CS446 Introduction to Machine Learning (Fall 2013)
University of Illinois at Urbana-Champaign
http://courses.engr.illinois.edu/cs446

LECTURE 11: LARGE MARGIN CLASSIFIERS

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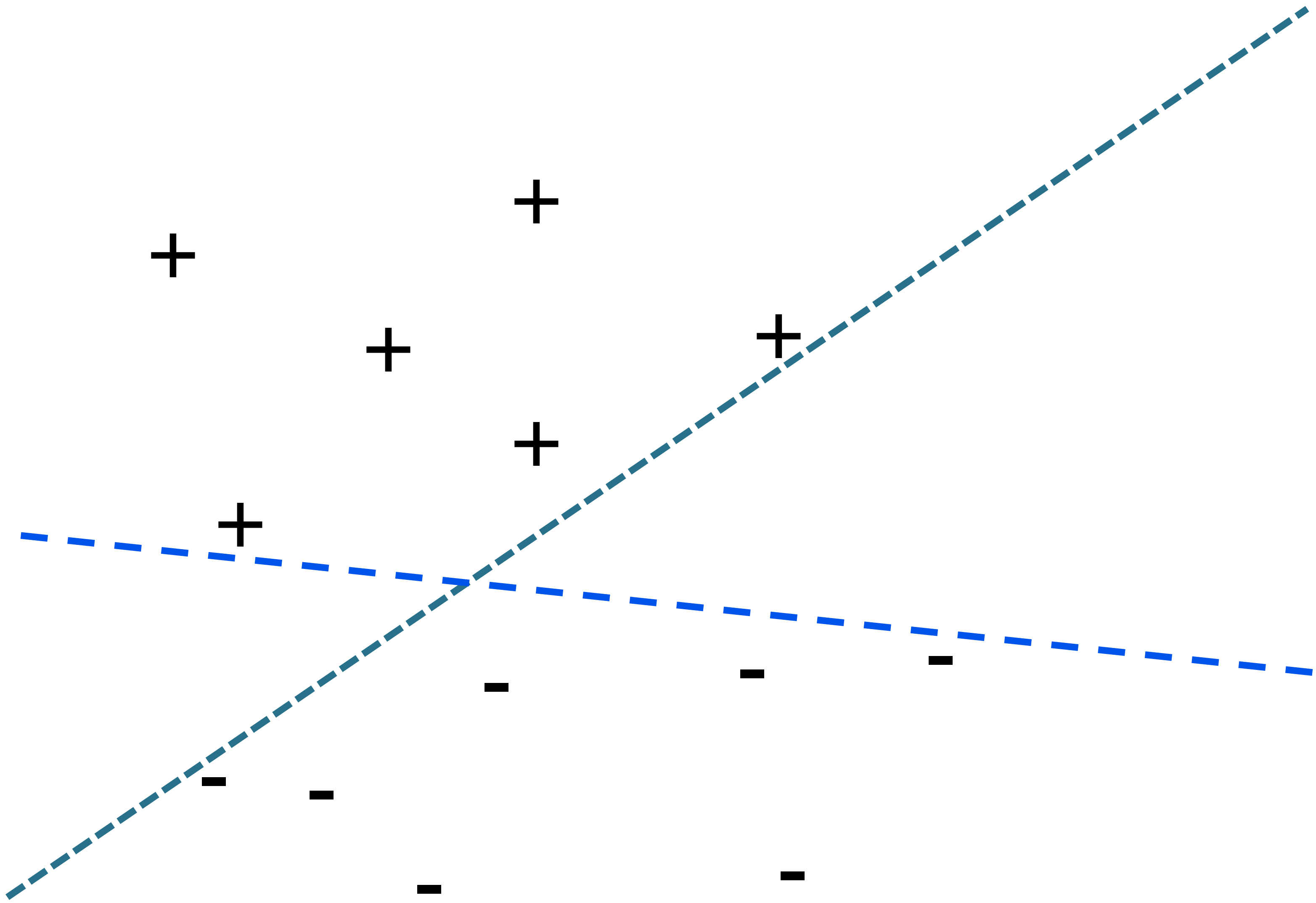
Large margin classifiers

What's the best separating hyperplane?



