Support Vector Machines, Kernel SVM

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Outline

1. Administration
2. Review of last lecture
3. SVM – Hinge loss (primal formulation)
4. Kernel SVM
Announcements

- Project proposal due now
- Graded HW3 and HW4 will be returned next Thursday
- HW5 has been posted online; due next Thursday
1. Administration

2. Review of last lecture
   - SVMs – Geometric interpretation

3. SVM – Hinge loss (primal formulation)

4. Kernel SVM
SVM Intuition: where to put the decision boundary?

Consider the following separable training dataset, i.e., we assume there exists a decision boundary that separates the two classes perfectly. There are an infinite number of decision boundaries \( \mathcal{H} : \mathbf{w}^T \phi(\mathbf{x}) + b = 0 \).

Which one should we pick? Idea: Find a decision boundary in the 'middle' of the two classes. In other words, we want a decision boundary that:

- Perfectly classifies the training data
- Is as far away from every training point as possible
The *unsigned* distance from a point $\phi(x)$ to decision boundary (hyperplane) $\mathcal{H}$ is

$$d_{\mathcal{H}}(\phi(x)) = \frac{|\mathbf{w}^T \phi(x) + b|}{\|\mathbf{w}\|_2}$$
Distance from a point to decision boundary

The *unsigned* distance from a point $\phi(x)$ to decision boundary (hyperplane) $\mathcal{H}$ is

$$d_{\mathcal{H}}(\phi(x)) = \frac{|w^T \phi(x) + b|}{\|w\|_2}$$

We can remove the absolute value $| \cdot |$ by exploiting the fact that the decision boundary classifies every point in the training dataset correctly. Namely, $(w^T \phi(x) + b)$ and $x$’s label $y$ must have the same sign, so:

$$d_{\mathcal{H}}(\phi(x)) = \frac{y[w^T \phi(x) + b]}{\|w\|_2}$$
Optimizing the Margin

**Margin** Smallest distance between the hyperplane and all training points

\[
MARGIN(w, b) = \min_n y_n \frac{w^T \phi(x_n) + b}{\|w\|_2}
\]

How should we pick \((w, b)\) based on its margin?

We want a decision boundary that is as far away from all training points as possible, so we maximize the margin!

\[
\max_{w, b} \min_n y_n \frac{w^T \phi(x_n) + b}{\|w\|_2} = \max_{w, b} \frac{1}{\|w\|_2}
\]
Optimizing the Margin

**Margin** Smallest distance between the hyperplane and all training points

\[
\text{MARGIN}(\mathbf{w}, b) = \min_n \frac{y_n[\mathbf{w}^T \phi(\mathbf{x}_n) + b]}{\|\mathbf{w}\|_2}
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How should we pick \((\mathbf{w}, b)\) based on its margin?
Optimizing the Margin

**Margin** Smallest distance between the hyperplane and all training points

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\]

How should we pick \((\mathbf{w}, b)\) based on its margin?

We want a decision boundary that is as far away from all training points as possible, so we to *maximize* the margin!

\[
\max_{\mathbf{w},b} \min_n \frac{y_n[\mathbf{w}^T \phi(\mathbf{x}_n) + b]}{\|\mathbf{w}\|} = \max_{\mathbf{w},b} \frac{1}{\|\mathbf{w}\|_2} \min_n y_n[\mathbf{w}^T \phi(\mathbf{x}_n) + b]
\]
Rescaled Margin

We can further constrain the problem by scaling \((w, b)\) such that

\[
\min_n y_n[w^T \phi(x_n) + b] = 1
\]
Rescaled Margin

We can further constrain the problem by scaling $(w, b)$ such that

$$\min_n y_n[w^T \phi(x_n) + b] = 1$$

We’ve fixed the numerator in the $\text{MARGIN}(w, b)$ equation, and we have:

$$\text{MARGIN}(w, b) = \frac{1}{\|w\|_2}$$
Rescaled Margin

We can further constrain the problem by scaling \((w, b)\) such that

\[
\min_n y_n [w^T \phi(x_n) + b] = 1
\]

We’ve fixed the numerator in the MARGIN\((w, b)\) equation, and we have:

\[
\text{MARGIN}(w, b) = \frac{1}{\|w\|_2}
\]

Hence the points closest to the decision boundary are at distance 1!
SVM: max margin formulation for separable data

