Support Vector Machine and Kernel Methods

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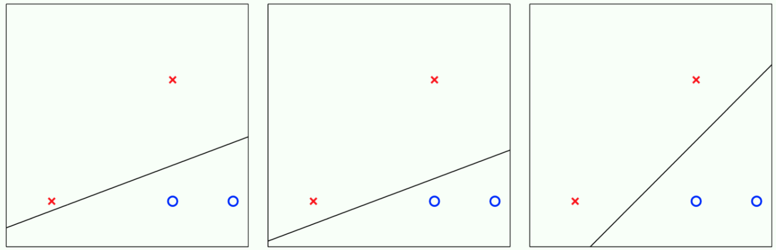
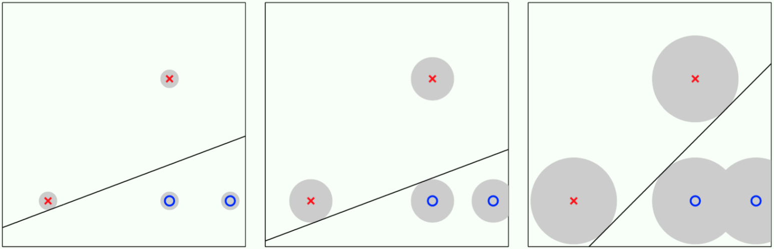
Which Separator Do You Pick?

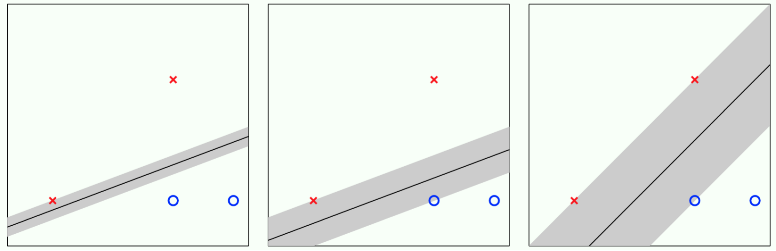


Robustness to Noisy Data



Being robust to noise (measurement error) is good (remember regularization).

Thicker Cushion Means More Robustness



We call such hyperplanes **fat**

Two Crucial Questions

1. Can we efficiently find the fattest separating hyperplane?
2. Is a fatter hyperplane better than a thin one?

Pulling Out the Bias

Before

$$\mathbf{x} \in \{1\} \times \mathbb{R}^d; \mathbf{w} \in \mathbb{R}^{d+1}$$

$$\mathbf{x} = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{bmatrix}; \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix}$$

$$\text{signal} = \mathbf{w}^T \mathbf{x}$$

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signal $= \mathbf{w}^T\mathbf{x}$

After

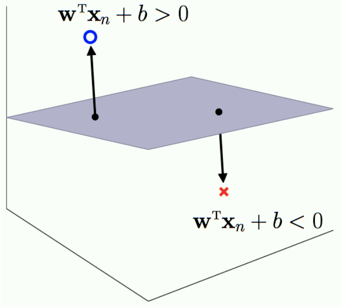
$$\mathbf{x} \in \mathbb{R}^d; b \in \mathbb{R}, \mathbf{w} \in \mathbb{R}^d$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}; \mathbf{w} = \begin{bmatrix} w_1 \\ \vdots \\ w_d \end{bmatrix}$$

bias b

signal $= \mathbf{w}^T\mathbf{x} + b$

Separating The Data


$\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b > 0$
$\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b < 0$

Hyperplane $h = (b, \mathbf{w})$
h separates the data means:

$$y_n(\mathbf{w}^T\mathbf{x}_n + b) > 0$$

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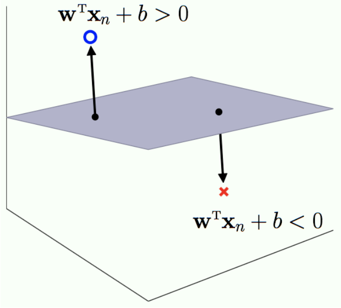
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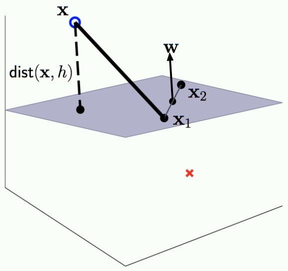
Hyperplane $h = (b, \mathbf{w})$
h separates the data means:

$$y_n(\mathbf{w}^T\mathbf{x}_n + b) > 0$$

By rescaling the weights and bias,

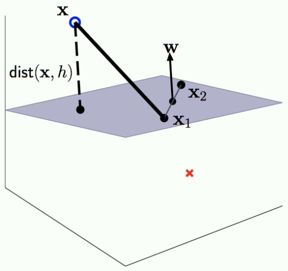
$$\min_{n=1,\ldots,N} y_n(\mathbf{w}^T\mathbf{x}_n + b) = 1$$

Distance to the Hyperplane



- $\mathbf{w}$ is normal to the hyperplane (why?)

Distance to the Hyperplane



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  $\mathbf{w}^T(\mathbf{x}_2 - \mathbf{x}_1) = \mathbf{w}^T\mathbf{x}_2 - \mathbf{w}^T\mathbf{x}_1 = -b + b = 0$

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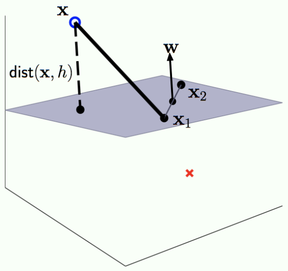

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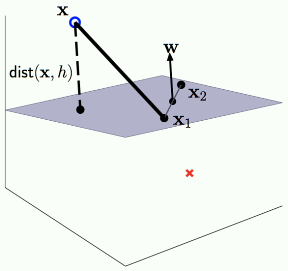
- Scalar projection:

$$\mathbf{a}^T\mathbf{b} = \|\mathbf{a}\|\|\mathbf{b}\|\cos(\mathbf{a},\mathbf{b})$$
$$\Rightarrow \mathbf{a}^T\mathbf{b}/\|\mathbf{b}\| = \|\mathbf{a}\|\cos(\mathbf{a},\mathbf{b})$$

Distance to the Hyperplane



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- let $\mathbf{x}_\perp$ be the orthogonal projection of $\mathbf{x}$ to h, distance to hyperplane is given by projection of $\mathbf{x} - \mathbf{x}_\perp$ to $\mathbf{w}$ (why?)

