Support Vector Machine Part 2

CS 760@UW-Madison

Goals for the lecture

you should understand the following concepts

- the kernel trick
- polynomial kernel
- Gaussian/RBF kernel

- valid kernels and kernel algebra
- kernels and neural networks

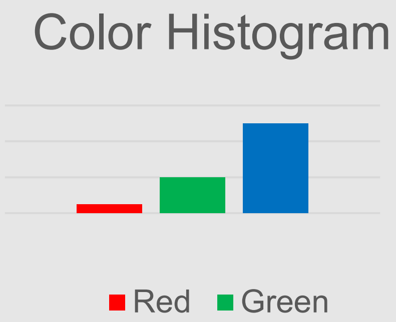
Kernel Methods

Features

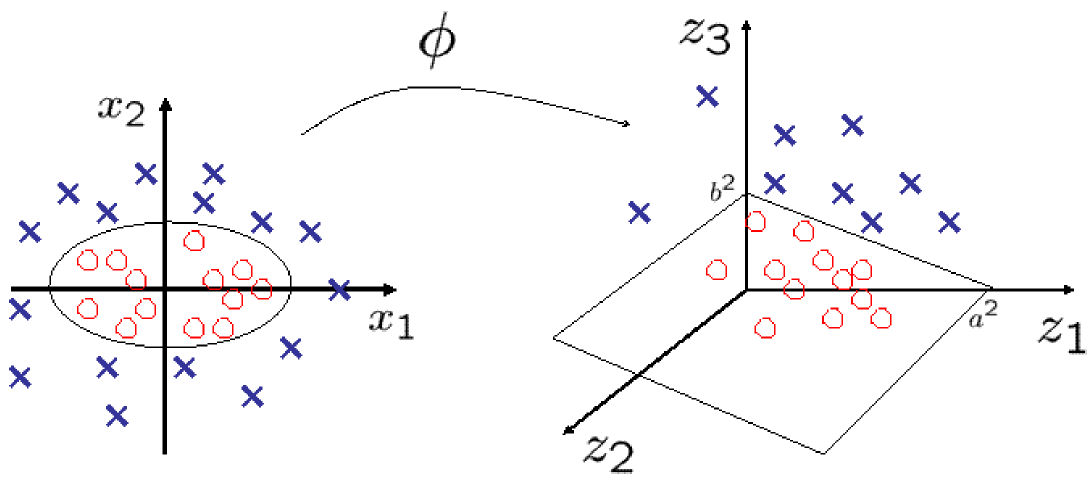
x

Extract features

$\phi(x)$



Features



$$\phi : (x_1, x_2) \longrightarrow (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$

$$\left(\frac{x_1}{a}\right)^2 + \left(\frac{x_2}{b}\right)^2 = 1 \longrightarrow \frac{z_1}{a^2} + \frac{z_3}{b^2} = 1$$

Proper feature mapping can make non-linear to linear!

Recall: SVM dual form

Only depend on inner products

- Reduces to dual problem:

$$\mathcal{L}(w, b, \boldsymbol{\alpha}) = \sum_i \alpha_i - \frac{1}{2}\sum_{ij} \alpha_i \alpha_j y_i y_j x_i^T x_j$$

$$\sum_i \alpha_i y_i = 0, \alpha_i \geq 0$$

- Since $w = \sum_i \alpha_i y_i x_i$, we have $f(x) = w^T x + b = \sum_i \alpha_i y_i x_i^T x + b$

Features

- Using SVM on the feature space $\{\phi(x_i)\}$: only need $\phi(x_i)^T\phi(x_j)$

- Conclusion: no need to design $\phi(\cdot)$, only need to design

$$k(x_i, x_j) = \phi(x_i)^T\phi(x_j)$$

Polynomial kernels

- Fix degree d and constant c:

$$k(x, x') = (x^T x' + c)^d$$

- What are $\phi(x)$?
- Expand the expression to get $\phi(x)$

Polynomial kernels

$$\forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^2, \quad K(\mathbf{x}, \mathbf{x}') = (x_1 x_1' + x_2 x_2' + c)^2 = \begin{bmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}\, x_1 x_2 \\ \sqrt{2c}\, x_1 \\ \sqrt{2c}\, x_2 \\ c \end{bmatrix} \cdot \begin{bmatrix} {x'}_1^2 \\ {x'}_2^2 \\ \sqrt{2}\, x_1' x_2' \\ \sqrt{2c}\, x_1' \\ \sqrt{2c}\, x_2' \\ c \end{bmatrix}$$