Assuming separable training data, we thus want to solve:

$$\max_{w,b} \frac{1}{\|w\|_2} \text{ such that } y_n[w^T \phi(x_n) + b] \geq 1, \ \forall \ n$$

This is equivalent to

$$\min_{w,b} \frac{1}{2} \|w\|_2^2 \text{ s.t. } y_n[w^T \phi(x_n) + b] \geq 1, \ \forall \ n$$

Given our geometric intuition, SVM is called a max margin (or large margin) classifier. The constraints are called large margin constraints.
SVM for non-separable data

Constraints in separable setting

\[ y_n [\mathbf{w}^T \phi(x_n) + b] \geq 1, \quad \forall \ n \]

Constraints in non-separable setting

Idea: modify our constraints to account for non-separability! Specifically, we introduce *slack variables* \( \xi_n \geq 0 \):

\[ y_n [\mathbf{w}^T \phi(x_n) + b] \geq 1 - \xi_n, \quad \forall \ n \]
SVM for non-separable data

Constraints in separable setting

\[ y_n [\mathbf{w}^T \phi(x_n) + b] \geq 1, \quad \forall \ n \]

Constraints in non-separable setting

Idea: modify our constraints to account for non-separability! Specifically, we introduce slack variables \( \xi_n \geq 0 \):

\[ y_n [\mathbf{w}^T \phi(x_n) + b] \geq 1 - \xi_n, \quad \forall \ n \]

- For “hard” training points, we can increase \( \xi_n \) until the above inequalities are met
- What does it mean when \( \xi_n \) is very large?
Soft-margin SVM formulation

We do not want $\xi_n$ to grow too large, and we can control their size by incorporating them into our optimization problem:

$$
\min_{w,b,\xi} \frac{1}{2} \|w\|^2 + C \sum_n \xi_n
$$

s.t. $y_n[w^T \phi(x_n) + b] \geq 1 - \xi_n$, $\forall n$

$\xi_n \geq 0$, $\forall n$

- $C$ is user-defined regularization hyperparameter that trades off between the two terms in our objective
- This is a convex quadratic program that can be solved with general purpose or specialized solvers
The SVM solution is only determined by a subset of the training samples (as we will see later in the lecture).

These samples are called *support vectors*, which are highlighted by the dotted orange lines in the figure.
Outline

1 Administration

2 Review of last lecture

3 SVM – Hinge loss (primal formulation)

4 Kernel SVM
Hinge loss

**Definition** Assume $y \in \{-1, 1\}$ and the decision rule is $h(x) = \text{SIGN}(f(x))$ with $f(x) = w^T \phi(x) + b$,

$$
\ell_{\text{HINGE}}(f(x), y) = \begin{cases} 
0 & \text{if } yf(x) \geq 1 \\
1 - yf(x) & \text{otherwise}
\end{cases}
$$

**Intuition**

No penalty if raw output, $f(x)$, has same sign and is far enough from decision boundary (i.e., if 'margin' is large enough) Otherwise pay a growing penalty, between 0 and 1 if signs match, and greater than one otherwise
Hinge loss

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- Otherwise pay a growing penalty, between 0 and 1 if signs match, and greater than one otherwise

**Convenient shorthand**

$$
\ell_{\text{Hinge}}(f(x), y) = \max(0, 1 - yf(x)) = (1 - yf(x))^+
$$
Visualization and Properties

We use hinge loss as a surrogate to \( \ell_0/\ell_1 \) loss – Why?

Hinge loss is convex, and thus easier to work with (though it's not differentiable at kink).
Visualization and Properties

- Upper-bound for 0/1 loss function (black line)
- We use hinge loss is a *surrogate* to 0/1 loss – Why?
Visualization and Properties

- Upper-bound for 0/1 loss function (black line)
- We use hinge loss is a surrogate to 0/1 loss – Why?
- Hinge loss is convex, and thus easier to work with (though it’s not differentiable at kink)
Other surrogate losses can be used, e.g., exponential loss for Adaboost (in blue), logistic loss (not shown) for logistic regression.

- Hinge loss less sensitive to outliers than exponential (or logistic) loss.
- Logistic loss has a natural probabilistic interpretation.
- We can greedily optimize exponential loss (Adaboost).
Primal formulation of support vector machines (SVM)

Minimizing the total hinge loss on all the training data

\[
\min_{w, b} \sum_n \max(0, 1 - y_n [w^T \phi(x_n) + b]) + \frac{\lambda}{2} \|w\|_2^2
\]

Analogous to regularized least squares, as we balance between two terms (the loss and the regularizer).
Primal formulation of support vector machines (SVM)

Minimizing the total hinge loss on all the training data

\[
\min_{\mathbf{w}, b} \sum_n \max(0, 1 - y_n[\mathbf{w}^T \phi(\mathbf{x}_n) + b]) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2
\]

Analogous to regularized least squares, as we balance between two terms (the loss and the regularizer).

