PS5841

Data Science in Finance & Insurance



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Geometry (2D)

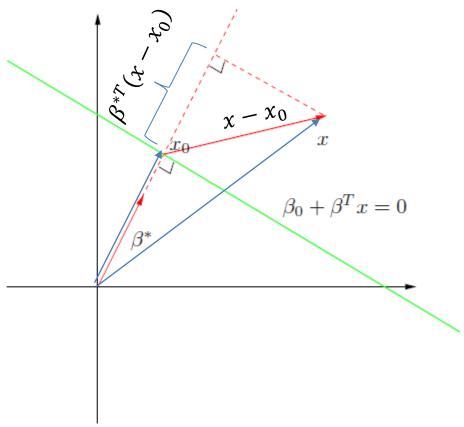
• Perpendicular lines $slope_1 \times slope_2 = -1$

Example

- The vector (β_1, β_2) has slope $\frac{\beta_2}{\beta_1}$
- The line $\beta_0+\beta_1x_1+\beta_2x_2=0$ has slope $-\frac{\beta_1}{\beta_2}$
- Are perpendicular to each other



Geometry (higher dimensions)



 β^* is a unit vector



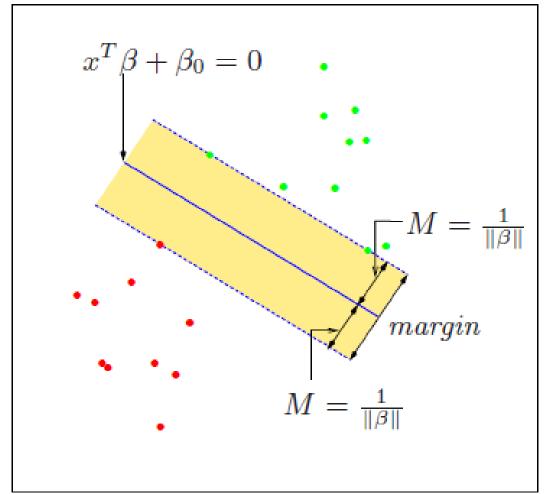
Geometry (higher dimensions)

- β is normal to the hyperplane L defined by $\{x|\beta_0 + \beta^T x = 0\}$
- For x_1 and x_2 on L, $\boldsymbol{\beta}^T(x_1-x_2)=0$
- The signed distance from x to L is

$$\left(\frac{\boldsymbol{\beta}}{\|\boldsymbol{\beta}\|}\right)^{T}(\boldsymbol{x}-\boldsymbol{x}_{0}) = \frac{1}{\|\boldsymbol{\beta}\|}(\boldsymbol{\beta}^{T}\boldsymbol{x}-\boldsymbol{\beta}^{T}\boldsymbol{x}_{0}) = \frac{1}{\|\boldsymbol{\beta}\|}(\boldsymbol{x}^{T}\boldsymbol{\beta}+\boldsymbol{\beta}_{0})$$

• $f(x) = x^T \beta + \beta_0$ is proportional to the signed distance from x to L

Separable Case



Optimal Separating Hyperplane

• Label y_i indicates where x_i is in relation to L

$$y_i = \begin{cases} +1, & \beta_0 + \boldsymbol{x}_i^T \boldsymbol{\beta} > 0 \\ -1, & \beta_0 + \boldsymbol{x}_i^T \boldsymbol{\beta} < 0 \end{cases}$$

•
$$\mathbf{x}_i$$
 is at least a distance M from L

$$y_i \frac{1}{\|\boldsymbol{\beta}\|} (\mathbf{x}_i^T \boldsymbol{\beta} + \beta_0) \ge M \to y_i (\mathbf{x}_i^T \boldsymbol{\beta} + \beta_0) \ge \|\boldsymbol{\beta}\| M$$

 The optimal separating hyperplane is the maximum margin hyperplane that maximizes M



Optimization Problem

• Maximizing M is equivalent to minimizing $\|\pmb{\beta}\|$. WLOG, set $\|\pmb{\beta}\| = \frac{1}{M}$

$$\min_{\beta_0, \beta} \frac{1}{2} \| \boldsymbol{\beta} \|^2$$

subject to

$$y_i(\mathbf{x}_i^T \boldsymbol{\beta} + \beta_0) \ge 1, \quad \forall i$$



Optimization (1)

