Introduction to Machine Learning

Maximum Margin Methods

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March 8, 2021

Outline

Contents

1 Training vs. Generalization Error

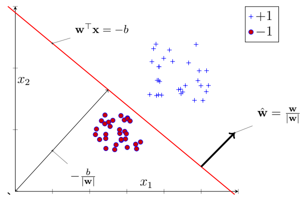
Training vs. Generalization Error

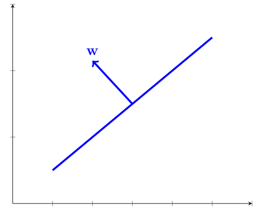
- Difference between training error and generalization error
- We can train a model to minimize the training error
- What we really want is a model that can minimize the generalization error
- But we do not have the *unseen* data to compute the generalization error
- What do we do?
  1. Focus on the training error and hope that generalization error is automatically minimized
  2. Incorporate some way to hedge (insure) against possible unseen issues

2 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 $\mathbf{w}$
- **But what is the best boundary?**



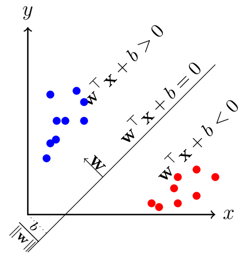


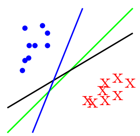
2.1 Linear Classification via Hyperplanes

- 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** $\mathbf{w}$?

For a hyperplane that passes through the origin, a point $\mathbf{x}$ will lie above the hyperplane if $\mathbf{w}^\top\mathbf{x} > 0$ and will lie below the plane if $\mathbf{w}^\top\mathbf{x} < 0$, otherwise. This can be further understood by understanding that $bfw^\top\mathbf{x}$ is essentially equal to $|\mathbf{w}||\mathbf{x}|\cos\theta$, where θ is the angle between $\mathbf{w}$ and $\mathbf{x}$.

- 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*
- Decision boundary represented by the hyperplane $\mathbf{w}$
- For binary classification, $\mathbf{w}$ points **towards** the positive class





Decision Rule

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

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

- **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

2.2 Concept of Margin

- The *Geometric* **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:
$$\gamma = -\frac{\mathbf{w}^\top \mathbf{x} + b}{\|\mathbf{w}\|}$$
- In general:
$$\gamma = y\frac{\mathbf{w}^\top \mathbf{x} + b}{\|\mathbf{w}\|}$$

To understand the margin from a geometric perspective, consider the projection of the vector connecting the origin to a point $\mathbf{x}$ on the decision line. Let the point be denoted as $\mathbf{x}'$. Obviously the vector $\mathbf{r}$ connecting $\mathbf{x}'$ and $\mathbf{x}$ is given by:

$$\mathbf{r} = \gamma\widehat{\mathbf{w}} = \gamma\frac{\mathbf{w}}{\|\mathbf{w}\|}$$

if $\mathbf{x}$ lies on the positive side of $\mathbf{w}$. But the same vector can be computed as:

$$\mathbf{r} = \mathbf{x} - \mathbf{x}'$$

Equating above two gives us $\mathbf{x}'$ as:

$$\mathbf{x}' = \mathbf{x} - \gamma\frac{\mathbf{w}}{\|\mathbf{w}\|}$$

Noting that, since $\mathbf{x}'$ lies on the hyperplane and hence:

$$\mathbf{w}^\top \mathbf{x}' + b = 0$$

Substituting $\mathbf{x}'$ from above:

$$\mathbf{w}^\top \mathbf{x} - \gamma\frac{\mathbf{w}^\top \mathbf{w}}{\|\mathbf{w}\|} + b = 0$$

Noting that $\frac{\mathbf{w}^\top \mathbf{w}}{\|\mathbf{w}\|} = \|\mathbf{w}\|$, we get γ as:

$$\gamma = \frac{\mathbf{w}^\top \mathbf{x} + b}{\|\mathbf{w}\|} \quad (1)$$

Similar analysis can be done for points on the negative side of $\mathbf{x}$. In general, one can write the expression for the margin as:

$$\gamma = y\frac{\mathbf{w}^\top \mathbf{x} + b}{\|\mathbf{w}\|} \quad (2)$$

where $y \in \{-1, +1\}$.

