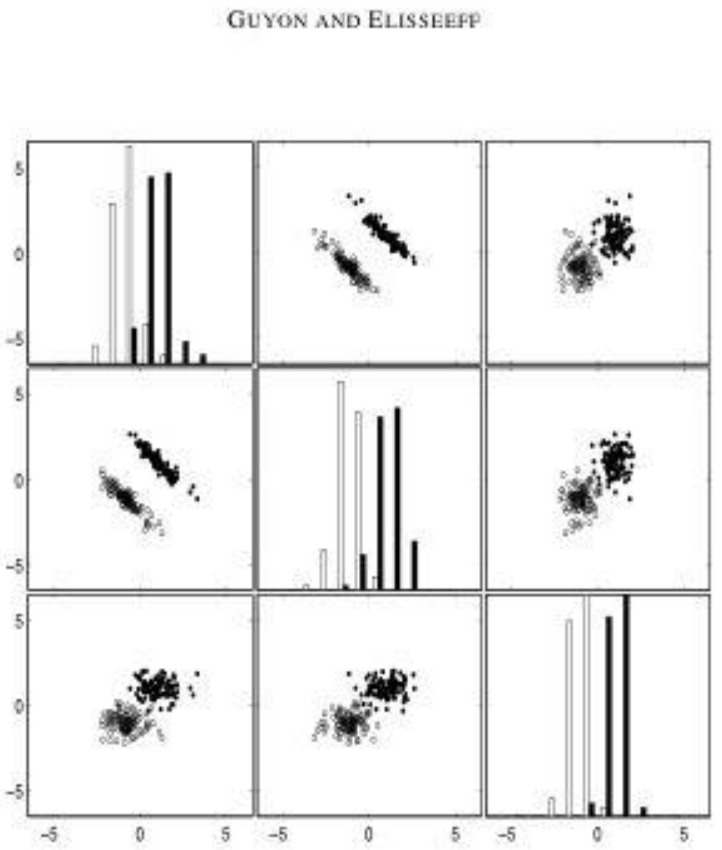


Search Method: sequential backward elimination



- **Forward or backward selection?** Of the three variables of this example, the third one separates the two classes best by itself (bottom right histogram). It is therefore the best candidate in a forward selection process. Still, the two other variables are better taken together than any subset of two including it. A backward selection method may perform better in this case.



Model search

- More sophisticated search strategies exist
  - Best-first search
  - Stochastic search
  - See "Wrappers for Feature Subset Selection", Kohavi and John 1997
- Other objective functions exist which add a model-complexity penalty to the training error
  - AIC, BIC

Regularization

- In certain cases, we can move model selection *into* the induction algorithm
  - Only have to fit one model; more efficient
- This is sometimes called an **embedded** feature selection algorithm

Regularization

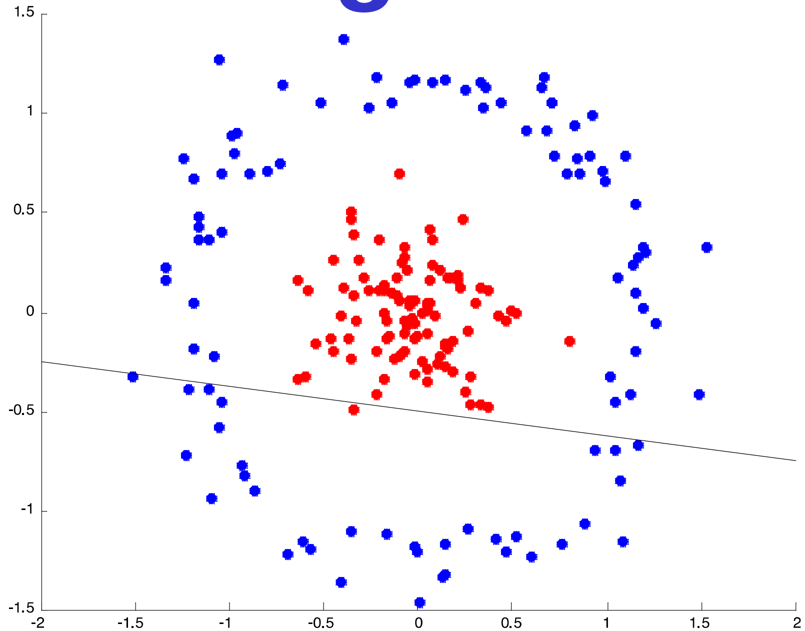
- Regularization: add model complexity penalty to training error.
- $J(\boldsymbol{w}) = L(\boldsymbol{w}) + C\|\boldsymbol{w}\|_p = \sum_{i=1}^{n}(y_i - \boldsymbol{w}^\top \boldsymbol{x}_i)^2 + C\|\boldsymbol{w}\|_p$

