CS420 Machine Learning, Lecture 3

Support Vector Machines and Kernel Methods

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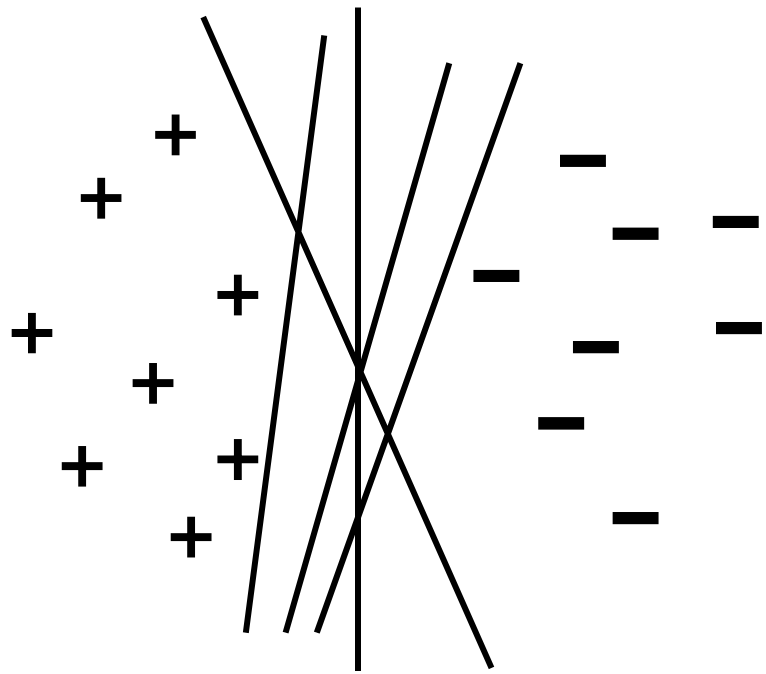
http://wnzhang.net/teaching/cs420/index.html

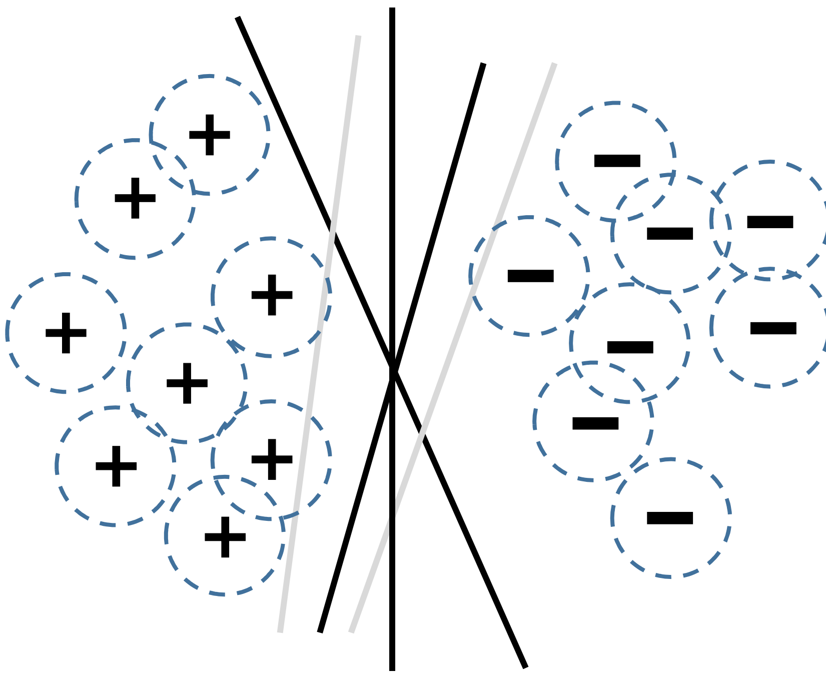
Linear Classification

- For linear separable cases, we have multiple decision boundaries



Linear Classification

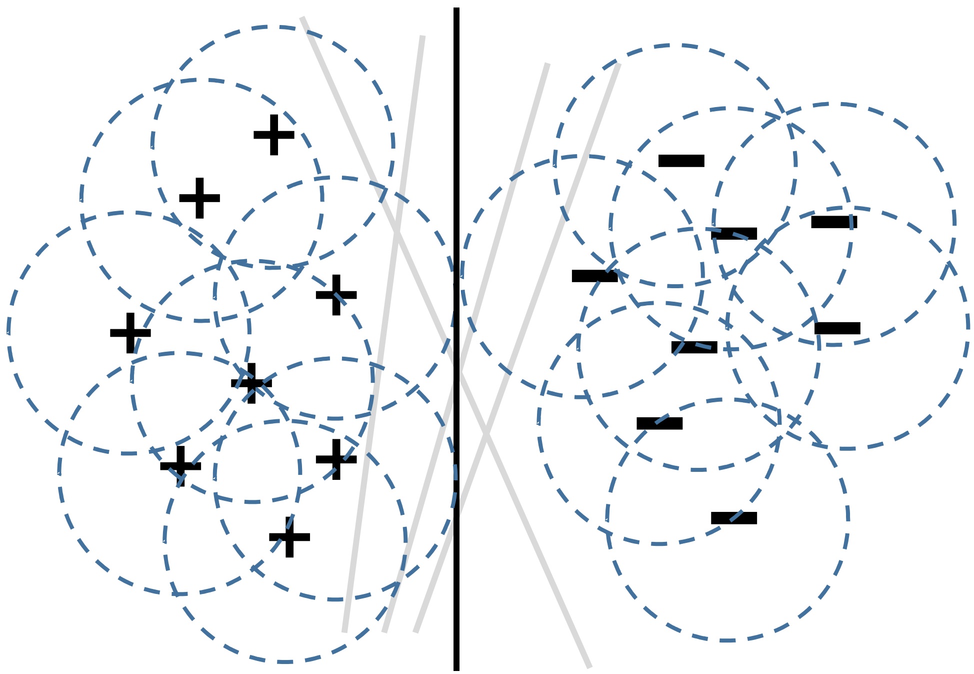
- For linear separable cases, we have multiple decision boundaries



- Ruling out some separators by considering data noise

Linear Classification

- For linear separable cases, we have multiple decision boundaries



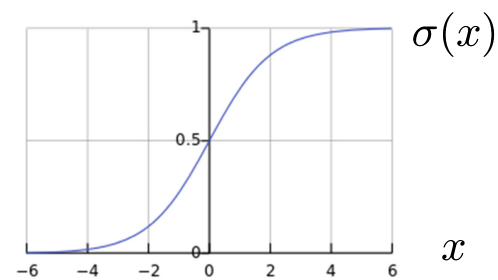
- The intuitive optimal decision boundary: the largest margin

Review: Logistic Regression

- Logistic regression is a binary classification model

$$p_\theta(y=1|x) = \sigma(\theta^\top x) = \frac{1}{1+e^{-\theta^\top x}}$$

$$p_\theta(y=0|x) = \frac{e^{-\theta^\top x}}{1+e^{-\theta^\top x}}$$



- Cross entropy loss function

$$\mathcal{L}(y, x, p_\theta) = -y \log \sigma(\theta^\top x) - (1-y)\log(1-\sigma(\theta^\top x))$$

- Gradient

$$\begin{aligned}\frac{\partial \mathcal{L}(y, x, p_\theta)}{\partial \theta} &= -y \frac{1}{\sigma(\theta^\top x)} \sigma(z)(1-\sigma(z))x - (1-y)\frac{-1}{1-\sigma(\theta^\top x)}\sigma(z)(1-\sigma(z))x \\ &= (\sigma(\theta^\top x) - y)x \\ \theta &\leftarrow \theta + \eta(y - \sigma(\theta^\top x))x\end{aligned}$$

$$\boxed{\frac{\partial \sigma(z)}{\partial z} = \sigma(z)(1-\sigma(z))}$$

Label Decision

- Logistic regression provides the probability

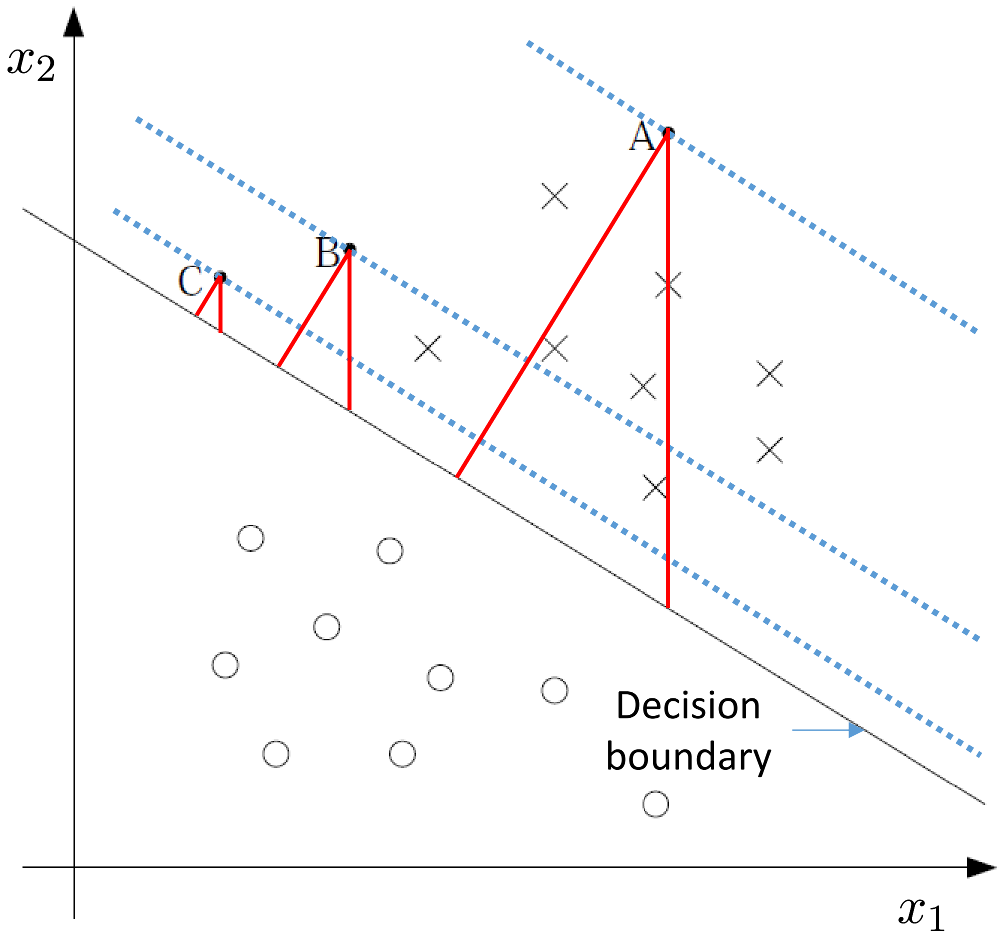
$$p_\theta(y=1|x) = \sigma(\theta^\top x) = \frac{1}{1+e^{-\theta^\top x}}$$

$$p_\theta(y=0|x) = \frac{e^{-\theta^\top x}}{1+e^{-\theta^\top x}}$$

- The final label of an instance is decided by setting a threshold h

$$\hat{y} = \begin{cases} 1, & p_\theta(y=1|x) > h \\ 0, & \text{otherwise} \end{cases}$$

