

# Support Vector Machines, Kernel SVM

Professor Ameet Talwalkar

Slide Credit: Professor Fei Sha

# Outline

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

# Announcements

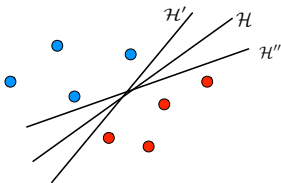
- Project proposal due now
- Graded HW3 and HW4 will be returned next Thursday
- HW5 has been posted online; due next Thursday

# Outline

- 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

# Distance from a point to decision boundary

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

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

# Distance from a point to decision boundary

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

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

We can remove the absolute value  $|\cdot|$  by exploiting the fact that the decision boundary classifies every point in the training dataset correctly.

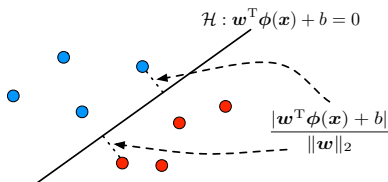
Namely,  $(\mathbf{w}^T \phi(\mathbf{x}) + b)$  and  $\mathbf{x}$ 's label  $y$  must have the same sign, so:

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

# Optimizing the Margin

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

$$\text{MARGIN}(\mathbf{w}, b) = \min_n \frac{y_n[\mathbf{w}^T \phi(\mathbf{x}_n) + b]}{\|\mathbf{w}\|_2}$$

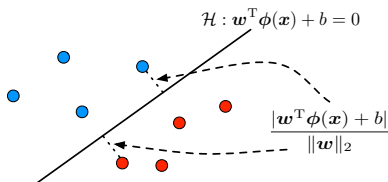




# Optimizing the Margin

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

$$\text{MARGIN}(\mathbf{w}, b) = \min_n \frac{y_n[\mathbf{w}^T \phi(\mathbf{x}_n) + b]}{\|\mathbf{w}\|_2}$$

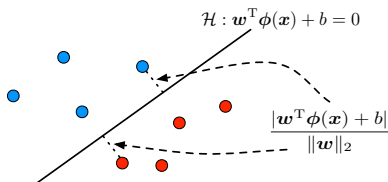


**How should we pick  $(\mathbf{w}, b)$  based on its margin?**

# Optimizing the Margin

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

$$\text{MARGIN}(\mathbf{w}, b) = \min_n \frac{y_n[\mathbf{w}^T \phi(\mathbf{x}_n) + b]}{\|\mathbf{w}\|_2}$$



## 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  $(\mathbf{w}, b)$  such that

$$\min_n y_n [\mathbf{w}^T \phi(\mathbf{x}_n) + b] = 1$$

## Rescaled Margin

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

$$\min_n y_n [\mathbf{w}^T \phi(\mathbf{x}_n) + b] = 1$$

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

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

## Rescaled Margin

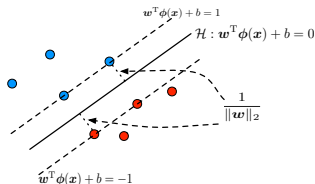
We can further constrain the problem by scaling  $(\mathbf{w}, b)$  such that

$$\min_n y_n [\mathbf{w}^T \phi(\mathbf{x}_n) + b] = 1$$

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

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

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:

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

This is equivalent to

$$\begin{aligned} \min_{\mathbf{w}, b} \quad & \frac{1}{2} \|\mathbf{w}\|_2^2 \\ \text{s.t.} \quad & y_n[\mathbf{w}^T \phi(\mathbf{x}_n) + b] \geq 1, \quad \forall n \end{aligned}$$

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

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

## Constraints in non-separable setting

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

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

# SVM for non-separable data

## Constraints in separable setting

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

## Constraints in non-separable setting

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

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

- 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?