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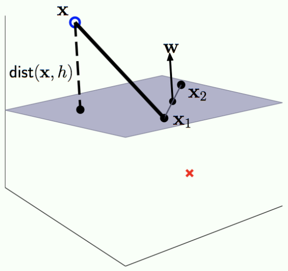

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- let $\mathbf{x}_\perp$ be the orthogonal projection of $\mathbf{x}$ to h, distance to hyperplane is given by projection of $\mathbf{x} - \mathbf{x}_\perp$ to $\mathbf{w}$ (why?)

$$\text{dist}(\mathbf{x}, h) = \frac{1}{\|\mathbf{w}\|} \cdot |\mathbf{w}^T\mathbf{x} - \mathbf{w}^T\mathbf{x}_\perp|$$
$$= \frac{1}{\|\mathbf{w}\|} \cdot |\mathbf{w}^T\mathbf{x} + b|$$

Fatness of a Separating Hyperplane

$$\text{dist}(\mathbf{x}, h) = \frac{1}{\|\mathbf{w}\|} \cdot |\mathbf{w}^T\mathbf{x} + b| = \frac{1}{\|\mathbf{w}\|} \cdot |y_n(\mathbf{w}^T\mathbf{x} + b)| = \frac{1}{\|\mathbf{w}\|} \cdot y_n(\mathbf{w}^T\mathbf{x} + b)$$

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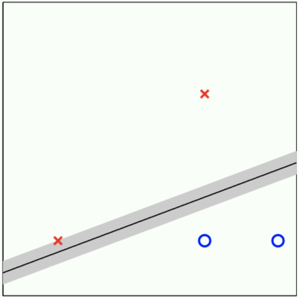
Fatness

$=$ Distance to the closest point



$$\begin{aligned} \text{Fatness} &= \min_n \text{dist}(\mathbf{x}_n, h) \\ &= \frac{1}{\|\mathbf{w}\|} \min_n y_n(\mathbf{w}^T\mathbf{x} + b) \\ &= \frac{1}{\|\mathbf{w}\|} \end{aligned}$$

Maximizing the Margin

- Formal definition of margin:

$$\text{margin: } \gamma(h) = \frac{1}{\|\mathbf{w}\|}$$

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$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

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- An equivalent objective:

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

$$\text{subject to: } y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1 \text{ for } n = 1, \ldots, N$$

Example - Our Toy Data Set

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

subject to: $y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1$ for $n = 1, \ldots, N$

Training Data:

$$X = \begin{bmatrix} 0 & 0 \\ 2 & 2 \\ 2 & 0 \\ 3 & 0 \end{bmatrix}, \mathbf{y} = \begin{bmatrix} -1 \\ -1 \\ +1 \\ +1 \end{bmatrix}$$

What is the margin?

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$$\begin{cases} (1) + (3) & \rightarrow w_1 \geq 1 \\ (2) + (3) & \rightarrow w_2 \leq -1 \end{cases} \Rightarrow \frac{1}{2}\mathbf{w}^T\mathbf{w} = \frac{1}{2}(w_1^2 + w_2^2) \geq 1$$

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Thus: $w_1 = 1, w_2 = -1, b = -1$

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- Given data $X = \begin{bmatrix} 0 & 0 \\ 2 & 2 \\ 2 & 0 \\ 3 & 0 \end{bmatrix}$
- Optimal solution

$$\mathbf{w}^* = \begin{bmatrix} w_1 = 1 \\ w_2 = -1 \end{bmatrix}, b^* = -1$$

- Optimal hyperplane
  $g(\mathbf{x}) = \mathsf{sign}(x_1 - x_2 - 1)$

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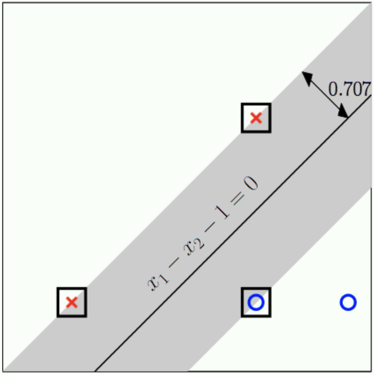

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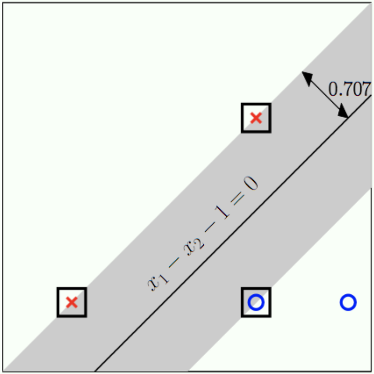

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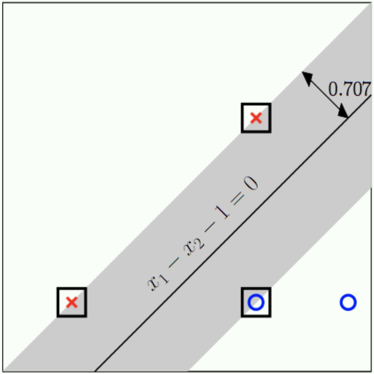

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Support Vectors

Solver: Quadratic Programming

$$\min_{\mathbf{u}\in\mathbb{R}^q} \quad \frac{1}{2}\mathbf{u}^T Q\mathbf{u} + \mathbf{p}^T\mathbf{u}$$

subject to: $A\mathbf{u} \geq \mathbf{c}$

$$\mathbf{u}^* \leftarrow QP(Q, \mathbf{p}, A, \mathbf{c})$$

($Q = 0$ is linear programming.)

`http://cvxopt.org/examples/tutorial/qp.html`

Maximum Margin Hyperplane is QP

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

subject to: $y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1, \forall n$

$$\min_{\mathbf{u}\in\mathbb{R}^q} \quad \frac{1}{2}\mathbf{u}^T Q\mathbf{u} + \mathbf{p}^T\mathbf{u}$$

subject to: $A\mathbf{u} \geq \mathbf{c}$

$$\mathbf{u} = \begin{bmatrix} b \\ \mathbf{w} \end{bmatrix} \in \mathbb{R}^{d+1} \Rightarrow \frac{1}{2}\mathbf{w}^T\mathbf{w} = [b, \mathbf{w}^T] \begin{bmatrix} 0 & \mathbf{0}_d^T \\ \mathbf{0}_d & I_d \end{bmatrix} \begin{bmatrix} b \\ \mathbf{w}^T \end{bmatrix} = \mathbf{u}^T \begin{bmatrix} 0 & \mathbf{0}_d^T \\ \mathbf{0}_d & I_d \end{bmatrix} \mathbf{u}$$

