EE3-23: Machine Learning

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Today

- Support Vector Machines

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- Kernels

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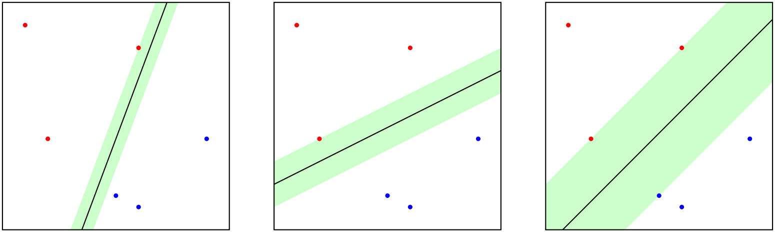

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- $x - p_x$ is parallel with $w \Rightarrow$ orthogonal to $H \Rightarrow p_x$ is the orthogonal projection
  More formally: any $u \in H$ is $p_x + v$ where $w^\top v = 0$ ($v \perp w$)

  $$\|x - u\|^2 = \|x - p_x + p_x - u\|^2 = \|\underbrace{x - p_x}_{const \cdot w} + v\|^2 = \|x - p_x\|^2 + \|v\|^2 \geq \|x - p_x\|^2$$

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Max-margin separator

$(w_*, b_*) = \text{argmax}_{w,b:\|w\|=1} \min_i |w^\top x_i + b|$ s.t. $y_i(w^\top x_i + b) > 0$ for all i

Hard-margin SVM

Equivalently derived from:

Hard-margin SVM

$$\begin{array}{ll} \text{minimize} & \|w\|^2 \\ \text{subject to} & y_i(w^\top x_i + b) \geq 1 \text{ for all } i \end{array}$$

Lagrangian formulation:

$$\mathcal{L}(w, b, \alpha) = \frac{1}{2}\|w\|^2 + \sum_{i=1}^{n} \alpha_i [1 - y_i(w^\top x_i + b)]$$

minimize in primal variables w, b, maximize in dual variables $\alpha_i \geq 0$

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- Support vectors: x_i with $\alpha_i \neq 0$
- $y_i(w_*^\top x_i + b_*) = 1$ for support vectors
- w is a linear combination of the support vectors

Hard-SVM - Dual Formulation:

$$\max_{\alpha} \mathcal{L}(\alpha) \triangleq \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j x_i^{\top} x_j$$

subject to $\alpha_i \geq 0$, $\sum_{i=1}^{n} \alpha_i y_i = 0$.

- Quadratic program
- Once α_is are solved:
  - $w^* = \sum_{i:\alpha_i^* > 0} \alpha_i^* y_i x_i$

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  - $b^* = 1 - y_i (w^*)^\top x_i$ for any support vector x_i (equivalently: $b^* = -\frac{\max_{i:y_i=-1}(w^*)^\top x_i + \min_{i:y_i=+1}(w^*)^\top x_i}{2}$)

Prediction with Hard-SVM

Assume we fit our model to a training dataset, and wish to make a prediction for a new data sample x.

- Predict $y = 1$ if and only if $w^T x + b > 0$

We have

$$\begin{aligned} w^T x + b &= \left(\sum_{i=1}^{n} \alpha_i y_i x_i \right)^T x + b \\ &= \sum_{i=1:\alpha_i>0}^{n} \alpha_i y_i (x_i^T x) + b \end{aligned}$$

We only need the inner products with the support vectors!

SVM with feature vectors

Let z be a feature vector for x

Use z instead of x:

$$\mathcal{L}(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j z_i^\top z_j$$

with constraints $\alpha_i \geq 0$, $\sum_{i=1}^{n} \alpha_i y_i = 0$.

What do we need?

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- $b = 1 - y_i w^\top z_i$ (z_i support vector)
- Only need to compute $z_i^\top z_j$!

Generalized inner product

The kernel: $\mathbf{z}^\top \mathbf{z}' = K(\mathbf{x}, \mathbf{x}')$

- Example: $\mathbf{x} = (x_1, x_2)$

  $\mathbf{z} = \Phi(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_2^2)$

  $\mathbf{z}^\top \mathbf{z}' = K(\mathbf{x}, \mathbf{x}') = 1 + x_1 x_1' + x_2 x_2' + x_1^2 {x_1'}^2 + x_2^2 {x_2'}^2$

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Computing $\mathbf{z}$ is not needed! – Kernel trick

Kernel trick

$$\mathcal{L}(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j z_i^\top z_j$$

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Indeed, no need to transform the features as long as we can compute K!

