GeoX Young Academy: Machine Learning in Remote Sensing Best practice and recent developments

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Part 2: Classical Learning

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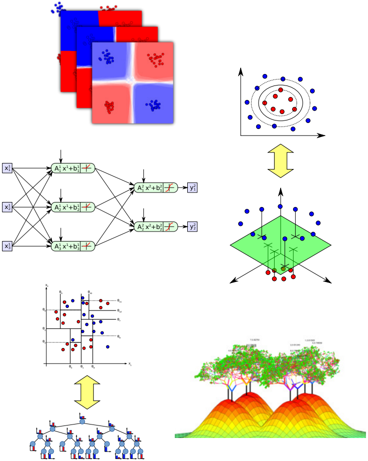
Overview

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



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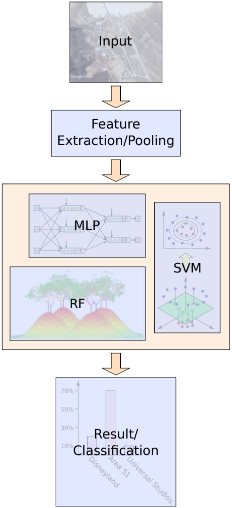
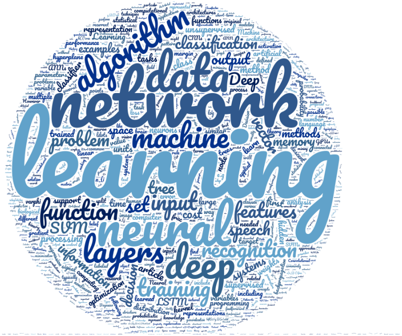
Classical Learning

- Features extract very basic, low level information
- We want very high level information (e.g. land-use class)
- 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!
- For now we stay away from complex data (eg., images)
  - Images in Part 3



Methods

- Choice of method not always rational
- Different pros/cons
- Speed, memory, scalability of training data, ease of implementation, ease of hyper parameter tuning, ...
- We'll try to get an intuitive understanding of the problems first, then present 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)

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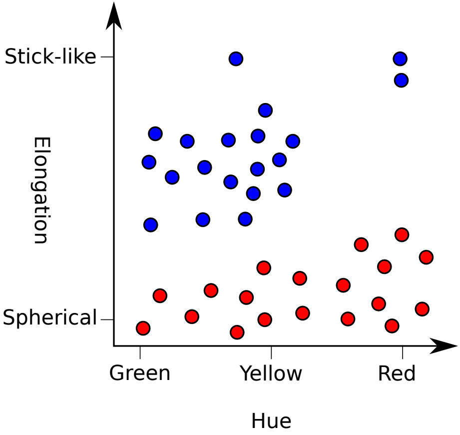
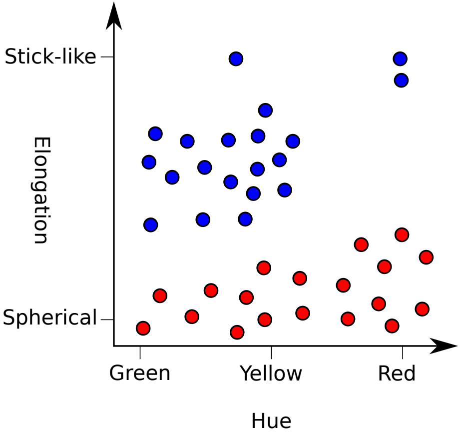
Some training data

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



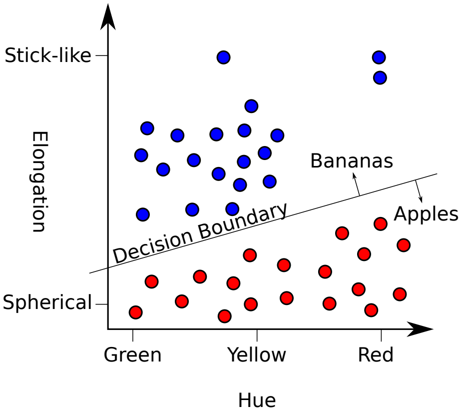
Some training data

- 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?



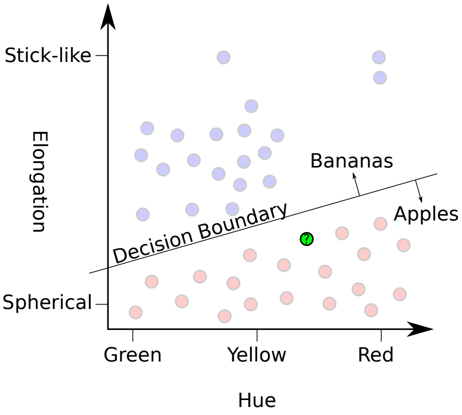
Decision boundary

- (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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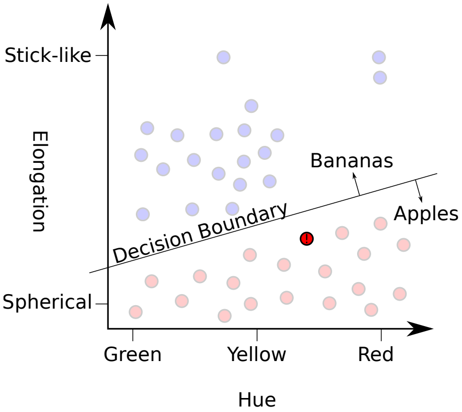
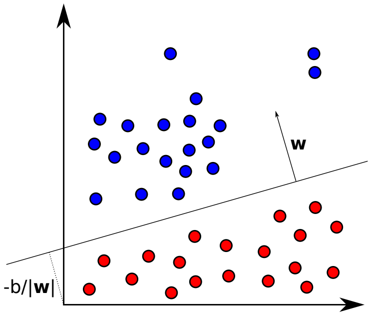


Perceptron

Perceptron

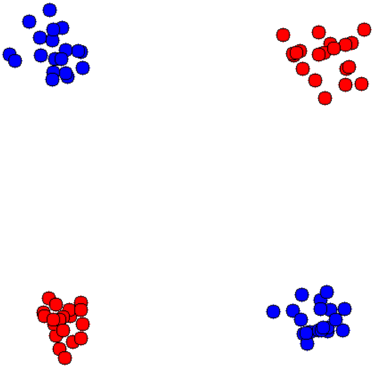
$$y = \text{sign}(\mathbf{w}^T \mathbf{x} + b) \qquad (1)$$

- $y \in \{-1, 1\}$: 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)



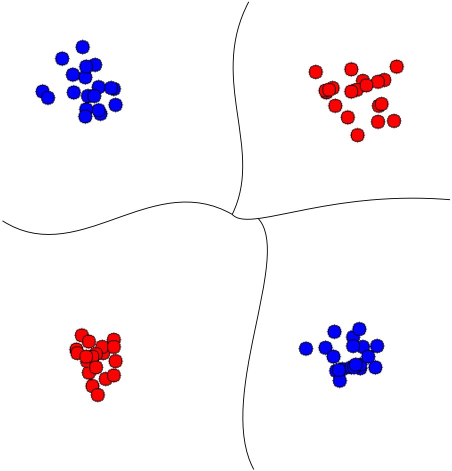
Linear Separability

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



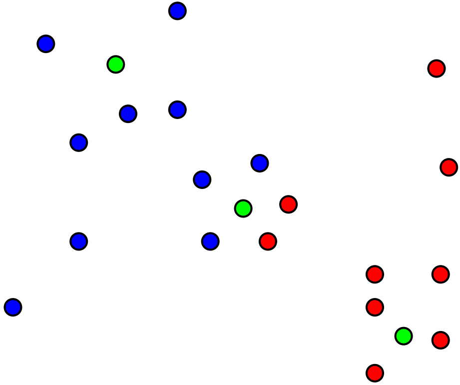
Non-linear Decision Boundary

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



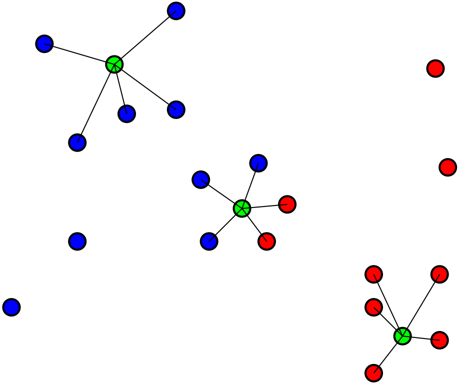
kNN

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



kNN

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



kNN

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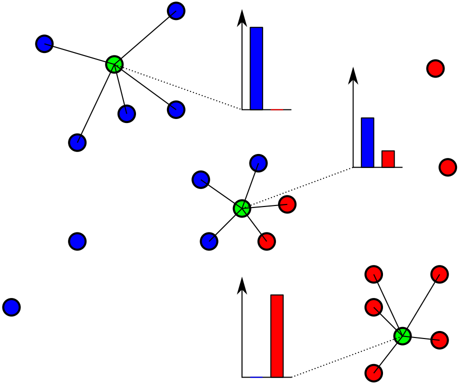
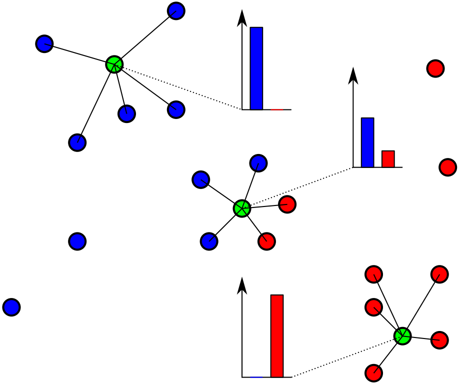