Maximum Margin Hyperplane is QP

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} \qquad\qquad \min_{\mathbf{u}\in\mathbb{R}^q} \quad \frac{1}{2}\mathbf{u}^T Q\mathbf{u} + \mathbf{p}^T\mathbf{u}$$

subject to: $y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1, \forall n$ subject to: $A\mathbf{u} \geq \mathbf{c}$

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$$Q = \begin{bmatrix} 0 & \mathbf{0}_d^T \\ \mathbf{0}_d & I_d \end{bmatrix}, \mathbf{p} = \mathbf{0}_{d+1}$$

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$$y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1 = [y_n, y_n\mathbf{x}_n^T]\mathbf{u} \geq 1 \Rightarrow \begin{bmatrix} y_1 & y_1\mathbf{x}_1^T \\ \vdots & \vdots \\ y_N & y_N\mathbf{x}_N^T \end{bmatrix} \mathbf{u} \geq \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

Maximum Margin Hyperplane is QP

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subject to: $y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1, \forall n$

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$$A = \begin{bmatrix} y_1 & y_1\mathbf{x}_1^T \\ \vdots & \vdots \\ y_N & y_N\mathbf{x}_N^T \end{bmatrix}, \boldsymbol{c} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

Back To Our Example

Exercise:

$$X = \begin{bmatrix} 0 & 0 \\ 2 & 2 \\ 2 & 0 \\ 3 & 0 \end{bmatrix}, \mathbf{y} = \begin{bmatrix} -1 \\ -1 \\ +1 \\ +1 \end{bmatrix} \qquad \begin{cases} (1) : -b \geq 1 \\ (2) : -(2w_1 + 2w_2 + b) \geq 1 \\ (3) : 2w_1 + b \geq 1 \\ (4) : 3w_1 + b \geq 1 \end{cases}$$

Show the corresponding $Q, \mathbf{p}, A, \mathbf{c}$.

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$$Q = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \mathbf{p} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, A = \begin{bmatrix} -1 & 0 & 0 \\ -1 & -2 & -2 \\ 1 & 2 & 0 \\ 1 & 3 & 0 \end{bmatrix}, \mathbf{c} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

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Use your QP-solver to give

$$\boldsymbol{u}^* = [b^*, w_1^*, w_2^*]^T = [-1, 1, -1]$$

Primal QP algorithm for linear-SVM

1. Let $\boldsymbol{p} = \mathbf{0}_{d+1}$ be the $(d+1)$-vector of zeros and $\boldsymbol{c} = \mathbf{1}_N$ the N-vector of ones. Construct matrices Q and A, where

$$A = \begin{bmatrix} y_1 & -y_1\mathbf{x}_1^T- \\ \vdots & \vdots \\ y_N & -y_N\mathbf{x}_N^T- \end{bmatrix}, Q = \begin{bmatrix} 0 & \mathbf{0}_d^T \\ \mathbf{0}_d & I_d \end{bmatrix}$$

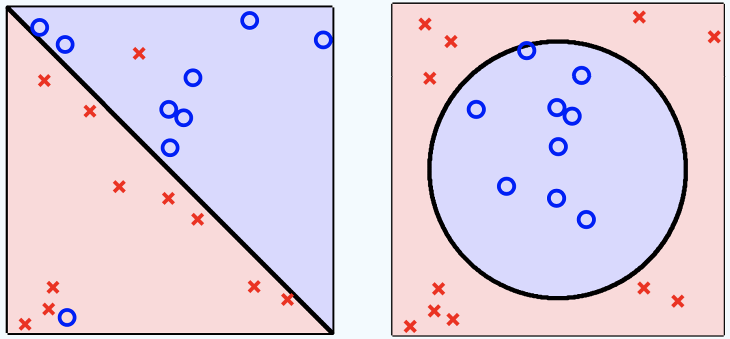
2. Return $\begin{bmatrix} b^* \\ \mathbf{w}^* \end{bmatrix} = \boldsymbol{u}^* \leftarrow QP(Q, \boldsymbol{p}, A, \boldsymbol{c})$.
3. The final hypothesis is $g(\mathbf{x}) = \text{sign}(\mathbf{x}^T\mathbf{w}^* + b^*)$.

Link to Regularization

$$\min_{\mathbf{w}} \quad E_{in}(\mathbf{w})$$
$$\text{subject to: } \mathbf{w}^T\mathbf{w} \leq C$$

	optimal hyperplane	regularization
minimize	$\mathbf{w}^T\mathbf{w}$	E_{in}
subject to	$E_{in} = 0$	$\mathbf{w}^T\mathbf{w} \leq C$

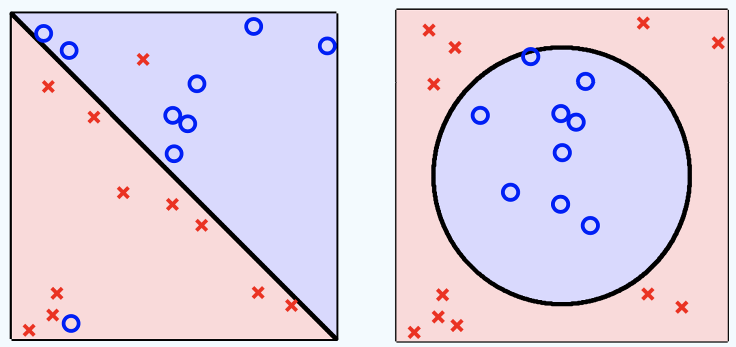
How to Handle Non-Separable Data?



(a) Few noisy data.

(b) Nonlinearly separable.

How to Handle Non-Separable Data?



(a) Few noisy data.

(b) Nonlinearly separable.

(a) Tolerate noisy data points: soft-margin SVM.

(b) Inherent nonlinear boundary: non-linear transformation.

