18-661 Introduction to Machine Learning

Support Vector Machines (SVM) – I

Spring 2024

- Homework 2 due today!
- Homework 3 is posted and due Feb 23.

Today:

- (Linear) Support Vector Machines
- Max-margin and hinge loss formulations

Next Class:

- Duality
- Kernel Machines and the "Kernel Trick"

1. Why SVM?

- 2. Max-Margin Formulation
- 3. Hinge Loss Formulation
- 4. Summary



Why Do We Need SVM?

Naïve Bayes (circa 1750):

•
$$\Pr(Y|x_1...x_n) = \Pr(Y) \prod_{i=1}^n \Pr(x_i|Y)$$

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Logistic Regression (circa 1950):

• arg min_w -
$$\sum_{i} (y_i \log \sigma(\mathbf{w}^T \mathbf{x}_n) + (1 - y_n \log(1 - \sigma(\mathbf{w}^T \mathbf{x}))))$$

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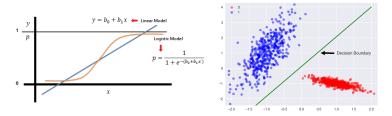
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The problem (circa 1990):

- Logistic regression and Naïve Bayes train over the whole dataset.
- These can require a lot of memory in high-dimensional settings.
- Neither can be easily generalized to nonlinear settings.

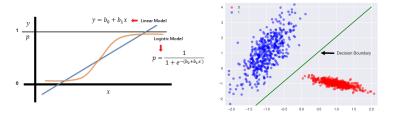
Can we do better?

Binary Logistic Regression



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- We don't (always) need to know how far x is from this boundary.

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How can we use this insight to improve the classification algorithm?

- What if we just looked at the boundary?
- Maybe then we could ignore some of the samples?

Work done by researchers at AT&T Bell Labs in the 1990s.

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- Still extremely popular today

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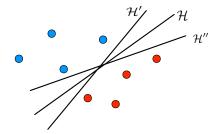
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We will see that SVM:

- Is less sensitive to outliers.
- Maximizes distance of training data from the boundary.
- Only requires a subset of the training points.
- Generalizes well to many nonlinear models.
- Scales better with high-dimensional data.

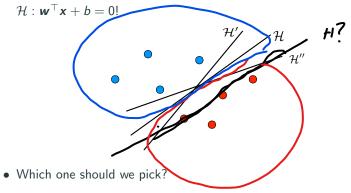
Max-Margin Formulation

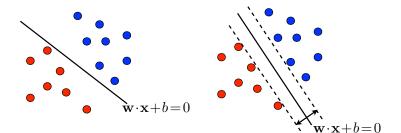
Binary Classification: Finding a Linear Decision Boundary

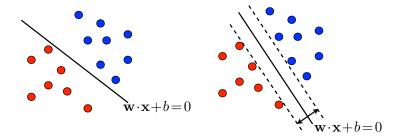


- Input features x.
- Decision boundary is a hyperplane $\mathcal{H} : \boldsymbol{w}^{\top} \boldsymbol{x} + b = 0$.

- Consider a separable training dataset (e.g., with two features)
- There are an infinite number of decision boundaries

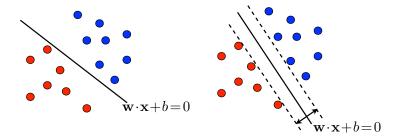






Find a decision boundary in the 'middle' of the two classes that:

- Perfectly classifies the training data
- Is as far away from every training point as possible

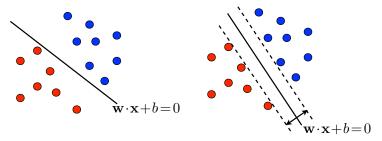


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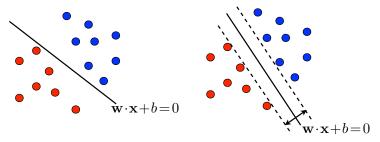
Let us apply this intuition to build a classifier that maximizes the margin between training points and the decision boundary.

What is a hyperplane?



- General equation is $\boldsymbol{w}^{\top}\boldsymbol{x} + b = 0$
- Divides the space in half, i.e., $\boldsymbol{w}^{\top}\boldsymbol{x} + b > 0$ and $\boldsymbol{w}^{\top}\boldsymbol{x} + b < 0$

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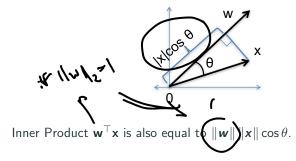
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- Divides the space in half, i.e., $\boldsymbol{w}^{\top}\boldsymbol{x} + b > 0$ and $\boldsymbol{w}^{\top}\boldsymbol{x} + b < 0$
- A hyperplane is a line in 2D and a plane in 3D
- $\pmb{w} \in \mathbb{R}^d$ is a non-zero normal vector

Given two vectors \mathbf{w} and \mathbf{x} , what is their inner product?

