Universität Konstanz

Lecture 4 Support Vector Machine (SVM) – Part 1

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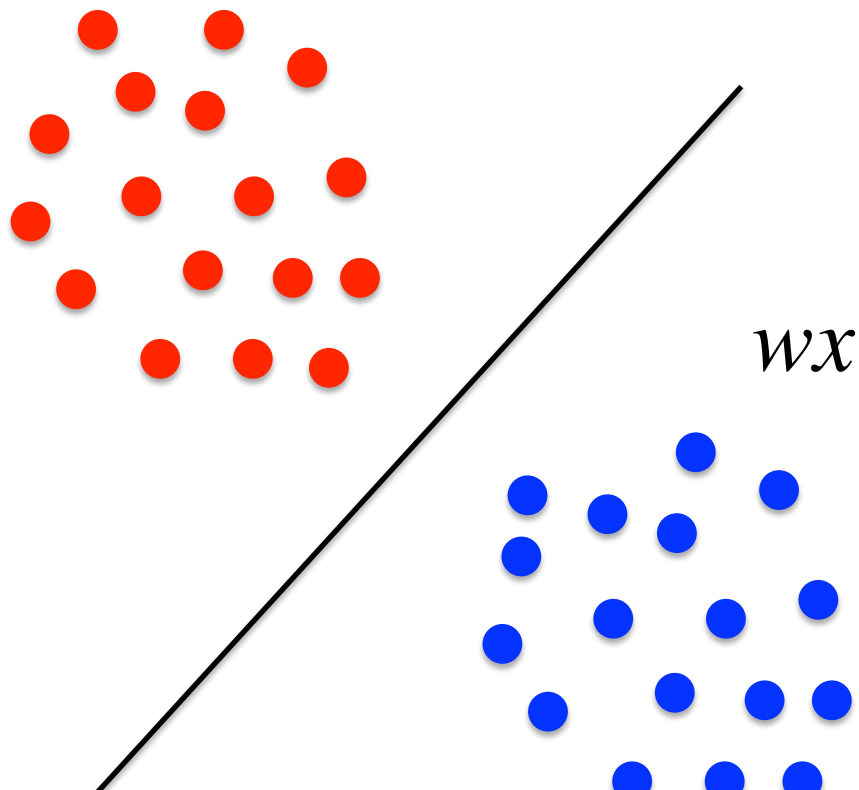
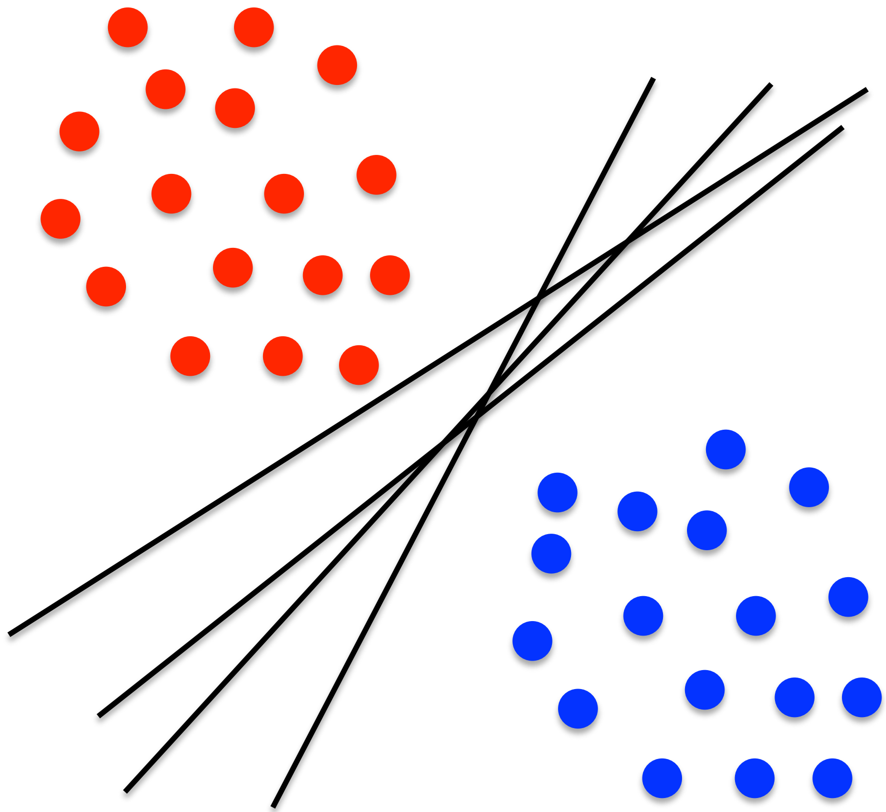
Intuition – binary classification

$$f(x) = \mathrm{sgn}(wx + b)$$

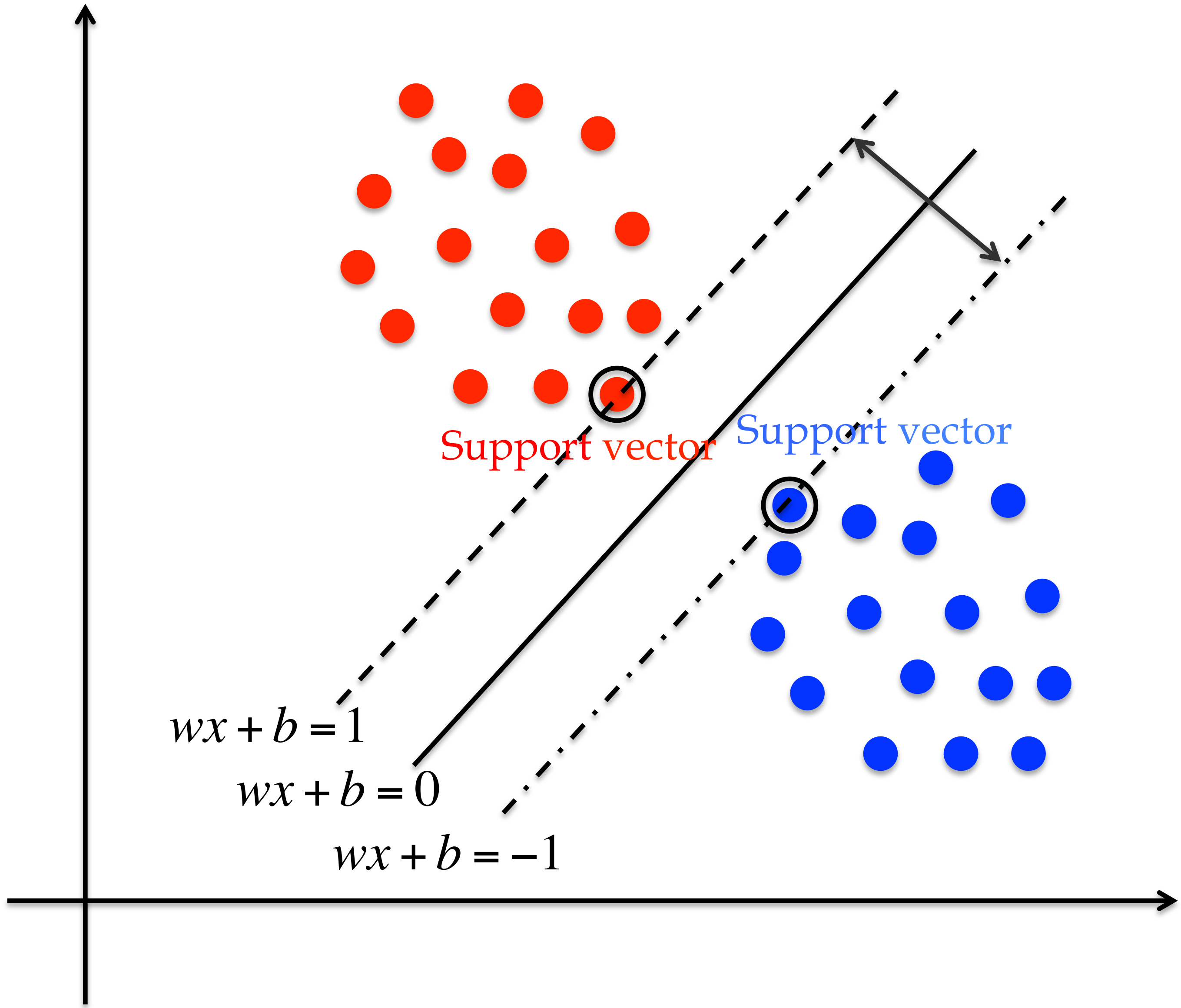


Intuition – binary classification

Which of the linear classifier is optimal?



