Motivation

Problem: Find a linear decision surface (Hyperplane) that can separate two classes, and has the largest distance between border line classes.

- borderline class (sample) = support vectors
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- If the convex hull of two classes form non-intersecting convex sets, then there exists a separating hyperplane[1]
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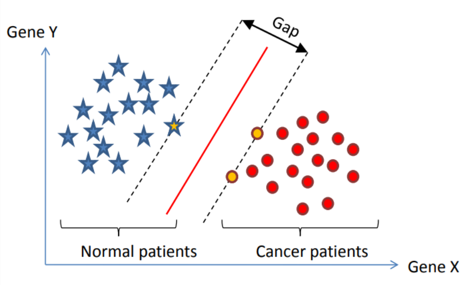

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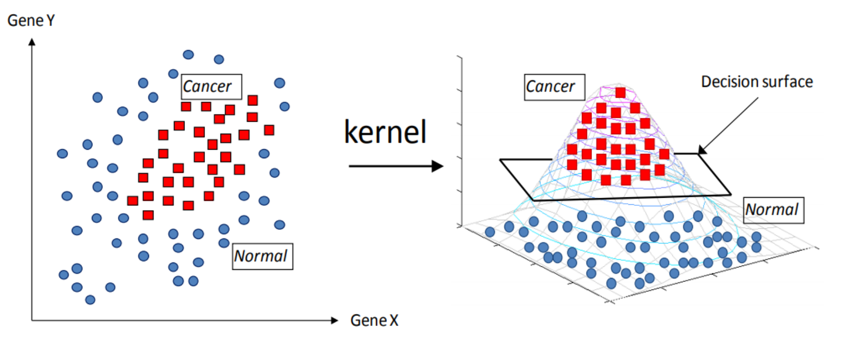

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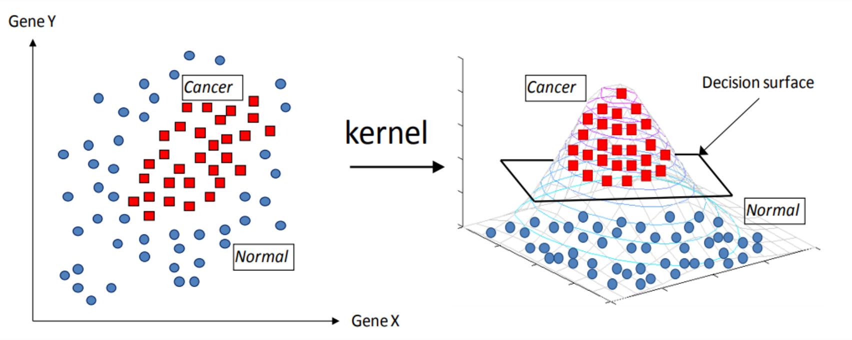

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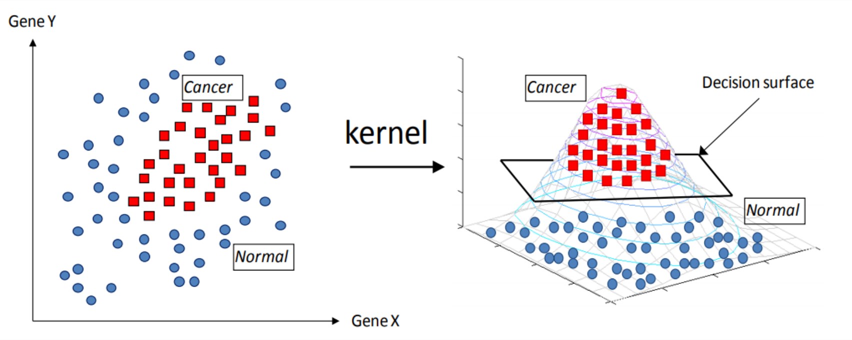

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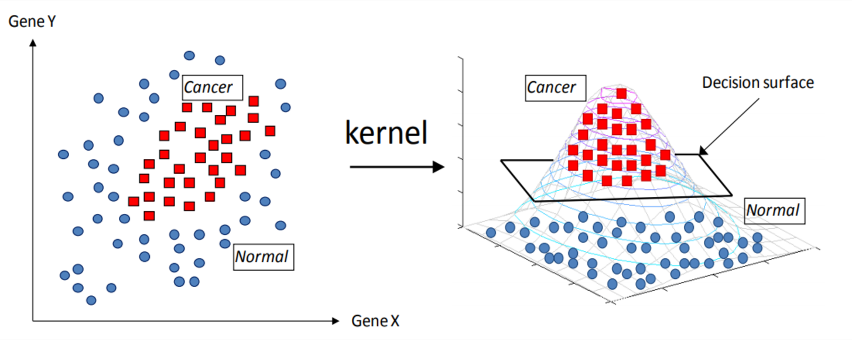

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- Such a mapping is achieved using clever so-called Kernel trick!
- Note dimension of the space increases: price to pay for linear separation

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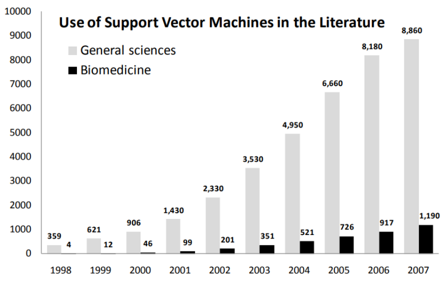

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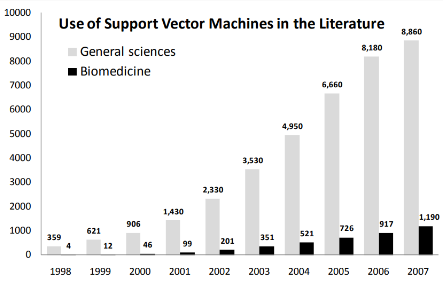

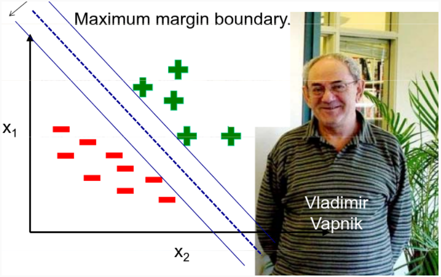

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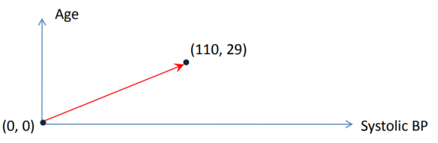

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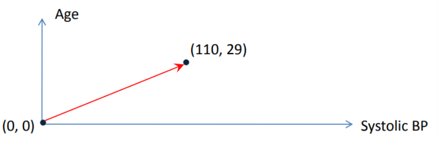
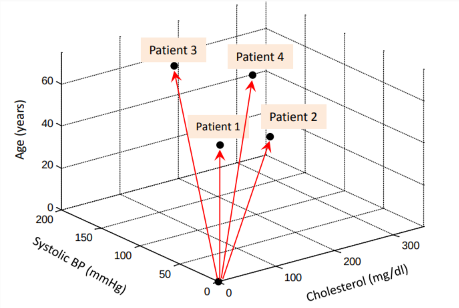
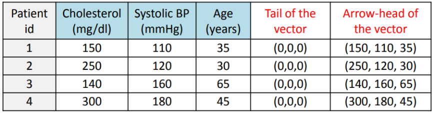
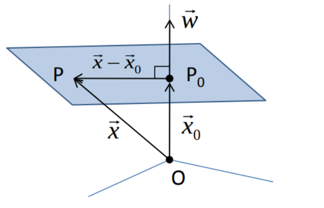


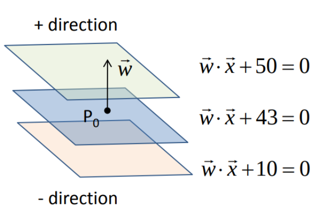




Patient id	Cholesterol (mg/dl)	Systolic BP (mmHg)	Age (years)	Tail of the vector	Arrow-head of the vector
1	150	110	35	(0,0,0)	(150, 110, 35)
2	250	120	30	(0,0,0)	(250, 120, 30)
3	140	160	65	(0,0,0)	(140, 160, 65)
4	300	180	45	(0,0,0)	(300, 180, 45)

Recall: Equation of Hyperplane

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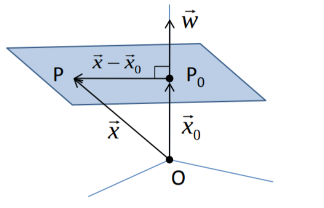

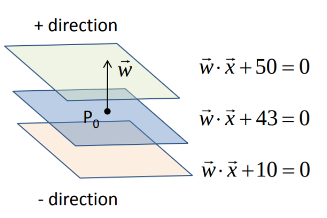
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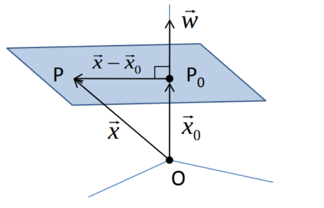

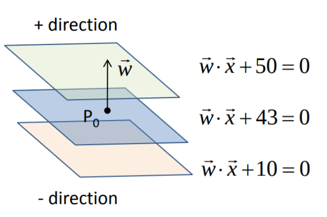
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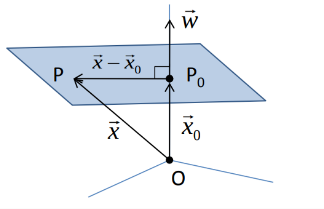

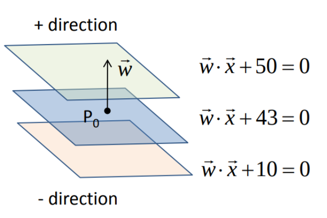
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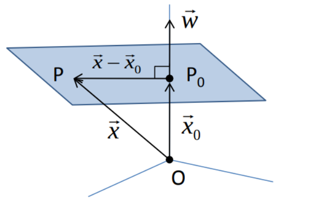

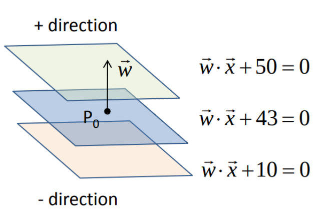

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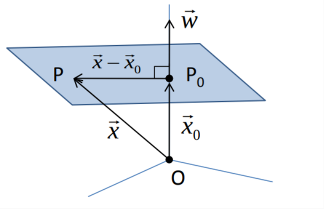

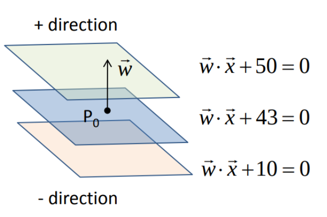
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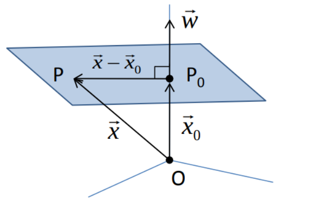

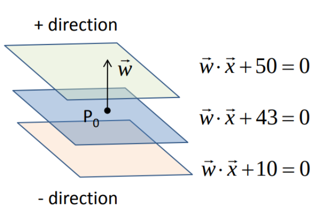

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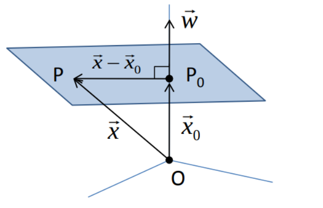