kNN

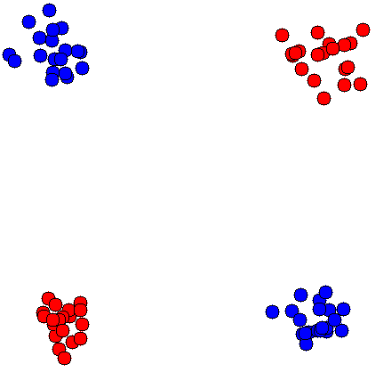
- Very simple idea:
  k-Nearest-Neighbors for classification
- For a sample find the k (e.g. 5) closest data points in the training dataset
- Look at the labels of those neighbors
- Fast lookup through trees/approximate methods
- Needs to keep all training data around



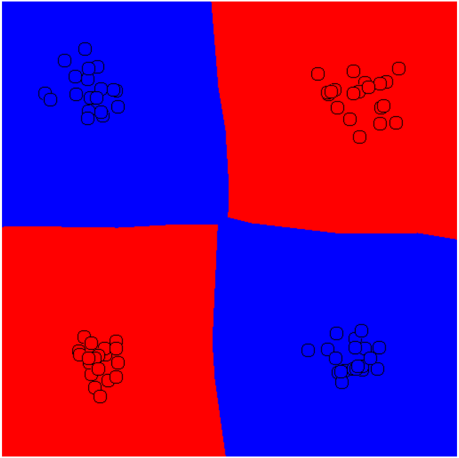
kNN Example

Exercise: kNN

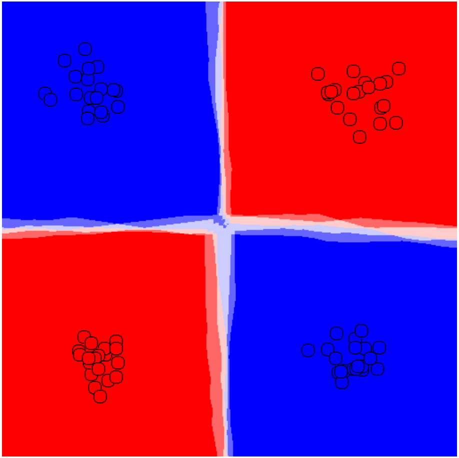
kNN Example - Simple



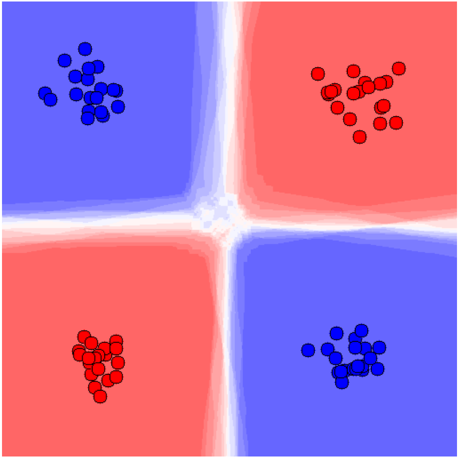
kNN Example - Simple - kNN K=1



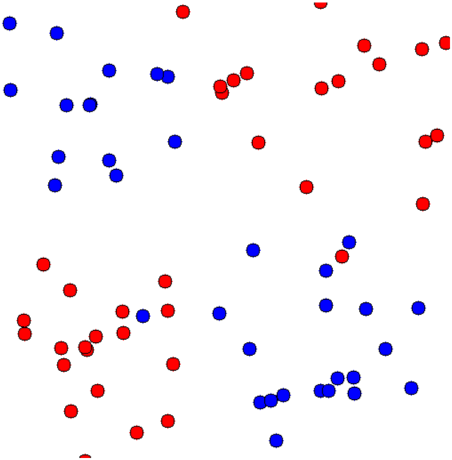
kNN Example - Simple - kNN K=5



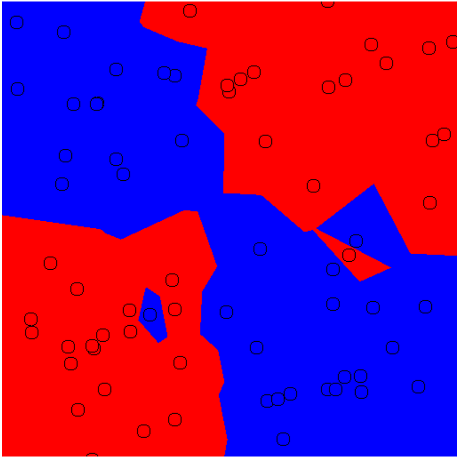
kNN Example - Simple - kNN K=25



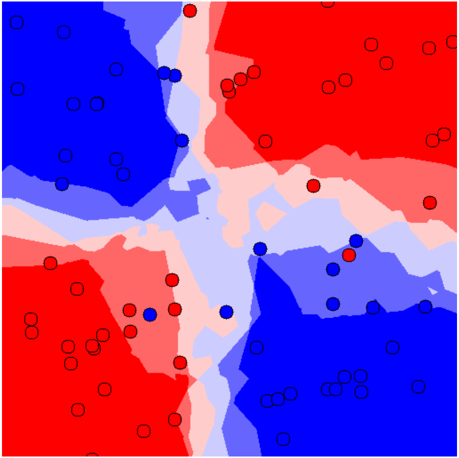
kNN Example - Hard



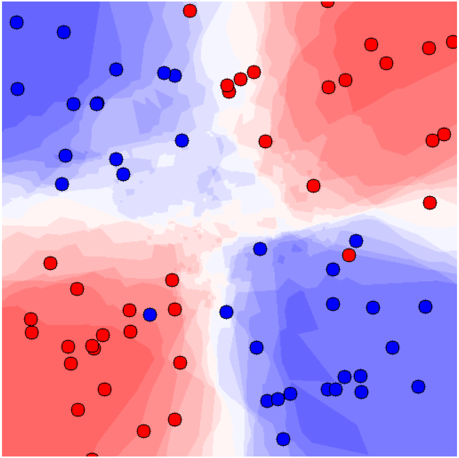
kNN Example - Hard - kNN K=1



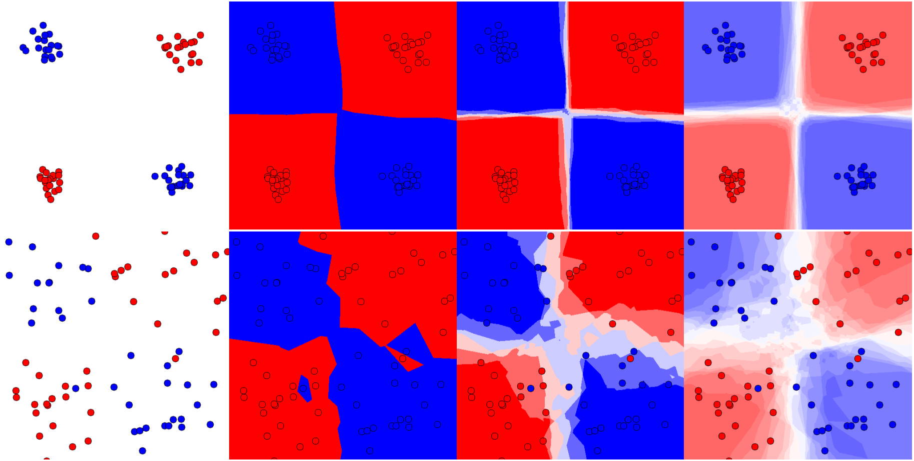
kNN Example - Hard - kNN K=5



kNN Example - Hard - kNN K=25

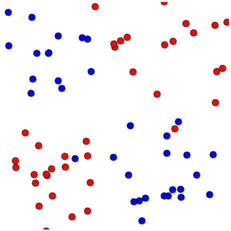


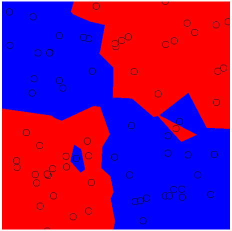
kNN Example



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





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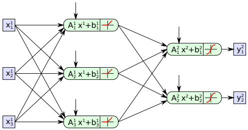