Previously, we used geometric arguments to derive:

\[
\min_{\mathbf{w}, b, \xi} \frac{1}{2} \|\mathbf{w}\|_2^2 + C \sum_n \xi_n
\]

s.t. \( y_n[\mathbf{w}^T \phi(\mathbf{x}_n) + b] \geq 1 - \xi_n \) and \( \xi_n \geq 0, \quad \forall \ n \)

Do these the yield the same solution?
Recovering our previous SVM formulation

Define $C = 1/\lambda$:

$$\min_{w,b} C \sum_n \max(0, 1 - y_n [w^T \phi(x_n) + b]) + \frac{1}{2} \|w\|_2^2$$
Recovering our previous SVM formulation

Define $C = 1/\lambda$:

$$
\min_{w,b} \quad C \sum_n \max(0, 1 - y_n[w^T \phi(x_n) + b]) + \frac{1}{2} \|w\|_2^2
$$

Define $\xi_n \geq \max(0, 1 - y_n f(x_n))$

$$
\min_{w,b,\xi} \quad C \sum_n \xi_n + \frac{1}{2} \|w\|_2^2
$$

s.t. $\max(0, 1 - y_n[w^T \phi(x_n) + b]) \leq \xi_n, \quad \forall n$

At optimal solution constraints are active so we have equality! Why?
Recovering our previous SVM formulation

Define $C = 1/\lambda$:

$$\min_{w,b} C \sum_n \max(0, 1 - y_n[w^T \phi(x_n) + b]) + \frac{1}{2} \|w\|_2^2$$

Define $\xi_n \geq \max(0, 1 - y_n f(x_n))$

$$\min_{w,b,\xi} C \sum_n \xi_n + \frac{1}{2} \|w\|_2^2$$

s.t. $\max(0, 1 - y_n[w^T \phi(x_n) + b]) \leq \xi_n, \quad \forall n$

At optimal solution constraints are active so we have equality! Why?
- If $\xi_n^* > \max(0, 1 - y_n f(x_n))$, we could choose $\bar{\xi}_n < \xi_n^*$ and still satisfy the constraint while reducing our objective function!
- Since $c \geq \max(a, b) \iff c \geq a, c \geq b$, we recover previous formulation
Outline

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2 Review of last lecture

3 SVM – Hinge loss (primal formulation)

4 Kernel SVM
   - Lagrange duality theory
   - SVM Dual Formulation and Kernel SVM
   - SVM Dual Derivation and Support Vectors
Kernel SVM Roadmap

**Key concepts we’ll cover**

- Brief review of constrained optimization with inequality constraints
  - “Primal” and “Dual” problems
  - Strong Duality and KKT conditions
- Dual SVM problem and Kernel SVM
- Dual SVM problem and support vectors
Constrained Optimization – Equality Constraints

$$\min_x f(x)$$

s.t. $h_j(x) = 0, \quad \forall j$

The Lagrangian is defined as follows:

$$L(x, \beta) = f(x) + \sum_j \beta_j h_j(x)$$

When problem is convex, we can find the optimal solution by

- Computing partial derivatives of $L$
- Setting them to zero
- Solving the corresponding system of equations
Constrained Optimization – Inequality Constraints

\[
\begin{align*}
\min_{\mathbf{x}} & \quad f(\mathbf{x}) \\
\text{s.t.} & \quad g_i(\mathbf{x}) \leq 0, \quad \forall \ i \\
& \quad h_i(\mathbf{x}) = 0, \quad \forall \ j
\end{align*}
\]

This is the ‘primal’ problem
Constrained Optimization – Inequality Constraints

\[
\min_x f(x) \\
\text{s.t. } g_i(x) \leq 0, \quad \forall \ i \\
h_i(x) = 0, \quad \forall \ j
\]