Figure from Foundations of Machine Learning, by M. Mohri, A. Rostamizadeh, and A. Talwalkar

SVMs with polynomial kernels

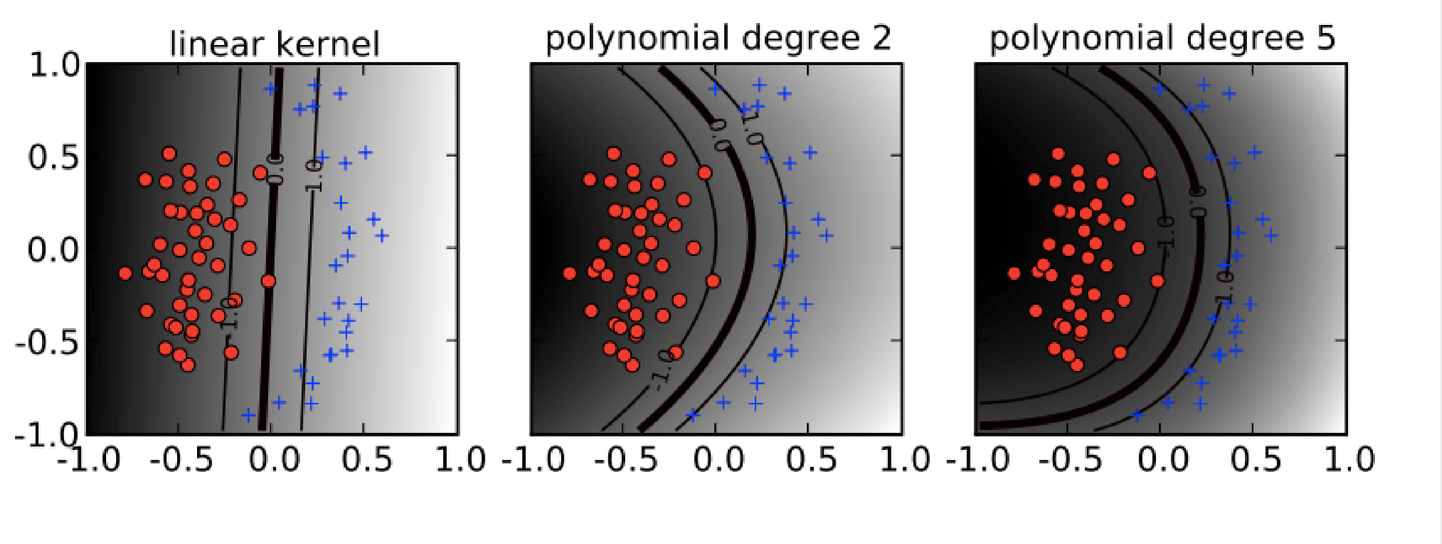


Figure from Ben-Hur & Weston,
Methods in Molecular Biology 2010

Gaussian/RBF kernels

- Fix bandwidth σ:

