

# Mathematics for Machine Learning

## — Classification with Support Vector Machines

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Fall 2025

## Credits for the resource

- The slides are based on the textbooks:
  - *Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong: Mathematics for Machine Learning. Cambridge University Press. 2020.*
  - *Arnold J. Insel, Lawrence E. Spence, Stephen H. Friedberg: Linear Algebra, 4th Edition. Prentice Hall. 2013.*
  - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra, 12th Edition. Wiley. 2019.*
- We could partially refer to the monograph:  
*Francesco Orabona: A Modern Introduction to Online Learning.*  
<https://arxiv.org/abs/1912.13213>

# Outline

- 1 Introduction
- 2 Separating Hyperplanes
- 3 Primal Support Vector Machine
  - The Hard Margin SVM
  - The Soft Margin SVM
- 4 Dual Support Vector Machine
  - Convex Duality via Lagrange Multipliers
  - Kernels - A Sketch
- 5 Numerical Solution

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# Binary Classification


- **Focus:** predictors of the form:

$$f : \mathbb{R}^D \mapsto \{+1, -1\}.$$

- **Given:** a set of example-label pairs  $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\}$  as the training dataset.
- **Goal:** a model of parameters giving the smallest classification error.

**The model:** **Hyperplane** (an affine subspace of dimension  $D - 1$ ).

# Chih-Jen Lin's libsvm (<https://github.com/cjlin1>)



**Chih-Jen Lin**  
cjlin1

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**liblinear** Public

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C++ 972 342

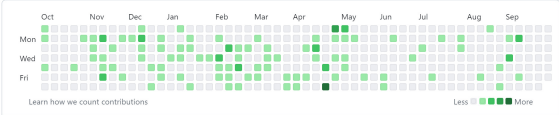
**libmf** Public

C++ 196 78

**simpleNN** Public

Python 47 16

195 contributions in the last year



Learn how we count contributions

Contribution activity

2023

October 2023

2022

2021

cjlin1 has no activity yet for this period.

# Purpose of Using SVM

- SVM allows for a geometric way of thinking (supervised learning).
- Resort to a variety of optimization tools.

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# Separating Hyperplanes

## Separating Hyperplane

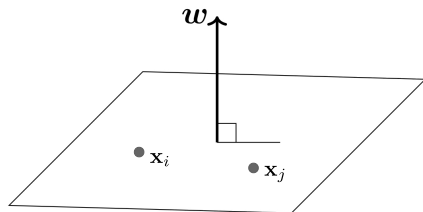
- Consider a function  $f : \mathbb{R}^D \mapsto \mathbb{R}$  such that

$$f(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle + b,$$

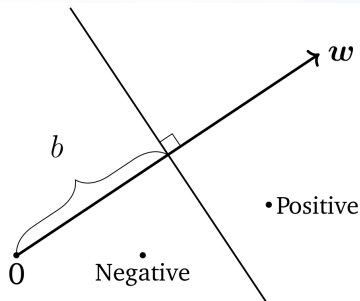
parametrized by  $\mathbf{w} \in \mathbb{R}^D$  and  $b \in \mathbb{R}$ .

- We define the hyperplane that separates the two classes in the binary classification problem as

$$\{\mathbf{x} \in \mathbb{R}^D : f(\mathbf{x}) = 0\}.$$

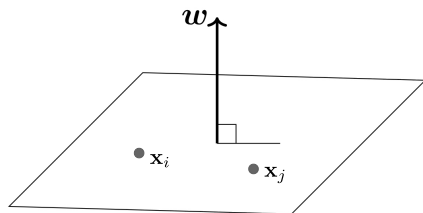


(a) Separating hyperplane in 3D

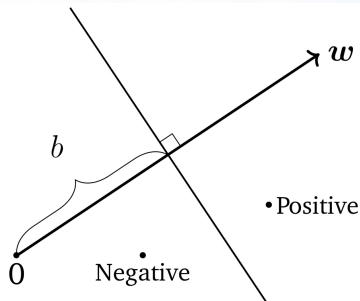


(b) Projection of the setting in (a) onto a plane

- $w$ : a normal vector to the hyperplane (?)