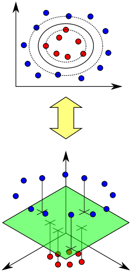

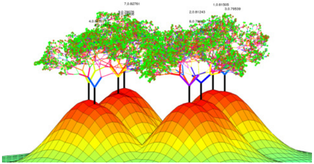

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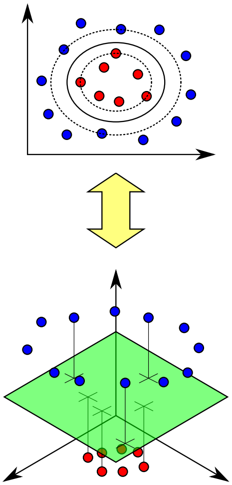
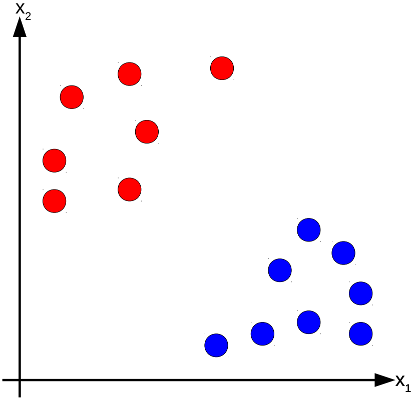


SVM

Reconsider the perceptron:

Perceptron

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



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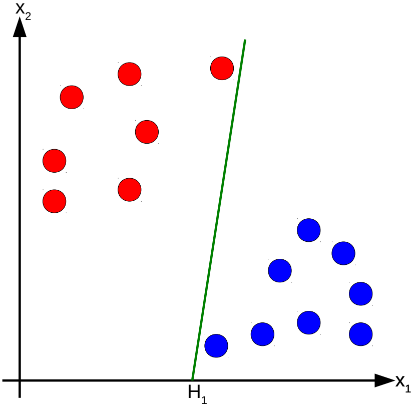

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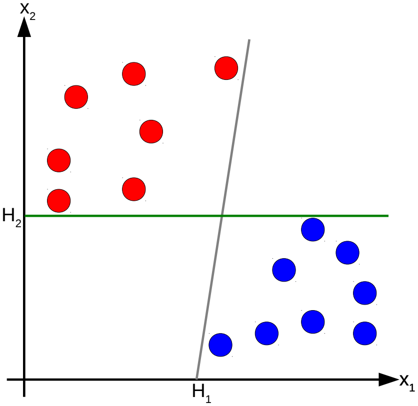

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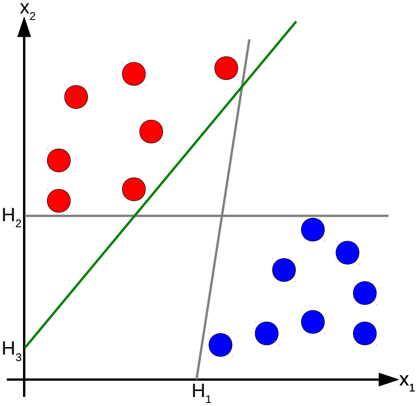

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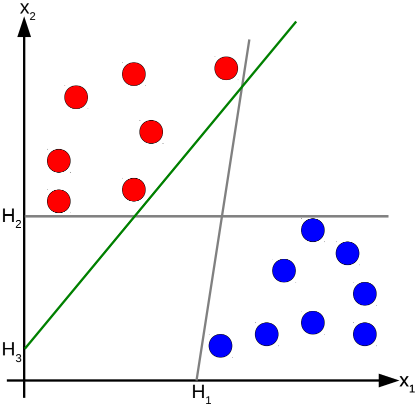

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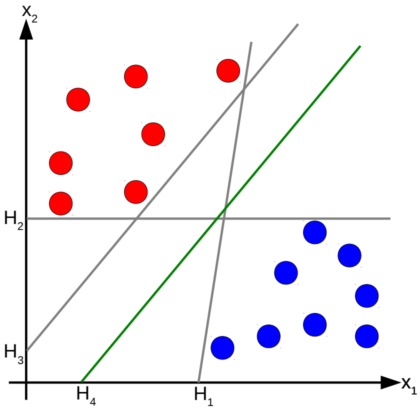

SVM

Reconsider the perceptron:

Perceptron

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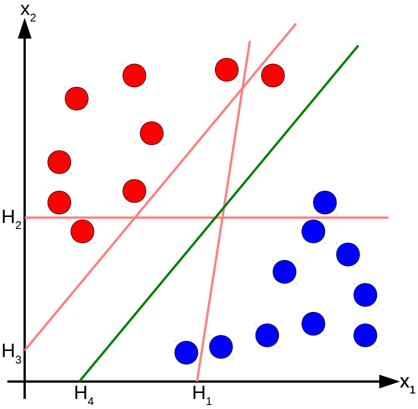
- Don't just pick any decision boundary
- Pick the one with the *maximal margin*
- Perceptron of maximal stability



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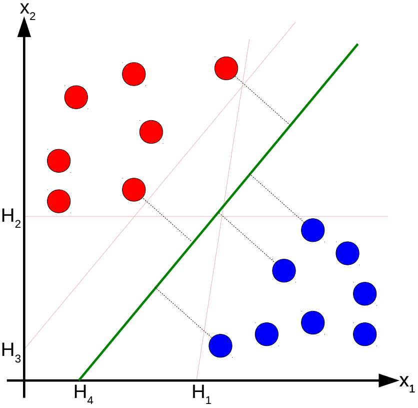
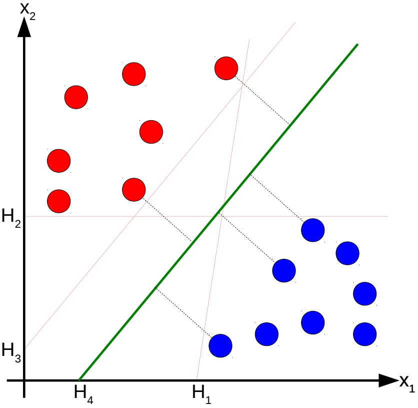


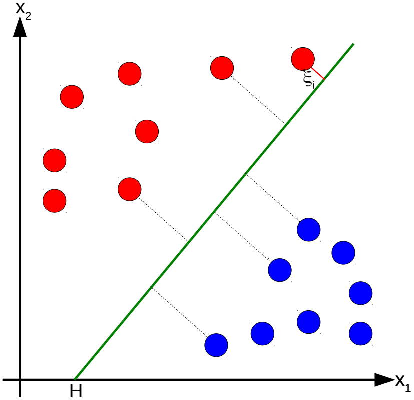
SVM

- 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 $\hat{y}_i(w^T\mathbf{x}_i - b) \geq 1 - \xi_i$
  $(\xi_i \geq 0)$

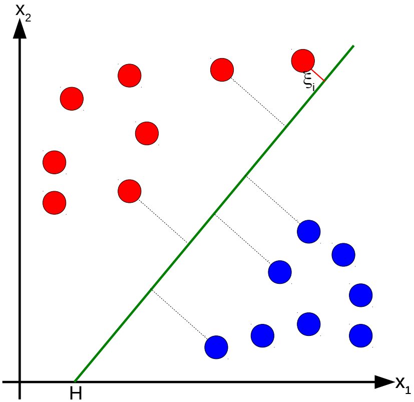


SVM

- 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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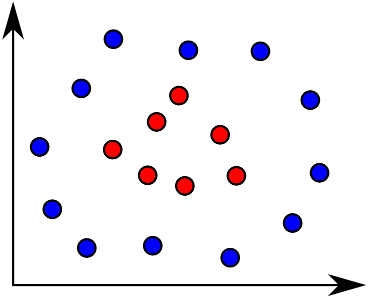
- What if $\mathbf{x}_i$ not linear separable at all?