This is the ‘primal’ problem with the *generalized* Lagrangian:

\[
L(x, \alpha, \beta) = f(x) + \sum_i \alpha_i g_i(x) + \sum_j \beta_j h_j(x)
\]
Constrained Optimization – Inequality Constraints

\[ \min_x f(x) \]
\[ \text{s.t. } g_i(x) \leq 0, \quad \forall \ i \]
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This is the ‘primal’ problem with the generalized Lagrangian:

\[ L(x, \alpha, \beta) = f(x) + \sum_i \alpha_i g_i(x) + \sum_j \beta_j h_j(x) \]

Consider the following function:

\[ \theta_P(x) = \max_{\alpha, \beta, \alpha_i \geq 0} L(x, \alpha, \beta) \]
Constrained Optimization – Inequality Constraints

\[
\begin{align*}
\min_x & \quad f(x) \\
\text{s.t.} & \quad g_i(x) \leq 0, \quad \forall \ i \\
& \quad h_i(x) = 0, \quad \forall \ j
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This is the ‘primal’ problem with the \textit{generalized} Lagrangian:

\[
L(x, \alpha, \beta) = f(x) + \sum_i \alpha_i g_i(x) + \sum_j \beta_j h_j(x)
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Consider the following function:

\[
\theta_P(x) = \max_{\alpha, \beta, \alpha_i \geq 0} L(x, \alpha, \beta)
\]

- If \( x \) violates a primal constraint, \( \theta_P(x) = \infty \);
Constrained Optimization – Inequality Constraints

\[
\begin{align*}
\min_x & \quad f(x) \\
\text{s.t.} & \quad g_i(x) \leq 0, \quad \forall \ i \\
& \quad h_i(x) = 0, \quad \forall \ j
\end{align*}
\]

This is the ‘primal’ problem with the \textit{generalized} Lagrangian:

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L(x, \alpha, \beta) = f(x) + \sum_i \alpha_i g_i(x) + \sum_j \beta_j h_j(x)
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- If \( x \) violates a primal constraint, \( \theta_P(x) = \infty \); otherwise \( \theta_P(x) = f(x) \)
Constrained Optimization – Inequality Constraints

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\min_x \quad f(x) \\
\text{s.t.} \quad g_i(x) \leq 0, \quad \forall \ i \\
\quad h_i(x) = 0, \quad \forall \ j
\]

This is the ‘primal’ problem with the generalized Lagrangian:

\[
L(x, \alpha, \beta) = f(x) + \sum_i \alpha_i g_i(x) + \sum_j \beta_j h_j(x)
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Consider the following function:

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\theta_P(x) = \max_{\alpha, \beta, \alpha_i \geq 0} L(x, \alpha, \beta)
\]

- If \(x\) violates a primal constraint, \(\theta_P(x) = \infty\); otherwise \(\theta_P(x) = f(x)\)
- Thus \(\min_x \theta_P(x) = \min_x \max_{\alpha, \beta, \alpha_i \geq 0} L(x, \alpha, \beta)\) has same solution as primal problem, which we denote as \(p^*\)
Constrained Optimization – Inequality Constraints

Primal Problem

\[ p^* = \min_{\mathbf{x}} \theta_P(\mathbf{x}) = \min_{\mathbf{x}} \max_{\alpha, \beta, \alpha_i \geq 0} L(\mathbf{x}, \alpha, \beta) \]

Dual Problem

Consider the function: \( \theta_D(\alpha, \beta) = \min_{\mathbf{x}} L(\mathbf{x}, \alpha, \beta) \)
Constrained Optimization – Inequality Constraints

Primal Problem

\[ p^* = \min_{x} \theta_P(x) = \min_{x} \max_{\alpha, \beta, \alpha_i \geq 0} L(x, \alpha, \beta) \]

Dual Problem

Consider the function: \( \theta_D(\alpha, \beta) = \min_{x} L(x, \alpha, \beta) \)

\[ d^* = \max_{\alpha, \beta, \alpha_i \geq 0} \theta_D(\alpha, \beta) = \max_{\alpha, \beta, \alpha_i \geq 0} \min_{x} L(x, \alpha, \beta) \]
Constrained Optimization – Inequality Constraints

**Primal Problem**

\[ p^* = \min_x \theta_P(x) = \min_x \max_{\alpha,\beta,\alpha_i \geq 0} L(x, \alpha, \beta) \]

**Dual Problem**

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Primal and dual are the same, except the max and min are exchanged!

