The Mathematics of Machine Learning 2025

Lecture 8

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Outline

Support Vector Machines

1. Intro
2. Optimal Separating Hyperplane
3. SVMs
4. Interpretation as Penalized ERM with Hinge Loss
5. Dual Formulation
6. Kernel Trick

History

Vapnik & Chervonenkis: foundational work on statistical learning starting in sixties and seventies, leading to SVMs around 1990

Vapnik, 1998: “Solve the problem directly and never solve a more general problem as an intermediate step.”

Intro

Plug-in Estimators:

	Estimate	Examples
Generative	$P^*(X, Y)$	Naive Bayes
Discriminative	$P^*(Y \mid X)$	LDA, logistic regression
Now	decision boundary directly	SVMs

Intro

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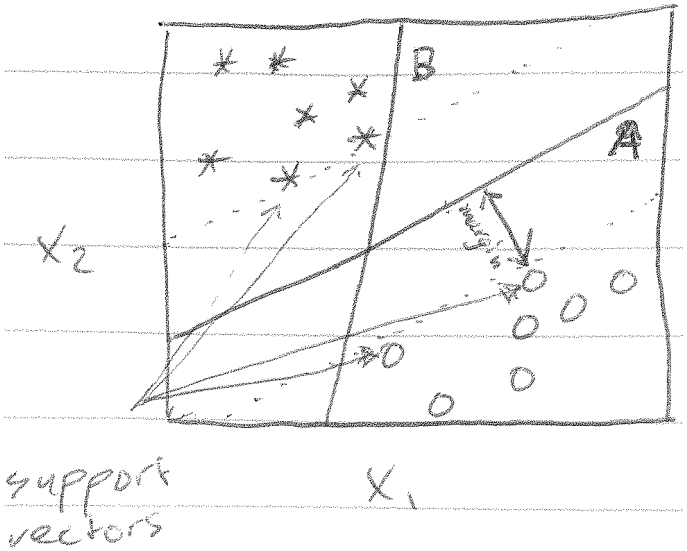
Binary Classification:

$$\begin{pmatrix} Y_1 \\ X_1 \end{pmatrix}, \ldots, \begin{pmatrix} Y_N \\ X_N \end{pmatrix} \qquad Y \in \{-1, +1\}$$

Linear Classifiers:

$$f_{\beta_0,\beta}(X) = X^\top \beta + \beta_0 \qquad \beta_0 \in \mathbb{R}, \beta \in \mathbb{R}^p$$

Optimal Separating Hyperplane I



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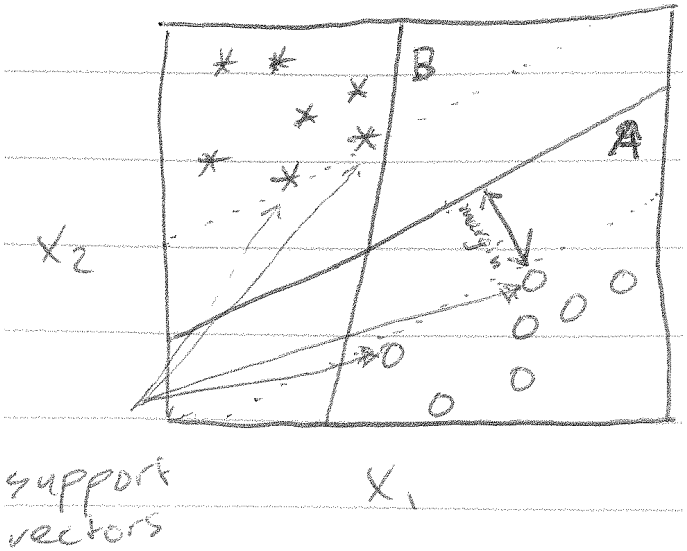

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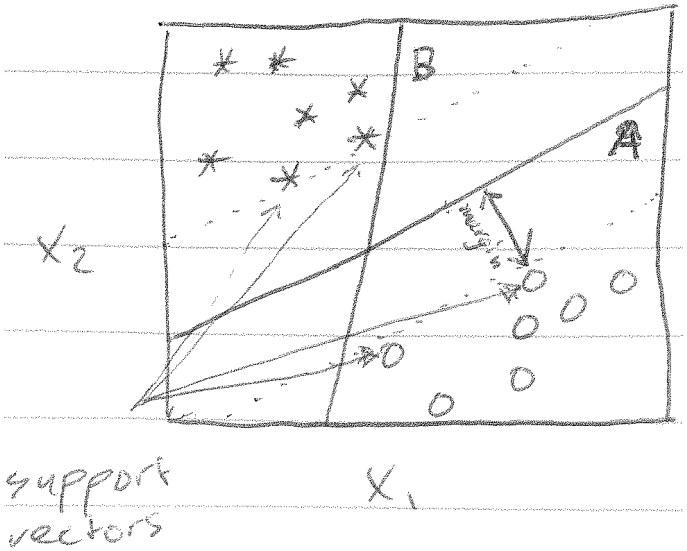

