Introduction to Machine Learning

Maximum Margin Methods

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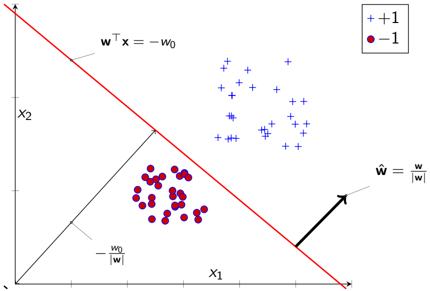
Outline

Maximum Margin Classifiers

$$y = \mathbf{w}^\top \mathbf{x} + b$$

- Remember the Perceptron!
- If data is linearly separable
  - Perceptron training guarantees learning the decision boundary
- There can be other boundaries
  - Depends on initial value for $\mathbf{w}$



Maximum Margin Classifiers

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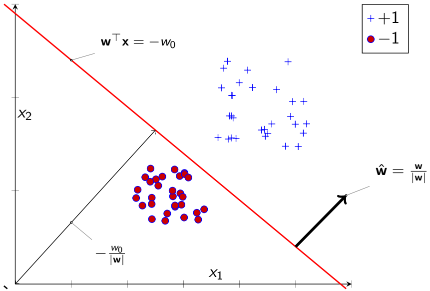
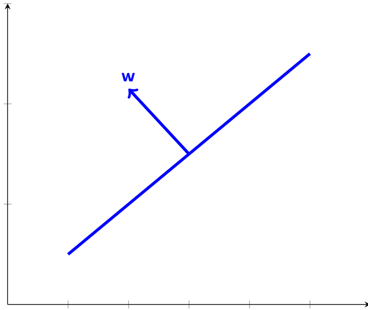
- Remember the Perceptron!
- If data is linearly separable
  - Perceptron training guarantees learning the decision boundary
- There can be other boundaries
  - Depends on initial value for $\mathbf{w}$
- **But what is the best boundary?**



Linear Hyperplane

- Separates a D-dimensional space into two half-spaces
- Defined by $\mathbf{w} \in \Re^D$
  - *Orthogonal* to the hyperplane
  - This $\mathbf{w}$ goes through the origin
  - How do you check if a point lies "above" or "below" $\mathbf{w}$?
  - What happens for points **on** $\mathbf{w}$?

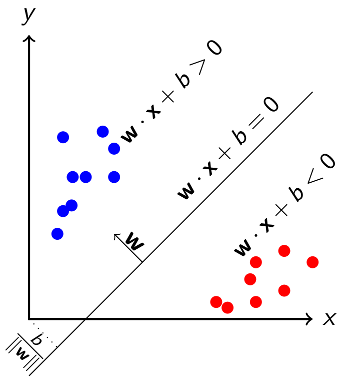


Make hyperplane not go through origin

- Add a bias b
  - $b > 0$ - move along $\mathbf{w}$
  - $b < 0$ - move opposite to $\mathbf{w}$
- How to check if point lies above or below $\mathbf{w}$?
  - If $\mathbf{w}^\top \mathbf{x} + b > 0$ then $\mathbf{x}$ is *above*
  - Else, *below*

Line as a Decision Surface

- Decision boundary represented by the hyperplane **w**
- For binary classification, **w** points **towards** the positive class



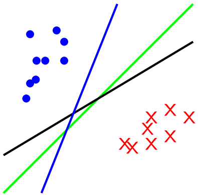
Decision Rule

$$y = sign(\mathbf{w}^\top \mathbf{x} + b)$$

- $\mathbf{w}^\top \mathbf{x} + b > 0 \Rightarrow y = +1$
- $\mathbf{w}^\top \mathbf{x} + b < 0 \Rightarrow y = -1$

What is Best Hyperplane Separator

- **Perceptron** can find a hyperplane that separates the data
  - ... if the data is linearly separable
- But there can be many choices!
- Find the one with best separability (largest margin)
- Gives better generalization performance



1. Intuitive reason
2. Theoretical foundations

What is a Margin?

