# Support Vector Machines

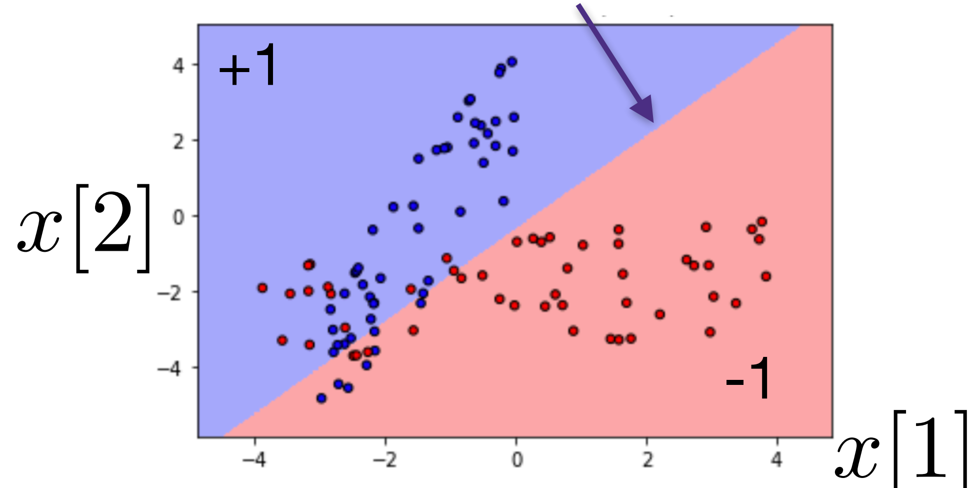
# Logistic regression for binary classification

- Data $\mathscr{D} = \{(x_i \in \mathbb{R}^d, y_i \in \{-1, +1\})\}_{i=1}^n$
- Model: $\hat{y} = x^T w + b$
- Loss function: logistic loss $\ell(\hat{y}, y) = \log(1 + e^{-y\hat{y}})$
- Optimization: solve for

$$(\widehat{b}, \widehat{w}) = \arg\min_{b,w} \sum_{i=1}^{n} \log(1 + e^{-y_i(b + x_i^T w)})$$

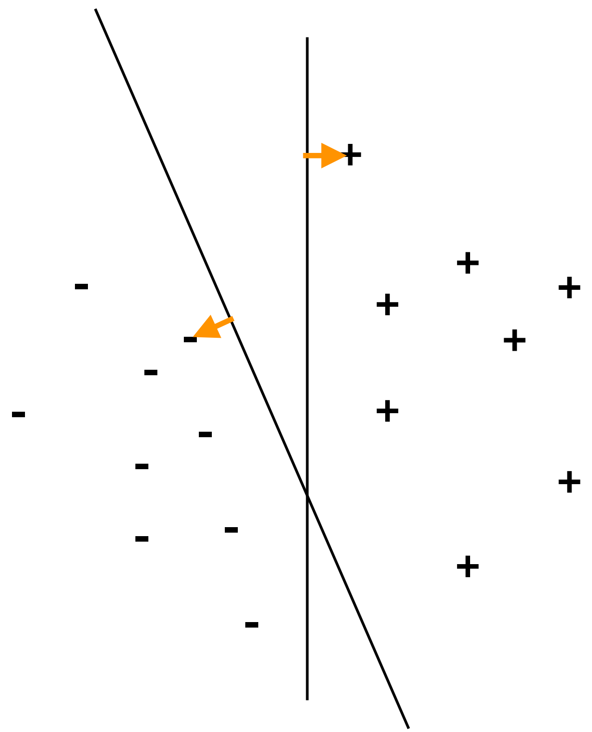
- As this is a **smooth convex** optimization, it can be solved efficiently using gradient descent
- Prediction: $\text{sign}(b + x^T w)$

decision boundary at $w^T x + b = 0$

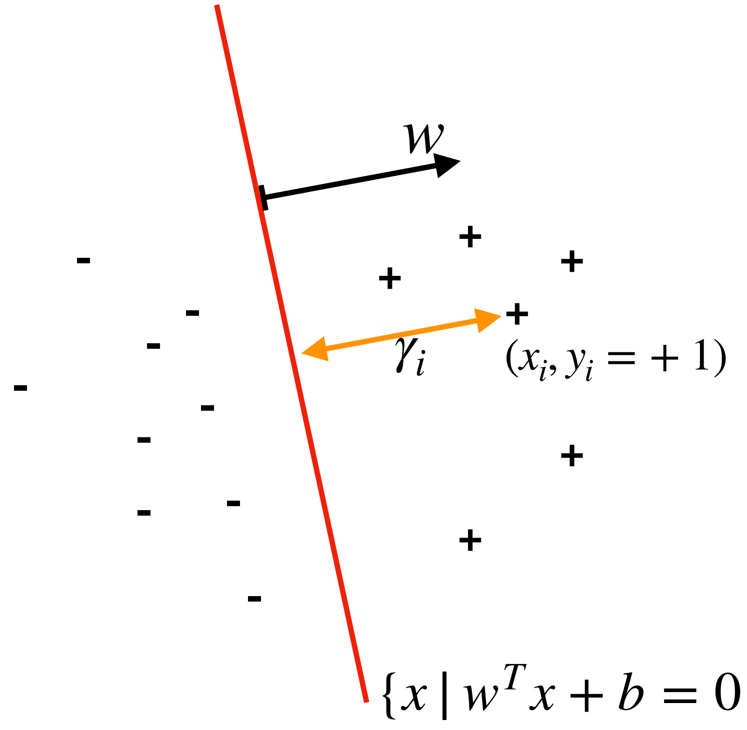


# How do we choose the best linear classifier?

- Informally, **margin** of a set of examples to a decision boundary is the distance to the closest point to the decision boundary
- For linearly separable datasets, **maximum margin** classifier is a natural choice
- Large margin implies that the decision boundary can change without losing accuracy, so the learned model is more robust against new data points



# Geometric margin



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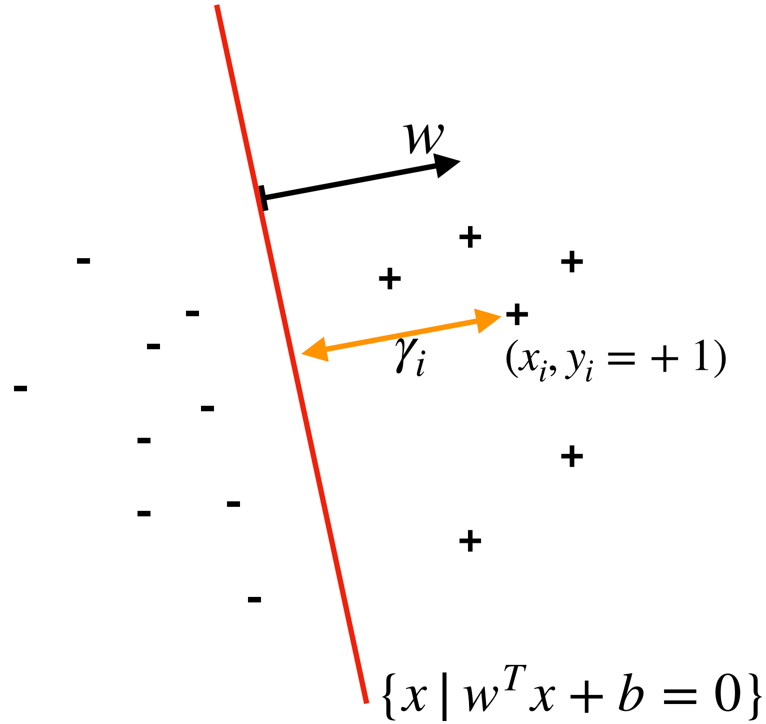