Logistic Regression Scores



$$s(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$$

$$p_\theta(y = 1|x) = \frac{1}{1 + e^{-s(x)}}$$

$$s(x) = \theta_0 + \theta_1 x_1^{(A)} + \theta_2 x_2^{(A)}$$

$$s(x) = \theta_0 + \theta_1 x_1^{(B)} + \theta_2 x_2^{(B)}$$

$$s(x) = \theta_0 + \theta_1 x_1^{(C)} + \theta_2 x_2^{(C)}$$

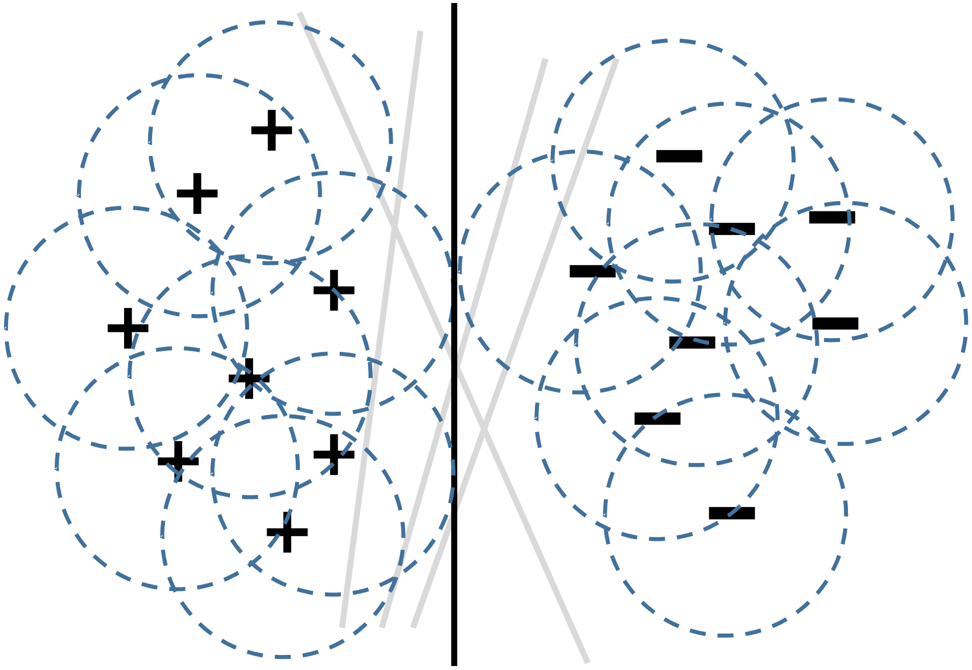
$$s(x) = 0$$

The higher score, the larger distance to the decision boundary, the higher confidence

Example from Andrew Ng

Linear Classification

- The intuitive optimal decision boundary: the highest confidence



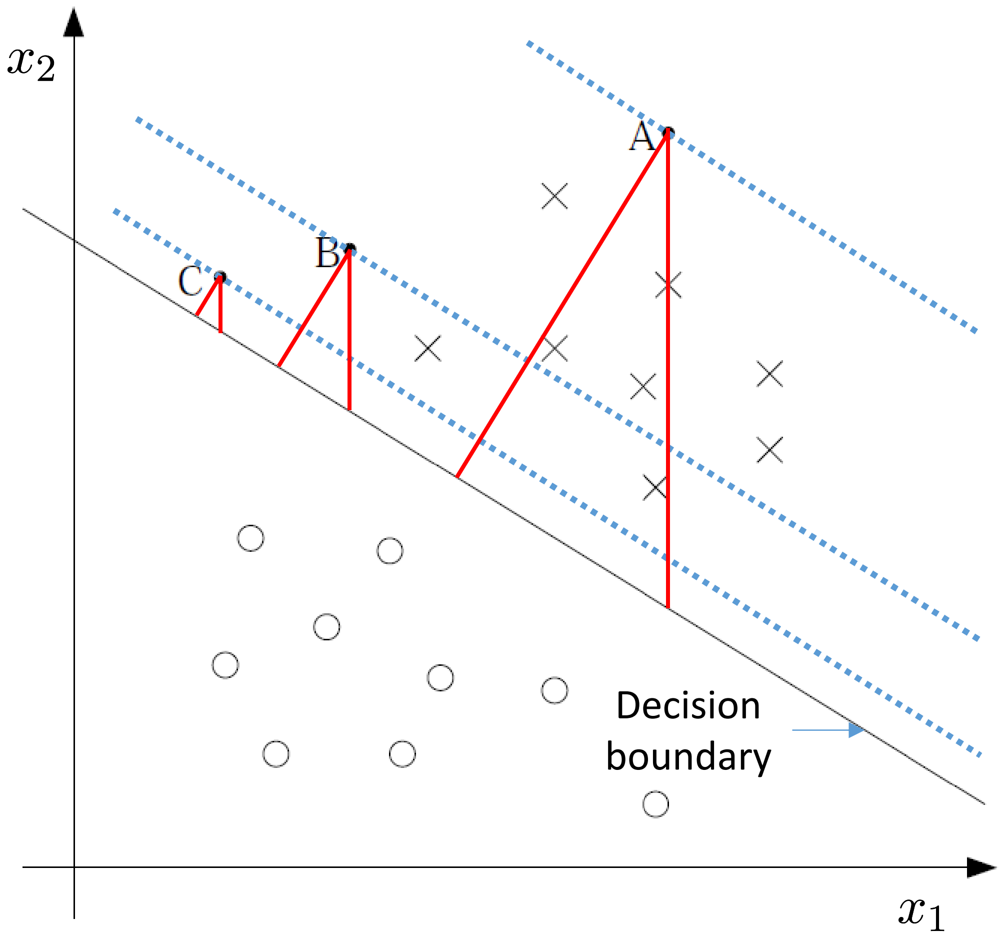
Notations for SVMs

- Feature vector x
- Class label $y \in \{-1, 1\}$
- Parameters
  - Intercept b
  - Feature weight vector w
- Label prediction

$$h_{w,b}(x) = g(w^\top x + b)$$

$$g(z) = \begin{cases} +1 & z \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

Logistic Regression Scores



$$s(x) = b + w_1 x_1 + w_2 x_2$$

$$p_\theta(y = 1|x) = \frac{1}{1 + e^{-s(x)}}$$

$$s(x) = b + w_1 x_1^{(A)} + w_2 x_2^{(A)}$$

$$s(x) = b + w_1 x_1^{(B)} + w_2 x_2^{(B)}$$

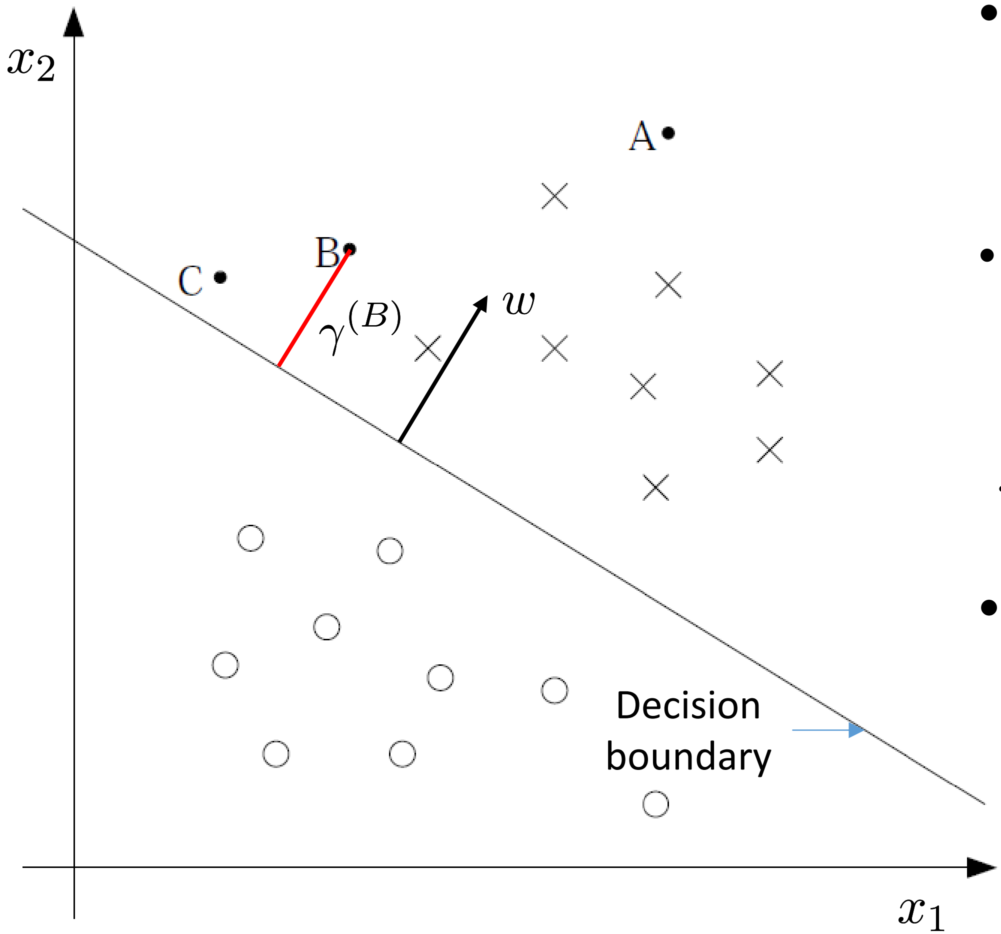
$$s(x) = b + w_1 x_1^{(C)} + w_2 x_2^{(C)}$$

$$s(x) = 0$$

The higher score, the larger distance to the separating hyperplane, the higher confidence