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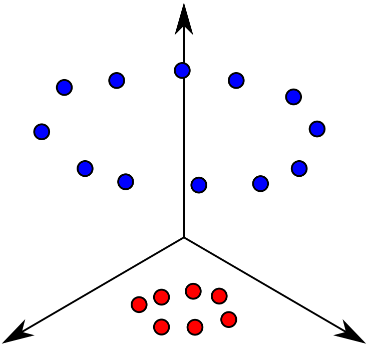
- What if $\mathbf{x}_i$ not linear separable at all?
  $\rightarrow$ Compute new features $\mathbf{x} \mapsto \phi(\mathbf{x})$



SVM

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- Support vectors: $\mathbf{x}_i$ if $\alpha_i \neq 0$
- Classification: $sign(\mathbf{w}^T \phi(\mathbf{x}) + b)$
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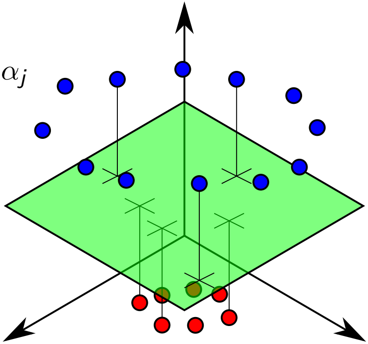
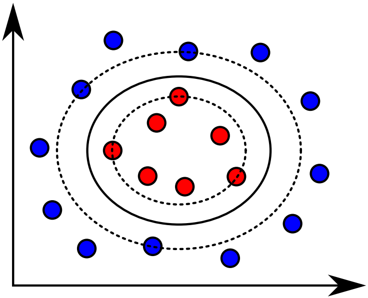


SVM

- 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

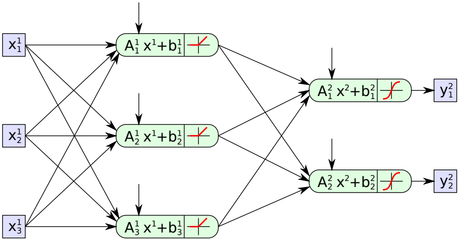
- Kernels can be designed to different purposes
- Hyperparameter tuning not easy
  $\rightarrow$ Usually grid search with cross validation
- Slow for large amounts of data
  $\rightarrow$ Potentially results in many support vectors and thus scalar products during prediction
- (Usually) all data needs 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

SVM Example

Exercise: SVM

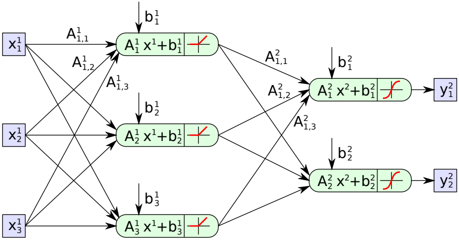
Models

1. Classification based on Features
   - Decision Boundary
   - Linear Decision Boundary
   - Non-linear Decision Boundary
2. 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

Building Blocks

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

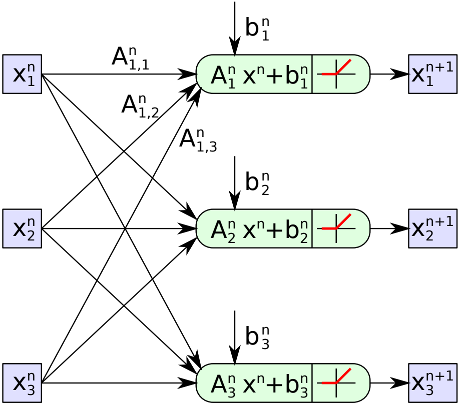
Special Layers (selection):

- 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

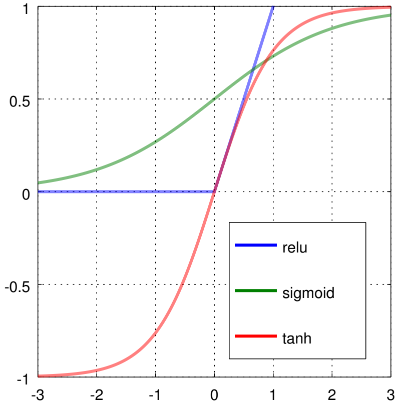
$$f(\mathbf{x}_i)_i = max(\mathbf{x}_i, 0) \tag{5}$$

Sigmoid / Logistic

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

TanH

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



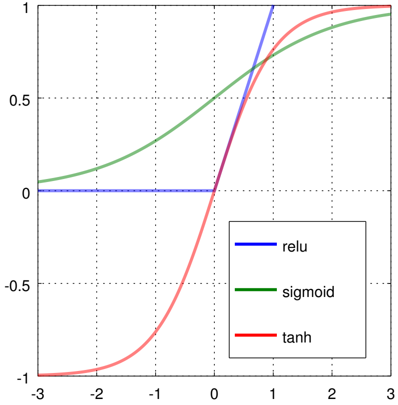
Activation Functions

Typical choices:

ReLU

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

- 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 descend $\Delta\boldsymbol{\theta} = -\lambda \cdot \frac{\partial E(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}$
  - 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 descend 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 Descend

- Exact gradient usually not needed or wanted
- Just empirical average over N samples anyways
- Stochastic Gradient Descend: 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

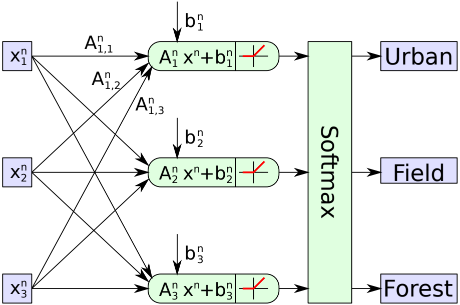
Special Layers

- 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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- Normalization can be important for learning
- Neither signal (forward) nor gradients (backward) must explode/shrink in magnitude

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- Local Response Normalization (LRN) [Krizhevsky et al., 2012]
    - Special layer placed at strategic locations
    - Let strong activations inhibit activations of other neurons in same layer
    - On images, alternatively also spatial inhibition (ConvNets, see Part 3)
    - Normalizes the otherwise unbounded output of ReLU

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  - On images, alternatively also spatial inhibition (ConvNets, see Part 3)
  - Normalizes the otherwise unbounded output of ReLU
- 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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  - e.g., add λ *cdot* $|\boldsymbol{\theta}|^2$ to optimization objective
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Handling Overfitting

- Dropout
- Weight regularization
  - Penalize large weight values
  - e.g., add λ $cdot\, |\boldsymbol{\theta}|^2$ 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 (for images, see ConvNets, Part 3)
    - 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
- More on this, and on how to apply it to images, in Part 3
- This is the book to read: Deep Learning [Goodfellow et al., 2016]

Complex-valued MLPs

- MLPs provide a functional mapping $f : \mathcal{X} \rightarrow \mathcal{Y}$
- 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 $\mathbb{R}$

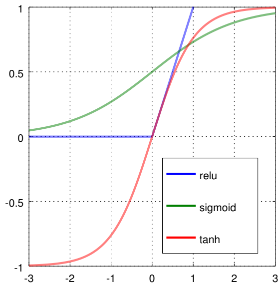
$$\begin{aligned} f &: \mathbb{R} \to \mathbb{R}, x \mapsto f(x) \\ \frac{\partial f}{\partial x} &= f'(x) \end{aligned}$$

Gradient in $\mathbb{C}$

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

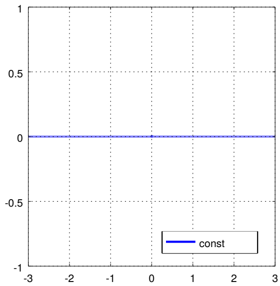
Complex-valued MLPs

Activation in $\mathbb{R}$



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

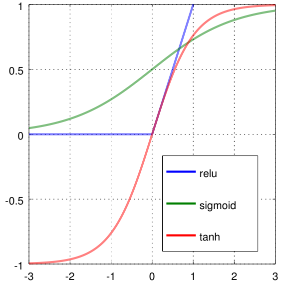
Activation in $\mathbb{C}$



Analytical and bounded?
$\rightarrow$ only constant functions

Complex-valued MLPs

Activation in $\mathbb{R}$



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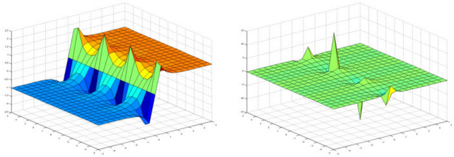
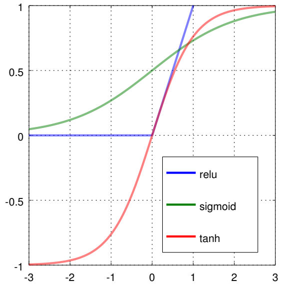


Analytical or bounded
$\rightarrow$ e.g. tanh

Complex-valued MLPs

Activation in $\mathbb{R}$



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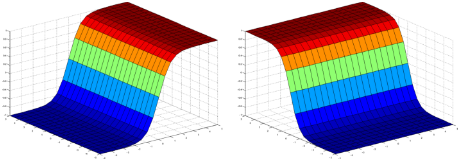
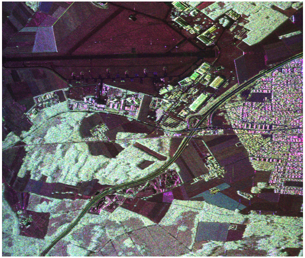


