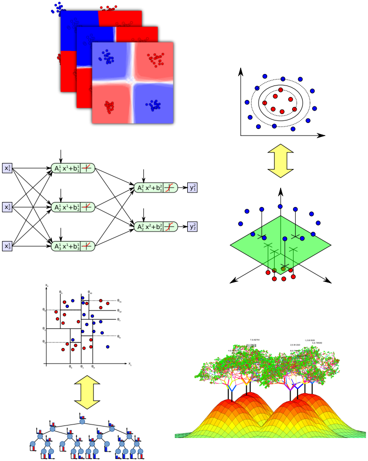
MVA - Discrete Inference and Learning
Lecture 6
-
Classical Learning

Yuliya Tarabalka
Inria Sophia Antipolis-Méditerranée - TITANE team
Université Côte d'Azur - France

Overview

1. Classification based on Features
   - Decision Boundary
   - Linear Decision Boundary
   - Non-linear Decision Boundary
2. Feature extraction
3. Machine Learning Methods
   - Support Vector Machine (SVM)
   - Multi-Layer Perceptron (MLP)
   - Random Forest (RF)



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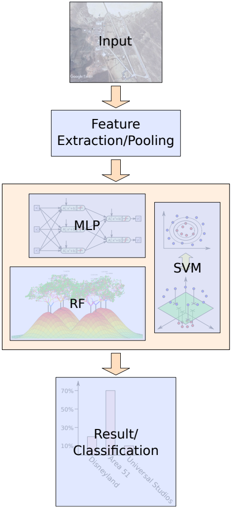
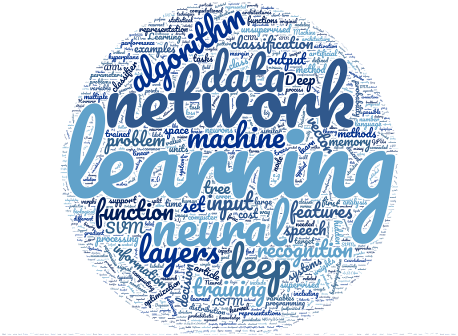
Classical Learning

- Features extract very basic, low level information
- We want very high level information (e.g. class of objects)
- Classical Learning: Learn the mapping between low level features and high level information



Classical Learning

- Machine Learning is a huge (growing) field
- Many different approaches for modeling/parametrizing this mapping!



Methods

- Choice of method not always rational
- Different pros/cons
- Speed, memory, scalability of training data, ease of implementation, ease of hyper parameter tuning, ...
- First intuitive understanding of the problems, then identifying methods

Decision based on features

Toy example

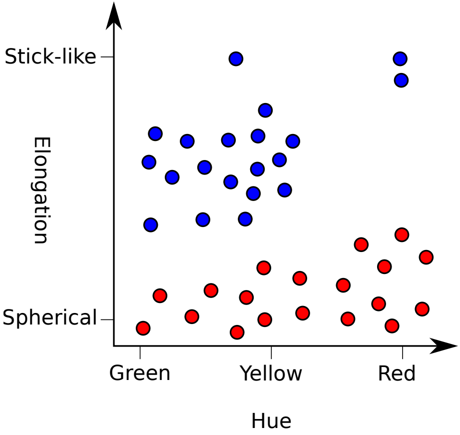
Task: Classify fruits into either bananas or apples

Extracted Feature Vector

- Hue (yellow to red)
- Elongation (max extend over min extend)

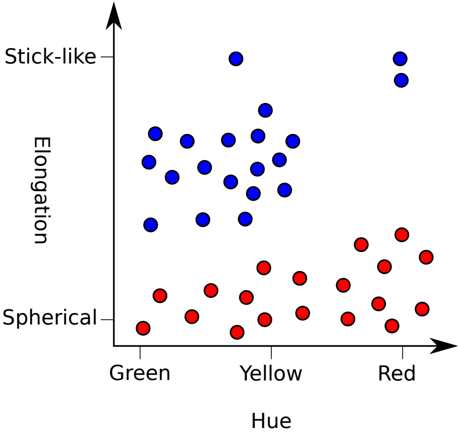
Some training data

- Feature space is just 2D
- Datapoints can be plotted as a scatter plot



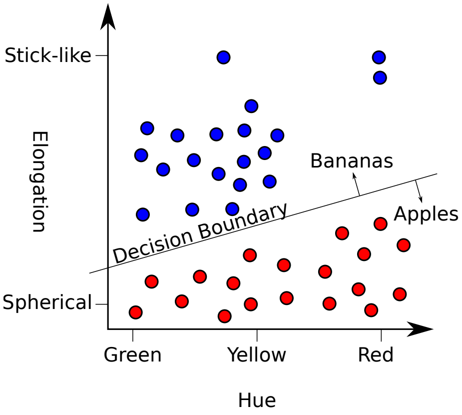
Some training data

- Feature space is just 2D
- Datapoints can be plotted as a scatter plot
- Can we "learn", which part of the feature space is bananas/apples?



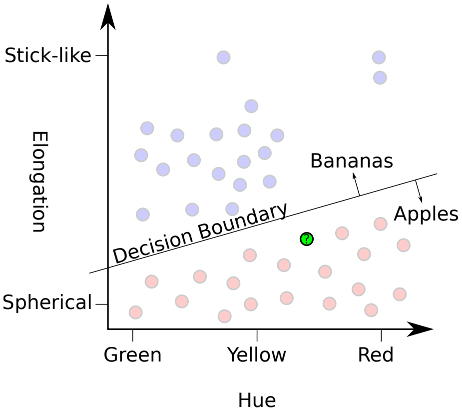
Decision boundary

- (Very) simple idea: Split the feature space into two half spaces



Decision boundary

- (Very) simple idea: Split the feature space into two half spaces
- During application, classify data based on this decision boundary



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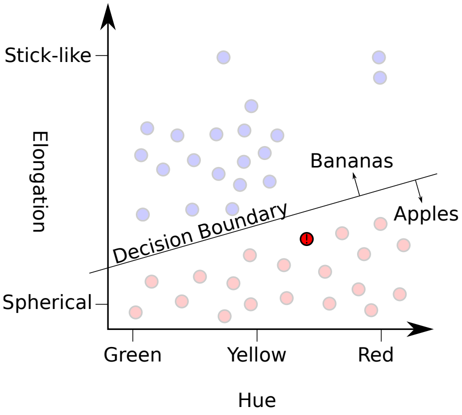
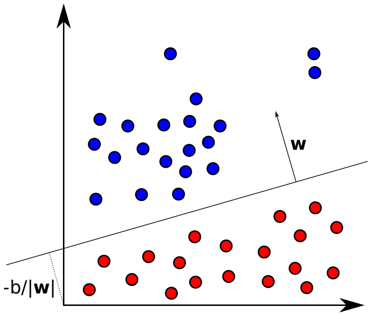


Perceptron

Perceptron

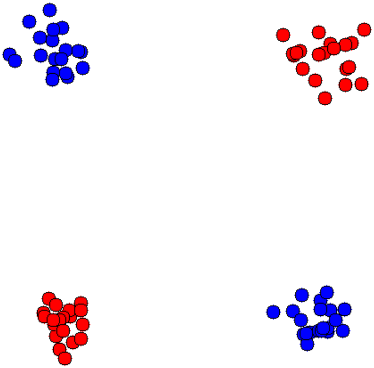
$$y = \text{sign}(\mathbf{w}^T \mathbf{x} + b) \qquad (1)$$

- $y \in \{-1, 1\}$: Predicted class
- $\mathbf{x} \in \mathbb{R}^2$: Feature vector
- $\mathbf{w} \in \mathbb{R}^2$: "Weight vector" (needs to be learned)
- $b \in \mathbb{R}$: "Bias" (needs to be learned)



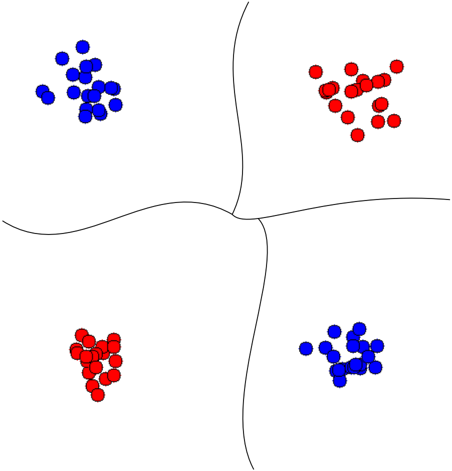
Linear Separability

- What if no such line exists?
- Quite often, problem not linearly separable
- Needs non-linear decision boundary



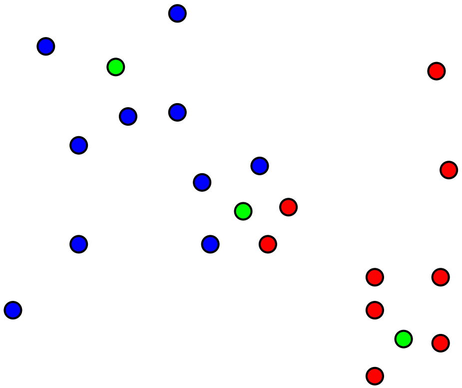
Non-linear Decision Boundary

- Decision boundaries of more complex ML techniques usually non-linear
- Regions need not be connected



kNN

- Very simple idea:
  k-Nearest-Neighbors for
  classification



kNN

- Very simple idea:
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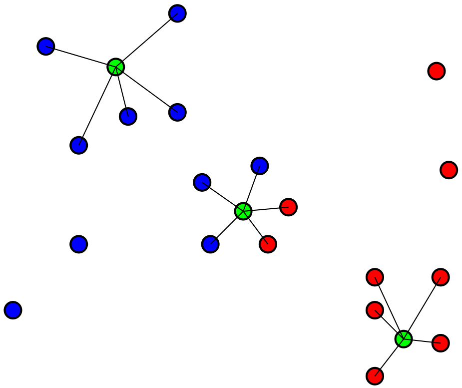
- For a sample find the k (e.g. 5) closest data points in the training dataset



kNN

- Very simple idea:
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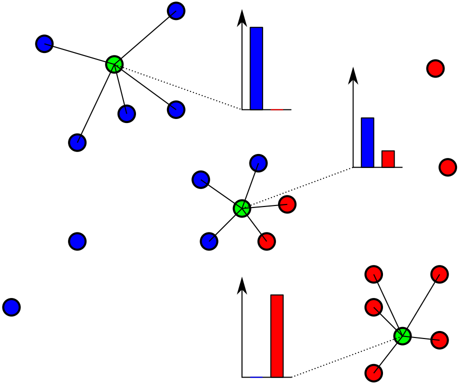
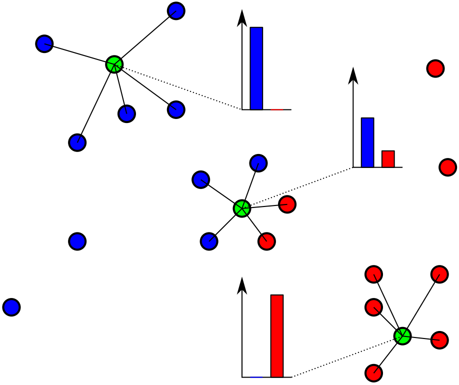
- For a sample find the k (e.g. 5) closest data points in the training dataset
- Look at the labels of those neighbors

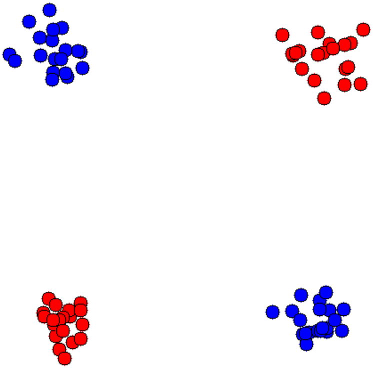


kNN

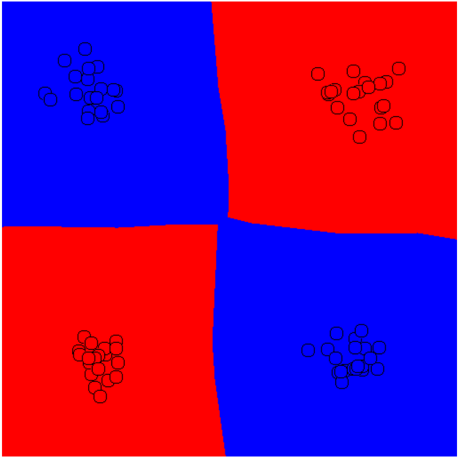
- Very simple idea: k-Nearest-Neighbors for classification
- For a sample find the k (e.g. 5) closest data points in the training dataset
- Look at the labels of those neighbors
- Fast lookup through trees/approximate methods
- Needs to keep all training data around