**Relationship between primal and dual?**
Constrained Optimization – Inequality Constraints

**Primal Problem**

\[ p^* = \min_x \theta_P(x) = \min_x \max_{\alpha, \beta, \alpha_i \geq 0} L(x, \alpha, \beta) \]

**Dual Problem**

Consider the function: \( \theta_D(\alpha, \beta) = \min_x L(x, \alpha, \beta) \)

\[ d^* = \max_{\alpha, \beta, \alpha_i \geq 0} \theta_D(\alpha, \beta) = \max_{\alpha, \beta, \alpha_i \geq 0} \min_x L(x, \alpha, \beta) \]

Primal and dual are the same, except the max and min are exchanged!

**Relationship between primal and dual?**

- \( p^* \geq d^* \) (weak duality)
- ‘min max’ of any function is always greater than the ‘max min’
- [https://en.wikipedia.org/wiki/Max%E2%80%93min_inequality](https://en.wikipedia.org/wiki/Max%E2%80%93min_inequality)
Strong Duality

When \( p^* = d^* \), we can solve the dual problem in lieu of the problem!
Strong Duality

When \( p^* = d^* \), we can solve the dual problem in lieu of the problem!

Sufficient conditions for strong duality:

- \( f \) and \( g_i \) are convex, \( h_i \) are affine (i.e., linear with offset)
- Inequality constraints are strictly ‘feasible,’ i.e., there exists some \( x \) such that \( g_i(x) < 0 \) for all \( i \)
- These conditions are all satisfied by the SVM optimization problem!
Strong Duality

When $p^* = d^*$, we can solve the dual problem in lieu of the problem!

Sufficient conditions for strong duality:

- $f$ and $g_i$ are convex, $h_i$ are affine (i.e., linear with offset)
- Inequality constraints are strictly ‘feasible,’ i.e., there exists some $x$ such that $g_i(x) < 0$ for all $i$
- These conditions are all satisfied by the SVM optimization problem!

Under these assumptions, there must exist $x^*, \alpha^*, \beta^*$ such that:

- $x^*$ is the solution to the primal and $\alpha^*, \beta^*$ is the solution to the dual
- $p^* = d^* = L(x^*, \alpha^*, \beta^*)$
- $x^*, \alpha^*, \beta^*$ satisfy the KKT conditions, and in fact are necessary and sufficient
Recap

- When working with constrained optimization problems with inequality constraints, we can write down primal and dual problems.
- The dual solution is always a lower bound on the primal solution (weak duality).
- The duality gap equals 0 under certain conditions (strong duality), and in such cases we can either solve the primal or dual problem.
- Strong duality holds for the SVM problem, and in particular the KKT conditions are necessary and sufficient for the optimal solution.
Dual formulation of SVM

Dual is also a convex quadratic programming

\[
\max_{\alpha} \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} y_m y_n \alpha_m \alpha_n \phi(x_m)^T \phi(x_n)
\]

s.t. \[ 0 \leq \alpha_n \leq C, \quad \forall \ n \]
\[ \sum_n \alpha_n y_n = 0 \]
Dual formulation of SVM

Dual is also a convex quadratic programming

\[
\max_\alpha \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} y_m y_n \alpha_m \alpha_n \phi(x_m)^T \phi(x_n)
\]

s.t. \(0 \leq \alpha_n \leq C, \quad \forall \ n\)

\[
\sum_n \alpha_n y_n = 0
\]

- There are \(N\) dual variable \(\alpha_n\), one for each constraint in the primal formulation
Kernel SVM

We replace the inner products $\phi(x_m)^T \phi(x_n)$ with a kernel function

$$\max_{\alpha} \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} y_m y_n \alpha_m \alpha_n k(x_m, x_n)$$

s.t. $0 \leq \alpha_n \leq C, \forall n$

$$\sum_n \alpha_n y_n = 0$$

We can define a kernel function to work with nonlinear features and learn a nonlinear decision surface.
Recovering solution to the primal formulation

Weights

\[ w = \sum_{n} y_n \alpha_n \phi(x_n) \leftarrow \text{Linear combination of the input features} \]
Recovering solution to the primal formulation

**Weights**

\[ w = \sum_{n} y_n \alpha_n \phi(x_n) \quad \leftarrow \quad \text{Linear combination of the input features} \]

**Offset**

\[ b = [y_n - w^T \phi(x_n)] = [y_n - \sum_{m} y_m \alpha_m k(x_m, x_n)], \quad \text{for any } C > \alpha_n > 0 \]
Recovering solution to the primal formulation

Weights

\[ w = \sum_n y_n \alpha_n \phi(x_n) \leftarrow \text{Linear combination of the input features} \]

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Prediction on a test point \( \mathbf{x} \)

\[ h(\mathbf{x}) = \text{SIGN}(\mathbf{w}^T \phi(\mathbf{x}) + b) = \text{SIGN}(\sum_n y_n \alpha_n k(x_n, x) + b) \]

At test time it suffices to know the kernel function!
Derivation of the dual

We will derive the dual formulation as the process will reveal some interesting and important properties of SVM. Particularly, why is it called “support vector”?