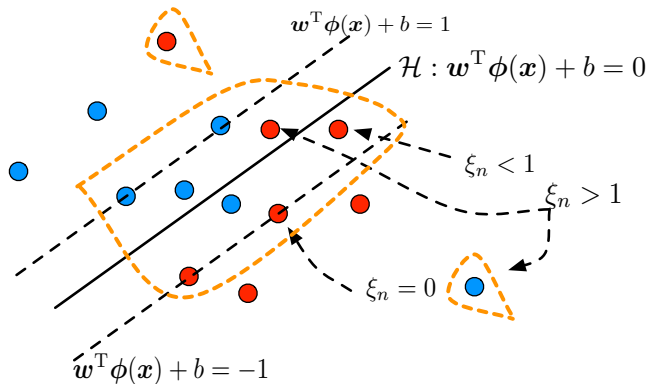
## Soft-margin SVM formulation

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

$$\begin{aligned} \min_{\mathbf{w}, b, \xi} \quad & \frac{1}{2} \|\mathbf{w}\|_2^2 + C \sum_n \xi_n \\ \text{s.t.} \quad & y_n [\mathbf{w}^T \phi(\mathbf{x}_n) + b] \geq 1 - \xi_n, \quad \forall n \\ & \xi_n \geq 0, \quad \forall n \end{aligned}$$

- $C$  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

# Visualization of how training data points are categorized



- 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  $h(\mathbf{x}) = \text{SIGN}(f(\mathbf{x}))$  with  $f(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b$ ,

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

## Intuition

# Hinge loss

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

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

## Intuition

- No penalty if raw output,  $f(\mathbf{x})$ , 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

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

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

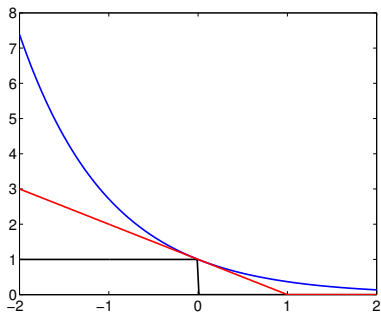
## Intuition

- No penalty if raw output,  $f(\mathbf{x})$ , 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

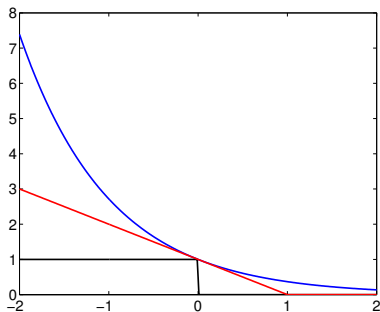
## Convenient shorthand

$$\ell^{\text{HINGE}}(f(\mathbf{x}), y) = \max(0, 1 - yf(\mathbf{x})) = (1 - yf(\mathbf{x}))_+$$

# Visualization and Properties



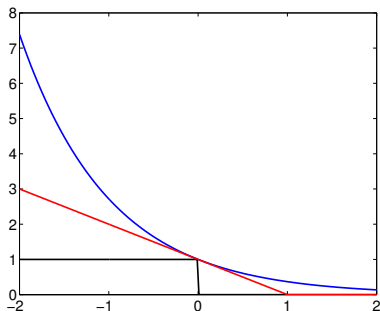
# Visualization and Properties



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

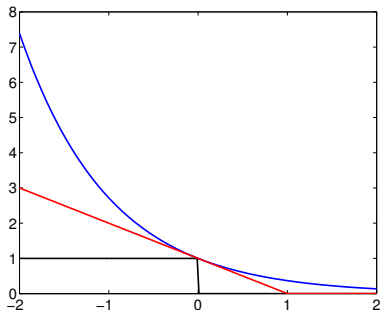


# Visualization and Properties



- 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)

## Visualization and Properties



- 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

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

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

# 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:

$$\begin{aligned} \min_{\mathbf{w}, b, \xi} \quad & \frac{1}{2} \|\mathbf{w}\|_2^2 + C \sum_n \xi_n \\ \text{s.t.} \quad & y_n[\mathbf{w}^T \phi(\mathbf{x}_n) + b] \geq 1 - \xi_n \quad \text{and} \quad \xi_n \geq 0, \quad \forall n \end{aligned}$$

*Do these yield the same solution?*

# Recovering our previous SVM formulation

**Define**  $C = 1/\lambda$ :

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

## Recovering our previous SVM formulation

**Define**  $C = 1/\lambda$ :

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

**Define**  $\xi_n \geq \max(0, 1 - y_n f(\mathbf{x}_n))$

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

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

At optimal solution constraints are active so we have equality! Why?

## Recovering our previous SVM formulation

**Define**  $C = 1/\lambda$ :

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

**Define**  $\xi_n \geq \max(0, 1 - y_n f(\mathbf{x}_n))$

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

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

At optimal solution constraints are active so we have equality! Why?

