UCLA Samueli Computer Science

CS M146 Discussion: Week 7
Kernels, SVM

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Friday, 02/19/2021

Roadmap

- Announcement
- Kernels
- SVM
- PyTorch Q&A (PS3)

Announcements

- **5:00 pm PST, Feb 19 (Friday):** Weekly Quiz 7 released on Gradescope.
- **11:59 pm PST, Feb 21 (Sunday):** Weekly quiz 4 closed on Gradescope!
    - Start the quiz before **11:00 pm PST, Feb 21** to have the full 60-minute time
- **Problem set 3** released on CCLE, submission on Gradescope.
    - Please assign pages of your submission with corresponding problem set outline items on GradeScope.
    - You need to submit code, similar to PS2
    - Due on next week, **11:59pm PST, Feb 26 (Friday)**

Late Submission of PS will NOT be accepted!

About Quiz 7

- Quiz release date and time: **Feb 19, 2021 (Friday) 05:00 PM PST**
- Quiz due/close date and time: **Feb 21, 2021 (Sunday) 11:59 PM PST**
- You will have up to **60 minutes** to take this exam. → Start before **11:00 PM** Sunday
- You can find the exam entry named "Week 7 Quiz" on GradeScope.
- Topics: **Kernels, SVM**
- Question Types
  - True/false, multiple choices
  - Some questions may include several subquestions.
- Some light calculations are expected. Some scratch paper and one scientific calculator (physical or online) are recommended for preparation.

Kernels

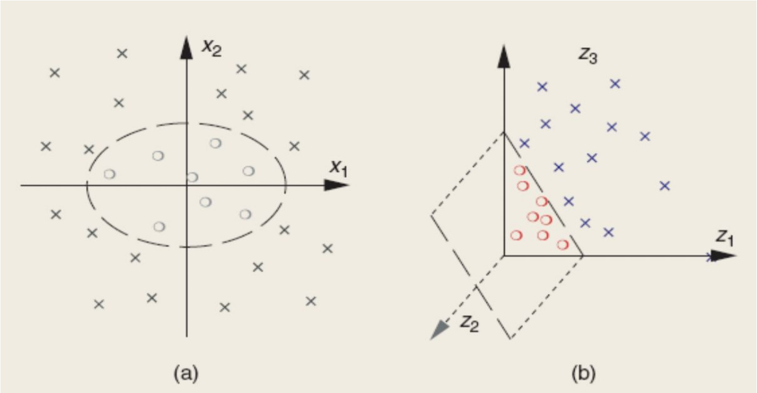
- Motivation: Transformed feature space

- Basic idea: Define K, called kernel, such that:

$$K : X \times X \to \mathbb{R} \qquad \Phi(x) \cdot \Phi(y) = K(x, y)$$

which is often as a similarity measure.

- Benefit:
  - Efficiency: is often more efficient to compute than and the dot product.
  - Flexibility: can be chosen arbitrarily so long as the existence of is guaranteed (Mercer’s condition).



Credit: https://cs.nyu.edu/~mohri/icml2011-tutorial/tutorial-icml2011-1.pdf

Polynomial Kernels

- **Definition:**

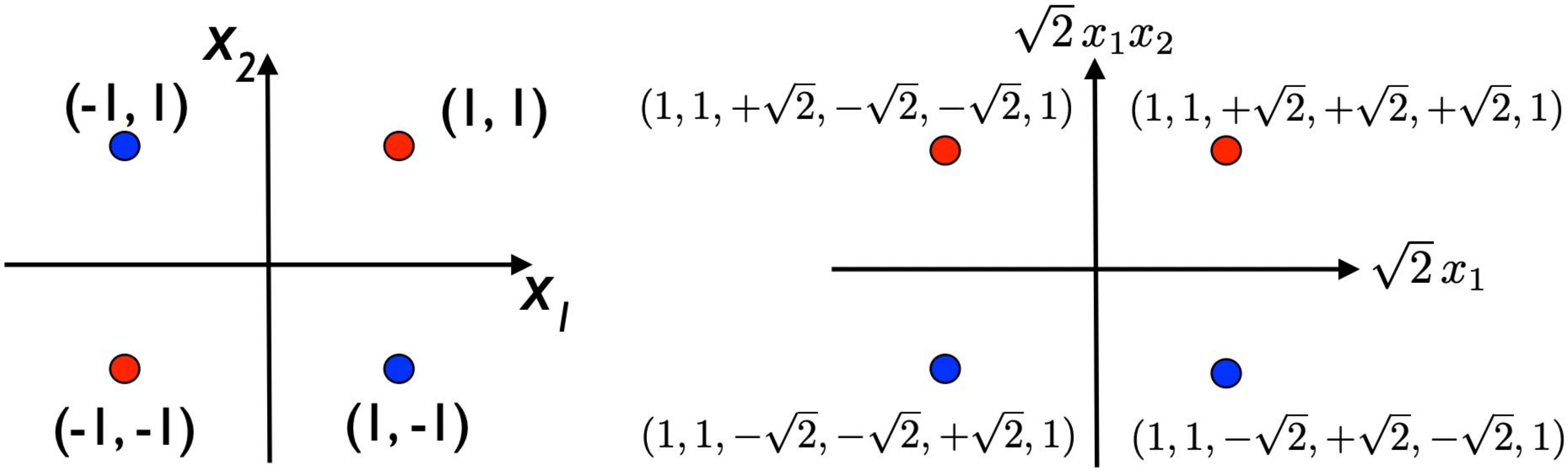
$$\forall x, y \in \mathbb{R}^N, \; K(x, y) = (x \cdot y + c)^d, \quad c > 0.$$