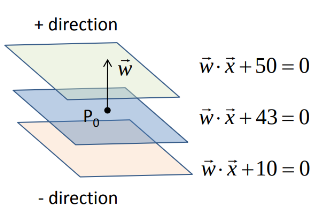
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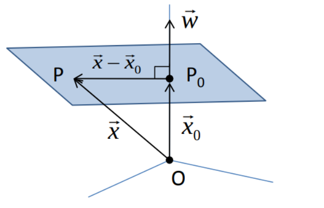

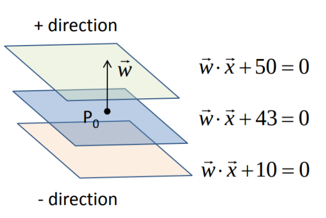

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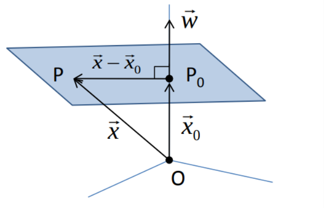

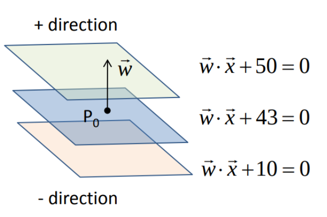
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$$D = |b_1 - b_2| / \|w\|_2$$

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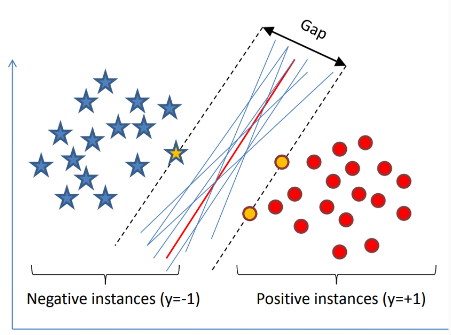

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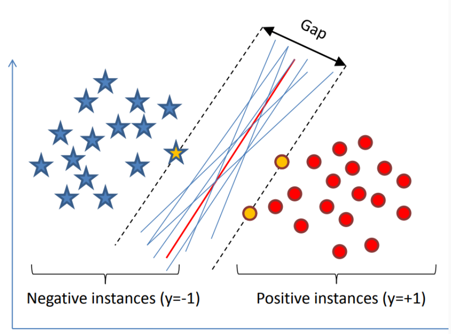

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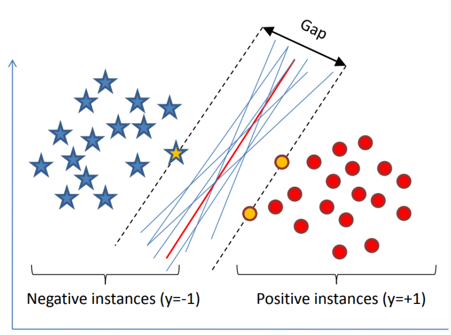

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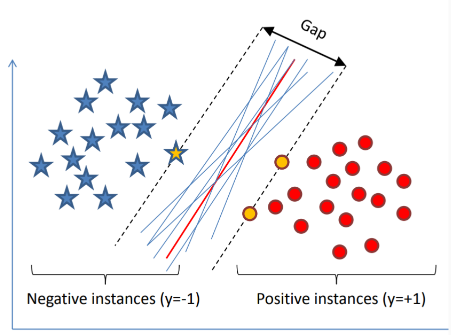

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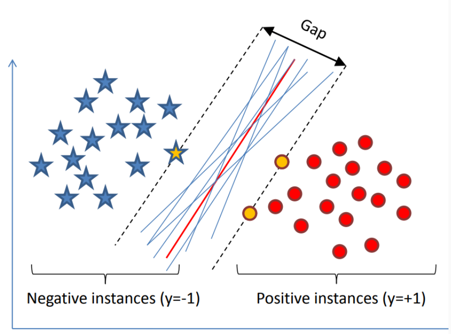

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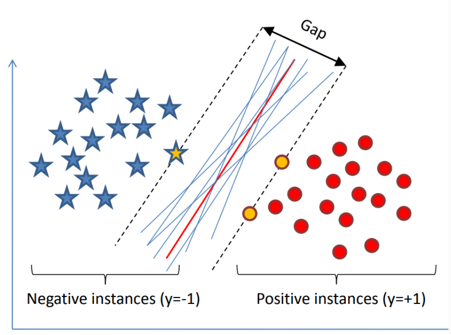

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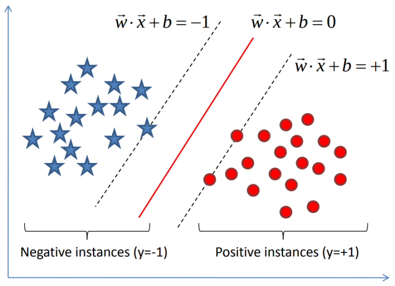
- If the support vectors are noisy, SVMs wont work well!

Particular Form of Hyperplanes Passing Through Support Vectors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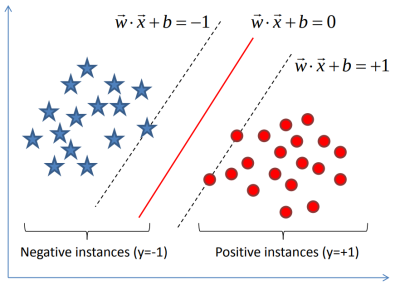
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- Quiz: Why dotted planes through support vectors are

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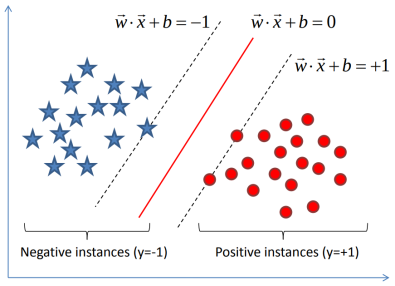
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$$w \cdot x + b = c \tag{4}$$

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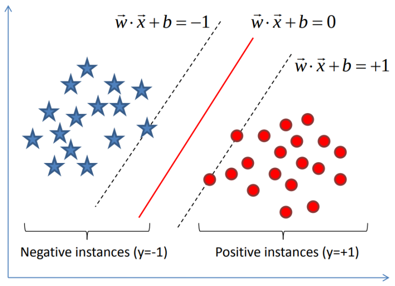
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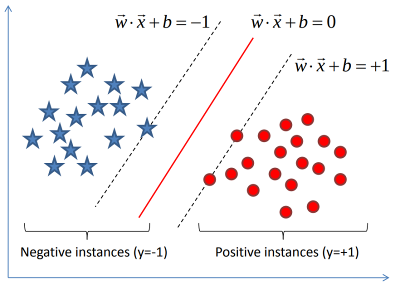
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- Divide $(3), (4), (5)$ by c to get

$$\tilde{w} \cdot x + \tilde{b} = 0$$
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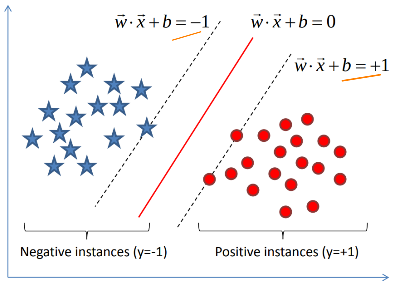

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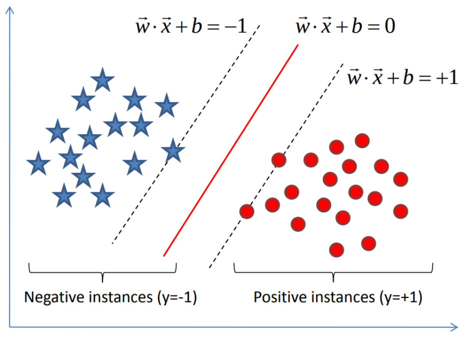
- Rename $\tilde{w}$ by w, and $\tilde{b}$ by b above!

SVM idea: Maximize the Margin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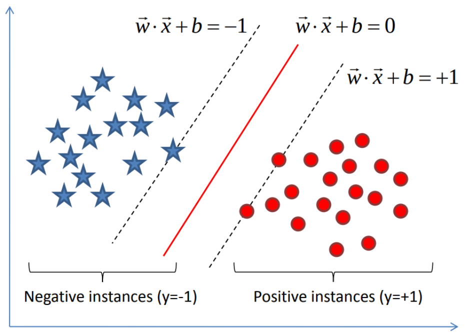
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Margin/Gap: Distance between parallel planes passing through support vectors

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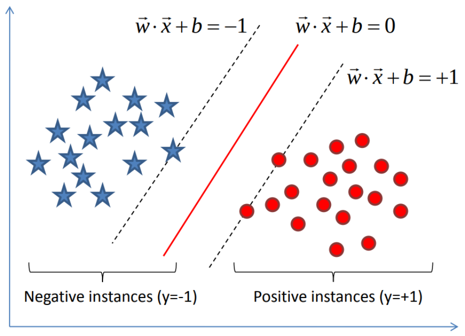
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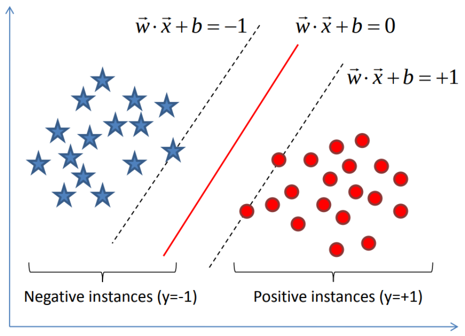
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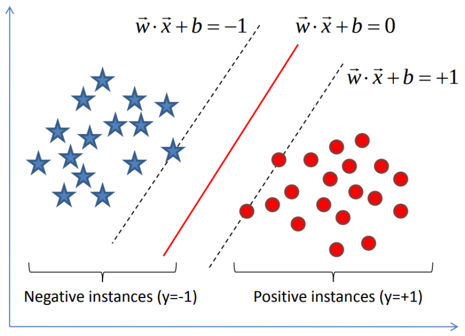

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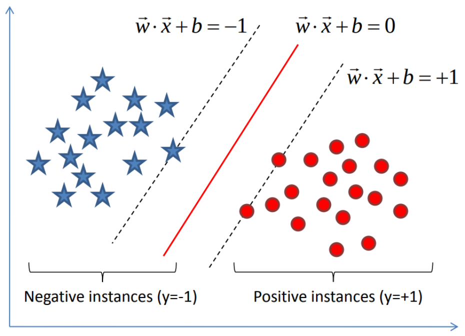
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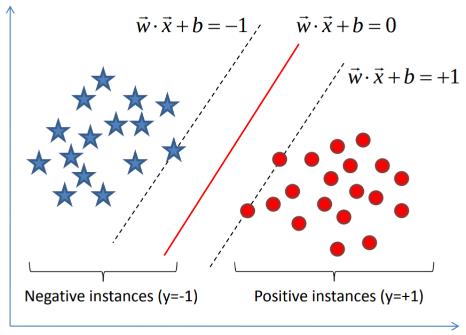
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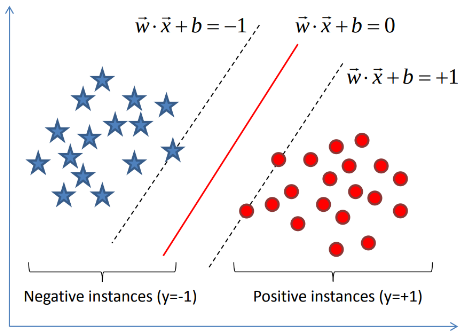

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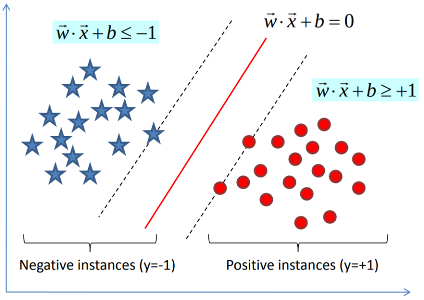
- Are there constraints?