- If  $\xi_n^* > \max(0, 1 - y_n f(\mathbf{x}_n))$ , 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

- 1 Administration
- 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

$$\begin{aligned} \min_{\mathbf{x}} \quad & f(\mathbf{x}) \\ \text{s.t.} \quad & h_j(\mathbf{x}) = 0, \quad \forall j \end{aligned}$$

The Lagrangian is defined as follows:

$$L(\mathbf{x}, \boldsymbol{\beta}) = f(\mathbf{x}) + \sum_j \beta_j h_j(\mathbf{x})$$

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

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

This is the 'primal' problem

# Constrained Optimization – Inequality Constraints

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

This is the 'primal' problem with the *generalized* Lagrangian:

$$L(\mathbf{x}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = f(\mathbf{x}) + \sum_i \alpha_i g_i(\mathbf{x}) + \sum_j \beta_j h_j(\mathbf{x})$$

# Constrained Optimization – Inequality Constraints

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

This is the 'primal' problem with the *generalized* Lagrangian:

$$L(\mathbf{x}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = f(\mathbf{x}) + \sum_i \alpha_i g_i(\mathbf{x}) + \sum_j \beta_j h_j(\mathbf{x})$$

Consider the following function:

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

# Constrained Optimization – Inequality Constraints

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

This is the 'primal' problem with the *generalized* Lagrangian:

$$L(\mathbf{x}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = f(\mathbf{x}) + \sum_i \alpha_i g_i(\mathbf{x}) + \sum_j \beta_j h_j(\mathbf{x})$$

Consider the following function:

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

- If  $\mathbf{x}$  violates a primal constraint,  $\theta_P(\mathbf{x}) = \infty$ ;

# Constrained Optimization – Inequality Constraints

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

This is the 'primal' problem with the *generalized* Lagrangian:

$$L(\mathbf{x}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = f(\mathbf{x}) + \sum_i \alpha_i g_i(\mathbf{x}) + \sum_j \beta_j h_j(\mathbf{x})$$

Consider the following function:

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

- If  $\mathbf{x}$  violates a primal constraint,  $\theta_P(\mathbf{x}) = \infty$ ; otherwise  $\theta_P(\mathbf{x}) = f(\mathbf{x})$

# Constrained Optimization – Inequality Constraints

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

This is the 'primal' problem with the *generalized* Lagrangian:

$$L(\mathbf{x}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = f(\mathbf{x}) + \sum_i \alpha_i g_i(\mathbf{x}) + \sum_j \beta_j h_j(\mathbf{x})$$

Consider the following function:

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

- If  $\mathbf{x}$  violates a primal constraint,  $\theta_P(\mathbf{x}) = \infty$ ; otherwise  $\theta_P(\mathbf{x}) = f(\mathbf{x})$
- Thus  $\min_{\mathbf{x}} \theta_P(\mathbf{x}) = \min_{\mathbf{x}} \max_{\boldsymbol{\alpha}, \boldsymbol{\beta}, \alpha_i \geq 0} L(\mathbf{x}, \boldsymbol{\alpha}, \boldsymbol{\beta})$  has same solution as primal problem, which we denote as  $p^*$



# Constrained Optimization – Inequality Constraints

## Primal Problem

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

## Dual Problem

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

# Constrained Optimization – Inequality Constraints

## Primal Problem

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

## Dual Problem

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

$$d^* = \max_{\boldsymbol{\alpha}, \boldsymbol{\beta}, \alpha_i \geq 0} \theta_D(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \max_{\boldsymbol{\alpha}, \boldsymbol{\beta}, \alpha_i \geq 0} \min_{\mathbf{x}} L(\mathbf{x}, \boldsymbol{\alpha}, \boldsymbol{\beta})$$

# 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:  $\theta_D(\alpha, \beta) = \min_{\mathbf{x}} L(\mathbf{x}, \alpha, \beta)$

$$d^* = \max_{\alpha, \beta, \alpha_i \geq 0} \theta_D(\alpha, \beta) = \max_{\alpha, \beta, \alpha_i \geq 0} \min_{\mathbf{x}} L(\mathbf{x}, \alpha, \beta)$$

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

## Relationship between primal and dual?

# Constrained Optimization – Inequality Constraints

## Primal Problem

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

## Dual Problem

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

$$d^* = \max_{\boldsymbol{\alpha}, \boldsymbol{\beta}, \alpha_i \geq 0} \theta_D(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \max_{\boldsymbol{\alpha}, \boldsymbol{\beta}, \alpha_i \geq 0} \min_{\mathbf{x}} L(\mathbf{x}, \boldsymbol{\alpha}, \boldsymbol{\beta})$$

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  $\mathbf{x}$  such that  $g_i(\mathbf{x}) < 0$  for all  $i$
- These conditions are all satisfied by the SVM optimization problem!