Intuition – binary classification



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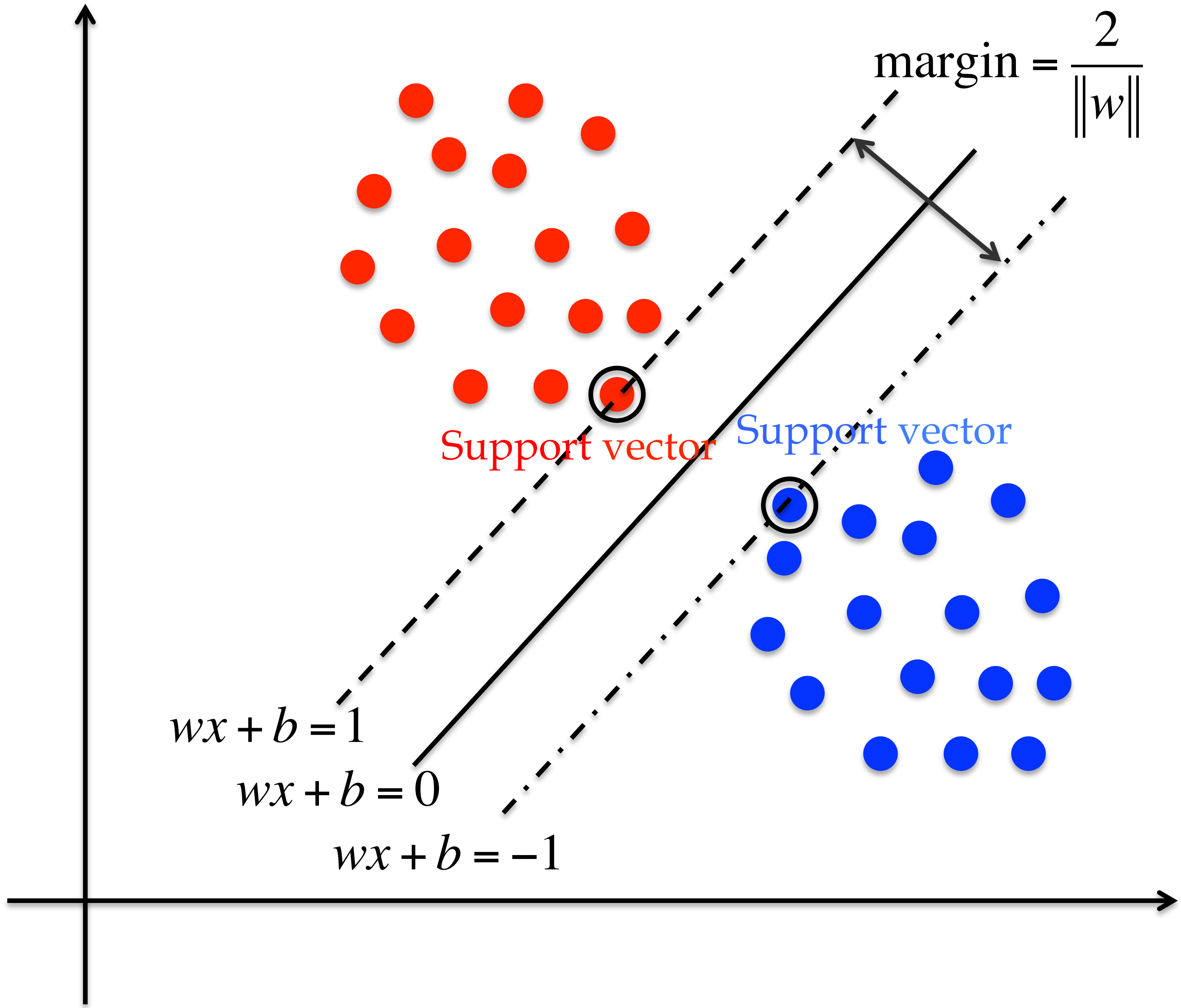
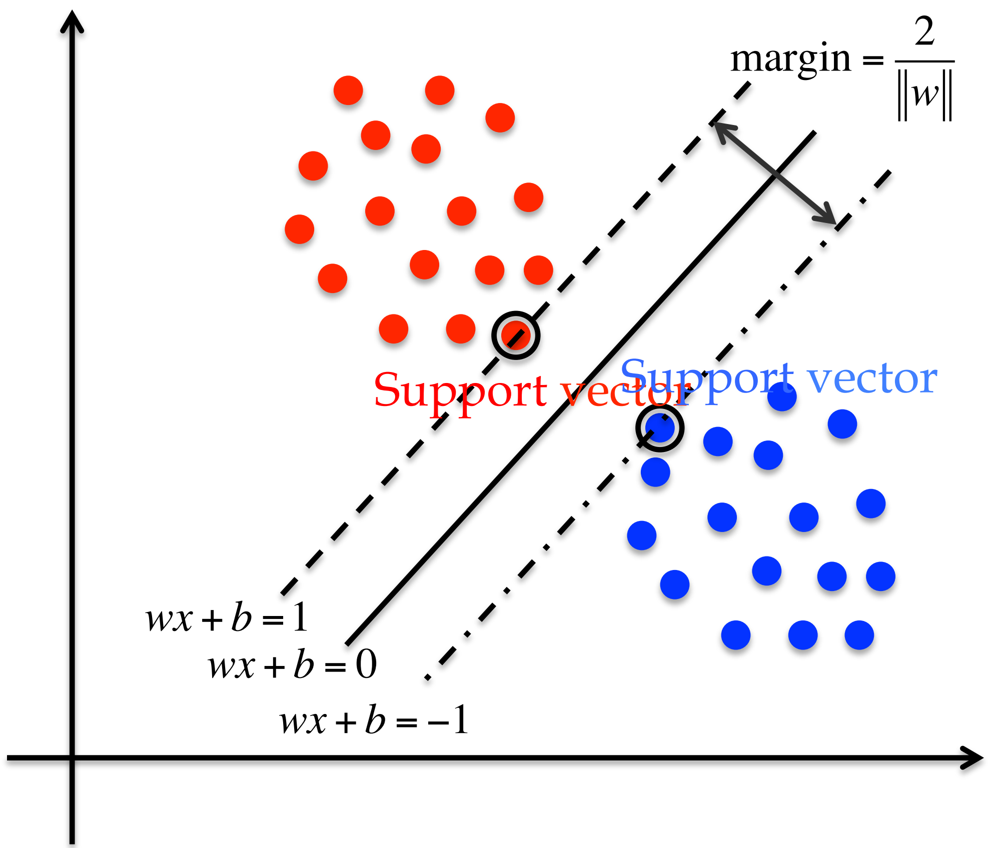


Maximum margin classifier

- Maximizing the margin is good according to tuition and Probably Approximately Correct learning (PAC) theory
- Implies that only support vectors are important; while other training examples are ignorable



“Hard” margin

- The maximum margin can be optimized as:

$$\max_{w,b} \frac{2}{\|w\|}$$

$$\text{s.t. } wx^{(i)} + b \begin{cases} \geq 1 \text{ if } y^{(i)} = 1 \\ \leq -1 \text{ if } y^{(i)} = -1 \end{cases}$$