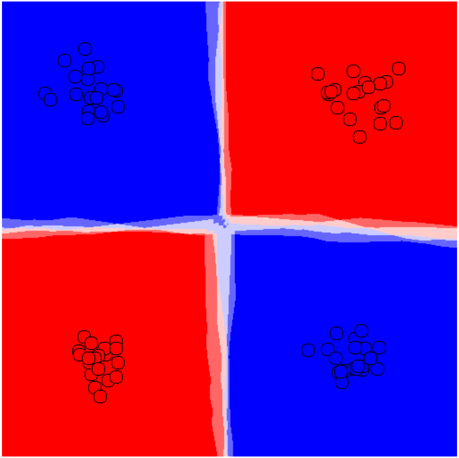
kNN Example - Simple



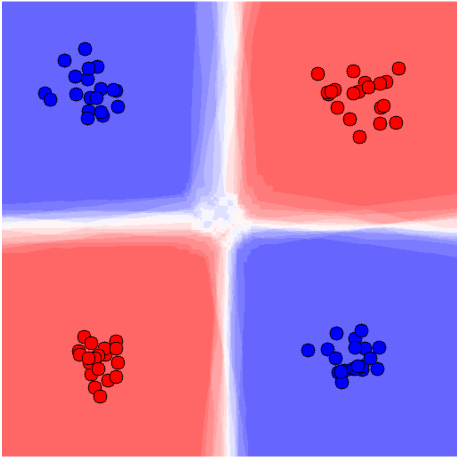
kNN Example - Simple - kNN K=1



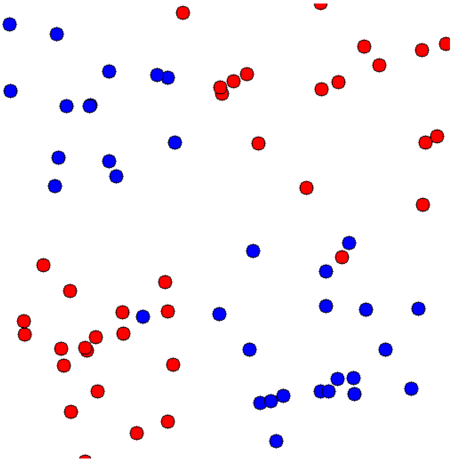
kNN Example - Simple - kNN K=5



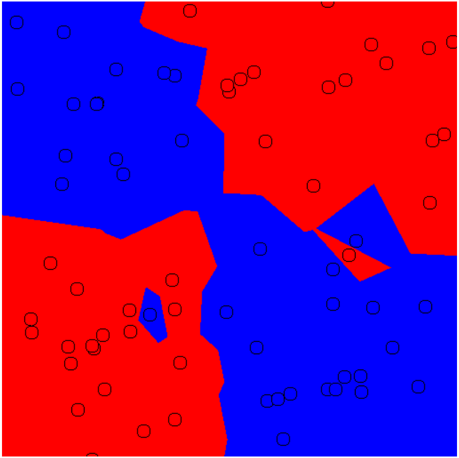
kNN Example - Simple - kNN K=25



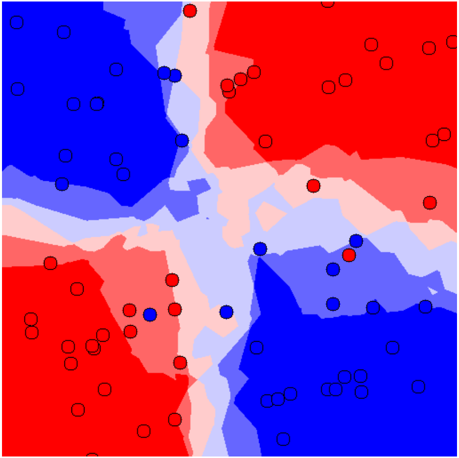
kNN Example - Hard



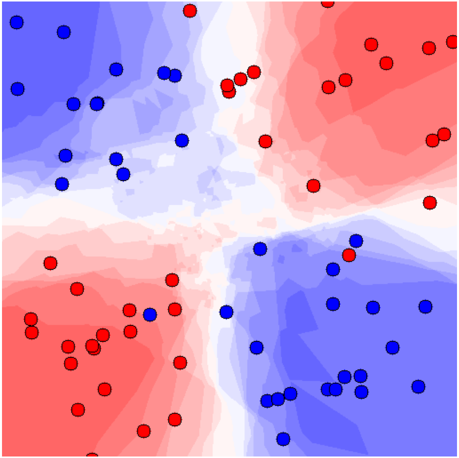
kNN Example - Hard - kNN K=1



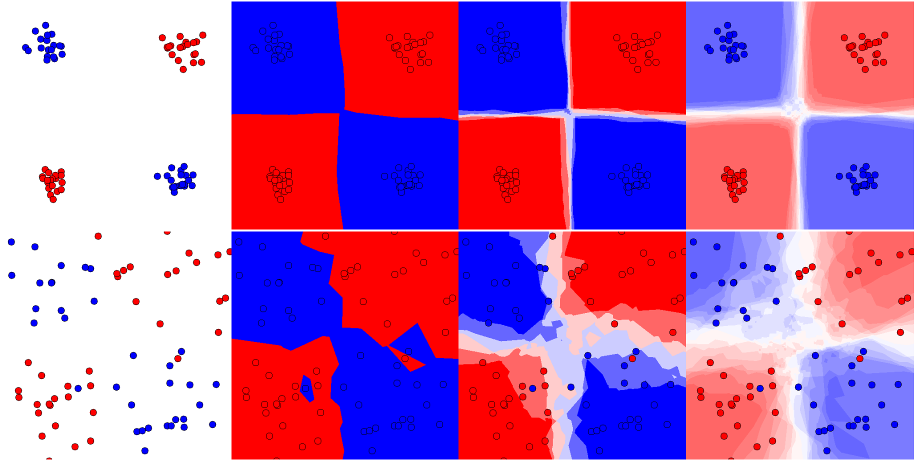
kNN Example - Hard - kNN K=5



kNN Example - Hard - kNN K=25

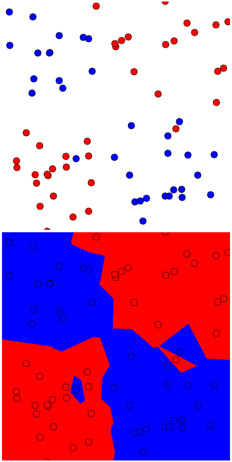


kNN Example

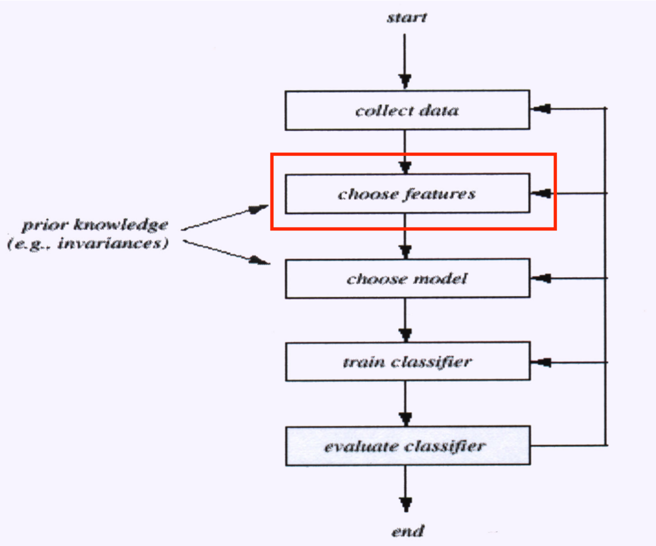


Model Complexity vs Overfitting

- With sufficient model complexity, it is often easy to get ZERO training error
- Generalization is what matters!
- **Test on data not used during training**
  - Disjoint train and test set
  - Non-overlapping samples if spatial features are used
  - Semi-manual parameter tuning (grid-search, etc.) needs third independent data set



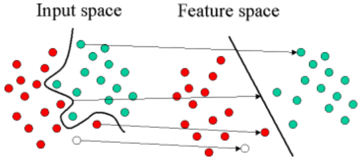
Why do we need feature extraction?



Motivation

- **Main motivation:** get out most of the data

- For classification task: find a space where samples from different classes are well separable

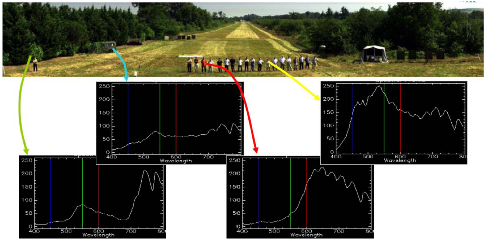


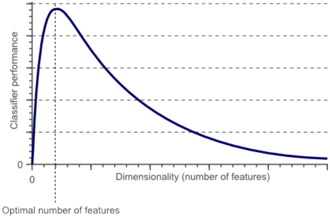
Objectives:

- Reduce computational load of the classifier
- Increase data consistency
- Incorporate different sources of information into a feature vector: spectral, spatial, multisource, ...

Motivation - Curse of dimensionality

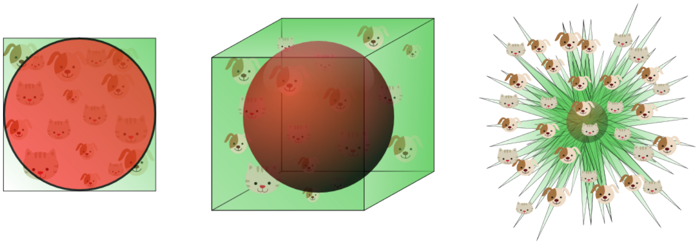
- Too few features do not allow to discriminate between classes
    - In the color image, both trees and a truck are green
- As the dimensionality of the feature space increases, the classifier's performance increases until the optimal number of features is reached
- Further increasing the dimensionality without increasing the number of training samples yields a performance decrease





Motivation - Curse of dimensionality

- As the dimensionality increases:
  - The volume of the hypersphere tends to zero
  - A larger percentage of the training data resides in the corners of the feature space
  - Distance measures start losing their effectiveness
  - Gaussian likelihoods become flat and heavy tailed distributions



How to reduce data dimensions?

Principal component analysis

Convert a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables, called **principal components**

Discriminant analysis

Find the best set of vectors which best separates the patterns

Principal component analysis

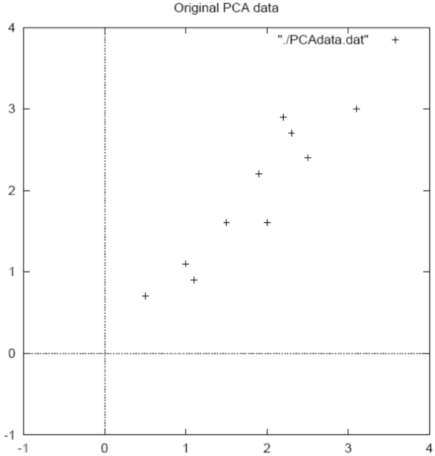
- **Goal**: represent data is a space that best describes the variation in a sum-squared error sense
- Projection onto eigenvectors that correspond to the first few largest eigenvalues of the covariance matrix
  - d-dimensional data are represented in a lower-dimensional space
  - Reduces the space and time complexities
- Intuitive introduction: `http://www.youtube.com/watch?v=BfTMmoDFXyE&feature=related`

Principal component analysis

- **Step 1**: Get some data

Data =

x	y
2.5	2.4
0.5	0.7
2.2	2.9
1.9	2.2
3.1	3.0
2.3	2.7
2	1.6
1	1.1
1.5	1.6
1.1	0.9



Principal component analysis

- **Step 2**: Subtract the mean
  - From each of the data dimensions (from x- and y-dimension)

Data =

x	y
2.5	2.4
0.5	0.7
2.2	2.9
1.9	2.2
3.1	3.0
2.3	2.7
2	1.6
1	1.1
1.5	1.6
1.1	0.9

DataAdjust =

x	y
.69	.49
-1.31	-1.21
.39	.99
.09	.29
1.29	1.09
.49	.79
.19	-.31
-.81	-.81
-.31	-.31
-.71	-1.01

Principal component analysis

- **Step 3**: Calculate the covariance matrix

Data =

x	y
2.5	2.4
0.5	0.7
2.2	2.9
1.9	2.2
3.1	3.0
2.3	2.7
2	1.6
1	1.1
1.5	1.6
1.1	0.9

$$\Rightarrow$$

$$cov = \begin{pmatrix} .616555556 & .615444444 \\ .615444444 & .716555556 \end{pmatrix}$$

Principal component analysis

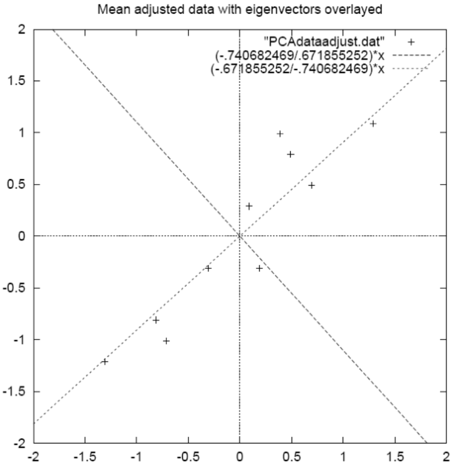
- **Step 4**: Calculate the unit eigenvectors and eigenvalues of the covariance matrix

$$cov = \begin{pmatrix} .616555556 & .615444444 \\ .615444444 & .716555556 \end{pmatrix}$$

$$\Downarrow$$

$$eigenvalues = \begin{pmatrix} .0490833989 \\ 1.28402771 \end{pmatrix}$$

$$eigenvectors = \begin{pmatrix} -.735178656 & -.677873399 \\ .677873399 & -.735178656 \end{pmatrix}$$



Principal component analysis

- The 1st eigenvector (principle component) shows how data in two dimensions are related along the eigenvector line
- The 2nd eigenvector shows that all the points are off to the side of the main line by some amount
- Eigenvectors are lines that characterize the data
- The next steps: transforming the data so that it is expressed in terms of these lines