Non-Linear Transformation

$$\mathbf{\Phi}_1(\mathbf{x}) = (x_1, x_2)$$
$$\mathbf{\Phi}_2(\mathbf{x}) = (x_1, x_2, x_1^2, x_1x_2, x_2^2)$$
$$\mathbf{\Phi}_3(\mathbf{x}) = (x_1, x_2, x_1^2, x_1x_2, x_2^2, x_1^3, x_1^2x_2, x_1x_2^2, x_2^3)$$

Non-Linear Transformation

- Using the nonlinear transform with the optimal hyperplane using a transform $\mathbf{\Phi}$: $\mathbb{R}^d \rightarrow \mathbb{R}^{\tilde{d}}$:

$$\mathbf{z}_n = \mathbf{\Phi}(\mathbf{x}_n)$$

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- Solve the hard-margin SVM in the $\mathcal{Z}$-space $(\tilde{\mathbf{w}}^*, \tilde{b}^*)$:

$$\min_{\tilde{b}, \tilde{\mathbf{w}}} \quad \frac{1}{2}\tilde{\mathbf{w}}^T\tilde{\mathbf{w}}$$

$$\text{subject to: } y_n(\tilde{\mathbf{w}}^T\mathbf{z}_n + \tilde{b}) \geq 1, \forall n$$

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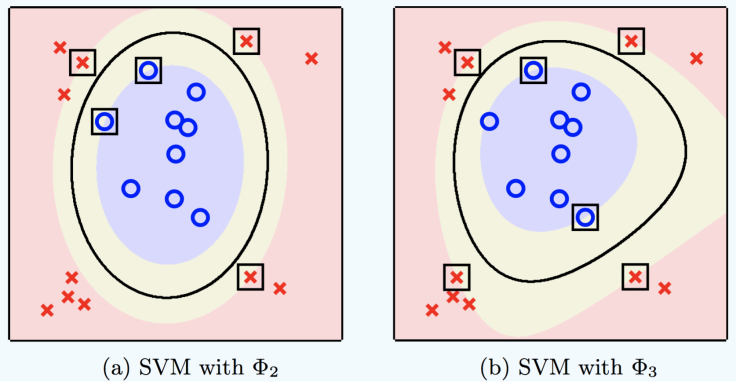
$$\text{subject to: } y_n(\tilde{\mathbf{w}}^T\mathbf{z}_n + \tilde{b}) \geq 1, \forall n$$

- Final hypothesis:

$$g(\mathbf{x}) = \text{sign}(\tilde{\mathbf{w}}^{*T}\mathbf{\Phi}(\mathbf{x}) + \tilde{b}^*)$$

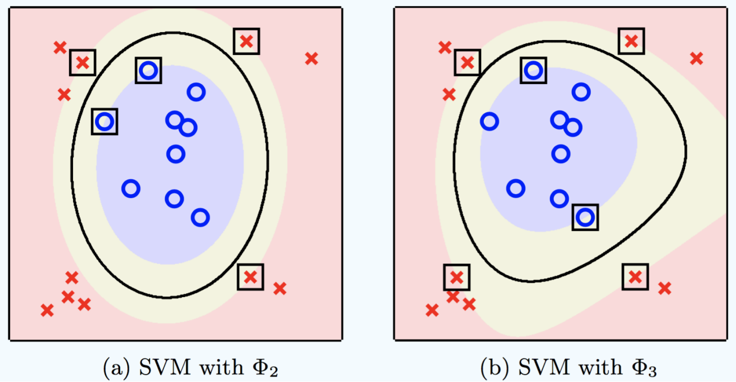
SVM and non-linear transformation


(a) SVM with Φ_2

(b) SVM with Φ_3

The margin is shaded in yellow, and the support vectors are boxed.

SVM and non-linear transformation

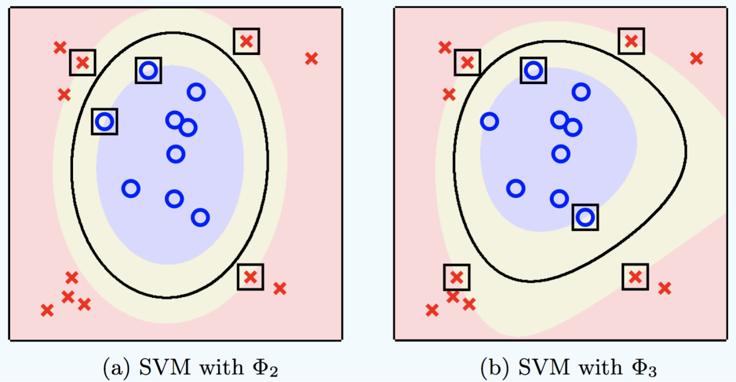


(a) SVM with Φ_2 (b) SVM with Φ_3

The margin is shaded in yellow, and the support vectors are boxed.

- For $\mathbf{\Phi}_2$, $\tilde{d}_2 = 5$ and for $\mathbf{\Phi}_3$, $\tilde{d}_3 = 9$

SVM and non-linear transformation



(a) SVM with Φ_2 (b) SVM with Φ_3

The margin is shaded in yellow, and the support vectors are boxed.

- For $\mathbf{\Phi}_2$, $\tilde{d}_2 = 5$ and for $\mathbf{\Phi}_3$, $\tilde{d}_3 = 9$
- $\tilde{d}_3$ is nearly double $\tilde{d}_2$, yet the resulting SVM separator is not severely overfitting with $\mathbf{\Phi}_3$ (regularization?).

Support Vector Machine Summary

- A very powerful, easy to use linear model which comes with automatic regularization.

Support Vector Machine Summary

- A very powerful, easy to use linear model which comes with automatic regularization.
- Fully exploit SVM: Kernel
    - potential robustness to overfitting even after transforming to a much higher dimension
    - How about infinite dimensional transforms?
    - Kernel Trick

SVM Dual: Formulation

- Primal and dual in optimization.

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SVM Dual: Formulation

- Primal and dual in optimization.
- The dual view of SVM enables us to exploit the kernel trick.
- In the primal SVM problem we solve $\mathbf{w} \in \mathbb{R}^d, b$, while in the dual problem we solve $\boldsymbol{\alpha} \in \mathbb{R}^N$

$$\begin{aligned} \max_{\boldsymbol{\alpha} \in \mathbb{R}^N} \ & \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m=1}^{N} \sum_{n=1}^{N} \alpha_n \alpha_m y_n y_m \mathbf{x}_n^T \mathbf{x}_m \\ \text{subject to } & \sum_{n=1}^{N} y_n \alpha_n = 0, \alpha_n \geq 0, \forall n \end{aligned}$$

which is also a QP problem.