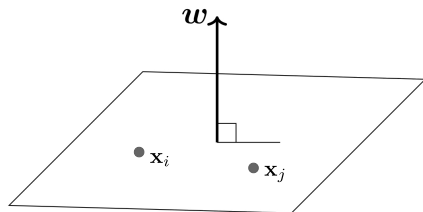


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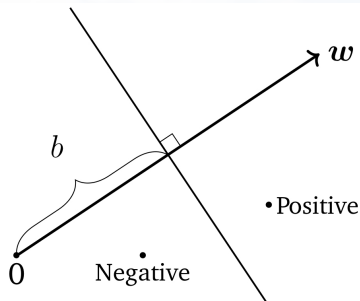


(b) Projection of the setting in (a) onto a plane

- $\mathbf{w}$ : a normal vector to the hyperplane (?)
- $f(\mathbf{x}_i) = f(\mathbf{x}_j) = 0$  &  $\mathbf{w} \perp (\mathbf{x}_i - \mathbf{x}_j)$  (?)



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- $\mathbf{w}$ : a normal vector to the hyperplane (?)
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  - $f(\mathbf{x}_i) - f(\mathbf{x}_j) = \langle \mathbf{w}, \mathbf{x}_i \rangle + b - (\langle \mathbf{w}, \mathbf{x}_j \rangle + b) = \langle \mathbf{w}, \mathbf{x}_i - \mathbf{x}_j \rangle$

# Classifier: Separating Hyperplanes

Ensure that the examples with **positive** labels are on the **positive** side of the hyperplane.

$$\langle \mathbf{w}, \mathbf{x}_i \rangle + b \geq 0 \text{ when } y_i = +1.$$

Ensure that the examples with **negative** labels are on the **negative** side of the hyperplane.

$$\langle \mathbf{w}, \mathbf{x}_i \rangle + b < 0 \text{ when } y_i = -1.$$

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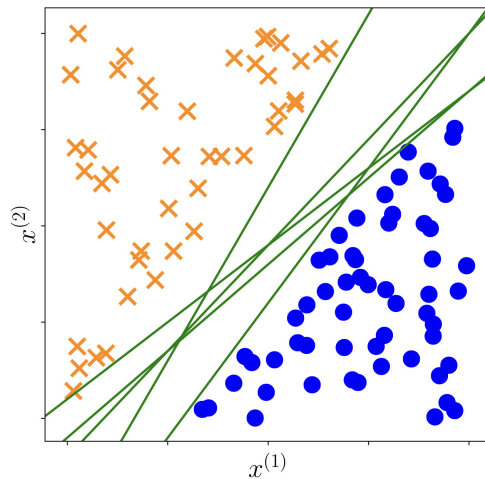
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Ensure that the examples with **negative** labels are on the **negative** side of the hyperplane.

$$\langle \mathbf{w}, \mathbf{x}_i \rangle + b < 0 \text{ when } y_i = -1.$$

- These two conditions  $\iff y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 0$ .

# Possible Separating Hyperplanes

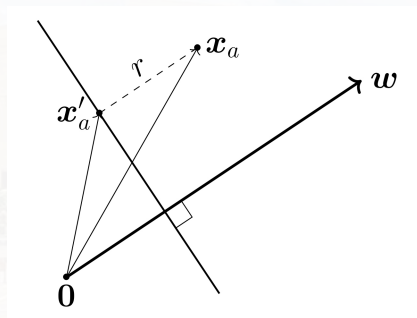


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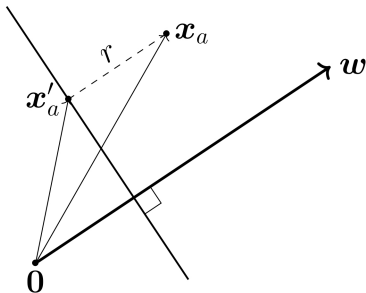
# Concept of the Margin



$$\mathbf{x}_a = \mathbf{x}'_a + r \frac{\mathbf{w}}{\|\mathbf{w}\|}.$$

- We can choose  $\mathbf{w}$  of unit length:  
 $\|\mathbf{w}\| = 1$  to simplify our discussion.
- The Euclidean norm:  
 $\|\mathbf{w}\| = \sqrt{\mathbf{w}^\top \mathbf{w}}.$