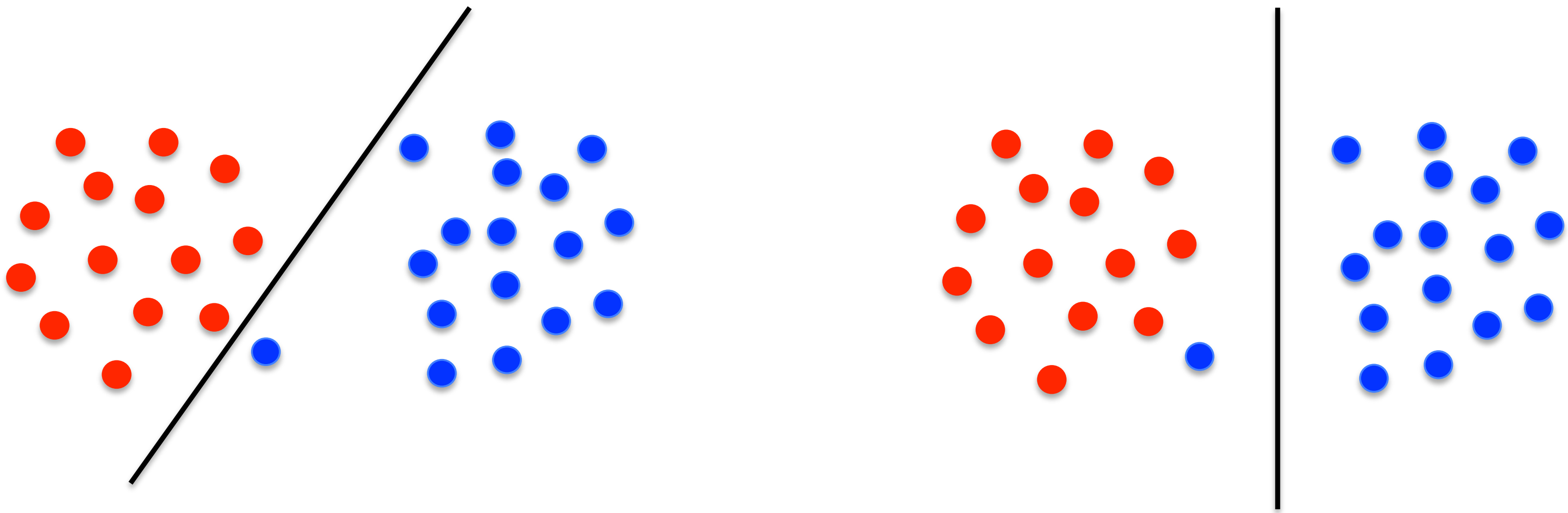
- Or equivalently:

$$\min_{w,b} \frac{1}{2} \|w\|^2$$

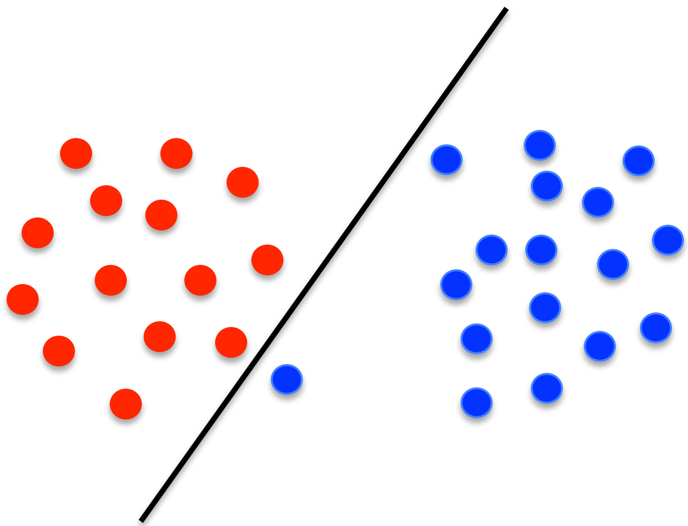
$$\text{s.t. } y^{(i)}(wx^{(i)} + b) \geq 1$$

- This is a quadratic optimization problem subject to linear constraints and there is a unique minimum

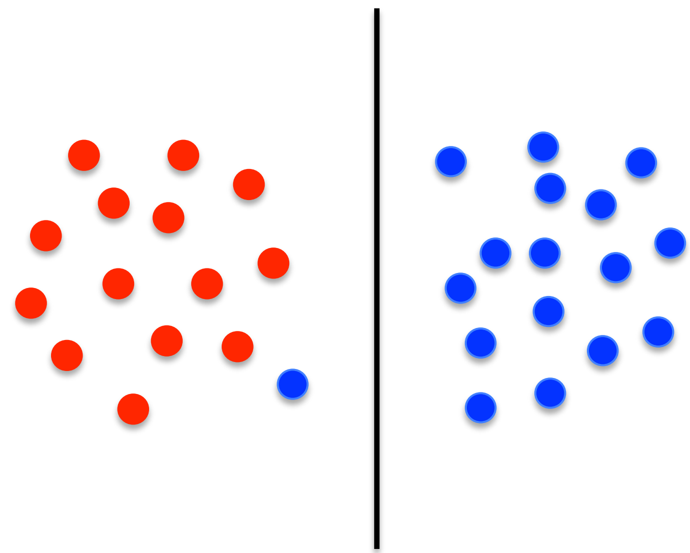
Which classifier is better?



Which classifier is better?

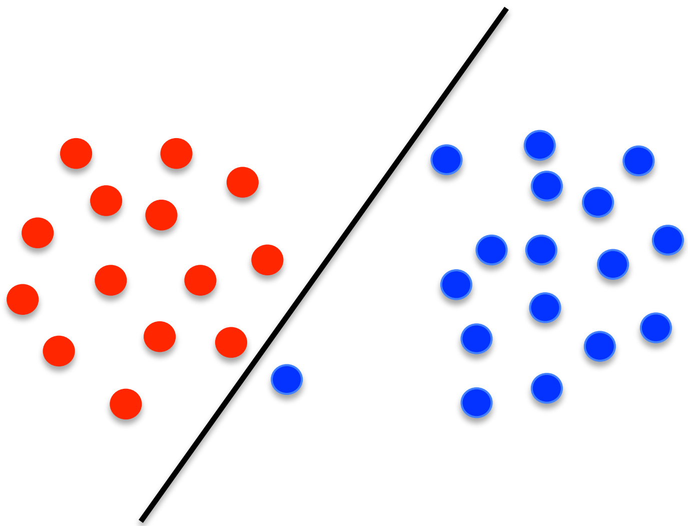


The points can be linearly separated but there is a very narrow margin



The large margin solution is better, even though one constraint is violated

Which classifier is better?



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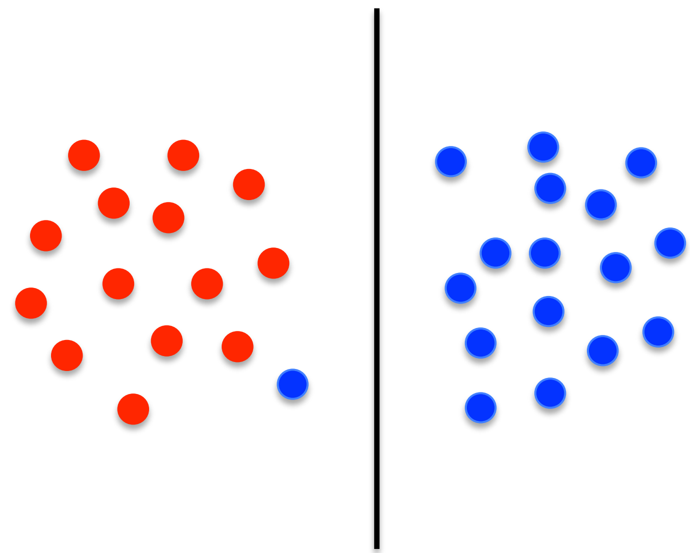