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

- $\mathbf{x}^*$  is the solution to the primal and  $\alpha^*, \beta^*$  is the solution to the dual
- $p^* = d^* = L(\mathbf{x}^*, \alpha^*, \beta^*)$
- $\mathbf{x}^*, \alpha^*, \beta^*$  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
- See <http://cs229.stanford.edu/notes/cs229-notes3.pdf> for details



# Dual formulation of SVM

## Dual is also a convex quadratic programming

$$\begin{aligned} \max_{\alpha} \quad & \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} y_m y_n \alpha_m \alpha_n \phi(\mathbf{x}_m)^T \phi(\mathbf{x}_n) \\ \text{s.t.} \quad & 0 \leq \alpha_n \leq C, \quad \forall n \\ & \sum_n \alpha_n y_n = 0 \end{aligned}$$

# Dual formulation of SVM

## Dual is also a convex quadratic programming

$$\begin{aligned} \max_{\alpha} \quad & \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} y_m y_n \alpha_m \alpha_n \phi(\mathbf{x}_m)^T \phi(\mathbf{x}_n) \\ \text{s.t.} \quad & 0 \leq \alpha_n \leq C, \quad \forall n \\ & \sum_n \alpha_n y_n = 0 \end{aligned}$$

- There are  $N$  dual variable  $\alpha_n$ , one for each constraint in the primal formulation

# Kernel SVM

We replace the inner products  $\phi(\mathbf{x}_m)^T \phi(\mathbf{x}_n)$  with a kernel function

$$\begin{aligned} \max_{\alpha} \quad & \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} y_m y_n \alpha_m \alpha_n k(\mathbf{x}_m, \mathbf{x}_n) \\ \text{s.t.} \quad & 0 \leq \alpha_n \leq C, \quad \forall n \\ & \sum_n \alpha_n y_n = 0 \end{aligned}$$

We can define a kernel function to work with nonlinear features and learn a nonlinear decision surface

# Recovering solution to the primal formulation

## Weights

$$\mathbf{w} = \sum_n y_n \alpha_n \phi(\mathbf{x}_n) \leftarrow \text{Linear combination of the input features}$$

# Recovering solution to the primal formulation

## Weights

$$\mathbf{w} = \sum_n y_n \alpha_n \phi(\mathbf{x}_n) \leftarrow \text{Linear combination of the input features}$$

## Offset

$$b = [y_n - \mathbf{w}^T \phi(\mathbf{x}_n)] = [y_n - \sum_m y_m \alpha_m k(\mathbf{x}_m, \mathbf{x}_n)], \quad \text{for any } C > \alpha_n > 0$$

# Recovering solution to the primal formulation

## Weights

$$\mathbf{w} = \sum_n y_n \alpha_n \phi(\mathbf{x}_n) \leftarrow \text{Linear combination of the input features}$$

## Offset

$$b = [y_n - \mathbf{w}^T \phi(\mathbf{x}_n)] = [y_n - \sum_m y_m \alpha_m k(\mathbf{x}_m, \mathbf{x}_n)], \quad \text{for any } C > \alpha_n > 0$$

## Prediction on a test point $\mathbf{x}$

$$h(\mathbf{x}) = \text{SIGN}(\mathbf{w}^T \phi(\mathbf{x}) + b) = \text{SIGN}\left(\sum_n y_n \alpha_n k(\mathbf{x}_n, \mathbf{x}) + b\right)$$

*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

$$\begin{aligned} \min \quad & \frac{1}{2}x^2 \\ \text{s.t.} \quad & -x \leq 0 \\ & 2x - 3 \leq 0 \end{aligned}$$

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

Consider the example of convex quadratic programming

$$\begin{aligned} \min \quad & \frac{1}{2}x^2 \\ \text{s.t.} \quad & -x \leq 0 \\ & 2x - 3 \leq 0 \end{aligned}$$

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  $\alpha_2 \geq 0$ . 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