SVM Dual: Prediction

- We can obtain the primal solution:

$$\mathbf{w}^* = \sum_{n=1}^{N} y_n \alpha_n^* \mathbf{x}_n$$

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SVM Dual: Prediction

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- The optimal hypothesis:

$$\begin{aligned} g(\mathbf{x}) &= \text{sign}(\mathbf{w}^{*T}\mathbf{x} + b^*) \\ &= \text{sign}\left(\sum_{n=1}^{N} y_n \alpha_n^* \mathbf{x}_n^T \mathbf{x} + b^*\right) \\ &= \text{sign}\left(\sum_{\alpha_n^* > 0} y_n \alpha_n^* \mathbf{x}_n^T \mathbf{x} + b^*\right) \end{aligned}$$

Dual SVM: Summary

$$\max_{\boldsymbol{\alpha}\in\mathbb{R}^N} \sum_{n=1}^{N}\alpha_n - \frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N}\alpha_n\alpha_m y_n y_m \mathbf{x}_n^T\mathbf{x}_m$$

$$\text{subject to } \sum_{n=1}^{N} y_n\alpha_n = 0, \alpha_n \geq 0, \forall n$$

$$\mathbf{w}^* = \sum_{n=1}^{N} y_n \alpha_n^* \mathbf{x}_n$$

Common SVM Basis Functions

- $\mathbf{z}_k$ = polynomial terms of $\mathbf{x}_k$ of degree 1 to q
- $\mathbf{z}_k$ = radial basis function of $\mathbf{x}_k$

$$\mathbf{z}_k(j) = \phi_j(\mathbf{x}_k) = \exp(-|\mathbf{x}_k - \mathbf{c}_j|^2/\sigma^2)$$

- $\mathbf{z}_k$ = sigmoid functions of $\mathbf{x}_k$

Quadratic Basis Functions

$$\boldsymbol{\Phi}(\mathbf{x}) = \begin{bmatrix} 1 \\ \sqrt{2}x_1 \\ \vdots \\ \sqrt{2}x_d \\ x_1^2 \\ \vdots \\ x_d^2 \\ \sqrt{2}x_1x_2 \\ \vdots \\ \sqrt{2}x_1x_d \\ \sqrt{2}x_2x_3 \\ \vdots \\ \sqrt{2}x_{d-1}x_d \end{bmatrix}$$

- Including Constant Term, Linear Terms, Pure Quadratic Terms, Quadratic Cross-Terms
- The number of terms is approximately $d^2/2$.
- You may be wondering what those $\sqrt{2}$s are doing. You'll find out why they're there soon.

Dual SVM: Non-linear Transformation

$$\max_{\boldsymbol{\alpha}\in\mathbb{R}^N} \sum_{n=1}^{N}\alpha_n - \frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N}\alpha_n\alpha_m y_n y_m \boldsymbol{\Phi}(\mathbf{x}_n)^T\boldsymbol{\Phi}(\mathbf{x}_m)$$

$$\text{subject to } \sum_{n=1}^{N} y_n\alpha_n = 0, \alpha_n \geq 0, \forall n$$

$$\mathbf{w}^* = \sum_{n=1}^{N} y_n\alpha_n^*\Phi(\mathbf{x}_n)$$

- Need to prepare a matrix Q, $Q_{nm} = y_n y_m \boldsymbol{\Phi}(\mathbf{x}_n)^T\boldsymbol{\Phi}(\mathbf{x}_m)$
- Cost?

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- Cost?
    - We must do $N^2/2$ dot products to get this matrix ready.
    - Each dot product requires $d^2/2$ additions and multiplications, The whole thing costs $N^2d^2/4$.

Quadratic Dot Products

$$\boldsymbol{\Phi}(\mathbf{a})^T\boldsymbol{\Phi}(\mathbf{b}) = \begin{bmatrix} 1 \\ \sqrt{2}a_1 \\ \vdots \\ \sqrt{2}a_m \\ a_1^2 \\ \vdots \\ a_m^2 \\ \sqrt{2}a_1a_2 \\ \vdots \\ \sqrt{2}a_1a_d \\ \sqrt{2}a_2a_3 \\ \vdots \\ \sqrt{2}a_{d-1}a_d \end{bmatrix}^T \begin{bmatrix} 1 \\ \sqrt{2}b_1 \\ \vdots \\ \sqrt{2}b_d \\ b_1^2 \\ \vdots \\ b_d^2 \\ \sqrt{2}b_1b_2 \\ \vdots \\ \sqrt{2}b_1b_d \\ \sqrt{2}b_2b_3 \\ \vdots \\ \sqrt{2}b_{d-1}b_d \end{bmatrix}$$

- Constant Term 1
- Linear Terms

$$\sum_{i=1}^{d} 2a_ib_i$$

- Pure Quadratic Terms

$$\sum_{i=1}^{d} a_i^2b_i^2$$

- Quadratic Cross-Terms

$$\sum_{i=1}^{d}\sum_{j=i+1}^{d} 2a_ia_jb_ib_j$$

Quadratic Dot Product

- Does $\mathbf{\Phi}(\mathbf{a})^T\mathbf{\Phi}(\mathbf{b})$ look familiar?

$$\mathbf{\Phi}(\mathbf{a})^T\mathbf{\Phi}(\mathbf{b}) = 1 + 2\sum_{i=1}^{d} a_i b_i + \sum_{i=1}^{d} a_i^2 b_i^2 + \sum_{i=1}^{d}\sum_{j=i+1}^{d} 2a_i a_j b_i b_j$$

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- Try this: $(\boldsymbol{a}^T\boldsymbol{b} + 1)^2$

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$$\begin{aligned}(\boldsymbol{a}^T\boldsymbol{b}+1)^2 &= (\boldsymbol{a}^T\boldsymbol{b})^2 + 2\boldsymbol{a}^T\boldsymbol{b} + 1\\ &= \left(\sum_{i=1}^{d} a_i b_i\right)^2 + 2\sum_{i=1}^{d} a_i b_i + 1\\ &= \sum_{i=1}^{d}\sum_{j=1}^{d} a_i b_i a_j b_j + 2\sum_{i=1}^{d} a_i b_i + 1\\ &= \sum_{i=1}^{d} a_i^2 b_i^2 + 2\sum_{i=1}^{d}\sum_{j=i+1}^{d} a_i a_j b_i b_j + 2\sum_{i=1}^{d} a_i b_i + 1\end{aligned}$$

Quadratic Dot Product

- Does $\mathbf{\Phi}(\mathbf{a})^T\mathbf{\Phi}(\mathbf{b})$ look familiar?