Principal component analysis

- **Step 5**: Choose components and form a feature vector
  - Order eigenvectors by eigenvalues
    - This gives the components in order of significance
    - You can decide to ignore the components of lesser significance $\Rightarrow$ final data will have less dimensions ($p < d$)
  - Form a feature vector (matrix of vectors):

$$FeatureVector = (eig_1 \;\; eig_2 \;\; eig_3)$$

- For our example, two feature vectors are possible:

$$eigenvalues = \begin{pmatrix} .0490833989 \\ 1.28402771 \end{pmatrix}$$

$$eigenvectors = \begin{pmatrix} -.735178656 & -.677873399 \\ .677873399 & -.735178656 \end{pmatrix}$$

$$\begin{pmatrix} -.677873399 & -.735178656 \\ -.735178656 & .677873399 \end{pmatrix}$$

or

$$\begin{pmatrix} -.677873399 \\ -.735178656 \end{pmatrix}$$

Principal component analysis

- **Step 6**: Derive the new dataset:

$$FinalData = FeatureVector^T \times RowDataAdjust$$

  where *RowDataAdjust* is the mean-adjusted data transposed

- It will give us the original data solely in terms of the vectors we chose

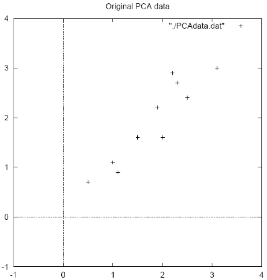
Principal component analysis

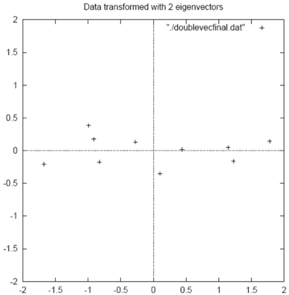
Data =

x	y
2.5	2.4
0.5	0.7
2.2	2.9
1.9	2.2
3.1	3.0
2.3	2.7
2	1.6
1	1.1
1.5	1.6
1.1	0.9

Transformed Data=

x	y
-.827970186	-.175115307
1.77758033	.142857227
-.992197494	.384374989
-.274210416	.130417207
-1.67580142	-.209498461
-.912949103	.175282444
.0991094375	-.349824698
1.14457216	.0464172582
.438046137	.0177646297
1.22382056	-.162675287



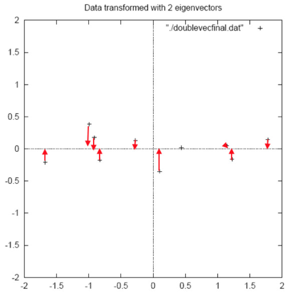


Principal component analysis (PCA)

Transformed Data=

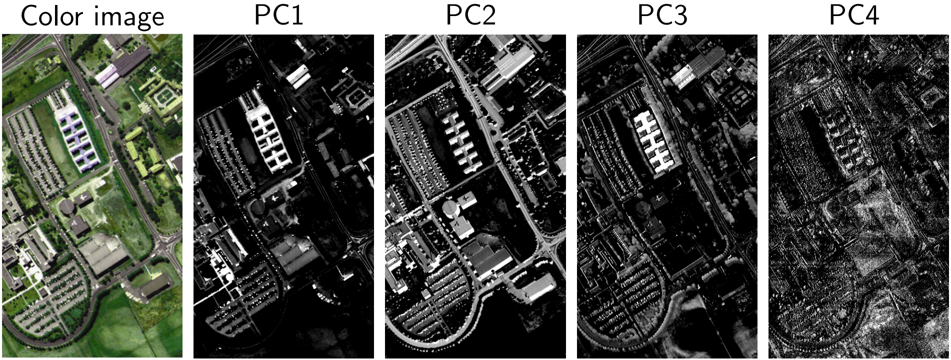
x	y
-.827970186	-.175115307
1.77758033	.142857227
-.992197494	.384374989
-.274210416	.130417207
-1.67580142	-.209498461
-.912949103	.175282444
.0991094375	-.349824698
1.14457216	.0464172582
.438046137	.0177646297
1.22382056	-.162675287

- If only one eigenvector was kept, the transformed data will have only one dimension



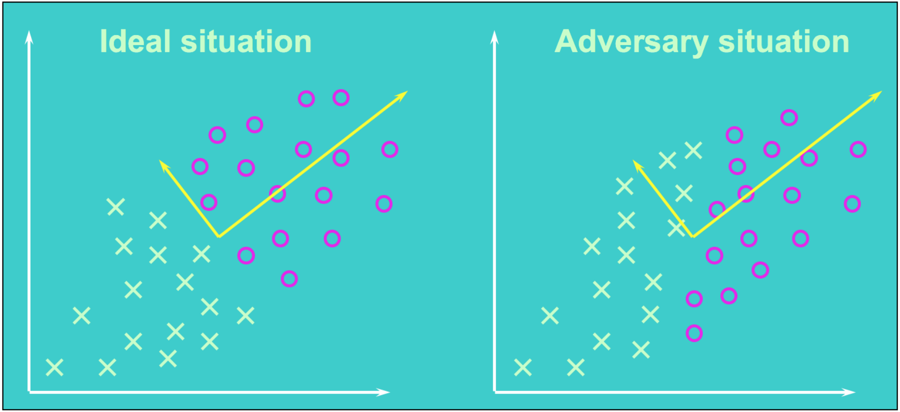
Example of PCA for hyperspectral image analysis

- Principal component analysis in the spectral space
  - Principal components (PCs) 1-3 contain 97% of information from original 103 channels



Principal component analysis

- Projection onto eigenvectors that correspond to the first few largest eigenvalues of the covariance matrix

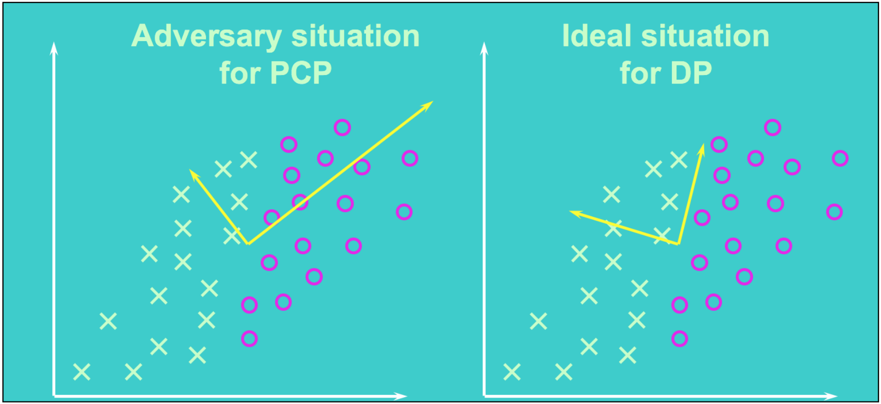


Discriminant analysis

- PCA seeks directions that are efficient for **representation**
  - *Unsupervised technique*
- Discriminant analysis seeks directions that are efficient for **discrimination**
  - *Supervised technique*

Discriminant analysis

- Projection onto directions that can best separate data of different classes



Discriminant analysis

- Theory of Fisher linear discriminant: `http://www.csd.uwo.ca/~olga/Courses//CS434a_541a//Lecture8.pdf`
- Project on line in the direction v which maximizes:

$$J(v) = \frac{\overbrace{(\tilde{\mu}_1 - \tilde{\mu}_2)^2}^{\text{want projected means are far from each other}}}{\tilde{s}_1^2 + \tilde{s}_2^2}$$

want scatter in class 1 is as small as possible, i.e. samples of class 1 cluster around the projected mean $\tilde{\mu}_1$

want scatter in class 2 is as small as possible, i.e. samples of class 2 cluster around the projected mean $\tilde{\mu}_2$

- Main drawback: in most real-life cases, projection to even the best line results in unseparable projected samples

Models

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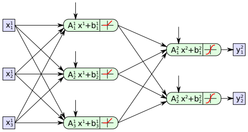

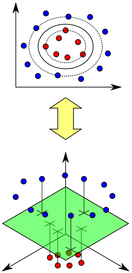

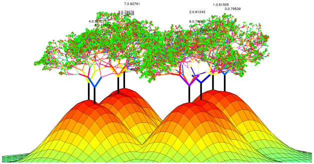

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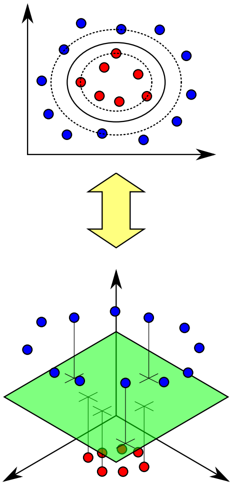
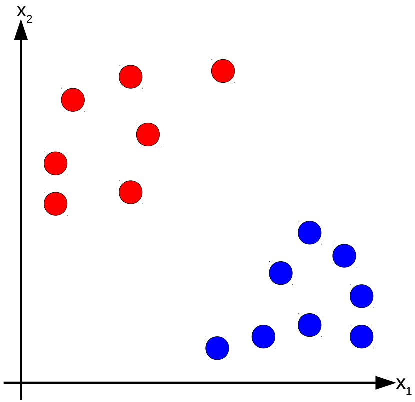


SVM

Reconsider the perceptron:

Perceptron

$$y = \text{sign}(\mathbf{w}^T \mathbf{x} + b) \qquad (2)$$

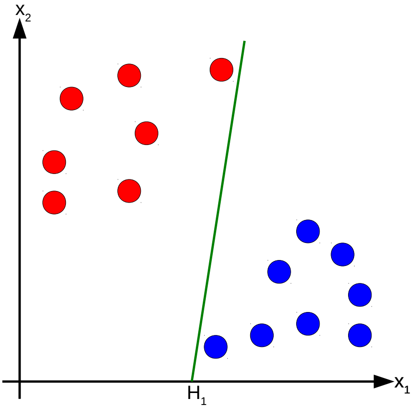


SVM

Reconsider the perceptron:

Perceptron

$$y = \text{sign}(\mathbf{w}^T\mathbf{x} + b) \qquad (2)$$



SVM

Reconsider the perceptron:

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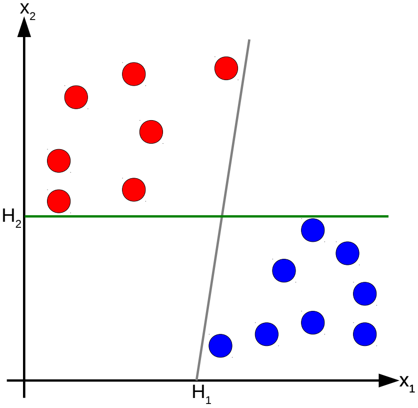

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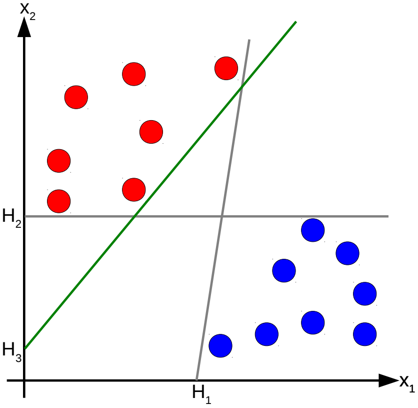

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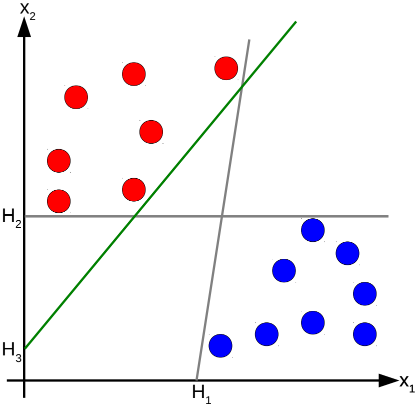

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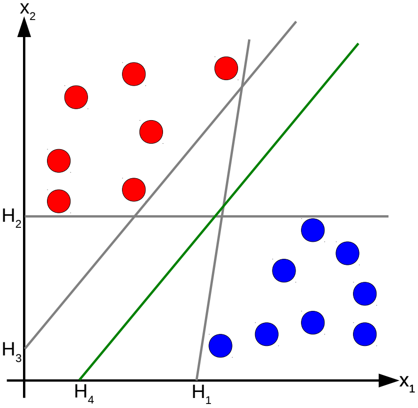

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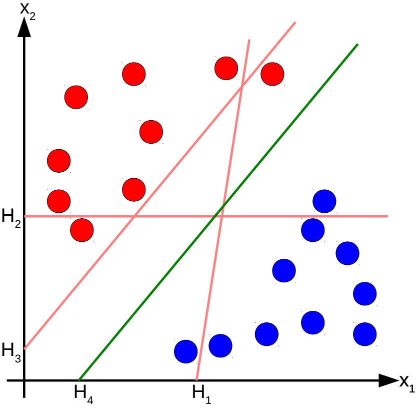
- Don't just pick any decision boundary
- Pick the one with the *maximal margin*
- Perceptron of maximal stability



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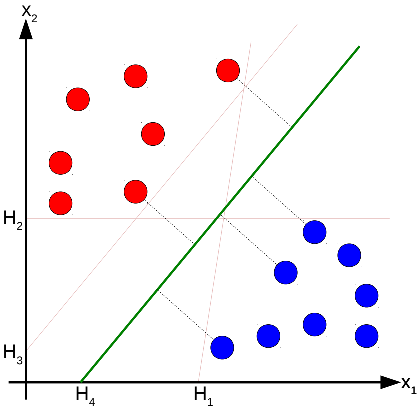
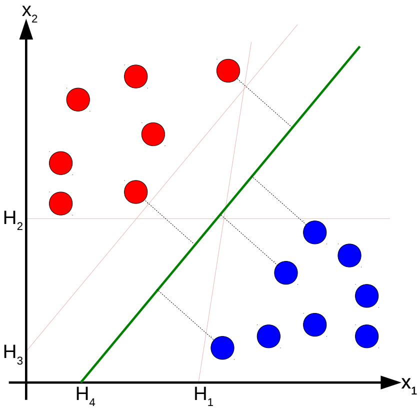