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

## Example (cont'd)

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

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

We next substitute the solution back into the Lagrangian:

$$g(\alpha) = \min_x \frac{1}{2}x^2 + (2\alpha_2 - \alpha_1)x - 3\alpha_2 = -\frac{1}{2}(2\alpha_2 - \alpha_1)^2 - 3\alpha_2$$

## Example (cont'd)

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

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

We next substitute the solution back into the Lagrangian:

$$g(\alpha) = \min_x \frac{1}{2}x^2 + (2\alpha_2 - \alpha_1)x - 3\alpha_2 = -\frac{1}{2}(2\alpha_2 - \alpha_1)^2 - 3\alpha_2$$

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

$$\begin{aligned} \min_{\mathbf{w}, b, \xi} \quad & \frac{1}{2} \|\mathbf{w}\|_2^2 + C \sum_n \xi_n \\ \text{s.t.} \quad & y_n [\mathbf{w}^T \phi(\mathbf{x}_n) + b] \geq 1 - \xi_n, \quad \forall n \\ & \xi_n \geq 0, \quad \forall n \end{aligned}$$

# Deriving the dual for SVM

## Primal SVM

$$\begin{aligned} \min_{\mathbf{w}, b, \xi} \quad & \frac{1}{2} \|\mathbf{w}\|_2^2 + C \sum_n \xi_n \\ \text{s.t.} \quad & y_n [\mathbf{w}^T \phi(\mathbf{x}_n) + b] \geq 1 - \xi_n, \quad \forall n \\ & \xi_n \geq 0, \quad \forall n \end{aligned}$$

## Lagrangian

$$\begin{aligned} L(\mathbf{w}, b, \{\xi_n\}, \{\alpha_n\}, \{\lambda_n\}) = & C \sum_n \xi_n + \frac{1}{2} \|\mathbf{w}\|_2^2 - \sum_n \lambda_n \xi_n \\ & + \sum_n \alpha_n \{1 - y_n [\mathbf{w}^T \phi(\mathbf{x}_n) + b] - \xi_n\} \end{aligned}$$

under the constraint that  $\alpha_n \geq 0$  and  $\lambda_n \geq 0$ .

# Minimizing the Lagrangian

## Taking derivatives with respect to the primal variables

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{w} - \sum_n y_n \alpha_n \phi(\mathbf{x}_n) = 0$$

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

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



# Minimizing the Lagrangian

## Taking derivatives with respect to the primal variables

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{w} - \sum_n y_n \alpha_n \phi(\mathbf{x}_n) = 0$$

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

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

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

$$\mathbf{w} = \sum_n y_n \alpha_n \phi(\mathbf{x}_n)$$

$$\sum_n \alpha_n y_n = 0$$

$$C - \lambda_n - \alpha_n = 0$$

## Substitute the solution back into the Lagrangian

$$g(\{\alpha_n\}, \{\lambda_n\}) = L(\mathbf{w}, b, \{\xi_n\}, \{\alpha_n\}, \{\lambda_n\})$$

## Substitute the solution back into the Lagrangian

$$\begin{aligned}g(\{\alpha_n\}, \{\lambda_n\}) &= L(\mathbf{w}, b, \{\xi_n\}, \{\alpha_n\}, \{\lambda_n\}) \\&= \sum_n (C - \alpha_n - \lambda_n) \xi_n + \frac{1}{2} \left\| \sum_n y_n \alpha_n \phi(\mathbf{x}_n) \right\|_2^2 + \sum_n \alpha_n \\&\quad + \left( \sum_n \alpha_n y_n \right) b - \sum_n \alpha_n y_n \left( \sum_m y_m \alpha_m \phi(\mathbf{x}_m) \right)^T \phi(\mathbf{x}_n)\end{aligned}$$

## Substitute the solution back into the Lagrangian

$$\begin{aligned}g(\{\alpha_n\}, \{\lambda_n\}) &= L(\mathbf{w}, b, \{\xi_n\}, \{\alpha_n\}, \{\lambda_n\}) \\&= \sum_n (C - \alpha_n - \lambda_n) \xi_n + \frac{1}{2} \left\| \sum_n y_n \alpha_n \phi(\mathbf{x}_n) \right\|_2^2 + \sum_n \alpha_n \\&\quad + \left( \sum_n \alpha_n y_n \right) b - \sum_n \alpha_n y_n \left( \sum_m y_m \alpha_m \phi(\mathbf{x}_m) \right)^T \phi(\mathbf{x}_n) \\&= \sum_n \alpha_n + \frac{1}{2} \left\| \sum_n y_n \alpha_n \phi(\mathbf{x}_n) \right\|_2^2 - \sum_{m,n} \alpha_n \alpha_m y_m y_n \phi(\mathbf{x}_m)^T \phi(\mathbf{x}_n)\end{aligned}$$