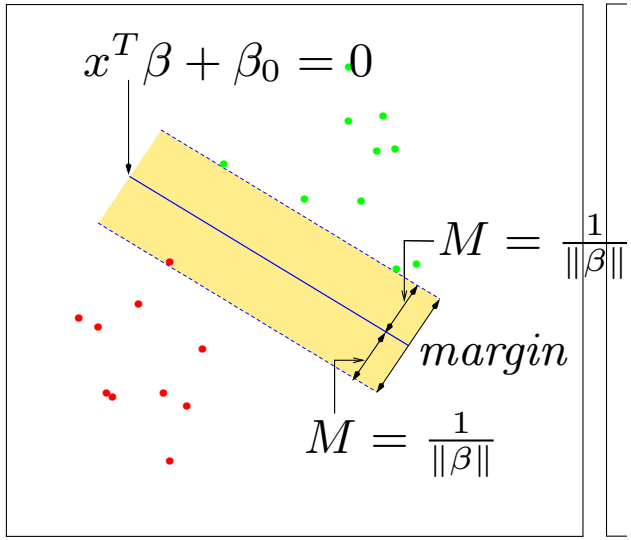

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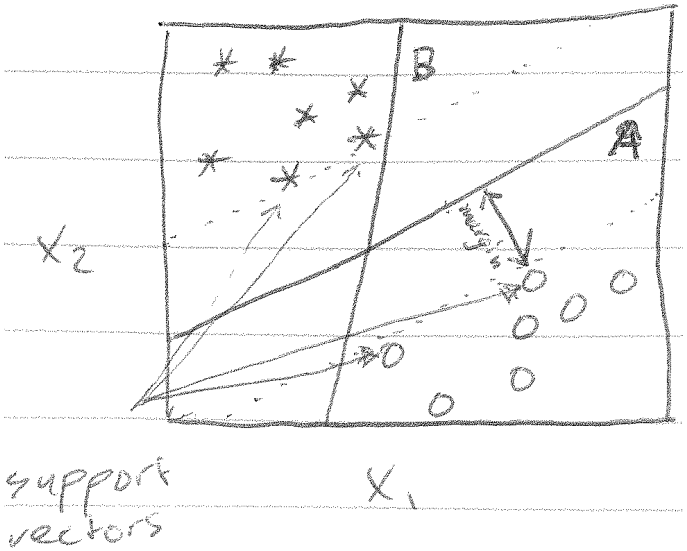

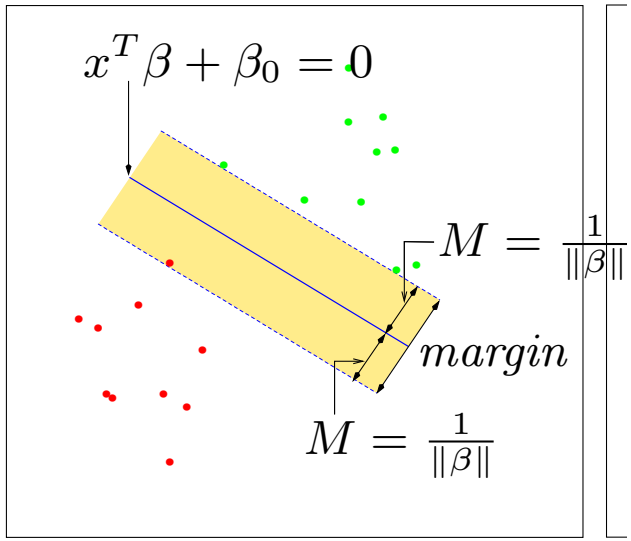

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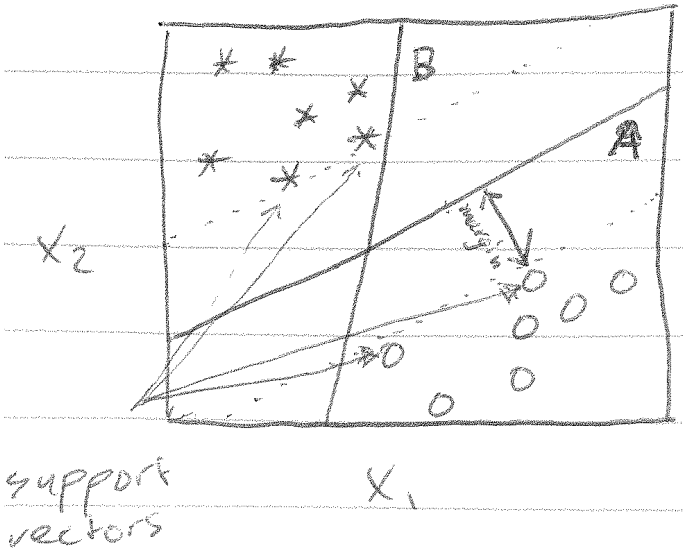