Impose Constraints, Optimization Model, Prediction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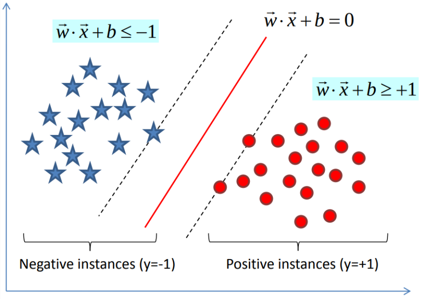
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Goal: Impose constraints such that all the data poitns are correctly classified.

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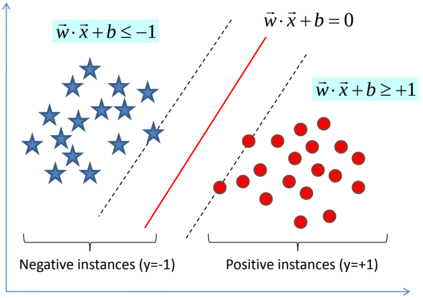
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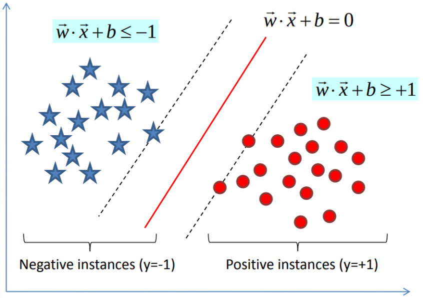
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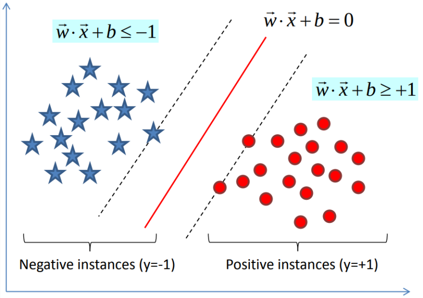

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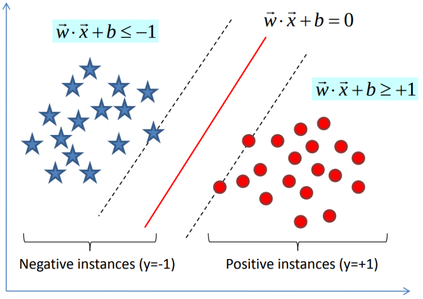
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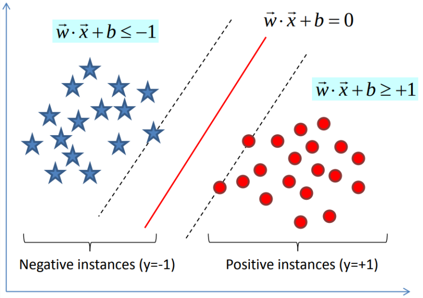
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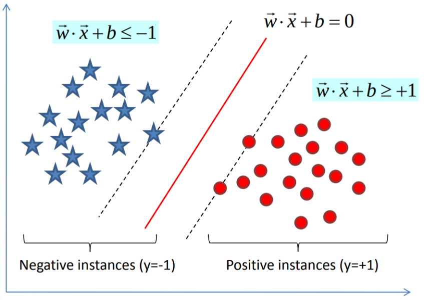

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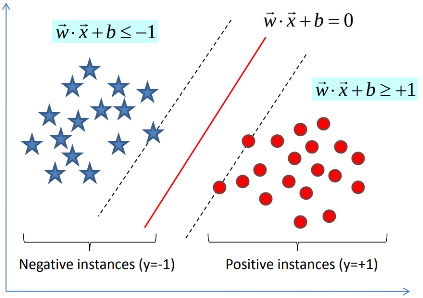
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Prediction:

$$f(x)=\text{sign}(w\cdot x+b)$$

Dual Formulation of SVM Optimization Problem

Standard form:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\|w\|^2 \\ \text{subject to} \quad & -y_i(w \cdot x + b) + 1 \leq 0, \quad i = 1, \ldots, m. \end{aligned}$$

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$$L(w, b, \lambda) = \underline{\frac{1}{2}\|w\|_2^2} + \sum_{i=1}^{m} \lambda_i(-\underline{y_i(w \cdot x} + b) + 1)$$

Dual Formulation of SVM Optimization Problem

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$$g(\lambda)=\inf_{\underset{x}{\boxed{w,b}}} L(\underbrace{w,b}_{x},\lambda)$$

3. $\underbrace{L(w,b,\lambda)}$ convex in w, b, minima given by

$$\nabla_{w,b}L(w,b,\lambda)=0$$

SVM-Dual Formulation

1. Setting the derivative of L w.r.t b to zero,

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$$\frac{\partial L(w, b, \lambda)}{\partial b} = 0 \implies \sum_{i=1}^{m} \lambda_i y_i = 0$$

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$$-\sum \lambda_i \lambda_j y_i y_j (x_i \cdot x_j)$$

$$+\sum \lambda_i + \cancel{\sum_{i=1}^{m} \lambda_i b y_i} \to 0$$

=

because

$$\boxed{\sum \lambda_i y_i = 0}$$

$$\frac{1}{2}\|w\|_2^2 = \frac{1}{2} w^T w = \frac{1}{2}\Big(\sum_{i=1}^{m} \lambda_i y_i x_i\Big)^T \Big(\sum_{j=1}^{m} \lambda_j y_j x_j\Big)$$

$$\frac{1}{2}\sum_{i=1}^{m} \lambda_i \lambda_j y_i y_j (x_i \cdot x_j)$$

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SVM Dual Problem:

maximize $\displaystyle \sum_{i=1}^{m} \lambda_i - \frac{1}{2}\sum_{i=1}^{m} \lambda_i \lambda_j y_i y_j (x_i \cdot x_j)$

subject to $\underline{\lambda_i \geq 0}, \quad \displaystyle \sum_{i=1}^{m} \lambda_i y_i = 0, \quad i = 1, \ldots, m$

SVM Primal Versus Dual Problem

SVM Primal Problem:

$$\text{minimize } \frac{1}{2}\|w\|^2, \quad w \in \mathbb{R}^n$$

$$\text{subject to } -y_i(w \cdot x + b) + 1 \leq 0, \; i = 1, \ldots, m.$$

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Primal:

- Variables are $\{\underline{w_1}, \underline{w_2}, \ldots, \underline{w_n}\}$

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$\frac{1}{2} w^T w$

$\boxed{P \succeq 0}$

constraint + objective fn all convex

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Dual:

- Variables are $\underline{\{\lambda_1, \lambda_2, \dots, \lambda_m\}}$

SVM Primal Versus Dual Problem

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$-\lambda_i \leq 0$

minimiz

$-\left(\quad (obj) \quad \right)$

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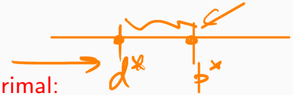

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- Variables are $\{\lambda_1, \lambda_2, \ldots, \lambda_m\}$
- m is number of data samples
- Dual is convex

Recommendation: Use dual when the number of samples m are significantly less relative to the number of features n, otherwise use primal.

Strong Duality and KKT Conditions for SVM

SVM Primal Problem:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\|w\|^2 \\ \text{subject to} \quad & -y_i(w \cdot x + b) + 1 \leq 0, \quad i = 1, \ldots, m. \end{aligned}$$

Strong Duality and KKT Conditions for SVM

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Recall Slater's condition from slide ~~12~~

Slater's condition when some f_i are affine. There exists $x \in \operatorname{int} \mathcal{D}$ with

$$\underbrace{f_i(x) \leq 0, \quad i = 1, \ldots, k,}_{\text{affine}} \quad \underbrace{f_i(x) < 0, \quad i = k+1, \ldots, m,}_{\text{non-affine}} \quad Ax = b.$$

12

Strong Duality and KKT Conditions for SVM

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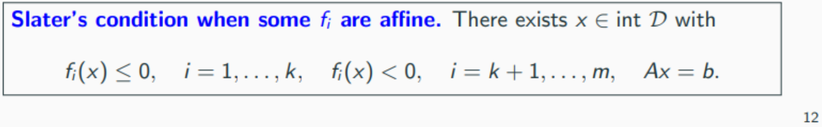
Recall Slater's condition from slide 12



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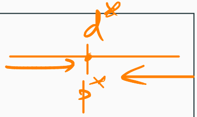
12

For SVM primal problem

- objective is quadratic and convex, and all inequality constraints are affine
- Slater's condition holds trivially, hence, strong duality holds

SVM Dual Problem:

$$\left.\begin{aligned}
\text{maximize} \quad & \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j y_i y_j (x_i \cdot x_j) \\
\text{subject to} \quad & \lambda_i \geq 0, \quad i = 1, \ldots, m, \\
& \sum_{i=1}^{m} \lambda_i y_i = 0.
\end{aligned}\right\}$$



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Solving primal from dual:

- Assume that the dual problem is solved to obtain the dual optimal $\underline{\lambda^*}$
- Recall: Setting the derivative of L w.r.t. w to zero, we got

SVM Dual Problem:

$$
\begin{aligned}
\underset{\lambda}{\text{maximize}} \quad & \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j y_i y_j (x_i \cdot x_j) \\
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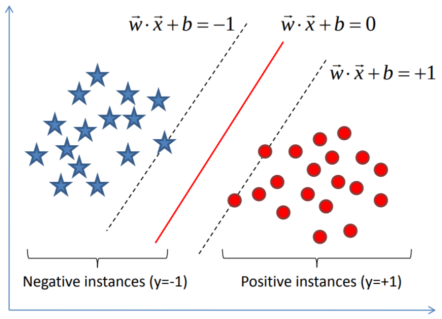
- Hence we get primal optimal w^* as

$$w^* = \sum_{i=1}^{m} \lambda_i^* y_i x_i$$

- The primal intercept b^* is

$$b^* = -\frac{\max_{i:y^{(i)}=-1} {w^*}^T x^{(i)} + \min_{i:y^{(i)}=+1} {w^*}^T x^{(i)}}{2}$$

Computing the optimal intercept b^*


$\vec{w} \cdot \vec{x} + b = -1$
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Negative instances (y=-1)
Positive instances (y=+1)

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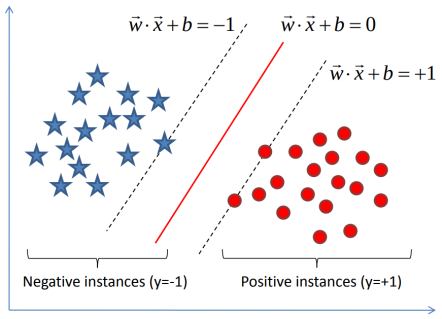
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- For all x in red plane:$w^* \cdot x = -b$