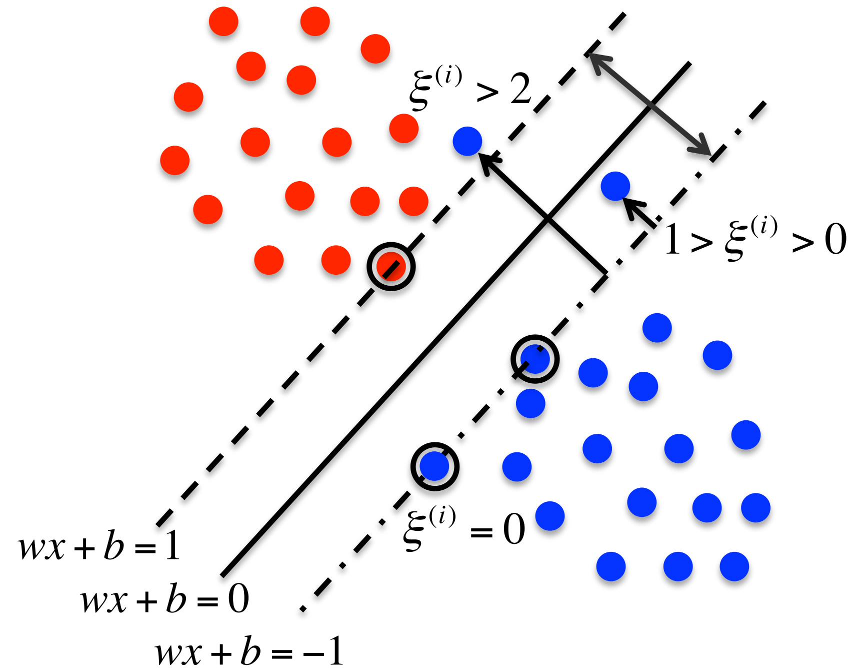
The large margin solution is better, even though one constraint is violated

Tradeoff between the margin and the number of mistakes in the training data

Introduce "slack" variables

$\xi^{(i)} \geq 0$

- For $1 > \xi^{(i)} > 0$ point is between margin and correct side of hyperplane. This is margin violation
- For $\xi^{(i)} > 1$ point is misclassified



“Soft” margin solution

The optimization problem becomes:

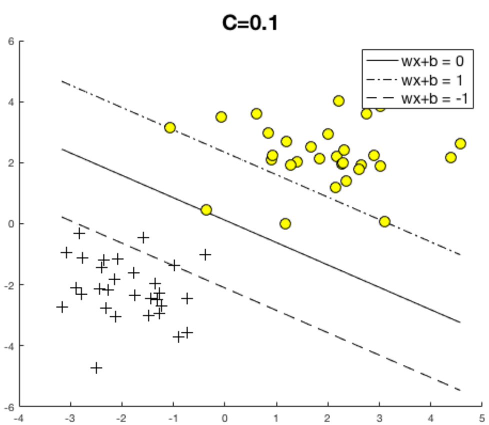
$$\min_{w,b} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m}\xi^{(i)}$$

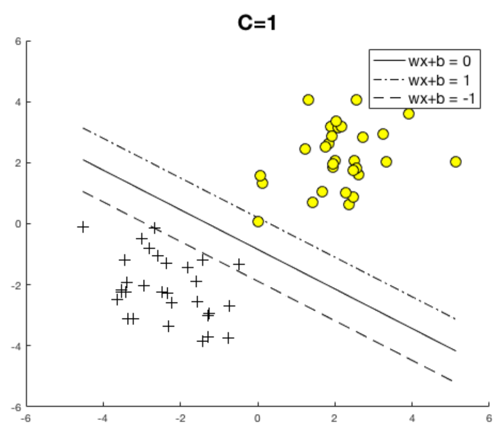
$$\text{s.t. } y^{(i)}(wx^{(i)} + b) \geq 1 - \xi^{(i)}, \xi^{(i)} \geq 0 \quad \forall i = 1,\ldots,m$$

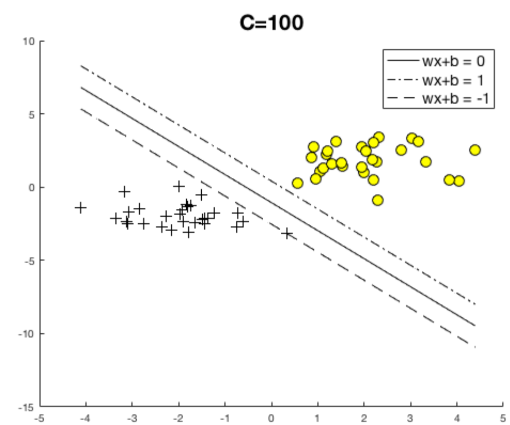
- Every constraint can be satisfied if $\xi^{(i)}$ is sufficiently large
- C is a regularization parameter:
  - Small C ➡ large margin
  - Large C ➡ narrow margin
  - C = ∞ ➡ hard margin
- It is called primal form of SVM

Still a quadratic optimization problem and there is a unique minimum

Example: different regularization







Soft margin

Hard margin

Primal form

The optimization problem becomes:

$$\min_{w,b} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m}\xi^{(i)}$$

$$\text{s.t. } y^{(i)}(wx^{(i)} + b) \geq 1 - \xi^{(i)}, \xi^{(i)} \geq 0 \quad \forall i = 1,\ldots,m$$

Can solve it more efficiently by taking the Lagrangian dual

- Duality is a common idea in optimization
- It transforms a difficult optimization problem into a simpler one
- Make SVM superior to logistic regression with kernel method

Optimization: Lagrange multiplier

- By introducing Lagrange multipliers $\alpha^{(i)}, \beta^{(i)} \geq 0$, the corresponding Lagrangian is formulated as:

$$L = \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m}\xi^{(i)} - \sum_{i=1}^{m}\alpha^{(i)}(y^{(i)}(wx^{(i)}+b)-1+\xi^{(i)}) - \sum_{i=1}^{m}\beta^{(i)}\xi^{(i)}$$

- To minimize it, its derivatives w.r.t to the variables are set to zeros:

$$\frac{\partial L}{\partial w} = w - \sum_{i=1}^{m}\alpha^{(i)}y^{(i)}x^{(i)} = 0 \Rightarrow w = \sum_{i=1}^{m}\alpha^{(i)}y^{(i)}x^{(i)}$$

$$\frac{\partial L}{\partial b} = \sum_{i=1}^{m}\alpha^{(i)}y^{(i)} = 0$$

$$\frac{\partial L}{\partial \xi^{(i)}} = C - \alpha^{(i)} - \beta^{(i)} = 0 \qquad C \geq \alpha^{(i)} \geq 0$$

Dual form

- Solve by a bunch of algebra and calculus, the dual form of SVM is:

$$\min_{\alpha} \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} x^{(i)} x^{(j)} - \sum_{i=1}^{m} \alpha^{(i)}$$

$$\text{s.t. } 0 \le \alpha^{(i)} \le C, \sum_{i=1}^{m} \alpha^{(i)} y^{(i)} = 0 \;\; \forall i = 1, \ldots, m$$

- The decision can also be rewritten as:

$$w = \sum_{i=1}^{m} \alpha^{(i)} y^{(i)} x^{(i)}$$

$$f(x) = wx + b \Rightarrow f(x) = \sum_{i=1}^{m} \alpha^{(i)} y^{(i)} x^{(i)} x + b$$

Understanding the dual

- Solve by a bunch of algebra and calculus, the dual form of SVM is:

$$\min_{\alpha} \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m}\alpha^{(i)}\alpha^{(j)}y^{(i)}y^{(j)}x^{(i)}x^{(j)} - \sum_{i=1}^{m}\alpha^{(i)}$$

$$\text{s.t.}\ \boxed{0 \le \alpha^{(i)} \le C}, \boxed{\sum_{i=1}^{m}\alpha^{(i)}y^{(i)} = 0}\ \forall i = 1,\ldots,m$$