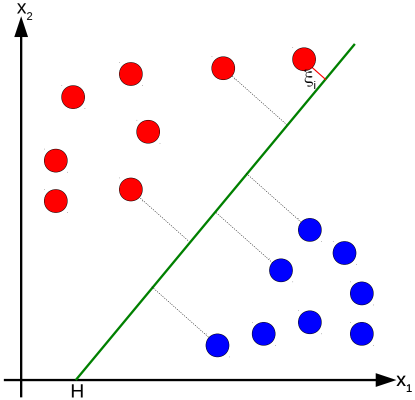
SVM

- Maximal margin equivalent to:
  Minimize $||w||^2$
  subject to $\hat{y}_i(w^T \mathbf{x}_i - b) \geq 1$



SVM

- Maximal margin equivalent to:
  Minimize $||\mathbf{w}||^2$
  subject to $\hat{y}_i(\mathbf{w}^T\mathbf{x}_i - b) \geq 1$
- Allow small errors (soft margin):
  Minimize $\lambda||w||^2 + \frac{1}{n}\sum_{i=1}^{n}\xi_i$
  subject to $\hat{y}_i(w^T\mathbf{x}_i - b) \geq 1 - \xi_i$
  $(\xi_i \geq 0)$

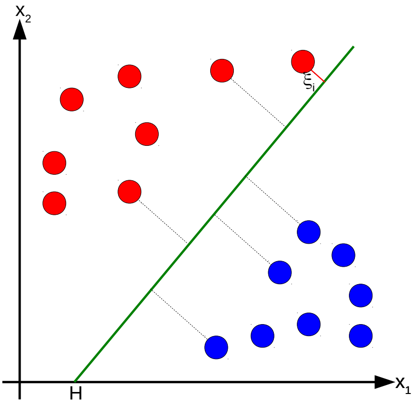


SVM

- The Lagrangian dual gives:
  Maximize

$$\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \hat{y}_i \alpha_i (\mathbf{x}_i \cdot \mathbf{x}_j) \hat{y}_j \alpha_j$$

  subject to $\sum_{i=1}^{n} \alpha_i \hat{y}_i = 0$
- Support vectors: $\mathbf{x}_i$ if $\alpha_i \neq 0$
- Classification: $sign(\mathbf{w}^T \mathbf{x} + b)$
  with $\mathbf{w} = \sum_{i=1}^{n} \alpha_i \hat{y}_i \mathbf{x}_i$



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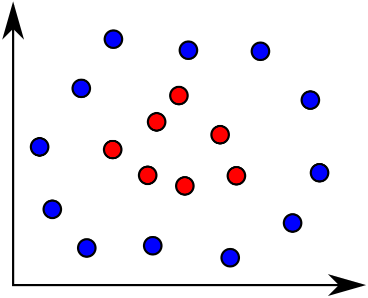

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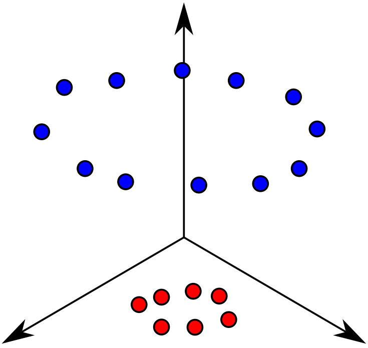
  with $\mathbf{w} = \sum_{i=1}^{n} \alpha_i \hat{y}_i \mathbf{x}_i$
- What if $\mathbf{x}_i$ not linear separable at all?
  $\rightarrow$ Compute new features $\mathbf{x} \mapsto \phi(\mathbf{x})$



SVM

- The Lagrangian dual gives:
  Maximize

$$\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \hat{y}_i \alpha_i (\phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j)) \hat{y}_j \alpha_j$$

  subject to $\sum_{i=1}^{n} \alpha_i \hat{y}_i = 0$
- Support vectors: $\mathbf{x}_i$ if $\alpha_i \neq 0$
- Classification: $sign(\mathbf{w}^T \phi(\mathbf{x}) + b)$
  with $\mathbf{w} = \sum_{i=1}^{n} \alpha_i \hat{y}_i \phi(\mathbf{x}_i)$
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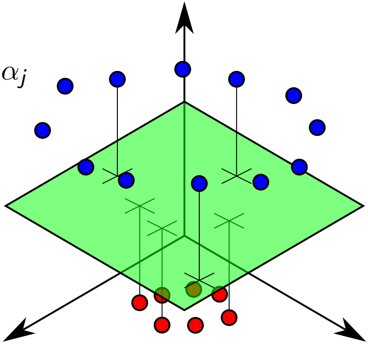
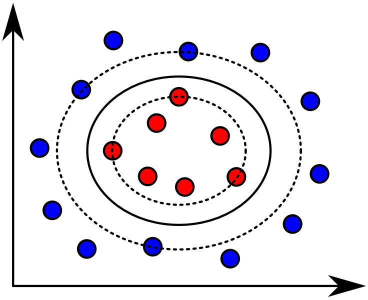


SVM

- The Lagrangian dual gives:
  Maximize

$$\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \hat{y}_i \alpha_i k(\mathbf{x}_i, \mathbf{x}_j) \hat{y}_j \alpha_j$$

  subject to $\sum_{i=1}^{n} \alpha_i \hat{y}_i = 0$
- Support vectors: $\mathbf{x}_i$ if $\alpha_i \neq 0$
- Classification:
  $sign(\sum_{i=1}^{n} \alpha_i \hat{y}_i k(\mathbf{x}_i, \mathbf{x}) + b)$
- What if $\mathbf{x}_i$ not linear separable at all?
  $\rightarrow$ Compute new features $\mathbf{x} \mapsto \phi(\mathbf{x})$
- Use $k(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j)$



SVM Kernels

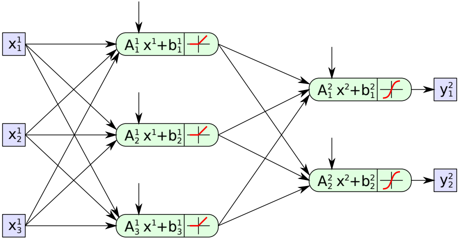
- Multiple kernels exist
  - Linear $k(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i \cdot \mathbf{x}_j$
  - Polynomial $k(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i \cdot \mathbf{x}_j)^d$
  - RBF $k(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\gamma||\mathbf{x}_i - \mathbf{x}_j)||^2$
  - Hyperbolic tangent $k(\mathbf{x}_i, \mathbf{x}_j) = \tanh(\kappa \cdot \mathbf{x}_i \cdot \mathbf{x}_j + c)$
- Linear kernel very fast and easy to train, but very simple
- RBF kernel very powerful and most often used
- Kernel can (should) be adapted to task and data
  $\rightarrow$ e.g. complex-valued kernels are possible [Moser and Serpico, 2014]
  $$k(\mathbf{z}, \mathbf{s}) = \Re\left[\exp\left(-\frac{1}{2\sigma^2}\sum_{r=1}^{d}(z_r - s_r^*)^2\right)\right]$$
- Kernels for different features can be fused into one common kernel

SVM Conclusion

- Kernels can be designed to different purposes
- Hyperparameter tuning not easy
  $\rightarrow$ Usually grid search with cross validation
- Slow for large amounts of data
  $\rightarrow$ Potentially results in many support vectors and thus scalar products during prediction
- (Usually) all data needs to be considered at once
  $\rightarrow$ No “streaming” of data
- Designed for binary tasks
  $\rightarrow$ Extension to multi-class problems usually decreases performance and increases computational load

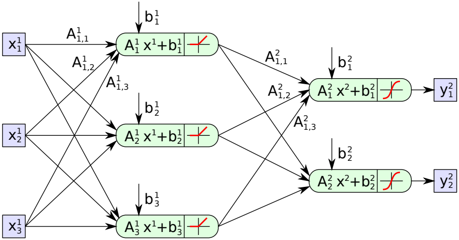
Models

1. Classification based on Features
   - Decision Boundary
   - Linear Decision Boundary
   - Non-linear Decision Boundary
2. Feature extraction
3. Machine Learning Methods
   - Support Vector Machine (SVM)
   - Multi-Layer Perceptron (MLP)
   - Random Forest (RF)



Multi-Layer Perceptron

- Feed forward neural network
- Neural networks “inspired by biology”
  - But work quite differently
- Core idea: concatenate multiple simple mappings to get one powerful mapping
- Multiple simple steps more powerful than one complex step
- Keep everything (mostly) differentiable
- Train by doing gradient descend on classification error



Building Blocks

Standard Layers:

- Fully connected layer with...
- ... activation function

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- Fully connected layer with...
- ... activation function

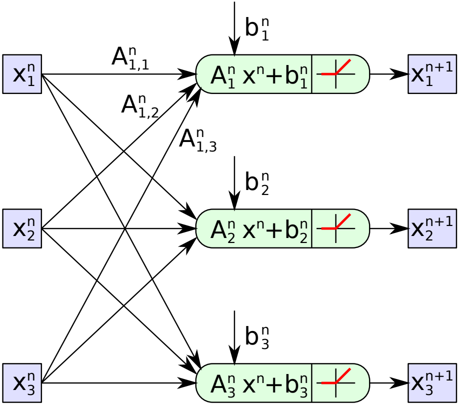
Special Layers (selection):

- Dropout (for regularization)
- Normalization (Improves training)
- Softmax (Produces nice classification output)

Fully Connected Layer

$$\mathbf{x}^{n+1} = \mathbf{y}^n = f(\mathbf{A}^n \cdot \mathbf{x}^n + \mathbf{b}^n) \quad (3)$$

- $\mathbf{x}^n$: Layer input
- $\mathbf{y}^n = \mathbf{x}^{n+1}$: Layer output
- $\mathbf{A}^n$: Weights
- $\mathbf{b}^n$: Bias
- $f(\cdot)$: Activation function



Activation Functions

$$\mathbf{y}^n = f(\mathbf{A}^n \cdot \mathbf{x}^n + \mathbf{b}^n) \tag{4}$$

- Assume $f(x) = x$
- Layer can assume any linear function (plus offset)

Activation Functions

$$\mathbf{y}^n = f(\mathbf{A}^n \cdot \mathbf{x}^n + \mathbf{b}^n) \tag{4}$$

- Assume $f(x) = x$
- Layer can assume any linear function (plus offset)
- Stacked layers can't improve that
- Activation function must be non-linear

Activation Functions

Typical choices:

ReLU

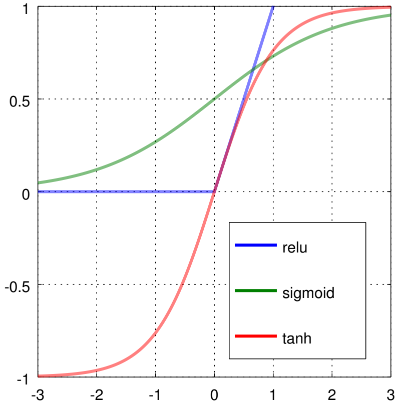
$$f(\mathbf{x}_i)_i = max(\mathbf{x}_i, 0) \tag{5}$$

Sigmoid / Logistic

$$f(\mathbf{x}_i)_i = \frac{1}{1 + e^{-\mathbf{x}_i}} \tag{6}$$

TanH

$$f(\mathbf{x}_i)_i = tanh(\mathbf{x}_i) = \frac{e^{\mathbf{x}_i} - e^{-\mathbf{x}_i}}{e^{\mathbf{x}_i} + e^{-\mathbf{x}_i}} \tag{7}$$



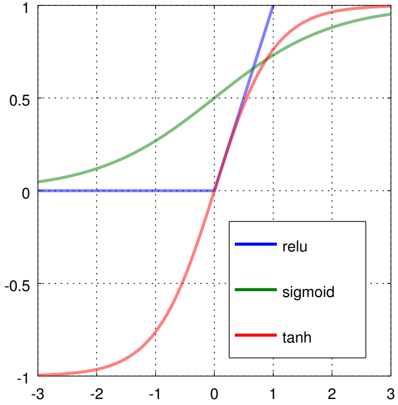
Activation Functions

Typical choices:

ReLU

$$f(\mathbf{x}_i)_i = max(\mathbf{x}_i, 0) \tag{8}$$

- ReLU (and variations of it) today the most common choice
- Better for deep networks
  - Derivative of activation function = 1 (in positive direction)
  - No saturation (in positive direction)
  - Gradients propagate better



Training

- How to find correct model parameters $\boldsymbol{\theta}$?
  - weight values
  - bias values
  - sometimes aux parameters

Training

- How to find correct model parameters $\boldsymbol{\theta}$?
  - weight values
  - bias values
  - sometimes aux parameters
- Setup/define energy function objective $E(\boldsymbol{\theta})$
- Derive analytic gradients $\frac{\partial E(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}$
- Perform gradient descent $\Delta\boldsymbol{\theta} = -\lambda \cdot \frac{\partial E(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}$
  - Usually slightly more sophisticated, more later

Training Objective

Empirical Risk Minimization (over N training samples)

$$E(\boldsymbol{\theta}) = \sum_{\alpha}^{N} e(\mathbf{y}^L(\underbrace{\boldsymbol{x}_\alpha}_{\text{Training sample}}, \boldsymbol{\theta}), \overbrace{\hat{\boldsymbol{y}}_\alpha}^{\text{Known/Desired value/label of } \boldsymbol{x}_\alpha}) \tag{9}$$

with, e.g.,:

$$e(\mathbf{y}^a, \mathbf{y}^b) = \left|\mathbf{y}^a - \mathbf{y}^b\right|^2 \tag{10}$$

Though bad for classification, see softmax layer later.