- **Margin** is the distance between an example and the decision line
- Denoted by γ
- For a positive point:

$$\gamma = \frac{\mathbf{w}^\top \mathbf{x} + b}{\|\mathbf{w}\|}$$

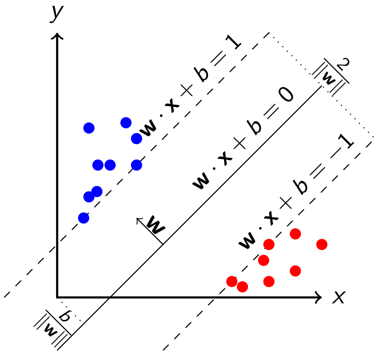
- For a negative point:

$$\gamma = -\frac{\mathbf{w}^\top \mathbf{x} + b}{\|\mathbf{w}\|}$$

Functional Interpretation

- Margin **positive** if prediction is **correct**; **negative** if prediction is **incorrect**

Maximum Margin Principle



Support Vector Machines

- A hyperplane based classifier defined by **w** and *b*
- Like perceptron
- Find hyperplane with *maximum separation margin* on the training data
- Assume that data is linearly separable (will relax this later)
  - Zero training error (loss)

SVM Prediction Rule

$$y = sign(\mathbf{w}^\top \mathbf{x} + b)$$

SVM Learning

- **Input**: Training data $\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_N, y_N)\}$
- **Objective**: Learn **w** and *b* that maximizes the margin

SVM Learning

- SVM learning task as an optimization problem
- Find $\mathbf{w}$ and b that gives zero training error
- Maximizes the margin $(= \frac{2}{\|w\|})$
- Same as minimizing $\|\mathbf{w}\|$

Optimization Formulation

$$\begin{aligned} \underset{\mathbf{w},b}{\text{minimize}} \quad & \frac{\|\mathbf{w}\|^2}{2} \\ \text{subject to} \quad & y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1,\ i = 1, \ldots, n. \end{aligned}$$

- **Optimization** with N linear inequality constraint

A Different Interpretation of Margin

- What impact does the margin have on $\mathbf{w}$?

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- Large margin $\Rightarrow$ Small $\|\mathbf{w}\|$
- Small $\|\mathbf{w}\|$ $\Rightarrow$ regularized/simple solutions
- Simple solutions $\Rightarrow$ Better generalizability (*Occam's Razor*)
- Computational Learning Theory provides a formal justification [1]

Solving the Optimization Problem

Optimization Formulation

$$\begin{aligned} \underset{\mathbf{w},b}{\text{minimize}} \quad & \frac{\|\mathbf{w}\|^2}{2} \\ \text{subject to} \quad & y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1, \; i = 1, \ldots, n. \end{aligned}$$

- There is an quadratic objective function to minimize with N inequality constraints
- "Off-the-shelf" packages - quadprog (MATLAB), CVXOPT
- Is that the best way?

Basic Optimization

$$\boxed{\underset{x,y}{\text{minimize}} \quad f(x,y) = \quad x^2 + 2y^2 - 2}$$

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$$\boxed{\begin{aligned} \underset{x,y}{\text{minimize}} \quad & f(x,y) = \quad x^2 + 2y^2 - 2 \\ \text{subject to} \quad & h(x,y) = \quad x + y - 1 = 0. \end{aligned}}$$

Lagrange Multipliers - A Primer

- Tool for solving constrained optimization problems of differentiable functions

$$
\boxed{
\begin{array}{lll}
\underset{x,y}{\text{minimize}} & f(x,y) = & x^2 + 2y^2 - 2 \\
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$$\boxed{\underset{x,y,\beta}{\text{minimize}} \quad L(x,y,\beta) = \quad f(x,y) + \beta h(x,y)}$$

Multiple Constraints

$$\begin{array}{lll} \underset{x,y,z}{\text{minimize}} & f(x,y,z) = & x^2 + 4y^2 + 2z^2 + 6y + z \\ \text{subject to} & h_1(x,y,z): & x + z^2 - 1 = 0 \\ & h_2(x,y,z): & x^2 + y^2 - 1 = 0. \end{array}$$

Multiple Constraints

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& h_2(x,y,z): & x^2 + y^2 - 1 = 0.
\end{aligned}$$

$$L(x,y,z,\beta) = f(x,y,z) + \sum_i \beta_i h_i(x,y,z)$$

Handling Inequality Constraints

$$\boxed{\begin{aligned} \underset{x,y}{\text{minimize}} \quad f(x,y) &= \quad x^3 + y^2 \\ \text{subject to} \quad g(x): &\quad x^2 - 1 \leq 0. \end{aligned}}$$