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- Given a set of training examples $\{(x_i, y_i)\}_{i=1}^n$, with $y_i \in \{-1, +1\}$
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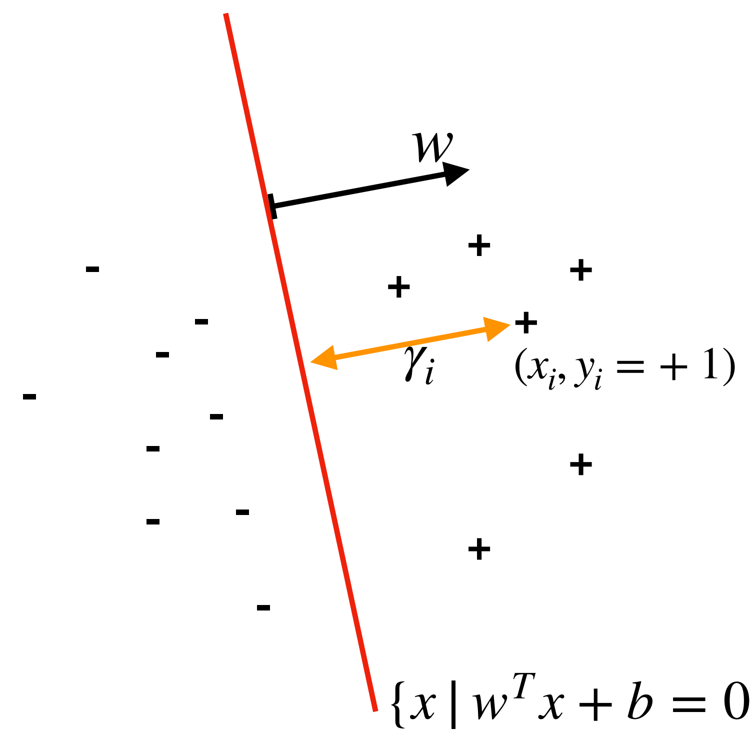

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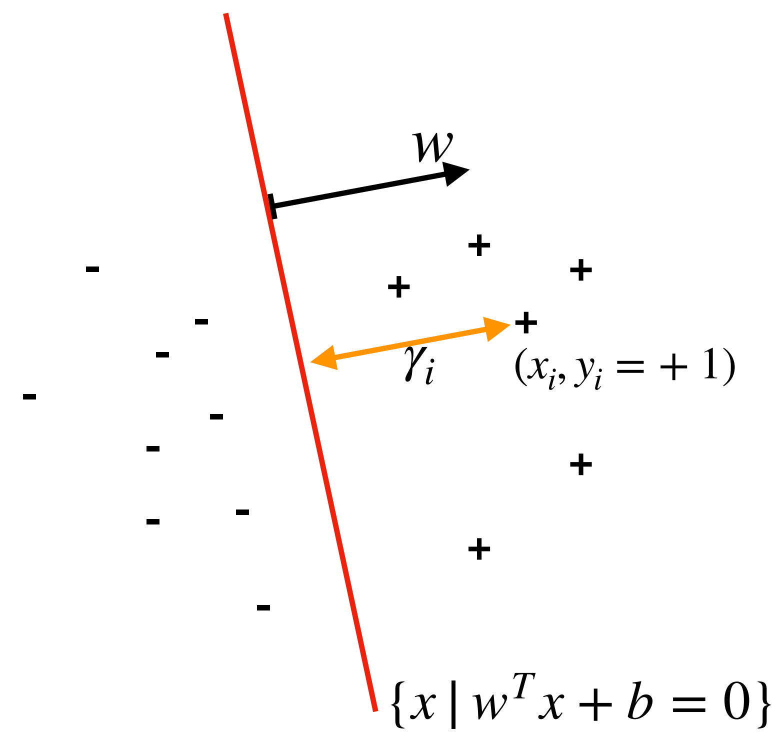
- such that the decision boundary is
  a separating hyperplane $\{x \mid \underbrace{b + w_1 x[1] + w_2 x[2] + \cdots + w_d x[d]}_{w^T x + b} = 0\}$,

  which is the hyperplane orthogonal to $w$ with a shift of $b$



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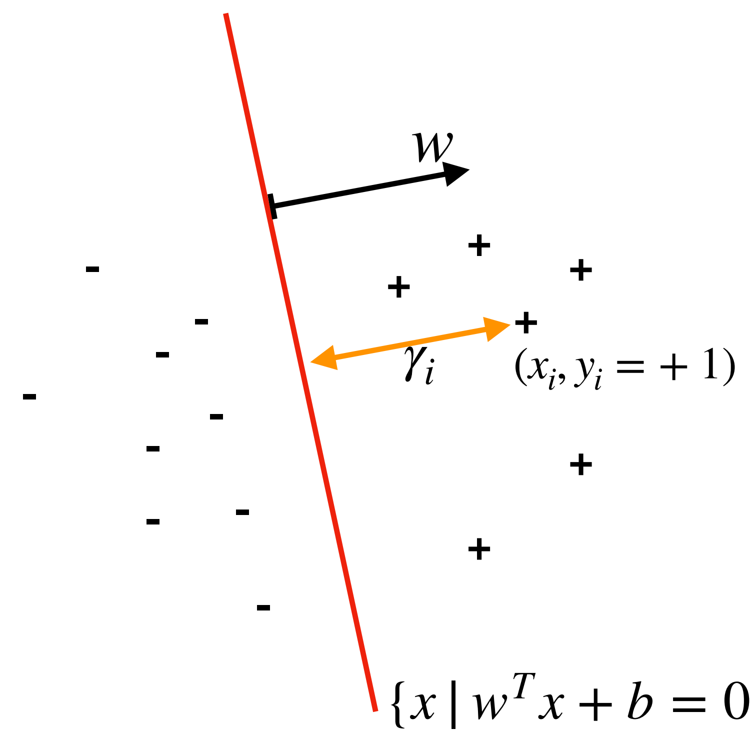
- we define **margin** of $(b, w)$
  with respect to a training example $(x_i, y_i)$ as
  the distance from the point $(x_i, y_i)$ to the
  decision boundary, which is

$$\gamma_i = y_i \frac{(w^T x_i + b)}{\|w\|_2}$$



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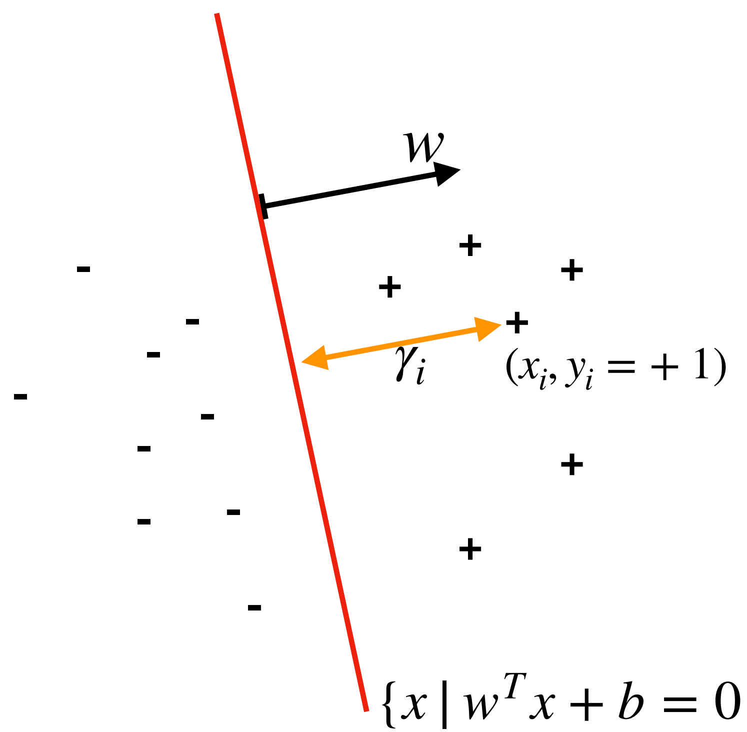
(The proof is on the next slide)