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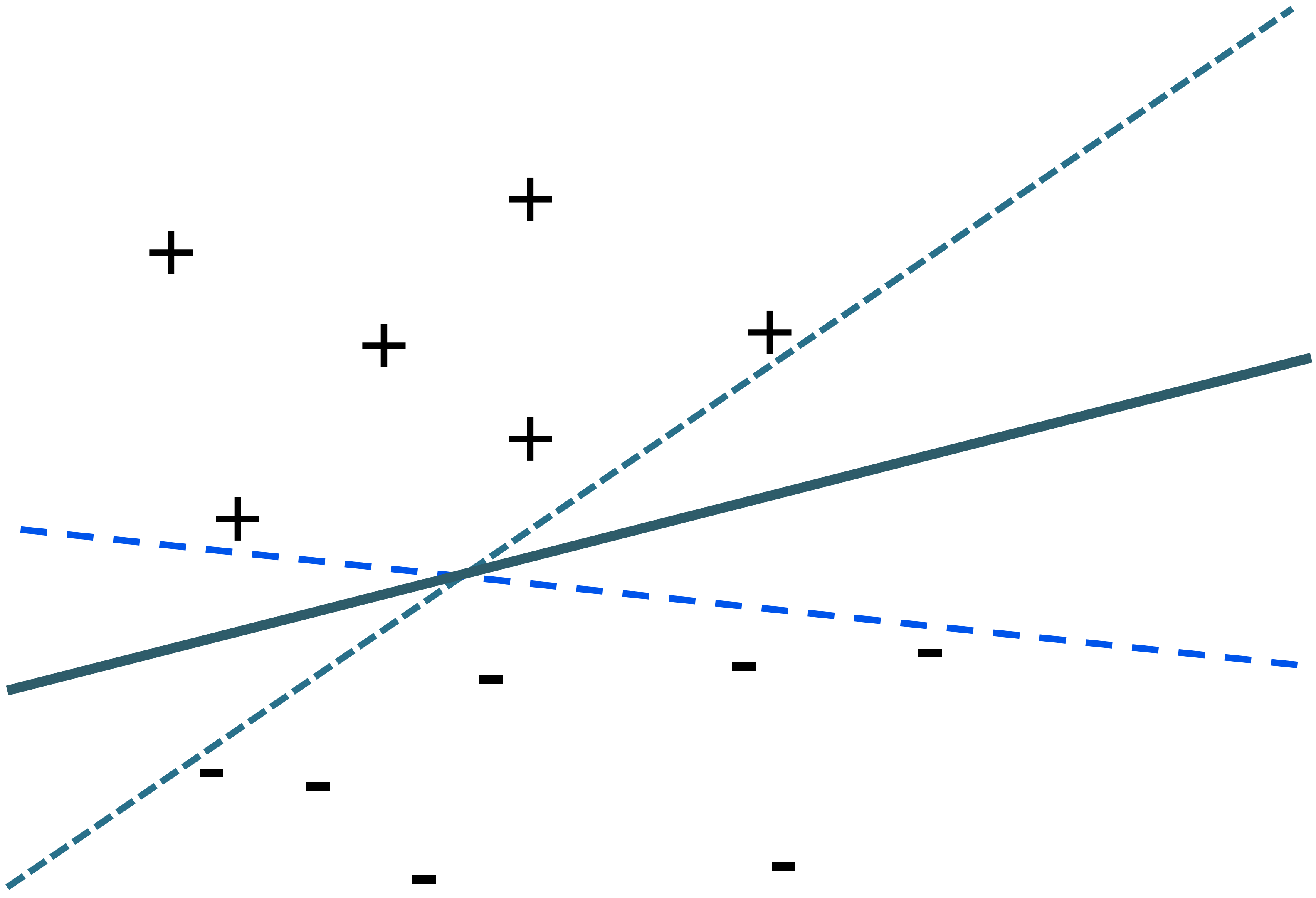