- **Example:** for $N=2$ and $d=2$,

$$K(x, y) = (x_1 y_1 + x_2 y_2 + c)^2$$

$$= \begin{bmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}\, x_1 x_2 \\ \sqrt{2c}\, x_1 \\ \sqrt{2c}\, x_2 \\ c \end{bmatrix} \cdot \begin{bmatrix} y_1^2 \\ y_2^2 \\ \sqrt{2}\, y_1 y_2 \\ \sqrt{2c}\, y_1 \\ \sqrt{2c}\, y_2 \\ c \end{bmatrix}.$$

Kernels: XOR Example



Linearly non-separable

Linearly separable by $x_1x_2 = 0.$

Other Kernel Options

Gaussian kernels:

$$K(x,y) = \exp\left(-\frac{||x-y||^2}{2\sigma^2}\right), \quad \sigma \neq 0.$$

Also known as "Radial Basis Function Kernel"

Sigmoid Kernels:

$$K(x,y) = \tanh(a(x \cdot y) + b), \;\; a, b \geq 0.$$

Note: The RBF/Gaussian kernel as a projection into infinite dimensions, commonly used in kernel SVM.

$$K(x, x') = \exp\left(-(x - x')^2\right)$$

$$= \exp\left(-x^2\right) \exp\left(-x'^2\right) \underbrace{\sum_{k=0}^{\infty} \frac{2^k (x)^k (x')^k}{k!}}_{\exp(2xx')}$$

Taylor Expansion

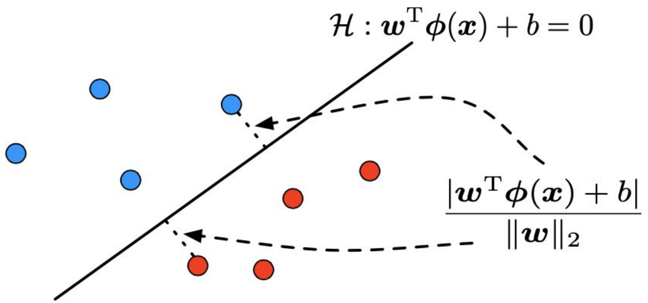
Credit: http://pages.cs.wisc.edu/~matthewb/pages/notes/pdf/svms/RBFKernel.pdf

SVM: Visual Tutorials

- Links: https://cs.stanford.edu/people/karpathy/svmjs/demo/

SVM: Margin

$$\text{MARGIN}(\boldsymbol{w}, b) = \min_n \frac{y_n[\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b]}{\|\boldsymbol{w}\|_2}$$



SVM: Start with the margin

Margin Lines

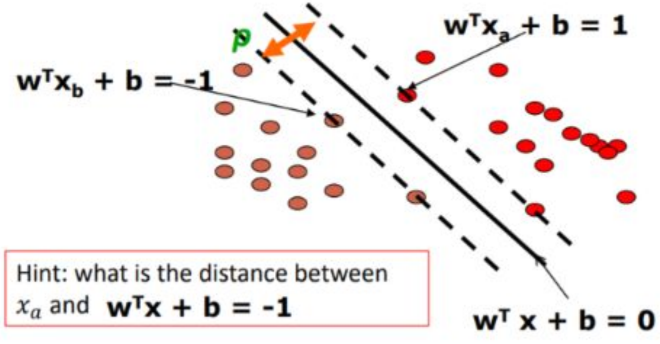
$$\boldsymbol{w}^T\mathbf{x}_a + \mathrm{b} = 1 \qquad \boldsymbol{w}^T\mathbf{x}_b + \mathrm{b} = -1$$

Distance between parallel lines of $ax_1+bx_2=c_1/c_2$)

$$d = \frac{|c_2 - c_1|}{\sqrt{a^2+b^2}}$$

Margin

$$\rho = \frac{|(b+1)-(b-1)|}{||w||} = \frac{2}{||w||}$$



Hint: what is the distance between x_a and $\mathbf{w^Tx + b = -1}$

SVM: Steps to understand SVM

1. Formulation of the Linear SVM problem: maximizing margin
2. Formulation of Quadratic Programming (optimization with linear constraints) → Primal problem
3. Solving linear SVM problem with “great” math*
   a. (Generalized) Lagrange function, lagrange multiplier
   b. Identify primal and dual problem (duality) → KKT conditions
   c. Solution to *w* and b regarding alpha
4. Support Vectors, SVM Classifier Inference
5. Non-linear SVM, Kernel tricks

SVM: Math Behind

- Slides: http://people.csail.mit.edu/dsontag/courses/ml13/slides/lecture6.pdf
- Notes: https://see.stanford.edu/materials/aimlcs229/cs229-notes3.pdf

**To show in hand notes*

Whiteboard for SVM Math Foundation

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Given labeled data and alpha values