$$k(x, x') = \exp(-\left||x - x'|\right|^2 / 2\sigma^2)$$

- Also called radial basis function (RBF) kernels

- What are $\phi(x)$? Consider the un-normalized version

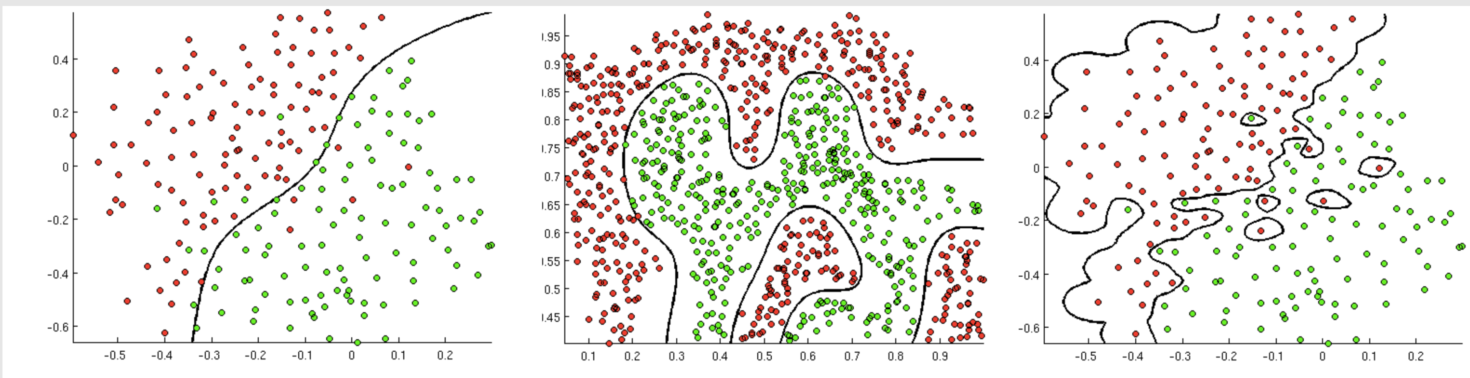
$$k'(x, x') = \exp(x^T x' / \sigma^2)$$

- Power series expansion:

$$k'(x, x') = \sum_{i}^{+\infty} \frac{(x^T x')^i}{\sigma^i i!}$$

The RBF kernel illustrated

$\gamma = 10$ $\gamma = 100$ $\gamma = 1000$



$$k(x, x') = \exp(-\gamma ||x - x'||^2)$$

Figures from openclassroom.stanford.edu (Andrew Ng)

Kernel Algebra

Polynomial and RBF kernels

- Polynomial kernel with degree d and constant c:

$$k(x, x') = (x^T x' + c)^d$$

- RBF kernels with bandwidth σ:

$$k(x, x') = \exp(-||x - x'||^2 / 2\sigma^2)$$

Mercer's condition for kernels

- Theorem: $k(x, x')$ has expansion

$$k(x, x') = \sum_{i}^{+\infty} a_i \phi_i(x) \phi_i(x')$$

for nonnegative a_i's, if and only if for any function $c(x)$,

$$\int \int c(x) c(x') k(x, x') dx dx' \geq 0$$

(Omit some math conditions for k and c)

Constructing new kernels

- Kernels are closed under positive scaling, sum, product, pointwise limit, and composition with a power series $\sum_i^{+\infty} a_i k^i(x, x')$

- Example: $k_1(x, x'), k_2(x, x')$ are kernels, then also is

$$k(x, x') = 2k_1(x, x') + 3k_2(x, x')$$

- Example: $k_1(x, x')$ is kernel, then also is

$$k(x, x') = \exp(k_1(x, x'))$$

Kernel algebra

- given a valid kernel, we can make new valid kernels using a variety of operators

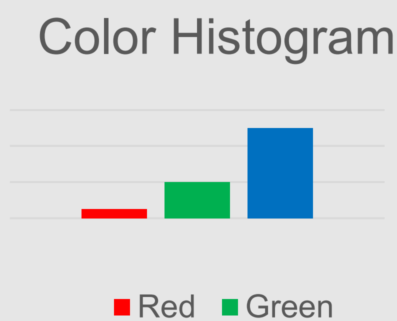
kernel composition	mapping composition
$k(\boldsymbol{x},\boldsymbol{v}) = k_a(\boldsymbol{x},\boldsymbol{v}) + k_b(\boldsymbol{x},\boldsymbol{v})$	$\phi(\boldsymbol{x}) = \left(\phi_a(\boldsymbol{x}),\ \phi_b(\boldsymbol{x})\right)$
$k(\boldsymbol{x},\boldsymbol{v}) = \gamma\ k_a(\boldsymbol{x},\boldsymbol{v}),\ \gamma > 0$	$\phi(\boldsymbol{x}) = \sqrt{\gamma}\ \phi_a(\boldsymbol{x})$
$k(\boldsymbol{x},\boldsymbol{v}) = k_a(\boldsymbol{x},\boldsymbol{v})k_b(\boldsymbol{x},\boldsymbol{v})$	$\phi_l(\boldsymbol{x}) = \phi_{ai}(\boldsymbol{x})\phi_{bj}(\boldsymbol{x})$
$k(\boldsymbol{x},\boldsymbol{v}) = \boldsymbol{x}^{\mathsf{T}} A\boldsymbol{v}$, A is p.s.d.	$\phi(\boldsymbol{x}) = L^{\mathsf{T}}\boldsymbol{x}$, where $A = LL^{\mathsf{T}}$
$k(\boldsymbol{x},\boldsymbol{v}) = f(\boldsymbol{x})f(\boldsymbol{v})k_a(\boldsymbol{x},\boldsymbol{v})$	$\phi(\boldsymbol{x}) = f(\boldsymbol{x})\phi_a(\boldsymbol{x})$