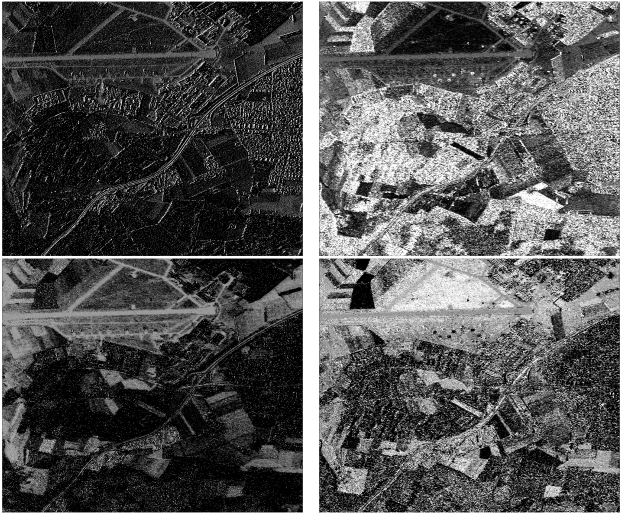
Analytical or **bounded**
$\rightarrow$ e.g. split-tanh

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

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. More in Part 3
- 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
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2. Machine Learning Methods
   - Support Vector Machine (SVM)
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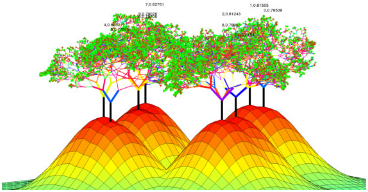
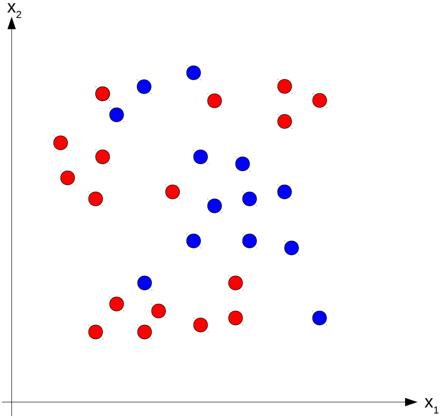


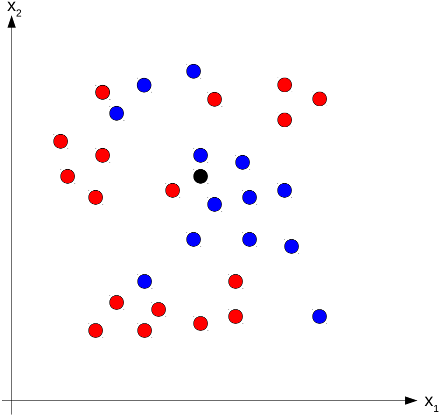
From kNN to Search Trees

- Data samples **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



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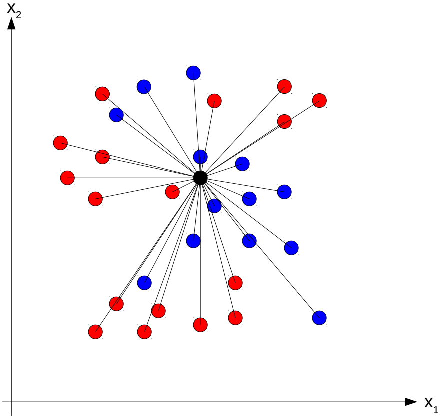

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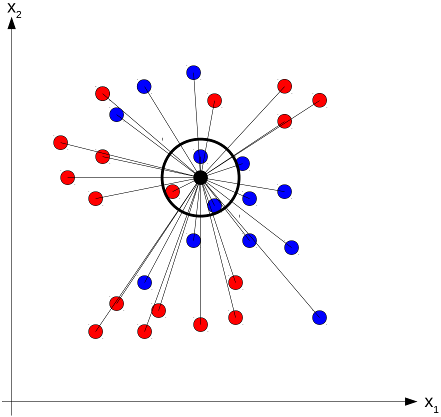
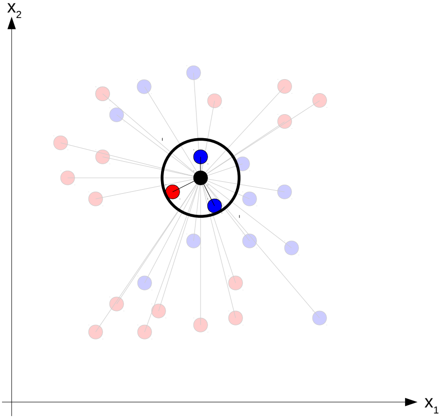


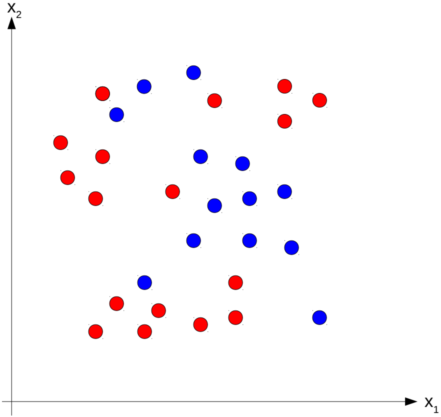
From kNN to Search Trees

- 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
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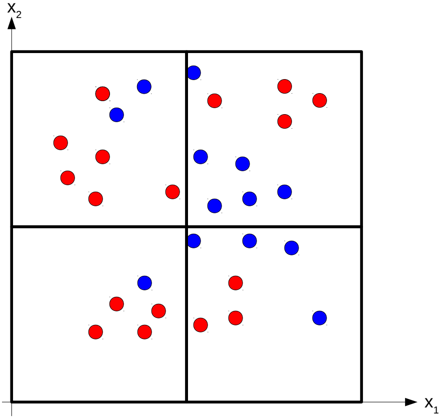
    - Divide space recursively into cells



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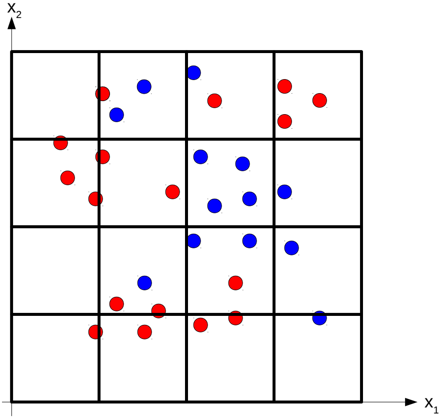

From kNN to Search Trees

- Search trees
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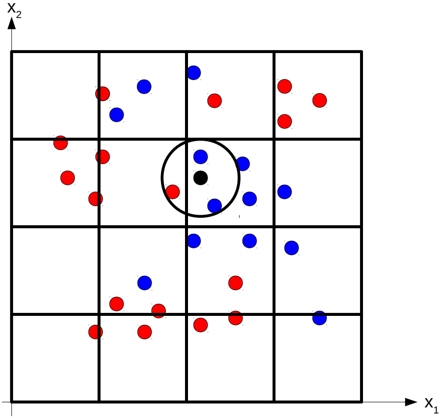
  - Divide space recursively into cells
  - Given a query, find relevant cells



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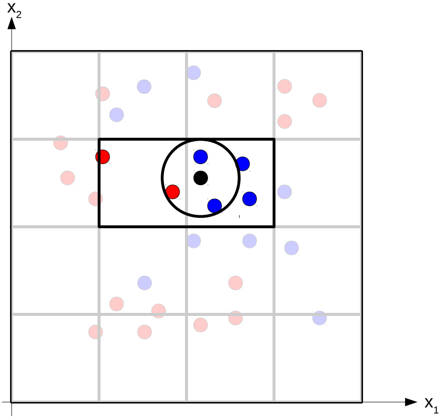

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- Search trees
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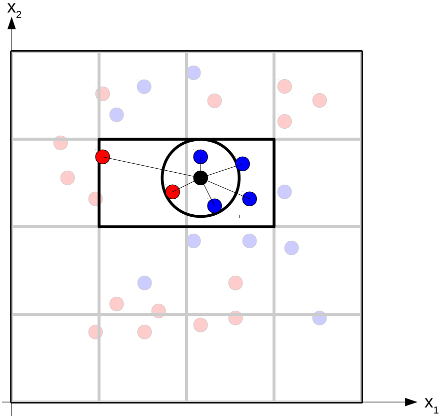

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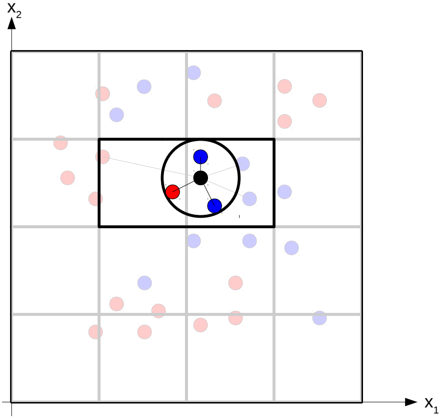