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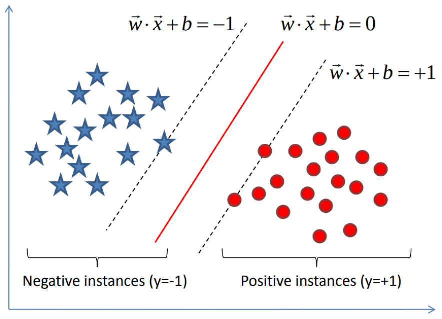
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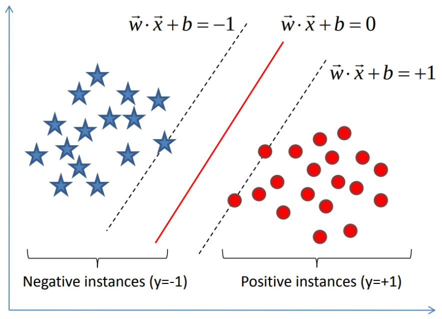
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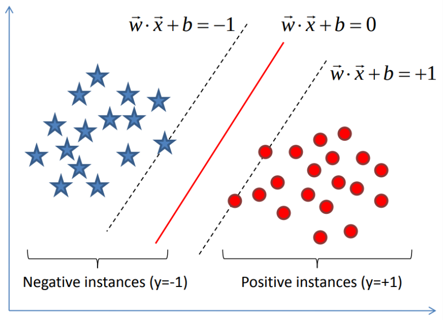
Computing the optimal intercept b^*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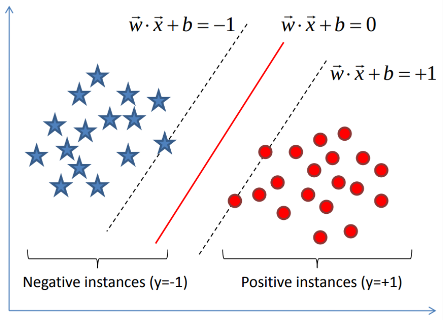
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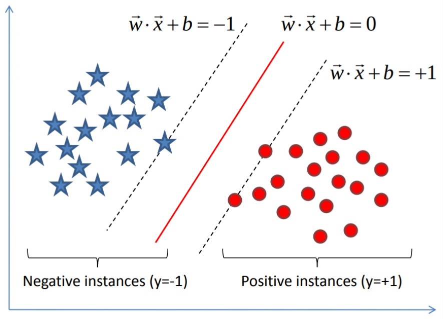
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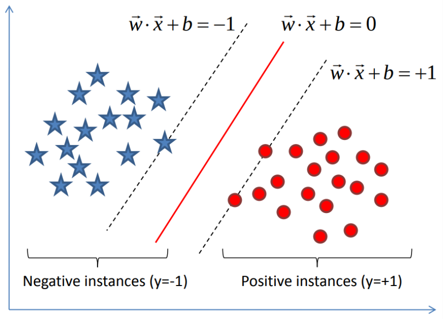
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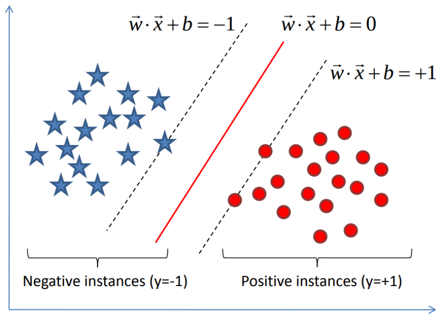
- Similarly, take projections of $x^{(i)}$ of negative class along $-w^*$, and find the farthest point

Computing the optimal intercept b^*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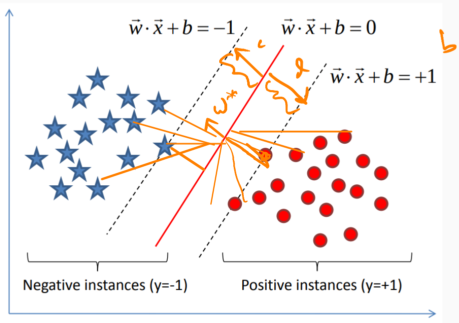

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c
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$b = \frac{c+d}{2}$

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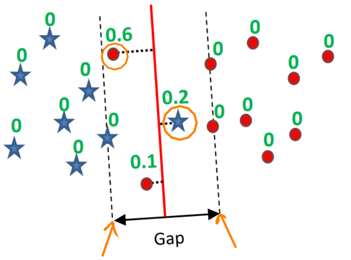
- Similarly, take projections of $x^{(i)}$ of negative class along $-w^*$, and find the farthest point

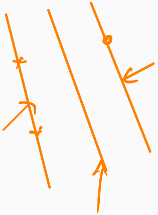
$$\min_{i:y^{(i)}=-1} -{w^*}^T x^{(i)} = \max_{i:y^{(i)}=-1} {w^*}^T x^{(i)}$$

$$\text{Hence, optimal intercept } b^* = -\frac{\overbrace{\max_{i:y^{(i)}=-1} {w^*}^T x^{(i)}}^{c} + \overbrace{\min_{i:y^{(i)}=+1} {w^*}^T x^{(i)}}^{d}}{2}$$

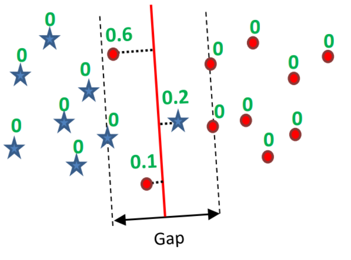
Linearly Separable with Noisy Data: Soft-Margin SVM

noisy?



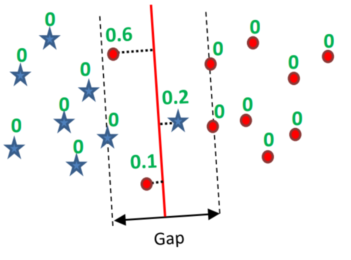


Linearly Separable with Noisy Data: Soft-Margin SVM



Two red and one blue samples noisy.

Linearly Separable with Noisy Data: Soft-Margin SVM



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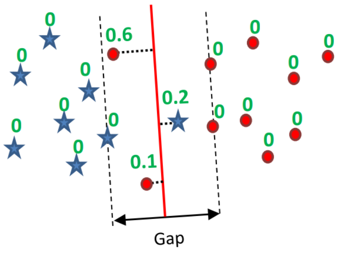
Goal: The data is noisy and it is not linearly separable. Modify SVM optimization model to allow for noisy data into account. Formulate optimization problem so that some noisy data is allowed bewteen gap/margin (region between dotted lines).

Linearly Separable with Noisy Data: Soft-Margin SVM



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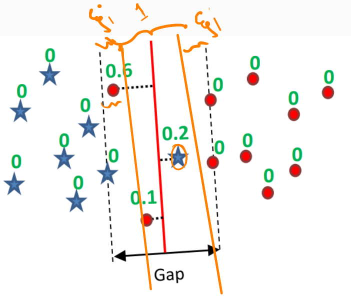
Linearly Separable with Noisy Data: Soft-Margin SVM



$y_i(w\cdot x_i+b)\geq 1$

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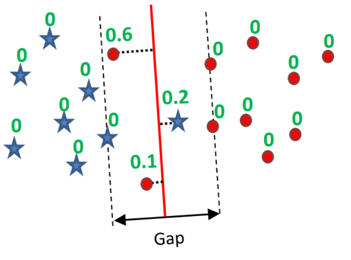
$$y_i(w\cdot x_i+b)\geq 1-\xi_i$$

Linearly Separable with Noisy Data: Soft-Margin SVM



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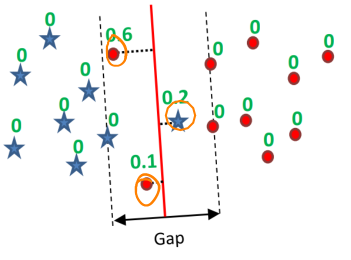
$$y_i(w \cdot x_i + b) \geq 1 - \xi_i$$

- Our margin is no longer strict or hard, it is now softened

Linearly Separable with Noisy Data: Soft-Margin SVM



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$$y_i(w \cdot x_i + b) \geq 1 - \xi_i$$
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- Also, don't want too many x_i to be between dotted planes, introduce penalty in objective

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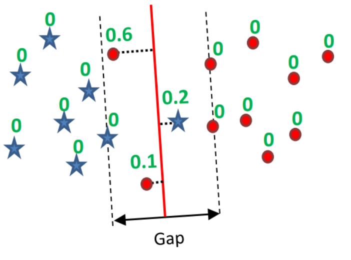

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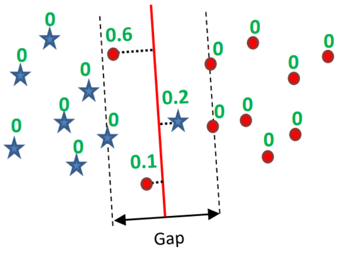
$$\min \quad \underbrace{\frac{1}{2}\|w\|^2} + C \underbrace{\sum_{i=1}^{m} \xi_i}$$

Linearly Separable with Noisy Data: Soft-Margin SVM



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$$y_i(w \cdot x_i + b) \geq 1 - \xi_i$$
- Our margin is no longer strict or hard, it is now softened
- Also, don't want too many x_i to be between dotted planes, introduce penalty in objective
$$\frac{1}{2}\|w\|^2 + C \sum_{i=1}^{m} \xi_i$$
- Since it is a minimization, large values of ξ_i will be discouraged

Primal and Dual Formulation of Soft-Margin SVM

Primal Soft-Margin SVM:

$$\begin{aligned}\text{minimize} \quad & \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m}\xi_i \\ \text{subject to} \quad & y_i(w \cdot x_i + b) \geq 1 - \xi_i, \quad i = 1, \ldots, m.\end{aligned}$$

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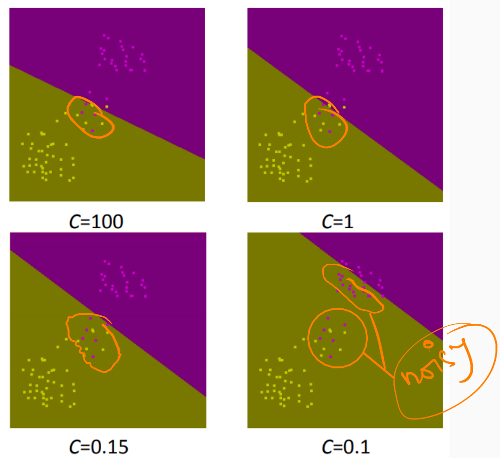
Dual Soft-Margin SVM:

$$\begin{aligned}
&\text{Maximize} \quad \sum_{i=1}^{m}\lambda_i - \frac{1}{2}\sum_{i,j=1}^{m}\lambda_i\lambda_j\, y_i y_j\, x_i \cdot x_j \\
&\text{subject to} \quad 0 \leq \lambda_i \leq C, \quad i = 1, \ldots, m, \\
&\qquad\qquad\quad \sum_{i=1}^{m}\lambda_i y_i = 0.
\end{aligned}$$

Quiz: How did we get the dual form? Try.

Effect of Parameter on soft-margin SVM

Minimize $\frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m}\xi_i$ subject to $y_i(w\cdot x_i + b) \geq 1 - \xi_i$ for $i = 1,\ldots,m$.