Kernels v.s. Neural Networks

Features

x

Extract features

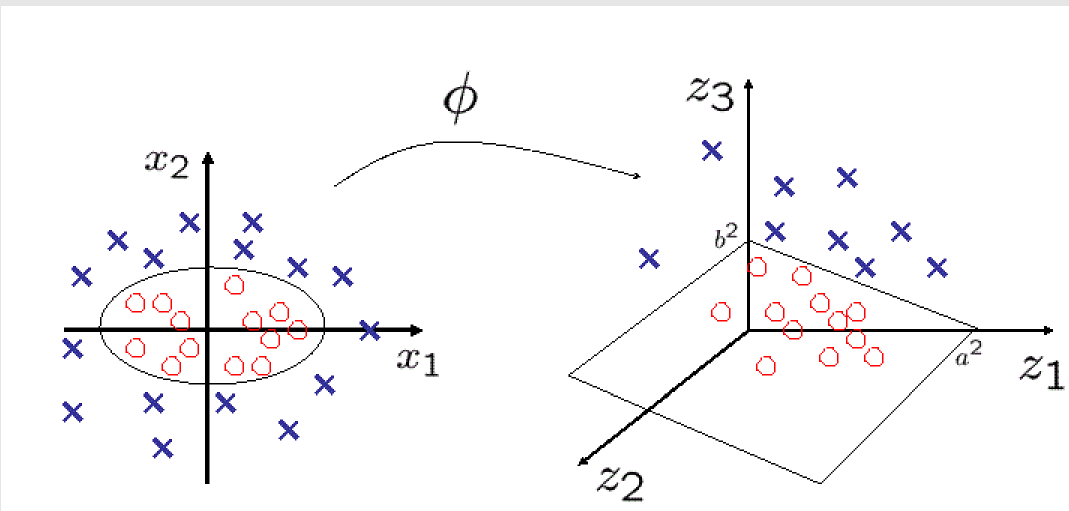


build hypothesis

$y = w^T \phi(x)$

Features: part of the model

Nonlinear model



build hypothesis

$y = w^T \phi(x)$

Linear model

Polynomial kernels

$$\forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^2, \quad K(\mathbf{x}, \mathbf{x}') = (x_1 x_1' + x_2 x_2' + c)^2 = \begin{bmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}\, x_1 x_2 \\ \sqrt{2c}\, x_1 \\ \sqrt{2c}\, x_2 \\ c \end{bmatrix} \cdot \begin{bmatrix} {x'}_1^2 \\ {x'}_2^2 \\ \sqrt{2}\, x_1' x_2' \\ \sqrt{2c}\, x_1' \\ \sqrt{2c}\, x_2' \\ c \end{bmatrix}$$