Recipe

- Formulate the generalized Lagrangian function that incorporates the constraints and introduces dual variables
- Minimize the Lagrangian function over the primal variables
- Substitute the primal variables for dual variables in the Lagrangian
- Maximize the Lagrangian with respect to dual variables
- Recover the solution (for the primal variables) from the dual variables
A simple example

Consider the example of convex quadratic programming

\[
\begin{align*}
\text{min} \quad & \frac{1}{2} x^2 \\
\text{s.t.} \quad & -x \leq 0 \\
& 2x - 3 \leq 0
\end{align*}
\]

The generalized Lagrangian is (note that we do not have equality constraints)

\[
L(x, \alpha) = \frac{1}{2} x^2 + \alpha_1 \times (-x) + \alpha_2 \times (2x - 3) = \frac{1}{2} x^2 + (2\alpha_2 - \alpha_1)x - 3\alpha_2
\]

under the constraint that \( \alpha_1 \geq 0 \) and \( \alpha_2 \geq 0 \).
A simple example

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\]

under the constraint that \(\alpha_1 \geq 0\) and \(\alpha_2 \geq 0\). Its dual problem is

\[
\max_{\alpha_1 \geq 0, \alpha_2 \geq 0} \min_x L(x, \alpha) = \max_{\alpha_1 \geq 0, \alpha_2 \geq 0} \min_x \frac{1}{2}x^2 + (2\alpha_2 - \alpha_1)x - 3\alpha_2
\]
Example (cont’d)

We now solve \( \min_x L(x, \alpha) \). The optimal \( x \) is attained by

\[
\frac{\partial}{\partial x} \left( \frac{1}{2} x^2 + (2 \alpha_2 - \alpha_1)x - 3\alpha_2 \right) = 0 \rightarrow x = -(2\alpha_2 - \alpha_1)
\]
Example (cont’d)

We now solve $\min_x L(x, \alpha)$. The optimal $x$ is attained by

$$\frac{\partial}{\partial x} \left( \frac{1}{2} x^2 + (2\alpha_2 - \alpha_1)x - 3\alpha_2 \right) = 0 \rightarrow x = -(2\alpha_2 - \alpha_1)$$

We next substitute the solution back into the Lagrangian:

$$g(\alpha) = \min_x \frac{1}{2} x^2 + (2\alpha_2 - \alpha_1)x - 3\alpha_2 = -\frac{1}{2} (2\alpha_2 - \alpha_1)^2 - 3\alpha_2$$
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Our dual problem can now be simplified:

$$\max_{\alpha_1 \geq 0, \alpha_2 \geq 0} -\frac{1}{2} (2\alpha_2 - \alpha_1)^2 - 3\alpha_2$$

We will solve the dual next.
Solving the dual

Note that,

\[ g(\alpha) = -\frac{1}{2}(2\alpha_2 - \alpha_1)^2 - 3\alpha_2 \leq 0 \]

for all \( \alpha_1 \geq 0, \alpha_2 \geq 0 \). Thus, to maximize the function, the optimal solution is

\[ \alpha_1^* = 0, \quad \alpha_2^* = 0 \]

This brings us back the optimal solution of \( x \)

\[ x^* = -(2\alpha_2^* - \alpha_1^*) = 0 \]

Namely, we have arrived at the same solution as the one we guessed from the primal formulation.
Deriving the dual for SVM

Primal SVM

\[
\begin{align*}
\min_{w,b,\xi} & \quad \frac{1}{2} \|w\|^2 + C \sum_n \xi_n \\
\text{s.t.} & \quad y_n [w^T \phi(x_n) + b] \geq 1 - \xi_n, \quad \forall \ n \\
\xi_n & \geq 0, \quad \forall \ n
\end{align*}
\]
Deriving the dual for SVM