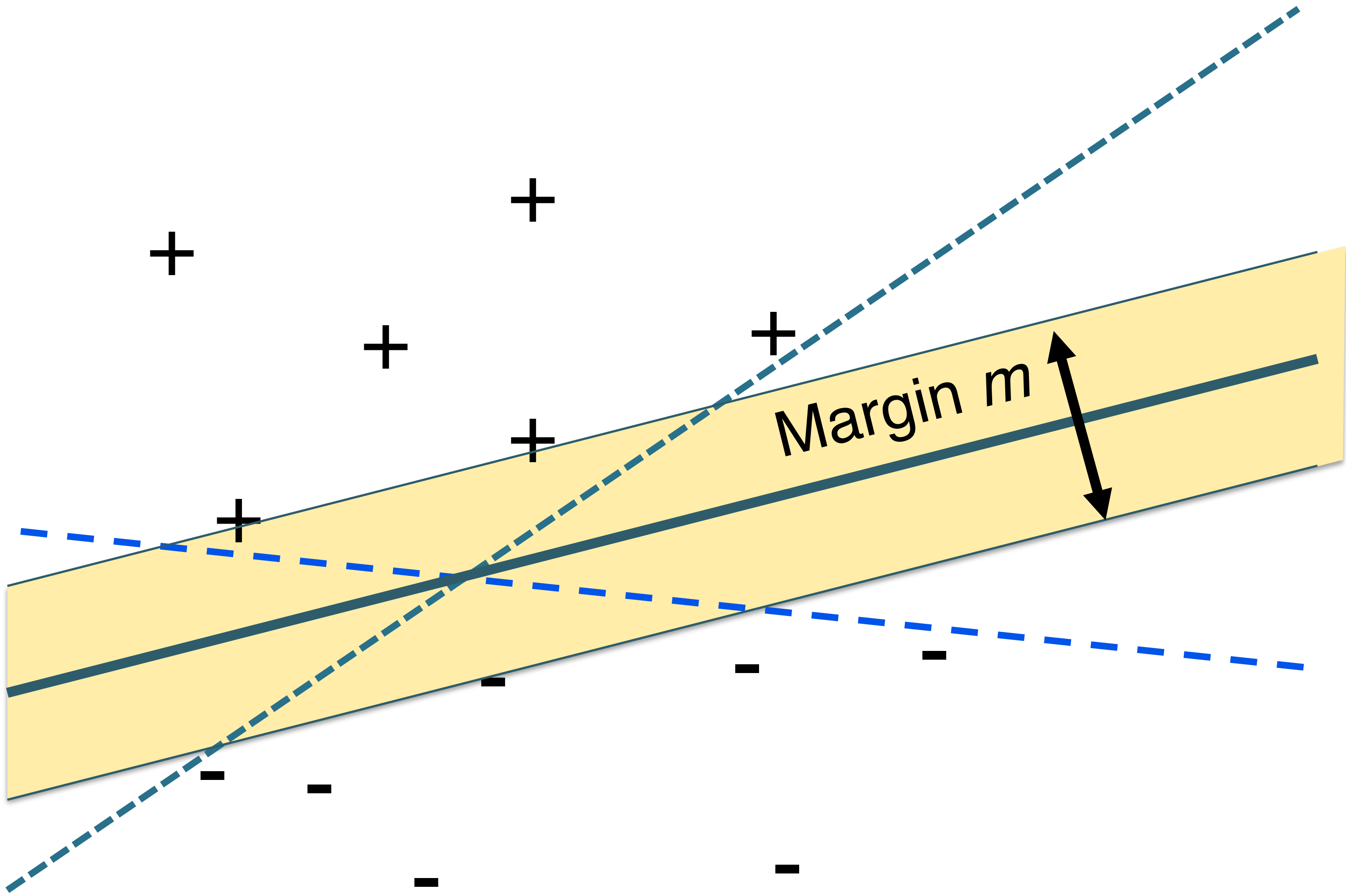
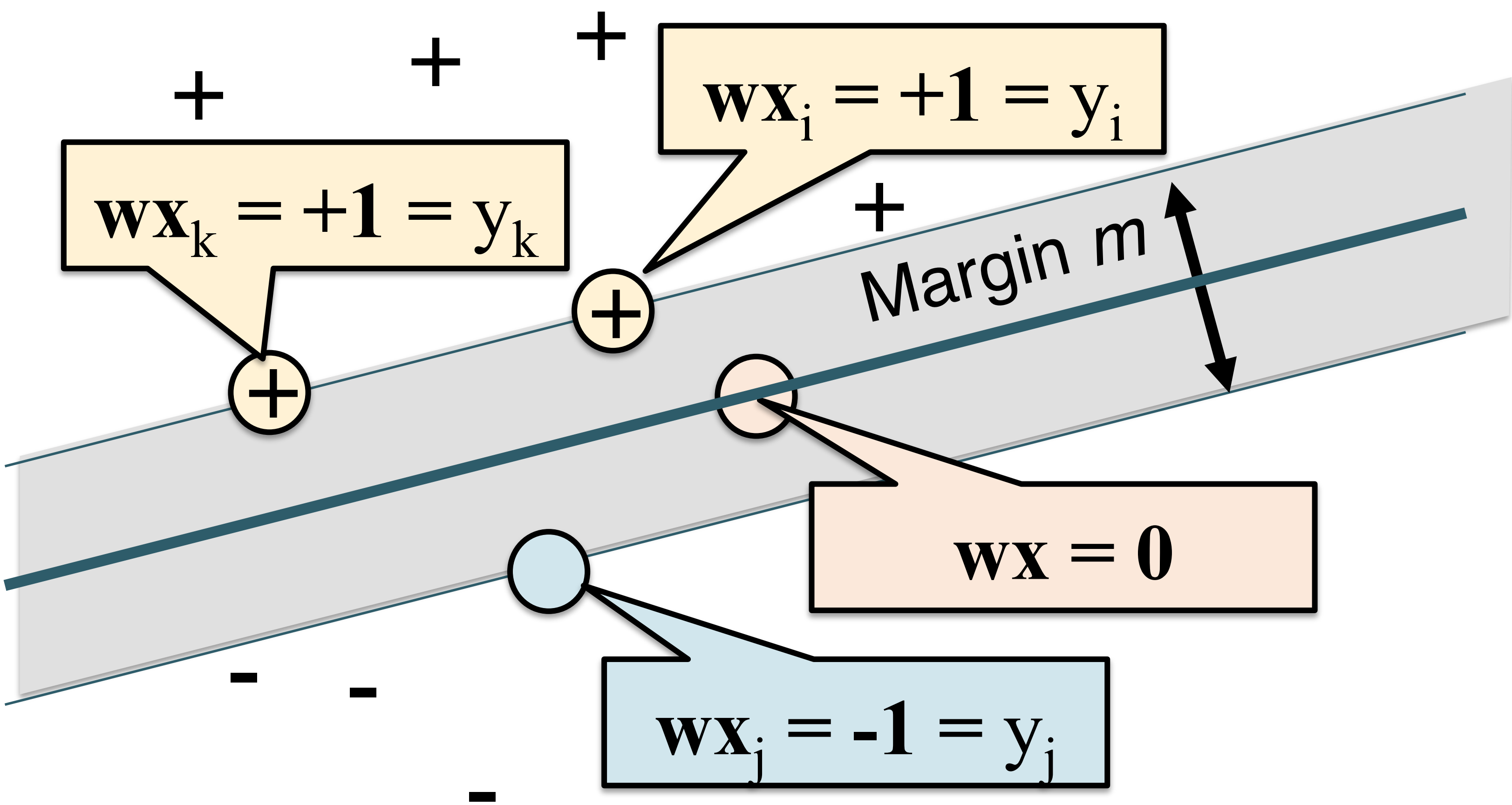


