

COMP 551 - Applied Machine Learning

Lecture 11 – SVMs continued

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(with slides and content from Joelle Pineau)

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MiniProject 2

#	Team Name	Kernel	Team Members	Score	Entries	Last
1	Group 80			0.94813	6	21h
2	Group 98			0.93813	3	8d
	📍 Prof. Hamilton's Benchmark			0.91866		
3	Group 12			0.91720	6	1d
4	Group 91			0.91493	2	2d
5	Group 3			0.91413	9	16h
6	Group 77			0.91173	5	19h
7	Group 73			0.91160	2	18h
8	Group 60			0.91013	7	2d
9	Group 95			0.91000	5	3d
10	Group 66			0.90920	5	2d
11	Group 10			0.90906	11	19h
12	Group Sixty8			0.90760	11	12h
13	Group 103			0.90493	1	6m
14	Group 101			0.90413	5	3d
15	Group 20			0.90200	3	4d
16	Group 17			0.90133	6	2d
17	Group 8			0.90106	6	13h

How to write a good project report?

- Read some good ML papers ☺
 - ACL and EMNLP publish short papers (4-5 pages).
 - Workshops are also good and have short papers (4-5 pages)
- Som examples:
 - <http://aclweb.org/anthology/D18-1546>
 - http://petar-v.com/dgi_nips18_camera.pdf
 - <http://emnlp2014.org/papers/pdf/EMNLP2014024.pdf>
 - <https://arxiv.org/pdf/1811.05868.pdf>
 - <http://www.aclweb.org/anthology/D13-1148>
 - <https://arxiv.org/pdf/1704.04008.pdf>

SVMs (Review)

- First suggestion:

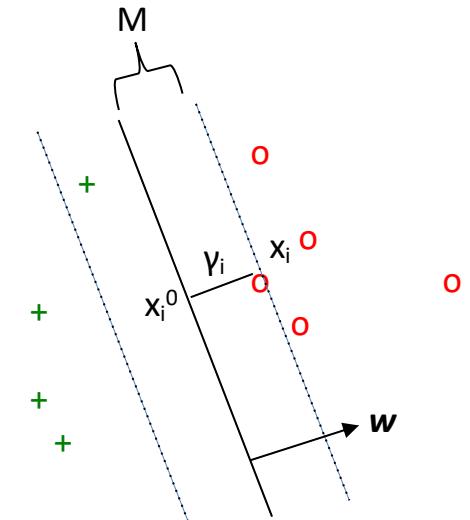
Maximize M

with respect to w

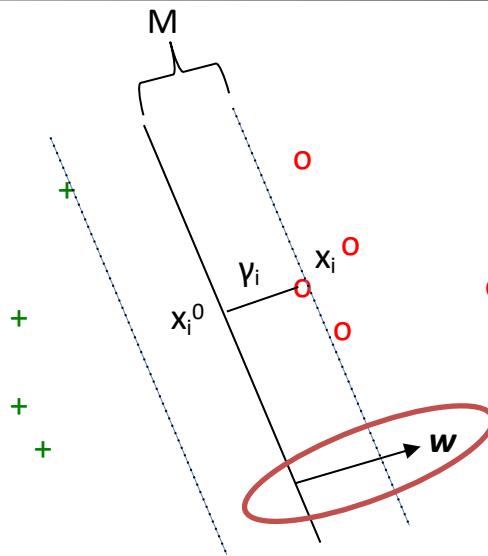
subject to $y_i w^T x_i / ||w|| \geq M, \forall i$

- This is not very convenient for optimization:

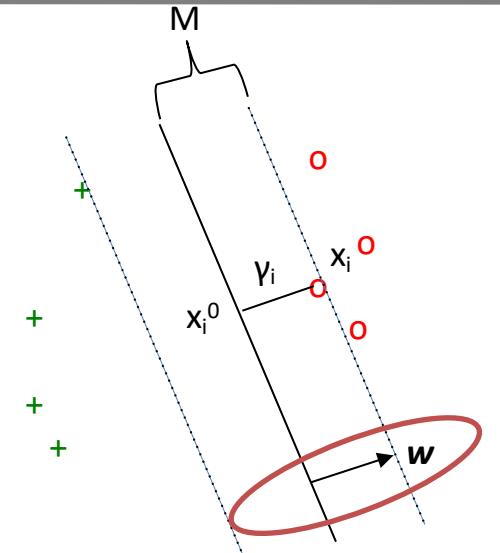
- w appears nonlinearly in the constraints.
- Problem is underconstrained. If (w, M) is optimal, so is $(\beta w, M)$, for any $\beta > 0$.
- Add a constraint:** $||w|| = 1/M$
 - Intuition: Changing $||w||$ doesn't change the decision hyperplane, so without loss of generality we say that $y_i w^T x_i = 1$ for points that are right on the margin.



SVMs (Review)



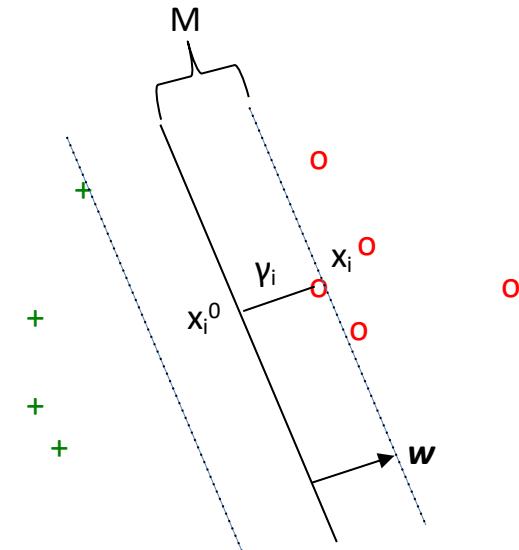
w specifies the orientation of the decision boundary, but $\|w\|$ is unconstrained and unrelated to M .



