Mathematics for Machine Learning

— Classification with Support Vector Machines

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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.*
  - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra. Wiley. 2019.*
- We could partially refer to the monograph:
  Francesco Orabona: A Modern Introduction to Online Learning.
  https://arxiv.org/abs/1912.13213

Outline

Outline

Binary Classification

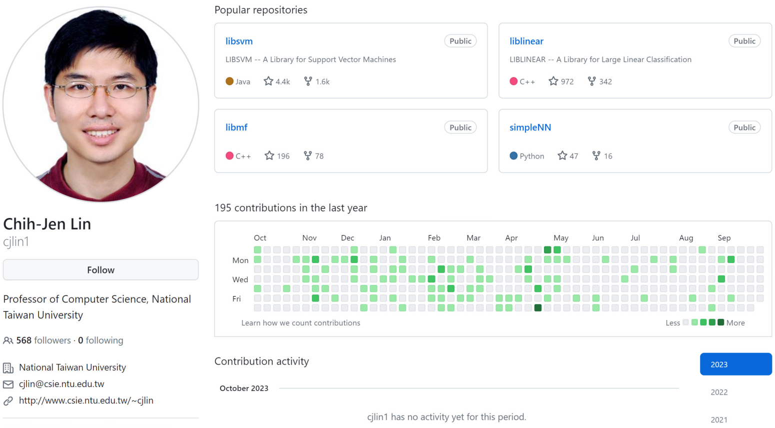
- **Focus:** predictors of the form:

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

- **Given:** a set of example-label pairs $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$ 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)



Purpose of Using SVM

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

Outline

Separating Hyperplanes

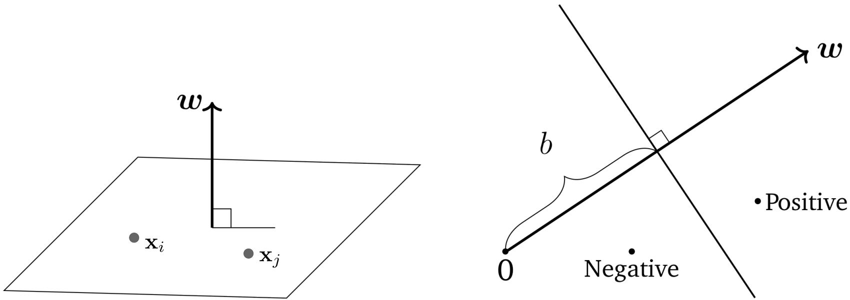
Separating Hyperplane

- 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

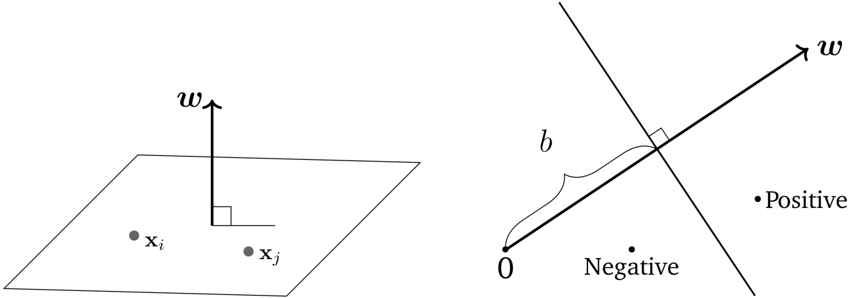
$$\{\mathbf{x} \in \mathbb{R}^D : f(\mathbf{x}) = 0\}.$$



(a) Separating hyperplane in 3D

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

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



(a) Separating hyperplane in 3D

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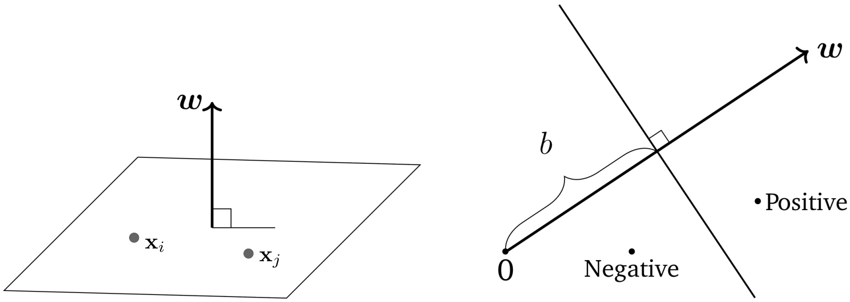