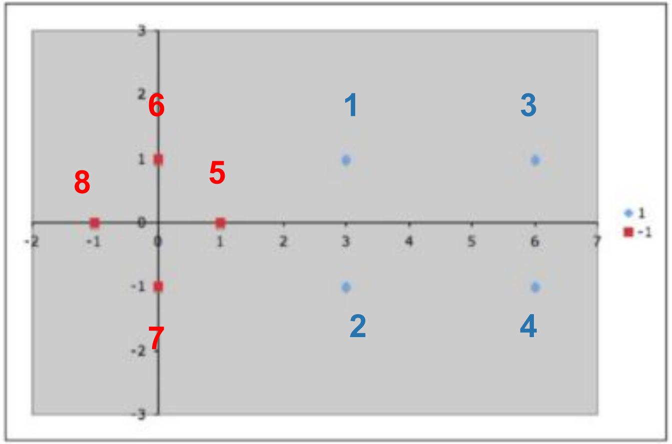
- Positively labeled data points (1 to 4)

$$\left\{\begin{pmatrix}3\\1\end{pmatrix},\begin{pmatrix}3\\-1\end{pmatrix},\begin{pmatrix}6\\1\end{pmatrix},\begin{pmatrix}6\\-1\end{pmatrix}\right\}$$

- Negatively labeled data points (5 to 8)

$$\left\{\begin{pmatrix}1\\0\end{pmatrix},\begin{pmatrix}0\\1\end{pmatrix},\begin{pmatrix}0\\-1\end{pmatrix},\begin{pmatrix}-1\\0\end{pmatrix}\right\}$$

- Alpha values
  - $\alpha_1 = \boxed{0.25}$
  - $\alpha_2 = \boxed{0.25}$
  - $\alpha_5 = \boxed{0.5}$
  - Others = 0

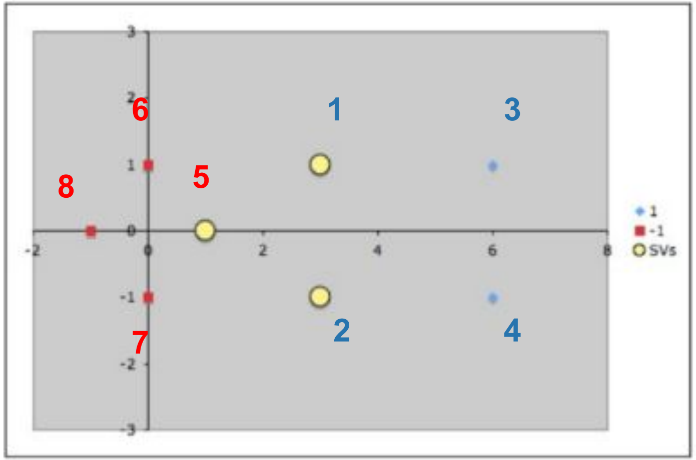


Linear SVM: Example for Practice

Questions

- Which points are support vectors?
- Calculate normal vector of hyperplane: $\boldsymbol{w}$
- Calculate the bias term
- What is the decision boundary?
- Predict class of new point (4, 1)

$$\boldsymbol{w} = \sum \alpha_i y_i \mathbf{x}_i \qquad b = \sum_{k:\alpha_k \neq 0} (y_k - \mathbf{w}^T \mathbf{x}_k)/N_k$$



Predictions for new data

$$y \leftarrow \text{sign}(\vec{w} \cdot \vec{x} + b)$$

Using dual solution

$$y \leftarrow \text{sign}\left[\sum_i \alpha_i y_i \underbrace{(\vec{x}_i \cdot \vec{x})}_{} + b\right]$$

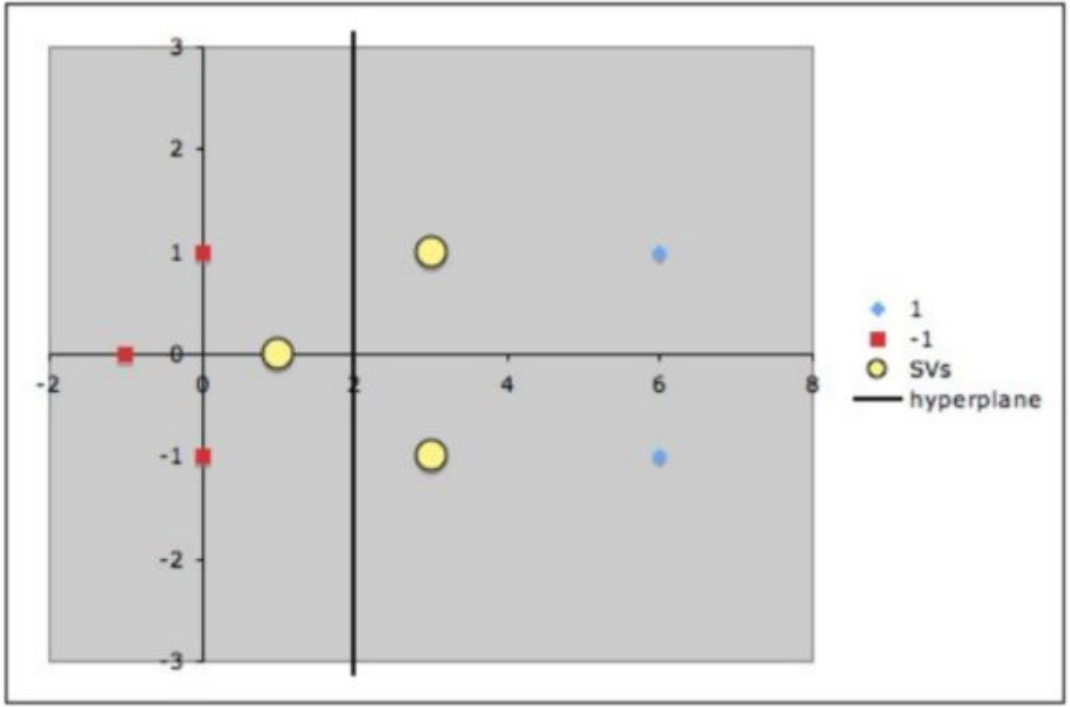
dot product of feature vectors of new example with support vectors