Example from Andrew Ng

Margins



- Functional margin

$$\hat{\gamma}^{(i)} = y^{(i)}(w^\top x^{(i)} + b)$$

- Note that the separating hyperplane won't change with the magnitude of (*w*, *b*)

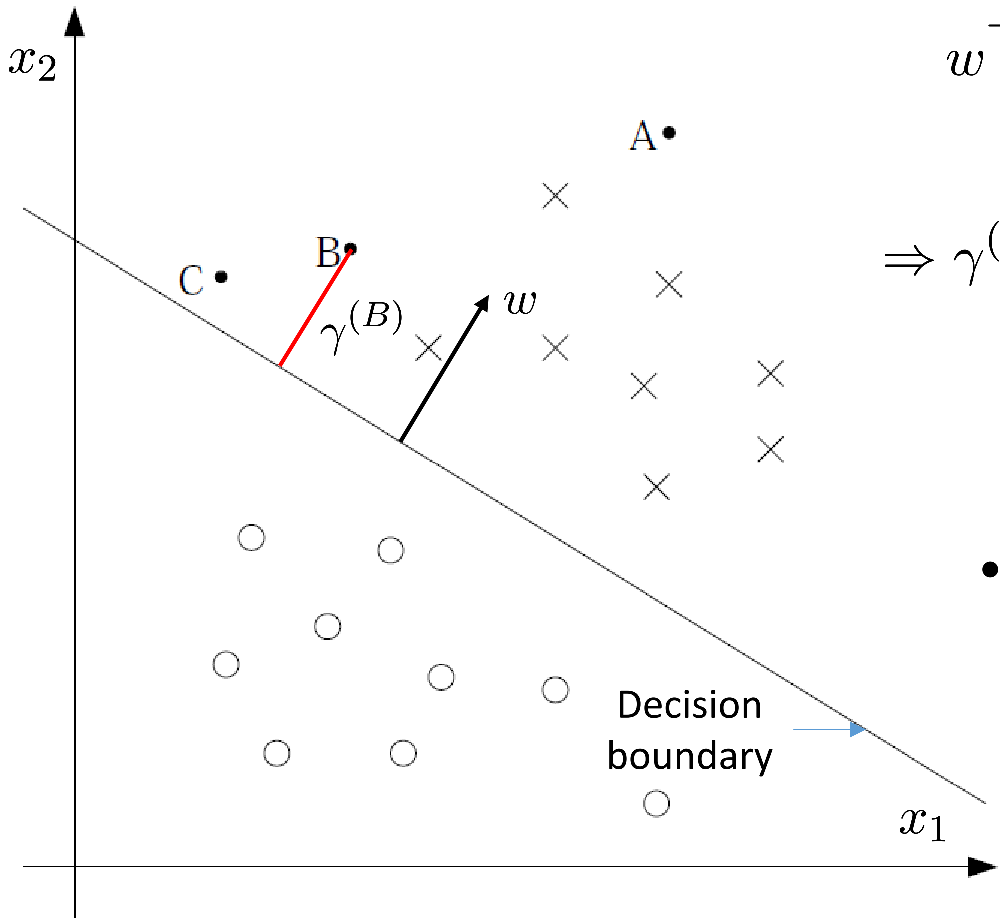
$$g(w^\top x + b) = g(2w^\top x + 2b)$$

- Geometric margin

$$\gamma^{(i)} = y^{(i)}(w^\top x^{(i)} + b)$$

$$\text{where } \|w\|^2 = 1$$

Margins



- Decision boundary

$$w^\top \left(x^{(i)} - \gamma^{(i)} y^{(i)} \frac{w}{\|w\|} \right) + b = 0$$

$$\Rightarrow \gamma^{(i)} = y^{(i)} \frac{w^\top x^{(i)} + b}{\|w\|}$$

$$= y^{(i)} \left(\left(\frac{w}{\|w\|} \right)^\top x^{(i)} + \frac{b}{\|w\|} \right)$$

- Given a training set

$$S = \{(x_i, y_i)\}_{i=1 \ldots m}$$

the smallest geometric margin

$$\gamma = \min_{i=1 \ldots m} \gamma^{(i)}$$

Objective of an SVM

- Find a separable hyperplane that maximizes the minimum geometric margin

$$\begin{aligned} \max_{\gamma,w,b} \quad & \gamma \\ \text{s.t.} \quad & y^{(i)}(w^\top x^{(i)} + b) \geq \gamma, \;\; i = 1, \ldots, m \\ & \|w\| = 1 \quad \text{(non-convex constraint)} \end{aligned}$$

- Equivalent to normalized functional margin

$$\begin{aligned} \max_{\hat{\gamma},w,b} \quad & \frac{\hat{\gamma}}{\|w\|} \qquad \text{(non-convex objective)} \\ \text{s.t.} \quad & y^{(i)}(w^\top x^{(i)} + b) \geq \hat{\gamma}, \;\; i = 1, \ldots, m \end{aligned}$$

Objective of an SVM

- Functional margin scales w.r.t. (*w*,*b*) without changing the decision boundary.
  - Let's fix the functional margin at 1.

$$\hat{\gamma} = 1$$

  - Objective is written as

$$\max_{w,b} \quad \frac{1}{\|w\|}$$
$$\text{s.t.} \quad y^{(i)}(w^\top x^{(i)} + b) \geq 1, \; i = 1, \ldots, m$$

  - Equivalent with

$$\min_{w,b} \quad \frac{1}{2}\|w\|^2$$
$$\text{s.t.} \quad y^{(i)}(w^\top x^{(i)} + b) \geq 1, \; i = 1, \ldots, m$$

A Digression of Lagrange Duality in Convex Optimization

Boyd, Stephen, and Lieven Vandenberghe. *Convex optimization*. Cambridge university press, 2004.

Lagrangian for Convex Optimization

- A convex optimization problem

$$\begin{aligned} \min_w \quad & f(w) \\ \text{s.t.} \quad & h_i(w) = 0, \quad i = 1, \ldots, l \end{aligned}$$

- The Lagrangian of this problem is defined as

$$\mathcal{L}(w, \beta) = f(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

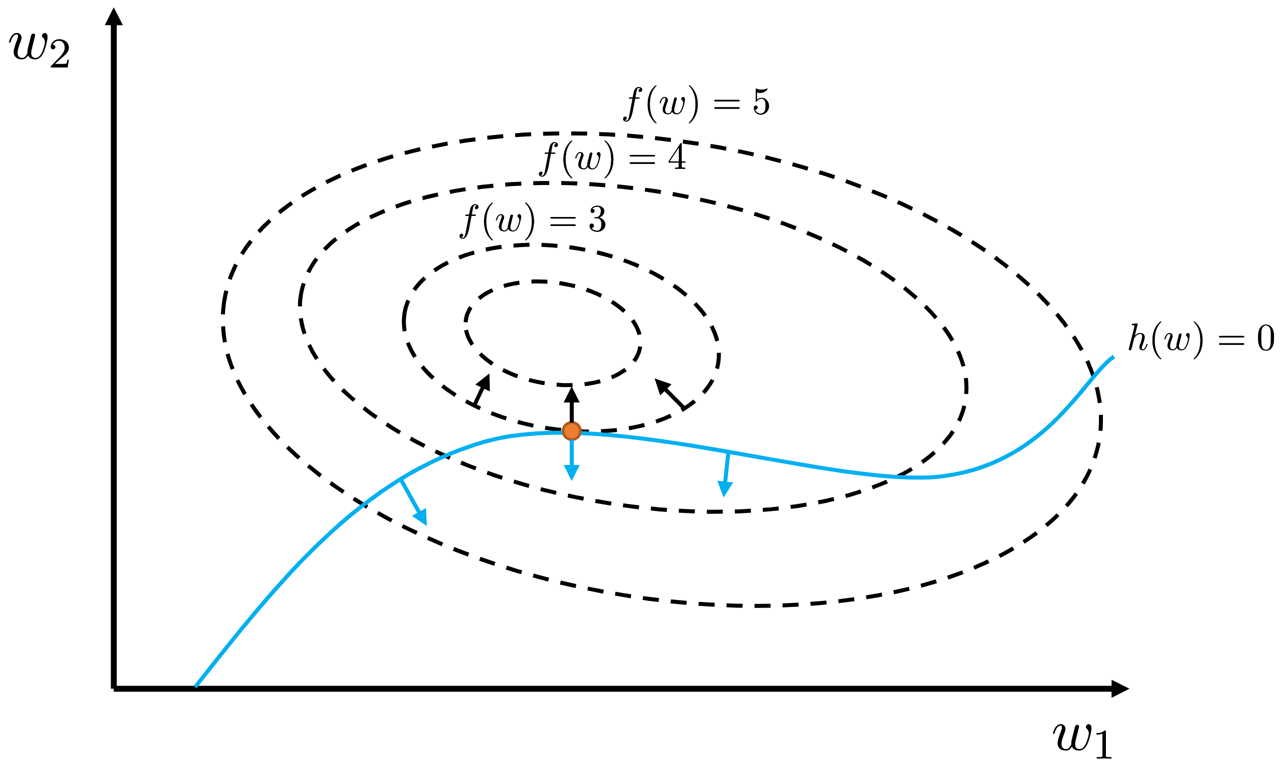
Lagrangian multipliers

  - Solving

$$\frac{\partial \mathcal{L}(w, \beta)}{\partial w} = 0 \qquad \frac{\partial \mathcal{L}(w, \beta)}{\partial \beta} = 0$$

yields the solution of the original optimization problem.