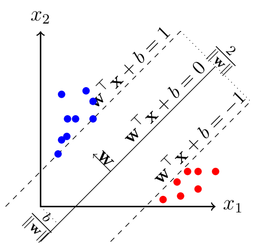
Functional Interpretation

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

Margin for a given line

- Geometric margin of a line $\mathbf{w}^\top \mathbf{x} + b$, with respect to a given data set is the smallest of the geometric margins over all examples:
$$\gamma = \arg\min_{i=1\dots n} \quad \gamma_i$$
- Consider the line parallel to the decision boundary that passes through the nearest training example
  - Assuming that the nearest example is positive, this line will be called the *positive margin*
  - A similar line on the other side of the decision boundary is called the *negative margin*
- We can rescale the weights, $\mathbf{w}$ and bias term b such that the equations of the positive and negative margins is given by:
$$\mathbf{w}^\top \mathbf{x} + b = +1$$
,and
$$\mathbf{w}^\top \mathbf{x} + b = -1$$

From the figure one can note that the size of the margin is $\frac{2}{\|\mathbf{w}\|}$. We can show this as follows. Since the data is separable, we can get two parallel lines represented by $\mathbf{w}^\top \mathbf{x} + b = +1$ and $\mathbf{w}^\top \mathbf{x} + b = -1$. Using result from (1) and (2), the distance between the two lines is given by $2\gamma = \frac{2}{\|\mathbf{w}\|}$.



3 Support Vector Machines

- A hyperplane based classifier defined by $\mathbf{w}$ 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 $\mathbf{w}$ and b that maximizes the margin

3.1 SVM Learning

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

- 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 constraints

3.2 Solving SVM Optimization Problem

Optimization Formulation

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

or

$$\begin{aligned} \underset{\mathbf{w},b}{\text{minimize}} \quad & \frac{\|\mathbf{w}\|^2}{2} \\ \text{subject to} \quad & 1 - [y_i(\mathbf{w}^\top \mathbf{x}_i + b)] \leq 0,\ i = 1, \ldots, N. \end{aligned}$$

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

4 Constrained Optimization and Lagrange Multipliers

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

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

- Method for solving constrained optimization problems of differentiable functions

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

- A Lagrange multiplier (β) lets you combine the two equations into one

$$\boxed{\underset{x,y,\beta}{\text{minimize}} \quad L(x,y,\beta) = \quad f(x,y)+\beta h(x,y)}$$

Solution 1. *Writing the objective as Lagrangian.*

$$L(x,y,\beta) = x^2+2y^2-2+\beta(x+y-1)$$

Setting the gradient to 0 with respect to x, y and β will give us the optimal values.

$$\frac{\partial L}{\partial x} = 2x+\beta = 0$$
$$\frac{\partial L}{\partial y} = 4y+\beta = 0$$
$$\frac{\partial L}{\partial \beta} = x+y-1 = 0$$

Multiple Constraints

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

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

Handling Inequality Constraints

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

- Inequality constraints are **transferred** as constraints on the generalized Lagrangian, using the multiplier, α
- Technically, α is a `Kahrun-Kuhn-Tucker` (KKT) multiplier
  - Lagrangian formulation is a special case of KKT formulation with no inequality constraints

Generalized Lagrangian

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

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

The Lagrangian in the above example becomes:

$$\begin{aligned} L(x,y,\alpha) &= f(x,y)+\alpha g(x,y) \\ &= x^3+y^2+\alpha(x^2-1) \end{aligned}$$

Solving for the gradient of the Lagrangian gives us:

$$\frac{\partial}{\partial x}L(x,y,\alpha) = 3x^2+2\alpha x = 0$$
$$\frac{\partial}{\partial y}L(x,y,\alpha) = 2y = 0$$
$$\frac{\partial}{\partial \alpha_1}L(x,y,\alpha) = x^2-1 = 0$$

Furthermore we require that:

$$\alpha \ge 0$$

From above equations we get $y = 0$, $x = \pm 1$ and $\alpha = \pm\frac{3}{2}$. But since $\alpha \ge 0$, hence $\alpha = \frac{3}{2}$. This gives $x = 1$, $y = 0$, and $f = 1$.