$$\mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i$$

$$b = y_k - \mathbf{w}.\mathbf{x}_k$$

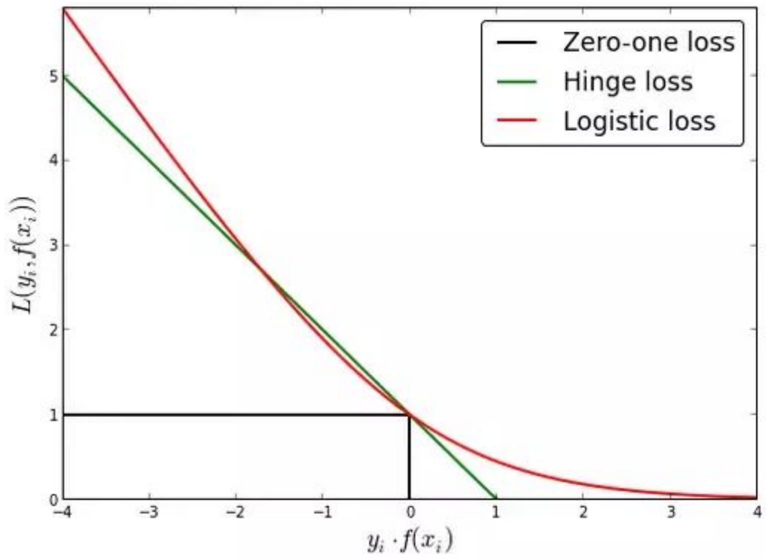
for any k where $C > \alpha_k > 0$

Plot



Linear SVM vs Logistic Regression

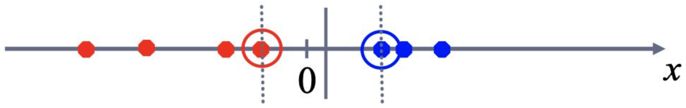
- Decision boundaries?
- Loss functions?



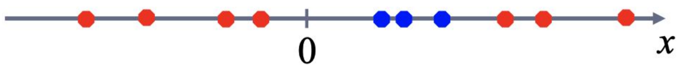
Reading: http://www.cs.toronto.edu/~kswersky/wp-content/uploads/svm_vs_lr.pdf

Non-linear SVM

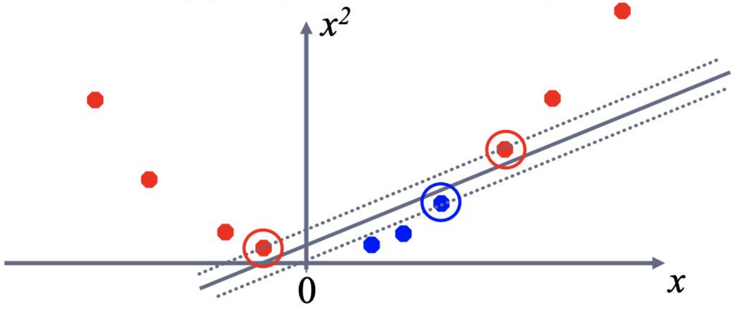
- Datasets that are linearly separable (with some noise) work out great:



- But what are we going to do if the dataset is just too hard?

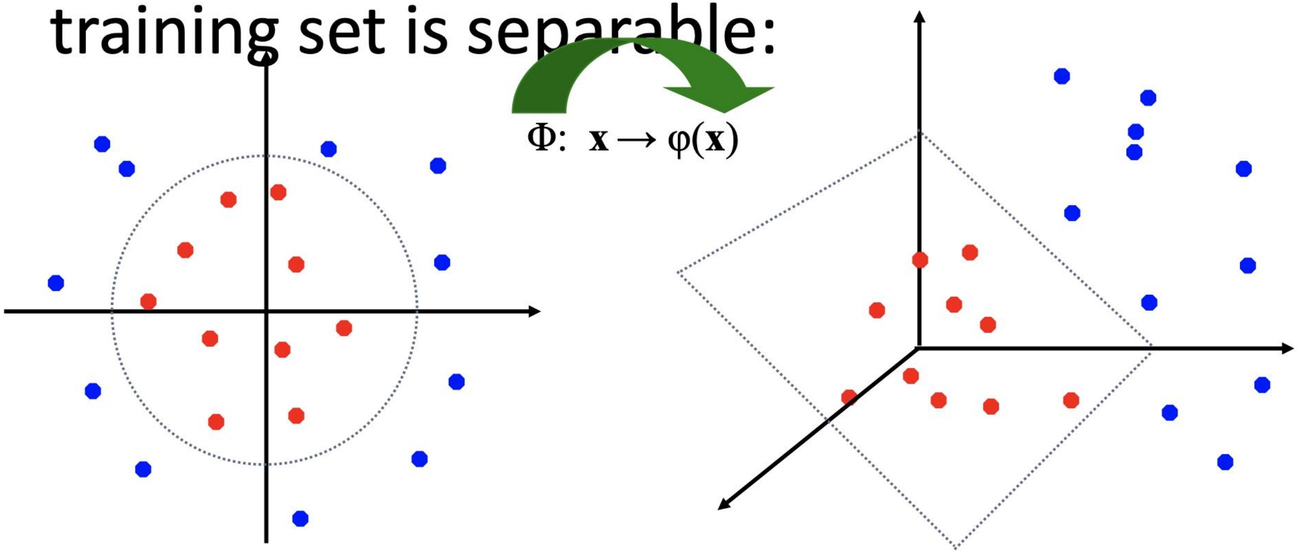


- How about … mapping data to a higher-dimensional space:

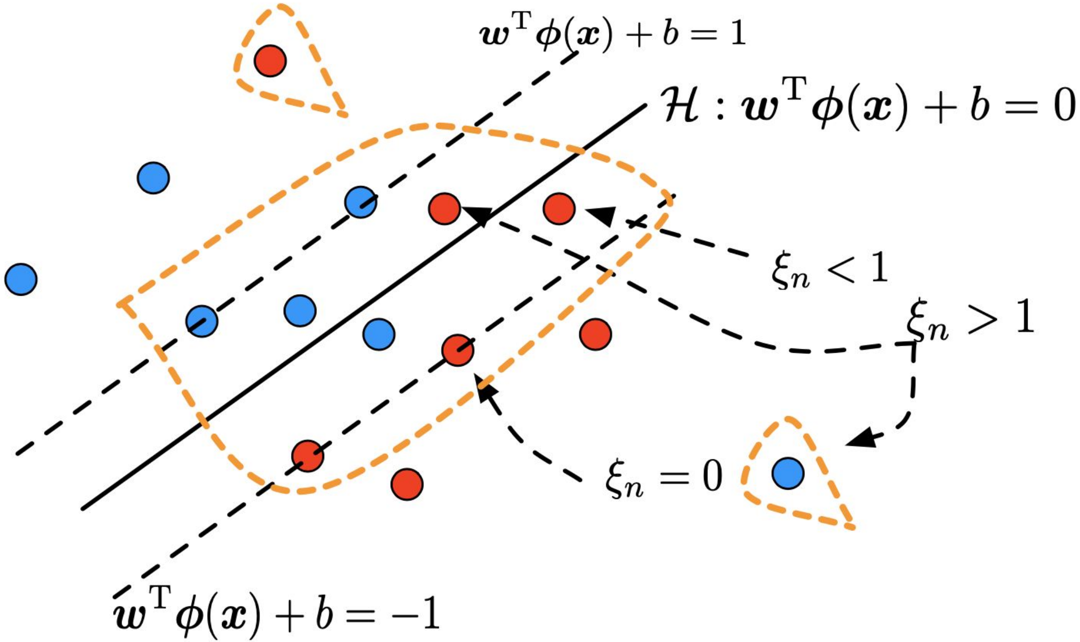


Non-linear SVM

- General idea: the original feature space can always be mapped to some higher-dimensional feature space where the training set is separable:



Support Vectors



SVM: Kernel

$$\text{maximize}_\alpha \quad \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \boxed{\mathbf{x}_i \mathbf{x}_j}$$

$$\sum_i \alpha_i y_i = 0$$

$$C \geq \alpha_i \geq 0$$

$$\text{maximize}_\alpha \quad \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \boxed{K(\mathbf{x}_i, \mathbf{x}_j)}$$

$$K(\mathbf{x}_i, \mathbf{x}_j) = \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j)$$

$$\sum_i \alpha_i y_i = 0$$

$$C \geq \alpha_i \geq 0$$

SVM: Kernel

- The linear SVM relies on an inner product between data vectors,

$$K(\mathbf{x_i}, \mathbf{x_j}) = \mathbf{x_i}^{\mathbf{T}} \mathbf{x_j}$$

- If every data point is mapped into high-dimensional space via transformation, the inner product becomes,

$$K(\mathbf{x_i}, \mathbf{x_j}) = \phi^T(\mathbf{x_i}) \cdot \phi(\mathbf{x_j})$$

- Do we need to compute ***ϕ(x)*** explicitly for each data sample? → **Directly compute kernel function *K(xi, xj)***

SVM: Kernel Function Example

$$
\begin{aligned}
k(\mathbf{x}, \mathbf{z}) &= (\mathbf{x}^T \mathbf{z} + c)^2 = \left(\sum_{j=1}^{n} x^{(j)} z^{(j)} + c \right) \left(\sum_{\ell=1}^{n} x^{(\ell)} z^{(\ell)} + c \right) \\
&= \sum_{j=1}^{n} \sum_{\ell=1}^{n} x^{(j)} x^{(\ell)} z^{(j)} z^{(\ell)} + 2c \sum_{j=1}^{n} x^{(j)} z^{(j)} + c^2 \\
&= \sum_{j,\ell=1}^{n} (x^{(j)} x^{(\ell)})(z^{(j)} z^{(\ell)}) + \sum_{j=1}^{n} (\sqrt{2c}\, x^{(j)})(\sqrt{2c}\, z^{(j)}) + c^2,
\end{aligned}
$$

Feature mapping given by:

$$
\mathbf{\Phi}(\mathbf{x}) = [x^{(1)2}, x^{(1)} x^{(2)}, ..., x^{(3)2}, \sqrt{2c}x^{(1)}, \sqrt{2c}x^{(2)}, \sqrt{2c}x^{(3)}, c]
$$