Lagrangian for Convex Optimization



$$\mathcal{L}(w, \beta) = f(w) + \beta h(w)$$

$$\frac{\partial \mathcal{L}(w, \beta)}{\partial w} = \frac{\partial f(w)}{\partial w} + \beta \frac{\partial h(w)}{\partial w} = 0$$

i.e two gradients on the same direction

With Inequality Constraints

- A convex optimization problem

$$\begin{aligned} \min_{w} \quad & f(w) \\ \text{s.t.} \quad & g_i(w) \leq 0, \quad i = 1, \ldots, k \\ & h_i(w) = 0, \quad i = 1, \ldots, l \end{aligned}$$

- The Lagrangian of this problem is defined as

$$\mathcal{L}(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

Lagrangian multipliers

Primal Problem

- The Lagrangian of this problem is defined as

$$\mathcal{L}(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \underbrace{\alpha_i}_{\uparrow} g_i(w) + \sum_{i=1}^{l} \underbrace{\beta_i}_{\uparrow} h_i(w)$$

Lagrangian multipliers

- The primal problem

$$\theta_{\mathcal{P}}(w) = \max_{\alpha, \beta : \alpha_i \geq 0} \mathcal{L}(w, \alpha, \beta)$$

  - If a given w violates any constraints, i.e.,

$$g_i(w) > 0 \quad \text{or} \quad h_i(w) \neq 0$$

  - Then $\theta_{\mathcal{P}}(w) = +\infty$

Primal Problem

- The Lagrangian of this problem is defined as

$$\mathcal{L}(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

Lagrangian multipliers

- The primal problem

$$\theta_{\mathcal{P}}(w) = \max_{\alpha,\beta:\alpha_i \geq 0} \mathcal{L}(w, \alpha, \beta)$$

  - Conversely, if all constraints are satisfied for w
  - Then $\theta_{\mathcal{P}}(w) = f(w)$

$$\theta_{\mathcal{P}}(w) = \begin{cases} f(w) & \text{if } w \text{ satisfies primal constraints} \\ +\infty & \text{otherwise} \end{cases}$$

Primal Problem

$$\theta_{\mathcal{P}}(w) = \begin{cases} f(w) & \text{if } w \text{ satisfies primal constraints} \\ +\infty & \text{otherwise} \end{cases}$$

- The minimization problem

$$\min_w \theta_{\mathcal{P}}(w) = \min_w \max_{\alpha,\beta:\alpha_i \geq 0} \mathcal{L}(w, \alpha, \beta)$$

is the same as the original problem

$$\begin{aligned} \min_w \quad & f(w) \\ \text{s.t.} \quad & g_i(w) \leq 0, \quad i = 1, \ldots, k \\ & h_i(w) = 0, \quad i = 1, \ldots, l \end{aligned}$$

- Define the value of the primal problem $p^* = \min_w \theta_{\mathcal{P}}(w)$

Dual Problem

- A slightly different problem

$$\theta_{\mathcal{D}}(\alpha, \beta) = \min_{w} \mathcal{L}(w, \alpha, \beta)$$

- Define the dual optimization problem

$$\max_{\alpha,\beta:\alpha_i \geq 0} \theta_{\mathcal{D}}(\alpha, \beta) = \max_{\alpha,\beta:\alpha_i \geq 0} \min_{w} \mathcal{L}(w, \alpha, \beta)$$

- Min & Max exchanged compared to the primal problem

$$\min_{w} \theta_{\mathcal{P}}(w) = \min_{w} \max_{\alpha,\beta:\alpha_i \geq 0} \mathcal{L}(w, \alpha, \beta)$$

- Define the value of the dual problem

$$d^* = \max_{\alpha,\beta:\alpha_i \geq 0} \min_{w} \mathcal{L}(w, \alpha, \beta)$$

Primal Problem vs. Dual Problem

$$d^* = \max_{\alpha,\beta:\alpha_i \geq 0} \min_w \mathcal{L}(w,\alpha,\beta) \leq \min_w \max_{\alpha,\beta:\alpha_i \geq 0} \mathcal{L}(w,\alpha,\beta) = p^*$$

- Proof

$$\min_w \mathcal{L}(w,\alpha,\beta) \leq \mathcal{L}(w,\alpha,\beta), \forall w, \alpha \geq 0, \beta$$

$$\Rightarrow \max_{\alpha,\beta:\alpha \geq 0} \min_w \mathcal{L}(w,\alpha,\beta) \leq \max_{\alpha,\beta:\alpha \geq 0} \mathcal{L}(w,\alpha,\beta), \forall w$$

$$\Rightarrow \max_{\alpha,\beta:\alpha \geq 0} \min_w \mathcal{L}(w,\alpha,\beta) \leq \min_w \max_{\alpha,\beta:\alpha \geq 0} \mathcal{L}(w,\alpha,\beta)$$

$$\square$$

- But under certain condition $d^* = p^*$

Karush-Kuhn-Tucker (KKT) Conditions

- If f and g_i's are convex and h_i's are affine, and suppose g_i's are all strictly feasible
- then there must exist w^*, α^*, β^*
  - w^* is the solution of the primal problem
  - α^*, β^* are the solutions of the dual problem
  - and the values of the two problems are equal $p^* = d^* = \mathcal{L}(w^*, \alpha^*, \beta^*)$
- And w^*, α^*, β^* satisfy the KKT conditions

$$\frac{\partial}{\partial w_i}\mathcal{L}(w^*, \alpha^*, \beta^*) = 0,\ i = 1, \ldots, n$$

$$\frac{\partial}{\partial \beta_i}\mathcal{L}(w^*, \alpha^*, \beta^*) = 0,\ i = 1, \ldots, l$$

KKT dual complementarity condition $\longrightarrow$

$$\alpha_i^* g_i(w^*) = 0,\ i = 1, \ldots, k$$

$$g_i(w^*) \leq 0,\ i = 1, \ldots, k$$

$$\alpha^* \geq 0,\ i = 1, \ldots, k$$

- Moreover, if some w^*, α^*, β^* satisfy the KKT conditions, then it is also a solution to the primal and dual problems.

Now Back to SVM Problem

Objective of an SVM

- SVM objective: finding the optimal margin classifier

$$\begin{aligned} \min_{w,b} \quad & \frac{1}{2}\|w\|^2 \\ \text{s.t.} \quad & y^{(i)}(w^\top x^{(i)} + b) \geq 1, \; i = 1, \ldots, m \end{aligned}$$

  - Re-wright the constraints as

$$g_i(w) = -y^{(i)}(w^\top x^{(i)} + b) + 1 \leq 0$$

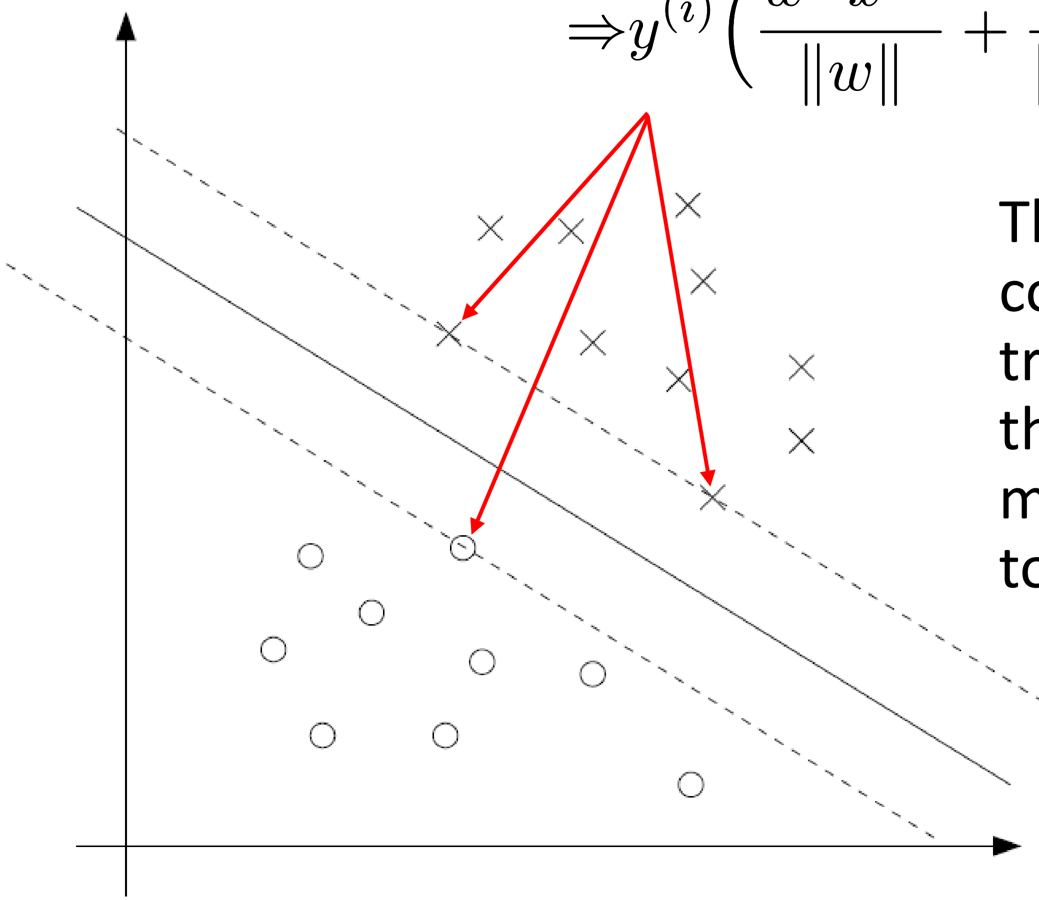
so as to match the standard optimization form

$$\begin{aligned} \min_{w} \quad & f(w) \\ \text{s.t.} \quad & g_i(w) \leq 0, \quad i = 1, \ldots, k \\ & h_i(w) = 0, \quad i = 1, \ldots, l \end{aligned}$$

Equality Cases

$$g_i(w) = -y^{(i)}(w^\top x^{(i)} + b) + 1 = 0$$

$$\Rightarrow y^{(i)}\left(\frac{w^\top x^{(i)}}{\|w\|} + \frac{b}{\|w\|}\right) = \frac{1}{\|w\|}$$



The g_i's = 0 cases correspond to the training examples that have functional margin exactly equal to 1.