Lagrange primal

$$L_{P} = \frac{1}{2} \|\boldsymbol{\beta}\|^{2} - \sum_{i=1}^{N} \alpha_{i} [y_{i}(\boldsymbol{x}_{i}^{T}\boldsymbol{\beta} + \beta_{0}) - 1]$$

$$= \frac{1}{2} (\beta_{1}^{2} + \dots + \beta_{p}^{2}) - \sum_{i=1}^{N} [\alpha_{i}y_{i}(\beta_{0} + \beta_{1}x_{i1} + \dots + \beta_{p}x_{ip}) - \alpha_{i}]$$

Set partial derivatives to zero

$$\frac{\partial L_p}{\partial \beta_0} = 0 \to \sum_{i=1}^N \alpha_i y_i = 0$$
$$\frac{\partial L_p}{\partial \beta_{j\neq 0}} = 0 \to \beta = \sum_{i=1}^N \alpha_i y_i x_i$$

• Get L_D by substitute these into L_P



Optimization (2)

Wolfe dual

$$L_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{N} \alpha_i \alpha_k y_i y_k \mathbf{x}_i^T \mathbf{x}_k$$
subject to $\alpha_i \ge 0$, $0 = \sum_{i=1}^{N} \alpha_i y_i$, $\forall i$

Solutions satisfy the Karush-Kuhn-Tucker (KKT) conditions

$$\sum_{i=1}^{N} \alpha_i y_i = 0$$

$$\boldsymbol{\beta} = \sum_{i=1}^{N} \alpha_i y_i \boldsymbol{x}_i$$

$$\alpha_i \ge 0, \forall i$$

$$\alpha_i [y_i (\boldsymbol{x}_i^T \boldsymbol{\beta} + \beta_0) - 1] = 0, \forall i$$



Support Vectors

- The margin around the linear decision boundary has thickness $M = \frac{1}{\|\beta\|}$
- For any \mathbf{x}_i more than M away from the boundary, $y_i(\mathbf{x}_i^T\boldsymbol{\beta} + \beta_0) > 1$ $\alpha_i \left[y_i(\mathbf{x}_i^T\boldsymbol{\beta} + \beta_0) 1 \right] = 0 \rightarrow \alpha_i = 0$
- The support vectors, those on the margin and $\alpha_i > 0$, define the decision boundary
- For SVs, $y_i(x_i^T \beta + \beta_0) 1 = 0$
- $\beta = \sum_{i=1}^{N} \alpha_i y_i x_i$ is a linear combination of support vectors

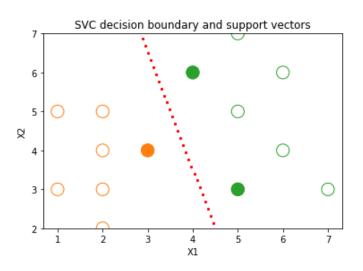


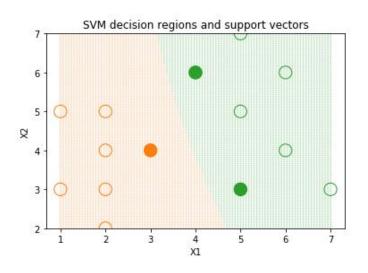
Maximal Margin Classifier

$$clf(\mathbf{x}) = sign[\mathbf{x}^T \widehat{\boldsymbol{\beta}} + \widehat{\beta}_0]$$



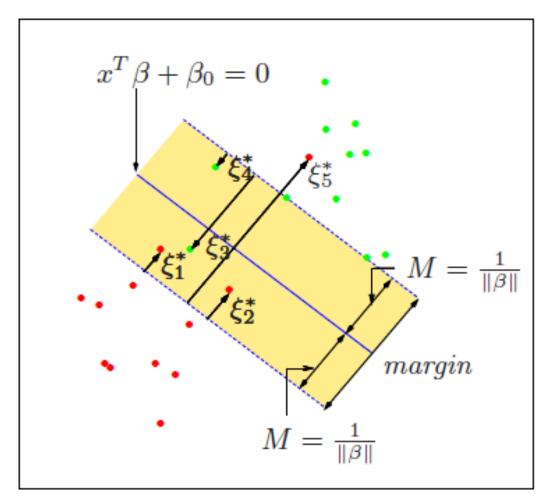
Decision Boundary separable case







Non-Separable Case



The Support Vector Classifier is the generalization of the Maximal Margin Classifier for the non-separable case.