# Concept of the Margin



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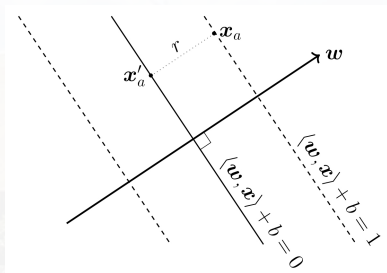
$$\mathbf{x}_a = \mathbf{x}'_a + r \frac{\mathbf{w}}{\|\mathbf{w}\|}.$$

- We can choose  $\mathbf{w}$  of unit length:  $\|\mathbf{w}\| = 1$  to simplify our discussion.
- The Euclidean norm:  $\|\mathbf{w}\| = \sqrt{\mathbf{w}^\top \mathbf{w}}.$
- We choose  $\mathbf{x}_a$  to be the point **closest** to the hyperplane, and the distance  $r$  is the **margin**.

# One single constrained optimization problem

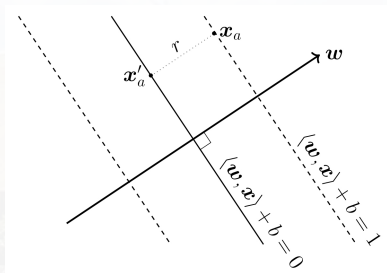
$$\begin{array}{ll} \max_{\mathbf{w}, b, r} & \underbrace{r}_{\text{margin}} \\ \text{subject to} & \underbrace{y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq r}_{\text{data fitting}}, \underbrace{\|\mathbf{w}\| = 1}_{\text{normalization}}, r > 0. \end{array}$$

# An alternative explanation



- Rescale the data such that  $\langle \mathbf{w}, \mathbf{x} \rangle + b = 1$  at the closest example  $\mathbf{x}$ .

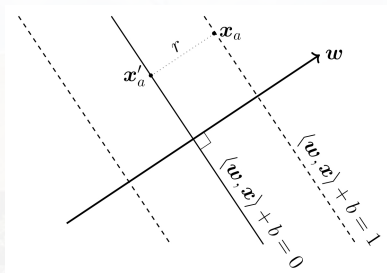
# An alternative explanation



- Rescale the data such that  $\langle w, x \rangle + b = 1$  at the closest example  $x$ .
- $x'_a$  is the orthogonal projection of  $x_a$  onto the hyperplane

$$\langle w, x'_a \rangle + b = 0.$$

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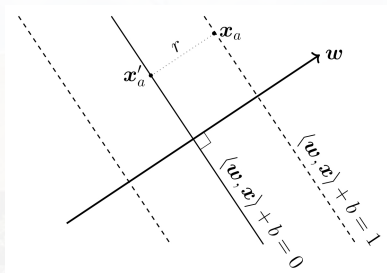


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$$\langle \mathbf{w}, \mathbf{x}'_a \rangle + b = 0.$$

$$\left\langle \mathbf{w}, \mathbf{x}_a - r \frac{\mathbf{w}}{\|\mathbf{w}\|} \right\rangle + b = 0.$$

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$$\langle \mathbf{w}, \mathbf{x}_a \rangle + b - r \frac{\langle \mathbf{w}, \mathbf{w} \rangle}{\|\mathbf{w}\|} = 0$$

$$\Rightarrow r = \frac{1}{\|\mathbf{w}\|}.$$

$$\left\langle \mathbf{w}, \mathbf{x}_a - r \frac{\mathbf{w}}{\|\mathbf{w}\|} \right\rangle + b = 0.$$

# Remark

We will show that setting the margin  $r = \frac{1}{\|\mathbf{w}\|}$  to be 1 is equivalent to assuming  $\|\mathbf{w}\| = 1$ .



# Combining the Two Conditions

$$\max_{\mathbf{w}, b} \quad \frac{1}{\|\mathbf{w}\|}$$

subject to  $y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1$  for all  $i = 1, \dots, N$ .

# Combining the Two Conditions

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Instead, we often do the minimization:

## Hard Margin SVM

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

subject to  $y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1$  for all  $i = 1, \dots, N$ .

- “Hard”: no violation of the margin condition is allowed.