C=100

C=1

C=0.15

C=0.1

- For C very large, soft margin is equivalent to hard margin.
- When C is small, we allow misclassification.
- Here C is a hyperparameter.
- In practice, cross-validations can be used.

Primal and Dual Formulation of Soft-Margin SVM

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Additional advantages of primal over dual

- We see $x_i \cdot x_j$ in dual.

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Additional advantages of ~~primal~~ dual over ~~dual~~ primal

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- Can we make use of this term?

Primal and Dual Formulation of Soft-Margin SVM

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- Fact that $x_i \cdot x_j$ appears only in dual objective and that too as dot product is useful.

Primal and Dual Formulation of Soft-Margin SVM

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$$
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\text{minimize} \quad & \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m} \xi_i \\
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$$

Dual Soft-Margin SVM:

$$
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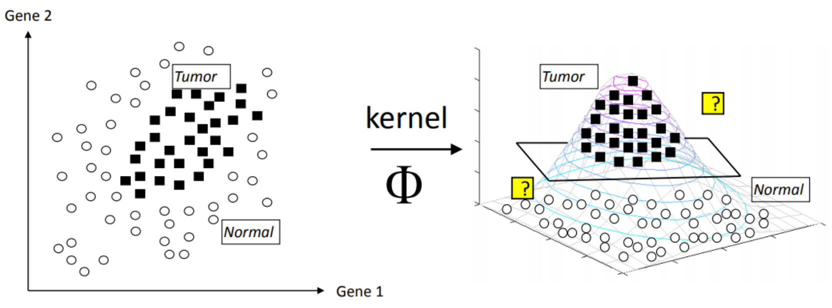
- We see $x_i \cdot x_j$ in dual.
- Can we make use of this term?
- Sample x_i also appears in constraint in primal. Is that useful?
- Fact that $x_i \cdot x_j$ appears only in dual objective and that too as dot product is useful.
- This allows mapping samples to a space where they may be linearly separated.

Non-Linearly Separable Data, Kernel Trick



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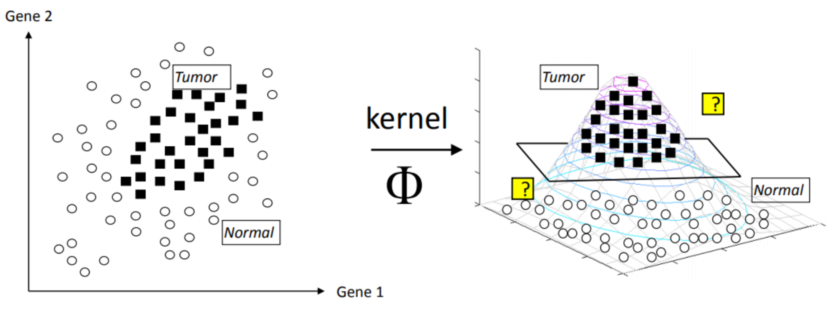

Here data is not linearly separable in the input space

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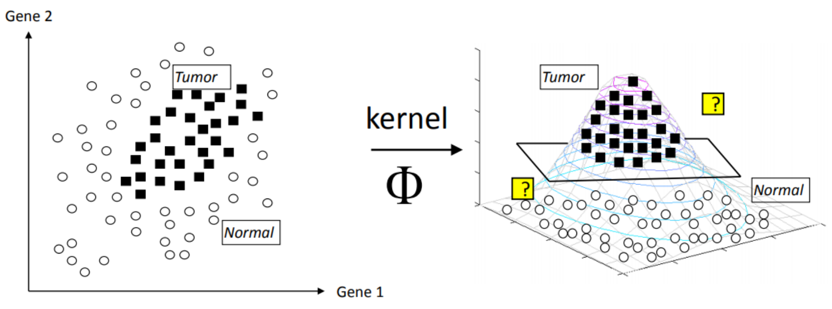

Here data is not linearly separable in the input space

After mapping to a new feature space, data is now linearly separable!

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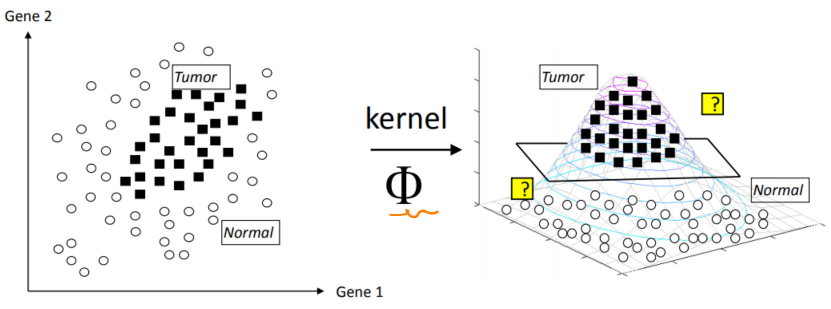

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After mapping to a new feature space, data is now linearly separable!

Quiz: How to find such map $\Phi : \mathbb{R}^N \to H$

Kernel Trick

For data in input space

$$f(x) = \text{sign}(w \cdot x + b)$$

$$w = \sum_{i=1}^{m} \alpha_i y_i x_i$$

Kernel Trick

$x \longrightarrow \phi(x)$

For data in input space

$$f(x) = \text{sign}(w \cdot x + b)$$

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Data in feature space $\Phi(x)$

$$f(x) = \text{sign}(w \cdot \Phi(x) + b)$$

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- Solve the dual problem for α_i

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- Compute w, b from above

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$$w = \sum_{i=1}^{m} \alpha_i y_i \Phi(x_i)$$

- Solve for α_i using dual
- Compute w, b (x_i by $\Phi(x_i)$)

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- Predict with $f(x)$. So what? Trick: substitute w in $f(x)$ above!

Kernel Trick:

$$f(x) = \text{sign}\left(\sum_{i=1}^{m} \alpha_i y_i \, \Phi(x_i) \cdot \Phi(x) + b\right) = \text{sign}\left(\sum_{i=1}^{m} \alpha_i y_i \, K(x_i, x) + b\right)$$

Kernel Trick

$x \longrightarrow \underline{\underline{\Phi(x)}}$

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Dont need to know Φ; Only a function $K(\cdot,\cdot) : \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R}$ will do!

Kernel Trick

$$\boxed{x \in \mathbb{R}^2} \rightarrow \boxed{\phi(x) \in \mathbb{R}^3}$$

$$\underbrace{\phi(x_i)}_{\in \mathbb{R}^3} \cdot \underbrace{\phi(x)}_{\mathbb{R}^3}$$

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Dont need to know Φ; Only a function $K(\cdot,\cdot) : \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R}$ will do!

→ Avoid explicit computation of features or infinite length vectors

Popular Kernels

Kernel: A kernel is a dot product in some feature space

$$\underline{K(x_i, x_j)} = \Phi(x_i) \cdot \Phi(x_j)$$

Popular Kernels

Kernel: A kernel is a dot product in some feature space

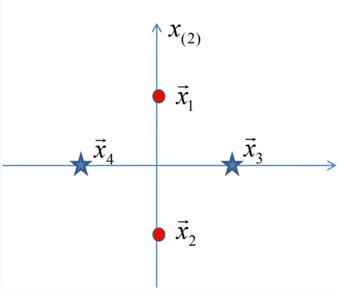
$$K(x_i, x_j) = \Phi(x_i) \cdot \Phi(x_j)$$

$$e^{-\gamma \underbrace{(x_i - x_j)^T (x_i - x_j)}}$$

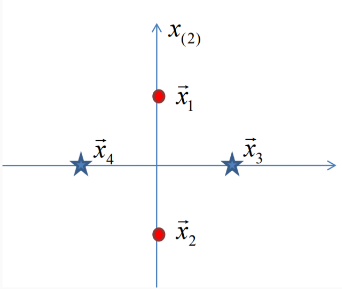
✓ $K(x_i, x_j) = \underline{x_i} \cdot \underline{x_j}$	Linear kernel
✓ $K(x_i, x_j) = \exp(-\gamma \lVert \underline{x_i - x_j} \rVert^2)$	Gaussian kernel
✓ $K(x_i, x_j) = \exp(-\gamma \lVert x_i - x_j \rVert)$	Exponential kernel
✓ $K(x_i, x_j) = (p + \underline{x_i \cdot x_j})^q$	Polynomial kernel
✓ $\underline{K(x_j, x_j)} = (p + \underline{x_i \cdot x_j})^q \exp(-\gamma \lVert x_i - x_j \rVert^2)$	Hybrid kernel
$K(x_i, x_j) = \tanh(kx_i \cdot x_j - \delta)$	Sigmoidal

Polynomial Kernel

Polynomial Kernel

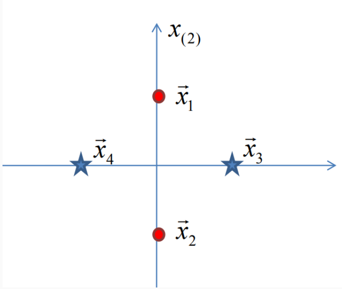


Polynomial Kernel



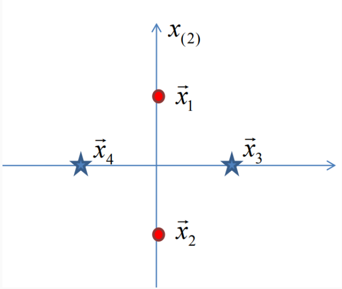
- Data is not linearly separable

Polynomial Kernel



- Data is not linearly separable
- Apply Kernel $\underline{K(x, z)} = (x \cdot z)^2$ to map data to higher dimension, to make it linearly separable

Polynomial Kernel



- Data is not linearly separable
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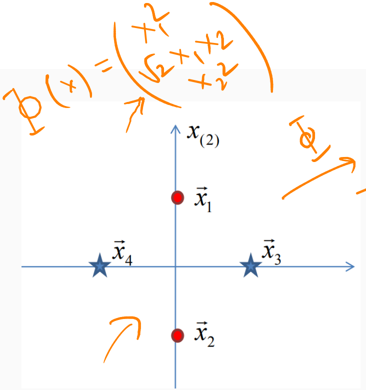
- $x_1 = [x_{(1)}, x_{(2)}]^T$, $z_1 = [z_{(1)}, z_{(2)}]^T$

Polynomial Kernel



- Data is not linearly separable
- Apply Kernel $K(x,z) = (x\cdot z)^2$ to map data to higher dimension, to make it linearly separable
- $x_1 = [x_{(1)}, x_{(2)}]^T, \ z_1 = [z_{(1)}, z_{(2)}]^T$

much cheaper than

Cost=4

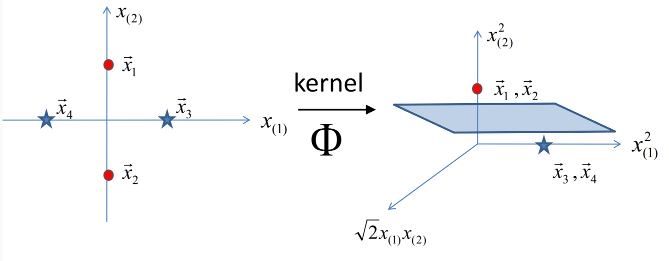
Cost=11

We have

$$K(x\cdot z) = (x\cdot z)^2 = \left(\begin{bmatrix}x_{(1)}\\x_{(2)}\end{bmatrix}\cdot\begin{bmatrix}z_{(1)}\\z_{(2)}\end{bmatrix}\right)^2 = (x_{(1)}z_{(1)} + x_{(2)}z_{(2)})^2$$

$$= x_{(1)}^2 z_{(1)}^2 + 2x_{(1)}z_{(1)}x_{(2)}z_{(2)} + x_{(2)}^2 z_{(2)}^2 = \begin{bmatrix}x_{(1)}^2\\ \sqrt{2}x_{(1)}x_{(2)}\\ x_{(2)}^2\end{bmatrix}\cdot\begin{bmatrix}z_{(1)}^2\\ \sqrt{2}z_{(1)}z_{(2)}\\ z_{(2)}^2\end{bmatrix} = \Phi(x)\cdot\Phi(z)$$

Separation Happens After Using Polynomial Kernel!