• Inner Product $\mathbf{w}^{\top}\mathbf{x} = w_1x_1 + w_2x_2 + \cdots + w_dx_d$

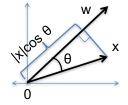
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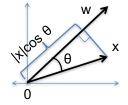
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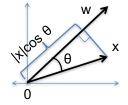


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- If $\mathbf{w} = \mathbf{x}$? $\theta = 0$, so $\mathbf{w}^{\top} \mathbf{w} = \|\mathbf{w}\|^2$.
- If $\mathbf{w} \perp \mathbf{x}$?

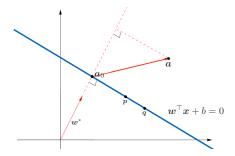
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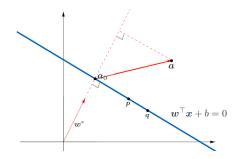


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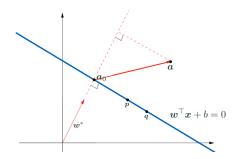
- If $\mathbf{w} = \mathbf{x}$? $\theta = 0$, so $\mathbf{w}^{\top} \mathbf{w} = \|\mathbf{w}\|^2$.
- If $\mathbf{w} \perp \mathbf{x}$? $\theta = \pi/2$, so $\mathbf{w}^T \mathbf{x} = 0$.



What is the meaning of w in the hyperplane $w^T x + b = 0$?

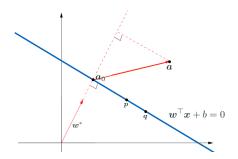


Vector w is normal to the hyperplane. Why?



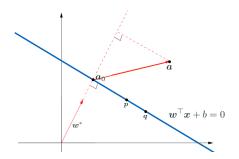
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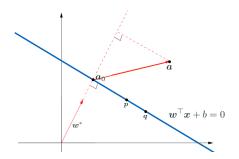
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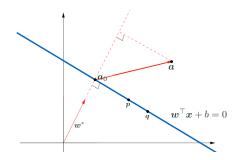
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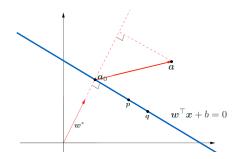
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Let $\mathbf{w}^* = \frac{\mathbf{w}}{\|\mathbf{w}\|_2}$ be the unit normal vector in the direction \mathbf{w} .



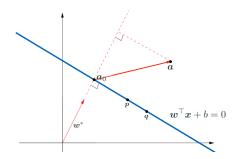
How to find the distance from *a* to the hyperplane?

• We want to find distance between a and line in the direction of w^* .



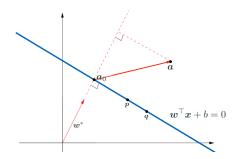
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- If we define point a_0 on the line, then this distance corresponds to length of $a a_0$ in direction of w^* , which equal $w^* (a a_0)$.
- We know $\boldsymbol{w}^{\top}\boldsymbol{a}_0 = -\boldsymbol{b}$ since $\boldsymbol{w}^{\top}\boldsymbol{a}_0 + \boldsymbol{b} = 0.$
- Then the distance equals $\left(\frac{1}{\|\boldsymbol{w}\|_2}(\boldsymbol{w}^{\mathsf{T}}\boldsymbol{a}+b)\right)$.

Distance from a Point to Decision Boundary

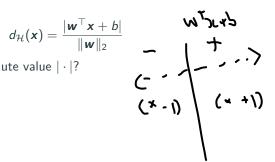
The *unsigned* distance from a point \boldsymbol{x} to the decision boundary (hyperplane) \mathcal{H} is

$$d_{\mathcal{H}}(\boldsymbol{x}) = rac{|\boldsymbol{w}^{ op} \boldsymbol{x} + b|}{\|\boldsymbol{w}\|_2}$$

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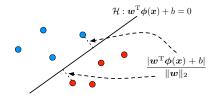
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Then, exploiting the fact that the decision boundary classifies every point in the training dataset correctly, we have $(w^{\top}x + b)$ and x's label y must have the same sign. So we get

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

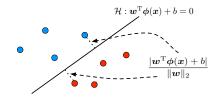
Margin: Smallest distance between the hyperplane and all training points

MARGIN
$$(\boldsymbol{w}, b) = \min_{n} \frac{y_{n}[\boldsymbol{w}^{\top}\boldsymbol{x}_{n} + b]}{\|\boldsymbol{w}\|_{2}}$$



How can we use this to find the SVM solution?

Optimizing the Margin

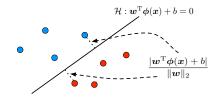


How should we pick (w, b) based on its margin?