(a) Separating hyperplane in 3D

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

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

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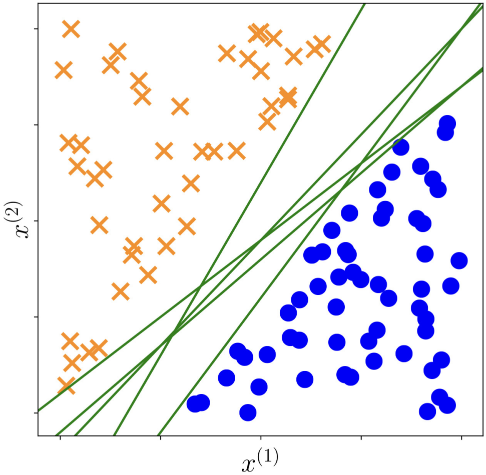
Ensure that the examples with negative labels are on the negative side of the hyperplane.

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

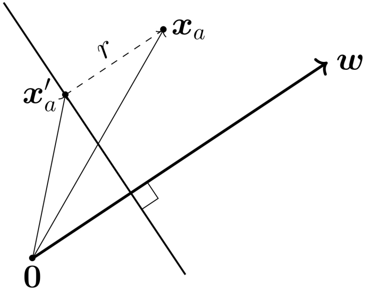
- These two conditions $\iff$ $y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 0$.

Possible Separating Hyperplanes



Outline

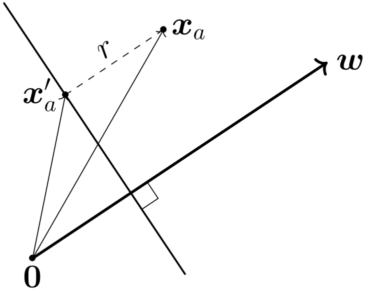
Concept of the Margin



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

- 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



$$y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq r.$$

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

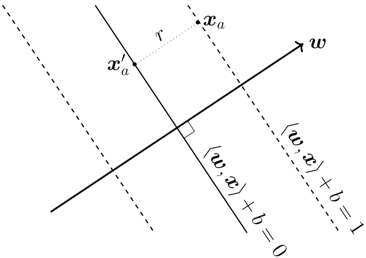
- We can choose $\mathbf{w}$ of unit length: $\|\mathbf{w}\| = 1$ to simplify our discussion.
  - The Euclidean norm: $\|\mathbf{w}\| = \sqrt{\mathbf{w}^\top \mathbf{w}}$.
- We choose $\mathbf{x}_a$ to be the point closest to the hyperplane, and the distance r is the margin.

One single constrained optimization problem

$$\max_{\mathbf{w},b,r} \underbrace{r}_{\text{margin}}$$

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

An alternative explanation



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

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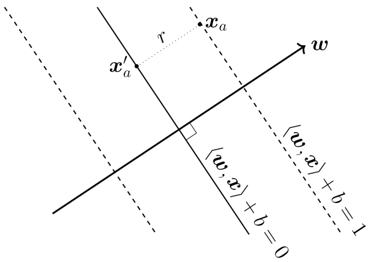

- Rescale the data such that $\langle \mathbf{w}, \mathbf{x} \rangle + b = 1$ at the closest example $\mathbf{x}$.
- $\mathbf{x}'_a$ is the orthogonal projection of $\mathbf{x}_a$ onto the hyperplane

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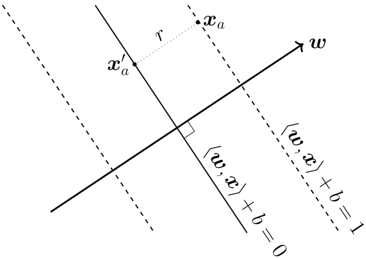