Constraint weights between 0 and C

Balances between the weight of constraints for different classes

Understanding the dual

- Solve by a bunch of algebra and calculus, the dual form of SVM is:

$$\min_{\alpha} \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha^{(i)} \alpha^{(j)} \boxed{y^{(i)} y^{(j)}} \boxed{x^{(i)} x^{(j)}} - \sum_{i=1}^{m} \alpha^{(i)}$$

$$\text{s.t. } 0 \leq \alpha^{(i)} \leq C, \quad \sum_{i=1}^{m} \alpha^{(i)} y^{(i)} = 0 \quad \forall i = 1, \ldots, m$$

Points with different labels decrease the sum
Points with same labels increase the sum

Measures the similarity between points

Understanding the dual

- Solve by a bunch of algebra and calculus, the dual form of SVM is:

$$\min_{\alpha} \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m}\alpha^{(i)}\alpha^{(j)}y^{(i)}y^{(j)}x^{(i)}x^{(j)} - \sum_{i=1}^{m}\alpha^{(i)}$$

$$\text{s.t. } 0 \le \alpha^{(i)} \le C, \sum_{i=1}^{m}\alpha^{(i)}y^{(i)} = 0 \;\; \forall i = 1,\ldots,m$$

$C \ge \alpha^{(i)} > 0$ point is a support vector

$\alpha^{(i)} = 0$ point is not a support vector

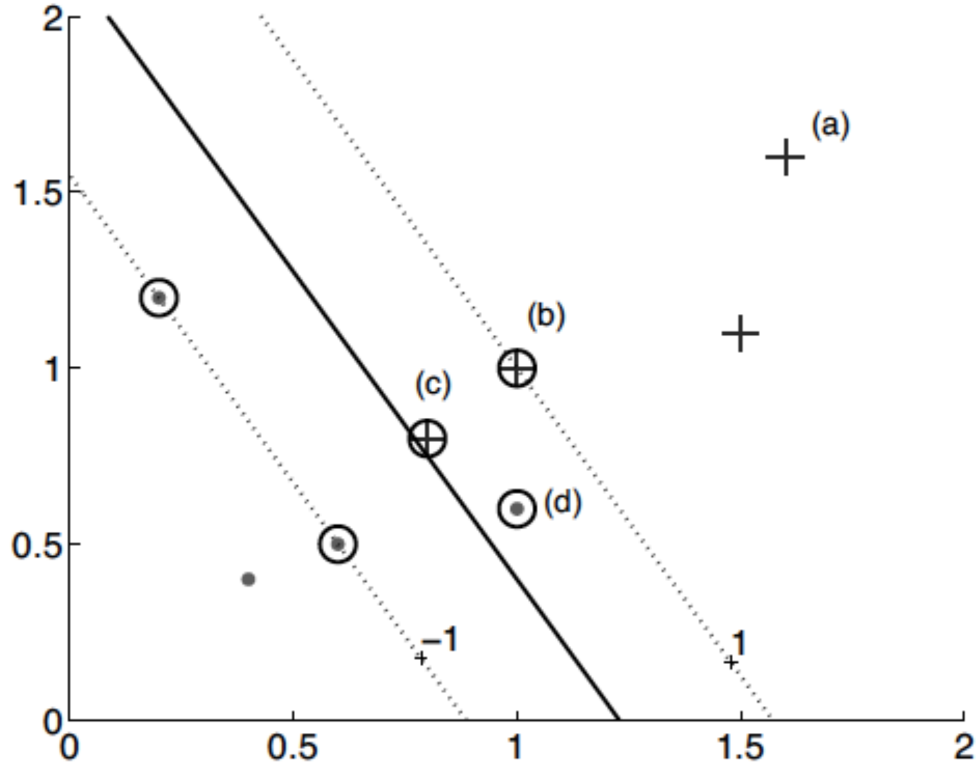
Q: support vectors

$\alpha^{(a)} = ?$

$\alpha^{(b)} = ?$

$\alpha^{(c)} = ?$

$\alpha^{(d)} = ?$



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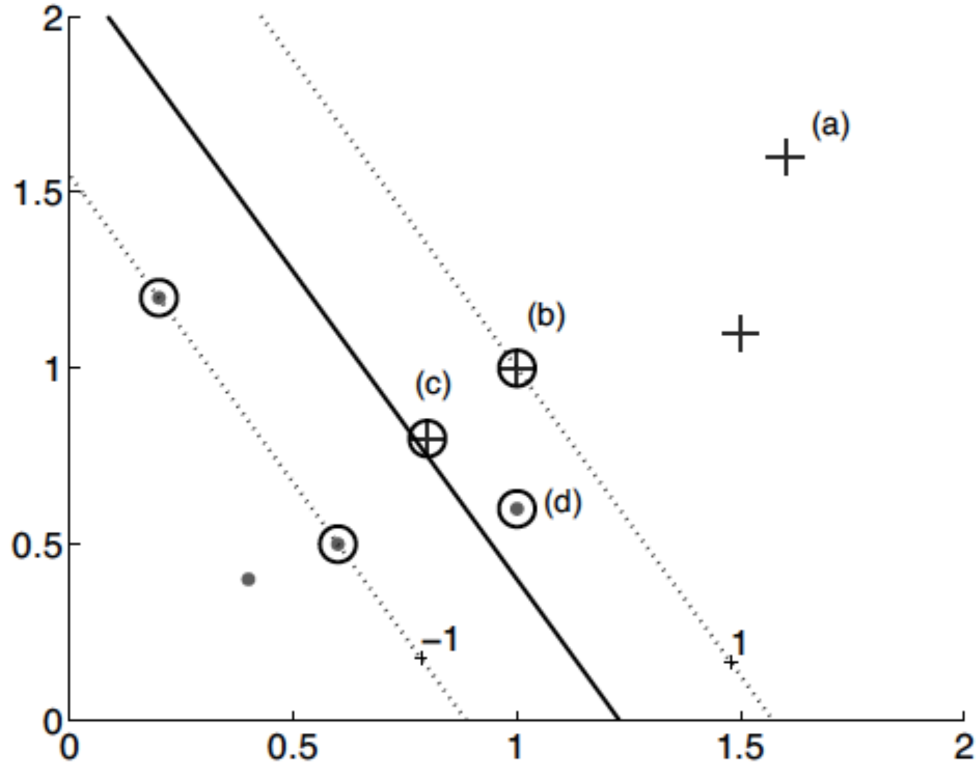