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$$\begin{aligned}(\boldsymbol{a}^T\boldsymbol{b} + 1)^2 &= (\boldsymbol{a}^T\boldsymbol{b})^2 + 2\boldsymbol{a}^T\boldsymbol{b} + 1\\ &= \left(\sum\nolimits_{i=1}^{d} a_i b_i\right)^2 + 2\sum\nolimits_{i=1}^{d} a_i b_i + 1\\ &= \sum\nolimits_{i=1}^{d}\sum\nolimits_{j=1}^{d} a_i b_i a_j b_j + 2\sum\nolimits_{i=1}^{d} a_i b_i + 1\\ &= \sum\nolimits_{i=1}^{d} a_i^2 b_i^2 + 2\sum\nolimits_{i=1}^{d}\sum\nolimits_{j=i+1}^{d} a_i a_j b_i b_j + 2\sum\nolimits_{i=1}^{d} a_i b_i + 1\end{aligned}$$

- They're the same! And this is only $O(d)$ to compute!

Dual SVM: Non-linear Transformation

$$\max_{\boldsymbol{\alpha}\in\mathbb{R}^N} \sum_{n=1}^{N} \alpha_n - \frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N} \alpha_n\alpha_m y_n y_m \mathbf{\Phi}(\mathbf{x}_n)^T \mathbf{\Phi}(\mathbf{x}_m)$$

$$\text{subject to } \sum_{n=1}^{N} y_n\alpha_n = 0, \alpha_n \geq 0, \forall n$$

$$\mathbf{w}^* = \sum_{n=1}^{N} y_n \alpha_n^* \Phi(\mathbf{x}_n)$$

- Need to prepare a matrix Q, $Q_{nm} = y_n y_m \mathbf{\Phi}(\mathbf{x}_n)^T \mathbf{\Phi}(\mathbf{x}_m)$
- Cost?
  - We must do $N^2/2$ dot products to get this matrix ready.
  - Each dot product requires d additions and multiplications.

Higher Order Polynomials

	$\mathbf{\Phi}(\mathbf{x})$	Cost	100dim
Quadratic	$d^2/2$ terms	$d^2N^2/4$	$2.5kN^2$
Cubic	$d^3/6$ terms	$d^3N^2/12$	$83kN^2$
Quartic	$d^4/24$ terms	$d^4N^2/48$	$1.96mN^2$
	$\Phi(\mathbf{a})^T\Phi(\mathbf{b})$	Cost	100dim
Quadratic	$(\mathbf{a}^T\mathbf{b}+1)^2$	$dN^2/2$	$50N^2$
Cubic	$(\mathbf{a}^T\mathbf{b}+1)^3$	$dN^2/2$	$50N^2$
Quartic	$(\mathbf{a}^T\mathbf{b}+1)^4$	$dN^2/2$	$50N^2$

Dual SVM with Quintic basis functions

$$\max_{\boldsymbol{\alpha}\in\mathbb{R}^N} \sum_{n=1}^{N}\alpha_n - \frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N}\alpha_n\alpha_m y_n y_m \underbrace{\boldsymbol{\Phi}(\mathbf{x}_n)^T\boldsymbol{\Phi}(\mathbf{x}_m)}_{(\mathbf{x}_n^T\mathbf{x}_m+1)^5}$$

$$\text{subject to } \sum_{n=1}^{N} y_n\alpha_n = 0, \alpha_n \geq 0, \forall n$$

Classification:

$$g(\mathbf{x}) = \text{sign}(\mathbf{w}^{*T}\boldsymbol{\Phi}(\mathbf{x}) + b^*) = \text{sign}\left(\sum\nolimits_{\alpha_n^*>0} y_n\alpha_n^*\boldsymbol{\Phi}(\mathbf{x}_n)^T\boldsymbol{\Phi}(\mathbf{x}) + b^*\right)$$

$$= \text{sign}\left(\sum\nolimits_{\alpha_n^*>0} y_n\alpha_n^*(\mathbf{x}_n^T\mathbf{x} + 1)^5 + b^*\right)$$

Dual SVM with general kernel functions

$$\max_{\boldsymbol{\alpha} \in \mathbb{R}^N} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m=1}^{N} \sum_{n=1}^{N} \alpha_n \alpha_m y_n y_m K(\mathbf{x}_n, \mathbf{x}_m)$$

$$\text{subject to} \sum_{n=1}^{N} y_n \alpha_n = 0, \alpha_n \geq 0, \forall n$$

Classification:

$$g(\mathbf{x}) = \text{sign}(\mathbf{w}^{*T} \boldsymbol{\Phi}(\mathbf{x}) + b^*) = \text{sign}\left(\sum\nolimits_{\alpha_n^* > 0} y_n \alpha_n^* \boldsymbol{\Phi}(\mathbf{x}_n)^T \boldsymbol{\Phi}(\mathbf{x}) + b^* \right)$$

$$= \text{sign}\left(\sum\nolimits_{\alpha_n^* > 0} y_n \alpha_n^* K(\mathbf{x}_n, \mathbf{x}_m) + b^* \right)$$

Kernel Tricks

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- Not all functions are kernel functions!
  - Need to be decomposable $K(\mathbf{a},\mathbf{b}) = \mathbf{\Phi}(\mathbf{a})^T\mathbf{\Phi}(\mathbf{b})$
  - Could $K(\mathbf{a},\mathbf{b}) = (\mathbf{a}-\mathbf{b})^3$ be a kernel function?
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  - To expand Kernel function $K(\mathbf{a},\mathbf{b})$ into a dot product, i.e., $K(\mathbf{a},\mathbf{b}) = \mathbf{\Phi}(\mathbf{a})^T \mathbf{\Phi}(\mathbf{b})$, $K(\mathbf{a},\mathbf{b})$ has to be positive semi-definite function.

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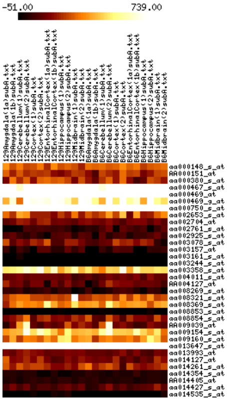
  - kernel matrix K is always symmetric PSD for any given $\mathbf{x}_1, \ldots, \mathbf{x}_N$.