Handling Inequality Constraints

$$\boxed{\begin{array}{lll} \underset{x,y}{\text{minimize}} & f(x,y) = & x^3 + y^2 \\ \text{subject to} & g(x): & x^2 - 1 \leq 0. \end{array}}$$

- Inequality constraints are **transferred** as constraints on the Lagrangian, α

Handling Both Types of Constraints

$$\begin{array}{lll} \underset{\mathbf{w}}{\text{minimize}} & f(\mathbf{w}) & \\ \text{subject to} & g_i(\mathbf{w}) \leq 0 & i = 1, \ldots, k \\ \text{and} & h_i(\mathbf{w}) = 0 & i = 1, \ldots, l. \end{array}$$

Generalized Lagrangian

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

subject to, $\alpha_i \geq 0, \forall i$

Primal and Dual Formulations

Primal Optimization

- Let θ_P be defined as:

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

- One can prove that the optimal value for the original constrained problem is same as:

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

Primal and Dual Formulations (II)

Dual Optimization

- Consider θ_D, defined as:

$$\theta_D(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \min_{\mathbf{w}} L(\mathbf{w}, \boldsymbol{\alpha}, \boldsymbol{\beta})$$

- The **dual** optimization problem can be posed as:

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

$d^* == p^*$?

- Note that $d^* \leq p^*$
- "Max min" of a function is always less than or equal to "Min max"
- When will they be equal?
  - $f(\mathbf{w})$ is convex
  - Constraints are affine

Relation between primal and dual

- In general $d^* \leq p^*$, for SVM optimization the equality holds
- Certain conditions should be true
- Known as the **Kahrun-Kuhn-Tucker** conditions
- For $d^* = p^* = L(\mathbf{w}^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)$:

$$
\begin{aligned}
\frac{\partial}{\partial \mathbf{w}} L(\mathbf{w}^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*) & &= 0 \\
\frac{\partial}{\partial \beta_i} L(\mathbf{w}^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*) &= 0, & i = 1, \ldots, l \\
\alpha_i^* g_i(\mathbf{w}^*) &= 0, & i = 1, \ldots, k \\
g_i(\mathbf{w}^*) &\leq 0, & i = 1, \ldots, k \\
\alpha_i^* &\geq 0, & i = 1, \ldots, k
\end{aligned}
$$

Lagrangian Multipliers for SVM

Optimization Formulation

$$
\begin{aligned}
\underset{\mathbf{w},b}{\text{minimize}} \quad & \frac{\|\mathbf{w}\|^2}{2} \\
\text{subject to} \quad & y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1, \; i = 1, \ldots, n.
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A Toy Example

- $\mathbf{x} \in \Re^2$
- Two training points:

$$\mathbf{x}_1, y_1 = (1, 1), -1$$

$$\mathbf{x}_2, y_2 = (2, 2), +1$$

- Find the best hyperplane $\mathbf{w} = (w_1, w_2)$

Optimization problem for the toy example

$$\begin{aligned}
\underset{\mathbf{w}}{\text{minimize}} \quad & f(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|^2 \\
\text{subject to} \quad & g_1(\mathbf{w}, b) = y_1(\mathbf{w}^\top \mathbf{x}_1 + b) - 1 \geq 0 \\
& g_2(\mathbf{w}, b) = y_2(\mathbf{w}^\top \mathbf{x}_2 + b) - 1 \geq 0.
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& g_2(\mathbf{w}, b) = & y_2(\mathbf{w}^\top \mathbf{x}_2 + b) - 1 \geq 0.
\end{aligned}$$

- Substituting actual values for $\mathbf{x}_1, y_1$ and $\mathbf{x}_2, y_2$.

$$\begin{aligned}
\underset{\mathbf{w}}{\text{minimize}} \quad & f(\mathbf{w}) = & \frac{1}{2}\|\mathbf{w}\|^2 \\
\text{subject to} \quad & g_1(\mathbf{w}, b) = & -(\mathbf{w}^\top \mathbf{x}_1 + b) - 1 \geq 0 \\
& g_2(\mathbf{w}, b) = & (\mathbf{w}^\top \mathbf{x}_2 + b) - 1 \geq 0.
\end{aligned}$$