- Energy function defines training loss
- Gradient descent will try to minimize this
- Usually not convex (as network not convex)

Backpropagation

- How to compute $\frac{\partial E(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}$?
- MLP is concatenation of "simple" functions
  $\mathbf{y}^L(\ldots \mathbf{y}^2(\mathbf{y}^1(\mathbf{x}^1, \boldsymbol{\theta}^1), \boldsymbol{\theta}^2), \ldots \boldsymbol{\theta}^L)$

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- Exploit chain rule

$$\frac{\partial E(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^1} = \frac{\partial E(\boldsymbol{\theta})}{\partial \mathbf{y}^L} \cdot \ldots \cdot \underbrace{\frac{\partial \mathbf{y}^3}{\partial \mathbf{y}^2}}_{\text{per layer output derivative}} \cdot \frac{\partial \mathbf{y}^2}{\partial \mathbf{y}^1} \cdot \overbrace{\frac{\partial \mathbf{y}^1}{\partial \boldsymbol{\theta}^1}}^{\text{per layer parameter derivative}} \tag{11}$$

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- Gradient computation happens in two passes:
  - Forward pass:
    - Feeds training data through network
    - Computes all $\mathbf{y}^n$ and training loss
  - Backward pass:
    - Feeds error gradient backward through network
    - Computes all $\frac{\partial E(\boldsymbol{\theta})}{\partial \mathbf{y}^n}$ and $\frac{\partial E(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^n}$

Stochastic Gradient Descent

- Exact gradient usually not needed or wanted
- Just empirical average over N samples anyways
- Stochastic Gradient Descent: Split into batches of $M < N$ samples and update weights after every batch

$$\Delta\boldsymbol{\theta} = -\lambda \cdot \frac{\partial \hat{E}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \frac{\partial}{\partial \boldsymbol{\theta}} \sum_{\alpha}^{M} e(\mathbf{y}^L(\boldsymbol{x}_\alpha, \boldsymbol{\theta}), \hat{\boldsymbol{y}}_\alpha) \tag{12}$$

- Usually small batch sizes (eg. around 128) sufficient
  - Stepsize limited by curvature of energy function, not by precision of gradient
  - Computation time increases with $O(M)$, precision of gradient only with $O(\sqrt{M})$
  - Large batch sizes lead to sharp minimizers that don't generalize
  - Further reading: [Keskar et al., 2016]

Parameter Update Rule

- $\Delta\boldsymbol{\theta} = -\lambda \cdot \frac{\partial \hat{E}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}$ most simple update rule
- Momentum
  - Accumulate "momentum" over time
  - Pick up speed in the valley direction, average out noise
- Adam [Kingma and Ba, 2014]/Adagrad/Adadelta [Zeiler, 2012]
  - Normalize based on average gradient variance in the past

Parameter Initialization

- How to initialize $\boldsymbol{\theta}$?
- Random Gaussian
- Xavier (and some variants) [Glorot and Bengio, 2010]
  - Draw weights randomly
  - Choose variance per layer depending on input/output size
  - Balance variance to keep signal/gradient variance constant

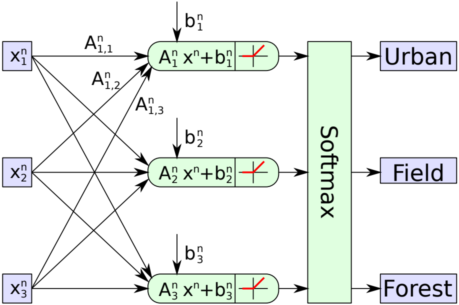
Special Layers

- Softmax
- Normalization
- Dropout

Softmax

$$f(x_i)_i = \frac{exp(x_i)}{\sum_j exp(x_j)} \qquad (13)$$

- Special (last) layer/activation for classification
- Creates vector that sums to one (read probabilities), one element per class
- Usually together with a specific optimization objective: Cross-entropy loss
    - Comparing the predicted probability mass distribution to the ground truth one



Dropout

- [Srivastava et al., 2014]
- During training, randomly disable neurons with probability p
- During application, scale output with $1 - p$
- Prevents co-adaptation
- Fosters redundancy throughout the network
- Reduces overfitting and improves generalization

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- Batch Normalization [Ioffe and Szegedy, 2015]
    - Special layer placed at strategic locations
    - Normalize mean and variance of activations across training batch (or accumulate running averages)
    - After learning, becomes fixed scale & offset

Handling Overfitting

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Handling Overfitting

- Dropout
- Weight regularization
  - Penalize large weight values
  - e.g., add $\lambda \cdot |\boldsymbol{\theta}|^2$ to optimization objective
  - Soft limit on model complexity
- Data Augmentation
  - Randomly modify training data
  - Based on what kind of invariances you want to have
    - Resistance to noise: add noise
    - Resistance to brightness/contrast/hue changes: Change those
    - Translation/Rotation (ex. for images)
    - Can also be applied to data before extracting features!

Increasing Depth

- Recent trend goes towards deeper networks
- Networks more powerful, but ...
- ... more difficult to train
  - Gradients collapse/explode/diffuse through the layers
- This is the book to read: Deep Learning [Goodfellow et al., 2016]

Complex-valued MLPs

- MLPs provide a functional mapping $f : \mathcal{X} \to \mathcal{Y}$
- f needs to be differentiable (due to backprop)
- Usually $\mathcal{X} \equiv \mathbb{R}^d$ (or $\mathbb{R}^{N \times M}$)
- But: (e.g.) PolSAR images are $\mathbb{C}^{N \times M}$
  - One solution: Compute real-valued features, then use standard MLP
    $\rightarrow$ Advantage: Usage of common MLPs and their extensions
    $\rightarrow$ Disadvantage: Dependency on feature extraction
  - Second solution: Use complex-valued MLP
    $\rightarrow$ Advantage: No dependency on feature extraction
    $\rightarrow$ Disadvantage: Math slightly more complicated

Complex-valued MLPs

Gradient in $\mathbb{R}$

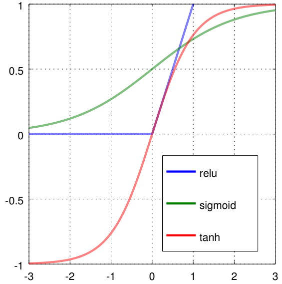
$$\begin{aligned} f &: \mathbb{R} \to \mathbb{R}, x \mapsto f(x) \\ \frac{\partial f}{\partial x} &= f'(x) \end{aligned}$$

Gradient in $\mathbb{C}$

$$\begin{aligned} f &: \mathbb{C} \to \mathbb{C}, z \mapsto f(z) \\ \frac{\partial f}{\partial z} &= \frac{1}{2}\left(\frac{\partial f}{\partial \Re z} - i\frac{\partial f}{\partial \Im z}\right) \\ \frac{\partial f}{\partial z^*} &= \frac{1}{2}\left(\frac{\partial f}{\partial \Re z} + i\frac{\partial f}{\partial \Im z}\right) \end{aligned}$$

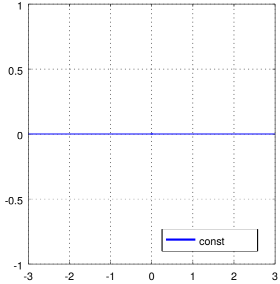
Complex-valued MLPs

Activation in $\mathbb{R}$



Analytical and bounded
$\rightarrow$ e.g. tanh, logistic function
(ReLU as exception)

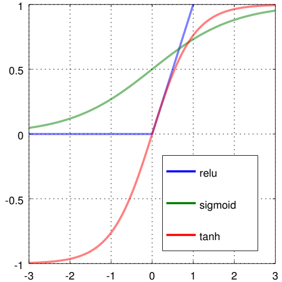
Activation in $\mathbb{C}$



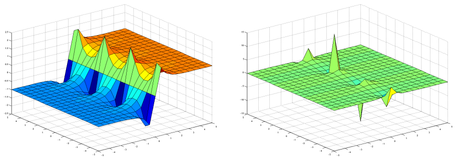
Analytical and bounded?
$\rightarrow$ only constant functions

Complex-valued MLPs

Activation in $\mathbb{R}$



Activation in $\mathbb{C}$

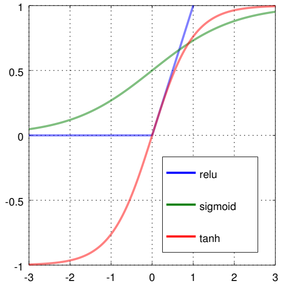


Analytical and bounded
$\rightarrow$ e.g. tanh, logistic function

Analytical or bounded
$\rightarrow$ e.g. tanh

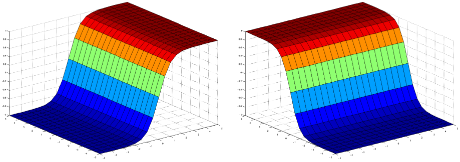
Complex-valued MLPs

Activation in $\mathbb{R}$



Analytical and bounded
$\rightarrow$ e.g. tanh, logistic function

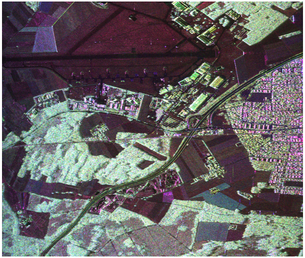
Activation in $\mathbb{C}$



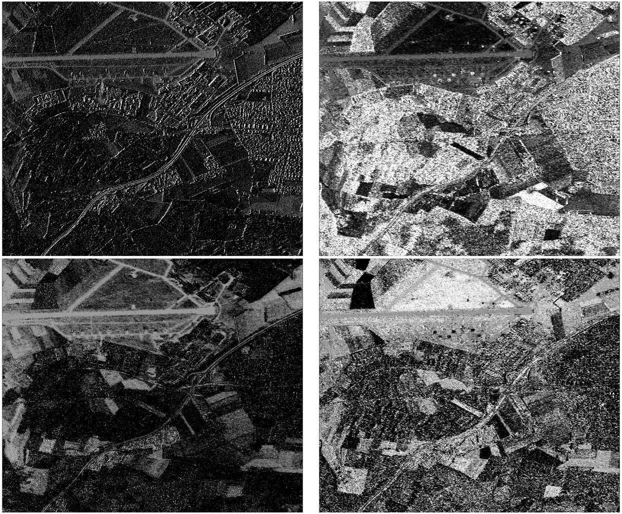
Analytical or **bounded**
$\rightarrow$ e.g. split-tanh

$$f(z) = \tanh(\Re(z)) + i \tanh(\Im(z))$$

Complex-valued MLPs



- PolSAR Data: $\mathbb{C}^{N\times M\times 3\times 3}$
- Input: Local patches, each pixel a Hermitan matrix (local covariance matrix of complex-valued scattering vector)
- Activation of few neurons in first layer is shown.

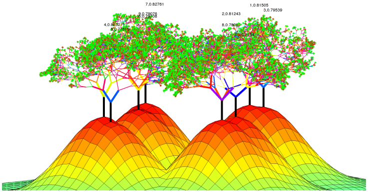


MLP Conclusion

- Architecture design a bit of an art
    - Though some tips/tricks exist
- Can ingest a lot of training data
- Training/Application not fast
- With modern tricks (ReLU, normalization, ...) scale surprisingly well
    - Up to very complex networks
    - Trained on lots of data

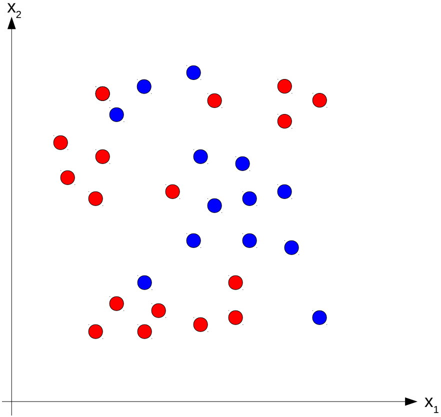
Models

1. Classification based on Features
   - Decision Boundary
   - Linear Decision Boundary
   - Non-linear Decision Boundary
2. Feature extraction
3. Machine Learning Methods
   - Support Vector Machine (SVM)
   - Multi-Layer Perceptron (MLP)
   - Random Forest (RF)



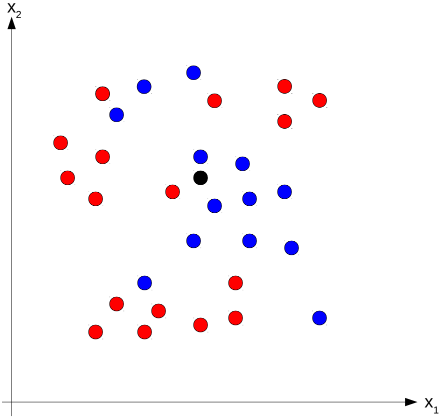
From kNN to Search Trees

- Data samples $\mathbf{x}$
  - Pixel information, image patch, feature vector, etc.
  - Often $\mathbf{x} \in \mathbb{R}^n$
- Classification:
  $\Rightarrow$ Estimate class label
- Training data: Values of target variable given e.g. class label