  for some constant C
- Now $\hat{\boldsymbol{w}} = \operatorname{argmin}_w J(w)$
- Regularization forces weights to be small, but does it force weights to be exactly *zero*?
  - $w_f = 0$ is equivalent to removing feature f from the model

Kernel Methods (Quick Review)

- Expanding feature space gives us new potentially useful features
- Kernel methods let us work implicitly in a high-dimensional feature space
  - All calculations performed quickly in low-dimensional space

Feature Engineering



- Linear models: convenient, fairly broad, but limited
- We can increase the expressiveness of linear models by expanding the feature space.
  - E.g.

$$\Phi([x_1\ x_2]) = [1\ \sqrt{2}x_1\ \sqrt{2}x_2\ \sqrt{2}x_1x_2\ x_1^2\ x_2^2]$$

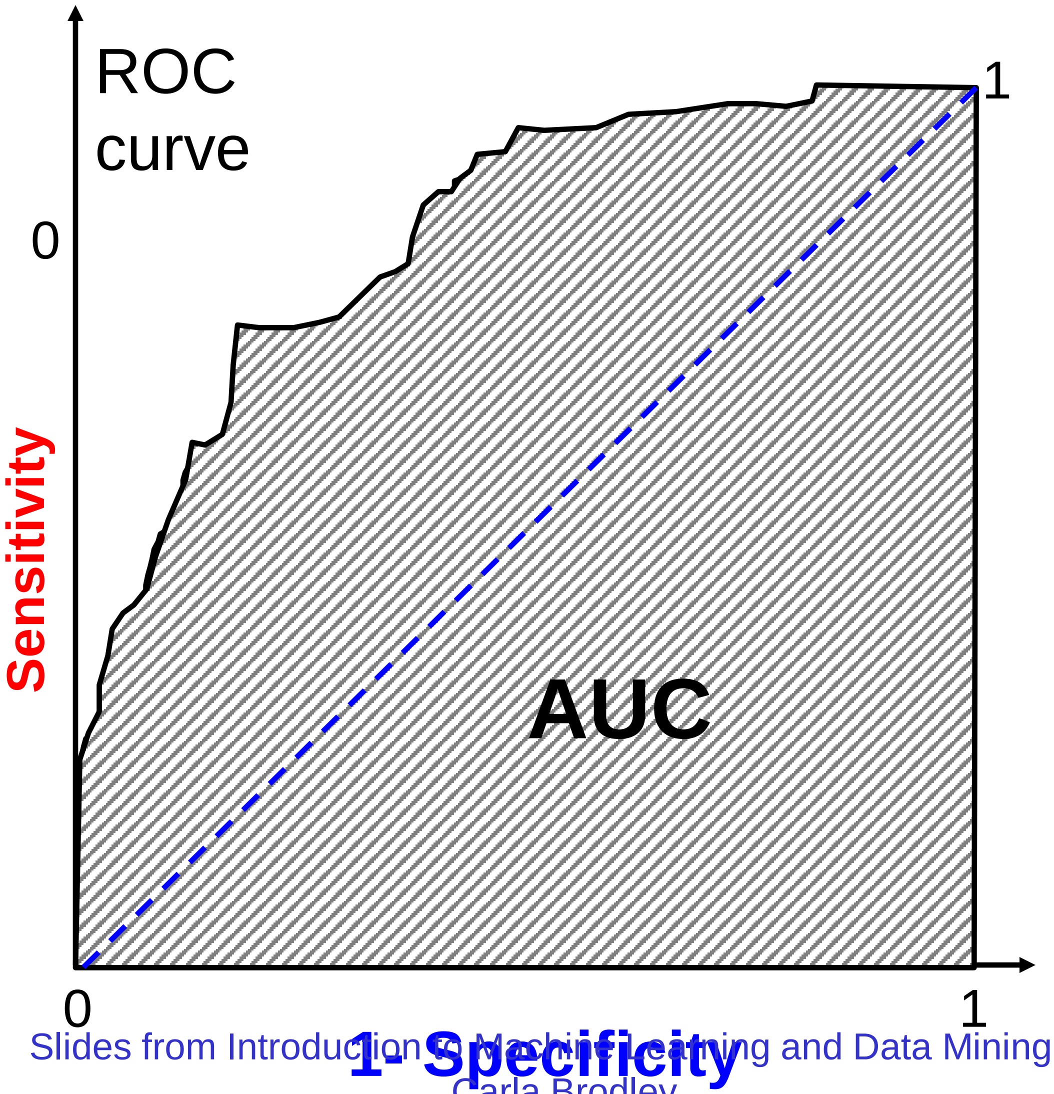
  - Now feature space is R^6 rather than R^2
  - Example *linear* predictor in these features:

