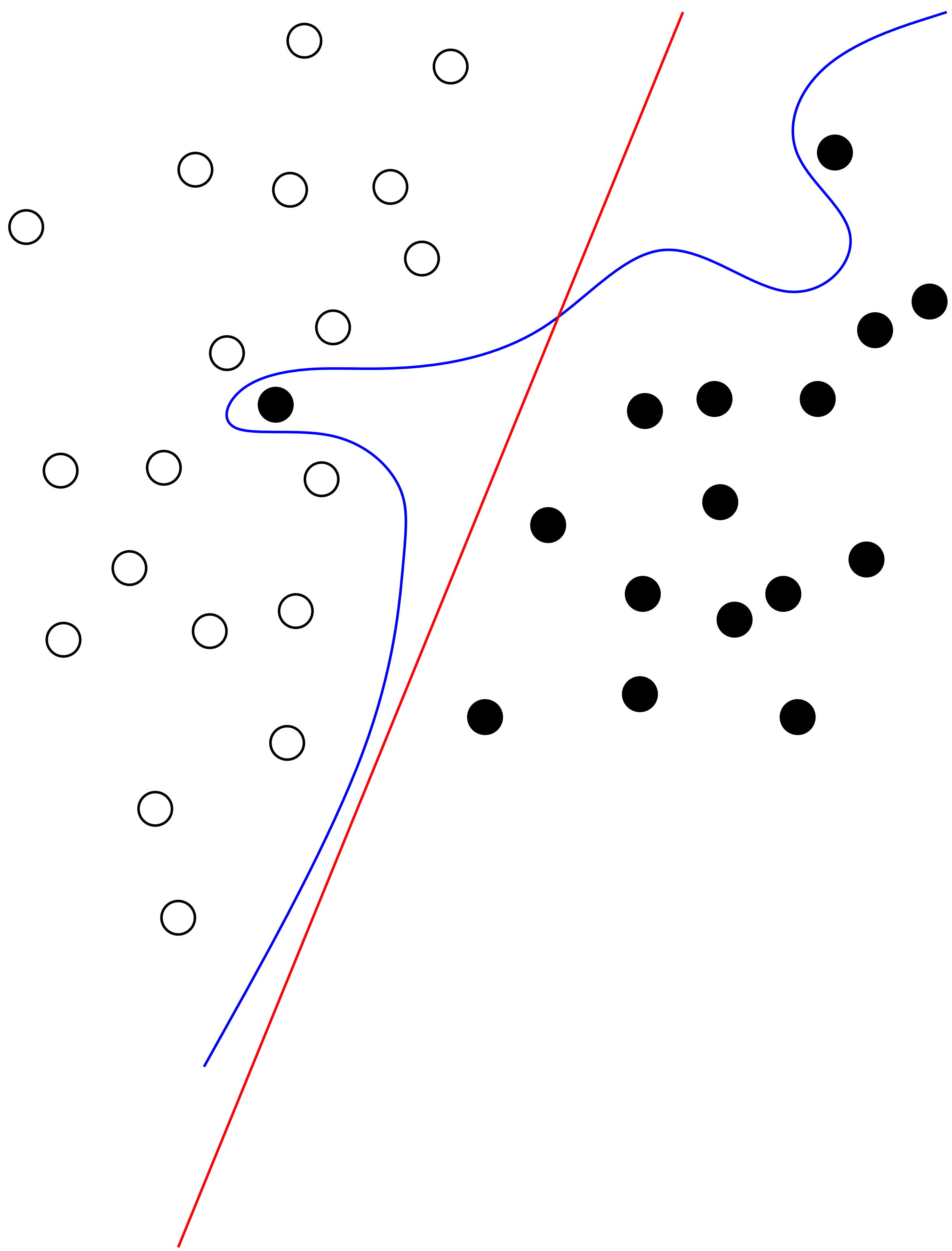
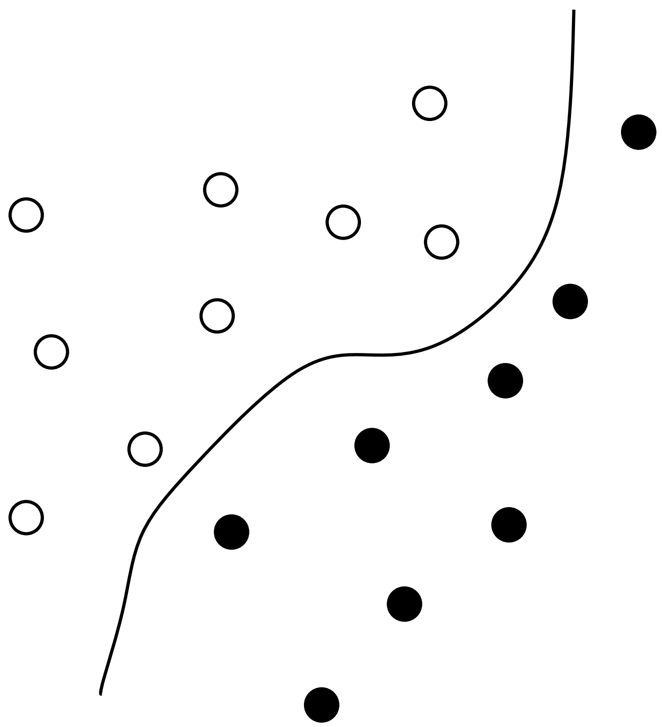
Recap of general problem