SVM: Kernel Function Example

$$\textbf{Polynomial kernel of degree } h: \quad K(\mathbf{X}_i, \mathbf{X}_j) = (\mathbf{X}_i \cdot \mathbf{X}_j + 1)^h$$

$$\textbf{Gaussian radial basis function kernel}: \quad K(\mathbf{X}_i, \mathbf{X}_j) = e^{-\|X_i - X_j\|^2/2\sigma^2}$$

$$\textbf{Sigmoid kernel}: \quad K(\mathbf{X}_i, \mathbf{X}_j) = \tanh(\kappa \mathbf{X}_i \cdot \mathbf{X}_j - \delta)$$

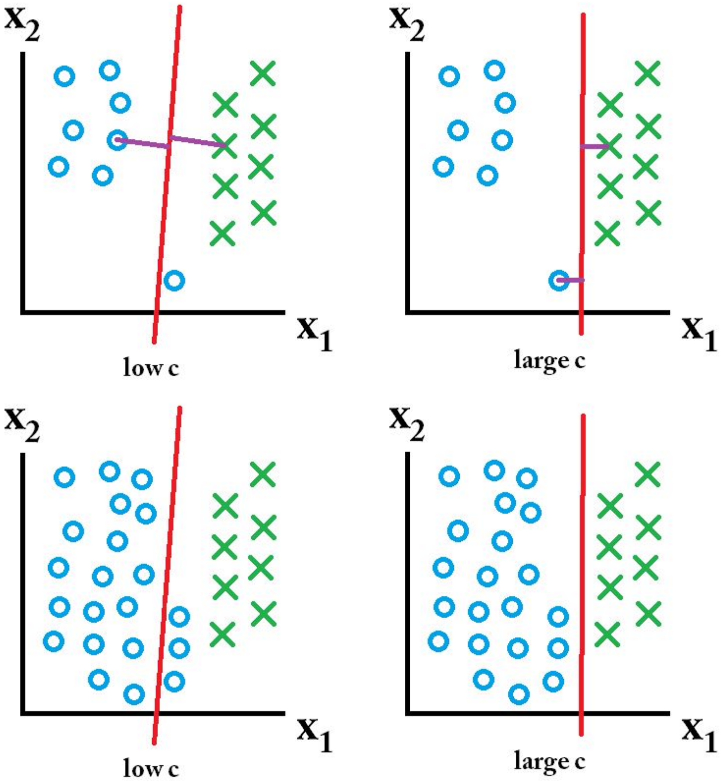
- Given the same data samples, what is the difference between linear kernel and non-linear kernel? Is the decision boundary linear (in original feature space)?

SVM: Overfitting

- Huge feature space with kernels: should we worry about overfitting?
  - SVM objective seeks a solution with large margin.
  - Theory says that large margin leads to good generalization.
  - But everything overfits sometimes.
  - Can control by:
    - Setting C
    - Choosing a better Kernel
    - Varying parameters of the Kernel (width of Gaussian, etc.)

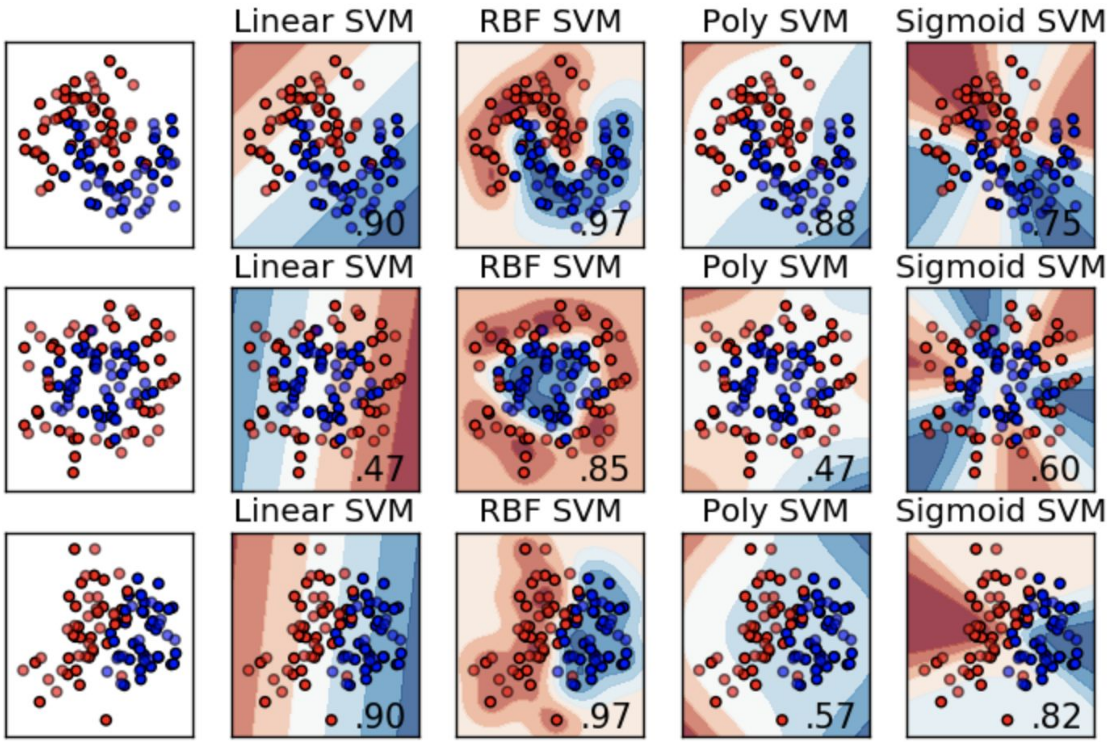
SVM: Understanding C

- The C parameter tells the SVM optimization how much you want to avoid misclassifying each training example.
- For large values of C, the optimization will choose **a smaller-margin hyperplane** if that hyperplane does a better job of getting all the training points classified correctly.
- Conversely, a very small value of C will cause the optimizer to look for **a larger-margin separating hyperplane**, even if that hyperplane misclassified more points.