Polynomial kernel

$$K(\mathbf{x}, \mathbf{x}') = (c + \mathbf{x}^\top \mathbf{x}')^q = \left(c + \sum_{j=1}^{d} x_i x_i'\right)^q$$

d^q terms if expanded! $\Rightarrow$ Computational benefits

Gaussian (Radial Basis Function - RBF) kernel

Assume the original instance space is R, and consider feature map

$$\Phi(x)_n = \frac{1}{\sqrt{n!}} \exp -x^2/2x^n$$

Then

$$\begin{aligned}
\Phi(x)^T \Phi(x') &= \sum_{n=0}^{\infty} \left(\frac{1}{\sqrt{n!}} e^{-x^2/2} x^n \right) \left(\frac{1}{\sqrt{n!}} e^{-(x')^2/2} (x')^n \right) \\
&= e^{-\frac{x^2+(x')^2}{2}} \sum_{n=0}^{\infty} \frac{(x \cdot x')^n}{n!} \\
&= e^{-\frac{\|x-x'\|^2}{2}}
\end{aligned}$$

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$$K_{x_1,\ldots,x_n} = \begin{bmatrix} K(x_1,x_1) & K(x_1,x_2) & \ldots & K(x_1,x_n) \\ K(x_2,x_1) & K(x_2,x_2) & \ldots & K(x_2,x_n) \\ \vdots & \ldots & \ddots & \vdots \\ K(x_n,x_1) & K(x_n,x_2) & \ldots & K(x_n,x_n) \end{bmatrix}$$

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    is symmetric and positive semidefinite (Mercer condition).
  - Indeed, if $Z^\top = (z_1, \dots, z_n)$ then $K_{x_1,\dots,x_n} = ZZ^\top$ and

$$u^\top K_{x_1,\dots,x_n} u = u^\top ZZ^\top u = (Z^\top u)^\top Z^\top u = \|Z^\top u\|^2 \geq 0$$

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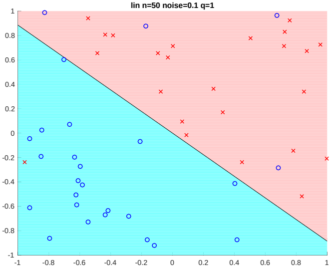
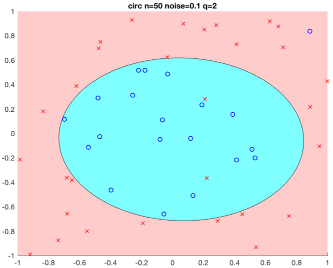
    is symmetric and positive semidefinite (Mercer condition).
  - Indeed, if $Z^\top = (z_1, \dots, z_n)$ then $K_{x_1,\dots,x_n} = ZZ^\top$ and

$$u^\top K_{x_1,\dots,x_n} u = u^\top ZZ^\top u = (Z^\top u)^\top Z^\top u = \|Z^\top u\|^2 \geq 0$$

- This is sufficient! $\mathcal{Z}$ exists as long as the Mercer conditions are satisfied.

Two non-separable cases



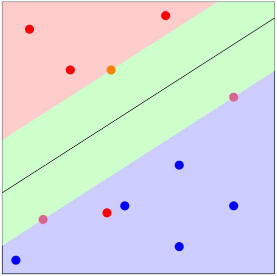


Soft-margin SVM

Non-separable case:

- Cannot guarantee

  $y_i(w^\top x_i + b) \geq 1$ for all i



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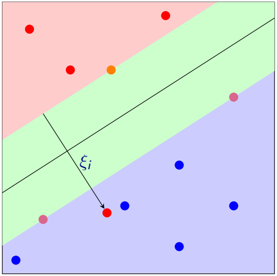

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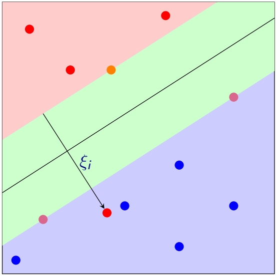