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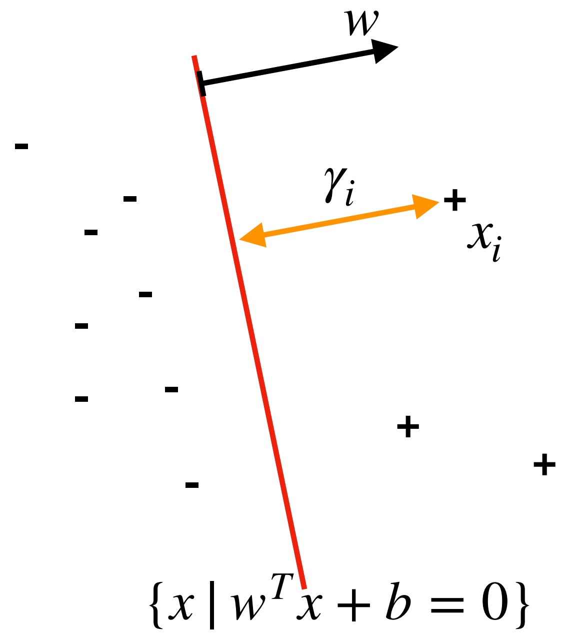
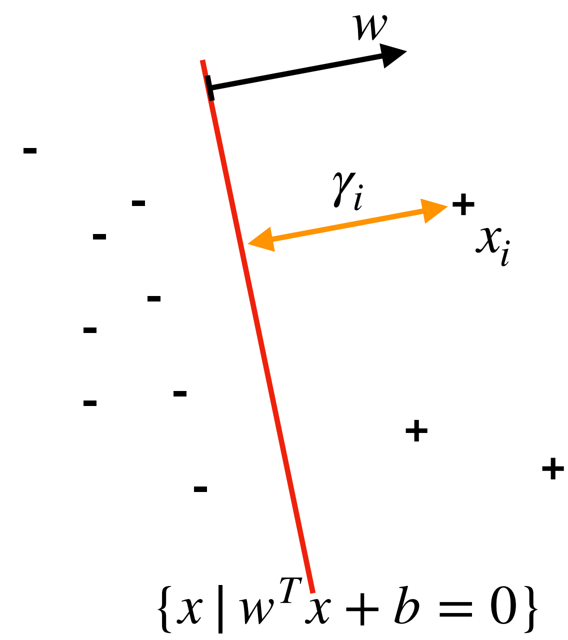


# Geometric margin

- The distance $\gamma_i$ from a hyperplane $\{x \,|\, w^T x + b = 0\}$ to a point $x_i$ can be computed geometrically as follows:



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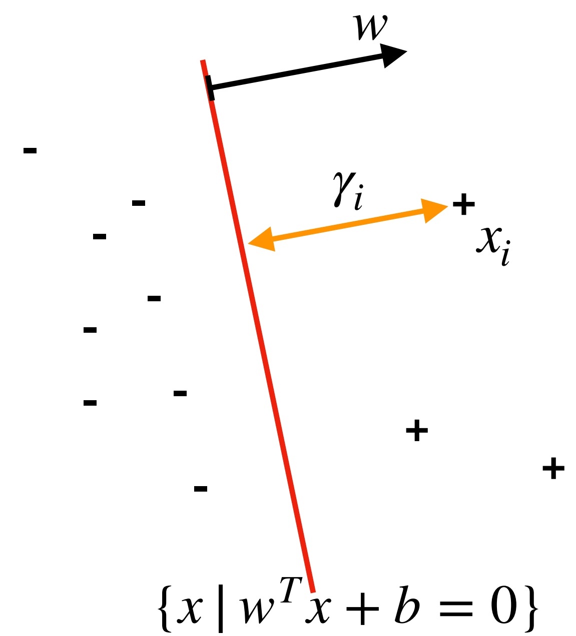
- The distance $\gamma_i$ from a hyperplane $\{x \mid w^T x + b = 0\}$ to a point $x_i$ can be computed geometrically as follows:
- We know that if you move from $x_i$ in the negative direction of $w$ by length $\gamma_i$, you arrive at the line, which can be written as

$$\left( x_i - \frac{w}{\|w\|_2} \gamma_i \right) \text{ is in } \{x \mid w^T x + b = 0\}$$



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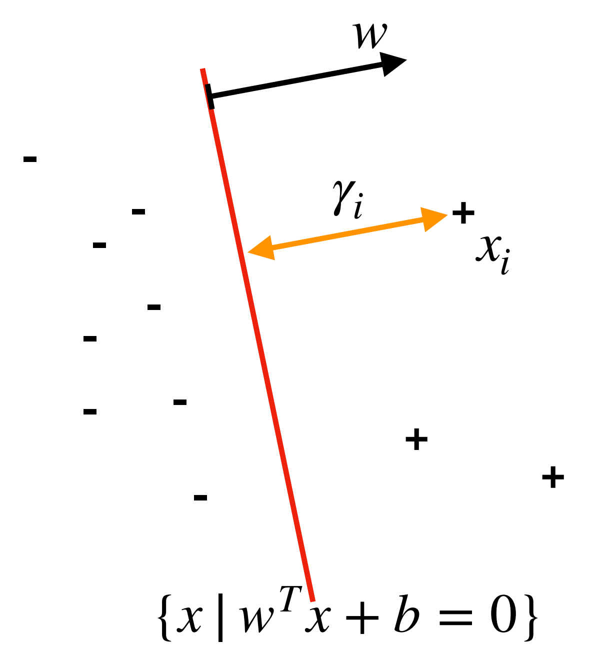



- So we can plug the point in the formula:

$$w^T \left( x_i - \frac{w}{\|w\|_2} \gamma_i \right) + b \;=\; 0$$

which is

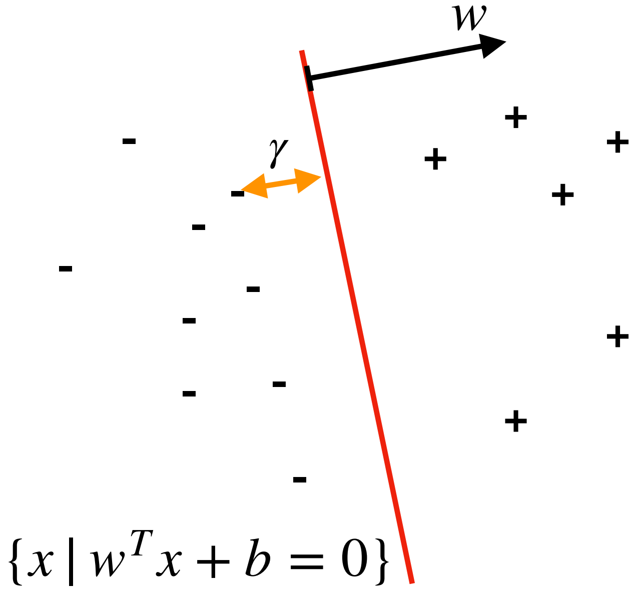
$$w^T x_i - \frac{\|w\|_2^2}{\|w\|_2} \gamma_i + b \;=\; 0$$

and hence

$$\gamma_i \;=\; \frac{w^T x_i + b}{\|w\|_2},$$

We multiply the formula by $y_i$ so that for negative samples we use the opposite direction of $-w$ instead of $w$