Reference: https://stats.stackexchange.com/questions/31066/what-is-the-influence-of-c-in-svms-with-linear-kernel

SVM: Demo of different kernels



Non-linear SVM: Example Practice

- Positively labeled data points (1 to 4)

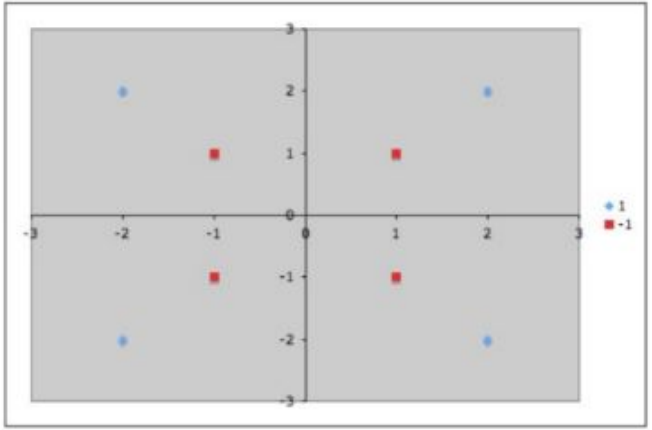
$$\left\{\begin{pmatrix}2\\2\end{pmatrix},\begin{pmatrix}2\\-2\end{pmatrix},\begin{pmatrix}-2\\-2\end{pmatrix},\begin{pmatrix}-2\\2\end{pmatrix}\right\}$$

- Negatively labeled data points (5 to 8)

$$\left\{\begin{pmatrix}1\\1\end{pmatrix},\begin{pmatrix}1\\-1\end{pmatrix},\begin{pmatrix}-1\\-1\end{pmatrix},\begin{pmatrix}-1\\1\end{pmatrix}\right\}$$

- Non-linear mapping

$$\Phi_1\begin{pmatrix}x_1\\x_2\end{pmatrix}=\begin{cases}\begin{pmatrix}4-x_2\\4-x_1\end{pmatrix} & \text{if } \sqrt{x_1^2+x_2^2}>2\\ \begin{pmatrix}x_1\\x_2\end{pmatrix} & \text{otherwise}\end{cases}$$



Non-linear SVM Example

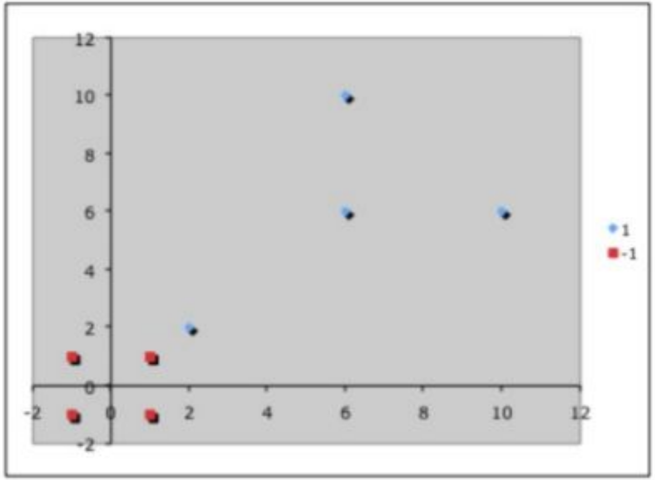
- New positively labeled data points (1 to 4)

$$\left\{\begin{pmatrix}2\\2\end{pmatrix},\begin{pmatrix}6\\2\end{pmatrix},\begin{pmatrix}6\\6\end{pmatrix},\begin{pmatrix}2\\6\end{pmatrix}\right\}$$

- New negatively labeled data points (5 to 8)

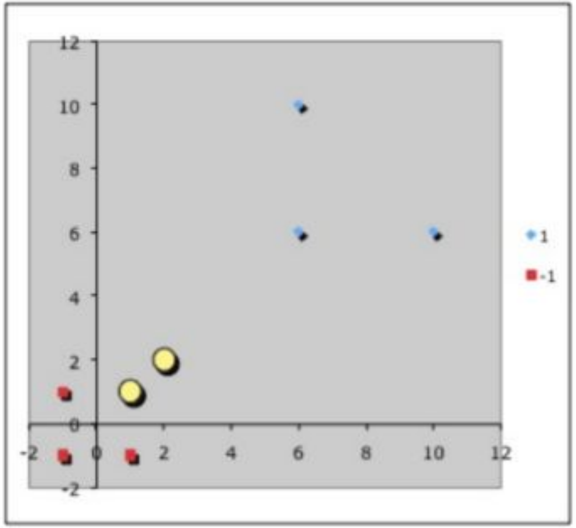
$$\left\{\begin{pmatrix}1\\1\end{pmatrix},\begin{pmatrix}1\\-1\end{pmatrix},\begin{pmatrix}-1\\-1\end{pmatrix},\begin{pmatrix}-1\\1\end{pmatrix}\right\}$$