$\|w\|=1/M$ so w specifies both the orientation of the decision boundary and the size of the margin.

SVMs (review)

- Revised formulation:
Min $\frac{1}{2} \|\mathbf{w}\|^2$
w.r.t. \mathbf{w}
s.t. $y_i \mathbf{w}^T \mathbf{x}_i \geq 1, \forall i$
- Note: we set $\|\mathbf{w}\| = 1/M$, so minimizing $\|\mathbf{w}\|^2$ is equivalent to maximizing M^2 , which is equivalent to maximizing M .



Lagrangian optimization

- Consider $P(\mathbf{w}) = \max_{\alpha: \alpha_i \geq 0} L(\mathbf{w}, \alpha) = \max_{\alpha: \alpha_i \geq 0} f(\mathbf{w}) + \sum_{i=1:k} \alpha_i g_i(\mathbf{w})$

(P stands for “primal”)

- Recall: $L(\mathbf{w}, \alpha) =$ Observe that the following is true:

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

- Hence, instead of computing $\min_{\mathbf{w}} f(\mathbf{w})$ subject to the original constraints, we can compute:

$$p^* = \min_{\mathbf{w}} P(\mathbf{w}) = \min_{\mathbf{w}} \max_{\alpha: \alpha_i \geq 0} L(\mathbf{w}, \alpha) \quad \textit{Primal}$$

- Alternately, invert max and min to get:

$$d^* = \max_{\alpha: \alpha_i \geq 0} \min_{\mathbf{w}} L(\mathbf{w}, \alpha) \quad \textit{Dual}$$

SVMs (review)

- We wanted to solve:

$$\begin{array}{ll} \text{Min} & \frac{1}{2} \|\mathbf{w}\|^2 \\ \text{w.r.t.} & \mathbf{w} \\ \text{s.t.} & y_i \mathbf{w}^T \mathbf{x}_i \geq 1 \end{array}$$

- The Lagrangian:

$$L(\mathbf{w}, \alpha) = \frac{1}{2} \|\mathbf{w}\|^2 + \sum_i \alpha_i (1 - y_i (\mathbf{w}^T \mathbf{x}_i))$$

$$\max_{\alpha: \alpha_i \geq 0} L(\mathbf{w}, \alpha) = \left\{ \begin{array}{l} \frac{1}{2} \|\mathbf{w}\|^2 \text{ if all constraints are satisfied, } +\infty \text{ otherwise } \end{array} \right.$$

- The **primal problem** is:

$$\min_{\mathbf{w}} \max_{\alpha: \alpha_i \geq 0} L(\mathbf{w}, \alpha)$$

- The **dual problem** is:

$$\max_{\alpha: \alpha_i \geq 0} \min_{\mathbf{w}} L(\mathbf{w}, \alpha)$$

SVMs (review)

- Consider both solutions:

$$\begin{aligned} p^* &= \min_w \max_{\alpha: \alpha_i \geq 0} L(w, \alpha) \\ d^* &= \max_{\alpha: \alpha_i \geq 0} \min_w L(w, \alpha) \end{aligned}$$

Primal
Dual

- If f and g_i are convex and the g_i can all be satisfied simultaneously for some w , then we have equality: $d^* = p^* = L(w^*, \alpha^*)$.
 - w^* is the optimal weight vector (= primal solution)
 - α^* is the optimal set of support vectors (= dual solution)
- For SVMs, we have a quadratic objective and linear constraints so both f and g_i are convex.
- For linearly separable data, all g_i can be satisfied simultaneously.
- Note: w^*, α^* solve the primal and dual if and only if they satisfy the Karush-Kuhn-Tucker conditions (see Section 7.1 of the Bishop book).

SVMs (review)

- Taking derivatives of $L(\mathbf{w}, \alpha)$ wrt \mathbf{w} , setting to 0, and solving for \mathbf{w} :

$$L(\mathbf{w}, \alpha) = \frac{1}{2} \|\mathbf{w}\|^2 + \sum_i \alpha_i (1 - y_i (\mathbf{w}^T \mathbf{x}_i))$$

$$\delta L / \delta \mathbf{w} = \mathbf{w} - \sum_i \alpha_i y_i \mathbf{x}_i = 0$$

$$\mathbf{w}^* = \sum_i \alpha_i y_i \mathbf{x}_i$$

- The optimal solution \mathbf{w}^* is a linear combination of the \mathbf{x}_i .
- Plugging this back into L we get the dual: $\max_{\alpha} \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} y_i y_j \alpha_i \alpha_j (\mathbf{x}_i \cdot \mathbf{x}_j)$ with constraints $\alpha_i \geq 0$ and $\sum_i \alpha_i y_i = 0$. (Quadratic programming problem).