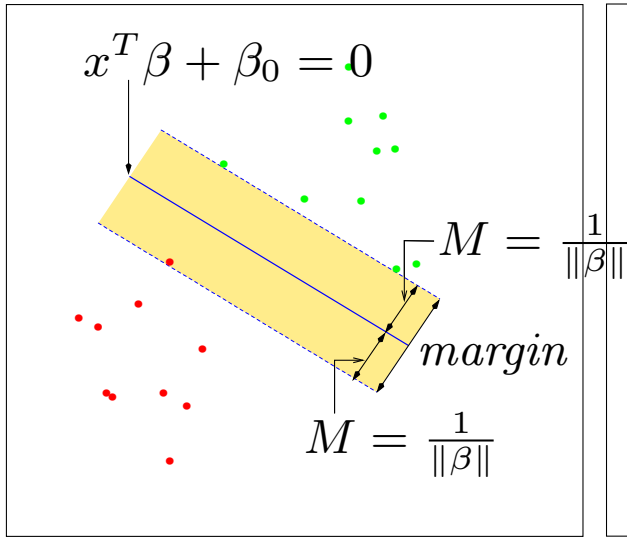

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Distance of X_i to decision boundary: $\frac{|X_i^\top \beta + \beta_0|}{\|\beta\|} = \frac{|f_{\beta_0,\beta}(X_i)|}{\|\beta\|}$

Margin: $\frac{Y_i f_{\beta_0,\beta}(X_i)}{\|\beta\|} = \begin{cases} \text{distance if } X_i \text{ classified correctly} \\ \text{negative distance if } X_i \text{ classified incorrectly} \end{cases}$

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How do we express optimal separating hyperplane mathematically?

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$$\text{subject to:} \quad \frac{Y_i(X_i^\top \beta + \beta_0)}{\|\beta\|} \geq M \qquad \text{for } i = 1, \ldots, N.$$

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Same decision boundary and margin if we multiply β_0, β by a constant $c > 0$, so we can always choose c such that $\|\beta\| = 1/M$:

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solution achieved by same parameters

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Convex optimization problem: **can solve efficiently!**

- NB We cannot efficiently compute an ERM solution for 0/1-loss in general, but, for separable data, this gives an efficient way to find one of the ERM solutions!

Support Vector Machines

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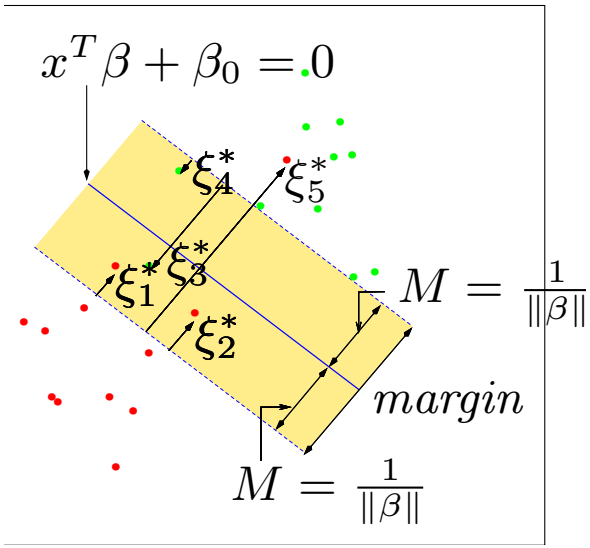

Greek letter "Xi"

Introduce slack variable $\xi_i \geq 0$ for each data point $i = 1, \ldots, N$.

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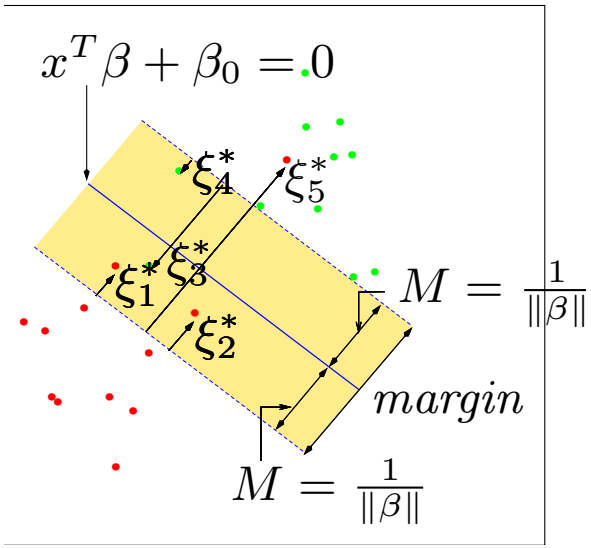