# Why We Can Set the Margin to 1? (1/3)

Recall the original setting:

$$\begin{aligned} & \max_{\mathbf{w}, b, r} \underbrace{r}_{\text{margin}} \\ & \text{subject to } \underbrace{y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b)}_{\text{data fitting}} \geq r, \underbrace{\|\mathbf{w}\| = 1}_{\text{normalization}}, r > 0. \end{aligned}$$

Reparametrize the equation with a new weight vector  $\mathbf{w}'$ :

$$\begin{aligned} & \max_{\mathbf{w}', b, r} r^2 \\ & \text{subject to } y_i \left( \left\langle \frac{\mathbf{w}'}{\|\mathbf{w}'\|}, \mathbf{x}_i \right\rangle + b \right) \geq r, r > 0. \end{aligned}$$

# Why We Can Set the Margin to 1? (2/3)

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Divide the constraint by  $r$ :

$$\begin{aligned} & \max_{\mathbf{w}', b, r} \quad r^2 \\ & \text{subject to} \quad y_i \left( \left\langle \frac{\mathbf{w}'}{\|\mathbf{w}'\| r}, \mathbf{x}_i \right\rangle + \frac{b}{r} \right) \geq 1, r > 0. \end{aligned}$$

$$\mathbf{w}'' = \mathbf{w}' / (\|\mathbf{w}'\| r), \quad b'' = b / r.$$

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$$\mathbf{w}'' = \mathbf{w}' / (\|\mathbf{w}'\| r), \quad b'' = b/r. \quad \text{So, } \|\mathbf{w}''\| = 1/r.$$

# Why We Can Set the Margin to 1? (3/3)

Finally,

$$\begin{aligned} & \max_{\mathbf{w}'', b''} \quad \frac{1}{\|\mathbf{w}''\|^2} \\ & \text{subject to} \quad y_i(\langle \mathbf{w}'', \mathbf{x}_i \rangle + b'') \geq 1. \end{aligned}$$

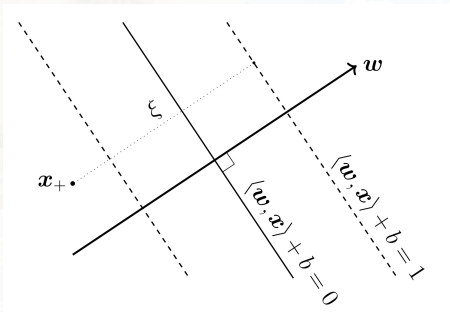
That is,

$$\begin{aligned} & \min_{\mathbf{w}'', b''} \quad \frac{1}{2} \|\mathbf{w}''\|^2 \\ & \text{subject to} \quad y_i(\langle \mathbf{w}'', \mathbf{x}_i \rangle + b'') \geq 1. \end{aligned}$$

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# Soft Margin?



- When the data is NOT linearly separable, we wish to allow some examples to **fall within** the margin region.
- We subtract the value  $\xi_i$  from the margin, constraining  $\xi_i$  to be non-negative.
- Purpose: Encourage correct classification



Add  $\xi_i$ 's to the objective, we get

## The Soft Margin SVM

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

$$\begin{aligned} \text{subject to} \quad & y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1 - \xi_i, \\ & \xi_i \geq 0 \end{aligned}$$

for  $i = 1, \dots, N$ .

$C$ : regularization parameter.  $\|\mathbf{w}\|^2$ : the regularizer.

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# Primal SVM

- The primal SVM: the SVM in terms of variables  $\mathbf{w}$  and  $b$ .
- The input  $\mathbf{x} \in \mathbb{R}^D$  with  $D$  features, while  $\mathbf{w}$  has the same dimension as  $\mathbf{x}$ .
  - The number of parameters grows linearly with the number of features.

# Equivalent Optimization Problem: The Dual View

- We consider the **dual problem**: Dual Support SVM, which is **independent** of the number of features.

# Equivalent Optimization Problem: The Dual View

- We consider the **dual problem**: Dual Support SVM, which is **independent** of the number of features.
- An additional advantage: Allow **kernels** to be applied easily.

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# Convex Duality

- We use  $\alpha_i \geq 0$  and  $\gamma_i \geq 0$  as the Lagrange multipliers.
  - $\alpha_i$ : w.r.t. the constraint that examples are correctly classified.
  - $\gamma_i$ : w.r.t. the non-negativity constraint of the slack variable.

$$\begin{aligned}\mathcal{L}(\mathbf{w}, b, \xi, \alpha, \gamma) &:= \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^N \xi_i \\ &\quad - \sum_{i=1}^N \alpha_i (y_i (\langle \mathbf{w}, \mathbf{x}_i \rangle + b) - 1 + \xi_i) - \sum_{i=1}^N \gamma_i \xi_i\end{aligned}$$

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- Then we derive the partial derivatives of  $\mathcal{L}$  w.r.t  $\mathbf{w}$ ,  $b$  and  $\xi_i$  for all  $i$ .