SVMs (review)

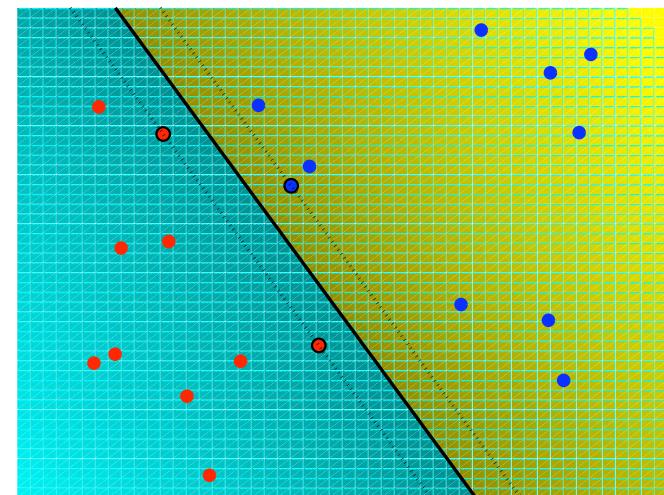
- Suppose we find the optimal α 's (e.g. using a QP package.)
- Constraint i is active when $\alpha_i > 0$. This corresponds for the points for which $(1-y_i\mathbf{w}^T\mathbf{x}_i)=0$.
- These are the points lying on the edge of the margin. We call them **support vectors**. They define the decision boundary.
- The output of the classifier for query point \mathbf{x} is computed as:

$$h_{\mathbf{w}}(\mathbf{x}) = \text{sign}(\sum_{i=1:n} \alpha_i y_i (\mathbf{x}_i \cdot \mathbf{x}))$$

- I.e., it is determined by computing the dot product of the query point with the support vectors.

SVMs (review)

- See pages 325-343 in the Bishop textbook for a detailed review of these derivations.
- You should know this material, but you are not responsible for anything in the Appendix.



Non-linearly separable data

- A linear boundary might be too simple to capture the data.
- Option 1: **Relax the constraints** and allow some points to be misclassified by the margin.
- Option 2: **Allow a nonlinear decision boundary** in the input space by finding a linear decision boundary in an **expanded space** (*similar to adding polynomial terms in linear regression.*)
 - Here \mathbf{x}_i is replaced by $\Phi(\mathbf{x}_i)$, where Φ is called a **feature mapping**.

Soften the primal objective

- We wanted to solve:

$$\begin{aligned} \min_w & \quad \frac{1}{2} \|w\|^2 \\ \text{s.t.} & \quad y_i w^T x_i \geq 1 \end{aligned}$$

- This can be re-written:

$$\begin{aligned} \min_w & \quad \sum_i L_{0-\infty}(w^T x_i, y_i) + \frac{1}{2} \|w\|^2 \\ \text{s.t.} & \quad y_i w^T x_i \geq 1 \end{aligned}$$

where $\sum_i L_{0-\infty}(w^T x_i, y_i) = (\infty \text{ for a misclassification, } 0 \text{ correct classification})$

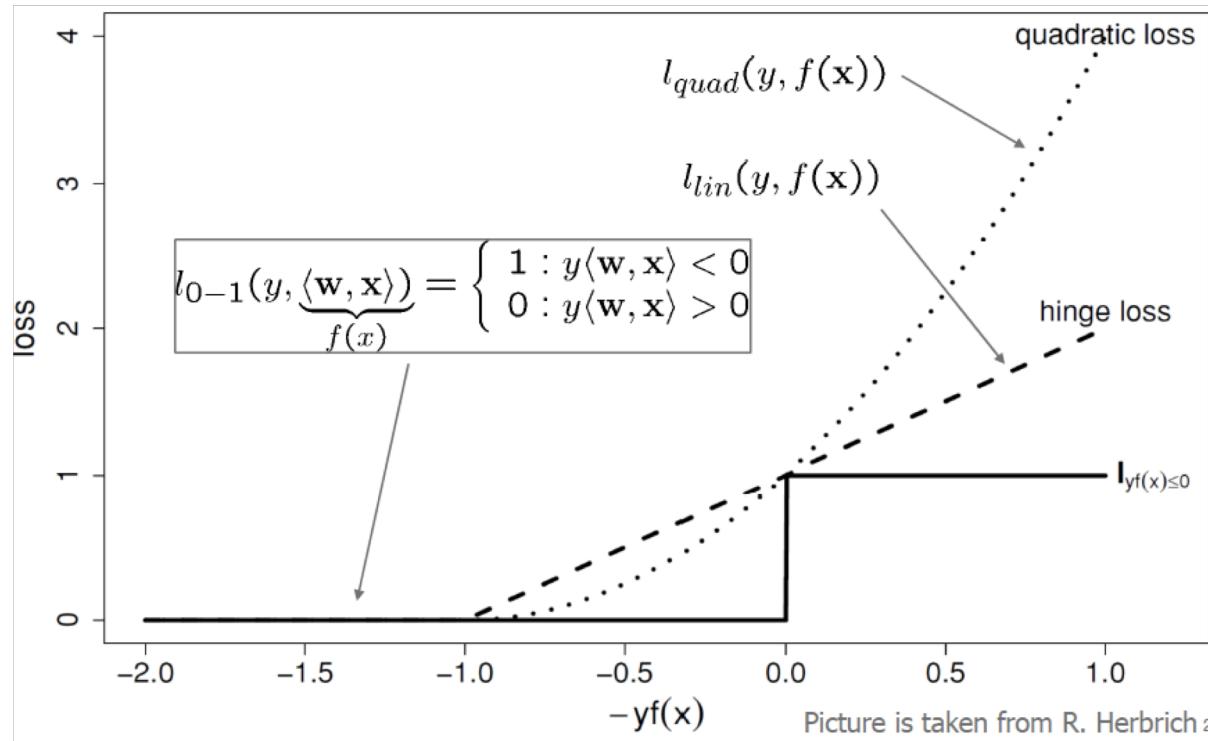
- Soften misclassification cost:

$$\begin{aligned} \min_w & \quad \sum_i L_{0-1}(w^T x_i, y_i) + \frac{1}{2} \|w\|^2 \\ \text{s.t.} & \quad y_i w^T x_i \geq 1 \end{aligned}$$

where $\sum_i L_{0-1}(w^T x_i, y_i) = (1 \text{ for a misclassification, } 0 \text{ correct classification})$

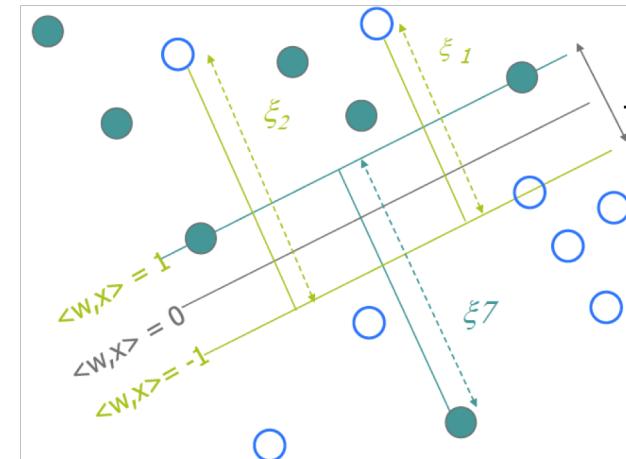
- But this is a **non-convex** objective!

Approximation of the L_{0-1} function



SVM with hinge loss

- Hinge loss: $L_{\text{hin}}(w^T x_i, y_i) = \max\{1 - y_i w^T x_i, 0\}$
- Softens misclassification cost: $\min_w C \sum_i L_{\text{hin}}(w^T x_i, y_i) + \frac{1}{2} \|w\|^2$
where C controls trade-off between slack penalty and margin.
- The hinge loss upper-bounds the 0-1 loss.
 $\xi_i \geq 1 - y_i w^T x_i \geq L_{0-1}(w^T x_i, y_i)$



Primal Soft SVM problem

- Define slack variables $\xi_i = L_{\text{hin}}(w^T x_i, y_i) = \max \{1 - y_i w^T x_i, 0\}$
- Solve: $\hat{w}_{\text{soft}} = \operatorname{argmin}_{w, \xi} C \sum_{i=1:n} \xi_i + \frac{1}{2} \|w\|^2$
s. t. $y_i w^T x_i \geq 1 - \xi_i, \quad i = 1, \dots, n$
 $\xi_i \geq 0, \quad i = 1, \dots, n$
where $w \in \mathbb{R}^m, \xi \in \mathbb{R}^n$

Primal Soft SVM problem

- Define slack variables $\xi_i = L_{\text{hin}}(w^T x_i, y_i) = \max \{1 - y_i w^T x_i, 0\}$
- Solve: $\hat{w}_{\text{soft}} = \operatorname{argmin}_{w, \xi} C \sum_{i=1:n} \xi_i + \frac{1}{2} \|w\|^2$ Add Lagrange mult:

$$\text{s. t.} \quad y_i w^T x_i \geq 1 - \xi_i, \quad i = 1, \dots, n \quad <= \text{Call this } \alpha_i$$

$$\xi_i \geq 0, \quad i = 1, \dots, n \quad <= \text{Call this } \beta_i$$

where $w \in R^m, \xi \in R^n$

- Introduce Lagrange multipliers: $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_n)^T, 0 \leq \alpha_i$
 $\beta = (\beta_1, \beta_2, \dots, \beta_n)^T, 0 \leq \beta_i$

Soft SVM: Adding Lagrange multipliers

- **Primal** objective: $(\mathbf{w}, \xi, \alpha, \beta) = \arg \min_{\mathbf{w}, \xi} \max_{\alpha, \beta} L(\mathbf{w}, \xi, \alpha, \beta)$
where $L(\mathbf{w}, \xi, \alpha, \beta) = \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1:n} \xi_i - \sum_{i=1:n} \alpha_i (y_i \mathbf{w}^T \mathbf{x}_i - 1 + \xi_i) - \sum_{i=1:n} \beta_i \xi_i$

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- **Dual** (invert min and max): $(\mathbf{w}, \xi, \alpha, \beta) = \arg \max_{\alpha, \beta} \min_{\mathbf{w}, \xi} L(\mathbf{w}, \xi, \alpha, \beta)$

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- Solve: $\delta L / \delta \mathbf{w} = \mathbf{w} - \sum_i \alpha_i y_i \mathbf{x}_i = 0 \Rightarrow \mathbf{w}^* = \sum_i \alpha_i y_i \mathbf{x}_i$
- $\delta L / \delta \xi = C \mathbf{1}_n - \alpha - \beta = 0 \Rightarrow \beta = C \mathbf{1}_n - \alpha$
- Lagrange multipliers are positive, so we have: $0 \leq \beta_i, 0 \leq \alpha_i \leq C$

Soft SVM: Adding Lagrange multipliers

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- $\delta L / \delta \xi = C \mathbf{1}_n - \alpha - \beta = 0 \Rightarrow \beta = C \mathbf{1}_n - \alpha$
- Lagrange multipliers are positive, so we have: $0 \leq \beta_i, 0 \leq \alpha_i \leq C$
- Plug into dual : $\max_{\alpha} \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} y_i y_j \alpha_i \alpha_j (\mathbf{x}_i \cdot \mathbf{x}_j)$
with constraints $0 \leq \alpha_i \leq C$ and $\sum_i \alpha_i y_i = 0$.
- This is a **quadratic programming problem** (similar to Hard SVM).