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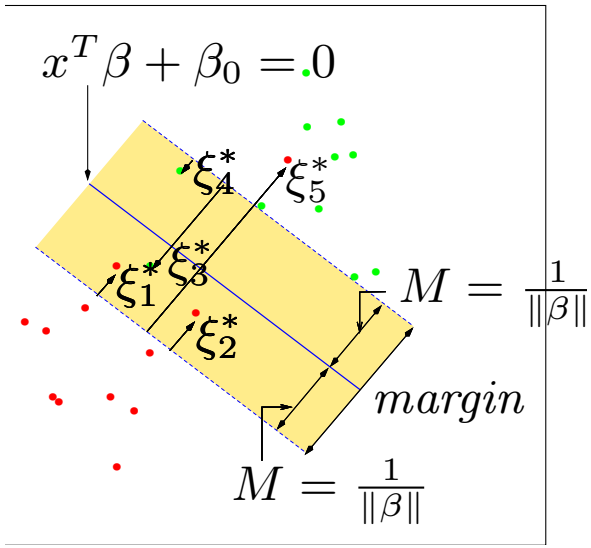

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subject to: $\xi_i \geq 0$, $\dfrac{Y_i(X_i^\top \beta + \beta_0)}{\|\beta\|} \geq M(1 - \xi_i)$ for $i = 1, \ldots, N$

$$\sum_{i=1}^{N} \xi_i \leq t$$

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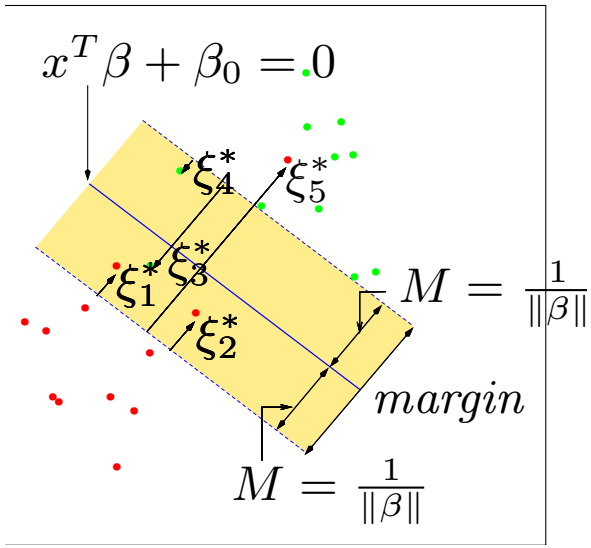

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t is hyperparameter of the algorithm (assume we take large enough to have a solution)

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equivalent: varying t above gives same set of solutions as varying C below

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$$\min_{\beta_0,\beta,\xi_1,\ldots,\xi_N} \quad \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{N} \xi_i$$

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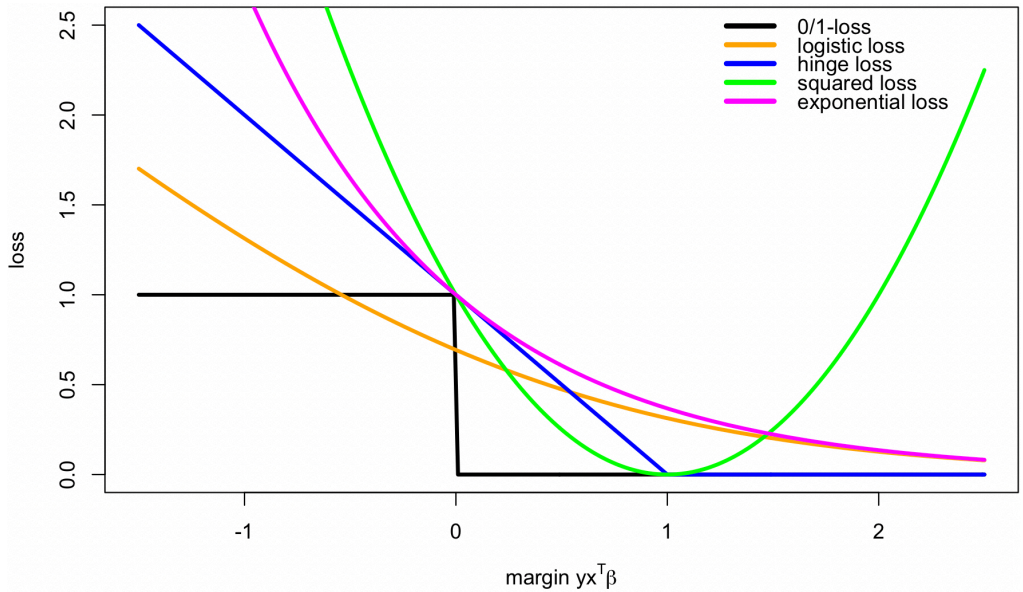
Interpretation as Penalized ERM with Hinge Loss