What's the best separating hyperplane?

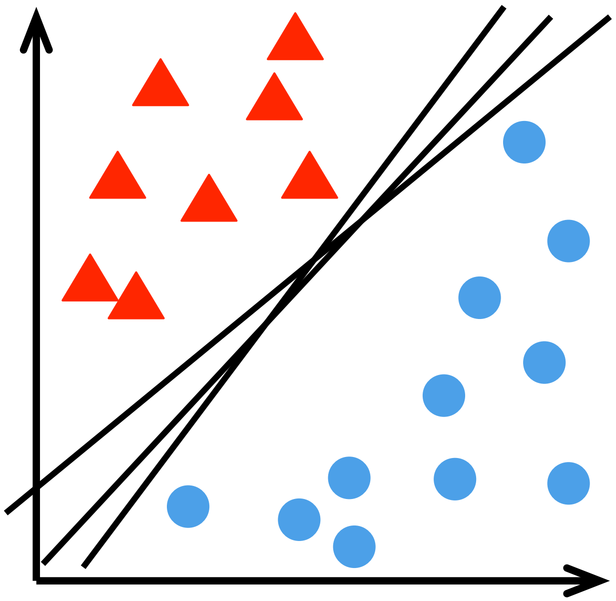


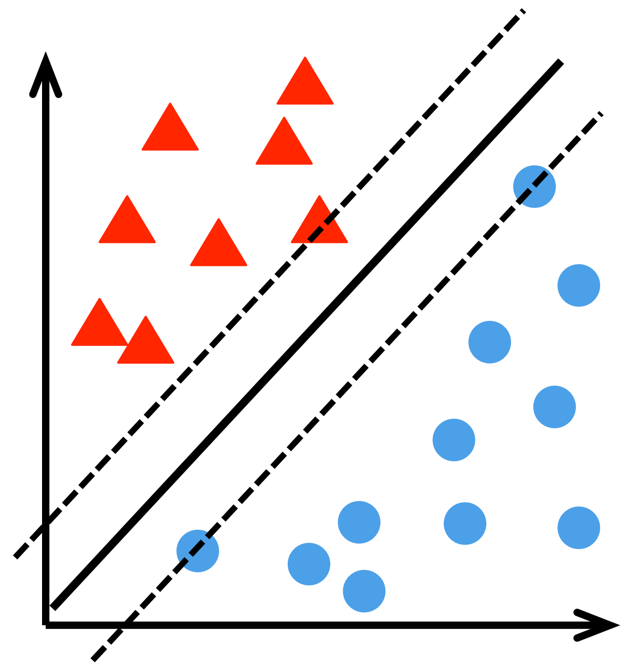
The maximum margin decision boundary



Margins

Maximum margin classifiers





Maximum margin classifier

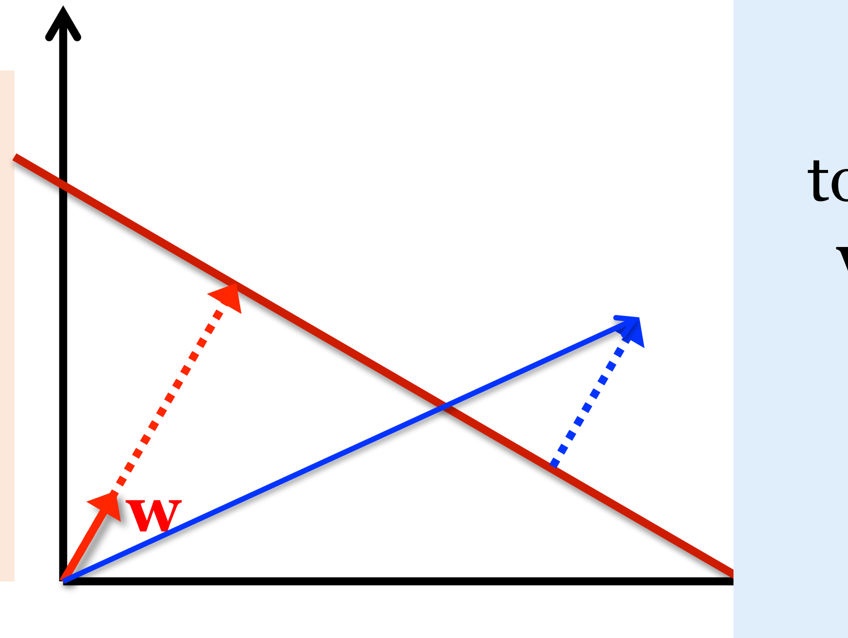
We want to find the classifier whose decision boundary is furthest away from any data point. (this classifier has the largest margin).

This additional requirement (*bias)* reduces the *variance* (i.e. reduces overfitting).

Margins

Distance of hyperplane $\mathbf{w}\mathbf{x} + b = 0$ to origin:

$$\frac{-b}{\|\mathbf{w}\|}$$



Absolute distance of point $\mathbf{x}$ to hyperplane $\mathbf{w}\mathbf{x} + b = 0$:

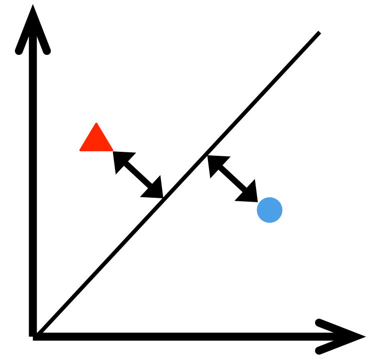
$$\frac{|\mathbf{w}\mathbf{x} + b|}{\|\mathbf{w}\|}$$

Decision boundary:

Hyperplane with $f(\mathbf{x}) = 0$

i.e. $\mathbf{w}\mathbf{x} + b = 0$

Margin



If the data are linearly separable,

$y^{(i)}(\mathbf{w}\mathbf{x}^{(i)} + b) > 0$

Euclidean distance of $\mathbf{x}^{(i)}$ to the decision boundary:

$$\frac{y^{(i)} f(\mathbf{x}^{(i)})}{\|\mathbf{w}\|} = \frac{y^{(i)}(\mathbf{w}\mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|}$$