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

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

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

Karush-Kuhn-Tucker (KKT) Conditions

- A set of conditions that are necessary for a solution ($\mathbf{w}^*$) to be optimal
- The are necessary conditions, but not always sufficient
  - In some cases they are sufficient (SVMs being one of them)
- **Stationarity**:

$$\nabla L(\mathbf{w}^*) = \nabla(\mathbf{w}^*) + \nabla \sum_{i=1}^{k} \alpha_i g_i(\mathbf{w}^*) + \nabla \sum_{i=1}^{l} \beta_i h_i(\mathbf{w}^*) = \mathbf{0}$$

- **Primal feasibility**:

$$g_i(\mathbf{w}^*) \leq 0, \forall i$$
$$h_i(\mathbf{w}^*) = 0, \forall i$$

- **Dual feasibility**:

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

- **Complementary slackness**

$$\sum_{i=1}^{k} \alpha_i g_i(\mathbf{w}^*) = 0$$

Optimization Formulation

$$\begin{array}{ll} \underset{\mathbf{w},b}{\text{minimize}} & \dfrac{\|\mathbf{w}\|^2}{2} \\ \text{subject to} & 1 - [y_i(\mathbf{w}^\top \mathbf{x}_i + b)] \leq 0,\ i = 1, \ldots, N. \end{array}$$

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 $\mathbf{w} = (w_1, w_2)$

4.1 Toy SVM Example

Optimization problem for a toy example

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

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

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

The above problem can be also written as:

$$\begin{array}{lll} \underset{w_1, w_2, b}{\text{minimize}} & f(w_1, w_2) = & \frac{1}{2}(w_1^2 + w_2^2) \\ \text{subject to} & g_1(w_1, w_2, b) = & 1 + (w_1 + w_2 + b) \leq 0 \\ & g_2(w_1, w_2, b) = & 1 - (2w_1 + 2w_2 + b) \leq 0. \end{array}$$

To solve the toy optimization problem, we rewrite it in the Lagrangian form:

$$L(w_1, w_2, b, \alpha) = \frac{1}{2}(w_1^2 + w_2^2) + \alpha_1(1 + w_1 + w_2 + b) + \alpha_2(1 - (2w_1 + 2w_2 + b))$$

Setting $\nabla L = 0$, we get:

$$\begin{aligned}
\frac{\partial}{\partial w_1} L(w_1, w_2, b, \alpha) &= w_1 + \alpha_1 - 2\alpha_2 = 0 \\
\frac{\partial}{\partial w_2} L(w_1, w_2, b, \alpha) &= w_2 + \alpha_1 - 2\alpha_2 = 0 \\
\frac{\partial}{\partial b} L(w_1, w_2, b, \alpha) &= \alpha_1 - \alpha_2 = 0 \\
\frac{\partial}{\partial \alpha_1} L(w_1, w_2, b, \alpha) &= w_1 + w_2 + b + 1 = 0 \\
\frac{\partial}{\partial \alpha_2} L(w_1, w_2, b, \alpha) &= 2w_1 + 2w_2 + b - 1 = 0
\end{aligned}$$

Solving the above equations, we get, $w_1 = w_2 = 1$ and $b = -3$.

Primal and Dual Formulations

Generalized Lagrangian

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

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

Primal Optimization

- Let θ_P be defined as:

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

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

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

Consider

$$\begin{aligned}
\theta_P(\mathbf{w}) &= \underset{\boldsymbol{\alpha},\boldsymbol{\beta}:\alpha_i \geq 0}{max} L(\mathbf{w}, \boldsymbol{\alpha}, \boldsymbol{\beta}) \\
&= \underset{\boldsymbol{\alpha},\boldsymbol{\beta}:\alpha_i \geq 0}{max} f(\mathbf{w}) + \sum_{i=1}^{k} \alpha_i g_i(\mathbf{w}) + \sum_{i=1}^{l} \beta_i h_i(\mathbf{w})
\end{aligned}$$

It is easy to show that if any constraints are not satisfied, i.e., if either $g_i(\mathbf{w}) > 0$ or $h_i(\mathbf{w}) \neq 0$, then $\theta_P(\mathbf{w}) = \infty$. Which means that:

$$\theta_P(\mathbf{w}) = \begin{cases} f(\mathbf{w}) & \text{if primal constraints are satisfied} \\ \infty & \text{otherwise,} \end{cases}$$

Primal and Dual Formulations (II)

Dual Optimization

- Consider θ_D, defined as:

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

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

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

$d^* == p^*$?

- 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
  - $\exists \mathbf{w}, s.t., g_i(\mathbf{w}) < 0, \forall i$
- For SVM optimization the equality holds

Kahrun-Kuhn-Tucker (KKT) Conditions

- First derivative tests to check if a solution for a non-linear optimization problem is *optimal*
- For $d^* = p^* = L(\mathbf{w}^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)$:

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

Back to SVM Optimization

Optimization Formulation

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

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

Rewriting as a (primal) Lagrangian

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

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

Dual Lagrangian Formulation

$$
\begin{aligned}
&\underset{b,\boldsymbol{\alpha}}{\text{maximize}} \quad L_D(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n (\mathbf{x}_m^\top \mathbf{x}_n) \\
&\text{subject to} \quad \sum_{i=1}^{N} \alpha_i y_i = 0, \alpha_i \geq 0 \; i = 1, \ldots, N.
\end{aligned}
$$

- 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?