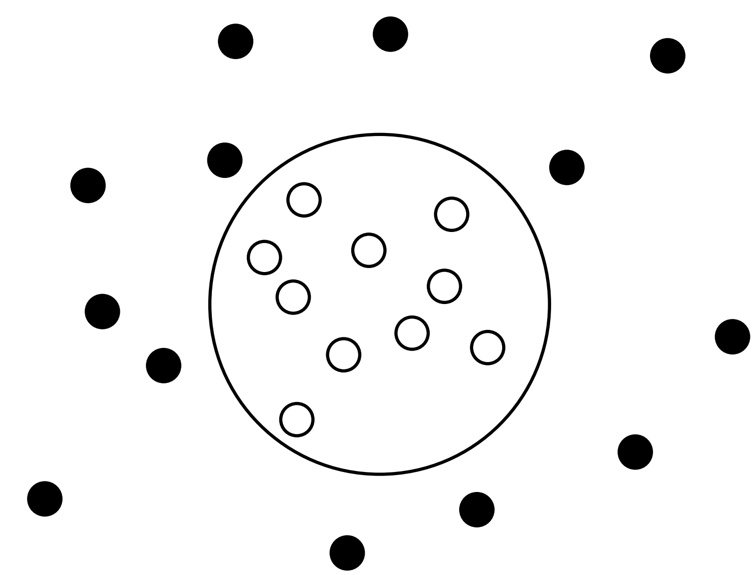


- we wanted to pick a function f amongst a class $\mathcal{F}$ of functions which hopefully not only classifies some given *sample* S (picked according to some probability distribution) but also future points that come along according to the same prob. dist.
- it seemed reasonable not to pick a very complicated function that fits the sample S exactly as this might decrease performance on future points that come along
- $\Rightarrow$ need some measure of complicatedness of function class $\mathcal{F}$ (Jochen: Rademacher complexity)

What to do with data not separable linearly ?

- Some data does not look linearly separable at all





- idea: apply some mapping to the points before trying the linear classifier; e.g. for points separated by $f : x \mapsto x^3$, use mapping $(x, y) \rightarrow (x, y^{1/3})$

- mapping might go to some higher dimension where linear classifiers are also more powerful (in terms of VC dimension) e.g. $(x, y) \rightarrow (x, y, x^2 + y^2)$

- Kernel methods: do not apply the mapping explicitly, but instead of applying dot products using some *kernel function*

The kernel method

- we are interested in functions $k(x, y)$ that replace $x \cdot y$

- Mercer's theorem characterizes functions $k(x, y)$ for which there exists a mapping ϕ to some strange space such that $k(x, y) = \phi(x) \cdot \phi(y)$

- typical kernel methods that can be realized as dot products in some higher dimensional space are

  - polynomials of degree d': $k(x, y) = (x^T y + c)^{d'}$
  - Gaussian functions: $k(x, y) = e^{-c||x-y||^2}$
  - Sigmoid functions $k(x, y) = \tanh(x^T y + c)$