Functional vs. Geometric margin

Geometric margin (Euclidean distance) of hyperplane $\mathbf{w}\mathbf{x} + b = 0$ to point $\mathbf{x}^{(i)}$:

$$\frac{y^{(i)} f(\mathbf{x}^{(i)})}{\|\mathbf{w}\|} = \frac{y^{(i)}(\mathbf{w}\mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|}$$

Functional margin of hyperplane $\mathbf{w}\mathbf{x} + b = 0$ to point $\mathbf{x}^{(i)}$:

$$\gamma = y^{(i)} \, \mathrm{f}(\mathbf{x}^{(i)})$$

i.e. $\gamma = y^{(i)} \, (\mathbf{w}\mathbf{x}^{(i)} + b)$

Rescaling **w** and *b*

Rescaling **w** and b by a factor k to $k\boldsymbol{w}$ and kb
does not change the geometric margin
(Euclidean distance):

$$\frac{y^{(i)}(\mathbf{w}\mathbf{x}^{(i)}+b)}{\|\mathbf{w}\|} = \frac{y^{(i)}\left(\sum_n w_n x_n^{(i)} + b\right)}{\sqrt{\sum_n w_n w_n}} = \frac{k y^{(i)}\left(\sum_n w_n x_n^{(i)} + b\right)}{k\sqrt{\sum_n w_n w_n}}$$

$$= \frac{y^{(i)}\left(\sum_n k w_n x_n^{(i)} + kb\right)}{\sqrt{\sum_n k w_n k w_n}} = \frac{y^{(i)}(k\mathbf{w}\mathbf{x}^{(i)}+kb)}{\|k\mathbf{w}\|}$$

Rescaling **w** and *b*

- Rescaling **w** and b by a factor k changes the functional margin γ by a factor k:

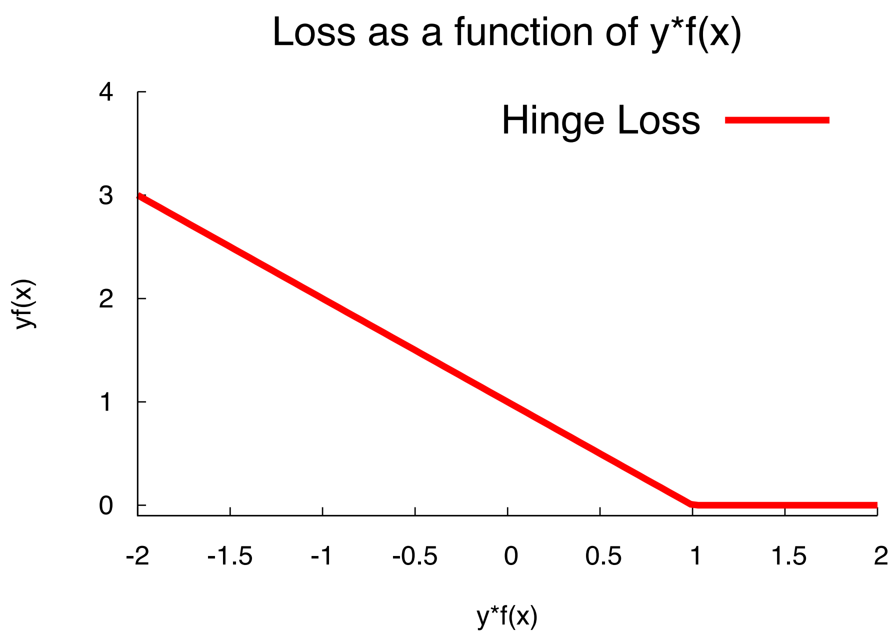
$$\gamma = y^{(i)}\,(\mathbf{w}\mathbf{x}^{(i)} + b)$$

$$k\gamma = y^{(i)}\,(k\mathbf{w}\mathbf{x}^{(i)} + kb)$$

- The point that is closest to the decision boundary has functional margin γ_{min}
- **w** and b can be rescaled so that $\gamma_{min} = 1$
- When learning **w** and b, we can set $\gamma_{min} = 1$ (and still get the same decision boundary)

Hinge loss

$$L(y, f(\mathbf{x})) = \max(0, 1 - yf(\mathbf{x}))$$



Perceptron with margin

Perceptron with Margin

Standard Perceptron update:

Update **w** if $y_m \cdot \mathbf{w} \cdot \mathbf{x_m} < 0$

Perceptron with Margin update:

Define a functional margin $\gamma > 0$

Update **w** if $y_m \cdot \mathbf{w} \cdot \mathbf{x_m} < \gamma$

Support Vector Machines

The maximum margin decision boundary…

… is defined by two parallel hyperplanes:

– one that goes through the **positive** data points ($y_j = +1$) that are closest to the decision boundary, and

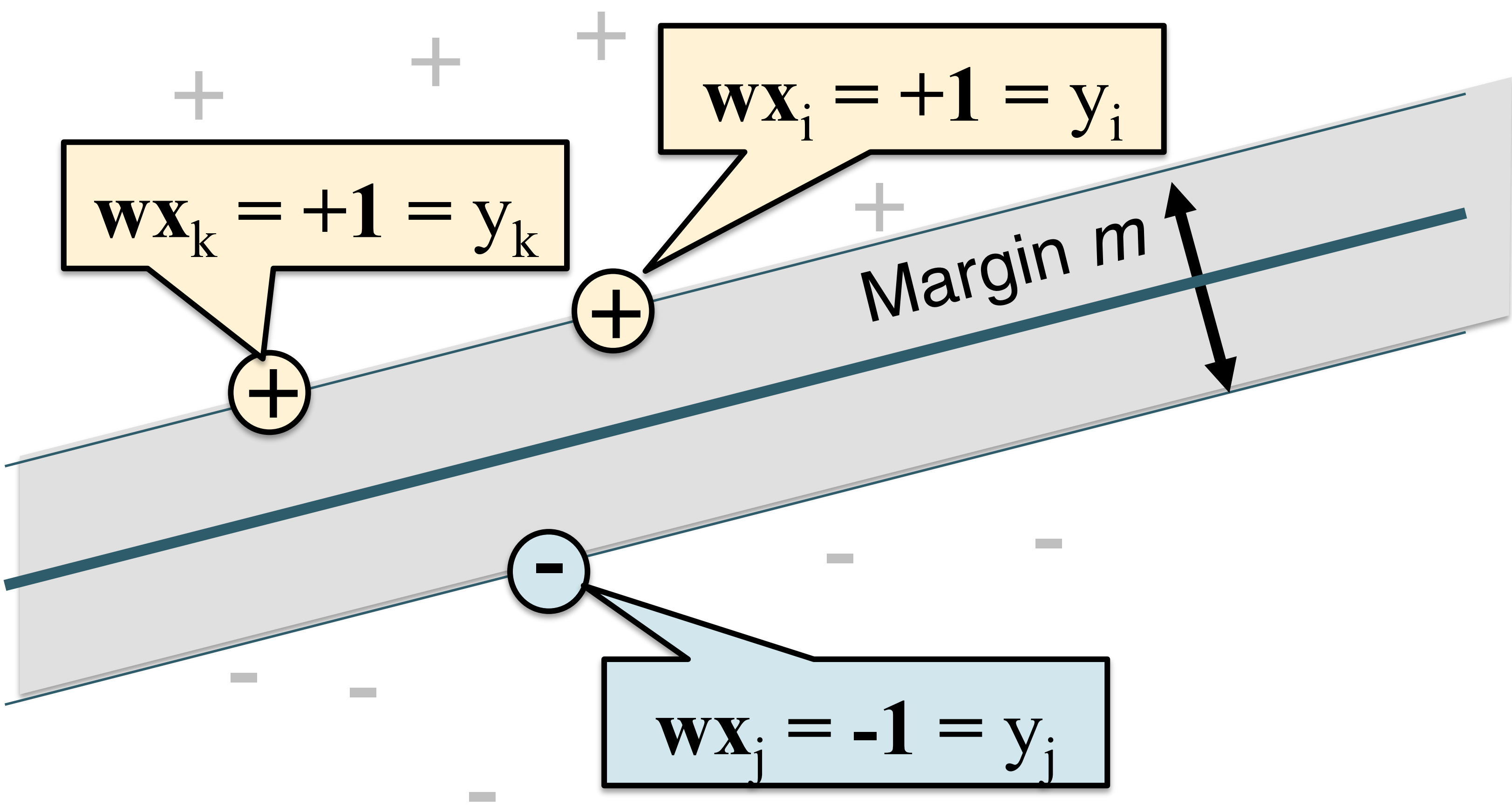
– one that goes through the **negative** data points ($y_j = -1$) that are closest to the decision boundary.