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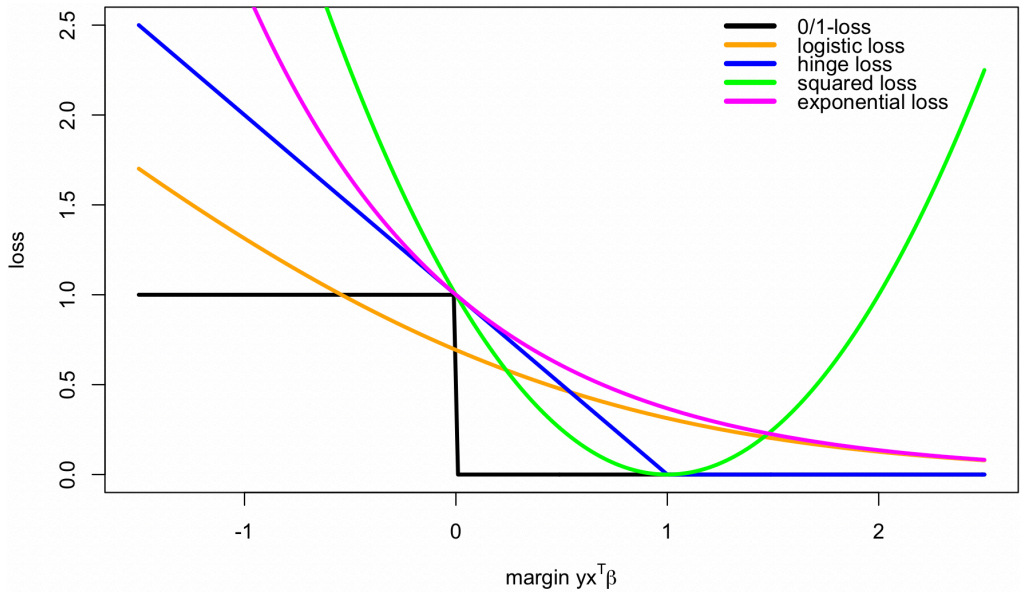

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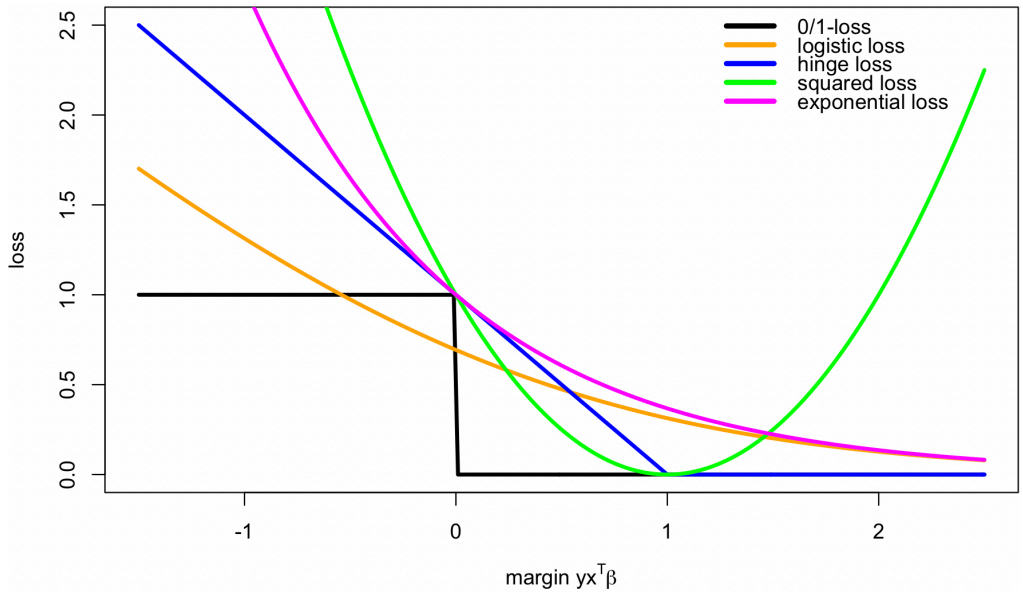

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$$\min_{\beta_0,\beta} \quad \sum_{i=1}^{N} L(Y_i, X_i^\top\beta + \beta_0) + \frac{1}{2C}\|\beta\|^2$$

ERM for hinge loss with ℓ_2-penalty, $\lambda = \frac{1}{2C}$.

Dual Formulation

$$\min_{\alpha_1,\ldots,\alpha_N} \quad \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{N} \alpha_i \alpha_k Y_i Y_k \langle X_i, X_k \rangle$$

$X_i^\top X_k$

subject to: $\quad 0 \leq \alpha_i \leq C \qquad$ for $i = 1, \ldots, N$

$$\sum_{i=1}^{N} \alpha_i Y_i = 0$$

[1] Proof in next lecture

Dual Formulation

$X_i^\top X_k$

$$\min_{\alpha_1,\ldots,\alpha_N} \quad \sum_{i=1}^N \alpha_i - \frac{1}{2}\sum_{i=1}^N\sum_{k=1}^N \alpha_i\alpha_k Y_i Y_k \langle X_i, X_k\rangle$$