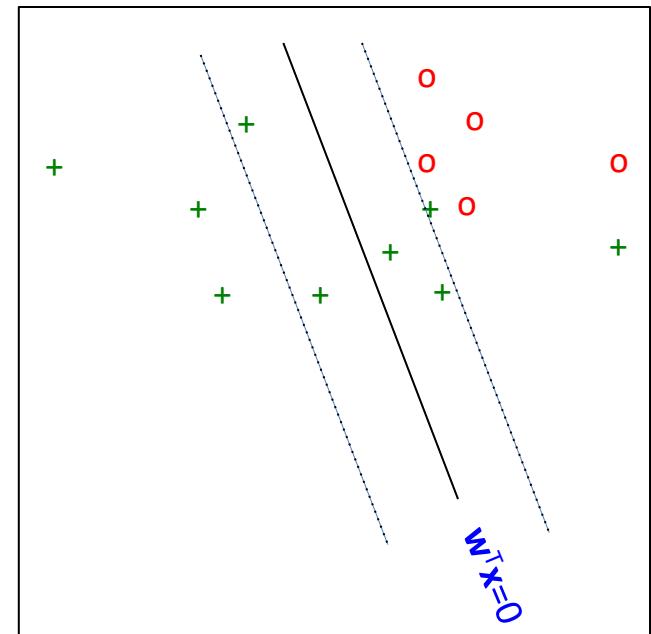
Soft SVM: Adding Lagrange multipliers

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- **Dual** (invert min and max): $(\mathbf{w}, \xi, \alpha, \beta) = \arg \max_{\alpha, \beta} \min_{\mathbf{w}, \xi} L(\mathbf{w}, \xi, \alpha, \beta)$

See Section 7.1.1 in the
Bishop book for detailed
derivations.

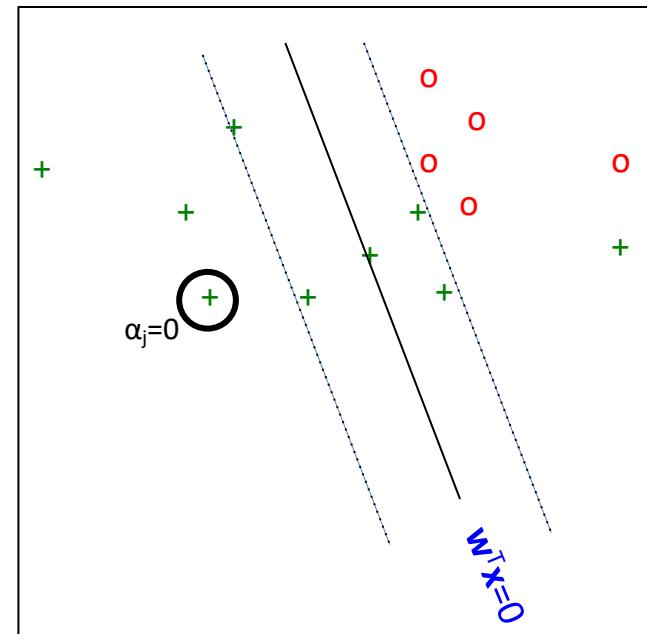
Soft SVM solution

- Soft-SVM has one more constraint $0 \leq a_i \leq C$ (vs $0 \leq a_i$ in Hard SVM).
- When $C \rightarrow \infty$, then Soft-SVM=>Hard-SVM.



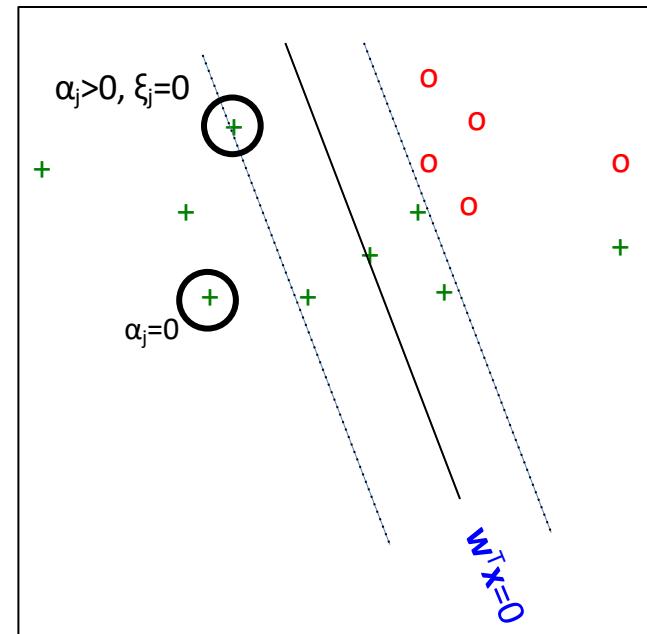
Soft SVM solution

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- When $C=>\infty$, then Soft-SVM=>Hard-SVM.
- Points away from margin have $a_i = 0$.
- Points on the margin have $a_i > 0$ and $\xi_i=0$.
- Points within the margin have $0 < \xi_i < 1$
 $a_j>0, \xi_j=0$
- Points on the decision line have $\xi_i = 1$.
- Misclassified points have $\xi_i > 1$.