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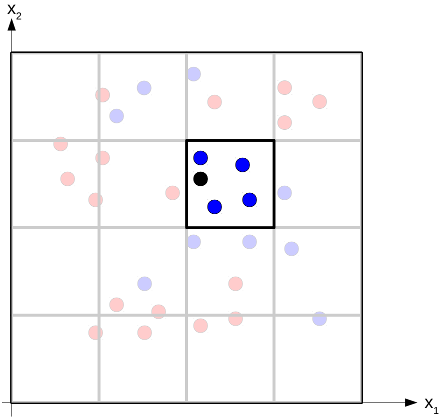
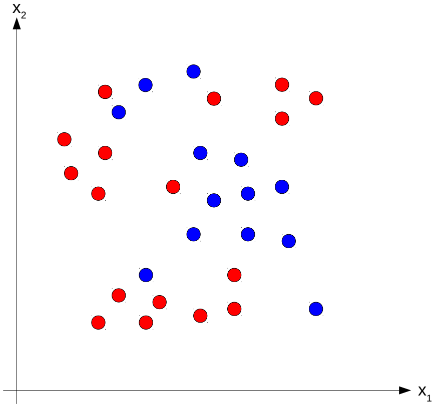
- Exact search: Leads to equivalent results
- Approximation: Use samples within query cell directly



From Search Trees to (Random) Decision Trees

- Cell construction



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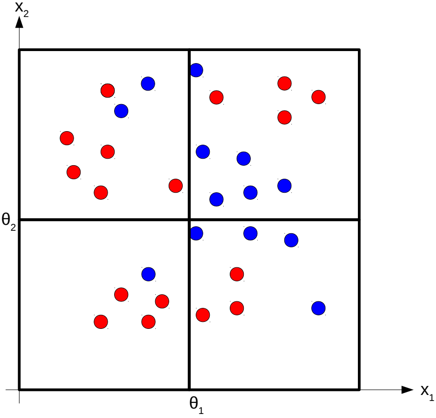
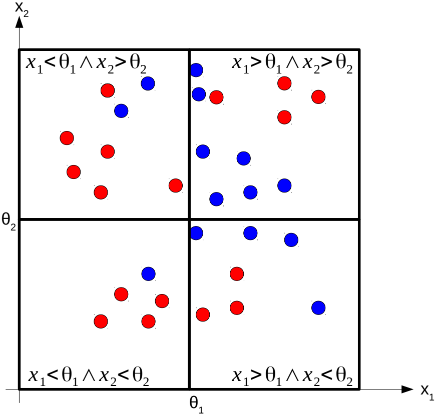


From Search Trees to (Random) Decision Trees

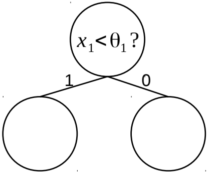
- Cell construction
  $\rightarrow$ Simple threshold operation
  $\rightarrow$ Different threshold definitions (e.g. equi-sized cells, threshold as data median) lead to different search tree variants (e.g. quad-tree, k-D tree).

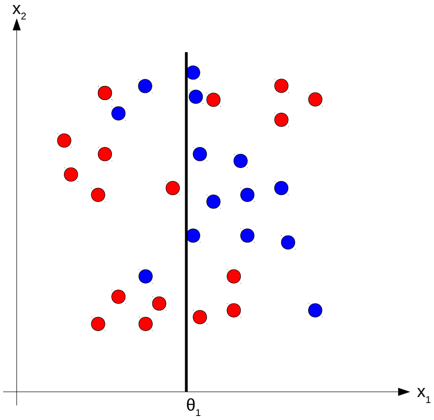


From Search Trees to (Random) Decision Trees

- 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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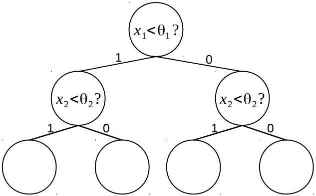

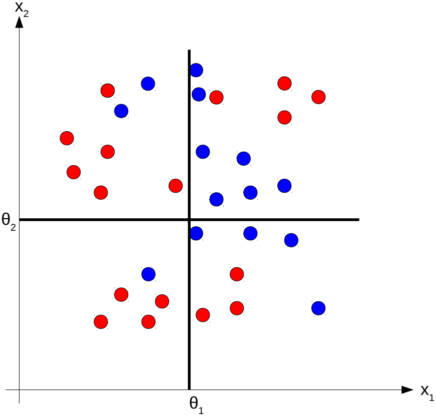

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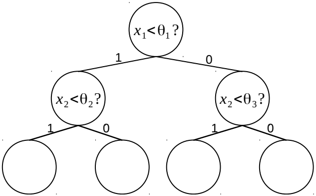
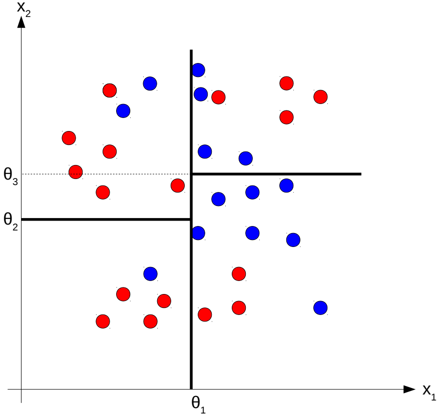
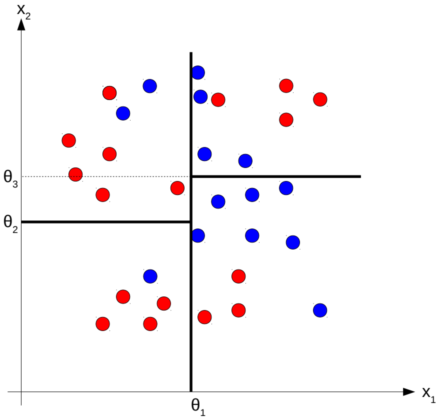




From Search Trees to (Random) Decision Trees

- 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 (c.f. Part-3)



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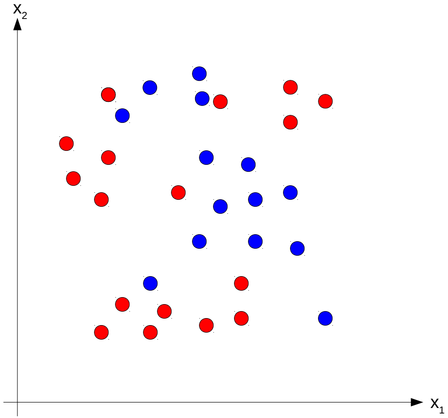

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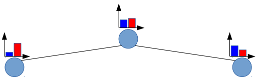

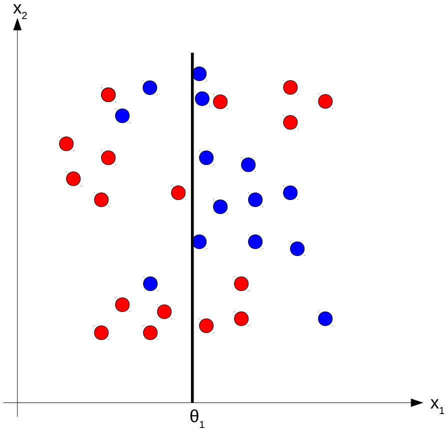

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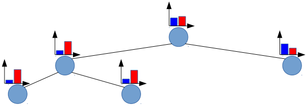

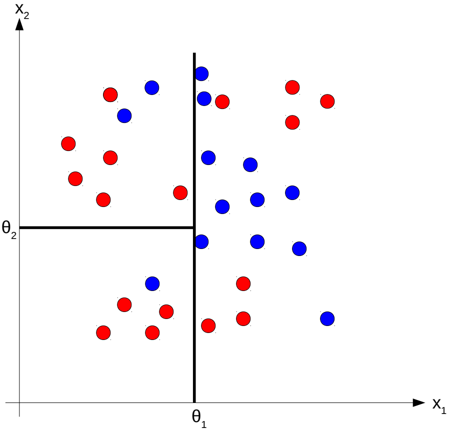

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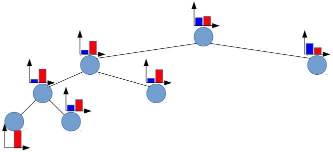

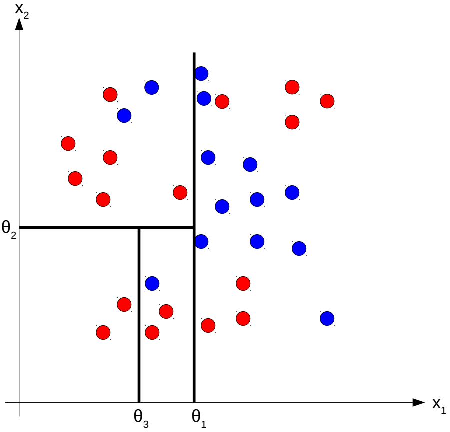

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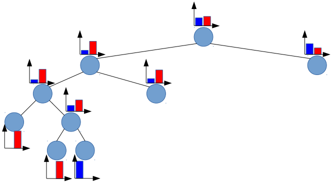