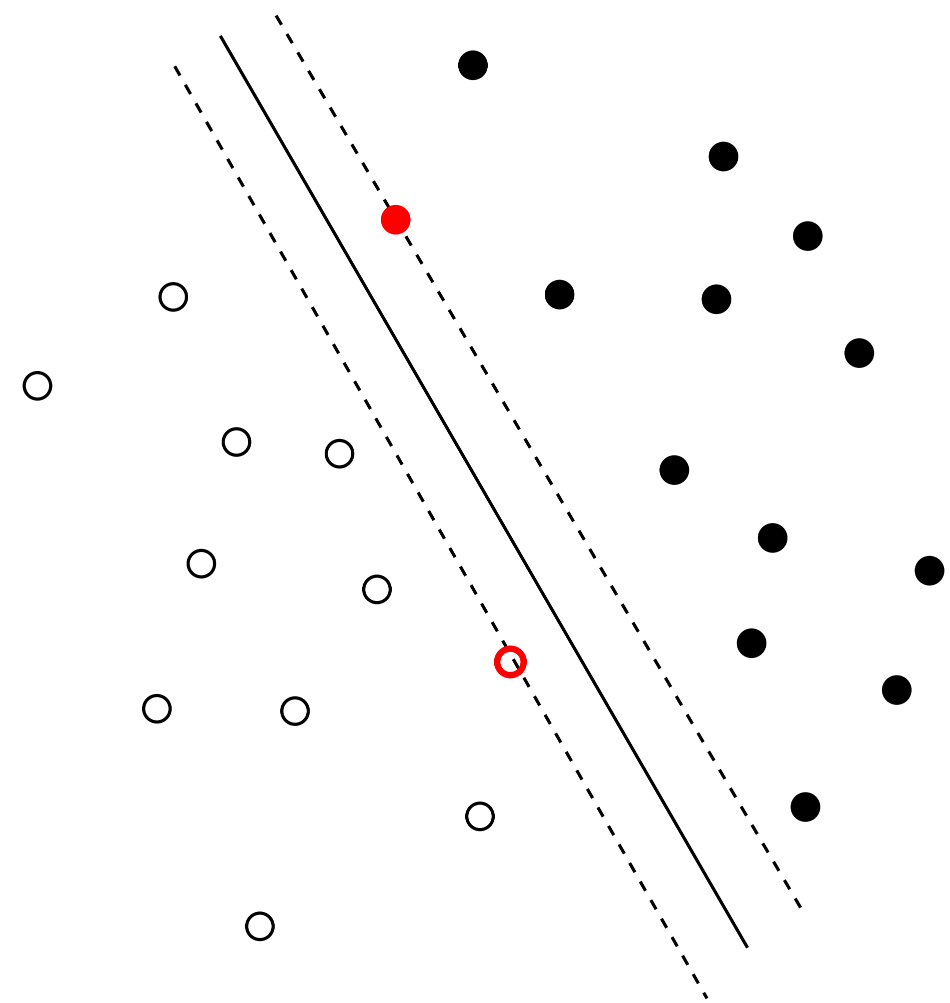
Linear Support Vector Machines

- we want to determine a hyperplane of the form $\mathbf{w} \cdot x + \mathbf{b} = 0$ which separates the $+1$ from the -1 points, maximizing the 'margin', i.e.

  $x_i \cdot \mathbf{w} + \mathbf{b} \geq 1$ for $y_i = +1$
  $x_i \cdot \mathbf{w} + \mathbf{b} \leq -1$ for $y_i = -1$

  $\Leftrightarrow$
  $\min ||\mathbf{w}||^2$ such that
  $y_i(x_i \cdot \mathbf{w} + \mathbf{b}) - 1 \geq 0$

- for x_i with tight constraints, distance to origin is $\frac{|1-b|}{||\mathbf{w}||}$, $\frac{|-1-b|}{||\mathbf{w}||}$ respectively, so the margin is $2/||\mathbf{w}||$



Lagrangian Formulation

- We replace the original problem

$$\min ||\mathbf{w}||^2 \text{ s.t.}$$
$$y_i(x_i \cdot \mathbf{w} + \mathbf{b}) - 1 \geq 0$$

  (penalizing violations of the constraint) by

- its Lagrangian formulation
  $L_P \equiv \frac{1}{2}||\mathbf{w}||^2 - \sum_{i=1}^{l} \alpha_i y_i(x_i \cdot \mathbf{w} + b) + \sum_{i=1}^{l} \alpha_i$
  which needs to be minimized (wrt $\mathbf{w}, \mathbf{b}$; requiring that the derivatives wrt α_i vanish and $\alpha_i \geq 0$)

- in the respective dual we *maximize* L_P s.t. the gradients wrt to w, b vanish and $\alpha_i \geq 0$; hence the respective dual is
  $L_D = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j x_i \cdot x_j$ s.t. $\sum \alpha_i y_i = 0$, $\alpha_i \geq 0$