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$$\langle \mathbf{w}, \mathbf{x}'_a\rangle + b = 0.$$

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

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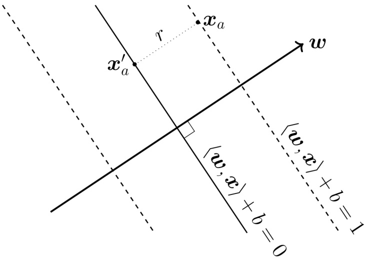

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$$\left\langle \mathbf{w}, \mathbf{x}_a - r\frac{\mathbf{w}}{\|\mathbf{w}\|} \right\rangle + b = 0.$$

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

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

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

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

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

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Instead, we often do the minimization:

Hard Margin SVM

$$\min_{\mathbf{w},b} \quad \frac{1}{2}\|\mathbf{w}\|^2$$
$$\text{subject to} \quad y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1 \quad \text{for all} \quad i = 1, \ldots, N.$$

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

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

Recall the original setting:

$$\max_{\mathbf{w},b,r} \underbrace{r}_{\text{margin}}$$

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

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

$$\max_{\mathbf{w}',b,r} r^2$$

$$\text{subject to} \quad y_i \left(\left\langle \frac{\mathbf{w}'}{\|\mathbf{w}'\|}, \mathbf{x}_i \right\rangle + b \right) \geq r, r > 0.$$

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

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Divide the constraint by r:

$$\max_{\mathbf{w}',b,r} \quad r^2$$

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

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

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

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

Finally,

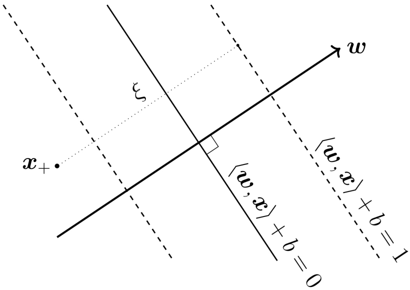
$$\max_{\mathbf{w}'', b''} \frac{1}{\|\mathbf{w}''\|^2}$$
$$\text{subject to} \quad y_i(\langle \mathbf{w}'', \mathbf{x}_i \rangle + b'') \geq 1.$$

That is,

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

Outline

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 ξ_i from the margin, constraining ξ_i to be non-negative.
- Purpose: Encourage correct classification

Add ξ_i's to the objective, we get

The Soft Margin SVM

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

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

$$\xi_i \geq 0$$

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

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

Outline

Primal SVM

- The primal SVM: the SVM interms 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.

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- An additional advantage: Allow kernels to be applied easily.

Outline

Convex Duality

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

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

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

Partial Derivatives of the Lagrangian

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

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

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

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

- 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 **w** into the Lagrangian, we have

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

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- No terms involving the primal variable **w**.

Partial Derivatives of the Lagrangian

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

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

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

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

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

The Dual SVM

The Dual SVM

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

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

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

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

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

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

Efficient to implement numerically!

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

From Dual to Primal

- Once we obtain $\boldsymbol{\alpha}$, we can recover $\mathbf{w}$.
    - Recall that $\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$.

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  - Recall that $\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$.
- Call the optimal primal parameter $\mathbf{w}^*$.

From Dual to Primal

- Once we obtain $\boldsymbol{\alpha}$, we can recover $\mathbf{w}$.
  - Recall that $\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$.
- Call the optimal primal parameter $\mathbf{w}^*$.
- Consider an example $\mathbf{x}_i$ that lies exactly on the margin's boundary: $y_i(\langle \mathbf{w}^*, \mathbf{x}_i \rangle + b^*) = 1$, where y_i is either $+1$ or -1.