Objective of an SVM

- SVM objective: finding the optimal margin classifier

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

$$\text{s.t.} \quad -y^{(i)}(w^\top x^{(i)} + b) + 1 \leq 0, \; i = 1, \ldots, m$$

- Lagrangian

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

  - No β^* or equality constraints in SVM problem

Solving

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

- Derivatives

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

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

- Then Lagrangian is re-written as

$$\mathcal{L}(w,b,\alpha) = \frac{1}{2}\Big\| \sum_{i=1}^{m} \alpha_i y^{(i)} x^{(i)} \Big\|^2 - \sum_{i=1}^{m} \alpha_i [y^{(i)}(w^\top x^{(i)} + b) - 1]$$

$$= \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j {x^{(i)}}^\top x^{(j)} \boxed{- b \sum_{i=1}^{m} \alpha_i y^{(i)}} = 0$$

Solving α^*

- Dual problem

$$\max_{\alpha \geq 0} \theta_{\mathcal{D}}(\alpha) = \max_{\alpha \geq 0} \min_{w,b} \mathcal{L}(w, b, \alpha)$$

$$\begin{aligned}
\max_{\alpha} \quad & W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j {x^{(i)}}^\top x^{(j)} \\
\text{s.t.} \quad & \alpha_i \geq 0, \; i = 1, \ldots, m \\
& \sum_{i=1}^{m} \alpha_i y^{(i)} = 0
\end{aligned}$$

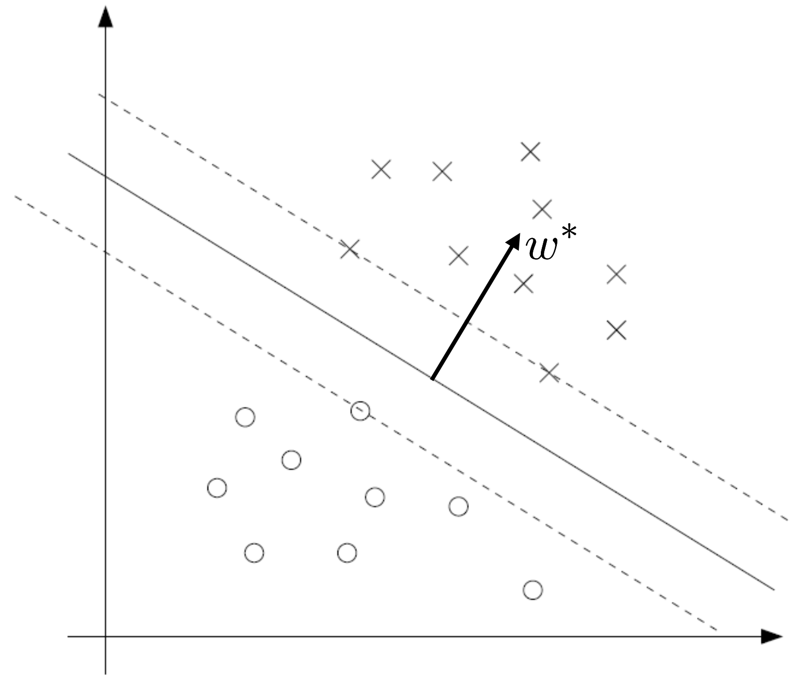
- To solve α^*

Solving w^* and b^*

- With α^* solved, w^* is obtained by

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

  - Only supporting vectors with $\alpha > 0$



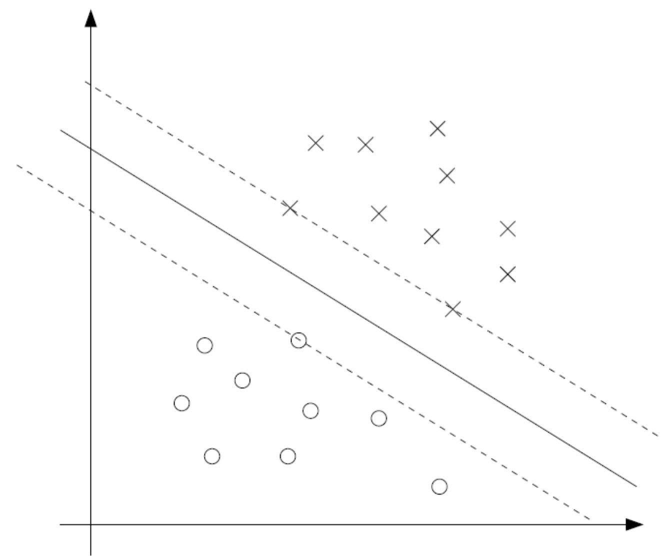
- With w^* solved, b^* is obtained by

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

Predicting Values

- With the solutions of w^* and b^* , the predicting value (i.e. functional margin) of each instance is

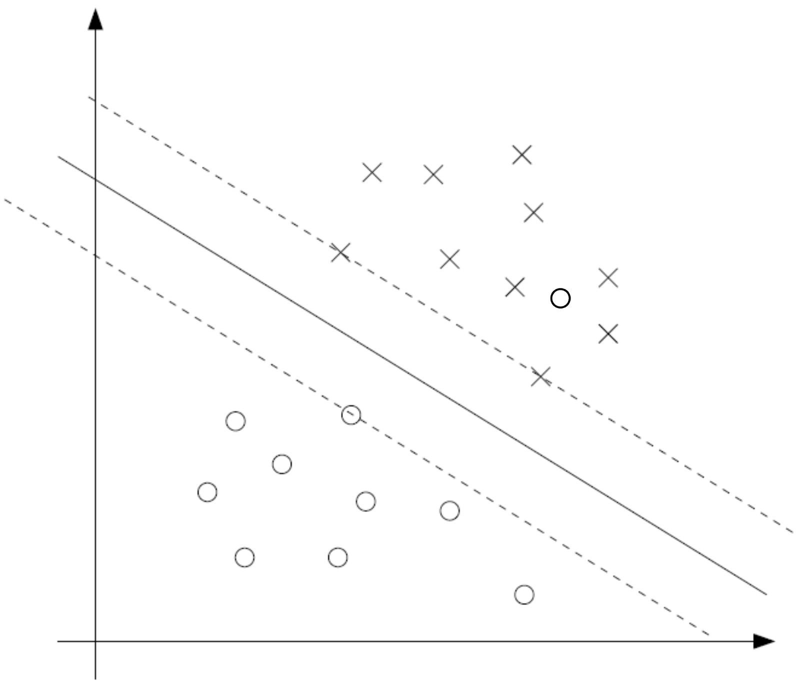
$$
\begin{aligned}
{w^*}^\top x + b^* &= \Big(\sum_{i=1}^{m} \alpha_i y^{(i)} x^{(i)}\Big)^\top x + b^* \\
&= \sum_{i=1}^{m} \alpha_i y^{(i)} \langle x^{(i)}, x \rangle + b^*
\end{aligned}
$$

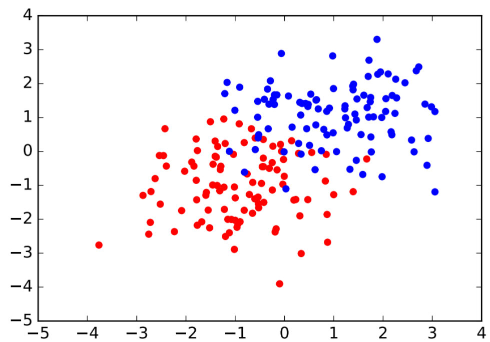


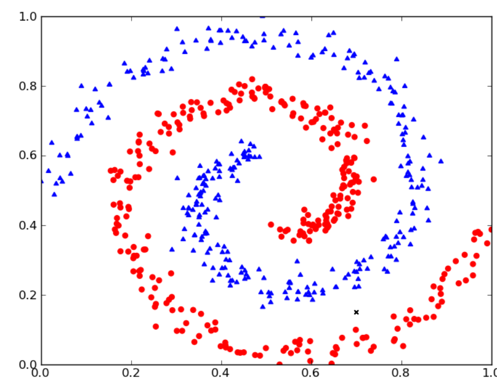
  - We only need to calculate the inner product of *x* with the supporting vectors

Non-Separable Cases

- The derivation of the SVM as presented so far assumed that the data is linearly separable.
- More practical cases are linearly non-separable.







Dealing with Non-Separable Cases

- Add slack variables

$$\min_{w,b} \quad \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m}\xi_i$$

L1 regularization

$$\text{s.t.} \quad y^{(i)}(w^\top x^{(i)} + b) \geq 1 - \xi_i, \;\; i = 1, \ldots, m$$

$$\xi_i \geq 0, \;\; i = 1, \ldots, m$$

- Lagrangian

$$\mathcal{L}(w, b, \xi, \alpha, r) = \frac{1}{2}w^\top w + C\sum_{i=1}^{m}\xi_i - \sum_{i=1}^{m}\alpha_i[y^{(i)}(x^\top w + b) - 1 + \xi_i] - \sum_{i=1}^{m} r_i\xi_i$$

- Dual problem

$$\max_{\alpha} \quad W(\alpha) = \sum_{i=1}^{m}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{m} y^{(i)}y^{(j)}\alpha_i\alpha_j {x^{(i)}}^\top x^{(j)}$$

$$\text{s.t.} \quad 0 \leq \alpha_i \leq C, \;\; i = 1, \ldots, m$$

Surprisingly, this is the only change

$$\sum_{i=1}^{m}\alpha_i y^{(i)} = 0$$

Efficiently solved by SMO algorithm

SVM Hinge Loss vs. LR Loss

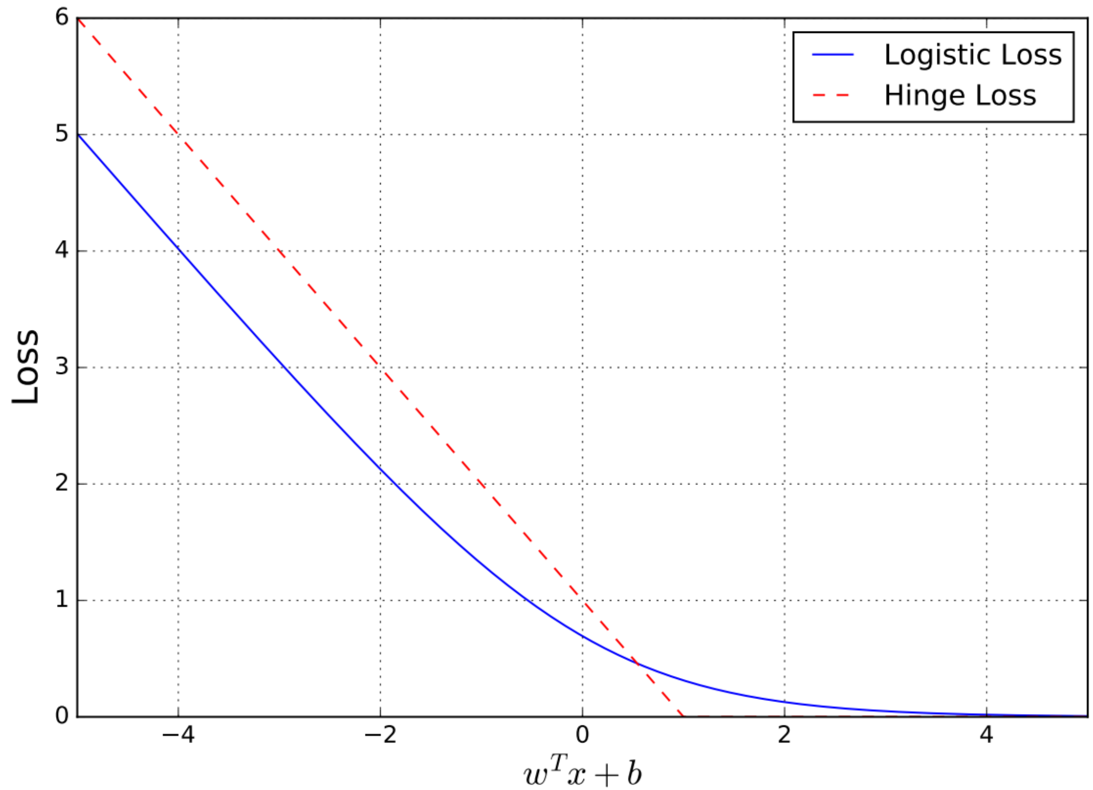
- SVM Hinge loss

$$\frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m}\max(0, 1 - y_i(w^\top x_i + b))$$