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Then solution to ★ is:[1]

$$\hat{\beta} = \sum_{i=1}^N \hat{\alpha}_i Y_i X_i$$

$$\hat{\beta}_0 = Y_i - X_i^\top \hat{\beta} \qquad \text{for any } i \text{ s.t. } 0 < \hat{\alpha}_i < C.$$

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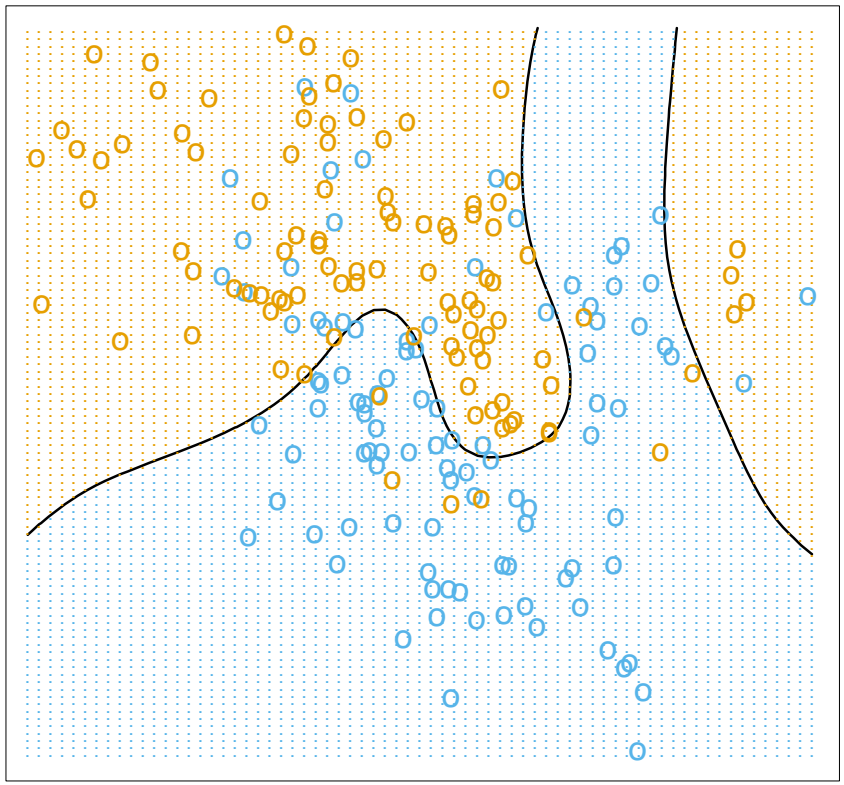
$\hat{\alpha}_i = 0$	for X_i outside margin and correctly classified
$0 < \hat{\alpha}_i < C$	for X_i exactly on margin and correctly classified
$\hat{\alpha}_i = C$	for X_i strictly inside margin or misclassified