From Dual to Primal

- Once we obtain α, we can recover $\mathbf{w}$.
  - Recall that $\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$.
- Call the optimal primal parameter $\mathbf{w}^*$.
- Consider an example $\mathbf{x}_i$ that lies exactly on the margin's boundary: $y_i(\langle \mathbf{w}^*, \mathbf{x}_i \rangle + b^*) = 1$, where y_i is either $+1$ or -1.
  - $\langle \mathbf{w}^*, \mathbf{x}_i \rangle + b^* = y_i$.

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  - Hence, we can compute $b^* = y_i - \langle \mathbf{w}^*, \mathbf{x}_i \rangle$.

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  - Hence, we can compute $b^* = y_i - \langle \mathbf{w}^*, \mathbf{x}_i \rangle$.

Remark

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

The Dual SVM

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

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

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

- 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

Revisit Soft SVM as an Example

The Soft Margin SVM

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

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

$$\xi_i \geq 0$$

A revised form:

Revisit Soft SVM as an Example

The Soft Margin SVM

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

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$$\xi_i \geq 0$$

A revised form:

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

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

$$-\xi_i \leq 0$$

Concatenating the variables (Primal SVM)

$$\min_{\mathbf{w},b,\boldsymbol{\xi}} \frac{1}{2}\begin{bmatrix}\mathbf{w}\\ b\\ \boldsymbol{\xi}\end{bmatrix}^{\top}\begin{bmatrix}\boldsymbol{I}_D & \mathbf{0}_{D,N+1}\\ \mathbf{0}_{N+1,D} & \mathbf{0}_{N+1,N+1}\end{bmatrix}\begin{bmatrix}\mathbf{w}\\ b\\ \boldsymbol{\xi}\end{bmatrix} + \begin{bmatrix}\mathbf{0}_{D+1,1} & C\mathbf{1}_{N,1}\end{bmatrix}^{\top}\begin{bmatrix}\mathbf{w}\\ b\\ \boldsymbol{\xi}\end{bmatrix}$$

$$\text{subject to} \begin{bmatrix}-\boldsymbol{YX} & -\mathbf{y} & -\boldsymbol{I}_N\\ \mathbf{0}_{N,D+1} & & -\boldsymbol{I}_N\end{bmatrix}\begin{bmatrix}\mathbf{w}\\ b\\ \boldsymbol{\xi}\end{bmatrix} \leq \begin{bmatrix}-\mathbf{1}_{N,1}\\ \mathbf{0}_{N,1}\end{bmatrix}.$$

- $[\mathbf{w}^{\top}, b, \boldsymbol{\xi}^{\top}]^{\top} \in \mathbb{R}^{D+1+N}$.
- $\boldsymbol{I}_m \in \mathbb{R}^{m\times m}$: 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 $m \times n$.
- $\mathbf{y} = [y_1, \cdots, y_N]^{\top}$
- $\boldsymbol{Y} = \text{diagonal}(\mathbf{y}) \in \mathbb{R}^{N\times N}$.
- $\boldsymbol{X} \in \mathbb{R}^{N\times D}$: concatenating all the examples.

Recall the Dual SVM

The Dual SVM

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

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

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

Concatenating the variables (Dual SVM)

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

$$\min_{\boldsymbol{\alpha}} \quad \frac{1}{2}\boldsymbol{\alpha}^\top \boldsymbol{YKY}\boldsymbol{\alpha} - \mathbf{1}_{N,1}^\top \boldsymbol{\alpha}$$

$$\text{subject to} \quad \begin{bmatrix} \mathbf{y}^\top \\ -\mathbf{y}^\top \\ -\boldsymbol{I}_N \\ \boldsymbol{I}_N \end{bmatrix} \boldsymbol{\alpha} \leq \begin{bmatrix} \mathbf{0}_{N+2,1} \\ C\mathbf{1}_{N,1} \end{bmatrix}.$$

- Note that for equality constraints:

$$\boldsymbol{A}\mathbf{x} = \mathbf{b} \;\text{ is replaced by }\; \boldsymbol{A}\mathbf{x} \leq \mathbf{b} \text{ and } -\boldsymbol{A}\mathbf{x} \leq -\mathbf{b}.$$

Discussions