Optimal Separating Hyperplane

• Label y_i indicates where x_i is in relation to L

$$y_i = \begin{cases} +1, & \beta_0 + \boldsymbol{x}_i^T \boldsymbol{\beta} > 0 \\ -1, & \beta_0 + \boldsymbol{x}_i^T \boldsymbol{\beta} < 0 \end{cases}$$

• x_i is at least a distance M from L, with allowance for some margin violation

$$y_i \frac{1}{\|\boldsymbol{\beta}\|} (\boldsymbol{x}_i^T \boldsymbol{\beta} + \beta_0) \ge M(1 - \epsilon_i) \to y_i (\boldsymbol{x}_i^T \boldsymbol{\beta} + \beta_0) \ge \|\boldsymbol{\beta}\| M(1 - \epsilon_i)$$

- The slack variable $\epsilon_i \geq 0$, is the proportional amount by which $\mathbf{x}_i^T \mathbf{\beta} + \beta_0$ is on the wrong side of its margin
- The decision boundary is one that maximizes M

Slack Variable

• The slack variable $\epsilon_i \geq 0$, is the proportional amount by which $oldsymbol{x}_i^T oldsymbol{eta} + eta_0$ is on the wrong side of its margin

$$\epsilon_i = \begin{cases} = 0, \\ > 0, \\ > 1, \end{cases}$$

 $\epsilon_i = \begin{cases} = 0, & \textit{OK wrt margin and L} \\ > 0, & \textit{violates margin, OK wrt L} \\ > 1, & \end{cases}$



Optimization Problem

• Maximizing M is equivalent to minimizing $\|\boldsymbol{\beta}\|$. WLOG, set $\|\boldsymbol{\beta}\| = \frac{1}{M}$

$$\min_{\boldsymbol{\beta}_0,\boldsymbol{\beta}} \frac{1}{2} \|\boldsymbol{\beta}\|^2 + C \sum_{i=1}^{N} \epsilon_i$$

subject to

$$y_i(\mathbf{x}^T \boldsymbol{\beta} + \beta_0) \ge 1 - \epsilon_i, \quad \forall i$$
$$\epsilon_i \ge 0$$

- cost parameter C
 - Replaces the constant in the constraint $\sum_{i=1}^{N} \epsilon_i \leq \text{constant}$
 - Penalty for margin violation
 - $-C=\infty$ is for the separable case



Optimization

Lagrange primal

$$L_{P} = \frac{1}{2} \|\boldsymbol{\beta}\|^{2} + C \sum_{i=1}^{N} \epsilon_{i} - \sum_{i=1}^{N} \alpha_{i} [y_{i} (\boldsymbol{x}_{i}^{T} \boldsymbol{\beta} + \beta_{0}) - (1 - \epsilon_{i})] - \sum_{i=1}^{N} \mu_{i} \epsilon_{i}$$

Wolfe dual

$$L_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{N} \alpha_i \alpha_k y_i y_k \mathbf{x}_i^T \mathbf{x}_k$$

Solutions satisfy

$$\sum_{i=1}^{N} \alpha_i y_i = 0, \qquad \boldsymbol{\beta} = \sum_{i=1}^{N} \alpha_i y_i \boldsymbol{x}_i$$

$$\alpha_i = C - \mu_i,$$

$$\alpha_i [y_i (\boldsymbol{x}_i^T \boldsymbol{\beta} + \beta_0) - (1 - \epsilon_i)] = 0$$

$$\mu_i \epsilon_i = 0$$

$$y_i (\boldsymbol{x}_i^T \boldsymbol{\beta} + \beta_0) - (1 - \epsilon_i) \ge 0$$

$$\alpha_i, \mu_i, \epsilon_i \ge 0$$



Support Vectors

- Support vectors alone define the decision boundary
- Support vectors are those on or violate the margin
- Support vectors satisfy