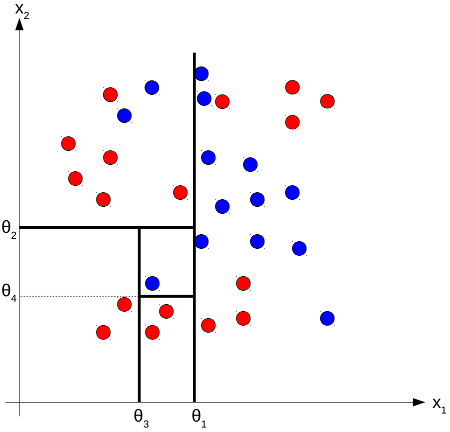

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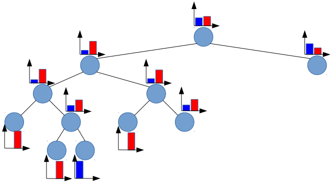

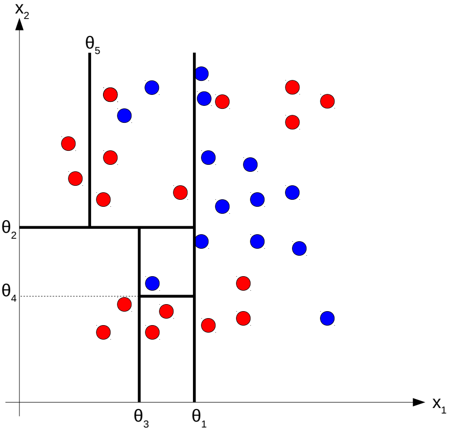

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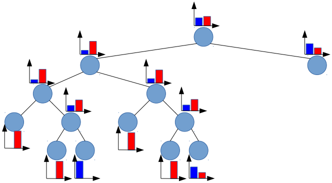

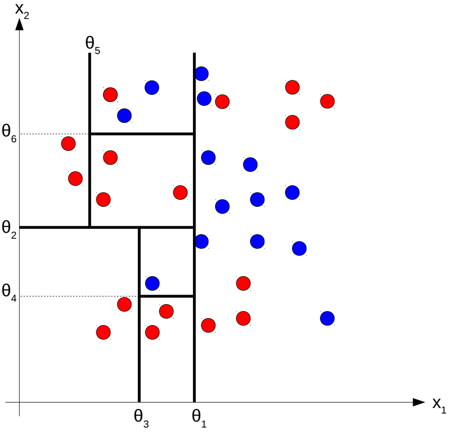

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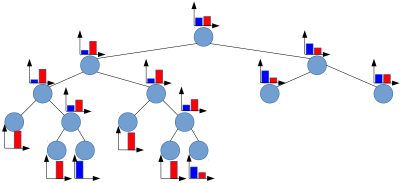

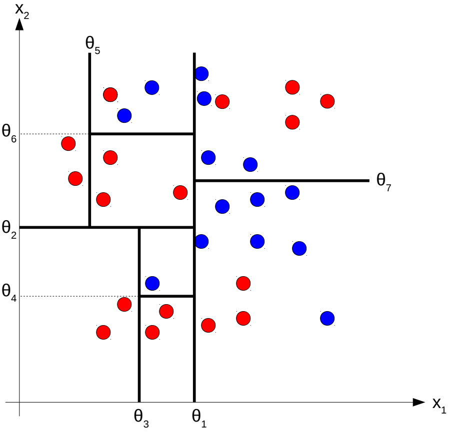

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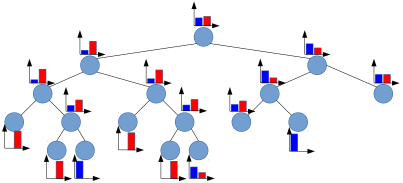

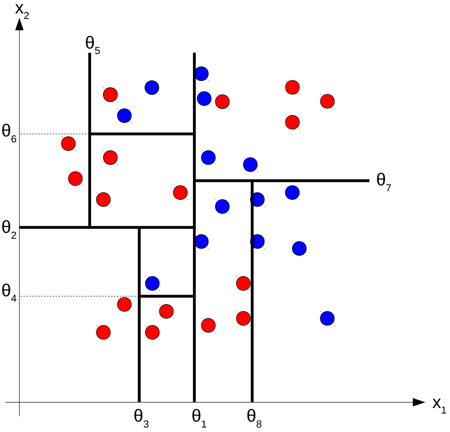

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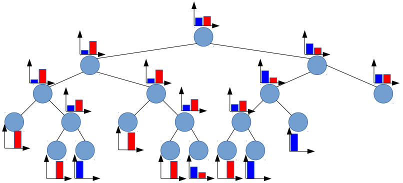

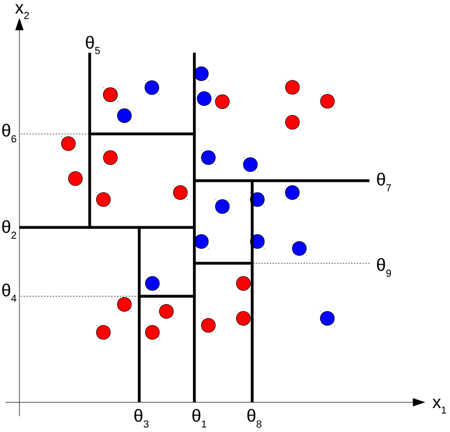

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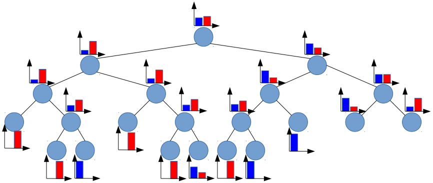

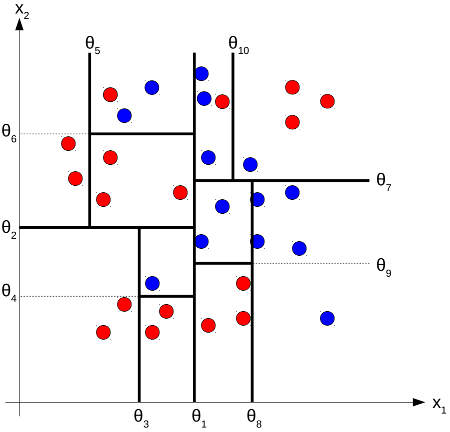

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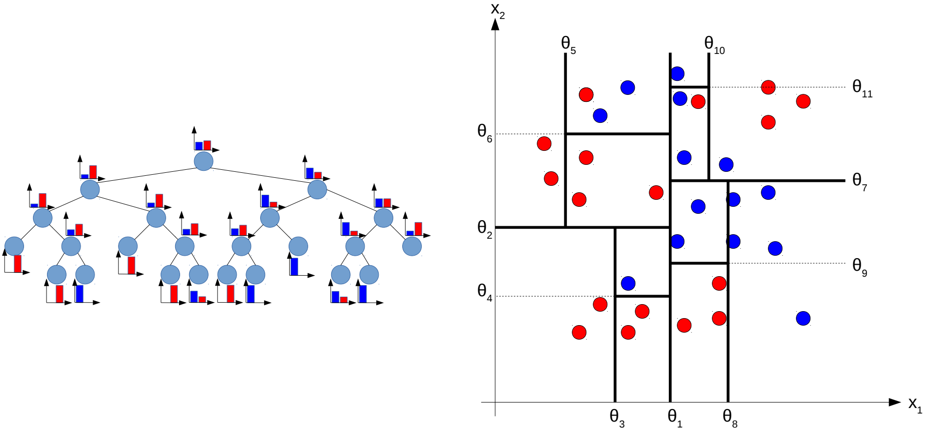

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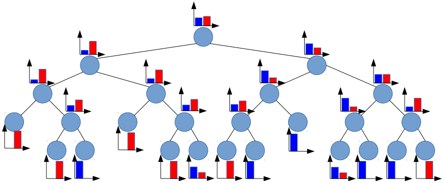
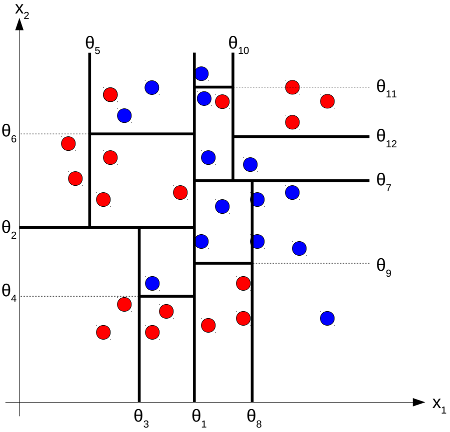
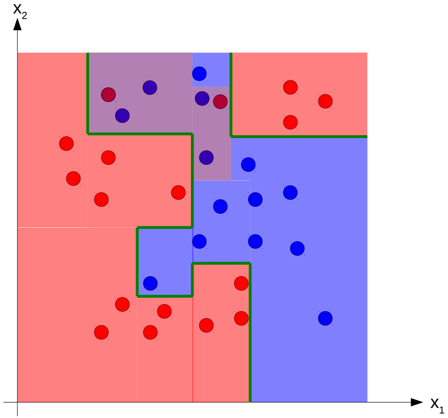