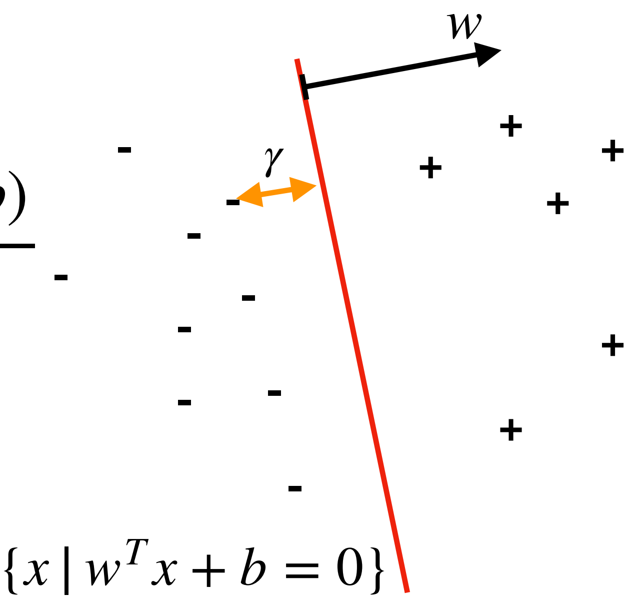
# Maximum margin classifiers



# Maximum margin classifiers

- The **margin** with respect to a set is defined as

$$\gamma = \min_{i \in \{1,\ldots,n\}} \gamma_i = \min_i y_i \frac{(w^T x_i + b)}{\|w\|_2}$$



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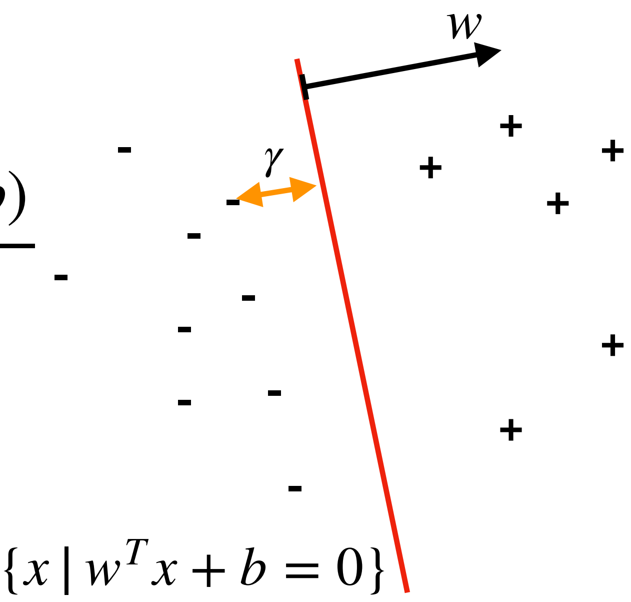

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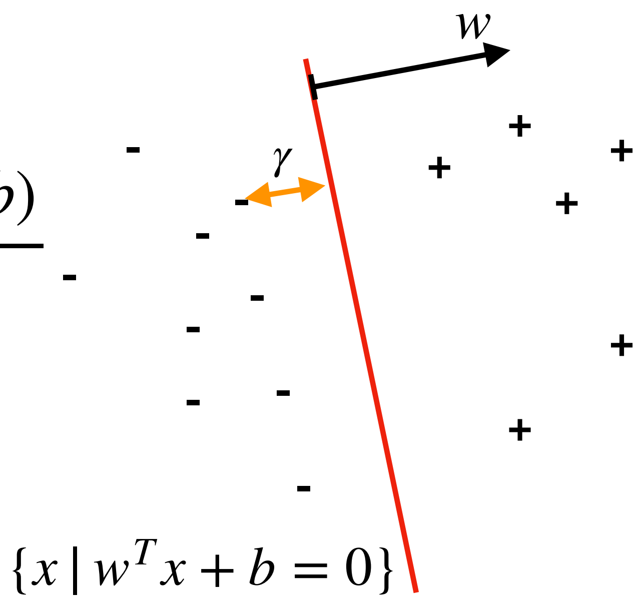


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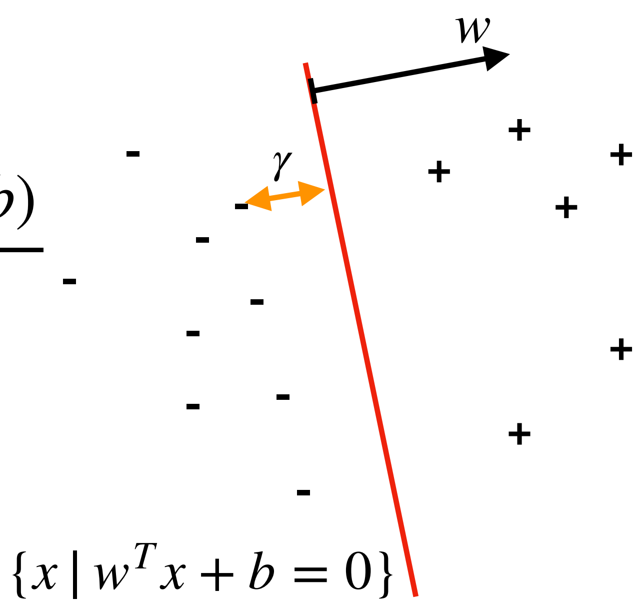


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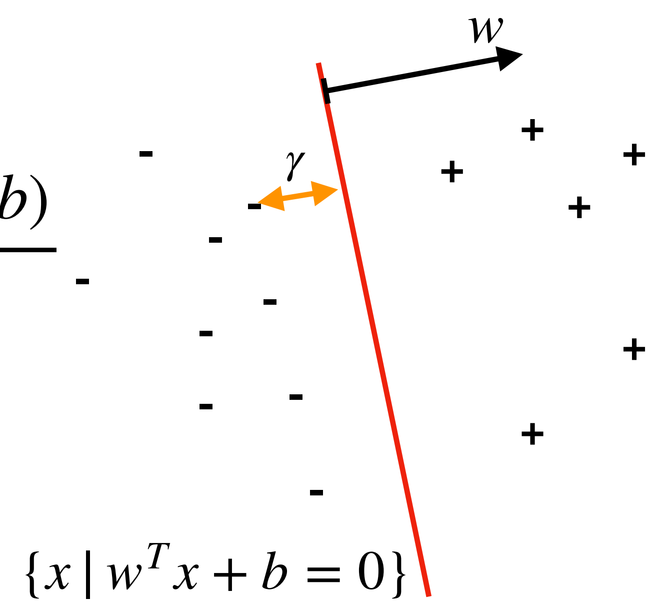



- Among all linear classifiers, we would like to find one that has the **maximum margin**