Kernel Design: expression kernel



- mRNA expression data:
  - Each matrix entry is an mRNA expression measurement.
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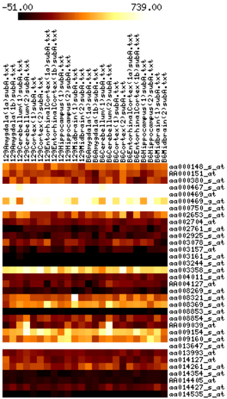

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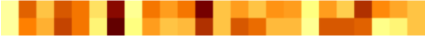
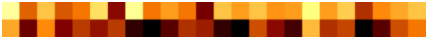


Similar



Dissimilar

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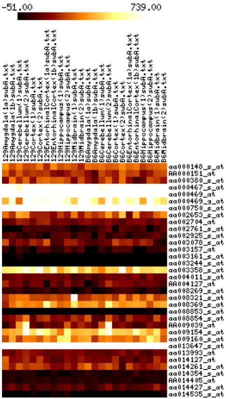

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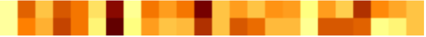
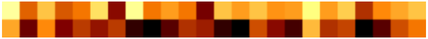


Similar



Dissimilar

- Kernel

$$K(x, y) = \frac{\sum_i x_i y_i}{\sqrt{\sum_i x_i x_i}\sqrt{\sum_i y_i y_i}}$$

Kernel Design: sequence kernel

- Work with non-vectorial data
- Scalar product on a pair of variable-length, discrete strings?

```
>ICYA_MANSE
GDIFYPGYCPDVKPVNDFDLSAFAGAWHEIAKLPLENENQGKCTIAEYKY
DGKKASVYNSFVSNGVKEYMEGDLEIAPDAKYTKQGKYVMTFKFGQRVVN
LVPWVLATDYKNYAINYMENSHPDKKAHSIHAWILSKSKVLEGNTKEVVD
NVLKTFSHLIDASKFISNDFSEAACQYSTTYSLTGPDRH

>LACB_BOVIN
MKCLLLALALTCGAQALIVTQTMKGLDIQKVAGTWYSLAMAASDISLLDA
QSAPLRVYVEELKPTPEGDLEILLQKWENGECAQKKIIAEKTKIPAVFKI
DALNENKVLVLDTDYKKYLLFCMENSAEPEQSLACQCLVRTPEVDDEALE
KFDKALKALPMHIRLSFNPTQLEEQCHI
```

Commonly Used SVM Kernel Functions

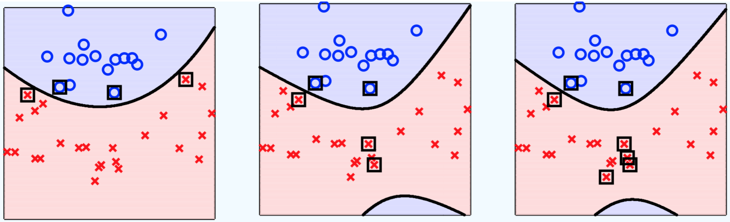
- $K(\mathbf{a}, \mathbf{b}) = (\alpha \cdot \mathbf{a}^T\mathbf{b} + \beta)^Q$ is an example of a SVM kernel function.
- Beyond polynomials there are other very high dimensional basis functions that can be made practical by finding the right Kernel Function
  - Radial-basis style kernel (RBF)/Gaussian kernel function

$$K(\mathbf{a}, \mathbf{b}) = \exp\left(-\gamma\|\mathbf{a} - \mathbf{b}\|^2\right)$$

  - Sigmoid functions

2nd Order Polynomial Kernel

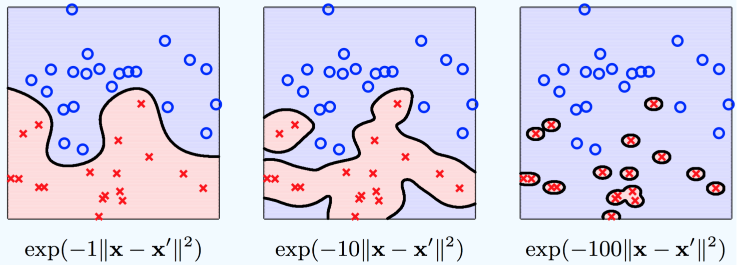
$$K(\mathbf{a}, \mathbf{b}) = (\alpha \cdot \mathbf{a}^T \mathbf{b} + \beta)^2$$



$(1 + 0.001\mathbf{x}^{\mathrm{T}}\mathbf{x}')^2$ $1 + (\mathbf{x}^{\mathrm{T}}\mathbf{x}') + (\mathbf{x}^{\mathrm{T}}\mathbf{x}')^2$ $(1 + 1000\mathbf{x}^{\mathrm{T}}\mathbf{x}')^2$

Gaussian Kernels

$$K(\mathbf{a},\mathbf{b}) = \exp\left(-\gamma\|\mathbf{a}-\mathbf{b}\|^2\right)$$



$\exp(-1\|\mathbf{x}-\mathbf{x}'\|^2)$ $\exp(-10\|\mathbf{x}-\mathbf{x}'\|^2)$ $\exp(-100\|\mathbf{x}-\mathbf{x}'\|^2)$

Gaussian Kernels

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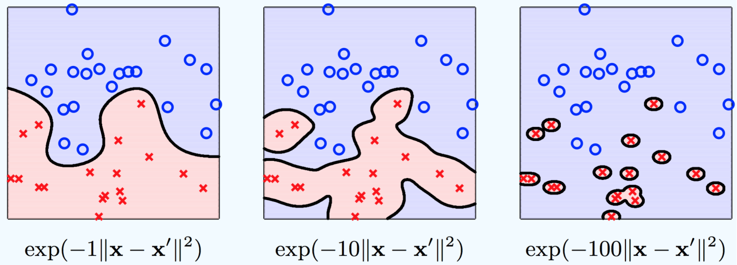
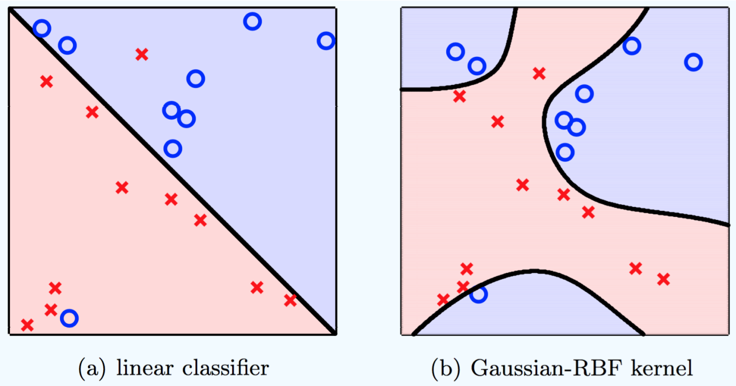


When γ is large, we clearly see that even the protection of a large margin cannot suppress overfitting. However, for a reasonably small γ, the sophisticated boundary discovered by SVM with the Gaussian-RBF kernel looks quite good.