Back to SVM Optimization

Optimization Formulation

$$\underset{\mathbf{w},b}{\text{minimize}} \quad \frac{\|\mathbf{w}\|^2}{2}$$
$$\text{subject to} \quad y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1, \ i = 1, \ldots, n.$$

- Introducing Lagrange Multipliers,α_i, $i = 1, \ldots, n$

Rewriting as a (primal) Lagrangian

$$\underset{\mathbf{w},b,\alpha}{\text{minimize}} \quad L_P(\mathbf{w}, b, \alpha) = \frac{\|\mathbf{w}\|^2}{2} + \sum_{i=1}^{n} \alpha_i\{1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b)\}$$
$$\text{subject to} \quad \alpha_i \geq 0 \ i = 1, \ldots, n.$$

Solving the Lagrangian

- Set gradient of L_P to 0

$$\frac{\partial L_P}{\partial \mathbf{w}} = 0 \Rightarrow \boxed{\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i}$$

$$\frac{\partial L_P}{\partial b} = 0 \Rightarrow \boxed{\sum_{i=1}^{n} \alpha_i y_i = 0}$$

- Substituting in L_P to get the dual L_D

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$$\frac{\partial L_P}{\partial b} = 0 \Rightarrow \boxed{\sum_{i=1}^{n} \alpha_i y_i = 0}$$

- Substituting in L_P to get the dual L_D

Dual Lagrangian Formulation

$$\underset{b,\alpha}{\text{maximize}} \quad L_D(\mathbf{w}, b, \alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_i y_m y_i (\mathbf{x}_m^\top \mathbf{x}_i)$$

$$\text{subject to} \quad \sum_{i=1}^{n} \alpha_i y_i = 0, \alpha_i \geq 0 \; i = 1, \ldots, n.$$

Solving the Dual

- Dual Lagrangian is a *quadratic programming problem* in α_i's
  - Use "off-the-shelf" solvers
- Having found α_i's

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

- What will be the bias term b?

Investigating Kahrun Kuhn Tucker Conditions

- For the primal and dual formulations
- We can optimize the dual formulation (as shown earlier)
- Solution should satisfy the **Karush-Kuhn-Tucker** (KKT) Conditions

The Kahrun-Kuhn-Tucker Conditions

$$\frac{\partial}{\partial \mathbf{w}} L_P(\mathbf{w}, b, \alpha) = \mathbf{w} - \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i = 0 \tag{1}$$

$$\frac{\partial}{\partial b} L_P(\mathbf{w}, b, \alpha) = -\sum_{i=1}^{n} \alpha_i y_i = 0 \tag{2}$$

$$1 - y_i\{\mathbf{w}^\top \mathbf{x}_i + b\} \leq 0 \tag{3}$$

$$\alpha_i \geq 0 \tag{4}$$

$$\alpha_i(1 - y_i\{\mathbf{w}^\top \mathbf{x}_i + b\}) = 0 \tag{5}$$

Estimating Bias b

- Use KKT condition #5
- For $\alpha_i > 0$

$$(y_i\{\mathbf{w}^\top \mathbf{x}_i + b\} - 1) = 0$$

- Which means that:

$$b = -\frac{\max\limits_{n:y_i=-1} \mathbf{w}^\top \mathbf{x}_i + \min\limits_{n:y_i=1} \mathbf{w}^\top \mathbf{x}_i}{2}$$

Key Observation from Dual Formulation

Most α_i's are 0

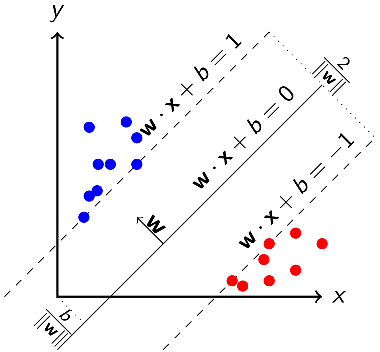
- KKT condition #5:

$$\alpha_i(1 - y_i\{\mathbf{w}^\top \mathbf{x}_i + b\}) = 0$$

- If $\mathbf{x}_i$ **not** on margin

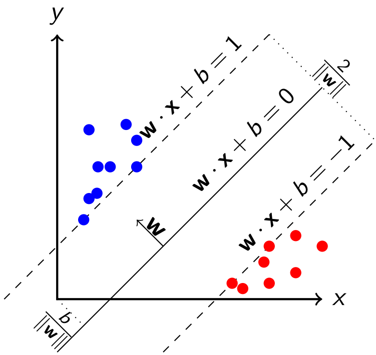
$$y_i\{\mathbf{w}^\top \mathbf{x}_i + b\} > 1$$
$$\Rightarrow \quad \alpha_i = 0$$