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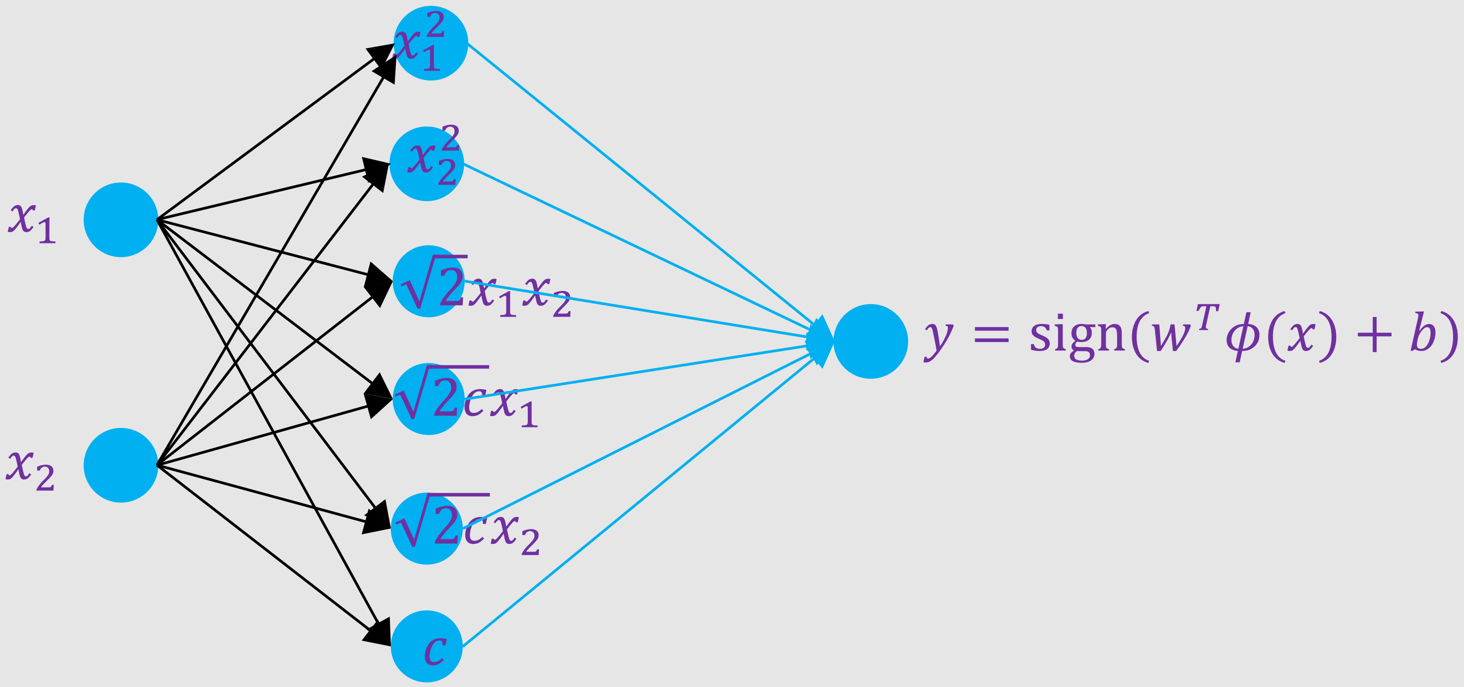
Polynomial kernel SVM as two layer neural network



First layer is fixed. If also learn first layer, it becomes two layer neural network

Comments on SVMs

- we can find solutions that are globally optimal (maximize the margin)
  - because the learning task is framed as a convex optimization problem
  - no local minima, in contrast to multi-layer neural nets

- there are two formulations of the optimization: *primal* and *dual*
  - dual represents classifier decision in terms of support vectors
  - dual enables the use of kernel functions

- we can use a wide range of optimization methods to learn SVM
  - standard quadratic programming solvers
  - SMO [Platt, 1999]
  - linear programming solvers for some formulations
  - etc.

Comments on SVMs

- kernels provide a powerful way to
  - allow nonlinear decision boundaries
  - represent/compare complex objects such as strings and trees
  - incorporate domain knowledge into the learning task
- using the kernel trick, we can implicitly use high-dimensional mappings without explicitly computing them
- one SVM can represent only a binary classification task; multi-class problems handled using multiple SVMs and some encoding
- empirically, SVMs have shown (close to) state-of-the art accuracy for many tasks
- the kernel idea can be extended to other tasks (anomaly detection, regression, etc.)

THANK YOU

Some of the slides in these lectures have been adapted/borrowed from materials developed by Mark Craven, David Page, Jude Shavlik, Tom Mitchell, Nina Balcan, Elad Hazan, Tom Dietterich, and Pedro Domingos.