$\alpha^{(a)} = 0$

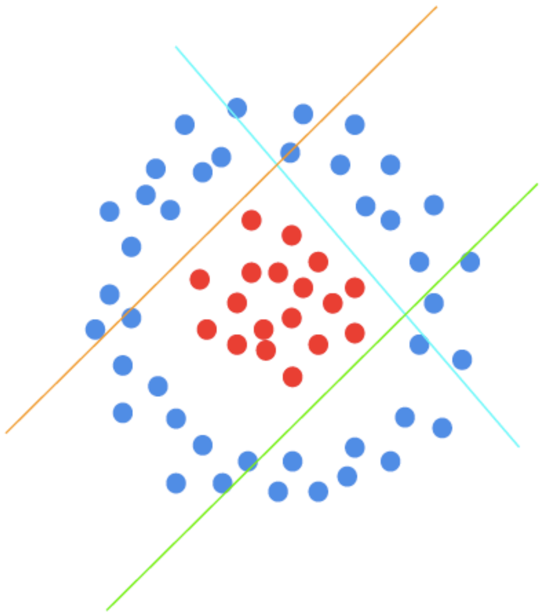
$C > \alpha^{(b)} > 0$

$\alpha^{(c)}, \alpha^{(d)} = C$

Prediction is very fast as most α are zeros

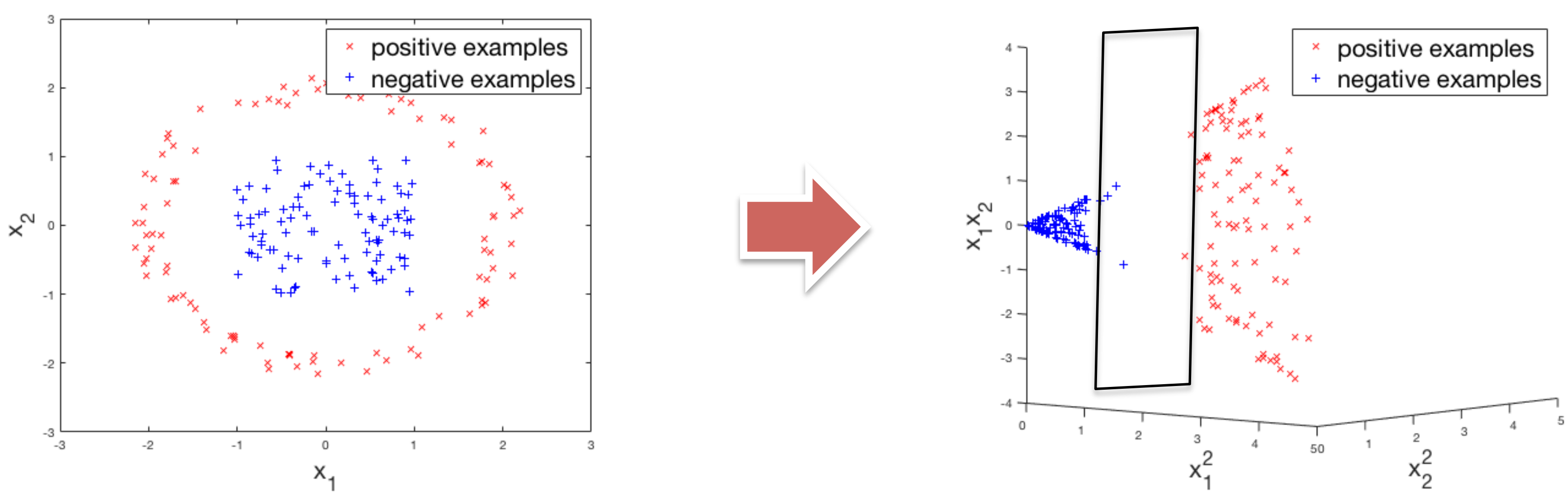
What if the data is not linearly separable?

- What's the advantage of SVM over logistic regression?
- In logistic regression, we add more parameters to make the decision boundary nonlinearly
- Expensive to compute and store when parameters are very large



Mapping data into a higher dimensional feature space

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} x_1^2 \\ x_2^2 \\ x_1 x_2 \end{pmatrix}$$



Feature map

- By mapping data from n-dimensional to N-dimensional space (n<N), we can still learn a linear classifier
- Feature map: $\Phi : x \rightarrow \Phi(x)$
- What if $\Phi(x)$ is really big?

Feature map

- By mapping data from n-dimensional to N-dimensional space (n<N), we can still learn a linear classifier
- Feature map: $\Phi : x \rightarrow \Phi(x)$
- What if $\Phi(x)$ is really big?

  A: use kernels to compute it implicitly

Kernel method: motivation

- Inefficient features:
  - Non-linearly separable data requires high dimensional representation
  - Might prohibitively expensive to compute or store

Kernel representation

- Kernel computing:

$$k(x^{(i)}, x^{(j)}) = \Phi(x^{(i)})\Phi(x^{(j)})$$

- Computing kernel should be efficient, much more than computing feature maps separately

Transformed feature in primal form

Classifier: $f(x) = w\Phi(x) + b$

Optimization:

$$\min_{w,b} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m} \xi^{(i)}$$

$$\text{s.t. } y^{(i)}(w\Phi(x^{(i)}) + b) \geq 1 - \xi^{(i)}, \xi^{(i)} \geq 0 \quad \forall i = 1, \ldots, m$$

- Simply map x to $\Phi(x)$ where data is separable
- Solve for w in high dimensional feature space
- Still troublesome when $\Phi(x)$ is very large

Transformed feature in dual form

Classifier: $f(x) = \sum_{i=1}^{m} \alpha^{(i)} y^{(i)} \Phi(x^{(i)}) \Phi(x) + b$

Optimization:

$$\min_{\alpha} \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} \Phi(x^{(i)}) \Phi(x^{(j)}) - \sum_{i=1}^{m} \alpha^{(i)}$$

$$\text{s.t. } 0 \le \alpha^{(i)} \le C, \sum_{i=1}^{m} \alpha^{(i)} y^{(i)} = 0 \;\; \forall i = 1, \ldots, m$$

- In dual form, $\Phi(x)$ only occurs in pairs
- Only the m dimensional vector $\alpha^{(i)}$ needs to be learnt

Kernel SVM in dual form

Classifier:

$$f(x) = \sum_{i=1}^{m} \alpha^{(i)} y^{(i)} k(x^{(i)}, x) + b$$

Optimization:

$$\min_{\alpha} \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} k(x^{(i)}, x^{(j)}) - \sum_{i=1}^{m} \alpha^{(i)}$$

$$\text{s.t. } 0 \le \alpha^{(i)} \le C, \sum_{i=1}^{m} \alpha^{(i)} y^{(i)} = 0 \ \ \forall i = 1, \ldots, m$$

Solve by quadratic programming!

The kernel trick

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{pmatrix}$$

$$\Phi(x)\Phi(z) = \begin{pmatrix} x_1^2 & x_2^2 & \sqrt{2}x_1x_2 \end{pmatrix} \begin{pmatrix} z_1^2 \\ z_2^2 \\ \sqrt{2}z_1z_2 \end{pmatrix} = (x_1z_1 + x_2z_2)^2 = (xz)^2$$

- Classifier can be learnt and applied without explicitly computing
- All that is required to compute the kernel function $k(x^{(i)}, x^{(j)})$
- Complexity of learning depends on number of training examples m rather than the dimensions of feature space N.

The kernel trick

- "Given an algorithm which is formulated in terms of a positive definite kernel K_1, one can construct an alternative algorithm by replacing K_1 with another positive kernel K_2"

Common kernels

- Linear kernel: $k(x^{(i)}, x^{(j)}) = x^{(i)} x^{(j)}$
- Polynomial kernel:

$$k(x^{(i)}, x^{(j)}) = (1 + x^{(i)} x^{(j)})^d$$

Contains all polynomials terms up to degree d

- Gaussian kernel: $k(x^{(i)}, x^{(j)}) = \exp\left(-\frac{\left\| x^{(i)} - x^{(j)} \right\|^2}{2\sigma^2}\right)$

Infinite dimensional feature space

- Many more…
  - Cosine similarity kernel
  - Chi-squared kernel
  - String/tree/graph kernel

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Infinite dimensional feature space

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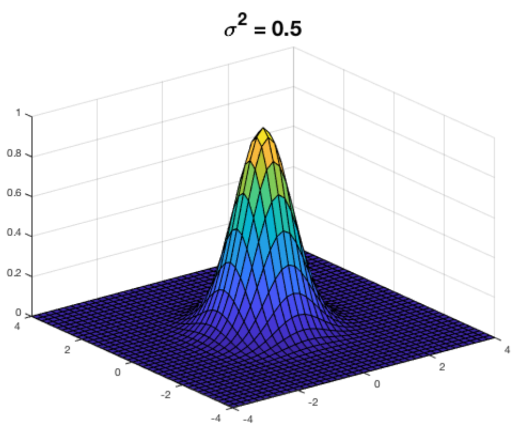
Q: how many hyper-parameters do you need to tune?