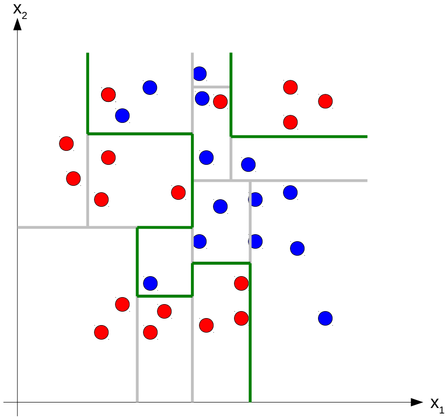
From Search Trees to (Random) Decision Trees

- 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



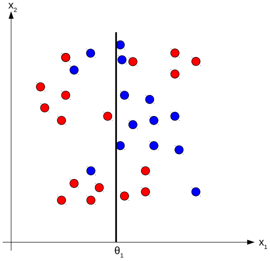
From Search Trees to (Random) Decision Trees

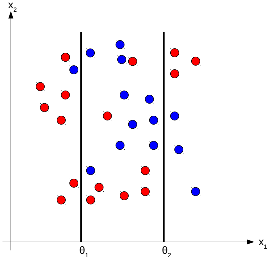
Other node tests are possible:

- 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

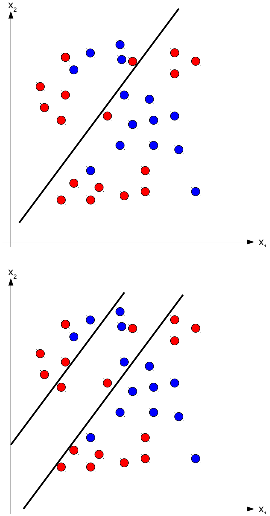
Other node tests are possible:

- 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:

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

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

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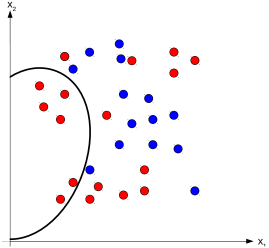
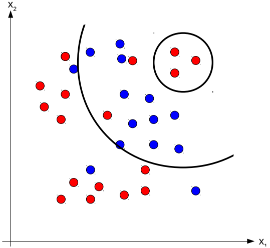


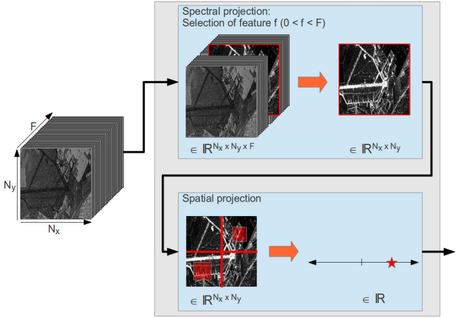


From Search Trees to (Random) Decision Trees

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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  → Few samples lead to small trees: Only few questions can be asked.
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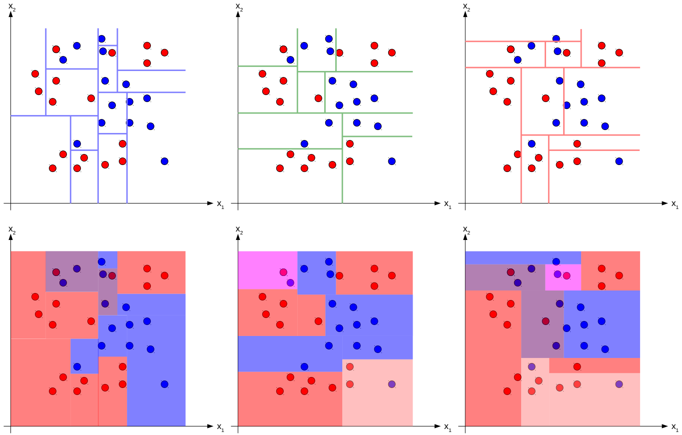
How to
→ keep (most) of the advantages
→ getting rid of (most) disadvantages?

From (Random) Decision Trees to Random Forests



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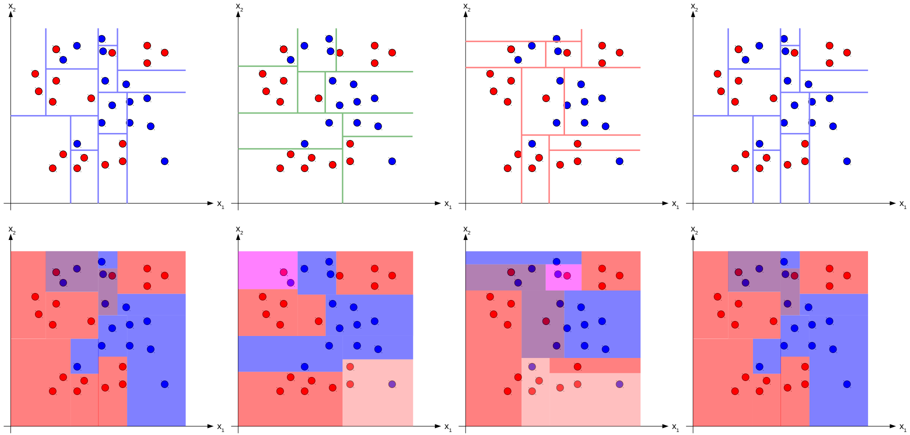

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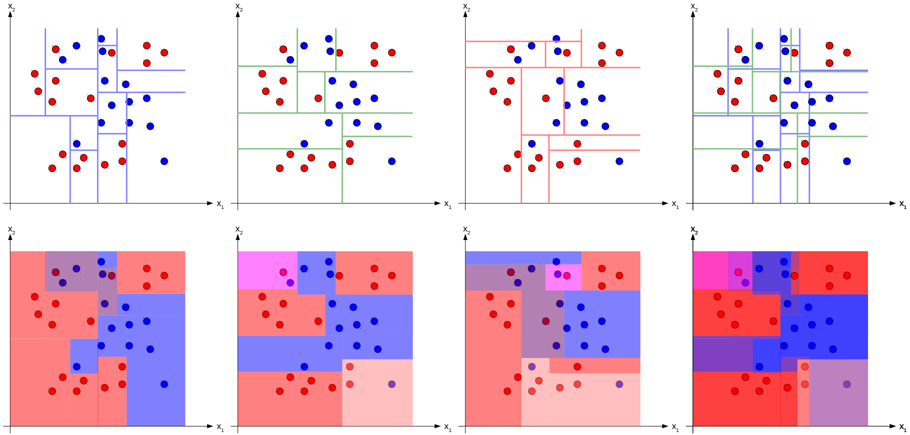

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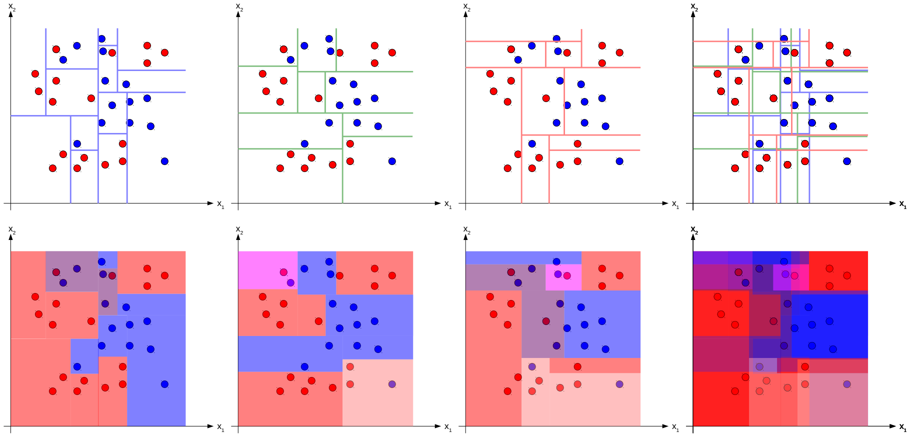

Random Forests

- 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

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

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
- Variant: Subagging $\equiv$ Sample without replacement

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.

Glorot, X. and Bengio, Y. (2010). Understanding the difficulty of training deep feedforward neural networks. In *Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics, AISTATS 2010, Chia Laguna Resort, Sardinia, Italy, May 13-15, 2010*, pages 249–256.

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