- LR log loss

$$-y_i \log \sigma(w^\top x_i + b) - (1 - y_i)\log(1 - \sigma(w^\top x_i + b))$$

- If $y = 1$



Coordinate Ascent (Descent)

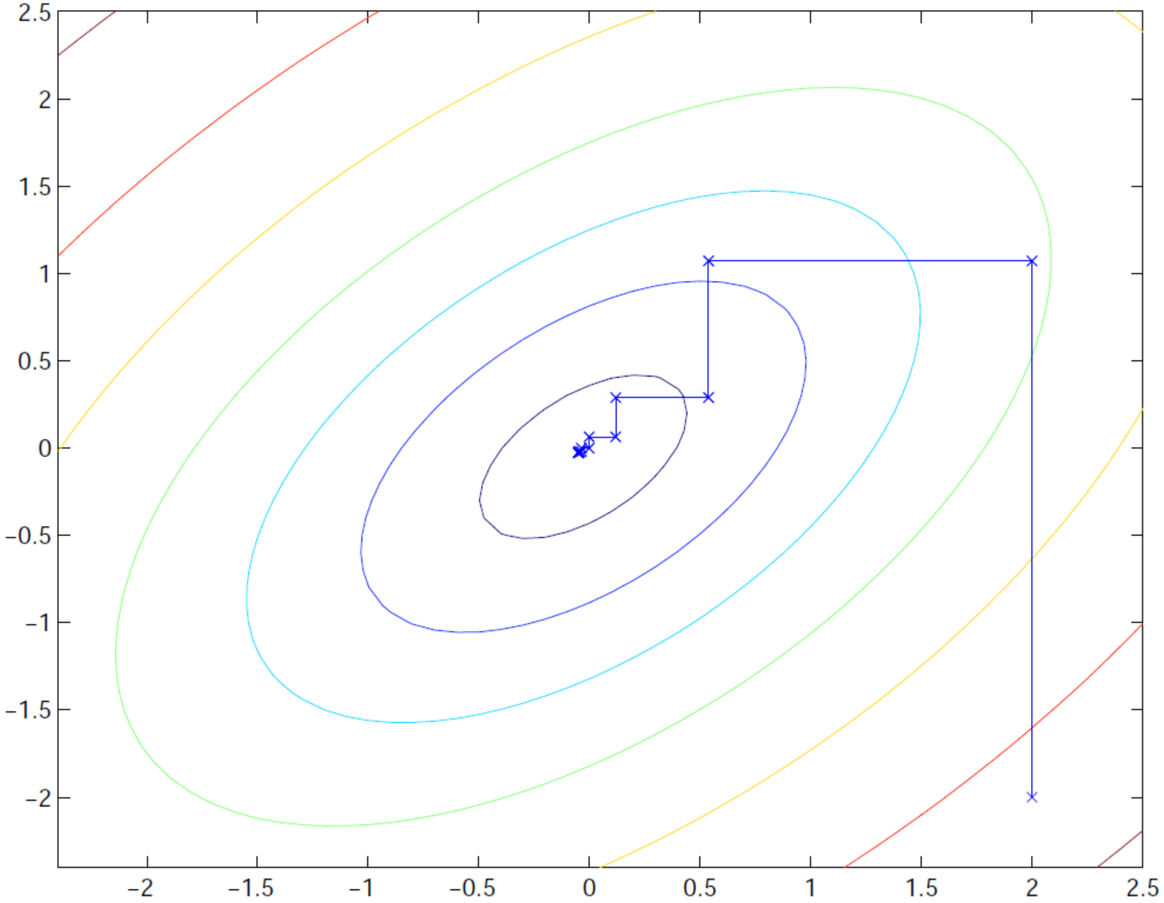
- For the optimization problem

$$\max_{\alpha} W(\alpha_1, \alpha_2, \ldots, \alpha_m)$$

- Coordinate ascent algorithm

$$
\begin{array}{l}
\text{Loop until convergence: } \{ \\
\quad \text{For } i = 1, \ldots, m \ \{ \\
\quad\quad \alpha_i := \arg\max_{\hat{\alpha}_i} W(\alpha_1, \ldots, \alpha_{i-1}, \hat{\alpha}_i, \alpha_{i+1}, \ldots, \alpha_m) \\
\quad \} \\
\}
\end{array}
$$

Coordinate Ascent (Descent)



A two-dimensional coordinate ascent example

SMO Algorithm

- SMO: sequential minimal optimization
- SVM optimization problem

$$\max_{\alpha} \quad W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j x^{(i)\top} x^{(j)}$$

$$\text{s.t.} \quad 0 \le \alpha_i \le C, \; i = 1, \ldots, m$$

$$\sum_{i=1}^{m} \alpha_i y^{(i)} = 0$$

- Cannot directly apply coordinate ascent algorithm because

$$\sum_{i=1}^{m} \alpha_i y^{(i)} = 0 \;\Rightarrow\; \alpha_i y^{(i)} = -\sum_{j \ne i} \alpha_j y^{(j)}$$

SMO Algorithm

- Update two variable each time

  Loop until convergence {
  1. Select some pair α_i and α_j to update next
  2. Re-optimize $W(\alpha)$ w.r.t. α_i and α_j

  }

- Convergence test: whether the change of $W(\alpha)$ is smaller than a predefined value (e.g. 0.01)
- Key advantage of SMO algorithm is the update of α_i and α_j (step 2) is efficient

SMO Algorithm

$$\max_{\alpha} \quad W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j {x^{(i)}}^\top x^{(j)}$$

$$\text{s.t.} \quad 0 \le \alpha_i \le C, \; i = 1, \ldots, m$$

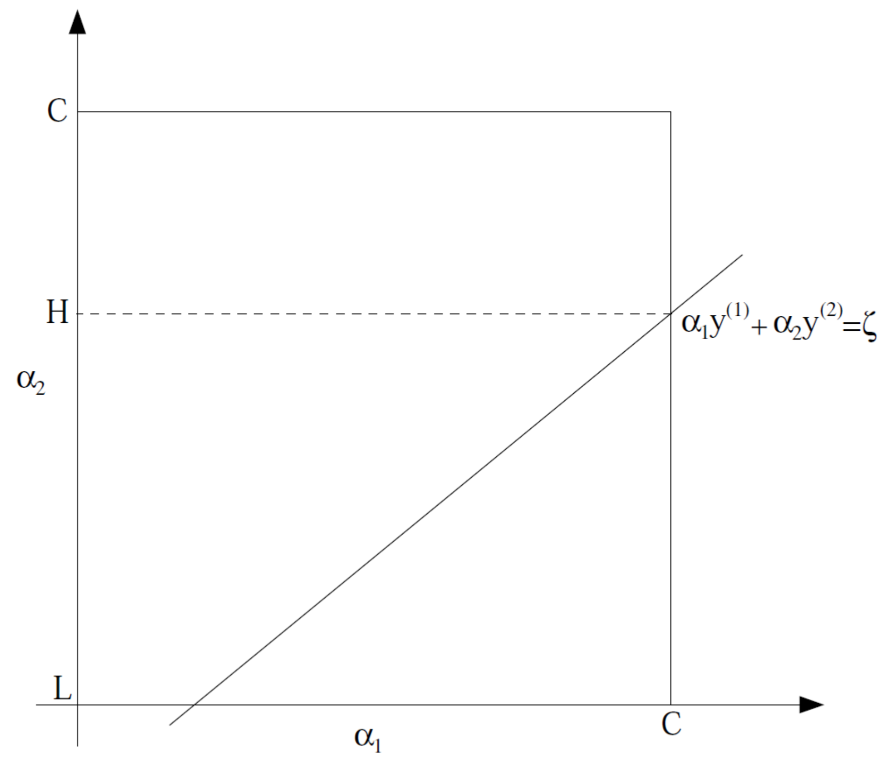
$$\sum_{i=1}^{m} \alpha_i y^{(i)} = 0$$

- Without loss of generality, hold α_3 … α_m and optimize $W(\alpha)$ w.r.t. α_1 and α_2

$$\alpha_1 y^{(1)} + \alpha_2 y^{(2)} = -\sum_{i=3}^{m} \alpha_i y^{(i)} = \zeta$$

$$\Rightarrow \quad \alpha_2 = -\frac{y^{(1)}}{y^{(2)}} \alpha_1 + \frac{\zeta}{y_2}$$

$$\alpha_1 = (\zeta - \alpha_2 y^{(2)}) y^{(1)}$$



SMO Algorithm

- With $\alpha_1 = (\zeta - \alpha_2 y^{(2)})y^{(1)}$, the objective is written as

$$W(\alpha_1, \alpha_2, \ldots, \alpha_m) = W((\zeta - \alpha_2 y^{(2)})y^{(1)}, \alpha_2, \ldots, \alpha_m)$$