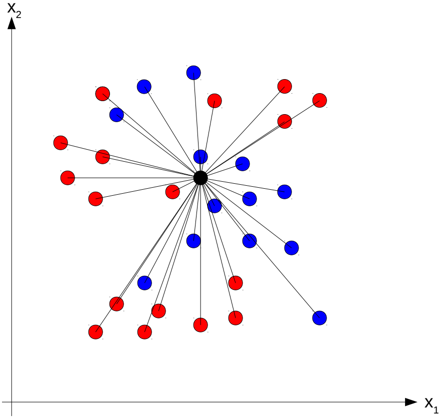
From kNN to Search Trees

- Task: Given training data, estimate label of query sample



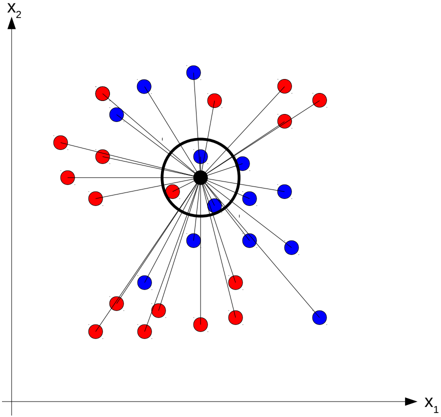
From kNN to Search Trees

- Task: Given training data, estimate label of query sample
- kNN/Parzen Window:
  - Compute distance to **all** samples



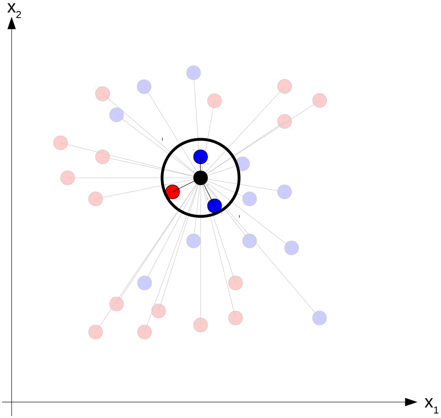
From kNN to Search Trees

- Task: Given training data, estimate label of query sample
- kNN/Parzen Window:
  - Compute distance to **all** samples
  - Select samples within window of given size (Parzen)



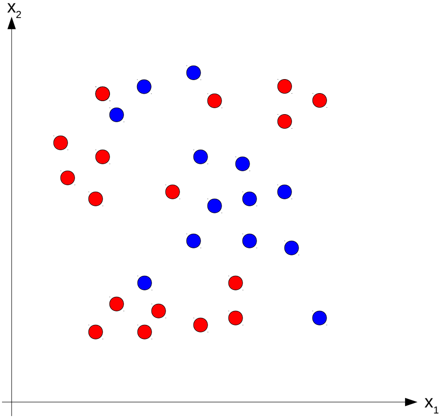
From kNN to Search Trees

- Task: Given training data, estimate label of query sample
- kNN/Parzen Window:
    - Compute distance to **all** samples
    - Select samples within window of given size (Parzen)
    - Use these samples to estimate target variable, e.g. class label
- Problem: Computationally expensive (exhaustive search)



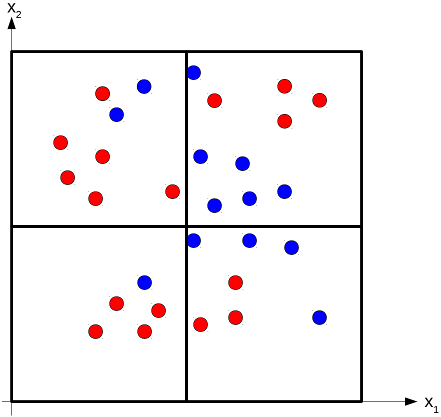
From kNN to Search Trees

- Search trees
  $\rightarrow$ Quad/Octree, KD tree, etc.



From kNN to Search Trees

- Search trees
  $\rightarrow$ Quad/Octree, KD tree, etc.
  - Divide space recursively into cells



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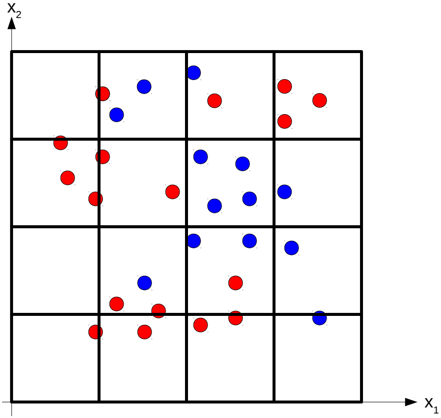
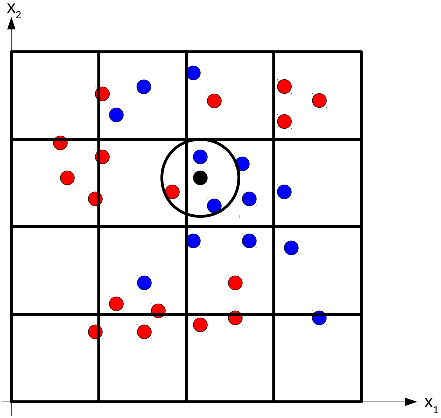


From kNN to Search Trees

- Search trees
  $\rightarrow$ Quad/Octree, KD tree, etc.
  - Divide space recursively into cells
  - Given a query, find relevant cells



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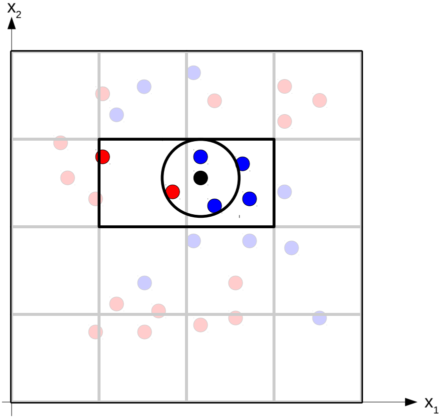

From kNN to Search Trees

- Search trees
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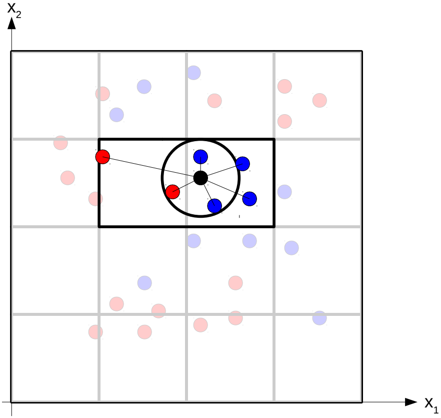
  - Given a query, find relevant cells
  - Perform exhaustive search in these cells ONLY



From kNN to Search Trees

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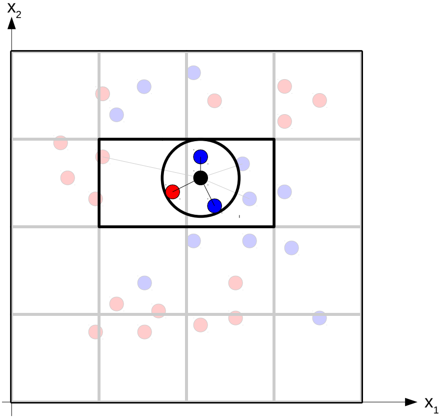
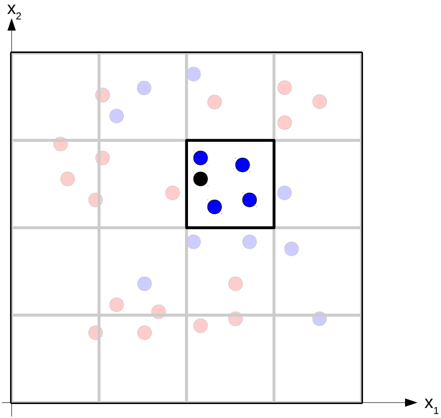
  - Perform exhaustive search in these cells ONLY
- Exact search: Leads to equivalent results



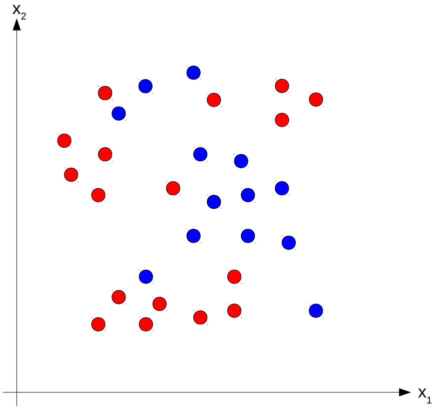
From kNN to Search Trees

- Search trees
  $\rightarrow$ Quad/Octree, KD tree, etc.
  - Divide space recursively into cells
  - Given a query, find relevant cells
  - Perform exhaustive search in these cells ONLY
- Exact search: Leads to equivalent results
- Approximation: Use samples within query cell directly



From Search Trees to (Random) Decision Trees

- Cell construction



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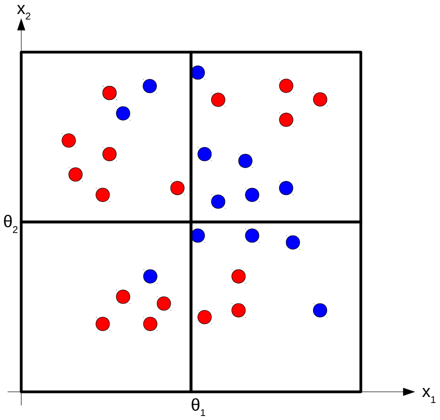
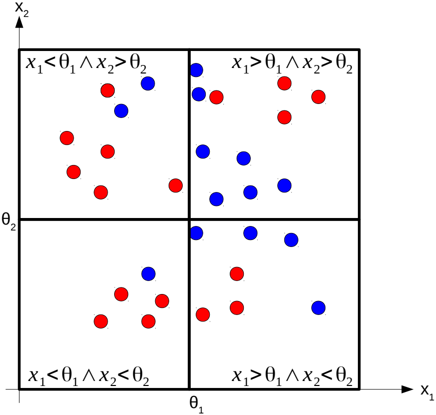


From Search Trees to (Random) Decision Trees

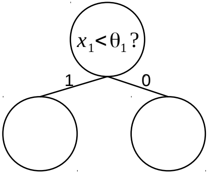
- Cell construction
  → Simple threshold operation
  → Different threshold definitions (e.g. equi-sized cells, threshold as data median) lead to different search tree variants (e.g. quad-tree, k-D tree).

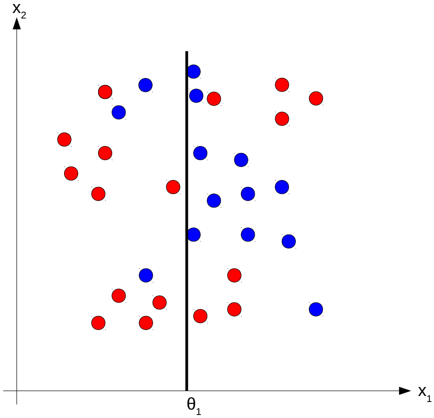


From Search Trees to (Random) Decision Trees

- Cell construction
  $\rightarrow$ Simple threshold operation
- Decision stump:

$$t(\mathbf{x}) = \begin{cases} 0 & \text{if } x_1 < \theta_1 \\ 1 & \text{otherwise.} \end{cases}$$





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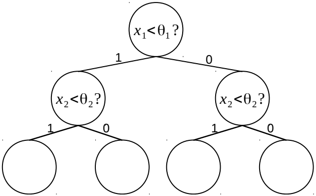

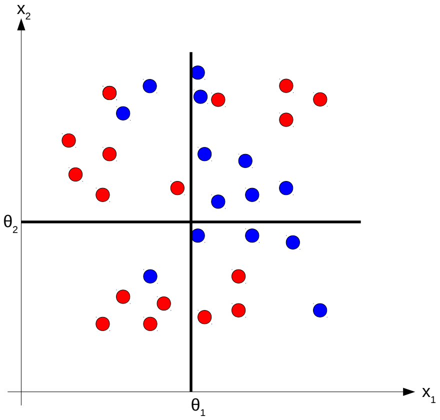

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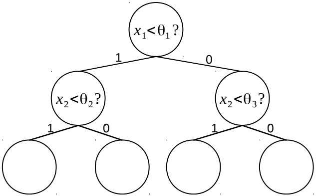
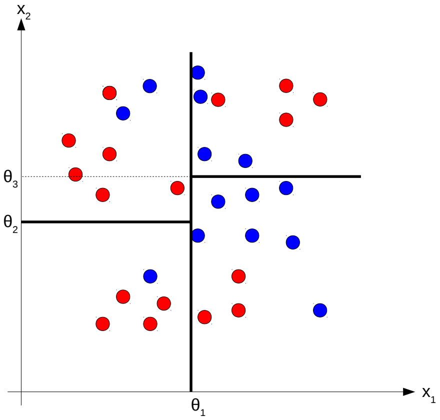
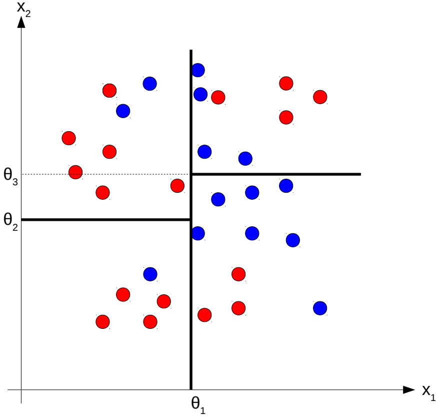