Support vectors

We can express the separating hyperplane in terms of the data points $\mathbf{x}_j$ closest to the decision boundary.

These data points are called the **support vectors.**

Support vectors



Perceptrons and SVMs: Differences in notation

Perceptrons:

- Weight vector has bias term w_0 (x_0 = dummy value 1)
- Decision boundary: $\mathbf{wx} = 0$

SVMs/Large Margin classifiers:

- Explicit bias term b; weight vector $\mathbf{w} = (w_1 \ldots w_n)$
- Decision boundary $\mathbf{wx} + b = 0$

Support Vector Machines

The functional margin of the data for (**w**, b) is determined by the points closest to the hyperplane

$$\gamma_{\min} = \min_n \left[y^{(n)} (\mathbf{wx}^{(n)} + b) \right]$$

Distance of $\mathbf{x}^{(n)}$ to hyperplane $\mathbf{wx} = 0$: $\dfrac{|\mathbf{wx} + b|}{\|\mathbf{w}\|}$

Learn **w** in an SVM = maximize the margin:

$$\underset{\mathbf{w},\, b}{\operatorname{argmax}} \left\{ \frac{1}{\|\mathbf{w}\|} \min_n \left[y^{(n)} (\mathbf{wx} + b) \right] \right\}$$

Support Vector Machines

Learn **w** in an SVM = maximize the margin:

$$\underset{\mathbf{w},\, b}{\operatorname{argmax}} \left\{ \frac{1}{\|\mathbf{w}\|} \min_{n} \left[y^{(n)} (\mathbf{w}\mathbf{x} + b) \right] \right\}$$

This is difficult to optimize.
Let's convert it to an equivalent problem that is easier.

Support Vector Machines

Learn $\mathbf{w}$ in an SVM = maximize the margin:

$$\underset{\mathbf{w},\, b}{\operatorname{argmax}} \left\{ \frac{1}{\|\mathbf{w}\|} \min_{n} \left[y^{(n)} (\mathbf{w}\mathbf{x} + b) \right] \right\}$$

Easier equivalent problem:

- We can always rescale $\mathbf{w}$ and b without affecting Euclidian distances.
- This allows us to set the functional margin to 1: $\min_n(y^{(n)}(\mathbf{w}\mathbf{x}^{(n)} + b) = 1$

Support Vector Machines

Learn **w** in an SVM = maximize the margin:

$$\underset{\mathbf{w},\, b}{\operatorname{argmax}} \left\{ \frac{1}{\|\mathbf{w}\|} \min_{n} \left[y^{(n)} (\mathbf{wx} + b) \right] \right\}$$

Easier equivalent problem: a quadratic program

- Setting $\min_n (y^{(n)}(\mathbf{wx}^{(n)} + b) = 1$ implies $(y^{(n)}(\mathbf{wx}^{(n)} + b) \geq 1$ for all n
- argmax(1/**ww**)= argmin(**ww**) = argmin(1/2·**ww**)

$$\underset{\mathbf{w}}{\operatorname{argmin}} \frac{1}{2} \mathbf{w} \cdot \mathbf{w}$$
$$\textit{subject to}$$
$$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1 \;\; \forall i$$