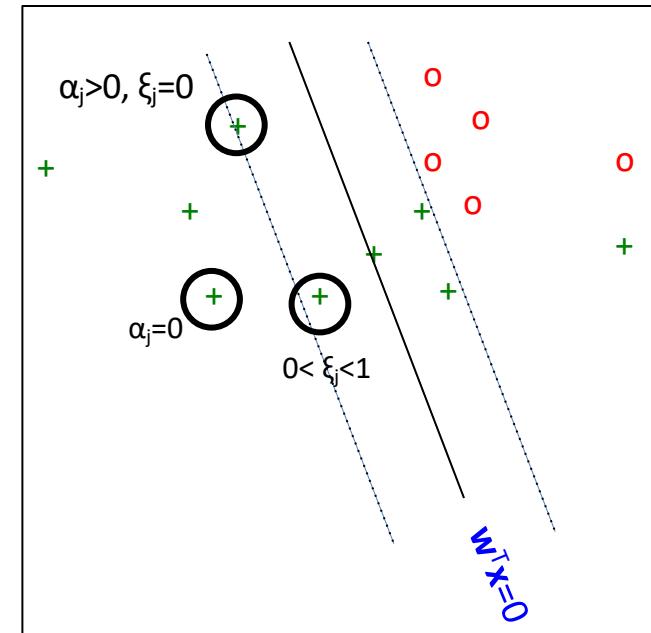
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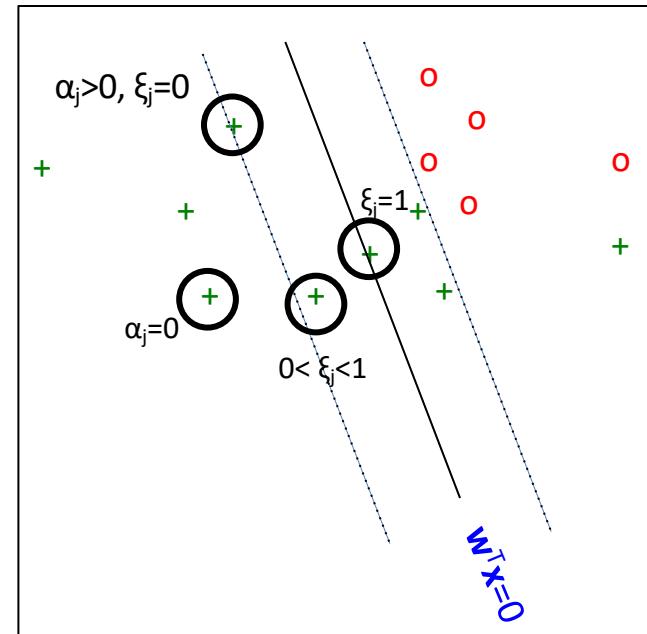
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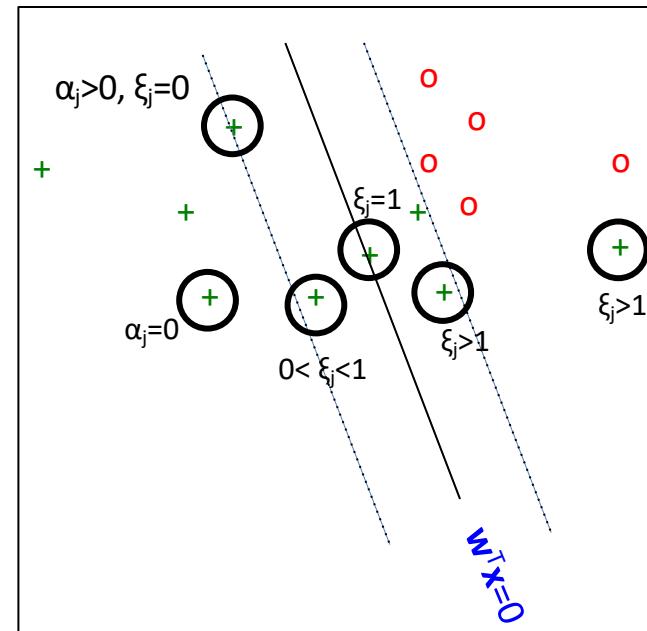
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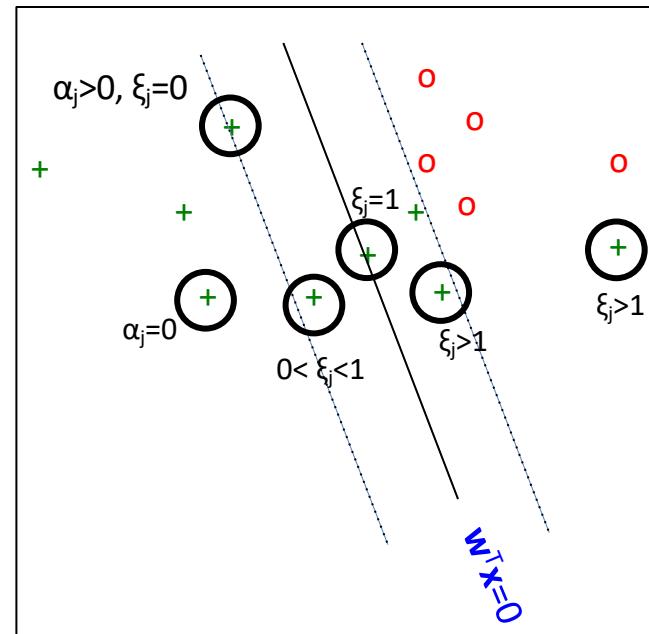
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Soft SVM solution