[1] Proof in next lecture

Kernel Trick I



How to learn something like this with **linear classifier?**

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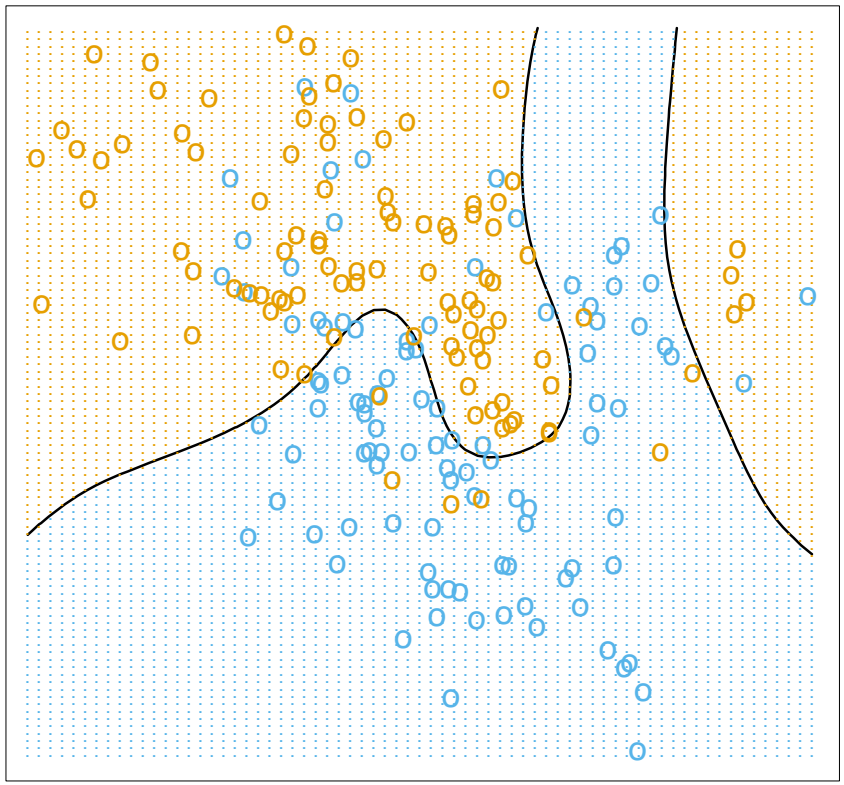
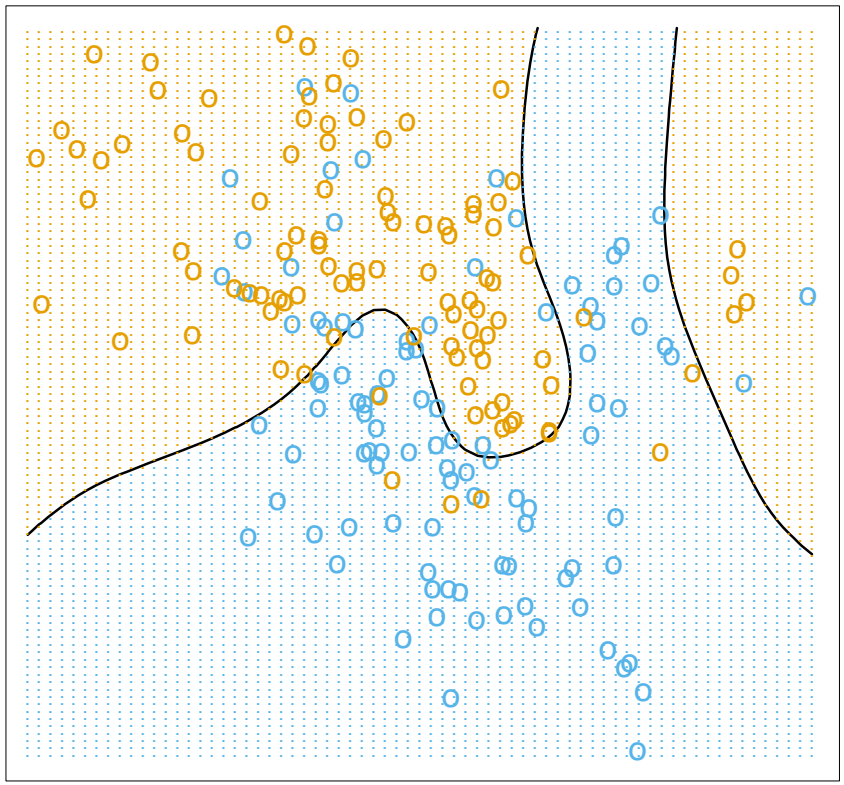


How to learn something like this with **linear classifier?**

Map features X to a larger set of features $h(X)$! For instance,

$$h\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \begin{pmatrix} X_1 \\ X_2 \\ X_1 X_2 \\ X_1^2 \\ X_2^2 \end{pmatrix}$$

Kernel Trick I



How to learn something like this with **linear classifier?**

Map features X to a larger set of features $h(X)$! For instance,

$$h\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \begin{pmatrix} X_1 \\ X_2 \\ X_1 X_2 \\ X_1^2 \\ X_2^2 \end{pmatrix}$$

Then $\langle X_i, X_k \rangle$ in dual formulation becomes $\langle h(X_i), h(X_k) \rangle$.

Kernel Trick II

$$h\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \begin{pmatrix} X_1 \\ X_2 \\ X_1 X_2 \\ X_1^2 \\ X_2^2 \end{pmatrix}$$

Then $\langle X_i, X_k \rangle$ in dual formulation becomes $\langle h(X_i), h(X_k) \rangle$.

Kernel Trick II

$$h\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \begin{pmatrix} X_1 \\ X_2 \\ X_1X_2 \\ X_1^2 \\ X_2^2 \end{pmatrix}$$

Then $\langle X_i, X_k \rangle$ in dual formulation becomes $\langle h(X_i), h(X_k) \rangle$.

Kernel Trick: Do not need to specify h, only need to know the **kernel function**

$$K(X_i, X_k) = \langle h(X_i), h(X_k) \rangle \tag{1}$$

$h(X)$ may even be infinite-dimensional!

Kernel Trick II

$$h\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \begin{pmatrix} X_1 \\ X_2 \\ X_1X_2 \\ X_1^2 \\ X_2^2 \end{pmatrix}$$

Then $\langle X_i, X_k \rangle$ in dual formulation becomes $\langle h(X_i), h(X_k) \rangle$.

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$h(X)$ may even be infinite-dimensional!

- Measure of similarity: larger if X_i and X_k more similar

Kernel Trick II

$$h\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \begin{pmatrix} X_1 \\ X_2 \\ X_1 X_2 \\ X_1^2 \\ X_2^2 \end{pmatrix}$$

Then $\langle X_i, X_k \rangle$ in dual formulation becomes $\langle h(X_i), h(X_k) \rangle$.

Kernel Trick: Do not need to specify h, only need to know the **kernel function**

$$K(X_i, X_k) = \langle h(X_i), h(X_k) \rangle \tag{1}$$

$h(X)$ may even be infinite-dimensional!