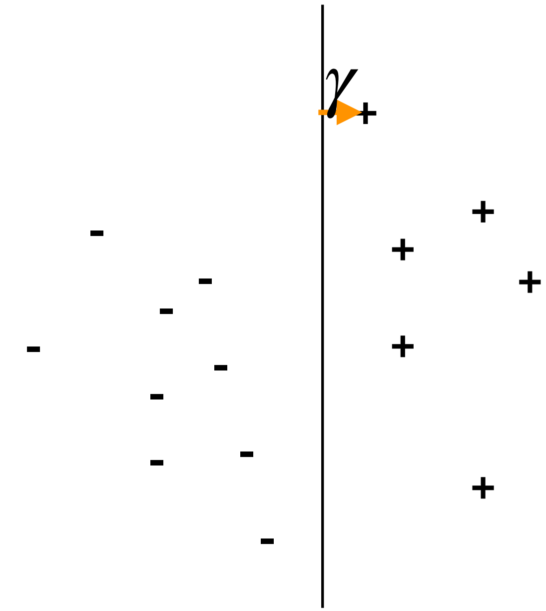
- We will derive an algorithm that finds the maximum margin classifier, by transforming a difficult to solve optimization into an efficient one

# Maximum margin classifier

(we transform the optimization into an efficient one)

**(maximize the margin)**

**(s.t. $\gamma$ is a lower bound on the margin)**



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- We propose the following optimization problem:

$$\text{maximize}_{w \in \mathbb{R}^d, b \in \mathbb{R}, \gamma \in \mathbb{R}} \quad \gamma$$

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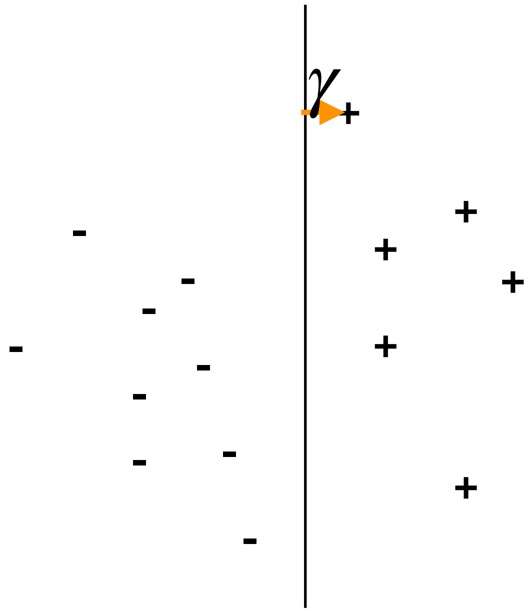

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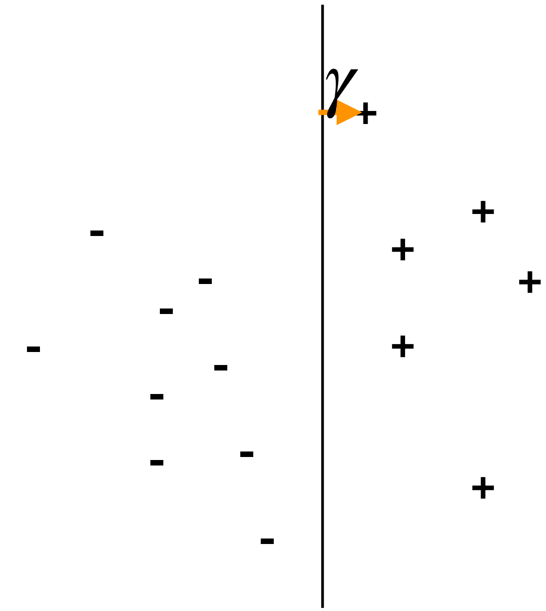

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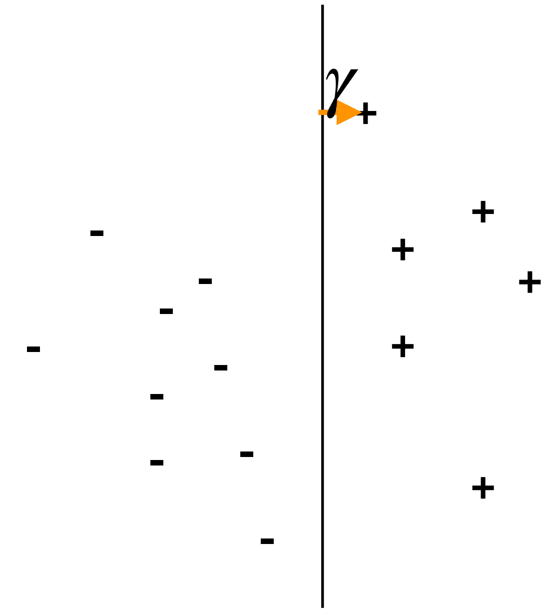

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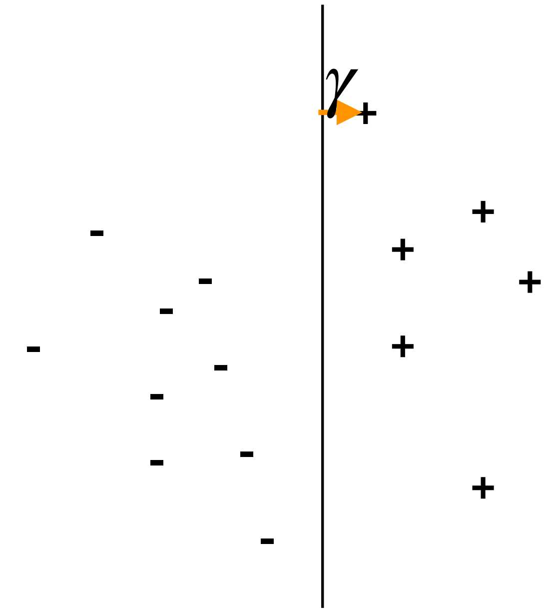

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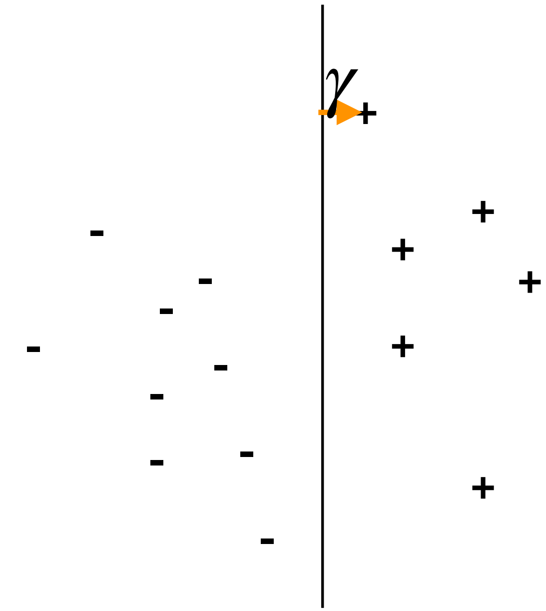

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- The above optimization looks difficult, so we transform it using **reparametrization**