- Thus the original optimization problem

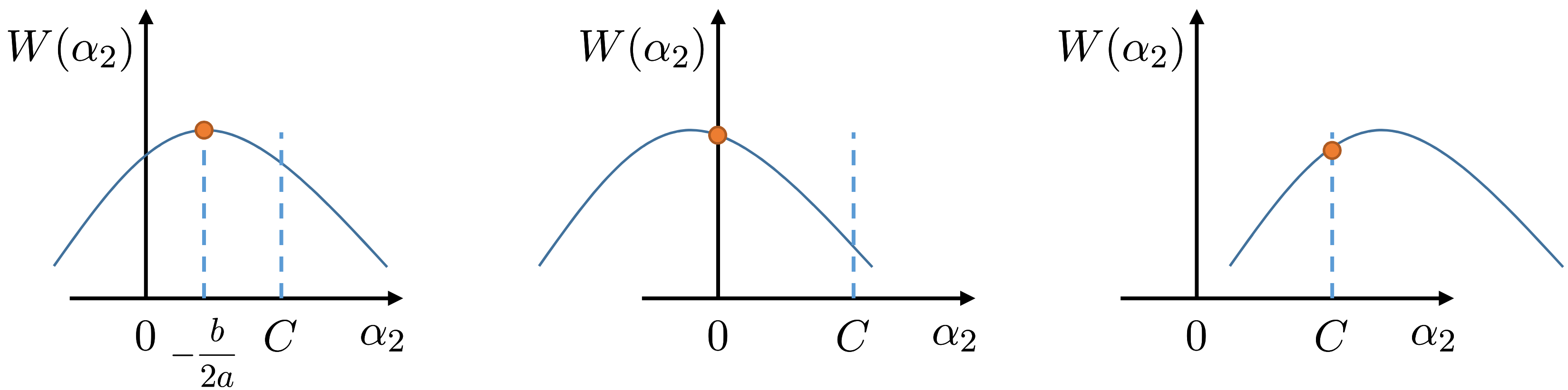
$$\begin{aligned} \max_{\alpha} \quad & W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j {x^{(i)}}^\top x^{(j)} \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C, \; i = 1, \ldots, m \\ & \sum_{i=1}^{m} \alpha_i y^{(i)} = 0 \end{aligned}$$

is transformed into a quadratic optimization problem w.r.t. α_2

$$\begin{aligned} \max_{\alpha_2} \quad & W(\alpha_2) = a\alpha_2^2 + b\alpha_2 + c \\ \text{s.t.} \quad & 0 \leq \alpha_2 \leq C \end{aligned}$$

SMO Algorithm

- Optimizing a quadratic function is much efficient

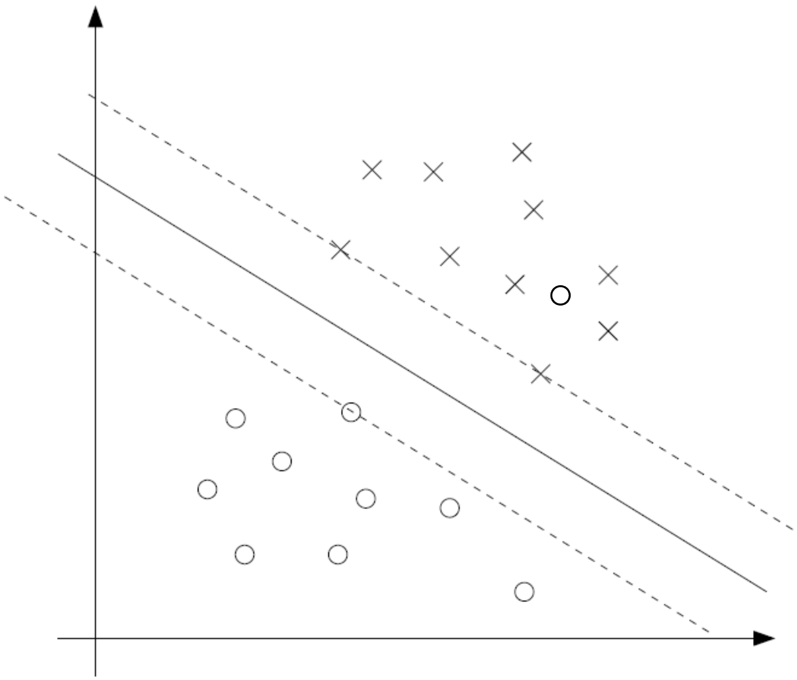


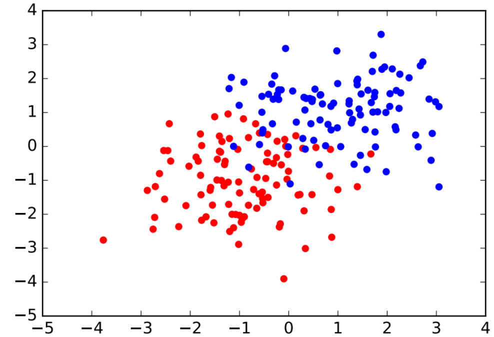
$$\max_{\alpha_2} \quad W(\alpha_2) = a\alpha_2^2 + b\alpha_2 + c$$
$$\text{s.t.} \quad 0 \le \alpha_2 \le C$$

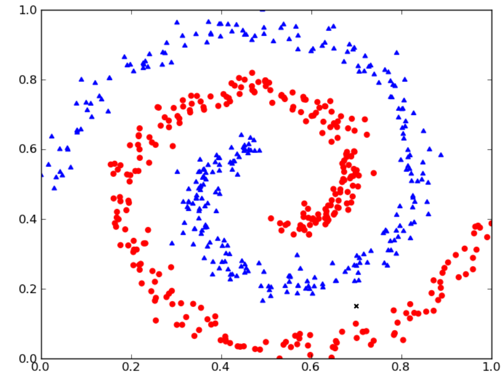
Kernel Methods

Non-Separable Cases

- More practical cases are linearly non-separable.

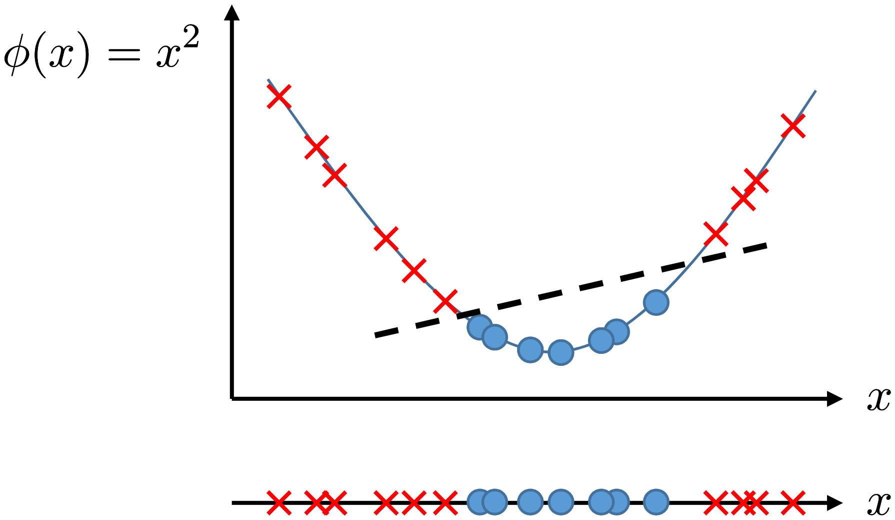






Non-Separable Cases

- More practical cases are linearly non-separable.

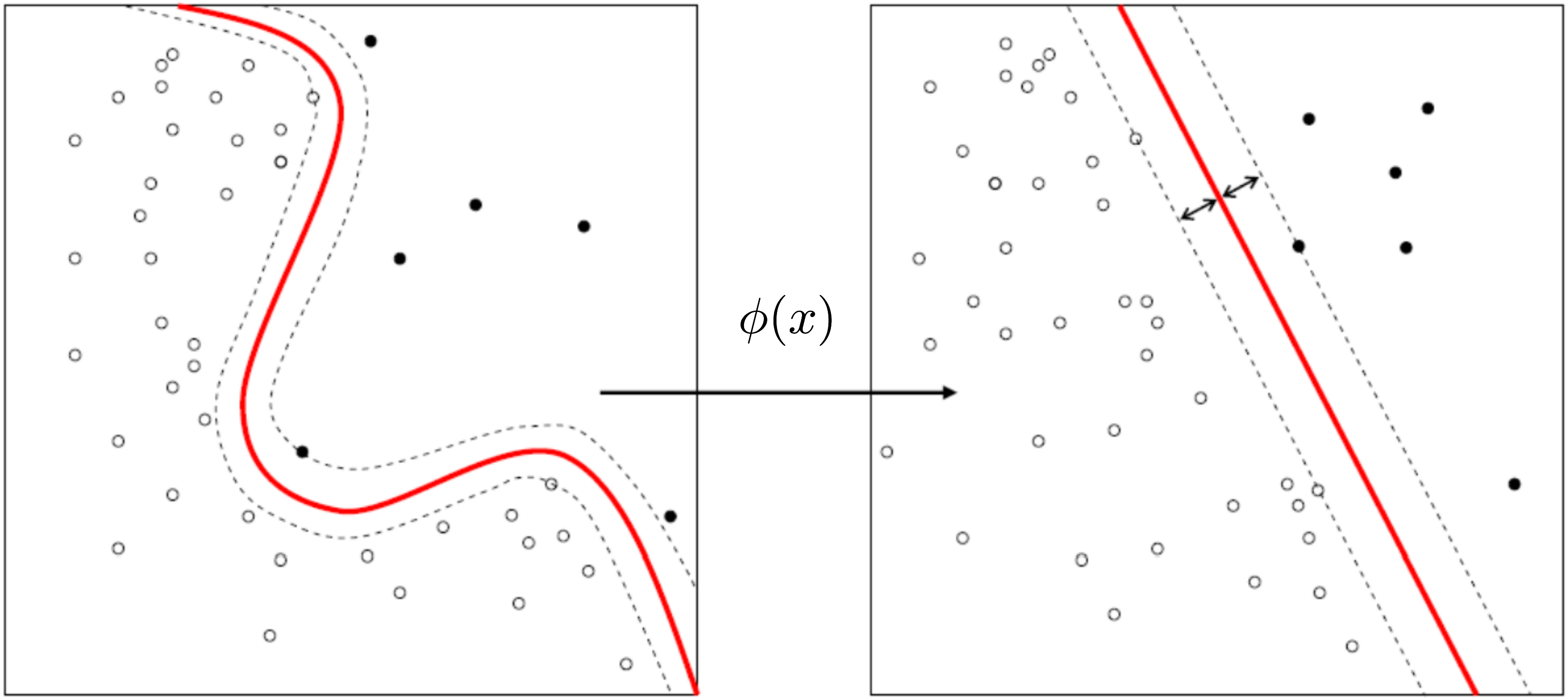


- Solution: mapping feature vectors to a higher-dimensional space

$$\phi(x)$$

Non-Separable Cases

- More generally, mapping feature vectors to a different space



Figures from Stuart Russell

Feature Mapping Functions

- SVM only cares about the inner products

$$W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j {x^{(i)}}^\top x^{(j)}$$

- With the feature mapping function $\phi(x)$

$$W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j K(x^{(i)}, x^{(j)})$$

- Kernel $K(x^{(i)}, x^{(j)}) = \phi(x^{(i)})^\top \phi(x^{(j)})$

Kernel

- With the example feature mapping function

$$\phi(x) = \begin{bmatrix} x \\ x^2 \\ x^3 \end{bmatrix}$$

- The corresponding kernel is

$$\begin{aligned} K(x^{(i)}, x^{(j)}) &= \phi(x^{(i)})^\top \phi(x^{(j)}) \\ &= x^{(i)} x^{(j)} + {x^{(i)}}^2 {x^{(j)}}^2 + {x^{(i)}}^3 {x^{(j)}}^3 \end{aligned}$$