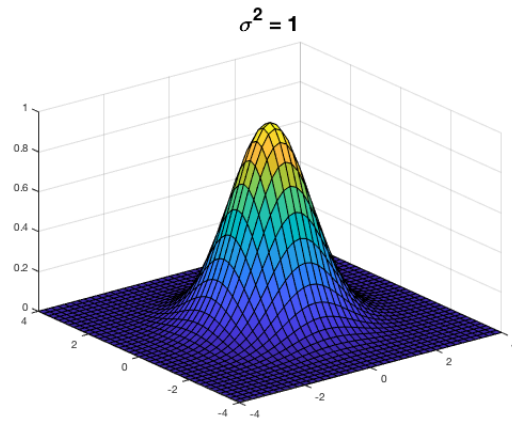
Gaussian kernel

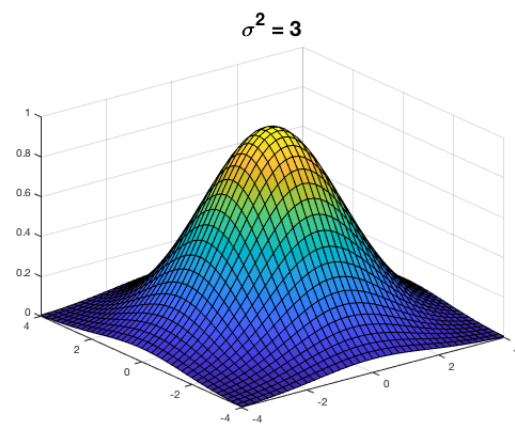
- Also called Radial Basis Function (RBF) kernel

$$k(x^{(i)}, x^{(j)}) = \exp\left(-\frac{\left\|x^{(i)} - x^{(j)}\right\|^2}{2\sigma^2}\right)$$

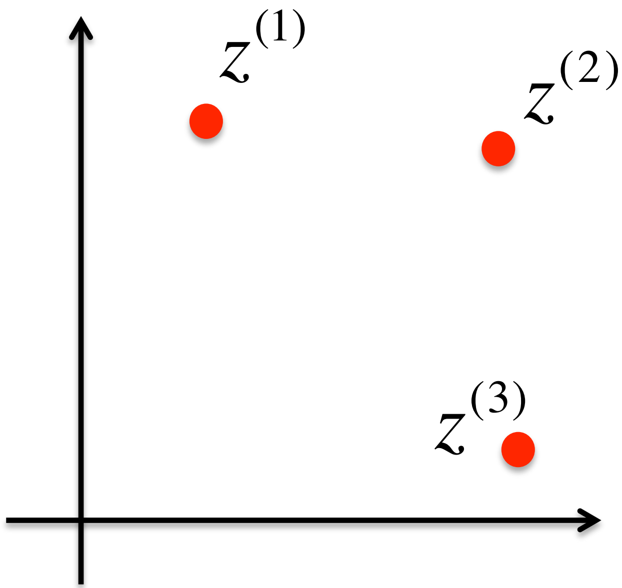
  - Has value 1 when $x^{(i)} = x^{(j)}$
  - Value falls off to 0 with increasing distance
  - Note: need to do feature normalization before using Gaussian kernel, why?







Gaussian kernel example



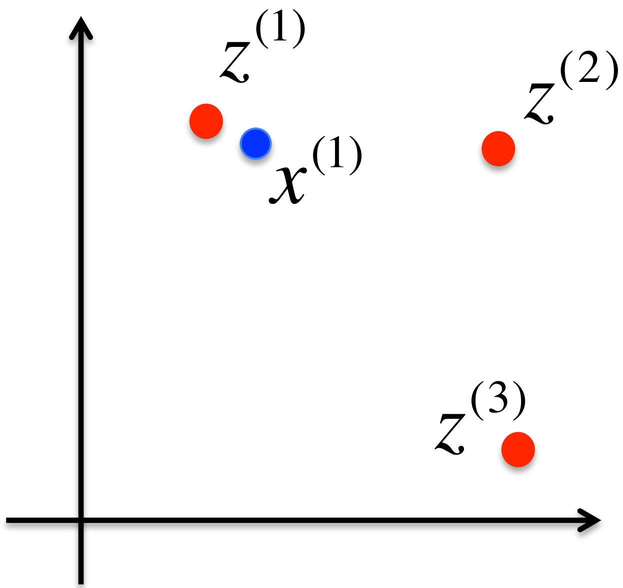
$$k(x^{(i)}, x^{(j)}) = \exp\left(-\frac{\left\|x^{(i)} - x^{(j)}\right\|^2}{2\sigma^2}\right)$$

Imagine we've learned that:

$$\alpha = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \quad b = -0.5$$

Predict $+1$ if $\alpha_1 k(x, z^{(1)}) + \alpha_2 k(x, z^{(2)}) + \alpha_3 k(x, z^{(3)}) + b \geq 0$

Gaussian kernel example



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Imagine we've learned that:

$$\alpha = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \quad b = -0.5$$

Predict $+1$ if $\alpha_1 k(x, z^{(1)}) + \alpha_2 k(x, z^{(2)}) + \alpha_3 k(x, z^{(3)}) + b \geq 0$

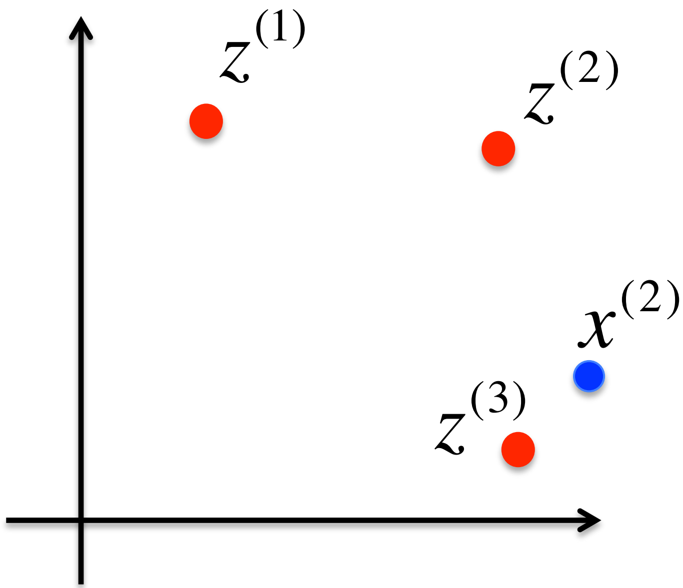
For $x^{(1)}$, we have $k(x^{(1)}, z^{(1)}) \approx 1,\ k(x^{(1)}, z^{(2)}) \approx 0,\ k(x^{(1)}, z^{(3)}) \approx 0$

$\alpha_1(1) + \alpha_2(0) + \alpha_3(0) + b$

$= 1(1) + 1(0) + 0(0) - 0.5$

$= 0.5,$ so predict $+1$

Gaussian kernel example



$$k(x^{(i)}, x^{(j)}) = \exp\left(-\frac{\left\| x^{(i)} - x^{(j)} \right\|^2}{2\sigma^2}\right)$$

Imagine we've learned that:

$$\alpha = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \quad b = -0.5$$

Predict $+1$ if $\alpha_1 k(x, z^{(1)}) + \alpha_2 k(x, z^{(2)}) + \alpha_3 k(x, z^{(3)}) + b \geq 0$

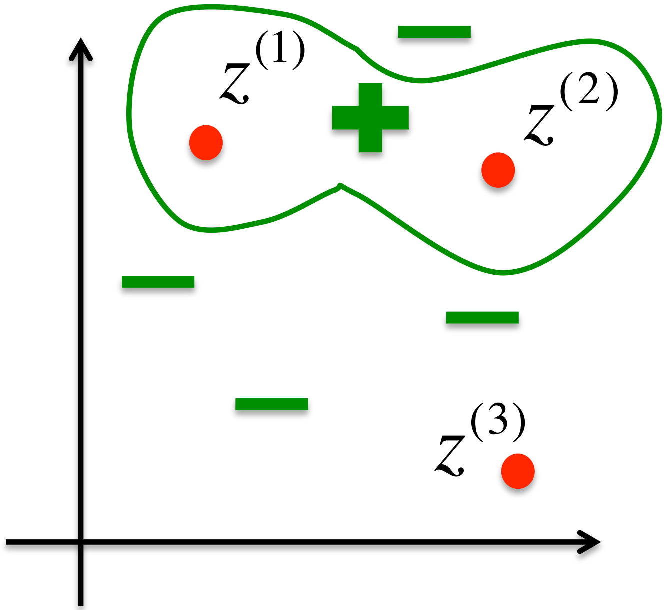
For $x^{(2)}$, we have $k(x^{(1)}, z^{(1)}) \approx 0,\ k(x^{(1)}, z^{(2)}) \approx 0,\ k(x^{(1)}, z^{(3)}) \approx 1$