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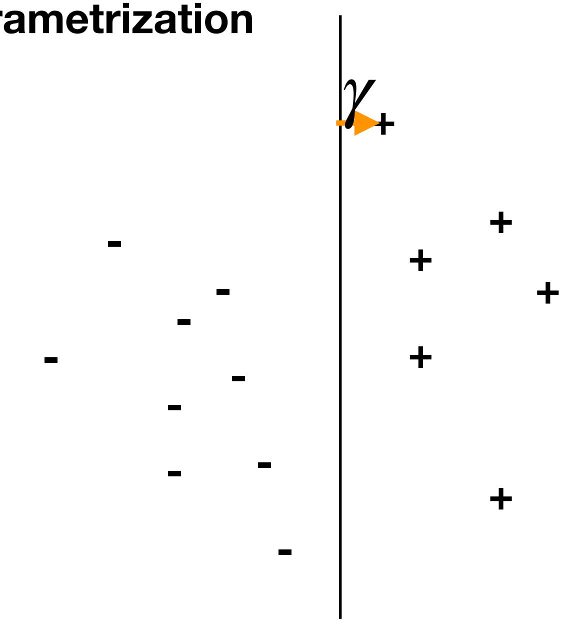
$$\|w\|_2 = \frac{1}{\gamma}$$



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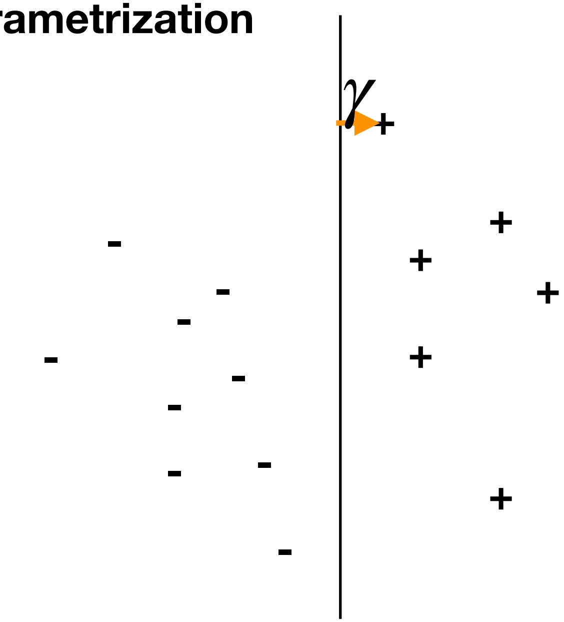


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- Because of scale invariance, the optimal solution does not change, as the solutions to the original problem did not depend on $\|w\|_2$, and only depends on the direction of $w$

**(maximize the margin)**

**(now** $\frac{1}{\|w\|_2}$ **plays the role of a lower bound on the margin)**

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- The above optimization still looks difficult, but can be transformed into

  $\text{maximize}_{w \in \mathbb{R}^d, b \in \mathbb{R}} \quad \dfrac{1}{\|w\|_2}$ **(maximize the margin)**

  subject to $\dfrac{y_i(w^T x_i + b)}{\|w\|_2} \geq \dfrac{1}{\|w\|_2}$ for all $i \in \{1, \ldots, n\}$ **(now $\dfrac{1}{\|w\|_2}$ plays the role of a lower bound on the margin)**

  which simplifies to

  $\text{minimize}_{w \in \mathbb{R}^d, b \in \mathbb{R}} \quad \|w\|_2^2$

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- This is a **quadratic program with linear constraints**, which can be easily solved

- $$\text{maximize}_{w \in \mathbb{R}^d, b \in \mathbb{R}, \gamma \in \mathbb{R}} \quad \gamma$$

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- This is a **quadratic program with linear constraints**, which can be easily solved
- Once the optimal solution is found, the margin of that classifier $(w, b)$ is $\frac{1}{\|w\|_2}$

# What if the data is not separable?

$$\text{minimize}_{w \in \mathbb{R}^d, b \in \mathbb{R}} \quad \|w\|_2^2$$

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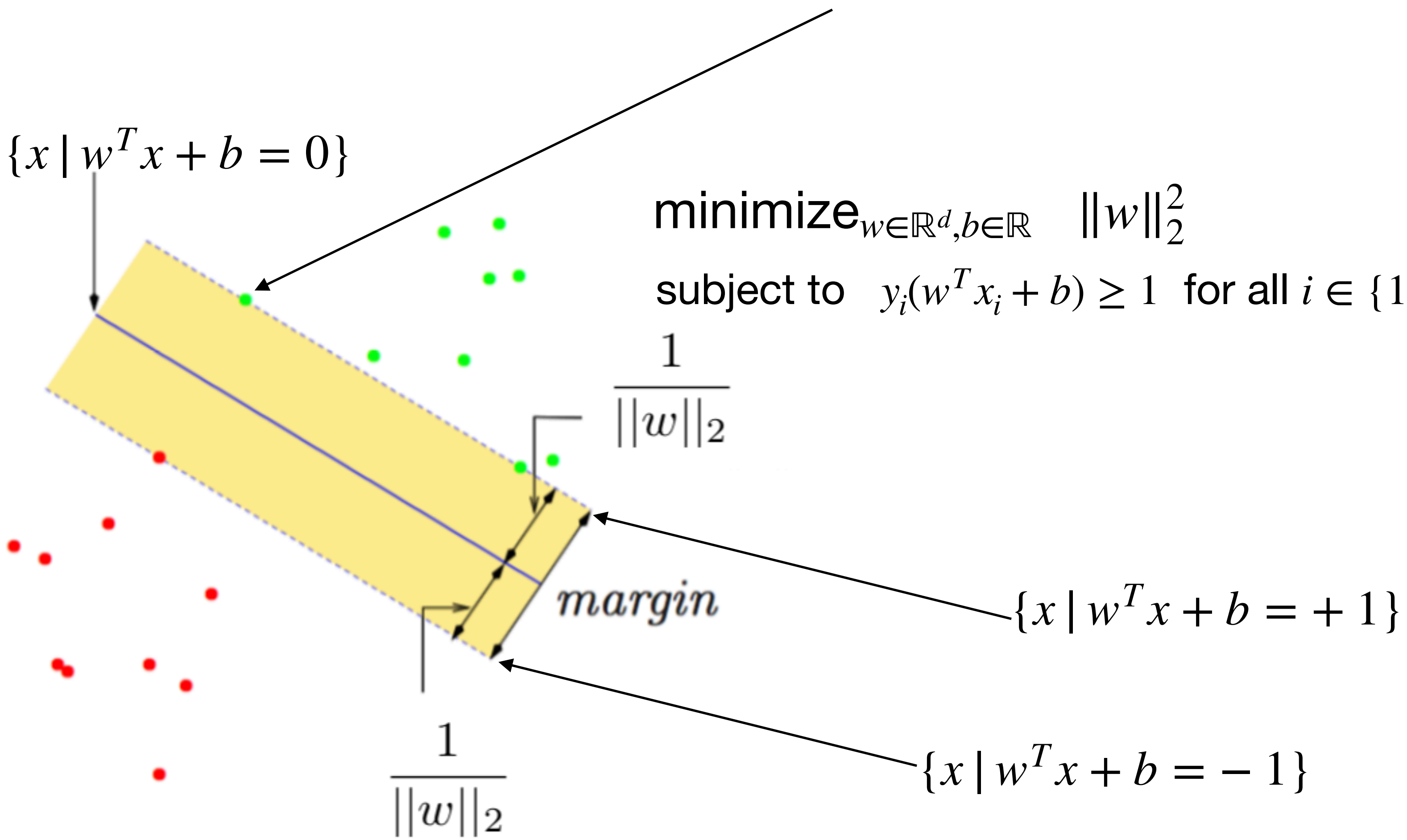