# Partial Derivatives of the Lagrangian

$$\mathcal{L} = \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^N \xi_i - \sum_{i=1}^N \alpha_i (y_i (\langle \mathbf{w}, \mathbf{x}_i \rangle + b) - 1 + \xi_i) - \sum_{i=1}^N \gamma_i \xi_i$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \mathbf{w}^\top - \sum_{i=1}^N \alpha_i y_i \mathbf{x}_i^\top$$

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- Maximizing the Lagrangian by setting  $\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \mathbf{0}^\top$ ,

$$\mathbf{w} = \sum_{i=1}^N \alpha_i y_i \mathbf{x}_i.$$

- The optimal weight vector is a linear combination of the examples  $\mathbf{x}_i$ 's.
- $\mathbf{x}_i$ 's with  $\alpha_i > 0$ : **support vectors**.

Substituting the expression for  $\mathbf{w}$  into the Lagrangian, we have

$$\begin{aligned}\mathcal{D}(\xi, \alpha, \gamma) &:= \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N y_i y_j \alpha_i \alpha_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle - \sum_{i=1}^N y_i \alpha_i \left\langle \sum_{j=1}^N y_j \alpha_j \mathbf{x}_j, \mathbf{x}_i \right\rangle \\ &+ C \sum_{i=1}^N \xi_i - b \sum_{i=1}^N y_i \alpha_i - \sum_{i=1}^N \alpha_i - \sum_{i=1}^N \alpha_i \xi_i - \sum_{i=1}^N \gamma_i \xi_i.\end{aligned}$$

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- No terms involving the primal variable  $\mathbf{w}$ .

# Partial Derivatives of the Lagrangian

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$$\frac{\partial \mathcal{L}}{\partial b} = - \sum_{i=1}^N \alpha_i y_i$$

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- Maximizing the Lagrangian by setting  $\frac{\partial \mathcal{L}}{\partial b} = 0$ ,

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

With terms simplified, we obtain the Lagrangian

$$\mathfrak{D}(\xi, \alpha, \gamma) = -\frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N y_i y_j \alpha_i \alpha_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle + \sum_{i=1}^N \alpha_i + \sum_{i=1}^N (C - \alpha_i - \gamma_i) \xi_i.$$

Setting  $\frac{\partial \mathfrak{L}}{\partial \xi_i} = 0$ , we see that

$$C = \alpha_i + \gamma_i \Rightarrow \sum_{i=1}^N (C - \alpha_i - \gamma_i) \xi_i = 0.$$



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Since  $\gamma_i \geq 0$ , we have that  $\alpha_i \leq C$ .

# The Dual SVM

## The Dual SVM

$$\min_{\alpha} \quad \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N y_i y_j \alpha_i \alpha_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle - \sum_{i=1}^N \alpha_i$$

$$\text{subject to} \quad \sum_{i=1}^N y_i \alpha_i = 0,$$

$$0 \leq \alpha_i \leq C \text{ for all } i = 1, \dots, N.$$

- $\alpha = [\alpha_1, \dots, \alpha_N]^T \in \mathbb{R}^N$ : Lagrange multipliers.
- The set of **inequality constraints**: **box constraints**.

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Efficient to implement numerically!

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# From Dual to Primal

- Once we obtain  $\alpha$ , we can recover  $\mathbf{w}$ .

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## Remark

- The primal SVM: # optimization variables: **feature dimension  $D$** .
- The dual SVM: # optimization variables: **the number  $N$  of examples**.

## The Dual SVM

$$\begin{aligned} \min_{\alpha} \quad & \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N y_i y_j \alpha_i \alpha_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle - \sum_{i=1}^N \alpha_i \\ \text{subject to} \quad & \sum_{i=1}^N y_i \alpha_i = 0, \\ & 0 \leq \alpha_i \leq C \text{ for all } i = 1, \dots, N. \end{aligned}$$

- We can see the inner product occurs only between examples. No inner products between examples and parameters!
- Kernel trick: consider  $\phi(\mathbf{x}_i)$  to represent  $\mathbf{x}_i$  ( $\phi : \mathcal{X} \mapsto \mathcal{H}$ ).