We want a decision boundary that is as far away from all training points as possible, so we to *maximize* the margin!

$$\max_{\boldsymbol{w},b} \left(\min_{n} \frac{y_{n}[\boldsymbol{w}^{\top}\boldsymbol{x}_{n}+b]}{\|\boldsymbol{w}\|_{2}} \right) = \max_{\boldsymbol{w},b} \left(\frac{1}{\|\boldsymbol{w}\|_{2}} \min_{n} y_{n}[\boldsymbol{w}^{\top}\boldsymbol{x}_{n}+b] \right)$$

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Only involves points near the boundary (more on this later).

Scale of w

Margin: Smallest distance between the hyperplane and all training points

MARGIN
$$(\boldsymbol{w}, b) = \min_{n} \frac{y_{n}[\boldsymbol{w}^{\top}\boldsymbol{x}_{n} + b]}{\|\boldsymbol{w}\|_{2}}$$

Consider three hyperplanes

$$(w, b)$$
 $(2w, 2b)$ $(.5w, .5b)$

Which one has the largest margin?

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Which one has the largest margin?

- The MARGIN doesn't change if we scale (w, b) by a constant c
- $\mathbf{w}^{\top}\mathbf{x} + b = 0$ and $(c\mathbf{w})^{\top}\mathbf{x} + (cb) = 0$: same decision boundary!

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- $\mathbf{w}^{\top}\mathbf{x} + b = 0$ and $(c\mathbf{w})^{\top}\mathbf{x} + (cb) = 0$: same decision boundary!
- Can we further constrain the problem so as to get a unique solution (*w*, *b*)?

Rescaled Margin

We can further constrain the problem by scaling (w, b) such that

$$\min_n y_n[\boldsymbol{w}^\top \boldsymbol{x}_n + b] = 1.$$

Note that there always exists a scaling for which this is true.

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MARGIN
$$(\boldsymbol{w}, b)$$

$$\underbrace{\min_{n} y_{n}[\boldsymbol{w}^{\top}\boldsymbol{x}_{n} + b]}_{\|\boldsymbol{w}\|_{2}} = \frac{1}{\|\boldsymbol{w}\|_{2}}$$

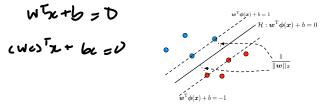
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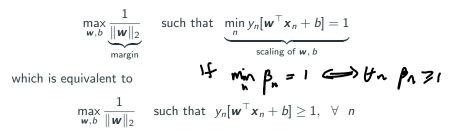
MARGIN
$$(\boldsymbol{w}, b) = \frac{\min_n y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b]}{\|\boldsymbol{w}\|_2} = \frac{1}{\|\boldsymbol{w}\|_2}$$

Hence the points closest to the decision boundary are at distance $\frac{1}{\|\mathbf{w}\|_2}$.



SVM: Max-margin Formulation for Separable Data

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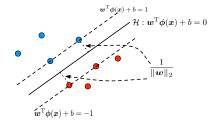
$$\max_{\boldsymbol{w},b} \frac{1}{\|\boldsymbol{w}\|_2} \quad \text{ such that } y_n[\boldsymbol{w}^\top \boldsymbol{x}_n + b] \ge 1, \ \forall \ n$$

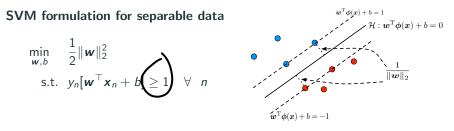
This is further equivalent to

$$\begin{split} \min_{\boldsymbol{w},b} & \frac{1}{2} \|\boldsymbol{w}\|_2^2 \\ \text{s.t.} & y_n[\boldsymbol{w}^\top \boldsymbol{x}_n + b] \geq 1, \quad \forall \quad n \end{split}$$

Given our geometric intuition, SVM is called a **max margin** (or large margin) classifier. The constraints are called **large margin constraints**.

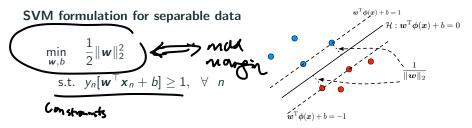
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Two types of training data, based on the situations of the constraint:

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- "=": y_n[w[⊤]x_n + b] = 1. These training data points are called "support vectors", which have the minimum distance (1/||w||) to the boundary.
- ">": y_n[w[⊤]x_n + b] > 1. Distance to the boundary is larger than the minimum. Removing these data points does not affect the optimal solution (more on this next lecture).

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Non-separable setting

In practice our training data may not be separable. What issues arise with the optimization problem above when data is not separable?

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• For every \boldsymbol{w} there exists a training point \boldsymbol{x}_i such that

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• There is no feasible (*w*, *b*) as at least one of our constraints is violated!