- Lagrange multiplier α_i for each training point x_i; $\alpha_i > 0 \Leftrightarrow x_i$ is support vector

- $\mathbf{w}$ can be computed as $\sum \alpha_i y_i x_i$

- KKT conditions guarantee equality of primal and dual solution and allow to compute b

Non-linear SVMs

- Recall we need to maximize the following:
  $L_D = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j x_i \cdot x_j$ s.t. $\sum \alpha_i y_i = 0$, $\alpha_i \geq 0$

- only operation on the training points is dot product

- we could replace the dot product by any other function $k(x_i, x_j)$ that is "justifiable", e.g.
  $\exists \phi : \mathbb{R}^d \rightarrow \mathcal{H}$ s.t.
  $k(x_i, x_j) = \Phi(x_i) \cdot \Phi(x_j)$
  i.e. the result of $k(x_i, x_j)$ equals dot product in some other space $\mathcal{H}$ (feature space)

- we don't even need to know about Φ or $\mathcal{H}$ provided we know that such exists

- from VC-dimension we know that linear classifiers become more powerful in higher dimensions $\Rightarrow$ this kernel trick might allow to separate more complicated data

Using the SVM

- the separating hyperplane unfortunately also lives in that highdimensional space $\mathcal{H}$!
- there need not exist some $\mathbf{w}'$ living in the original space that maps via Φ to the above
- but we can evaluate the learned SVM using
  $f(x) = \mathbf{w} \cdot \Phi(x) = \sum \alpha_i y_i \Phi(s_i) \cdot \Phi(x) + b = \sum \alpha_i y_i k(s_i, x) + b$
  so no need to compute $\Phi(x)$ explicitly

Characterization of valid kernel functions

- let us first consider a kernel function for which we can explicitly construct the mapping Φ
- data in $\mathbb{R}^2$, $k(x, x') = (x \cdot x')^2$
- we need to find $\Phi : \mathbb{R}^2 \to \mathcal{H}$ such that $(x \cdot y)^2 = \Phi(x) \cdot \Phi(y)$
- let's choose $\mathcal{H} = \mathbb{R}^3$ and $\Phi(x) = \begin{pmatrix} x_1^2 \\ \sqrt{2}x_1 x_2 \\ x_2^2 \end{pmatrix}$
- $\mathcal{H}$ and $\Phi(x)$ are not unique for $k(.)$
- $\Phi(x) = \begin{pmatrix} x_1^2 \\ x_1 x_2 \\ x_1 x_2 \\ x_2^2 \end{pmatrix}$, $\mathcal{H} = \mathbb{R}^4$
  would have worked as well

Mercer's Theorem

- characterizes for which kernel functions $\mathcal{H}, \Phi$ exist.
- for $k(x, y)$ there exists a mapping Φ such that
  $k(x, y) = \sum \Phi(x)_i \Phi(y)_i$
  if and only if for any $g(x)$ with
  $\int g(x)^2 dx$ finite
  we have that $\int k(x, y) g(x) g(y) dx dy \geq 0$
- again example for $k(x, y) = (x \cdot y)^2$ in $\mathbb{R}^2$
- generalizes to $k(x, y) = (x \cdot y)^p$
- Mercer's Theorem does not reveal anything about $\mathcal{H}$ or Φ

Discussion

- e.g. 16×16 images ($d = 256$) and a degree $p = 4$ polynomial, the dimension of $\mathcal{H}$ is > 180000000!
- there are kernels for which Mercer's Theorem does not hold, still they seem to work in practice
- due to the often high dimension of $\mathcal{H}$, the VC dimension 'justification' seems pointless; generalization performance should be very bad
- some handwaving arguments why things still work out nicely:
  - mapped surface still lives in some sort of low-dimensional subspace
  - looking for the maximum margin hyperplane also seems to help
- in general there is no theory which guarantees good generalization properties of SVMs!

Examples: Polynomial Classifiers

- $k(x, y) = (x \cdot y + 1)^p$
- kernel functions with implicit high-dimensional $\mathcal{H}$ don't seem to perform too badly on linearly separable examples (no overfitting observed) really high dimension leads to overfitting, though
- high-dimensional kernel really necessary to separate more difficult data

Examples: Radial Basis functions

- $k(x, y) = e^{-||x-y||^2/2\sigma^2}$

Examples: Sigmoidal Neural Network

- $k(x, y) = \tanh(\kappa x \cdot y - \delta)$