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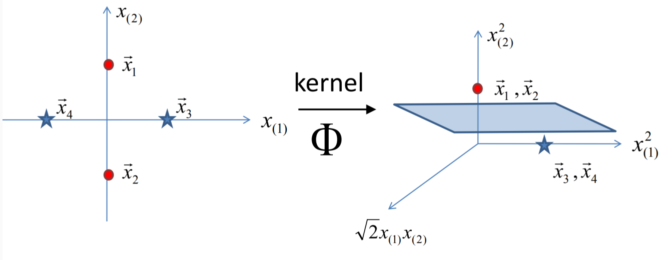
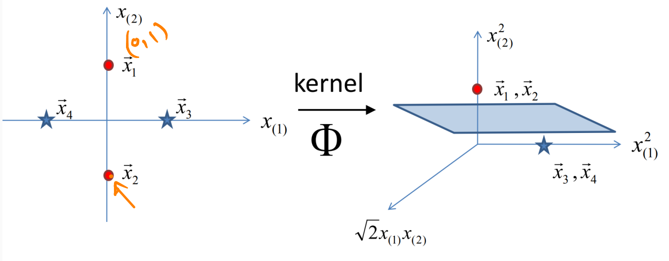


- In last slide: $\Phi(x) = \begin{bmatrix} x_{(1)}^2 \\ \sqrt{2}x_{(1)}x_{(2)} \\ x_{(2)}^2 \end{bmatrix}$

Separation Happens After Using Polynomial Kernel!



- In last slide: $\Phi(x) = \begin{bmatrix} x_{(1)}^2 \\ \sqrt{2}x_{(1)}x_{(2)} \\ x_{(2)}^2 \end{bmatrix}$
- The points in figure above are

$$x_1 = (0,1), \quad x_2 = (0,-1)$$
$$x_3 = (1,0), \quad x_4 = (-1,0)$$

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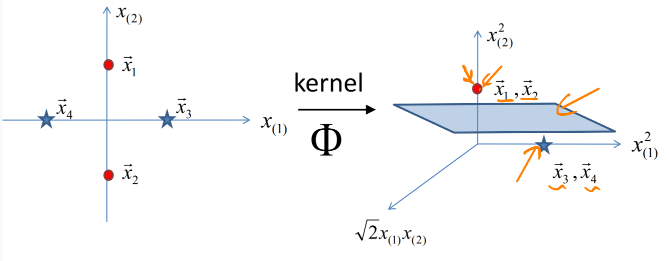


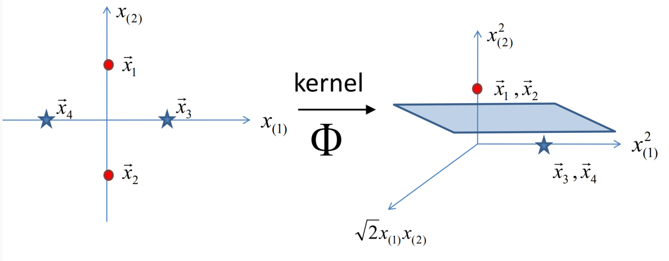
- In last slide: $\Phi(x) = \begin{bmatrix} x_{(1)}^2 \\ \sqrt{2}x_{(1)}x_{(2)} \\ x_{(2)}^2 \end{bmatrix} \begin{matrix} 0 \\ 0 \\ 1 \end{matrix}$
- The points in figure above are

$$x_1 = (0, 1), \quad x_2 = (0, -1)$$
$$x_3 = (1, 0), \quad x_4 = (-1, 0)$$

- We have

$$\Phi(x_1) = [0, 0, 1]^T$$
$$\Phi(x_2) = [0, 0, 1]^T$$
$$\Phi(x_3) = [1, 0, 0]^T$$
$$\Phi(x_4) = [1, 0, 0]^T$$

Separation Happens After Using Polynomial Kernel!



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- After Φ transformation, points are now linearly separable!

Same Kernel Function but Different Features

Note: Feature space might not be unique for the same kernel function.

Same Kernel Function but Different Features

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Example-1: Consider $\Phi : \mathbb{R}^2 \to \mathbb{R}^3$

$$\begin{aligned}
\Phi(x_1, x_2) &= (x_1^2, x_2^2, \sqrt{2}x_2x_2) \\
\Phi(x) \cdot \Phi(z) &= (x_1^2, x_2^2, \sqrt{2}x_1x_2) \cdot (z_1^2, z_2^2, \sqrt{2}z_1z_2) \\
&= (x_1z_1 + x_2z_2)^2 = (x \cdot z)^2 = \underline{K(x, z)}.
\end{aligned}$$

Same Kernel Function but Different Features

Note: Feature space might not be unique for the same kernel function.

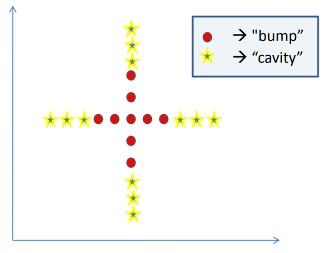
Example-1: Consider $\Phi : \mathbb{R}^2 \to \mathbb{R}^3$

$$\begin{aligned}\Phi(x_1, x_2) &= (x_1^2, x_2^2, \sqrt{2}x_2x_2)\\ \Phi(x) \cdot \Phi(z) &= (x_1^2, x_2^2, \sqrt{2}x_1x_2) \cdot (z_1^2, z_2^2, \sqrt{2}z_1z_2)\\ &= (x_1z_1 + x_2z_2)^2 = (x \cdot z)^2 = K(x, z).\end{aligned}$$

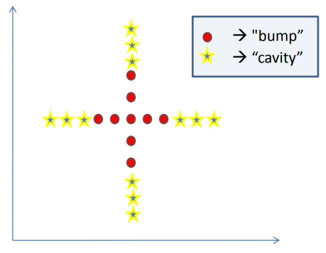
Example-2: Consider $\Phi : \mathbb{R}^2 \to \mathbb{R}^4$

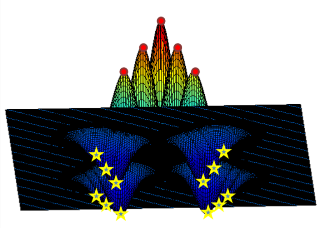
$$\begin{aligned}\Phi(x_1, x_2) &= (x_1^2, x_2^2, x_1x_2, x_2x_1)\\ \Phi(x) \cdot \Phi(z) &= (x_1^2, x_2^2, x_1x_2, x_2x_1) \cdot (z_1^2, z_2^2, z_1z_2, z_2z_1)\\ &= (x \cdot z)^2 = \underline{K(x, z)}.\end{aligned}$$

RBF or Gaussian Kernel

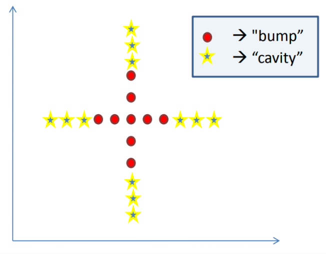


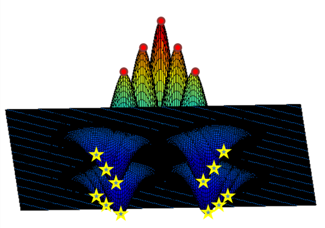
RBF or Gaussian Kernel

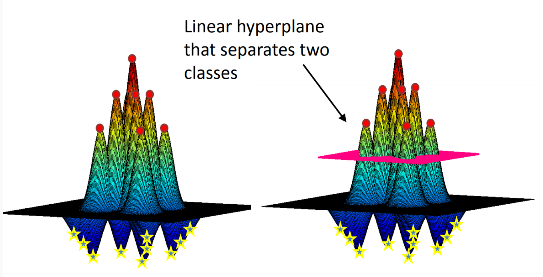




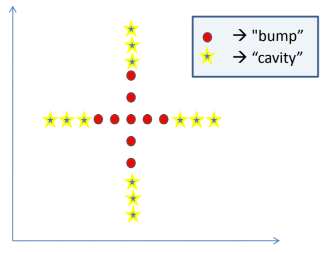
RBF or Gaussian Kernel

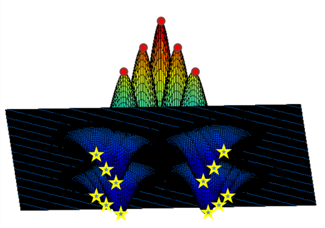


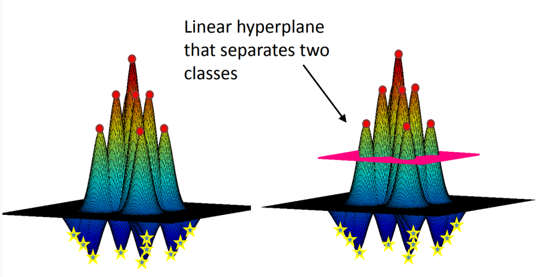



Linear hyperplane that separates two classes

RBF or Gaussian Kernel

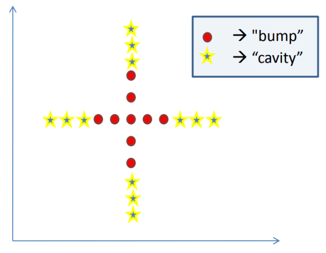


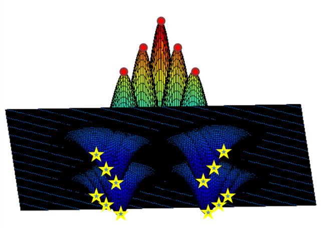


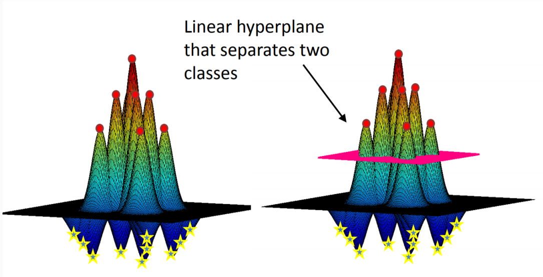


After applying the kernel, we observe:

RBF or Gaussian Kernel



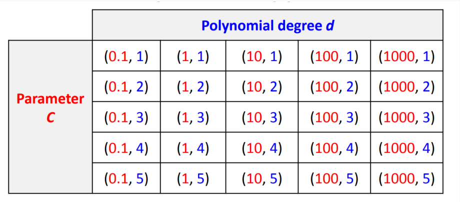



Linear hyperplane that separates two classes

After applying the kernel, we observe:

- red data points are bumped up
- yellow data points are pushed to cavity

Model Selection: Which Kernels with which parameter?