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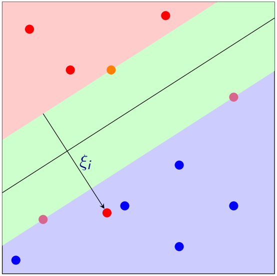

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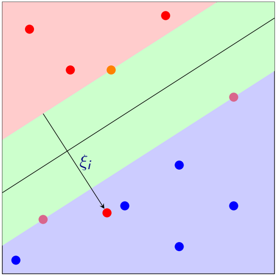

$$
\begin{array}{ll}
\text{minimize} & \frac{1}{2}\|w\|^2 + C\sum_{i=1}^n \xi_i \\
\text{subject to} & y_i(w^\top x_i + b) \geq 1 - \xi_i \text{ and } \xi_i \geq 0 \text{ for all } i
\end{array}
$$

Parameter C provides a balance between minimizing $\|w\|^2$ (large margin) and ensuring that most samples have functional margin at least 1 (minimum number of misclassified samples)

Lagrangian formulation:

$$\mathcal{L}(w, b, \alpha) = \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi_i + \sum_{i=1}^{n}\alpha_i[1 - \xi_i - y_i(w^\top x_i + b)] - \sum_{i=1}^{n}\beta_i\xi_i$$

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Soft-margin SVM – dual

Minimize

$$\mathcal{L}(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j x_i^\top x_j$$

subject to $0 \leq \alpha_i \leq C$, $\sum_{i=1}^{n} \alpha_i y_i = 0$

$b = y_i - \sum_{i=j}^{n} \alpha_j y_j x_j^\top x_i$
when $0 < \alpha_i < C$.

Parameter tuning

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    - ★ $K_j(x, x') = \phi_j^\top(x)\phi_j(x')$, and $K(x, x') = \sum_{j=1}^{J} \gamma_j K_j(x, x')$

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- Training time with QP typically $\Theta(n^3)$–can be much faster with GD/SGD with an approximate solution

Gaussian–RBF kernels

Gaussian RBF (radial basis function) kernel:

$$K(x, x') = \exp\Big(-\gamma \underbrace{\|x - x'\|^2}_{\textit{radial}} \Big)$$

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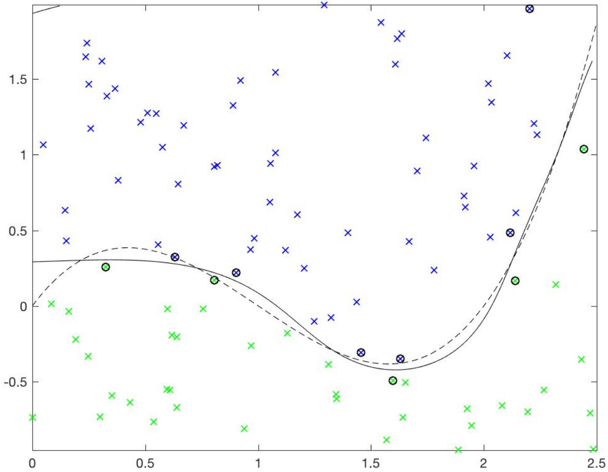
SVM predictor

$$g(x) = \text{sign}\left(\sum_{x_i \text{ is SV}} \alpha_i y_i K(x_i, x) + b \right) = \text{sign}\left(\sum_{x_i \text{ is SV}} \alpha_i y_i e^{-\gamma \|x - x_i\|^2} + b \right)$$