- Measure of similarity: larger if X_i and X_k more similar
- Would be computationally nice if this were a simple function...
- ... so turn things around and **start by defining** $K(X_i, X_k)$; then find h to satisfy (1)!

Kernel Function

Examples:

- Degree d polynomial: $K(X, X') = \left(1 + \langle X, X' \rangle\right)^d$
  - E.g. the case of $d = 2$ and $X \in \mathbb{R}^2$ corresponds to:

$$h(X) = \begin{pmatrix} 1 \\ \sqrt{2}X_1 \\ \sqrt{2}X_2 \\ X_1^2 \\ X_2^2 \\ \sqrt{2}X_1X_2 \end{pmatrix}$$

Kernel Function

Examples:

- Degree d polynomial: $K(X, X') = \left(1 + \langle X, X' \rangle\right)^d$
- Radial basis: $K(X, X') = e^{-\gamma \|X - X'\|^2}$ for $\gamma > 0$
- Neural network: $K(X, X') = \tanh\left(a\langle X, X' \rangle + b\right)$ for $a > 0, b \in \mathbb{R}$, $\tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$

Kernel Function

Examples:

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If K satisfies certain **technical conditions** (symmetric, positive definite), then there always exists some mapping h s.t.

$$K(X_i, X_k) = \langle h(X_i), h(X_k) \rangle.$$

Kernel Function

Examples:

- Degree d polynomial: $K(X, X') = \left(1 + \langle X, X' \rangle\right)^d$
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If K satisfies certain **technical conditions** (symmetric, positive definite), then there always exists some mapping h s.t.

$$K(X_i, X_k) = \langle h(X_i), h(X_k) \rangle.$$

- In general this requires h to map to "infinite-dimensional vectors"
- Details in the homework, where we will represent such vectors as elements of a so-called **reproducing kernel Hilbert space**

Kernel Trick: Classifying a New X

- If h maps X to an "infinite-dimensional vector", then β also becomes infinite-dimensional.
- How do we then compute $f_{\hat{\beta}_0,\hat{\beta}}(X)$ for a new input X?

Kernel Trick: Classifying a New X

- If h maps X to an "infinite-dimensional vector", then β also becomes infinite-dimensional.
- How do we then compute $f_{\hat{\beta}_0,\hat{\beta}}(X)$ for a new input X?

Classifying a new X:

$$\begin{aligned} f_{\hat{\beta}_0,\hat{\beta}}(X) &= \langle h(X), \hat{\beta} \rangle + \hat{\beta}_0 \\ &= \langle h(X), \sum_{i=1}^{N} \hat{\alpha}_i Y_i h(X_i) \rangle + \hat{\beta}_0 \\ &= \sum_{i=1}^{N} \hat{\alpha}_i Y_i \langle h(X), h(X_i) \rangle + \hat{\beta}_0 \\ &= \sum_{i=1}^{N} \hat{\alpha}_i Y_i K(X, X_i) + \hat{\beta}_0 \end{aligned}$$

Again no need to compute h, only need to know kernel function!

Support Vector Machines in Action

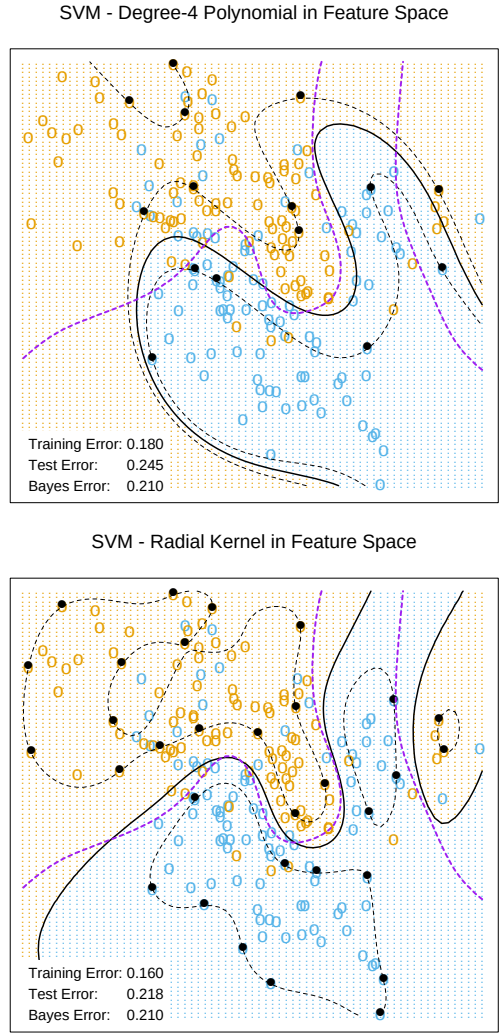

FIGURE 12.3. *Two nonlinear SVMs for the mixture data. The upper plot uses a 4th degree polynomial*

To be continued next week!

- I still owe you a derivation for the relation between $\star$ and the dual formulation
- This will require additional background on convex optimization