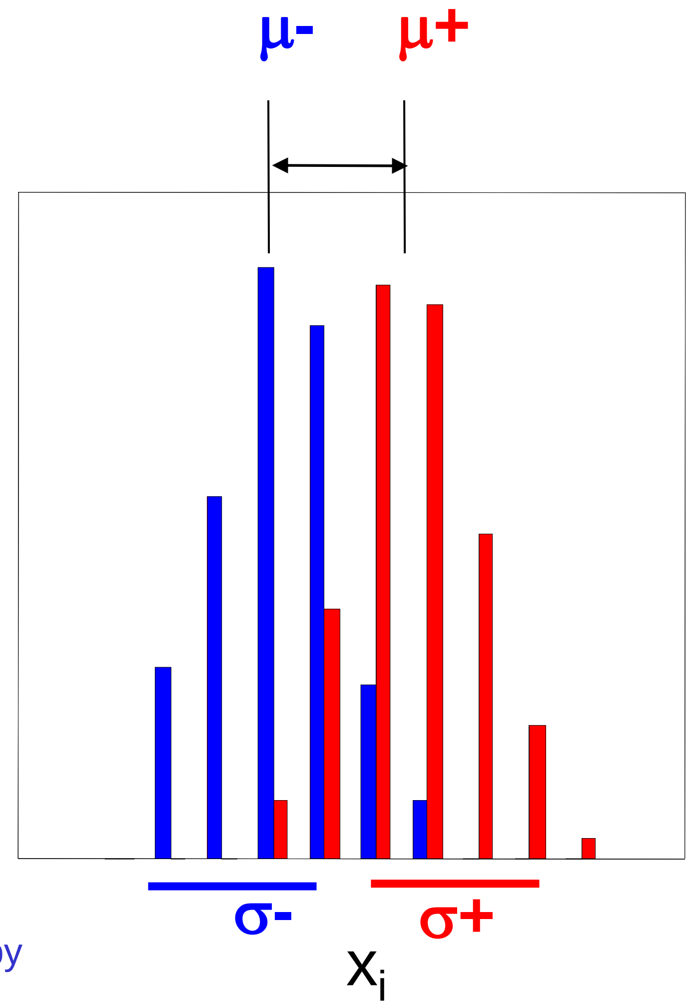
$$\mathrm{y} = [1\ 0\ 0\ 0\ \text{-}1\ \text{-}1] \cdot \Phi(\boldsymbol{x}) = 1 - x_1^2 - x_2^2$$

END OF MATERIAL

- Follow up slides require knowledge of ROC and L1, L2 Norms – have not yet covered these ideas in Fall 2012

Individual Feature Relevance





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L_1 versus L_2 Regularization

$$||\boldsymbol{w}||_1 = \sum_{f=0}^{d} |w_f| \qquad ||\boldsymbol{w}||_2 = \sqrt{\sum_{f=0}^{d} w_f^2}$$