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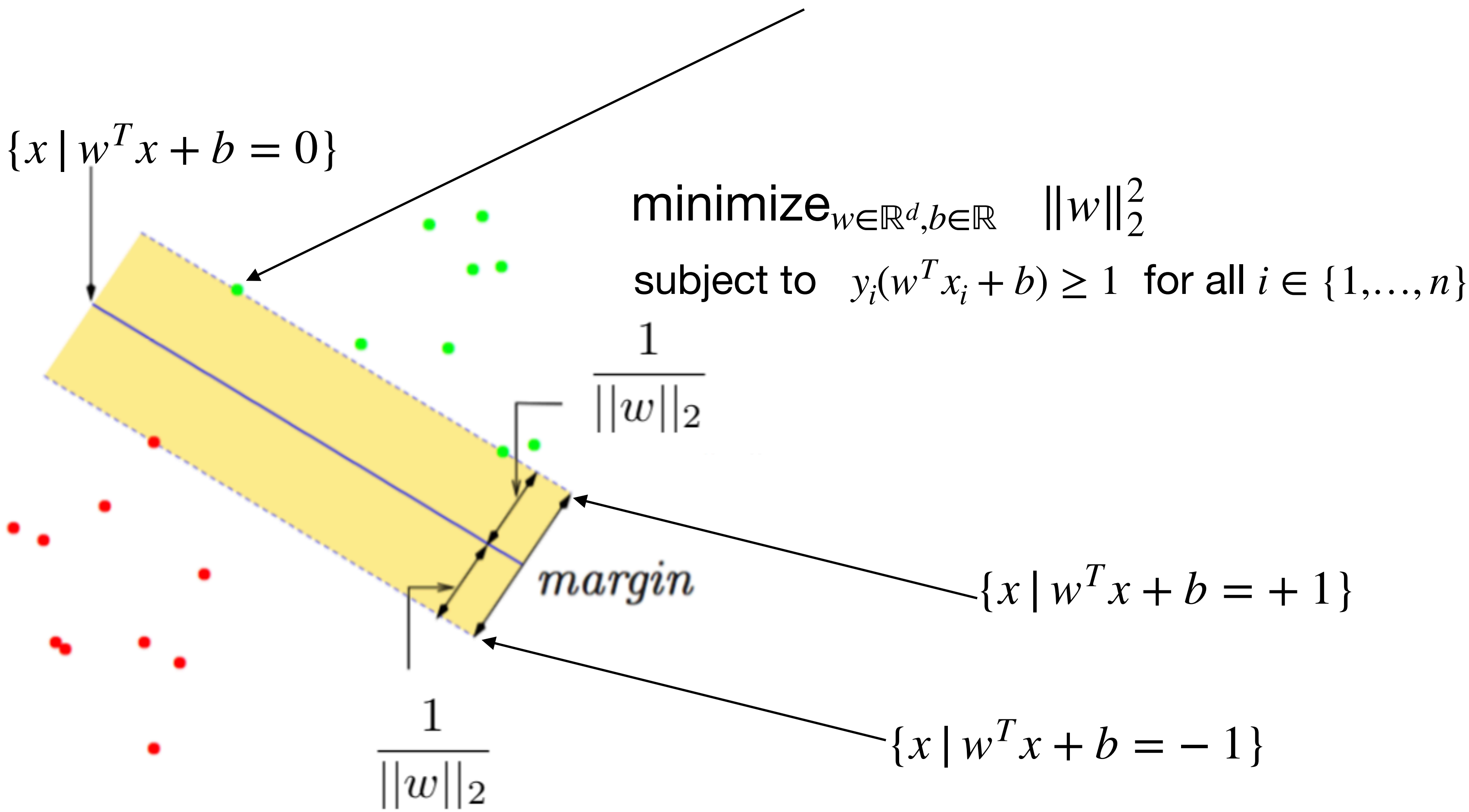

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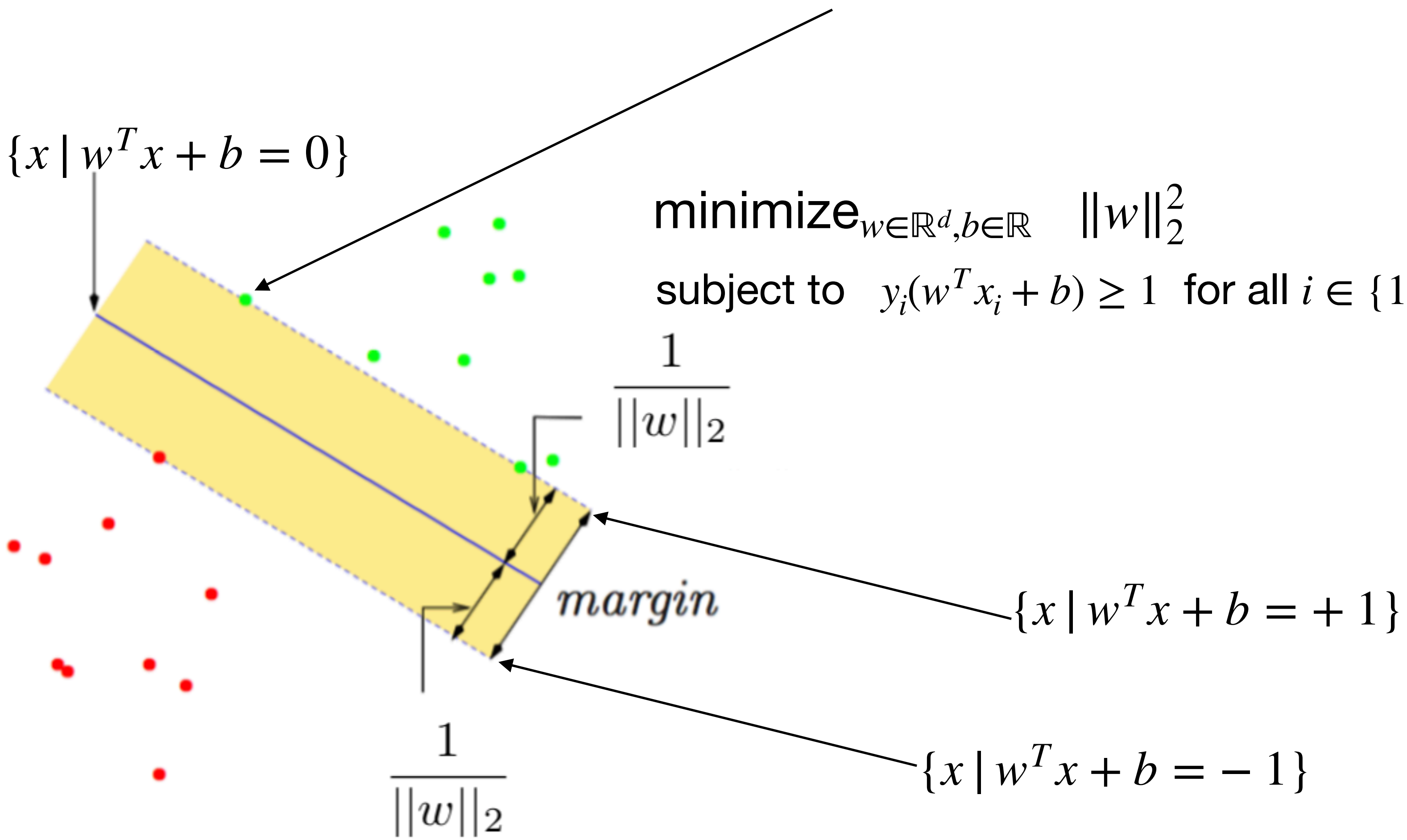