$$y_i(\mathbf{x}_i^T \boldsymbol{\beta} + \beta_0) - (1 - \epsilon_i) = 0$$

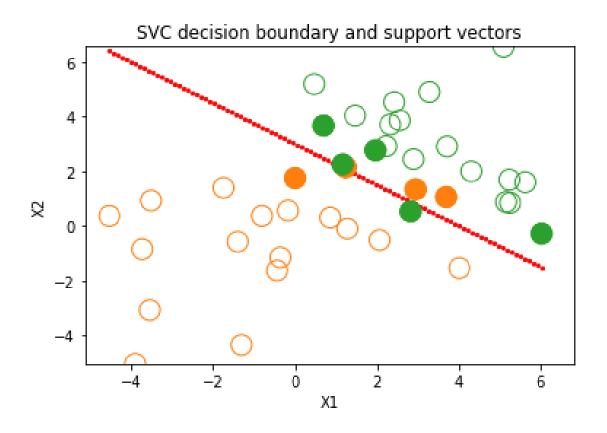


Support Vector Classifier

$$clf(\mathbf{x}) = sign[\mathbf{x}^{T}\widehat{\boldsymbol{\beta}} + \widehat{\boldsymbol{\beta}}_{0}]$$



Decision Boundary (SVC) non-separable case





SVC

$$L_{D} = \sum_{i=1}^{N} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{N} \alpha_{i} \alpha_{k} y_{i} y_{k} x_{i}^{T} x_{k}$$

$$\hat{f}(\mathbf{x}) = \mathbf{x}^T \hat{\boldsymbol{\beta}} + \hat{\beta}_0 = \sum_{i=1}^{N} \hat{\alpha}_i y_i \mathbf{x}^T \mathbf{x}_i + \hat{\beta}_0$$
$$\boldsymbol{\beta} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$$



SVC with Kernel Function (1)

Generalize the inner products to kernel functions

$$L_{D} = \sum_{i=1}^{N} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{N} \alpha_{i} \alpha_{k} y_{i} y_{k} x_{i}^{T} x_{k}$$

$$= \sum_{i=1}^{N} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{N} \alpha_{i} \alpha_{k} y_{i} y_{k} < x_{i}, x_{k} >$$

$$\rightarrow L_{D} = \sum_{i=1}^{N} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{N} \alpha_{i} \alpha_{k} y_{i} y_{k} < h(x_{i}), h(x_{k}) >$$

$$= \sum_{i=1}^{N} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{N} \alpha_{i} \alpha_{k} y_{i} y_{k} K(x_{i}, x_{k})$$

• For the linear kernel function, $K(x, x') = \langle h(x), h(x') \rangle = x^T x'$



SVC with Kernel Function (2)

Generalize the inner products to kernel functions

$$\hat{f}(\mathbf{x}) = \mathbf{x}^T \hat{\boldsymbol{\beta}} + \hat{\beta}_0 = \sum_{i=1}^N \hat{\alpha}_i y_i \mathbf{x}^T \mathbf{x}_i + \hat{\beta}_0 = \sum_{i=1}^N \hat{\alpha}_i y_i < \mathbf{x}, \mathbf{x}_i > + \hat{\beta}_0$$

$$\rightarrow \hat{f}(\mathbf{x}) = \sum_{i=1}^N \hat{\alpha}_i y_i < h(\mathbf{x}), h(\mathbf{x}_i) > + \hat{\beta}_0$$

$$= \sum_{i=1}^N \hat{\alpha}_i y_i K(\mathbf{x}, \mathbf{x}_i) + \hat{\beta}_0$$

• For the linear kernel function, $K(x,x') = \langle h(x), h(x') \rangle = x^T x'$