Gaussian Kernels



(a) linear classifier

(b) Gaussian-RBF kernel

For (a) a noisy data set that linear classifier appears to work quite well, (b) using the Gaussian-RBF kernel with the hard-margin SVM leads to overfitting.

From hard-margin to soft-margin

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- Remedy: a soft formulation that allows small violation of the margins or even some classification errors.
- Soft-margin: margin violation $\varepsilon_n \geq 0$ for each data point $(\mathbf{x}_n, y_n)$ and require that

$$y_n(\mathbf{w}^T \mathbf{x}_n + b) \geq 1 - \varepsilon_n$$

  - ε_n captures by how much $(\mathbf{x}_n, y_n)$ fails to be separated.

Soft-Margin SVM

We modify the hard-margin SVM to the soft-margin SVM by allowing margin violations but adding a penalty term to discourage large violations:

$$\min_{b,\mathbf{w},\boldsymbol{\varepsilon}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{n=1}^{N}\varepsilon_n$$

$$\text{subject to: } y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1 - \varepsilon_n \text{ for } n = 1, \ldots, N$$

$$\varepsilon_n \geq 0, \text{ for } n = 1, \ldots, N$$

The meaning of C?

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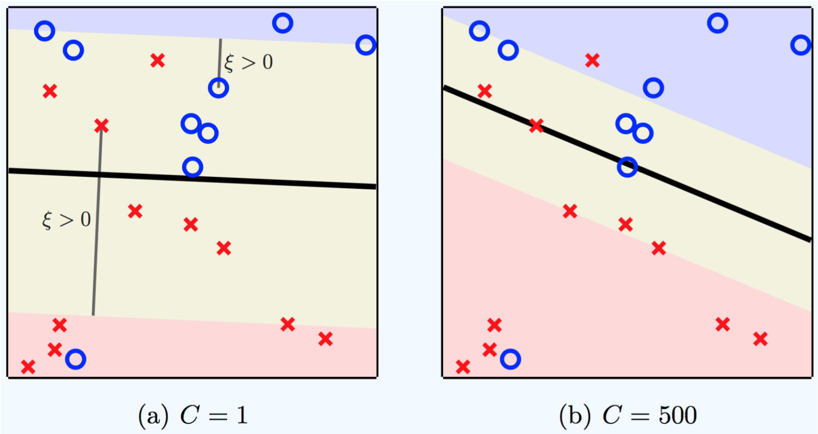
The meaning of C?

- When C is large, it means we care more about violating the margin, which gets us closer to the hard-margin SVM.
- When C is small, on the other hand, we care less about violating the margin.

Soft Margin Example

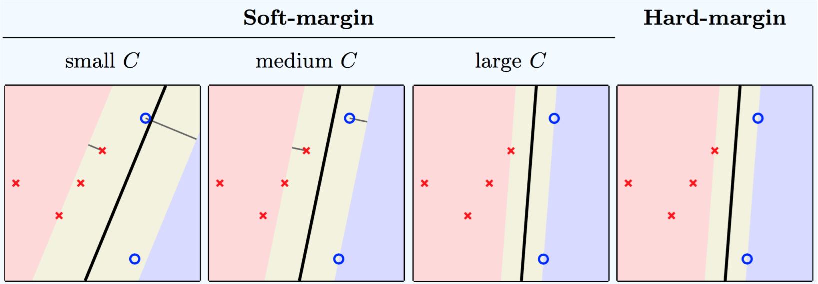


(a) $C = 1$ (b) $C = 500$

Soft Margin and Hard Margin

$$\min_{b,\mathbf{w},\boldsymbol{\varepsilon}} \quad \underbrace{\frac{1}{2}\mathbf{w}^T\mathbf{w}}_{\text{margin}} + \underbrace{C\sum\nolimits_{n=1}^{N}\varepsilon_n}_{\text{error tolerance}}$$

subject to: $y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1 - \varepsilon_n, \varepsilon_n \geq 0, \forall N$



The Hinge Loss

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- The soft-margin SVM can be re-written as the following optimization problem:

$$\min_{b,\mathbf{w}} E_{\mathsf{SVM}}(b, \mathbf{w}) + \lambda \mathbf{w}^T\mathbf{w}$$

Dual Soft-Margin SVM

$$\max_{\boldsymbol{\alpha}\in\mathbb{R}^N} \sum_{n=1}^{N}\alpha_n - \frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N}\alpha_n\alpha_m y_n y_m \mathbf{x}_n^T\mathbf{x}_m$$

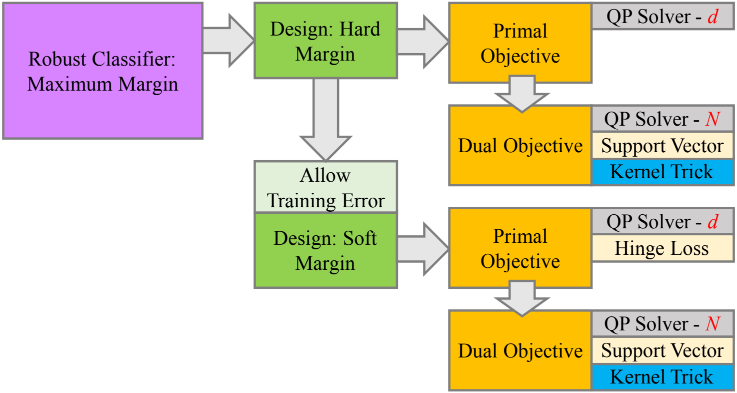
$$\text{subject to } \sum_{n=1}^{N} y_n\alpha_n = 0, 0 \le \alpha_n \le C, \forall n$$

$$\mathbf{w}^* = \sum_{n=1}^{N} y_n\alpha_n^*\mathbf{x}_n$$

Summary of Dual SVM

- Deliver a large-margin hyperplane, and in so doing it can control the effective model complexity.
- Deal with high- or infinite-dimensional transforms using the kernel trick.
- Express the final hypothesis $g(\mathbf{x})$ using only a few support vectors, their corresponding dual variables (Lagrange multipliers), and the kernel.
- Control the sensitivity to outliers and regularize the solution through setting C appropriately.

Support Vector Machine



Robust Classifier: Maximum Margin
Design: Hard Margin
Primal Objective
QP Solver - d
Dual Objective
QP Solver - N
Support Vector
Kernel Trick
Allow Training Error
Design: Soft Margin
Primal Objective
QP Solver - d
Hinge Loss
Dual Objective
QP Solver - N
Support Vector
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