- Alpha values
  - $\alpha_1 =$ 1.0
  - $\alpha_5 =$ 1.0
  - Others = 0

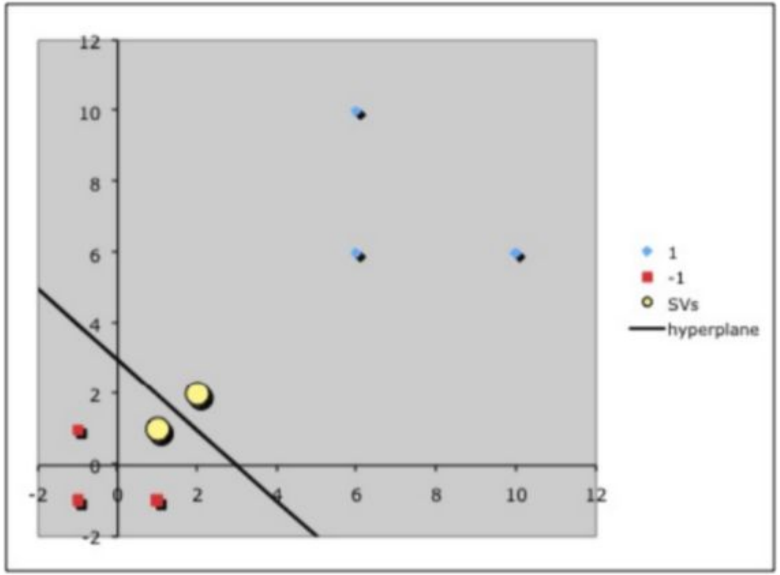


Non-linear SVM Example

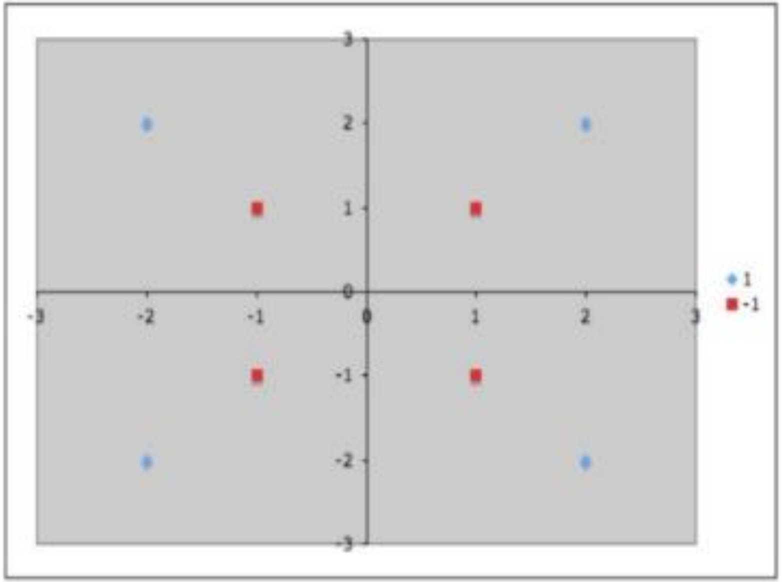
- Which points are support vectors?
- Calculate normal vector of hyperplane: $\boldsymbol{w}$
- Calculate the bias term
- What is the decision boundary?
- Predict class of new point (4, 5)



Plot



12
10
8
6
4
2
0
-2
-2
0
2
4
6
8
10
12
1
-1
SVs
hyperplane



3
2
1
0
-1
-2
-3
-3
-2
-1
0
1
2
3
1
-1

Non-linear SVM Solution

- Decision Boundary

$$y \leftarrow \text{sign}\left[\sum_i \alpha_i y_i K(x_i, x) + b\right]$$

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Thank you!

Q & A

SVM Dual Problem: How to optimize?

- The answer is Sequential Minimal Optimization (SMO) Algorithm.
- Basic idea: optimization problem of multiple variables is decomposed into a series of subproblems each optimizing an objective function of a small number of variables, typically only one, while all other variables are treated as constants that remain unchanged in the subproblem.
- Formulation:

$$
\begin{aligned}
\textbf{maximize:} \quad & L(\alpha_i, \alpha_j) = \alpha_i + \alpha_j - \frac{1}{2}\left(\alpha_i^2 \mathbf{x}_i^T \mathbf{x}_i + \alpha_j^2 \mathbf{x}_j^T \mathbf{x}_j + 2\alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j\right) \\
& -\alpha_i y_i \left(\sum_{n \neq i} \alpha_n y_n \mathbf{x}_n^T\right) \mathbf{x}_i - \alpha_j y_j \left(\sum_{n \neq j} \alpha_n y_n \mathbf{x}_n^T\right) \mathbf{x}_j \\
& = \alpha_i + \alpha_j - \frac{1}{2}\left(\alpha_1^2 K_{ii} + \alpha_2^2 K_{jj} + 2\alpha_i \alpha_j y_i y_j K_{ij}\right) \\
& -\alpha_i y_i \sum_{n \neq i,j} \alpha_n y_n K_{ni} - \alpha_j y_j \sum_{n \neq i,,j} \alpha_n y_n K_{nj} \\
\textbf{subject to:} \quad & 0 \leq \alpha_i, \alpha_j \leq C, \qquad \sum_{n=1}^{N} \alpha_n y_n = 0
\end{aligned}
$$

Whiteboard

- Content