## Substitute the solution back into the Lagrangian

$$\begin{aligned}g(\{\alpha_n\}, \{\lambda_n\}) &= L(\mathbf{w}, b, \{\xi_n\}, \{\alpha_n\}, \{\lambda_n\}) \\&= \sum_n (C - \alpha_n - \lambda_n) \xi_n + \frac{1}{2} \left\| \sum_n y_n \alpha_n \phi(\mathbf{x}_n) \right\|_2^2 + \sum_n \alpha_n \\&\quad + \left( \sum_n \alpha_n y_n \right) b - \sum_n \alpha_n y_n \left( \sum_m y_m \alpha_m \phi(\mathbf{x}_m) \right)^\top \phi(\mathbf{x}_n) \\&= \sum_n \alpha_n + \frac{1}{2} \left\| \sum_n y_n \alpha_n \phi(\mathbf{x}_n) \right\|_2^2 - \sum_{m,n} \alpha_n \alpha_m y_m y_n \phi(\mathbf{x}_m)^\top \phi(\mathbf{x}_n) \\&= \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} \alpha_n \alpha_m y_m y_n \phi(\mathbf{x}_m)^\top \phi(\mathbf{x}_n)\end{aligned}$$

*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

$$\max_{\alpha} g(\{\alpha_n\}, \{\lambda_n\}) = \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} y_m y_n \alpha_m \alpha_n k(\mathbf{x}_m, \mathbf{x}_n)$$

$$\text{s.t. } \alpha_n \geq 0, \quad \forall n$$

$$\sum_n \alpha_n y_n = 0$$

$$C - \lambda_n - \alpha_n = 0, \quad \forall n$$

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

# The dual problem

## Maximizing the dual under the constraints

$$\max_{\alpha} g(\{\alpha_n\}, \{\lambda_n\}) = \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} y_m y_n \alpha_m \alpha_n k(\mathbf{x}_m, \mathbf{x}_n)$$

$$\text{s.t. } \alpha_n \geq 0, \quad \forall n$$

$$\sum_n \alpha_n y_n = 0$$

$$C - \lambda_n - \alpha_n = 0, \quad \forall n$$

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

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:  $\alpha_n \leq C$ :

$$\begin{aligned} C - \lambda_n - \alpha_n = 0, \lambda_n \geq 0 &\iff \lambda_n = C - \alpha_n \geq 0 \\ &\iff \alpha_n \leq C \end{aligned}$$

# Simplified Dual

$$\begin{aligned} \max_{\alpha} \quad & \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} y_m y_n \alpha_m \alpha_n \phi(\mathbf{x}_m)^T \phi(\mathbf{x}_n) \\ \text{s.t.} \quad & 0 \leq \alpha_n \leq C, \quad \forall n \\ & \sum_n \alpha_n y_n = 0 \end{aligned}$$



# Recovering solution to the primal formulation

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

$$\mathbf{w} = \sum_n \alpha_n y_n \phi(\mathbf{x}_n)$$

# Recovering solution to the primal formulation

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

$$\mathbf{w} = \sum_n \alpha_n y_n \phi(\mathbf{x}_n)$$

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:

$$\lambda_n \xi_n = 0$$

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

## Complementary slackness and support vectors

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

$$\begin{aligned}\lambda_n \xi_n &= 0 \\ \alpha_n \{1 - \xi_n - y_n[\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n) + b]\} &= 0\end{aligned}$$

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  $y_n \in \{-1, 1\}$ :

$$1 - y_n[\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n) + b] = 0 \rightarrow b = y_n - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n)$$

## Complementary slackness and support vectors

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

$$\begin{aligned}\lambda_n \xi_n &= 0 \\ \alpha_n \{1 - \xi_n - y_n [\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n) + b]\} &= 0\end{aligned}$$

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  $y_n \in \{-1, 1\}$ :

$$1 - y_n [\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n) + b] = 0 \rightarrow b = y_n - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n)$$

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

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