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- Kernel trick: consider  $\phi(\mathbf{x}_i)$  to represent  $\mathbf{x}_i$  ( $\phi : \mathcal{X} \mapsto \mathcal{H}$ ).
- Consider a similarity function  $k(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle_{\mathcal{H}}$  instead of defining  $\phi(\cdot)$  and computing the resulting inner product.

# Outline

- 1 Introduction
- 2 Separating Hyperplanes
- 3 Primal Support Vector Machine
  - The Hard Margin SVM
  - The Soft Margin SVM
- 4 Dual Support Vector Machine
  - Convex Duality via Lagrange Multipliers
  - Kernels - A Sketch
- 5 Numerical Solution

# Revisit Soft SVM as an Example

## The Soft Margin SVM

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

$$\begin{aligned} \text{subject to} \quad & y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1 - \xi_i, \\ & \xi_i \geq 0 \end{aligned}$$

A revised form:

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A revised form:

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

$$\begin{aligned} \text{subject to} \quad & -y_i \mathbf{x}_i^\top \mathbf{w} - y_i b - \xi_i \leq -1, \\ & -\xi_i \leq 0 \end{aligned}$$

# Concatenating the variables (Primal SVM)

$$\min_{\mathbf{w}, b, \xi} \frac{1}{2} \begin{bmatrix} \mathbf{w} \\ b \\ \xi \end{bmatrix}^T \begin{bmatrix} I_D & \mathbf{0}_{D, N+1} \\ \mathbf{0}_{N+1, D} & \mathbf{0}_{N+1, N+1} \end{bmatrix} \begin{bmatrix} \mathbf{w} \\ b \\ \xi \end{bmatrix} + [\mathbf{0}_{D+1, 1} \quad C\mathbf{1}_{N, 1}]^T \begin{bmatrix} \mathbf{w} \\ b \\ \xi \end{bmatrix}$$

$$\text{subject to } \begin{bmatrix} -\mathbf{Y}\mathbf{X} & -\mathbf{y} & -I_N \\ \mathbf{0}_{N, D+1} & & -I_N \end{bmatrix} \begin{bmatrix} \mathbf{w} \\ b \\ \xi \end{bmatrix} \leq \begin{bmatrix} -\mathbf{1}_{N, 1} \\ \mathbf{0}_{N, 1} \end{bmatrix}.$$

- $[\mathbf{w}^T, b, \xi^T]^T \in \mathbb{R}^{D+1+N}$ .
- $I_m \in \mathbb{R}^{m \times m}$ : identity matrix.
- $\mathbf{0}_{m, n} \in \mathbb{R}^{m \times n}$ : zeros of size  $m \times n$ ,  $\mathbf{1}_{m, n} \in \mathbb{R}^{m \times n}$ : ones of size  $m \times n$ .
- $\mathbf{y} = [y_1, \dots, y_N]^T$
- $\mathbf{Y} = \text{diagonal}(\mathbf{y}) \in \mathbb{R}^{N \times N}$ .
- $\mathbf{X} \in \mathbb{R}^{N \times D}$ : concatenating all the examples.

## Recall the Dual SVM

### The Dual SVM

$$\min_{\alpha} \quad \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N y_i y_j \alpha_i \alpha_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle - \sum_{i=1}^N \alpha_i$$

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## Concatenating the variables (Dual SVM)

$K$ : kernel matrix for which  $K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$  (or simply  $K_{ij} = \langle \mathbf{x}_i, \mathbf{x}_j \rangle$ ).

$$\begin{aligned} \min_{\alpha} \quad & \frac{1}{2} \alpha^\top \mathbf{Y} \mathbf{K} \mathbf{Y} \alpha - \mathbf{1}_{N,1}^\top \alpha \\ \text{subject to} \quad & \begin{bmatrix} \mathbf{y}^\top \\ -\mathbf{y}^\top \\ -I_N \\ I_N \end{bmatrix} \alpha \leq \begin{bmatrix} \mathbf{0}_{N+2,1} \\ C \mathbf{1}_{N,1} \end{bmatrix}. \end{aligned}$$

- Note that for equality constraints:

$\mathbf{Ax} = \mathbf{b}$  is replaced by  $\mathbf{Ax} \leq \mathbf{b}$  and  $-\mathbf{Ax} \leq -\mathbf{b}$ .

# Discussions