	Polynomial degree *d*				
Parameter *C*	(0.1, 1)	(1, 1)	(10, 1)	(100, 1)	(1000, 1)
	(0.1, 2)	(1, 2)	(10, 2)	(100, 2)	(1000, 2)
	(0.1, 3)	(1, 3)	(10, 3)	(100, 3)	(1000, 3)
	(0.1, 4)	(1, 4)	(10, 4)	(100, 4)	(1000, 4)
	(0.1, 5)	(1, 5)	(10, 5)	(100, 5)	(1000, 5)

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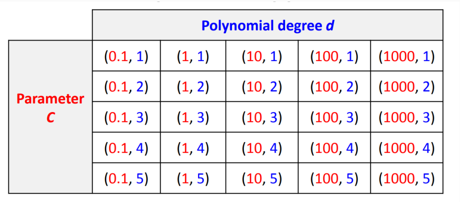

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- Consider polynomial kernel.

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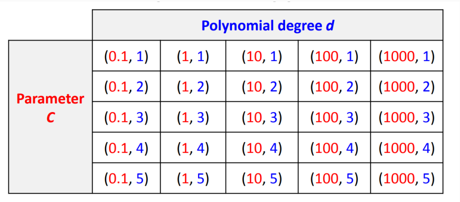

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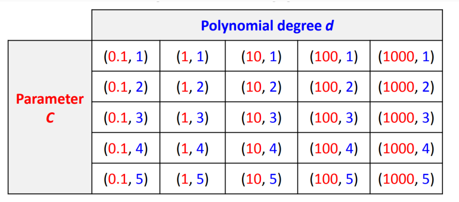
- Consider polynomial kernel.
- There are parameters: C, d.

Model Selection: Which Kernels with which parameter?



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- Consider polynomial kernel.
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- We can consider possible values.

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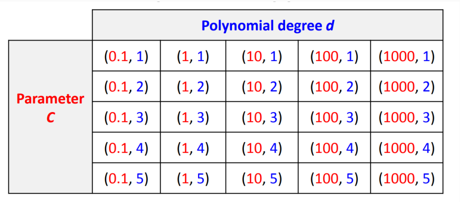

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- Check our choice by doing cross-validations.

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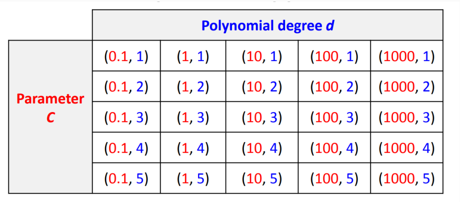

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- Consider polynomial kernel.
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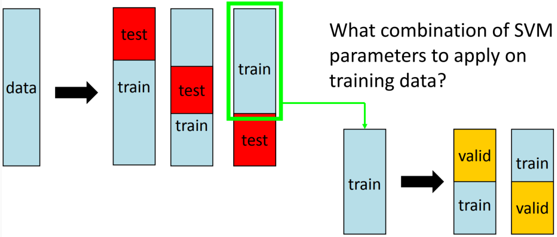
Recall the main idea of cross-validation:



What combination of SVM parameters to apply on training data?

Perform “grid search” using another nested loop of cross-validation.

SVM in Unconstrained Form: loss + penalty form

Primal Soft-Margin SVM:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m}\xi_i \\ \text{subject to} \quad & y_i(w \cdot x_i + b) \geq 1 - \xi_i, \\ & i = 1, \ldots, m. \end{aligned}$$

SVM in Unconstrained Form: loss + penalty form

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1. Write constraint as

$$y_i(w \cdot x_i + b) \geq 1 - \xi_i$$

$$\underbrace{\xi_i \geq -(w \cdot x_i}_{} + b)y_i + 1$$

SVM in Unconstrained Form: loss + penalty form

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1. Write constraint as

$$\begin{aligned} y_i(w\cdot x_i + b) &\geq 1 - \xi_i \\ \xi_i &\geq -\underbrace{(w\cdot x_i + b)}_{f(x_i)}y_i + 1 \end{aligned}$$

and $\xi_i \geq 0$.

2. Write constraints on ξ as function?

$$\xi_i = \max(0, 1 - y_i f(x_i))$$

max is not diff.

SVM in Unconstrained Form: loss + penalty form

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$$\xi_i = \max(0, 1 - y_i f(x_i))$$

3. Substituting ξ_i in objective

$$\begin{aligned} &= \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m}\max(0, 1 - y_i f(x_i)) \\ &= \frac{1}{2C}\|w\|^2 + \sum_{i=1}^{m}\max(0, 1 - y_i f(x_i)) \\ &= \lambda\|w\|^2 + \sum_{i=1}^{m}\max(0, 1 - y_i f(x_i)) \\ &= \lambda\|w\|^2 + \sum_{i=1}^{m}[0, 1 - y_i f(x_i)]_+ \end{aligned}$$

$\lambda\left\{\frac{1}{2C}\|w\|^2 + \sum\right.$

$\boxed{\lambda = \frac{1}{2C}}$

Unconstrained SVM: Find w, b s.t. minimize $\sum_{i=1}^{m}[1 - y_i f(x_i)]_+ + \lambda\|w\|_2^2$

w b

SVM in Unconstrained Form: loss + penalty form

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1. Write constraint as

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Unconstrained SVM: Find w, b s.t. minimize $\sum_{i=1}^{m}[1 - y_i f(x_i)]_+ + \lambda\|w\|_2^2$

Penalty: $\lambda\|w\|_2^2$.

Loss (Hinge Loss): $\sum_{i=1}^{m}[1 - y_i f(x_i)]_+$.

Variety of Loss+Penalty Formulations for SVM

Loss	Penalty function	Resulting algorithm
Hinge Loss: $\sum_{i=1}^{m}[1 - y_i f(x_i)]_+$	$\lambda \lVert w \rVert_2^2$	SVM
Mean Squared Error $\sum_{i=1}^{m}(y_i - f(x_i))^2$	$\lambda \lVert w \rVert_2^2$	Ridge Regression
Mean Squared Error $\sum_{i=1}^{m}(y_i - f(x_i))^2$	$\lambda \lVert w \rVert_1$	Lasso
Mean Squared Error $\sum_{i=1}^{m}(y_i - f(x_i))^2$	$\lambda_1 \lVert w \rVert_1 + \lambda_2 \lVert w \rVert_2^2$	Elastic Net
Hinge Loss: $\sum_{i=1}^{m}[1 - y_i f(x_i)]_+$	$\lambda \lVert w \rVert_1$	1-Norm SVM

Variety of Loss+Penalty Formulations for SVM

Loss	Penalty function	Resulting algorithm
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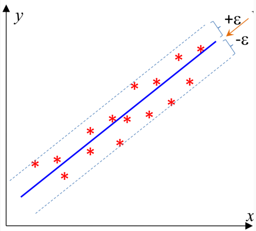
Mean Squared Error $\sum_{i=1}^{m}(y_i - f(x_i))^2$	$\lambda\|w\|_2^2$	Ridge Regression
Mean Squared Error $\sum_{i=1}^{m}(y_i - f(x_i))^2$	$\lambda\|w\|_1$	Lasso
Mean Squared Error $\sum_{i=1}^{m}(y_i - f(x_i))^2$	$\lambda_1\|w\|_1 + \lambda_2\|w\|_2^2$	Elastic Net
Hinge Loss: $\sum_{i=1}^{m}[1 - y_i f(x_i)]_+$	$\lambda\|w\|_1$	1-Norm SVM

Algorithm	Loss	Penalty
SVM	convex, non-differentiable	convex, differentiable
Ridge Regression	convex, differentiable	convex, differentiable
Lasso	convex, differentiable	convex, non-differentiable
Elastic Net	convex, differentiable	convex, non-differentiable
Hinge Loss	convex, non-differentaible	convex, non-differentiable

Hard Margin SVM Regression: ϵ-SVR



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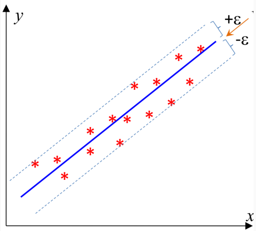
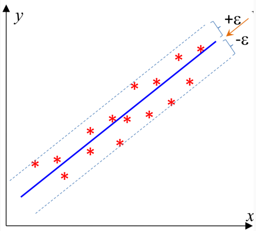


Goal: Find a linear function that fits the red data points.

Hard Margin SVM Regression: ϵ-SVR

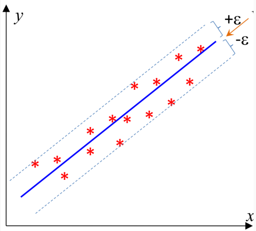


Goal: Find a linear function that fits the red data points.

Optimization Model:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\left\|w\right\|^2 \\ \text{subject to:} \quad & y_i(w \cdot x_i + b) \leq \epsilon, \\ & y_i(w \cdot x_i + b) \geq -\epsilon, \\ & i = 1, \dots, m. \end{aligned}$$

Hard Margin SVM Regression: ϵ-SVR



Goal: Find a linear function that fits the red data points.

Optimization Model:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\,\|w\|^2 \\ \text{subject to:} \quad & y_i(w \cdot x_i + b) \le \epsilon, \\ & y_i(w \cdot x_i + b) \ge -\epsilon, \\ & i = 1, \dots, m. \end{aligned}$$

Remark: Hence, the model suggests that the difference between y_i and fitted function should be smaller than ϵ (hyperparameter) and larger than $-\epsilon$. That is

$$|y_i - (w \cdot x_i + b)| \le \epsilon.$$

Here y_i is the height of the samples x_i, and not $+1$ or -1 labels!

Formlate Dual Margin Kernel SVM Problem for QP

Dual Soft-Margin Kernel SVM:

$$\begin{aligned}
\text{Maximize} \quad & \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j \, y_i y_j \, \Phi(x_i) \cdot \Phi(x_j) \\
\text{subject to} \quad & 0 \leq \lambda_i \leq C, \quad i = 1, \ldots, m, \\
& \sum_{i=1}^{m} \lambda_i y_i = 0.
\end{aligned}$$

Formlate Dual Margin Kernel SVM Problem for QP

Dual Soft-Margin Kernel SVM:

$$\begin{aligned} \text{Maximize} \quad & \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j \, y_i y_j \, \Phi(x_i) \cdot \Phi(x_j) \\ \text{subject to} \quad & 0 \le \lambda_i \le C, \quad i = 1, \dots, m, \\ & \sum_{i=1}^{m} \lambda_i y_i = 0. \end{aligned}$$

Recall QP:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2} x^T P x + q^T x, \\ \text{subject to} \quad & Gx \le h, \\ & Ax = b \end{aligned}$$

How to set: x, P, q, G, h, A, b?

Formlate Dual Margin Kernel SVM Problem for QP

Dual Soft-Margin Kernel SVM:

$$\begin{aligned} \text{Maximize} \quad & \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j \, y_i y_j \, \Phi(x_i) \cdot \Phi(x_j) \\ \text{subject to} \quad & 0 \leq \lambda_i \leq C, \quad i = 1, \ldots, m, \\ & \sum_{i=1}^{m} \lambda_i y_i = 0. \end{aligned}$$

Recall QP:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2} \underline{x}^T P x + q^T x, \\ \text{subject to} \quad & Gx \leq h, \\ & Ax = b \end{aligned}$$

How to set: x, P, q, G, h, A, b?