$\alpha_1(0) + \alpha_2(0) + \alpha_3(1) + b$

$= 1(0) + 1(0) + 0(1) - 0.5$

$= -0.5$, so predict -1

Gaussian kernel example



$$k(x^{(i)}, x^{(j)}) = \exp\left(-\frac{\left\| x^{(i)} - x^{(j)} \right\|^2}{2\sigma^2}\right)$$

Imagine we've learned that:

$$\alpha = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \quad b = -0.5$$

Predict $+1$ if $\alpha_1 k(x, z^{(1)}) + \alpha_2 k(x, z^{(2)}) + \alpha_3 k(x, z^{(3)}) + b \geq 0$

Rough sketch of decision boundary

Summary: Kernel methods

- Key idea:
  - Rewrite the algorithm so that we only work with dot products $x^{(i)}x^{(j)}$ of feature vectors
  - Replace the dot products $x^{(i)}x^{(j)}$ with a kernel function $k(x^{(i)}, x^{(j)})$
- Different kernel functions may be applied to different scenarios
- This “kernel trick” can be applied to many algorithms:
  - Kernel PCA
  - Kernel k-means
- Cons: the optimal parameters and kernel function have to be chosen empirically

SVM vs. Logistic regression

- Given training examples $(x^{(i)}, y^{(i)})$, SVM aims to find an optimal hyperplane so that:

$$f(x^{(i)}) = wx^{(i)} + b \begin{cases} \geq 1 \text{ if } y^{(i)} = 1 \\ \leq -1 \text{ if } y^{(i)} = -1 \end{cases}$$

- Which is equivalent to minimizing the following loss function

$$L(w,b) = \frac{1}{m}\sum_{i=1}^{m} \max(0, 1 - y^{(i)} \underbrace{(wx^{(i)} + b)}_{f(x^{(i)})}) + \frac{\lambda}{2}\|w\|^2$$

- Hinge loss: $\max(0, 1 - y^{(i)} f(x^{(i)}))$

$y^{(i)} f(x^{(i)}) \geq 1$ No contribution to loss

$y^{(i)} f(x^{(i)}) < 1$ Contributes to loss

Gradient computing

- The hinge loss is not differentiable, a sub-gradient is computed instead:

$$\frac{\partial}{\partial w} L(w,b) = \frac{1}{m}\sum_{i=1}^{m} \begin{cases} -y^{(i)}x^{(i)} \text{ if } 1\text{-}y^{(i)}f(x^{(i)}) > 0 \\ 0 \text{ else} \end{cases} + \lambda w$$

$$\frac{\partial}{\partial b} L(w,b) = \frac{1}{m}\sum_{i=1}^{m} \begin{cases} -y^{(i)} \text{ if } 1\text{-}y^{(i)}f(x^{(i)}) > 0 \\ 0 \text{ else} \end{cases}$$

SVM vs. Logistic regression

Logistic regression

- Label:

$$(x^{(i)}, y^{(i)})\ y^{(i)} \in \{0,1\}$$

- Hypothesis:

$$h(x) = \frac{1}{1 + e^{-(wx+b)}}$$

- Objective:

$$h(x)\begin{cases} \approx 1 \text{ if } y^{(i)} = 1 \\ \approx 0 \text{ if } y^{(i)} = 0 \end{cases}$$

SVM

- Label:

$$(x^{(i)}, y^{(i)})\ y^{(i)} \in \{-1,1\}$$

- Hypothesis:

$$f(x) = wx + b$$

- Objective:

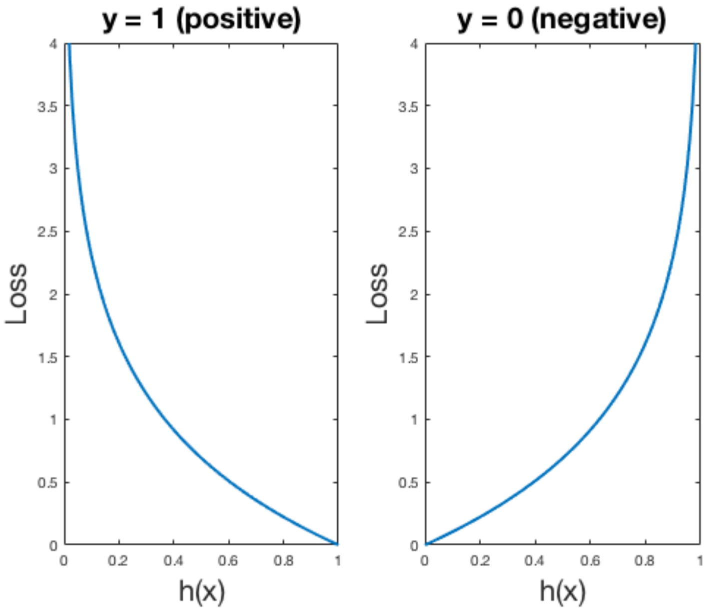
$$f(x^{(i)})\begin{cases} \geq 1 \text{ if } y^{(i)} = 1 \\ \leq -1 \text{ if } y^{(i)} = -1 \end{cases}$$

SVM vs. Logistic regression

Logistic regression

- Loss function

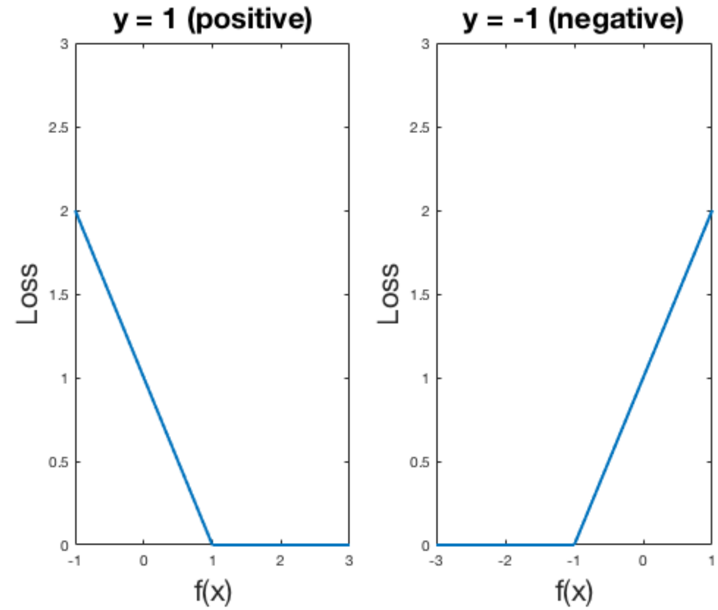
$$\text{Loss}(h(x), y) = \begin{cases} -\log(h(x)) \text{ if } y = 1 \\ -\log(1 - h(x)) \text{ if } y = 0 \end{cases}$$



SVM

- Loss function

$$\text{Loss}(f(x), y) = \begin{cases} \max(0, 1 - f(x)) \text{ if } y = 1 \\ \max(0, 1 + f(x)) \text{ if } y = -1 \end{cases}$$



SVM vs. Logistic regression

- Logistic regression:

$$L(w,b) = -\frac{1}{m}\sum_{i=1}^{m}\left(y^{(i)}\log(h(x^{(i)})) + (1-y^{(i)})\log(1-h(x^{(i)}))\right) + \frac{\lambda}{2m}\sum_{j=1}^{n} w_j^2$$

- SVM:

$$L(w,b) = \frac{1}{m}\sum_{i=1}^{m}\max(0,1-y^{(i)}f(x^{(i)})) + \frac{\lambda}{2}\sum_{j=1}^{n} w_j^2$$

Reading suggestion

- Chapter 13 Kernel machines in ‘Introduction to Machine Learning’