Feature Space Expansion

- A kernel function can expand the feature space.
- Example from 2D to 6D $\mathbf{x} = (x_1, x_2)^T \to h(\mathbf{x}) = (h_1(\mathbf{x}), ..., h_6(\mathbf{x}))^T$

$$K(x_i, x_k) = (1 + \langle x_i, x_k \rangle)^2$$



Example – from 2D to 6D (1)

$$\mathbf{x} = (x_1, x_2)^T \to h(\mathbf{x}) = (h_1(\mathbf{x}), \dots, h_6(\mathbf{x}))^T$$

$$K(\mathbf{x}_{i}, \mathbf{x}_{k}) = (1 + \langle \mathbf{x}_{i}, \mathbf{x}_{k} \rangle)^{2}$$

$$= (1 + x_{i1}x_{k1} + x_{i2}x_{k2})^{2}$$

$$= 1 + (x_{i1}x_{k1})^{2} + (x_{i2}x_{k2})^{2}$$

$$+2x_{i1}x_{k1} + 2x_{i2}x_{k2} + 2x_{i1}x_{k1}x_{i2}x_{k2}$$



Example – from 2D to 6D (2)

$$K(\mathbf{x}_i, \mathbf{x}_k) = 1 + (x_{i1}x_{k1})^2 + (x_{i2}x_{k2})^2 +2x_{i1}x_{k1} + 2x_{i2}x_{k2} + 2x_{i1}x_{k1}x_{i2}x_{k2} = \langle h(\mathbf{x}_i), h(\mathbf{x}_k) \rangle$$

•
$$h_1(\mathbf{x}) = 1 \to h_1(\mathbf{x}_i)h_1(\mathbf{x}_k) = 1$$

•
$$h_2(\mathbf{x}) = x_1^2 \to h_2(\mathbf{x}_i) h_2(\mathbf{x}_k) = (x_{i1} x_{k1})^2$$

•
$$h_3(\mathbf{x}) = x_2^2 \to h_3(\mathbf{x}_i)h_3(\mathbf{x}_k) = (x_{i2}x_{k2})^2$$

•
$$h_4(\mathbf{x}) = \sqrt{2}x_1 \to h_4(\mathbf{x}_i)h_4(\mathbf{x}_k) = 2x_{i1}x_{k1}$$

•
$$h_5(\mathbf{x}) = \sqrt{2}x_2 \to h_5(\mathbf{x}_i)h_5(\mathbf{x}_k) = 2x_{i2}x_{k2}$$

•
$$h_6(\mathbf{x}) = \sqrt{2}x_1x_2 \to h_6(\mathbf{x}_i)h_6(\mathbf{x}_k) = 2x_{i1}x_{k1}x_{i2}x_{k2}$$



Support Vector Machine

- The support vector machine is an extension of the support vector classifier, expanding the feature space using kernels
- Linear $K(x, x') = \langle x, x' \rangle = x^T x'$
- Polynomial $K(x, x') = (1 + \langle x, x' \rangle)^d$
- Radial basis $K(x, x') = \exp(-\gamma ||x x'||^2)$
- Neural Network

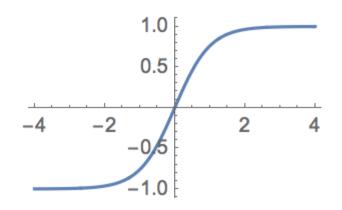
$$K(\mathbf{x}, \mathbf{x}') = \tanh(\kappa_1 < \mathbf{x}, \mathbf{x}' > +\kappa_2)$$



tanh

Neural Network

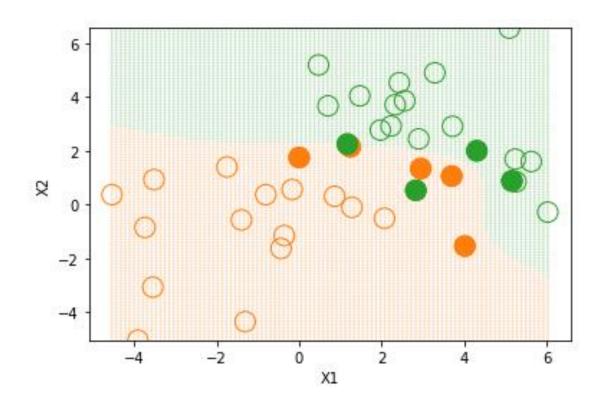
$$K(\mathbf{x}, \mathbf{x}') = \tanh(\kappa_1 < \mathbf{x}, \mathbf{x}' > + \kappa_2)$$





Decision Boundary (SVM) non-separable case

• Poly3, C=1





That was