From Search Trees to (Random) Decision Trees

- Cell construction
  $\rightarrow$ Simple threshold operation
- Decision stump:
  $$t(\mathbf{x}) = \begin{cases} 0 & \text{if } x_1 < \theta_1 \\ 1 & \text{otherwise.} \end{cases}$$
- When to stop? Minimal resolution reached, purity, ...
- How to select split points? Randomly, optimized selection



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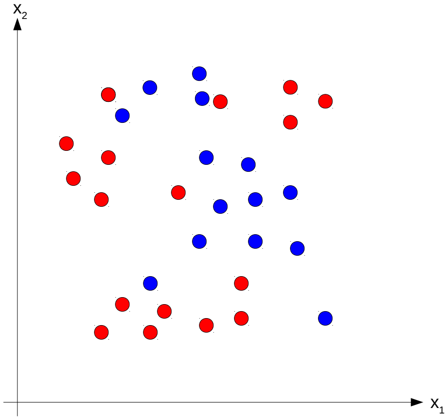

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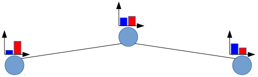

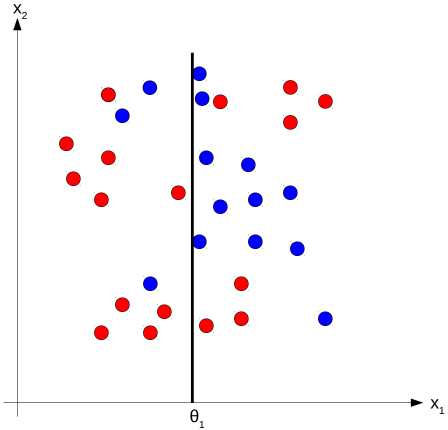

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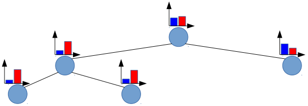

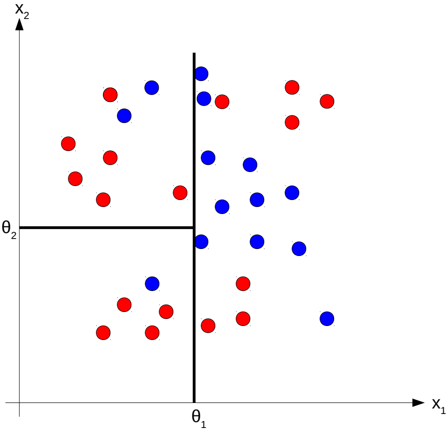

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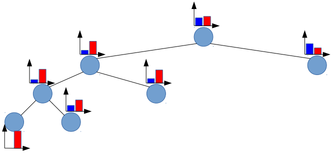

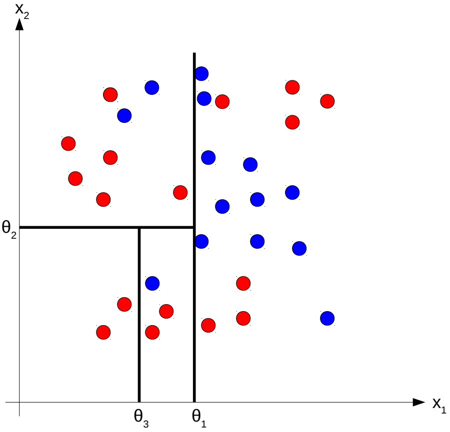

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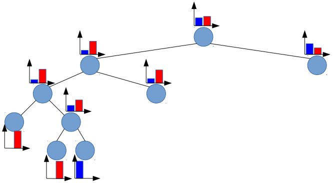

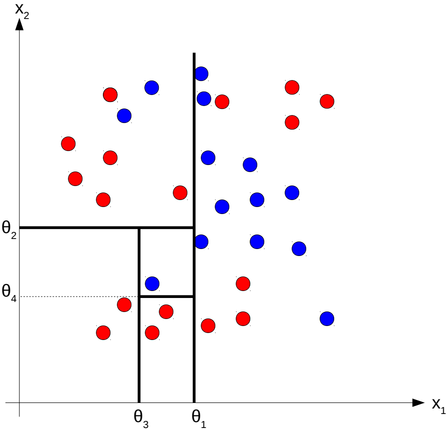

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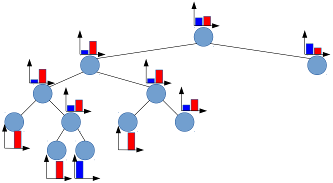

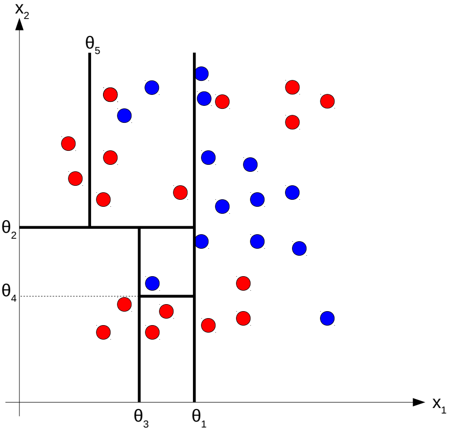

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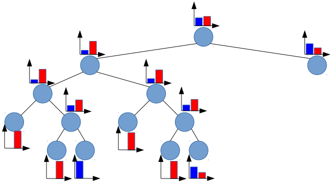

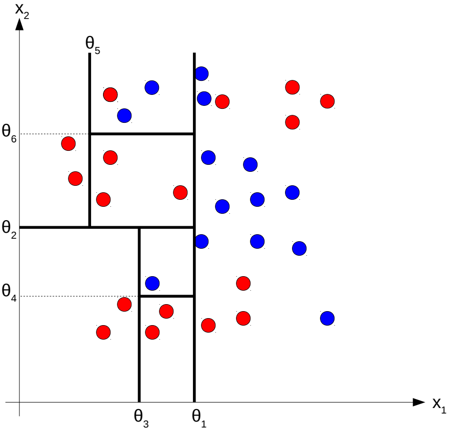

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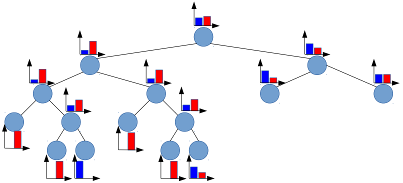

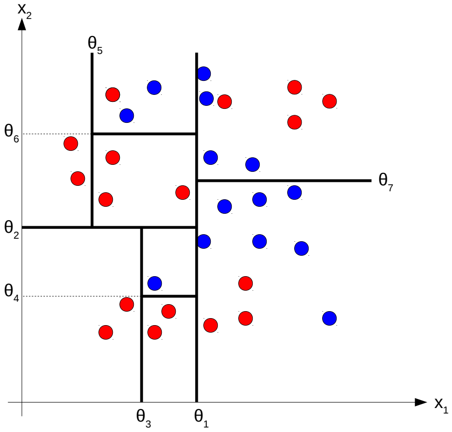

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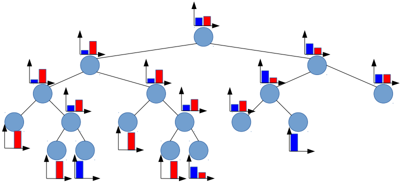

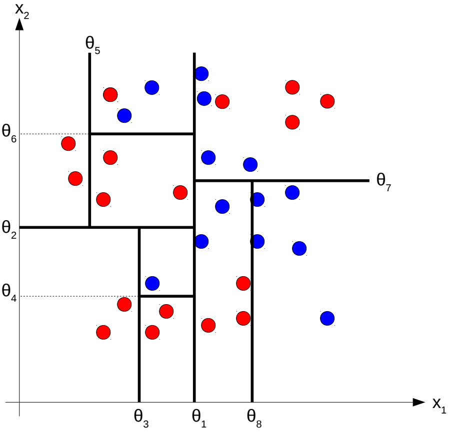

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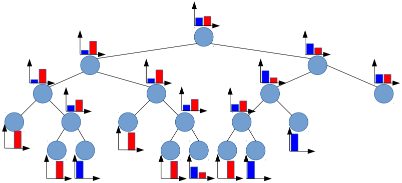

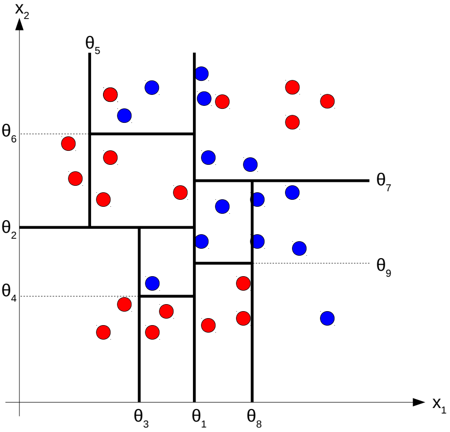

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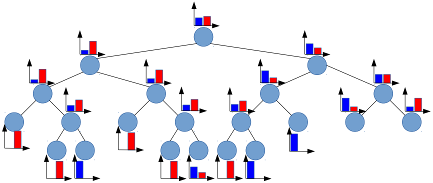

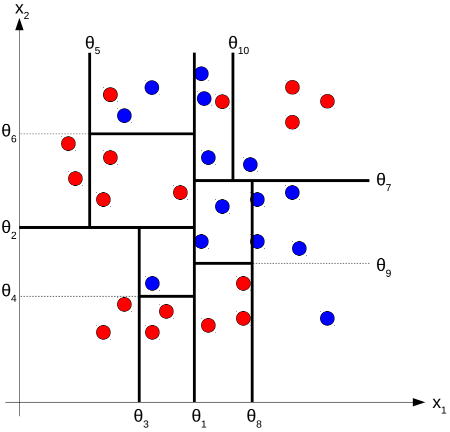

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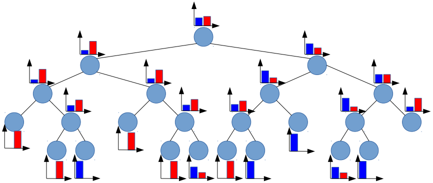

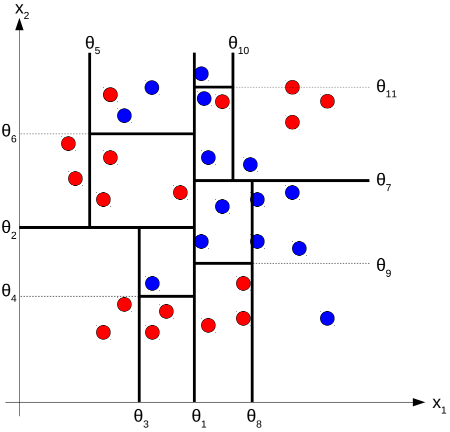

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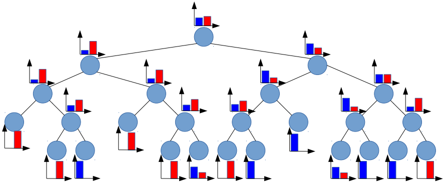
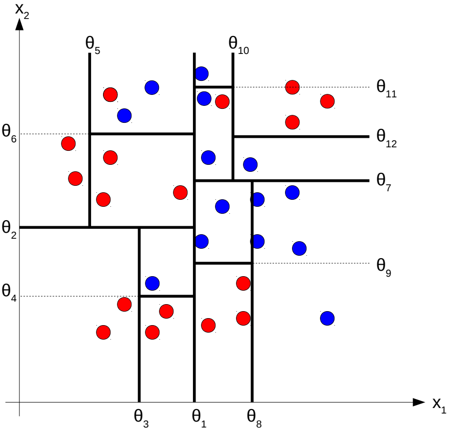
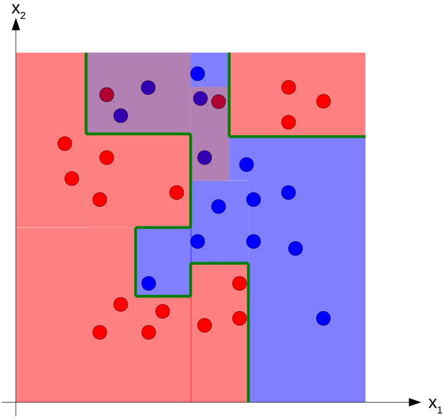




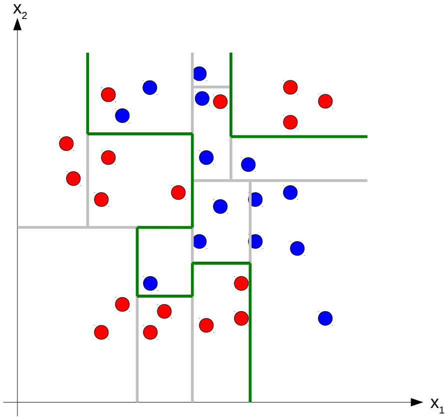
From Search Trees to (Random) Decision Trees

- Local estimate of the target variable (e.g. class posterior) is assigned to cells



From Search Trees to (Random) Decision Trees

- Local estimate of the target variable (e.g. class posterior) is assigned to cells
- Results in highly non-linear, even non-connected (but piece-wise constant) decision boundaries