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

- We are skipping the proof for this part.

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

4.2 Kahrun-Kuhn-Tucker Conditions

$$
\begin{aligned}
\frac{\partial}{\partial \mathbf{w}} L_P(\mathbf{w}, b, \alpha) &= \mathbf{w} - \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i = 0 && (1)\\
\frac{\partial}{\partial b} L_P(\mathbf{w}, b, \alpha) &= -\sum_{i=1}^{N} \alpha_i y_i = 0 && (2)\\
1 - y_i\{\mathbf{w}^\top \mathbf{x}_i + b\} &\leq 0 && (3)\\
\alpha_i &\geq 0 && (4)\\
\alpha_i(1 - y_i\{\mathbf{w}^\top \mathbf{x}_i + b\}) &= 0 && (5)
\end{aligned}
$$

4.3 Support Vectors

Most α_i's are 0

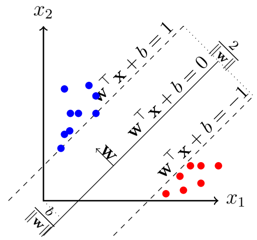
- KKT condition #5:

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

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

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

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



One can see from the prediction equation that:

$$y^* = sign(\sum_{i=1}^{N} \alpha_i y_i \boxed{(\mathbf{x}_i^\top \mathbf{x}^*)})$$

In the summation, the entries for $\mathbf{x}_i$ that do not lie on the margin will have no contribution to the sum because α_i for those $\mathbf{x}_i$'s will be 0. Hence we only need to the non-zero input examples to get the prediction.

- 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

Introducing Slack Variables

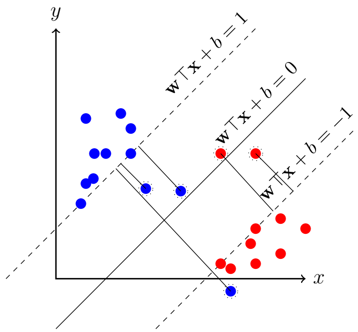
- **Separable Case**: To ensure zero training loss, constraint was

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

- **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, $\xi_i > 1$



4.4 Optimization Constraints

- 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

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

- 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 ($\xi_i \geq 1$)

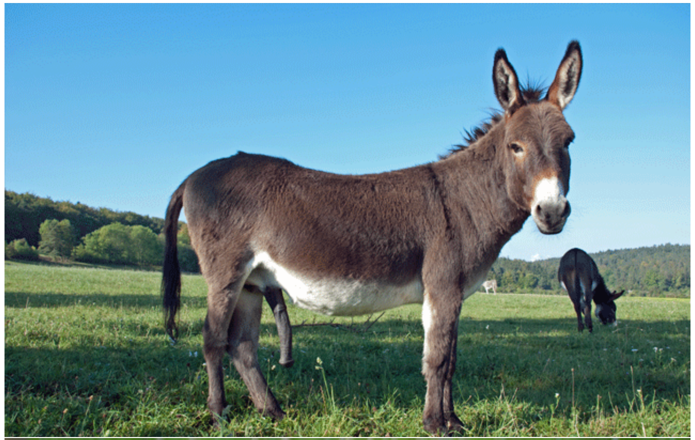
It is straightforward to see why the support vectors also includes points that are on the wrong side of the margin. The KKT condition #5, in this case will be:

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

For any point that is not on the margin, but is on the correct side of the margin, ξ_i will be 0, and $y_i\{\mathbf{w}^\top \mathbf{x}_i + b > 1$. Thus to satisfy the above condition, α_i will be 0. However, for the points on the margin, both ξ_i and $y_i\{\mathbf{w}^\top \mathbf{x}_i + b$ will be 0, thus, α_i will be non-zero. Finally, for the points that are on the wrong side of the margin, ξ_i will be equal to $1 - \{y_i\{\mathbf{w}^\top \mathbf{x}_i + b\}$, because that is how the slack is defined. Thus, α_i will have to be non-zero to satisfy the condition.

- C dictates if we focus more on maximizing the margin or reducing the training error.
- Controls the *bias-variance* tradeoff

5 The Bias-Variance Tradeoff



- C allows the model to be a mule or a sheep or something in between
- Question: What do you want the model to be?
- 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