RBF-kernel width



$$\gamma = 1$$

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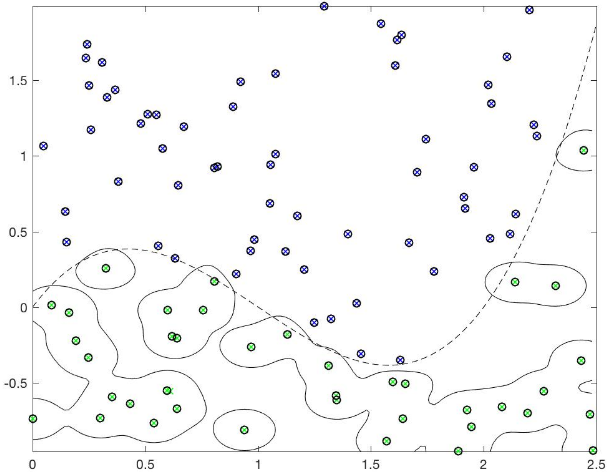
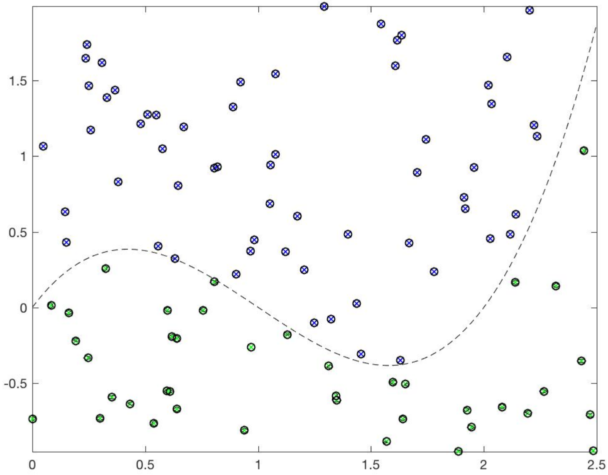


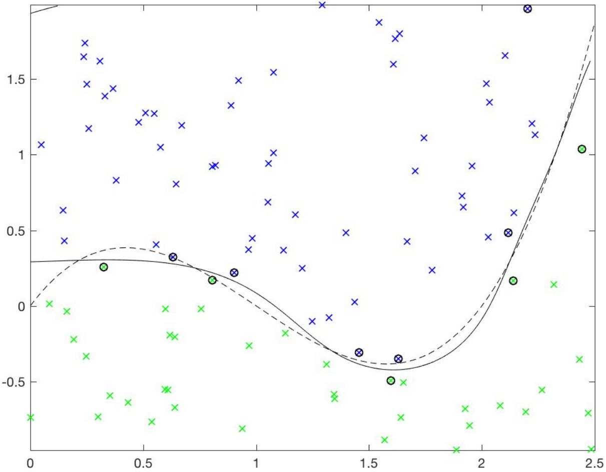
$\gamma = 10$

RBF-kernel width



$$\gamma = 100$$

RBF-kernel width



$\gamma = 1$

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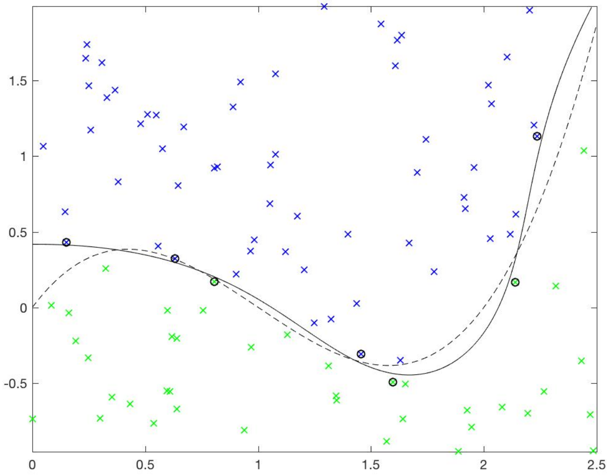

$$\gamma = 0.1$$

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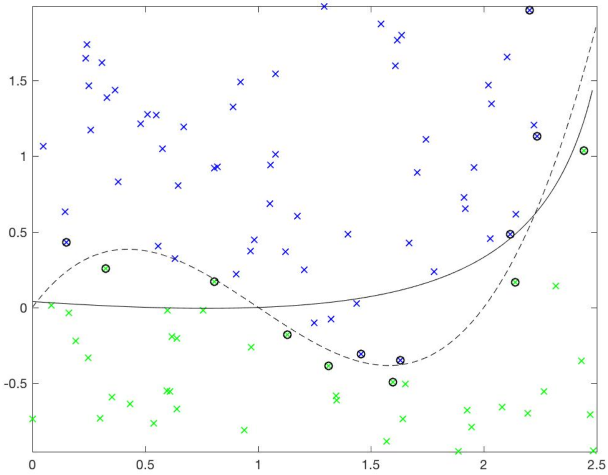

$$\gamma = 0.01$$