SVM for Non-separable Data

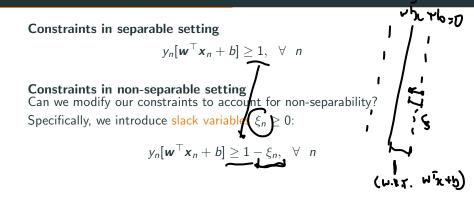
Constraints in separable setting

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

Constraints in non-separable setting

Can we modify our constraints to account for non-separability?

SVM for Non-separable Data



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Constraints in non-separable setting

Can we modify our constraints to account for non-separability? Specifically, we introduce slack variables $\xi_n \ge 0$:

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

 For "hard" training points, we can increase ξ_n until the above inequalities are met.

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- For "hard" training points, we can increase ξ_n until the above inequalities are met.
- What does it mean when $\xi_n = 0$? This data point is correctly classified.

$$y_n[\boldsymbol{w}^{\top}\boldsymbol{x}_n+b] \geq 1, \quad \forall \quad n$$

Constraints in non-separable setting

Can we modify our constraints to account for non-separability? Specifically, we introduce slack variables $\xi_n \ge 0$:

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

- For "hard" training points, we can increase ξ_n until the above inequalities are met.
- What does it mean when $\xi_n = 0$? This data point is correctly classified.
- What does it mean when ξ_n is very large?

$$y_n[\mathbf{w}^\top \mathbf{x}_n + b] \ge 1, \quad \forall \quad n \qquad (\mathbf{y}_1, \mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_2, \mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_2, \mathbf{y}_1, \mathbf{y}_$$

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- For "hard" training points, we can increase ξ_n until the above inequalities are met.
- What does it mean when $\xi_n = 0$? This data point is correctly classified.
- What does it mean when ξ_n is very large? We have violated the original constraints "by a lot."

$$\min_{\boldsymbol{w}, b, \boldsymbol{\xi}} \underbrace{\frac{1}{2} \|\boldsymbol{w}\|_2^2 + C \sum_n \xi_n}_{\text{s.t. } y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b] \ge 1 - \xi_n, \quad \forall \quad n \\ \xi_n \ge 0, \quad \forall \quad n \end{cases}$$

$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \quad \frac{1}{2} \|\boldsymbol{w}\|_2^2 + C \sum_n \xi_n$$
s.t. $y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b] \ge 1 - \xi_n, \quad \forall \quad n$
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What is the role of C?

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What is the role of C?

• User-defined hyperparameter

$$\min_{\boldsymbol{w}, b, \boldsymbol{\xi}} \quad \frac{1}{2} \|\boldsymbol{w}\|_2^2 + C \sum_n \xi_n$$
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What is the role of C?

- User-defined hyperparameter
- Trades off between the two terms in our objective

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 $\xi_n \ge 0, \quad \forall \quad n$

What is the role of C?

- User-defined hyperparameter
- Trades off between the two terms in our objective
- Same idea as the regularization term in ridge regression

How to Solve this Problem?

$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \quad \frac{1}{2} \|\boldsymbol{w}\|_2^2 + C \sum_n \xi_n$$
s.t. $y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b] \ge 1 - \xi_n, \quad \forall \quad n$
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 This is a convex quadratic program: the objective function is quadratic in *w* and linear in *ξ* and the constraints are linear (inequality) constraints in *w*, *b* and *ξ_n*.

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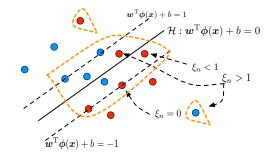
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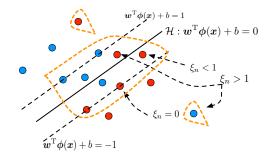
$$\begin{array}{l} \underset{\boldsymbol{w},\boldsymbol{b} \in \boldsymbol{\xi}}{\text{min}} \quad \frac{1}{2} \|\boldsymbol{w}\|_{2}^{2} + C \sum_{n} \xi_{n} \\ \text{s.t.} \quad y_{n} [\boldsymbol{w}^{\top} \boldsymbol{x}_{n} + b] \geq 1 - \xi_{n}, \quad \forall \quad n \\ \quad \xi_{n} \geq 0, \quad \forall \quad n \end{array}$$

- This is a convex quadratic program: the objective function is quadratic in *w* and linear in *ξ* and the constraints are linear (inequality) constraints in *w*, *b* and ξ_n.
- Early solvers were based on general-purpose quadratic program solvers (e.g. similar to scipy.optimize or Matlab's quadprog(), albeit in the 1990s)
- SVM solvers today are based on highly optimized search algorithms that exploit SVM-specific structure.

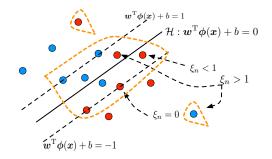
Support Vectors: Revisited



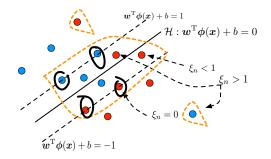
Support vectors are highlighted by the dotted orange lines. What does this mean mathematically?