The primal representation

The data items $\mathbf{x} = (x_1 \ldots x_n)$ have n features
The weight vector $\mathbf{w} = (w_1 \ldots w_n)$ has n elements

Learning:

Find a weight w_j for each feature x_j

Classification:

Evaluate $\mathbf{wx}$

The dual representation

$$\mathbf{w} = \sum_j \alpha_j \mathbf{x}_j$$

Learning:

Find a weight α_j (≥ 0) for each data point $\mathbf{x}_j$

This requires computing the inner product $\mathbf{x}_i\mathbf{x}_j$ between all data items $\mathbf{x}_i$ and $\mathbf{x}_j$

Support vectors = the set of data points $\mathbf{x}_j$ with non-zero weights α_j

Classifying test data with SVM

In the primal:

Compute inner product between weight vector and test item

$$\mathbf{wx} = \langle \mathbf{w}, \mathbf{x} \rangle$$

In the dual:

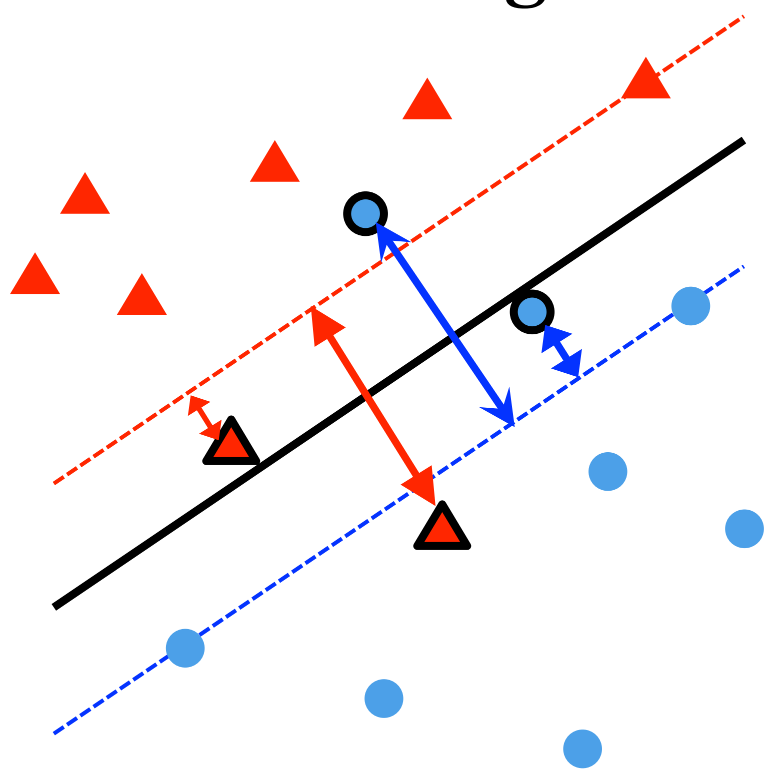
Compute inner product between support vectors and test item

$$\mathbf{wx} = \langle \mathbf{w}, \mathbf{x} \rangle = \langle \textstyle\sum_j \alpha_j x_j, \mathbf{x} \rangle = \textstyle\sum_j \alpha_j \langle x_j, \mathbf{x} \rangle$$

Hard vs. soft margins

Dealing with outliers: Slack variables ξ_i

ξ_i measures by how much example $(\mathbf{x}_i, y_i)$ fails to achieve margin δ



Dealing with outliers: Slack variables ξ_i

If $\mathbf{x}_i$ is on correct side of the margin:

$\xi_i = 0$

otherwise

$\xi_i = |y_i - \mathbf{w}\mathbf{x}_i|$

If $\xi_i = 1$: $\mathbf{x}_i$ is on the decision boundary $\mathbf{w}\mathbf{x}_i = 0$

If $\xi_i > 1$: $\mathbf{x}_i$ is misclassified

Replace $y^{(n)}(\mathbf{w}\mathbf{x}^{(n)} + b) \geq 1$ (hard margin)

with $y^{(n)}(\mathbf{w}\mathbf{x}^{(n)} + b) \geq 1 - \xi^{(n)}$ (soft margin)

Soft margins

$$\underset{\mathbf{w}}{\operatorname{argmin}} \frac{1}{2}\mathbf{w}\cdot\mathbf{w} + C\sum_{i=1}^{n}\xi_i$$

$$\textit{subject to}$$

$$\xi_i \geq 0 \quad \forall i$$

$$y_i(\mathbf{w}\cdot\mathbf{x}_i + b) \geq (1-\xi_i)\,\forall i$$

ξ_i (slack): how far off is $\mathbf{x}_i$ from the margin?

C (cost): how much do we have to pay for misclassifying $\mathbf{x}_i$

We want to minimize $C\sum_i \xi_i$ and maximize the margin

C controls the tradeoff between margin and training error