- For lots of cases, we only need $K(x^{(i)}, x^{(j)})$, thus we can directly define $K(x^{(i)}, x^{(j)})$ without explicitly defining $\phi(x^{(i)})$
  - For example, suppose $x^{(i)}, x^{(j)} \in \mathbb{R}^n$

$$K(x^{(i)}, x^{(j)}) = ({x^{(i)}}^\top x^{(j)})^2$$

Kernel Example

- For example, suppose $x^{(i)}, x^{(j)} \in \mathbb{R}^n$

If *n* = 3, the mapping function is

$$
\begin{aligned}
K(x^{(i)}, x^{(j)}) &= ({x^{(i)}}^\top x^{(j)})^2 \\
&= \Big(\sum_{k=1}^{n} x_k^{(i)} x_k^{(j)}\Big)\Big(\sum_{l=1}^{n} x_l^{(i)} x_l^{(j)}\Big) \\
&= \sum_{k=1}^{n}\sum_{l=1}^{n} x_k^{(i)} x_k^{(j)} x_l^{(i)} x_l^{(j)} \\
&= \sum_{k,l=1}^{n} (x_k^{(i)} x_l^{(i)})(x_k^{(j)} x_l^{(j)})
\end{aligned}
\quad \Rightarrow \quad
\phi(x) = \begin{bmatrix} x_1x_1 \\ x_1x_2 \\ x_1x_3 \\ x_2x_1 \\ x_2x_2 \\ x_2x_3 \\ x_3x_1 \\ x_3x_2 \\ x_3x_3 \end{bmatrix}
$$

- Note that calculating $\phi(x)$ takes *O*(*n*^{2}) time, while calculating $K(x^{(i)}, x^{(j)})$ only takes *O*(*n*) time

Kernel for Measuring Similarity

- Intuitively, for two instances *x* and *z*, if $\phi(x)$ and $\phi(z)$ are close together, then we expect

$$K(x,z) = \phi(x)^\top \phi(z)$$

  to be large, and vice versa.

- Gaussian kernel

$$K(x,z) = \exp\left(-\frac{\|x-z\|^2}{2\sigma^2}\right)$$

  - Also called radial basis function (RBF) kernel
  - Then what is the feature mapping function for this kernel?

Kernel Matrix

- Consider a finite set of instances $\{x^{(1)}, \ldots, x^{(m)}\}$
- The corresponding Kernel Matrix *K* is defined as $\{K_{ij}\}_{i,j=1,\ldots,m}$
- The kernel matrix *K* must be symmetric since

$$K_{ij} = K(x^{(i)}, x^{(j)}) = \phi(x^{(i)})^\top \phi(x^{(j)}) = \phi(x^{(j)})^\top \phi(x^{(i)}) = K(x^{(j)}, x^{(i)}) = K_{ji}$$

- If we define $\phi_k(x)$ as the *k*-th coordinate of the vector $\phi(x)$, then for any vector $z \in \mathbb{R}^m$, we have

$$\begin{aligned} z^\top K z &= \sum_i \sum_j z_i K_{ij} z_j \\ &= \sum_i \sum_j z_i \phi(x^{(i)})^\top \phi(x^{(j)}) z_j = \sum_i \sum_j z_i \sum_k \phi_k(x^{(i)}) \phi_k(x^{(j)}) z_j \\ &= \sum_k \sum_i \sum_j z_i \phi_k(x^{(i)}) \phi_k(x^{(j)}) z_j = \sum_k \Big(\sum_i z_i \phi_k(x^{(i)}) \Big)^2 \geq 0 \end{aligned}$$

- Therefore, *K* is semi-definite

Valid (Mercer) Kernel

James Mercer
UK Mathematician
1883-1932

- Theorem (Mercer)

  Let $K : \mathbb{R}^n \times \mathbb{R}^n \mapsto \mathbb{R}$ be given. Then for *K* to be a valid (Mercer) kernel, it is necessary and sufficient that for any $\{x^{(1)}, \ldots, x^{(m)}\},\ m < \infty$, the corresponding kernel matrix is symmetric positive semi-definite.

- Example valid kernels
  - RBF kernel $K(x, z) = \exp\left(-\frac{\|x - z\|^2}{2\sigma^2}\right)$
  - Simple polynomial kernel $K(x, z) = (x^\top z)^d$
  - Cosine similarity kernel $K(x, z) = \frac{x^\top z}{\|x\| \cdot \|z\|}$

Sigmoid Kernel

$$K(x, z) = \tanh(\alpha x^\top z + c)$$

- Neural networks use sigmoid as activation function
- SVM with a sigmoid kernel is equivalent to a 2-layer perceptron

(We shall return to this after the study of neural networks)

Generalized Linear Models

Review: Linear Regression

$$\boldsymbol{X} = \begin{bmatrix} \boldsymbol{x}^{(1)} \\ \boldsymbol{x}^{(2)} \\ \vdots \\ \boldsymbol{x}^{(n)} \end{bmatrix} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & x_3^{(1)} & \dots & x_d^{(1)} \\ x_1^{(2)} & x_2^{(2)} & x_3^{(2)} & \dots & x_d^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_1^{(n)} & x_2^{(n)} & x_3^{(n)} & \dots & x_d^{(n)} \end{bmatrix} \quad \boldsymbol{\theta} = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_d \end{bmatrix} \quad \boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

- Prediction $\hat{\boldsymbol{y}} = \boldsymbol{X}\boldsymbol{\theta} = \begin{bmatrix} \boldsymbol{x}^{(1)}\boldsymbol{\theta} \\ \boldsymbol{x}^{(2)}\boldsymbol{\theta} \\ \vdots \\ \boldsymbol{x}^{(n)}\boldsymbol{\theta} \end{bmatrix}$

- Objective $J(\boldsymbol{\theta}) = \frac{1}{2}(\boldsymbol{y} - \hat{\boldsymbol{y}})^\top(\boldsymbol{y} - \hat{\boldsymbol{y}}) = \frac{1}{2}(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta})^\top(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta})$

Review: Matrix Form of Linear Reg.

- Objective

$$J(\boldsymbol{\theta}) = \frac{1}{2}(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta})^\top(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}) \qquad \min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$$

- Gradient

$$\frac{\partial J(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = -\boldsymbol{X}^\top(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta})$$

- Solution

$$\frac{\partial J(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \boldsymbol{0} \;\rightarrow\; \boldsymbol{X}^\top(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}) = \boldsymbol{0}$$

$$\rightarrow\; \boldsymbol{X}^\top\boldsymbol{y} = \boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{\theta}$$

$$\rightarrow\; \hat{\boldsymbol{\theta}} = (\boldsymbol{X}^\top\boldsymbol{X})^{-1}\boldsymbol{X}^\top\boldsymbol{y}$$

Generalized Linear Models

- Dependence

$$y = f(\theta^\top \phi(x))$$

  - Feature mapping function $\phi(x) : \mathbb{R}^d \mapsto \mathbb{R}^h$
  - Mapped feature matrix $\Phi_{n\times h}$

$$\Phi = \begin{bmatrix} \phi(x^{(1)}) \\ \phi(x^{(2)}) \\ \vdots \\ \phi(x^{(i)}) \\ \vdots \\ \phi(x^{(n)}) \end{bmatrix} = \begin{bmatrix} \phi_1(x^{(1)}) & \phi_2(x^{(1)}) & \cdots & \phi_h(x^{(1)}) \\ \phi_1(x^{(2)}) & \phi_2(x^{(2)}) & \cdots & \phi_h(x^{(2)}) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(x^{(i)}) & \phi_2(x^{(i)}) & \cdots & \phi_h(x^{(i)}) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(x^{(n)}) & \phi_2(x^{(n)}) & \cdots & \phi_h(x^{(n)}) \end{bmatrix}$$

Matrix Form of Kernel Linear Regression

- Objective

$$J(\boldsymbol{\theta}) = \frac{1}{2}(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta})^\top(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta}) \qquad \min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$$

- Gradient

$$\frac{\partial J(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = -\boldsymbol{\Phi}^\top(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta})$$

- Solution

$$\begin{aligned} \frac{\partial J(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \mathbf{0} \;\; &\rightarrow \;\; \boldsymbol{\Phi}^\top(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta}) = \mathbf{0} \\ &\rightarrow \;\; \boldsymbol{\Phi}^\top \boldsymbol{y} = \boldsymbol{\Phi}^\top\boldsymbol{\Phi}\boldsymbol{\theta} \\ &\rightarrow \;\; \hat{\boldsymbol{\theta}} = (\boldsymbol{\Phi}^\top\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^\top\boldsymbol{y} \end{aligned}$$

Matrix Form of Kernel Linear Regression

- With the Algebra trick

$$(\boldsymbol{P}^{-1} + \boldsymbol{B}^\top \boldsymbol{R}^{-1} \boldsymbol{B})^{-1} \boldsymbol{B}^\top \boldsymbol{R}^{-1} = \boldsymbol{P}\boldsymbol{B}^\top (\boldsymbol{B}\boldsymbol{P}\boldsymbol{B}^\top + R)^{-1}$$

- The optimal parameters with L2 regularization

$$\begin{aligned} \hat{\boldsymbol{\theta}} &= (\boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \lambda \boldsymbol{I}_h)^{-1} \boldsymbol{\Phi}^\top \boldsymbol{y} \\ &= \boldsymbol{\Phi}^\top (\boldsymbol{\Phi}\boldsymbol{\Phi}^\top + \lambda \boldsymbol{I}_n)^{-1} \boldsymbol{y} \end{aligned}$$

for prediction, we never actually need access $\boldsymbol{\Phi}$

$$\begin{aligned} \hat{\boldsymbol{y}} = \boldsymbol{\Phi}\hat{\boldsymbol{\theta}} &= \boldsymbol{\Phi}\boldsymbol{\Phi}^\top (\boldsymbol{\Phi}\boldsymbol{\Phi}^\top + \lambda \boldsymbol{I}_n)^{-1} \boldsymbol{y} \\ &= \boldsymbol{K}(\boldsymbol{K} + \lambda \boldsymbol{I}_n)^{-1} \boldsymbol{y} \end{aligned}$$

where the kernel matrix $\boldsymbol{K} = \{K(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)})\}$

[http://www.ics.uci.edu/~welling/classnotes/papers_class/Kernel-Ridge.pdf]