Recall the constraints $y_n[\mathbf{w}^{\top}\mathbf{x}_n + b] \ge 1 - \xi_n$ from the soft-margin formulation. All the training points (\mathbf{x}_n, y_n) that satisfies the constraint with "=" are support vectors.

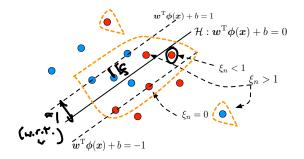


In other words, support vectors satisfy $y_n[\mathbf{w}^{\top}\mathbf{x}_n + b] = 1 - \xi_n$, which can be further divided into several categories:



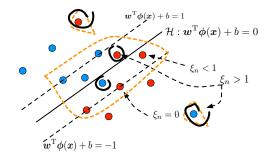
In other words, support vectors satisfy $y_n[\mathbf{w}^{\top}\mathbf{x}_n + b] = 1 - \xi_n$, which can be further divided into several categories:

• $\xi_n = 0$: $y_n[\mathbf{w}^\top \mathbf{x}_n + b] = 1$, the point is on the correct side with distance $\frac{1}{\|\mathbf{w}\|}$.



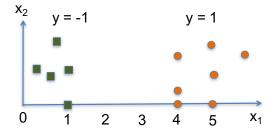
In other words, support vectors satisfy $y_n[\mathbf{w}^\top \mathbf{x}_n + b] = 1 - \xi_n$, which can be further divided into several categories:

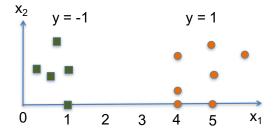
- $\xi_n = 0$: $y_n[\boldsymbol{w}^\top \boldsymbol{x}_n + b] = 1$, the point is on the correct side with distance $\frac{1}{\|\boldsymbol{w}\|}$.
- $0 < \xi_n \leq 1$: $y_n[\boldsymbol{w}^\top \boldsymbol{x}_n + b] \in [0, 1)$ on the correct side, but with distance less than $\frac{1}{\|\boldsymbol{w}\|}$.



In other words, support vectors satisfy $y_n[\mathbf{w}^\top \mathbf{x}_n + b] = \underline{1 - \xi_n}$, which can be further divided into several categories:

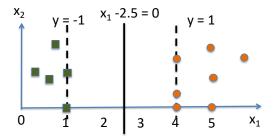
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- $0 < \xi_n \leq 1$: $y_n[\boldsymbol{w}^\top \boldsymbol{x}_n + b] \in [0, 1)$ on the correct side, but with distance less than $\frac{1}{\|\boldsymbol{w}\|}$.
- $\xi_n > 1$: $y_n[\mathbf{w}^\top \mathbf{x}_n + \ddot{b}] < 0$, on the wrong side of the boundary.





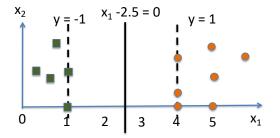
What will be the decision boundary learnt by solving the SVM optimization problem?

Example of SVM



Margin = 1.5; the decision boundary has $\mathbf{w} = [1, 0]^{\top}$, and b = -2.5.

Example of SVM

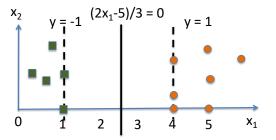


Margin = 1.5; the decision boundary has $\mathbf{w} = [1, 0]^{\top}$, and b = -2.5.

Not quite: we need the support vectors to satisfy to $y_n(\mathbf{w}^\top \mathbf{x}_n + b) = 1$. For example, for $\mathbf{x}_n = [1, 0]^\top$, we have

$$y_n(\mathbf{w}^{\top}\mathbf{x}_n+b)=(-1)[1-2.5]=1.5.$$

Example of SVM: Scaling

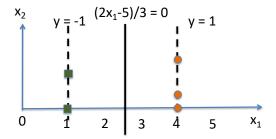


Thus, our optimization problem will re-scale \mathbf{w} and b to get this equation for the same decision boundary.

Margin = 1.5; the decision boundary has $\mathbf{w} = [2/3, 0]^{\top}$, and b = -5/3. For example, for $\mathbf{x}_n = [1, 0]^{\top}$, we have

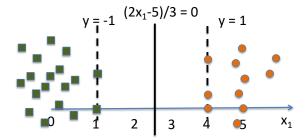
$$y_n(\mathbf{w}^{\top}\mathbf{x}_n+b)=(-1)[2/3-5/3]=1.$$

Example of SVM: Support Vectors

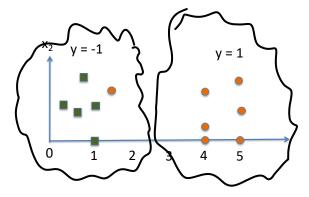


The solution to our optimization problem will be the **same** to the *reduced* dataset containing all the support vectors.