- Soft-SVM has one more constraint $0 \leq a_i \leq C$ (vs $0 \leq a_i$ in Hard SVM).
- When $C=>\infty$, then Soft-SVM=>Hard-SVM.
- To predict on test data:
$$h_w(\mathbf{x}) = \text{sign}(\sum_{i=1:n} \alpha_i y_i (\mathbf{x}_i \cdot \mathbf{x}))$$
- Only need to store the support vectors (i.e. points on the margin) to predict.



Multiple classes

- **One-vs-All:** Learn K separate binary classifiers.
 - Can lead to inconsistent results.
 - Training sets are imbalanced, e.g. assuming n examples per class, each binary classifier is trained with positive class having $1*n$ of the data, and negative class having $(K-1)*n$ of the data.

Multiple classes

- **One-vs-All:** Learn K separate binary classifiers.
 - Can lead to inconsistent results.
 - Training sets are imbalanced, e.g. assuming n examples per class, each binary classifier is trained with positive class having $1*n$ of the data, and negative class having $(K-1)*n$ of the data.
- **Multi-class SVM:** Define the margin to be the gap between the correct class and the nearest other class.

Non-linearly separable data

- A linear boundary might be too simple to capture the data.
- Option 1: **Relax the constraints** and allow some points to be misclassified by the margin.
- Option 2: **Allow a nonlinear decision boundary** in the input space by finding a linear decision boundary in an **expanded space** (*similar to adding polynomial terms in linear regression.*)
 - Here \mathbf{x}_i is replaced by $\Phi(\mathbf{x}_i)$, where Φ is called a **feature mapping**.

Margin optimization in feature space

- Replacing x_i by $\Phi(x_i)$, the optimization problem for w becomes:

- Primal form:** Min $\frac{1}{2} \|w\|^2$
w.r.t. w
s.t. $y_i w^T \Phi(x_i) \geq 1$

Margin optimization in feature space

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- Primal form:** Min $\frac{1}{2} \|w\|^2$
w.r.t. w
s.t. $y_i w^T \Phi(x_i) \geq 1$
- Dual form:** Max $\sum_i \alpha_i - \frac{1}{2} \sum_{i,j} y_i y_j \alpha_i \alpha_j (\Phi(x_i) \cdot \Phi(x_j))$
w.r.t. α_i
s.t. $\alpha_i \geq 0$
 $\sum_i \alpha_i y_i = 0$

Feature space solution

- The optimal weights, in the expended feature space, are

$$\mathbf{w} = \sum_{i=1:n} \alpha_i y_i \Phi(\mathbf{x}_i)$$

- Classification of an input \mathbf{x} is given by:

$$h_w(\mathbf{x}) = \text{sign}(\sum_{i=1:n} \alpha_i y_i (\phi(\mathbf{x}_i) \cdot \phi(\mathbf{x})))$$

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$$\mathbf{w} = \sum_{i=1:n} \alpha_i y_i \Phi(\mathbf{x}_i)$$

- Classification of an input \mathbf{x} is given by:

$$h_{\mathbf{w}}(\mathbf{x}) = \text{sign}\left(\sum_{i=1:n} \alpha_i y_i (\Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x})) \right)$$

- Note that to solve the SVM optimization problem in dual form and to make a prediction, we only ever need to **compute dot-products of feature vectors.**

Kernel functions

- Whenever a learning algorithm (such as SVMs) can be written in terms of dot-products, it can be generalized to kernels.
- A **kernel** is any function $K: \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R}$, which corresponds to a dot product for some feature mapping Φ :
$$K(\mathbf{x}_1, \mathbf{x}_2) = \phi(\mathbf{x}_1) \cdot \phi(\mathbf{x}_2) \text{ for some } \Phi$$
- Conversely, by choosing feature mapping Φ , we implicitly choose a kernel function.
- Recall that $\phi(\mathbf{x}_1) \cdot \phi(\mathbf{x}_2) = \cos\angle(\mathbf{x}_1, \mathbf{x}_2)$, where \angle denotes the angle between the vectors, so a kernel function can be thought of as a notion of **similarity**.

Example: Quadratic kernel

- Let $K(\mathbf{x}, \mathbf{z}) = (\mathbf{x} \cdot \mathbf{z})^2$.
- Is this a kernel?

$$\begin{aligned} K(\mathbf{x}, \mathbf{z}) &= \left(\sum_{i=1:m} x_i z_i \right) \left(\sum_{j=1:m} x_j z_j \right) \\ &= \sum_{i,j \in \{1..m\}} x_i z_i x_j z_j \\ &= \sum_{i,j \in \{1..m\}} (x_i x_j) (z_i z_j) \end{aligned}$$

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- We see it is a kernel, with feature mapping:

$$\phi(\mathbf{x}) = \langle x_1^2, x_1 x_2, \dots, x_1 x_m, x_2 x_1, x_2^2, \dots, x_m^2 \rangle$$

Feature vector includes all squares of elements and all cross terms.