- $\alpha_i \neq 0$ only for $\mathbf{x}_i$ on margin
- These are the **support vectors**
- Only need these for prediction



What have we seen so far?

- For linearly separable data, SVM learns a weight vector $\mathbf{w}$
- Maximizes the margin
- SVM training is a **constrained optimization problem**
  - Each training example should lie outside the margin
  - N constraints



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- Still learn a maximum margin hyperplane

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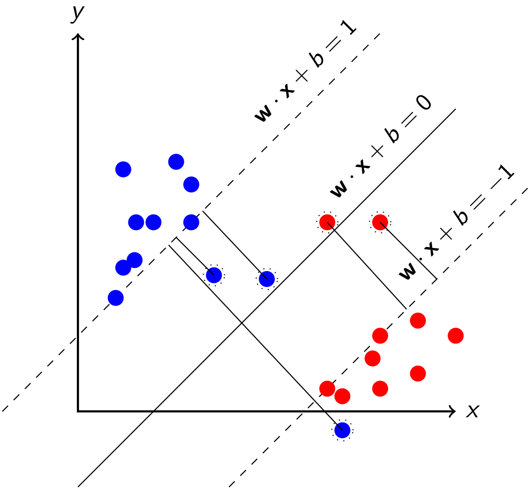
  2. Allow some examples to fall **inside** the margin

What if data is not linearly separable?

- Cannot go for zero training error
- Still learn a maximum margin hyperplane
  1. Allow some examples to be misclassified
  2. Allow some examples to fall **inside** the margin
- How do you set up the optimization for SVM training

Cutting Some Slack



Introducing Slack Variables

- **Separable Case**: To ensure zero training loss, constraint was

$$y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 \quad \forall i = 1 \ldots n$$

Introducing Slack Variables

- **Separable Case**: To ensure zero training loss, constraint was

$$y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 \quad \forall i = 1 \ldots n$$

- **Non-separable Case**: Relax the constraint

$$y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i \quad \forall i = 1 \ldots n$$

- ξ_i is called **slack variable** ($\xi_i \geq 0$)
- For misclassification, $\xi_i > 1$

Relaxing the Constraint

- It is OK to have some misclassified training examples
  - Some ξ_i's will be non-zero

Relaxing the Constraint

- It is OK to have some misclassified training examples
  - Some ξ_i's will be non-zero
- Minimize the number of such examples
  - Minimize $\sum_{i=1}^{n} \xi_i$
- Optimization Problem for Non-Separable Case

$$
\begin{aligned}
\underset{\mathbf{w},b}{\text{minimize}} \quad & f(\mathbf{w}, b) = \|\mathbf{w}\|^2 + C\sum_{i=1}^{n} \xi_i \\
\text{subject to} \quad & y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i, \xi_i \geq 0 \; i = 1, \ldots, n.
\end{aligned}
$$

- C controls the impact of margin and the margin error.

Estimating Weights

- What is the role of C?
- Similar optimization procedure as for the separable case (QP for the dual)
- Weights have the same expression

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

- Support vectors are slightly different
  1. Points on the margin ($\xi_i = 0$)
  2. Inside the margin but on the correct side ($0 < \xi_i < 1$)
  3. On the wrong side of the hyperplane ($\xi_i \geq 1$)

Concluding Remarks on SVM

- Training time for SVM training is $O(n^3)$
- Many *faster* but approximate approaches exist
  - Approximate QP solvers
  - Online training
- SVMs can be extended in different ways
  1. Non-linear boundaries (**kernel trick**)
  2. Multi-class classification
  3. Probabilistic output
  4. Regression (Support Vector Regression)

References

V. Vapnik.
Statistical learning theory.
Wiley, 1998.