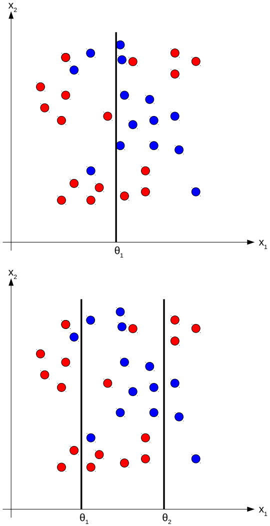
From Search Trees to (Random) Decision Trees

Other node tests are possible:

- Axis-aligned:

$$t(\mathbf{x}) = \begin{cases} 0 & \text{if } x_1 < \theta_1 \\ 1 & \text{otherwise.} \end{cases}$$

$$t(\mathbf{x}) = \begin{cases} 0 & \text{if } \theta_1 < x_1 < \theta_2 \\ 1 & \text{otherwise.} \end{cases}$$



From Search Trees to (Random) Decision Trees

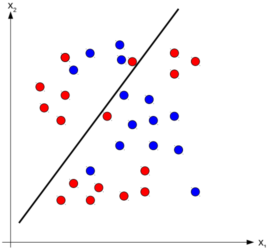
Other node tests are possible:

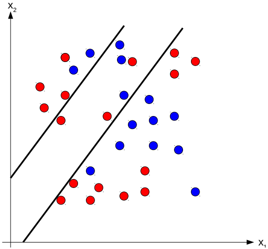
- Axis-aligned
- Linear:

  $\tilde{\mathbf{x}} = [\mathbf{x}, 1] \in \mathbb{R}^{d+1}, \psi \in \mathbb{R}^{d+1}$

  $$t(\mathbf{x}) = \begin{cases} 0 & \text{if } \psi^T \tilde{\mathbf{x}} < \theta_1 \\ 1 & \text{otherwise.} \end{cases}$$

  $$t(\mathbf{x}) = \begin{cases} 0 & \text{if } \theta_1 < \psi^T \tilde{\mathbf{x}} < \theta_2 \\ 1 & \text{otherwise.} \end{cases}$$



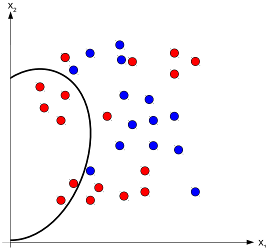


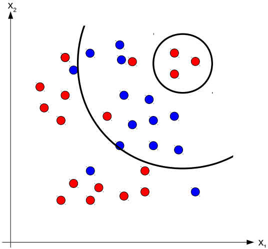
From Search Trees to (Random) Decision Trees

Other node tests are possible:

- Axis-aligned
- Linear
- Conic section:

$$
\begin{aligned}
\tilde{\mathbf{x}} &= [\mathbf{x}, 1] \in \mathbb{R}^{d+1}, \psi \in \mathbb{R}^{(d+1)\times(d+1)} \\
t(\mathbf{x}) &= \begin{cases} 0 & \text{if } \tilde{\mathbf{x}}^T \psi \tilde{\mathbf{x}} < \theta_1 \\ 1 & \text{otherwise.} \end{cases} \\
t(\mathbf{x}) &= \begin{cases} 0 & \text{if } \theta_1 < \tilde{\mathbf{x}}^T \psi \tilde{\mathbf{x}} < \theta_2 \\ 1 & \text{otherwise.} \end{cases}
\end{aligned}
$$



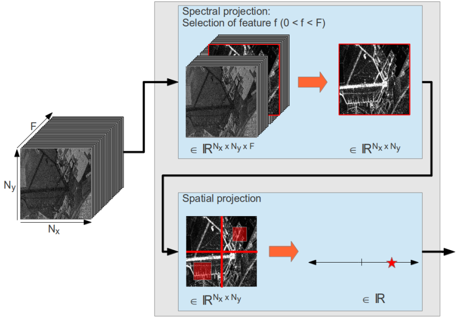


From Search Trees to (Random) Decision Trees

Other node tests are possible:

- Axis-aligned
- Linear
- Conic section
- Other data spaces than $\mathbb{R}^d$
  - PolSAR: $\mathbb{C}^3, \mathbb{C}^{3\times 3}$
  - Image patches: $\mathbb{R}^{n\times n}$
  - Non-scalar features, e.g. histograms, cardinal features such as pre-classification
  - ...

Spoiler alert
Part 3: ML and Images



From (Random) Decision Trees to Random Forests

Advantages

- Can deal with very heterogeneous data
  $\rightarrow$ Different, data-specific types of node tests
- Not prone to the curse of dimensionality
  $\rightarrow$ Each node only works on a very limited set of dimensions
- Very efficient
  $\rightarrow$ Each sample passes maximal H nodes (H = maximal height)
- Easy to implement
  $\rightarrow$ Binary trees are one of the most basic data structures
- Easy to interprete
  $\rightarrow$ Path through tree is a connected set of decision rules
- Well understood
  $\rightarrow$ Theoretical and practical implications of design decisions have been researched for more than 4 decades

From (Random) Decision Trees to Random Forests

Disadvantages

- Optimized by greedy algorithms
  $\rightarrow$ A chain of individually optimal decisions, might not lead to an overall optimum
- The optimal solution (i.e. decision boundary) might not be part of the model class (e.g. piece-wise linear and axis-aligned functions)
- Prone to overfitting
- Model capacity depends on amount of data
  $\rightarrow$ Few samples lead to small trees: Only few questions can be asked.
  $\rightarrow$ Many samples (might) lead to very high trees: Long processing times, large memory footprint.

From (Random) Decision Trees to Random Forests

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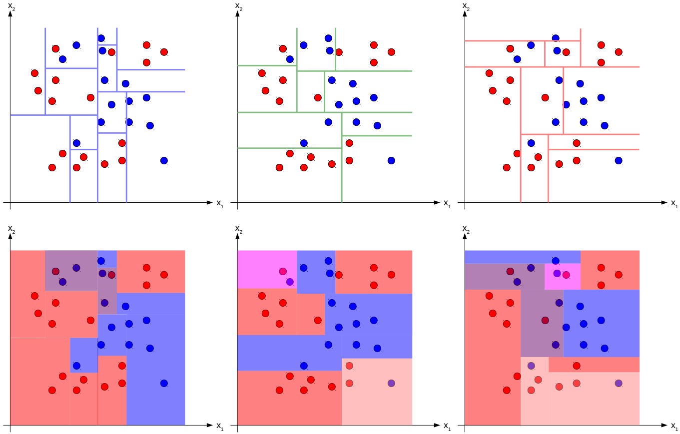
How to
$\rightarrow$ keep (most) of the advantages
$\rightarrow$ getting rid of (most) disadvantages?

From (Random) Decision Trees to Random Forests



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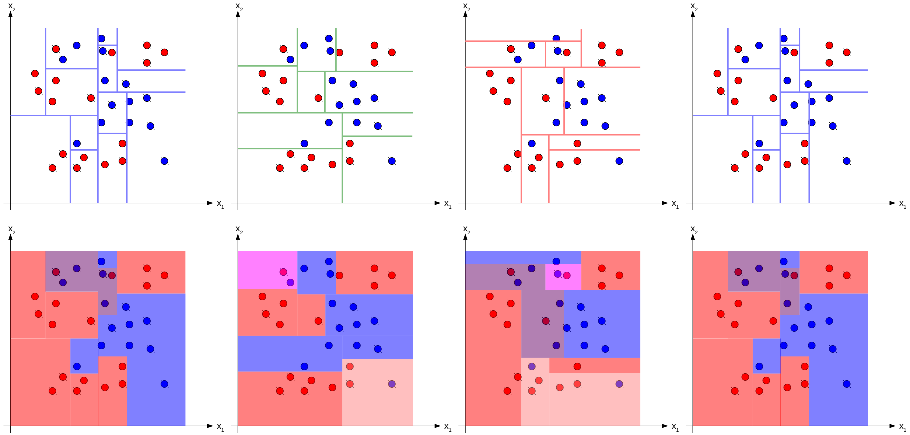
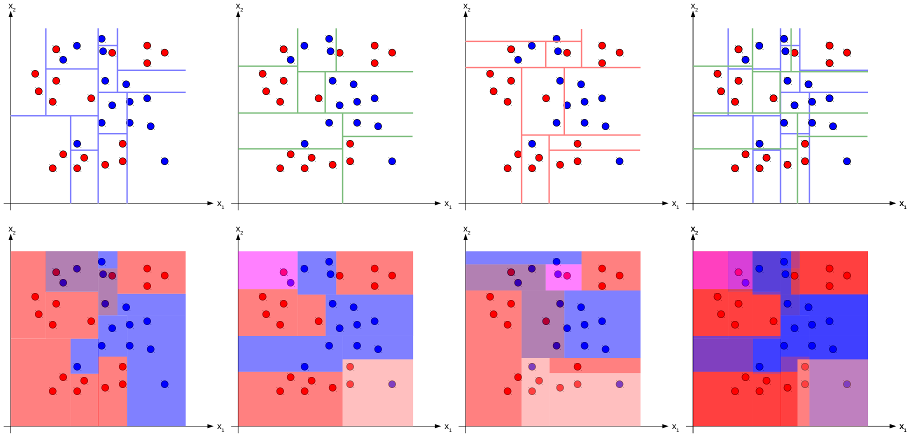
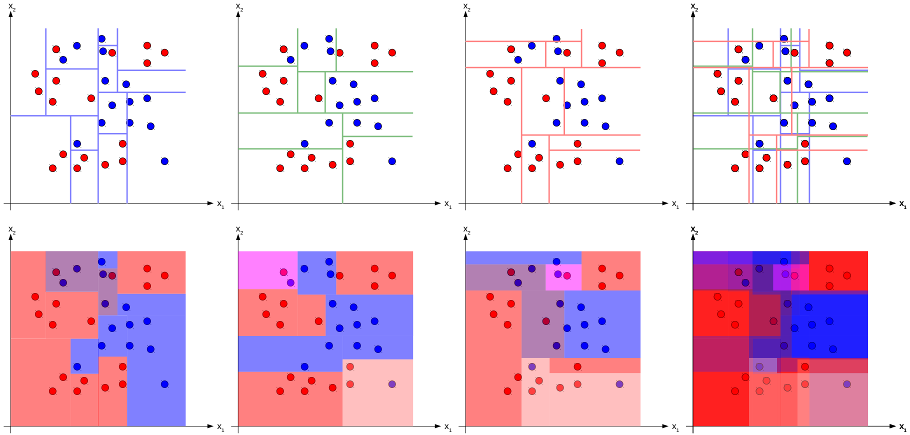


From (Random) Decision Trees to Random Forests



From (Random) Decision Trees to Random Forests



Random Forests

- Many (suboptimal) baselearners, i.e. decision trees
- Fusion of the individual output
- Minimization of the risk to use wrong model
- Extension of the model space
- Decreased dependence on initialization
- One name to rule them all
  - Bagged Decision Trees
  - Randomized Trees
  - Decision Forests
  - ERT, PERT, Rotation Forests, Hough Forests, Semantic Texton Forests, ...

Random Forests - Randomization through node tests

Before: $t(\mathbf{x}) = \begin{cases} 0 & \text{if } x_1 < \theta_1 \\ 1 & \text{otherwise.} \end{cases}$

Now: More general

$\rightarrow$ Concatenation of several functions with different tasks

$$t_\tau : \mathbb{D} \rightarrow \{0, 1\} \qquad \tau \in \mathrm{T} \equiv \text{Parameter set}$$

$$t_\tau = \xi \circ \psi \circ \phi$$

$$\begin{aligned}
\phi : \mathbb{D} \rightarrow \mathbb{R}^n &\equiv \text{Implicit feature extraction} \\
&\quad \text{e.g. } x \in \mathbb{R}^n : \ \phi : \mathbb{R}^n \rightarrow \mathbb{R}^2, x \mapsto (x_i, x_j)^T \\
\psi : \mathbb{R}^n \rightarrow \mathbb{R} &\equiv \text{Feature fusion} \\
&\quad \text{e.g. } \phi(x) \in \mathbb{R}^2 : \ \psi : \mathbb{R}^2 \rightarrow \mathbb{R}, \phi(x) \mapsto [\psi_i, \psi_j] \cdot \phi(x) \\
\xi : \mathbb{R} \rightarrow \{0, 1\} &\equiv \text{Child node assignment} \\
&\quad \text{e.g. thresholding}
\end{aligned}$$

Decision trees perform exhaustive search for optimal parameters τ in T
Random Forests use random subset $\tilde{\mathrm{T}}$ (Note: $|\tilde{\mathrm{T}}| = 1$ possible)

Random Forests - Randomization through Bagging

Given: Training set $\mathrm{D} \subset \mathbb{D}$ with $|\mathrm{D}| = N$ samples.
Bagging (**B**ootstrap **agg**regat**ing**):

1. Randomly sample M data sets D_m with replacement ($|\mathrm{D}_m| = N$).
2. Train M models where m-th model has only access to m-th dataset.
3. Average all models.

- Meta learning technique
- Works if small change in input data leads to large model variation
- Reduces variance (of final model), avoids overfitting.
- Leads to diverse decision trees, even if all other parameters are fixed

Random Forests - Key questions

- What kind of node tests?
  $\rightarrow$ For images, for other data spaces than $\mathbb{R}^n$
- How to select node tests?
  $\rightarrow$ How to measure good tests?
- What kind of target variables?
  $\rightarrow$ More than a single class label?
- How to limit model capacity (tree height, tree number)?
  $\rightarrow$ The more the better? What about overfitting?
- How to fuse tree decisions?
  $\rightarrow$ Whom to trust?
- How to interprete results?
  $\rightarrow$ Tree properties and visualization.

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