Important: Computing Φ takes $O(m^2)$ but computing K only takes $O(m)$.

Polynomial kernels

- More generally, $K(\mathbf{x}, \mathbf{z}) = (\mathbf{x} \cdot \mathbf{z})^d$ is a kernel, for any positive integer d :
$$K(\mathbf{x}, \mathbf{z}) = (\sum_{i=1:m} x_i z_i)^d$$
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- Terms are monomials (products of x_i and/or z_i) with total power equal to d .
- If we use the primal form of the SVM, each term gets a weight.
- **Curse of dimensionality**: it is very expensive both to optimize and to predict with an SVM in primal form.
- However, evaluating K can be done in $O(m)$.

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- If we work with the dual, we do not have to ever compute the feature mapping Φ . We just compute the similarity kernel \mathbf{K} .

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- We can solve the dual for the α_i :

$$\begin{array}{ll} \text{Max} & \sum_{i=1:n} \alpha_i - \frac{1}{2} \sum_{i,j=1:n} y_i y_j \alpha_i \alpha_j K(x_i, x_j) \\ \text{w.r.t.} & \alpha_i \\ \text{s.t.} & \alpha_i \geq 0 \text{ and } \sum_{i:1..n} \alpha_i y_i = 0 \end{array}$$

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- The class of a new input x is computed as:

$$h_w(x) = \text{sign}\left(\sum_{i=1:n} \alpha_i y_i K(x_i, x)\right)$$

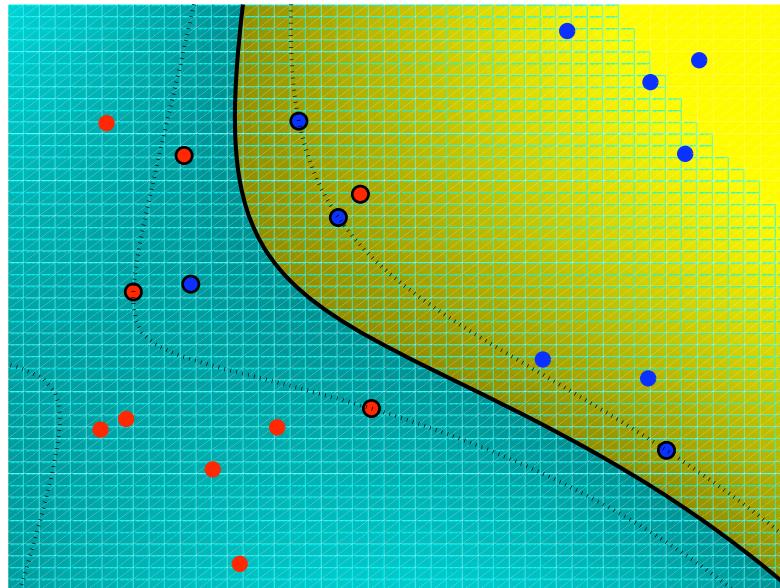
where x_i are the support vectors (defining the margin).

- Remember, $K(\cdot, \cdot)$ can be evaluated in $O(m)$ time = big savings!

Some other kernel functions

- $K(\mathbf{x}, \mathbf{z}) = (1 + \mathbf{x} \cdot \mathbf{z})^d$ - feature expansion has all monomial terms of total power.
- Radial basis / Gaussian kernel: $K(\mathbf{x}, \mathbf{z}) = \exp(-\|\mathbf{x} - \mathbf{z}\|^2 / 2\sigma^2)$
 - This kernel has an infinite-dimensional feature expansion, but dot-products can still be computed in $O(m)$ (where $m = \# \text{features}$)
- Sigmoidal kernel: $K(\mathbf{x}, \mathbf{z}) = \tanh(c_1 \mathbf{x} \cdot \mathbf{z} + c_2)$

Example: Gaussian Kernel



Note the non-linear decision boundary

Kernels beyond SVMs

- A lot of research related to defining kernel functions suitable to particular tasks, or types of inputs (e.g. words, graphs, images).
 - Many kernels are available:
 - Information diffusion kernels (Lafferty and Lebanon, 2002)
 - Diffusion kernels on graphs (Kondor and Jebara, 2003)
 - String kernels for text classification (Lodhi et al, 2002)
 - String kernels for protein classification (Leslie et al, 2002)
- ... and others!

Example: String kernels

- Very important for DNA matching, text classification, ...
- Often use a sliding window of length k over the two strings that we want to compare.
- Within the fixed-size window we can do many things:
 - Count exact matches.
 - Weigh mismatches based on how bad they are.
 - Count certain markers, e.g. AGT.
- The kernel is the sum of these similarities over the two sequences.

Kernelizing other ML algorithms

- Many other machine learning algorithms have a “**dual formulation**”, in which dot-products of features can be replaced by kernels.
- Examples:
 - Perceptron
 - Logistic regression
 - Linear regression

What you should know

From last class and from today:

- Perceptron algorithm.
- Margin definition for linear SVMs.
- Use of Lagrange multipliers to transform optimization problems.
- Primal and dual optimization problems for SVMs.
- Feature space version of SVMs.
- The kernel trick and examples of common kernels.