1. Set $\underline{x} = [\lambda_1, \lambda_2, \ldots, \lambda_m]^T$

Formlate Dual Margin Kernel SVM Problem for QP

Dual Soft-Margin Kernel SVM:

$$\begin{aligned} \text{Maximize} \quad & \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j \, y_i y_j \, \underline{\Phi(x_i) \cdot \Phi(x_j)} \\ \text{subject to} \quad & 0 \leq \lambda_i \leq C, \quad i = 1, \ldots, m, \\ & \sum_{i=1}^{m} \lambda_i y_i = 0. \end{aligned}$$

Recall QP:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2} x^T P x + q^T x, \\ \text{subject to} \quad & G x \leq h, \\ & A x = b \end{aligned}$$

How to set: x, P, q, G, h, A, b?

1. Set $x = [\lambda_1, \lambda_2, \ldots, \lambda_m]^T$
2. Let $\underline{K(x_i, x_j)} = \underline{\Phi(x_i) \cdot \Phi(x_j)}$

Formlate Dual Margin Kernel SVM Problem for QP

Dual Soft-Margin Kernel SVM:

$$\begin{aligned} \text{Maximize} \quad & \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j \, y_i y_j \, \underbrace{\Phi(x_i) \cdot \Phi(x_j)}_{K} \\ \text{subject to} \quad & 0 \le \lambda_i \le C, \quad i = 1, \ldots, m, \\ & \sum_{i=1}^{m} \lambda_i y_i = 0. \end{aligned}$$

Recall QP:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2} x^T P x + q^T x, \\ \text{subject to} \quad & Gx \le h, \\ & Ax = b \end{aligned}$$

How to set: x, P, q, G, h, A, b?

$$[\lambda_1 \cdot \ \lambda_m] \, P \begin{bmatrix} \lambda_1 \\ \vdots \\ \lambda_m \end{bmatrix}$$

1. Set $x = [\lambda_1, \lambda_2, \ldots, \lambda_m]^T$
2. Let $K(x_i, x_j) = \Phi(x_i) \cdot \Phi(x_j)$
3. Set matrix $P_{ij} = y_i y_j K(x_i, x_j)$

Formlate Dual Margin Kernel SVM Problem for QP

Dual Soft-Margin Kernel SVM:

$$\begin{aligned}
\text{Maximize} \quad & \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j \, y_i y_j \, \Phi(x_i) \cdot \Phi(x_j) \\
\text{subject to} \quad & 0 \le \lambda_i \le C, \quad i = 1, \ldots, m, \\
& \sum_{i=1}^{m} \lambda_i y_i = 0.
\end{aligned}$$

$$\min \boxed{-\sum \lambda_i} + \frac{1}{2} \sum \lambda_i \lambda_j y_i y_j \phi(x_i) \phi(x_j)$$

Recall QP:

$$\begin{aligned}
\underline{\text{minimize}} \quad & \frac{1}{2} x^T P x + \underline{q}^T x, \\
\text{subject to} \quad & Gx \le h, \\
& Ax = b
\end{aligned}$$

How to set: x, P, q, G, h, A, b?

1. Set $x = [\lambda_1, \lambda_2, \ldots, \lambda_m]^T$
2. Let $K(x_i, x_j) = \Phi(x_i) \cdot \Phi(x_j)$
3. Set matrix $P_{ij} = y_i y_j K(x_i, x_j)$
4. q is column vector containing $\underline{\text{-1}}$.

Formlate Dual Margin Kernel SVM Problem for QP

Dual Soft-Margin Kernel SVM:

$$\begin{aligned} \text{Maximize} \quad & \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j \, y_i y_j \, \Phi(x_i) \cdot \Phi(x_j) \\ \text{subject to} \quad & 0 \leq \lambda_i \leq C, \quad i = 1, \ldots, m, \\ & \sum_{i=1}^{m} \underset{x}{\boxed{\lambda_i}} y_i = \boxed{0}. \end{aligned}$$

Recall QP:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2} x^T P x + q^T x, \\ \text{subject to} \quad & Gx \leq h, \\ & \underline{Ax} = \underline{b} \end{aligned}$$

How to set: x, P, q, G, h, A, b?

1. Set $x = [\lambda_1, \lambda_2, \ldots, \lambda_m]^T$
2. Let $K(x_i, x_j) = \Phi(x_i) \cdot \Phi(x_j)$
3. Set matrix $P_{ij} = y_i y_j K(x_i, x_j)$
4. q is column vector containing -1.
5. For equality constraint, set
   $A = \underline{[y_1, y_2, \ldots, y_m]}^T, \; b = \underline{0}$

Formlate Dual Margin Kernel SVM Problem for QP

Dual Soft-Margin Kernel SVM:

$$\text{Maximize} \quad \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j \, y_i y_j \, \Phi(x_i) \cdot \Phi(x_j)$$

$$\text{subject to} \quad \underline{0 \le \lambda_i \le C}, \quad i = 1, \ldots, m,$$

$$\sum_{i=1}^{m} \lambda_i y_i = 0.$$

$\boxed{-\lambda_i \le 0}$

$\lambda_i \geq 0$

$\boxed{\lambda_i \le C}$

Recall QP:

$$\text{minimize} \quad \frac{1}{2} x^T P x + q^T x,$$

$$\text{subject to} \quad Gx \le h,$$

$$Ax = b$$

How to set: x, P, q, G, h, A, b?

1. Set $x = [\lambda_1, \lambda_2, \ldots, \lambda_m]^T$
2. Let $K(x_i, x_j) = \Phi(x_i) \cdot \Phi(x_j)$
3. Set matrix $P_{ij} = y_i y_j K(x_i, x_j)$
4. q is column vector containing -1.
5. For equality constraint, set $A = [y_1, y_2, \ldots, y_m]^T$, $b = 0$
6. Inequalities: $\underline{-\lambda_i \le 0}$, $\underline{\lambda_i \le C}$

Formlate Dual Margin Kernel SVM Problem for QP

Dual Soft-Margin Kernel SVM:

$$\begin{aligned} \text{Maximize} \quad & \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j \, y_i y_j \, \Phi(x_i) \cdot \Phi(x_j) \\ \text{subject to} \quad & 0 \leq \lambda_i \leq C, \quad i = 1, \ldots, m, \\ & \sum_{i=1}^{m} \lambda_i y_i = 0. \end{aligned}$$

Recall QP:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2} x^T P x + q^T x, \\ \text{subject to} \quad & Gx \leq h, \\ & Ax = b \end{aligned}$$

How to set: x, P, q, G, h, A, b?

1. Set $x = [\lambda_1, \lambda_2, \ldots, \lambda_m]^T$
2. Let $K(x_i, x_j) = \Phi(x_i) \cdot \Phi(x_j)$
3. Set matrix $P_{ij} = y_i y_j K(x_i, x_j)$
4. q is column vector containing -1.
5. For equality constraint, set
   $A = [y_1, y_2, \ldots, y_m]^T, \; b = 0$
6. Inequalities: $-\lambda_i \leq 0, \, \lambda_i \leq C$
7. Set G as

Formlate Dual Margin Kernel SVM Problem for QP

Dual Soft-Margin Kernel SVM:

$$\text{Maximize} \quad \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i,j=1}^{m} \lambda_i \lambda_j \, y_i y_j \, \Phi(x_i) \cdot \Phi(x_j)$$

$$\text{subject to} \quad 0 \leq \lambda_i \leq C, \quad i = 1, \ldots, m,$$

$$\sum_{i=1}^{m} \lambda_i y_i = 0.$$

Recall QP:

$$\text{minimize} \quad \frac{1}{2} x^T P x + q^T x,$$

$$\text{subject to} \quad Gx \leq h,$$

$$Ax = b$$

How to set: x, P, q, G, h, A, b?

1. Set $x = [\lambda_1, \lambda_2, \ldots, \lambda_m]^T$
2. Let $K(x_i, x_j) = \Phi(x_i) \cdot \Phi(x_j)$
3. Set matrix $P_{ij} = y_i y_j K(x_i, x_j)$
4. q is column vector containing -1.
5. For equality constraint, set $A = [y_1, y_2, \ldots, y_m]^T$, $b = 0$
6. Inequalities: $-\lambda_i \leq 0$, $\lambda_i \leq C$

$$h = \begin{bmatrix} C \\ C \\ C \\ \vdots \\ C \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

7. Set G as

$$G = \left[\begin{array}{cccc} 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \ddots & \ldots & \vdots \\ 0 & 0 & \ldots & 1 \\ \hline -1 & 0 & \ldots & 0 \\ \vdots & \ddots & \ldots & \vdots \\ 0 & 0 & \ldots & -1 \end{array}\right] \quad \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_m \end{bmatrix}$$

x

$-\lambda_1 \leq 0$

Formlate Dual Margin Kernel SVM Problem for QP

Dual Soft-Margin Kernel SVM:

$$\text{Maximize} \quad \sum_{i=1}^{m} \lambda_i - \frac{1}{2}\sum_{i,j=1}^{m} \lambda_i\lambda_j\, y_i y_j\, \Phi(x_i)\cdot\Phi(x_j)$$

$$\text{subject to} \quad 0 \le \lambda_i \le C, \quad i = 1,\dots,m,$$

$$\sum_{i=1}^{m} \lambda_i y_i = 0.$$

Recall QP:

$$\text{minimize} \quad \frac{1}{2}x^T P x + q^T x,$$

$$\text{subject to} \quad Gx \le h,$$

$$Ax = b$$

How to set: x, P, q, G, h, A, b?

1. Set $x = [\lambda_1, \lambda_2, \dots, \lambda_m]^T$
2. Let $K(x_i, x_j) = \Phi(x_i)\cdot\Phi(x_j)$
3. Set matrix $P_{ij} = y_i y_j K(x_i, x_j)$
4. q is column vector containing -1.
5. For equality constraint, set
   $A = [y_1, y_2, \dots, y_m]^T$, $b = 0$
6. Inequalities: $-\lambda_i \le 0$, $\lambda_i \le C$

$\lambda_1 \le C$

$\lambda_2 \le C$

$\lambda_m \le C$

$$I\begin{bmatrix}\lambda_1\\ \lambda_2\\ \lambda_m\end{bmatrix} \le \begin{bmatrix}C\\ C\\ C\end{bmatrix}$$

7. Set G as

$$G = \left[\begin{array}{cccc} 1 & 0 & \dots & 0\\ 0 & 1 & \dots & 0\\ \vdots & \ddots & \dots & \vdots\\ 0 & 0 & \dots & 1\\ \hline -1 & 0 & \dots & 0\\ \vdots & \ddots & \dots & \vdots\\ 0 & 0 & \dots & -1 \end{array}\right]$$

I

$-I$

8. $h = [C, C, \dots, C \,|\, 0, \dots, 0]^T$

Algorithms for Dual Soft Margin Kernel SVM

Algorithm 1 Algorithm for solving Dual Kernel SVM using QP

```
Initialization:
    • Compute $K = XX^T$, if possible using input space. ✓
    • For linear kernel, return $K$, for polynomial of degree $d$, return $\frac{1}{d}K^d$. ✓
    • For RBF kernel, compute $K = \exp(-(x - x')^2/2\sigma^2)$. ✓
Training: Assemble matrices and vectors to solve QP for dual
        $\min_x \quad (x^T P x + q^T x), \quad \text{subject to } Gx \leq h, \; Ax = b.$
    • Define $x, P, q, G, x, h, b$ as described in previous slide.
```

Pass to some solver.