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\min_{w, b, \xi} \quad \frac{1}{2} \|w\|^2 + C \sum_n \xi_n \\
\text{s.t.} \quad y_n [w^T \phi(x_n) + b] \geq 1 - \xi_n, \quad \forall \ n \\
\xi_n \geq 0, \quad \forall \ n
\]

Lagrangian

\[
L(w, b, \{\xi_n\}, \{\alpha_n\}, \{\lambda_n\}) = C \sum_n \xi_n + \frac{1}{2} \|w\|^2 - \sum_n \lambda_n \xi_n \\
+ \sum_n \alpha_n \{1 - y_n [w^T \phi(x_n) + b] - \xi_n\}
\]

under the constraint that \(\alpha_n \geq 0\) and \(\lambda_n \geq 0\).
Minimizing the Lagrangian

Taking derivatives with respect to the primal variables

\[ \frac{\partial L}{\partial w} = w - \sum_n y_n \alpha_n \phi(x_n) = 0 \]

\[ \frac{\partial L}{\partial b} = \sum_n \alpha_n y_n = 0 \]

\[ \frac{\partial L}{\partial \xi_n} = C - \lambda_n - \alpha_n = 0 \]
Minimizing the Lagrangian

Taking derivatives with respect to the primal variables

\[
\frac{\partial L}{\partial w} = w - \sum_n y_n \alpha_n \phi(x_n) = 0
\]

\[
\frac{\partial L}{\partial b} = \sum_n \alpha_n y_n = 0
\]

\[
\frac{\partial L}{\partial \xi_n} = C - \lambda_n - \alpha_n = 0
\]

These equations link the primal variables and the dual variables and provide new constraints on the dual variables:

\[
w = \sum_n y_n \alpha_n \phi(x_n)
\]

\[
\sum_n \alpha_n y_n = 0
\]

\[
C - \lambda_n - \alpha_n = 0
\]
Substitute the solution back into the Lagrangian

\[ g(\{\alpha_n\}, \{\lambda_n\}) = L(w, b, \{\xi_n\}, \{\alpha_n\}, \{\lambda_n\}) \]
Substitute the solution back into the Lagrangian

\[ g(\{\alpha_n\}, \{\lambda_n\}) = L(w, b, \{\xi_n\}, \{\alpha_n\}, \{\lambda_n\}) \]

\[ = \sum_n (C - \alpha_n - \lambda_n) \xi_n + \frac{1}{2} \left\| \sum_n y_n \alpha_n \phi(x_n) \right\|^2_2 + \sum_n \alpha_n \]

\[ + \left( \sum_n \alpha_n y_n \right) b - \sum_n \alpha_n y_n \left( \sum_m y_m \alpha_m \phi(x_m) \right)^T \phi(x_n) \]
Substitute the solution back into the Lagrangian

\[ g(\{\alpha_n\}, \{\lambda_n\}) = L(w, b, \{\xi_n\}, \{\alpha_n\}, \{\lambda_n\}) = \sum_n (C - \alpha_n - \lambda_n) \xi_n + \frac{1}{2} \| \sum_n y_n \alpha_n \phi(x_n) \|^2_2 + \sum_n \alpha_n + \left( \sum_n \alpha_n y_n \right) b - \sum_n \alpha_n y_n \left( \sum_m y_m \alpha_m \phi(x_m) \right)^T \phi(x_n) \]

\[ = \sum_n \alpha_n + \frac{1}{2} \| \sum_n y_n \alpha_n \phi(x_n) \|^2_2 - \sum_{m,n} \alpha_n \alpha_m y_m y_n \phi(x_m)^T \phi(x_n) \]
Substitute the solution back into the Lagrangian

\[ g(\{\alpha_n\}, \{\lambda_n\}) = L(w, b, \{\xi_n\}, \{\alpha_n\}, \{\lambda_n\}) \]

\[ = \sum_n (C - \alpha_n - \lambda_n)\xi_n + \frac{1}{2} \| \sum_n y_n \alpha_n \phi(x_n) \|_2^2 + \sum_n \alpha_n \]

\[ + \left( \sum_n \alpha_n y_n \right) b - \sum_n \alpha_n y_n \left( \sum_m y_m \alpha_m \phi(x_m) \right)^T \phi(x_n) \]

\[ = \sum_n \alpha_n + \frac{1}{2} \| \sum_n y_n \alpha_n \phi(x_n) \|_2^2 - \sum_{m,n} \alpha_n \alpha_m y_m y_n \phi(x_m)^T \phi(x_n) \]

\[ = \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} \alpha_n \alpha_m y_m y_n \phi(x_m)^T \phi(x_n) \]