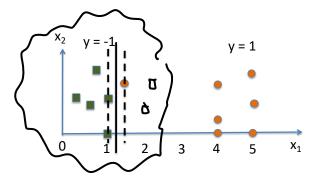
Example of SVM: Support Vectors



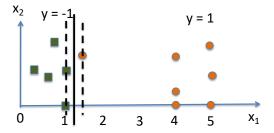
There can be many more data than the number of support vectors (so we can train on a smaller dataset).



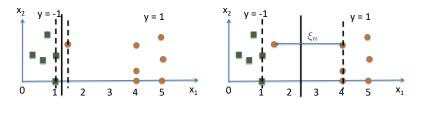
• Still linearly separable, but one of the orange dots is an "outlier".



• Naively applying the hard-margin SVM will result in a classifier with small margin.



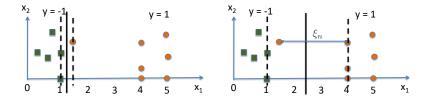
- Naively applying the hard-margin SVM will result in a classifier with small margin.
- So, better to use the soft-margin (or equivalently, hinge loss) formulation.



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

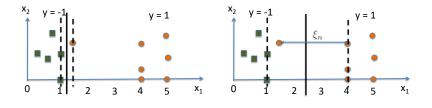
s.t. $y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b] \ge 1 - \xi_n, \quad \forall \quad n$
 $\xi_n \ge 0, \quad \forall \quad n$

Due to the flexibility provided by C, (properly tuned) SVM is less sensitive to outliers.



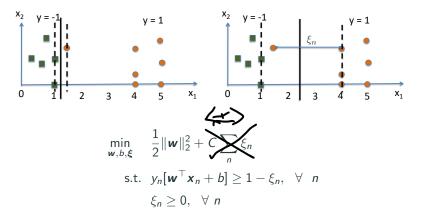
$$\begin{split} \min_{\boldsymbol{w},b,\boldsymbol{\xi}} & \frac{1}{2} \|\boldsymbol{w}\|_2^2 + C \sum_n \xi_n \\ \text{s.t.} & y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b] \geq 1 - \xi_n, \quad \forall \quad n \\ & \xi_n \geq 0, \quad \forall \ n \end{split}$$

• What happens if C is very small?

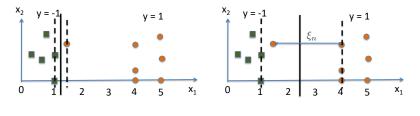


$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \quad \frac{1}{2} \|\boldsymbol{w}\|_2^2 + C \sum_n \xi_n$$
s.t. $y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b] \ge 1 - \xi_n, \quad \forall \quad n$
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• What happens if *C* is very small? More data points near the boundary are disregarded.

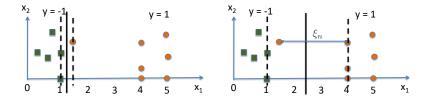


- What happens if *C* is very small? More data points near the boundary are disregarded.
- What happens if C is 0?



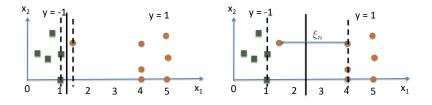
$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \quad \frac{1}{2} \|\boldsymbol{w}\|_2^2 + C \sum_n \xi_n$$
s.t. $y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b] \ge 1 - \xi_n, \quad \forall \quad n$
 $\xi_n \ge 0, \quad \forall \quad n$

- What happens if *C* is very small? More data points near the boundary are disregarded.
- What happens if C is 0? All data points will be ignored.



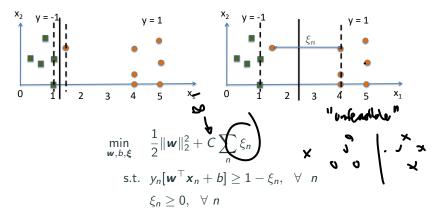
$$\begin{split} \min_{\boldsymbol{w},b,\boldsymbol{\xi}} & \frac{1}{2} \|\boldsymbol{w}\|_2^2 + C \sum_n \xi_n \\ \text{s.t.} & y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b] \geq 1 - \xi_n, \quad \forall \quad n \\ & \xi_n \geq 0, \quad \forall \ n \end{split}$$

• What happens if C is very large?

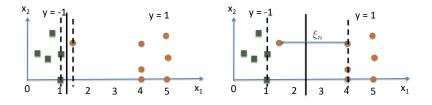


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• What happens if *C* is very large? Outliers near the decision boundary will have a greater impact.



- What happens if *C* is very large? Outliers near the decision boundary will have a greater impact.
- What happens if C is ∞ ?



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- What happens if *C* is very large? Outliers near the decision boundary will have a greater impact.
- What happens if C is ∞ ? We get hard margin SVM.