Several terms vanish because of the constraints \( \sum_n \alpha_n y_n = 0 \) and \( C - \lambda_n - \alpha_n = 0 \).
The dual problem

Maximizing the dual under the constraints

\[
\max_{\alpha} \quad g(\{\alpha_n\}, \{\lambda_n\}) = \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} y_m y_n \alpha_m \alpha_n k(x_m, x_n)
\]

s.t. \[\alpha_n \geq 0, \quad \forall \ n\]
\[\sum_n \alpha_n y_n = 0\]
\[C - \lambda_n - \alpha_n = 0, \quad \forall \ n\]
\[\lambda_n \geq 0, \quad \forall \ n\]
The dual problem

Maximizing the dual under the constraints

\[
\max_{\alpha} \ g(\{\alpha_n\}, \{\lambda_n\}) = \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} y_m y_n \alpha_m \alpha_n k(x_m, x_n)
\]

s.t. \quad \alpha_n \geq 0, \quad \forall \ n

\sum_n \alpha_n y_n = 0

\lambda_n \geq 0, \quad \forall \ n

We can simplify as the objective function does not depend on \( \lambda_n \).
Specifically, we can combine the constraints involving \( \lambda_n \) resulting in the following inequality constraint: \( \alpha_n \leq C' \):

\[ C - \lambda_n - \alpha_n = 0, \quad \lambda_n \geq 0 \iff \lambda_n = C - \alpha_n \geq 0 \iff \alpha_n \leq C \]
Simplified Dual

\[
\max_{\alpha} \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} y_m y_n \alpha_m \alpha_n \phi(x_m)^T \phi(x_n)
\]

s.t. \[0 \leq \alpha_n \leq C, \quad \forall \ n\]

\[\sum_n \alpha_n y_n = 0\]
Recovering solution to the primal formulation

We already identified the primal variable $\mathbf{w}$ as

$$
\mathbf{w} = \sum_{n} \alpha_n y_n \phi(x_n)
$$
Recovering solution to the primal formulation

We already identified the primal variable $w$ as

$$w = \sum_n \alpha_n y_n \phi(x_n)$$

To identify $b$, we need to appeal to one of the KKT conditions. See http://cs229.stanford.edu/notes/cs229-notes3.pdf for details.
Complementary slackness and support vectors

At the optimal solution to both primal and dual, the following condition must hold due to the KKT conditions:

$$\lambda_n \xi_n = 0$$
$$\alpha_n \{1 - \xi_n - y_n[w^T \phi(x_n) + b]\} = 0$$

Test Prediction:
$$h(x) = \text{sign}\left(\sum_n y_n \alpha_n k(x_n, x) + b\right)$$
Prediction only depends on support vectors, i.e., points with $$\alpha_n > 0$$!
Complementary slackness and support vectors

At the optimal solution to both primal and dual, the following condition must hold due to the KKT conditions:

\[ \lambda_n \xi_n = 0 \]
\[ \alpha_n \{1 - \xi_n - y_n[w^T \phi(x_n) + b]\} = 0 \]

From the first condition, if \( \alpha_n < C \), then

\[ \lambda_n = C - \alpha_n > 0 \rightarrow \xi_n = 0 \]

Thus, using the second condition, if \( C > \alpha_n > 0 \) and \( y_n \in \{-1, 1\} \):

\[ 1 - y_n[w^T \phi(x_n) + b] = 0 \rightarrow b = y_n - w^T \phi(x_n) \]
Complementary slackness and support vectors

At the optimal solution to both primal and dual, the following condition must hold due to the KKT conditions:

$$\lambda_n \xi_n = 0$$

$$\alpha_n \{1 - \xi_n - y_n [w^T \phi(x_n) + b]\} = 0$$

From the first condition, if $\alpha_n < C$, then

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Thus, using the second condition, if $C > \alpha_n > 0$ and $y_n \in \{-1, 1\}$:

$$1 - y_n [w^T \phi(x_n) + b] = 0 \rightarrow b = y_n - w^T \phi(x_n)$$

**Test Prediction:** $h(x) = \text{SIGN} (\sum_n y_n \alpha_n k(x_n, x) + b)$

Prediction only depends on support vectors, i.e., points with $\alpha_n > 0$!