Hinge Loss Formulation

SVM vs. Logistic Regression

SVM soft-margin formulation

$$\min_{\boldsymbol{w}, b, \boldsymbol{\xi}} \quad \frac{1}{2} \|\boldsymbol{w}\|_2^2 + C \sum_n \xi_n$$
s.t. $y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b] \ge 1 - \xi_n, \ \forall \ n$
 $\xi_n \ge 0, \ \forall \ n$

$$\begin{split} \min_{\boldsymbol{w}} &- \sum_{n} \{ y_{n} \log \sigma(\boldsymbol{w}^{\top} \boldsymbol{x}_{n}) \\ &+ (1 - y_{n}) \log[1 - \sigma(\boldsymbol{w}^{\top} \boldsymbol{x}_{n})] \} \\ &+ \frac{\lambda}{2} \|\boldsymbol{w}\|_{2}^{2} \end{split}$$

SVM vs. Logistic Regression

SVM soft-margin formulation

Logistic regression formulation

$$\min_{\boldsymbol{w}, b, \boldsymbol{\xi}} \quad \frac{1}{2} \|\boldsymbol{w}\|_{2}^{2} + C \sum_{n} \xi_{n} \qquad \min_{\boldsymbol{w}} - \sum_{n} \{y_{n} \log \sigma(\boldsymbol{w}^{\top} \boldsymbol{x}_{n}) \\ \text{s.t.} \quad y_{n} [\boldsymbol{w}^{\top} \boldsymbol{x}_{n} + b] \geq 1 - \xi_{n}, \ \forall \ n \qquad \qquad + (1 - y_{n}) \log[1 - \sigma(\boldsymbol{w}^{\top} \boldsymbol{x}_{n})]\} \\ \xi_{n} \geq 0, \ \forall \ n \qquad \qquad + \frac{\lambda}{2} \|\boldsymbol{w}\|_{2}^{2}$$

• Logistic regression defines a loss for each data point and minimizes the total loss plus a regularization term.

SVM soft-margin formulation

v

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- This is convenient for assessing the "goodness" of the model on each data point.

SVM soft-margin formulation

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- This is convenient for assessing the "goodness" of the model on each data point.
- Can we write SVMs in this form as well? The Hinge Loss formulation!

Here's the soft-margin formulation again:

$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \frac{1}{2} \|\boldsymbol{w}\|_{2}^{2} + C \sum_{n} \xi_{n} \text{ s.t. } y_{n} [\boldsymbol{w}^{\top} \boldsymbol{x}_{n} + b] \geq 1 - \xi_{n}, \ \xi_{n} \geq 0, \ \forall \ n$$

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Now since $y_n[\boldsymbol{w}^\top \boldsymbol{x}_n + b] \ge 1 - \xi_n \iff \xi_n \ge 1 - y_n[\boldsymbol{w}^\top \boldsymbol{x}_n + b]$:

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Now since
$$\underbrace{\mathbf{v}_{n}[\boldsymbol{w}^{\top}\boldsymbol{x}_{n} + b]}_{min} \geq 1 - \underbrace{\xi_{n}}_{n} \longleftrightarrow \xi_{n} \geq 1 - \underbrace{y_{n}[\boldsymbol{w}^{\top}\boldsymbol{x}_{n} + b]}_{min} \leq \sum_{n} \xi_{n} + \frac{1}{2} \|\boldsymbol{w}\|_{2}^{2} \text{ s.t. } \xi_{n} \geq \max(0, 1 - y_{n}[\boldsymbol{w}^{\top}\boldsymbol{x}_{n} + b]), \ \forall \ n$$

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$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \frac{1}{2} \|\boldsymbol{w}\|_2^2 + C \sum_n \xi_n \text{ s.t. } y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b] \ge 1 - \xi_n, \ \xi_n \ge 0, \ \forall \ n$$

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$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} C \sum_{n} \xi_{n} + \frac{1}{2} \|\boldsymbol{w}\|_{2}^{2} \text{ s.t. } \xi_{n} \geq \max(0, 1 - y_{n}[\boldsymbol{w}^{\top}\boldsymbol{x}_{n} + b]), \forall n$$

Now since the ξ_n should always be as small as possible, we obtain:

$$\min_{\boldsymbol{w},\boldsymbol{b}} C \sum_{n} \max(0, 1 - y_n[\boldsymbol{w}^\top \boldsymbol{x}_n + \boldsymbol{b}]) + \frac{1}{2} \|\boldsymbol{w}\|_2^2$$

Here's the soft-margin formulation again:

$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \frac{1}{2} \|\boldsymbol{w}\|_{2}^{2} + C \sum_{n} \xi_{n} \quad \text{s.t.} \quad y_{n} [\boldsymbol{w}^{\top} \boldsymbol{x}_{n} + b] \geq 1 - \xi_{n} , \boldsymbol{\xi}_{n} \geq 0, \forall n$$
Now since $y_{n} [\boldsymbol{w}^{\top} \boldsymbol{x}_{n} + b] \geq 1 - \xi_{n} \iff \xi_{n} \geq 1 - y_{n} [\boldsymbol{w}^{\top} \boldsymbol{x}_{n} + b]$:
$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} C \sum_{n} \xi_{n} + \frac{1}{2} \|\boldsymbol{w}\|_{2}^{2} \text{ s.t.} \quad \xi_{n} \geq \max(0, 1 - y_{n} [\boldsymbol{w}^{\top} \boldsymbol{x}_{n} + b]), \forall n$$

Now since the ξ_n should always be as small as possible, we obtain:

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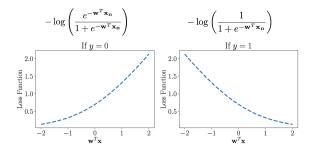
Divide by C and set $\lambda = \frac{1}{C}$, we get get Hinge Loss formulation:

$$\min_{\boldsymbol{w},b} \sum_{n} \underbrace{\max(0,1-y_n[\boldsymbol{w}^{\top}\boldsymbol{x}_n+b])}_{\text{Hinge Loss for } x_n,y_n} + \underbrace{\lambda_2}_{2} \|\boldsymbol{w}\|_2^2$$

Logistic Regression Loss vs Hinge Loss

Given training data (x_n, y_n) , the cross entropy loss was

$$-\{y_n \log \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n) + (1 - y_n) \log[1 - \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n)]\}$$

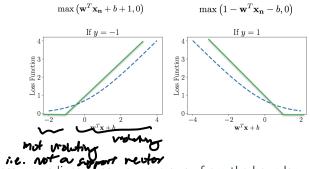


• What does the Hinge Loss Function look like?

Logistic Regression Loss vs Hinge Loss

Given training data (x_n, y_n) , the Hinge loss is

$$\max(0,1-y_n[\boldsymbol{w}^{\top}\boldsymbol{x}_n+b])$$



- Loss grows linearly as we move away from the boundary.
- No penalty if a point is more than 1 unit from the boundary.

Minimizing the total hinge loss on all the training data

$$\min_{\boldsymbol{w},b} \sum_{n} \underbrace{\max(0, 1 - y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b])}_{\text{hinge loss for sample } n} + \underbrace{\frac{\lambda}{2} \|\boldsymbol{w}\|_2^2}_{\text{regularizer}}$$

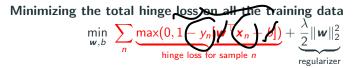
Analogous to regularized least squares or logistic regression, as we balance between two terms (the loss and the regularizer).

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• Can solve using gradient descent to get the optimal ${\bf w}$ and b



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- Can solve using gradient descent to get the optimal ${\bf w}$ and b
- Gradient of the first term will be either 0, \mathbf{x}_n or $-\mathbf{x}_n$ depending on y_n and $\mathbf{w}^\top \mathbf{x}_n + b$.
- Much easier to compute than in logistic regression, where we need to compute the sigmoid function σ(w^Tx_n + b) in each iteration.

Summary

Hard-margin (for separable data) $\min_{\boldsymbol{w}, b, \boldsymbol{\xi}} \frac{1}{2} \|\boldsymbol{w}\|_2^2 \text{ s.t. } y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b] \ge 1, \ \xi_n \ge 0, \ \forall \ n$ Hard-margin (for separable data) $\min_{\boldsymbol{w}, \boldsymbol{b}, \boldsymbol{\xi}} \ \frac{1}{2} \|\boldsymbol{w}\|_2^2 \text{ s.t. } y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b] \ge 1, \ \xi_n \ge 0, \ \forall \ n$

Soft-margin (add slack variables)

$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \ \frac{1}{2} \|\boldsymbol{w}\|_2^2 + C \sum_n \xi_n \text{ s.t. } y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b] \ge 1 - \xi_n, \ \xi_n \ge 0, \ \forall \ n$$

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Hinge loss (define a loss function for each data point) $\min_{\boldsymbol{w}, b} \sum_{n} \max(0, 1 - y_n [\boldsymbol{w}^\top \boldsymbol{x}_n + b]) + \frac{\lambda}{2} \|\boldsymbol{w}\|_2^2$ We've seen the geometric formulation of SVM and the equivalent formulation of minimizing the empirical hinge loss.

This explains why SVM:

- 1. Is less sensitive to outliers.
- 2. Maximizes distance of training data from the boundary.
- 3. Only requires a subset of the training points.
- 4. Generalizes well to many nonlinear models.
- 5. Scales better with high-dimensional data.

We will need to use duality to show the remaining properties.

You should know:

- Max-margin formulation for separable and non-separable SVMs.
- Definition and importance of support vectors.
- Hinge loss formulation of SVMs.
- Equivalence of the max-margin and hinge loss formulations.

Next class:

- Duality
- Nonlinear SVM