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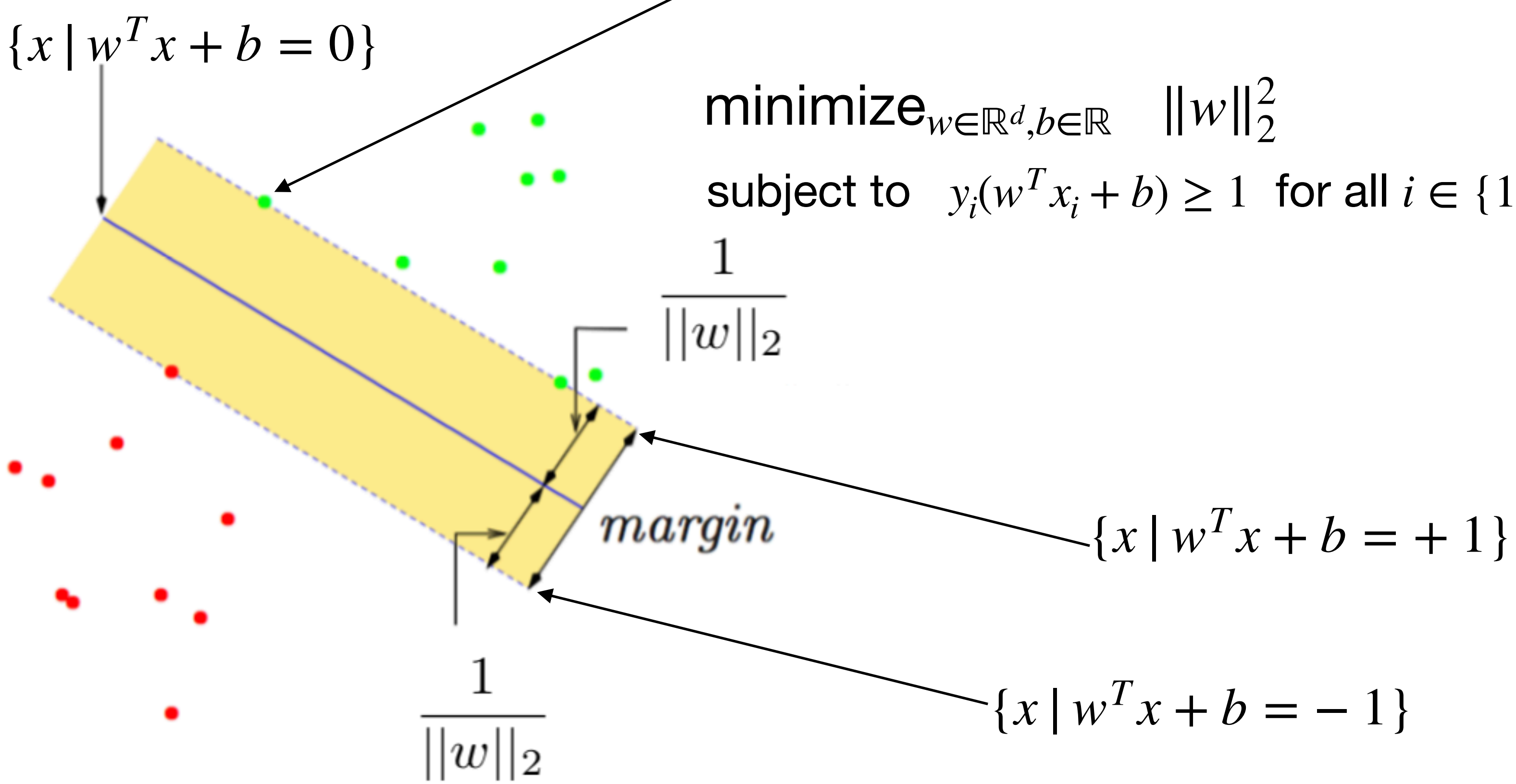

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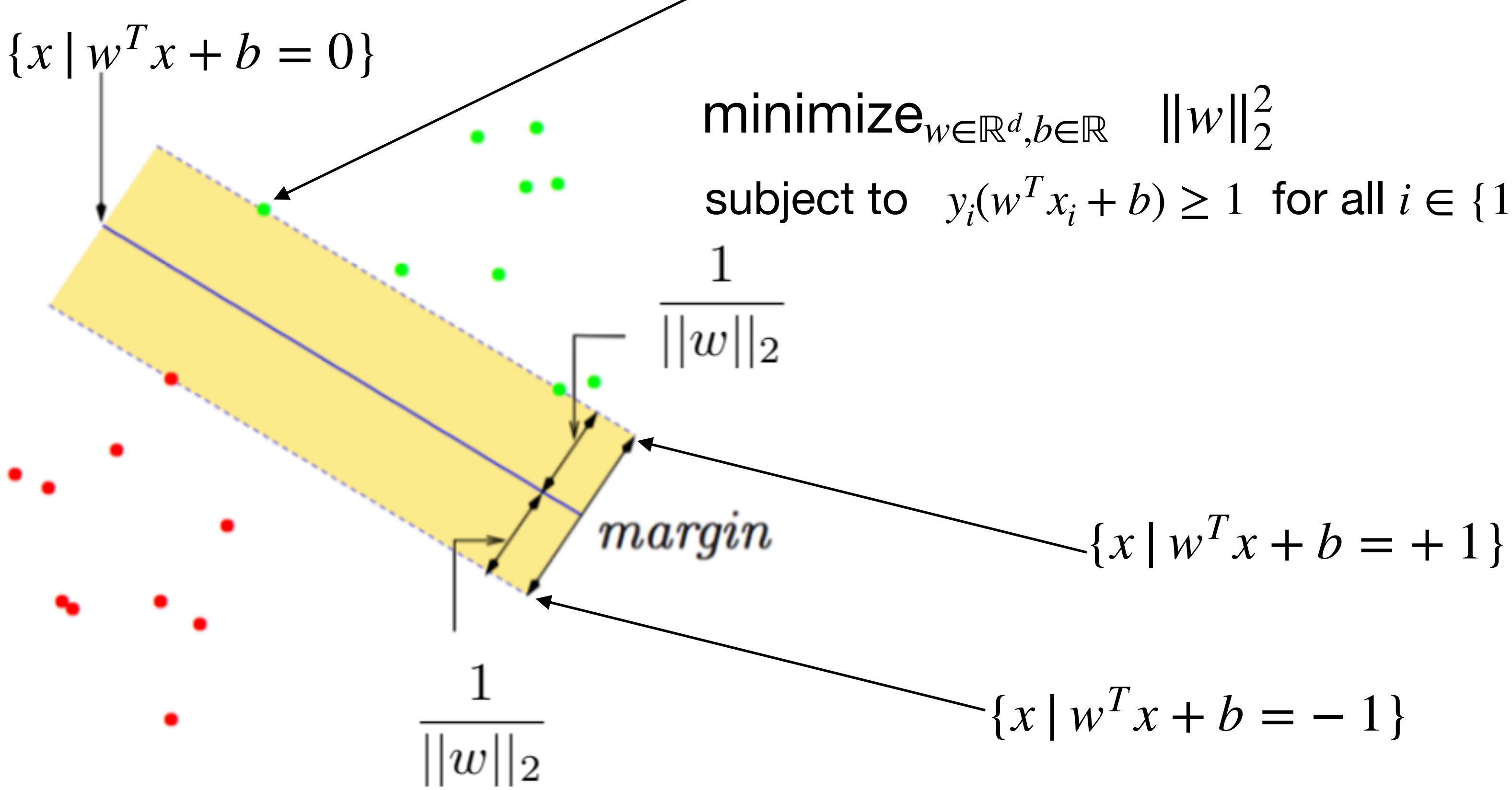

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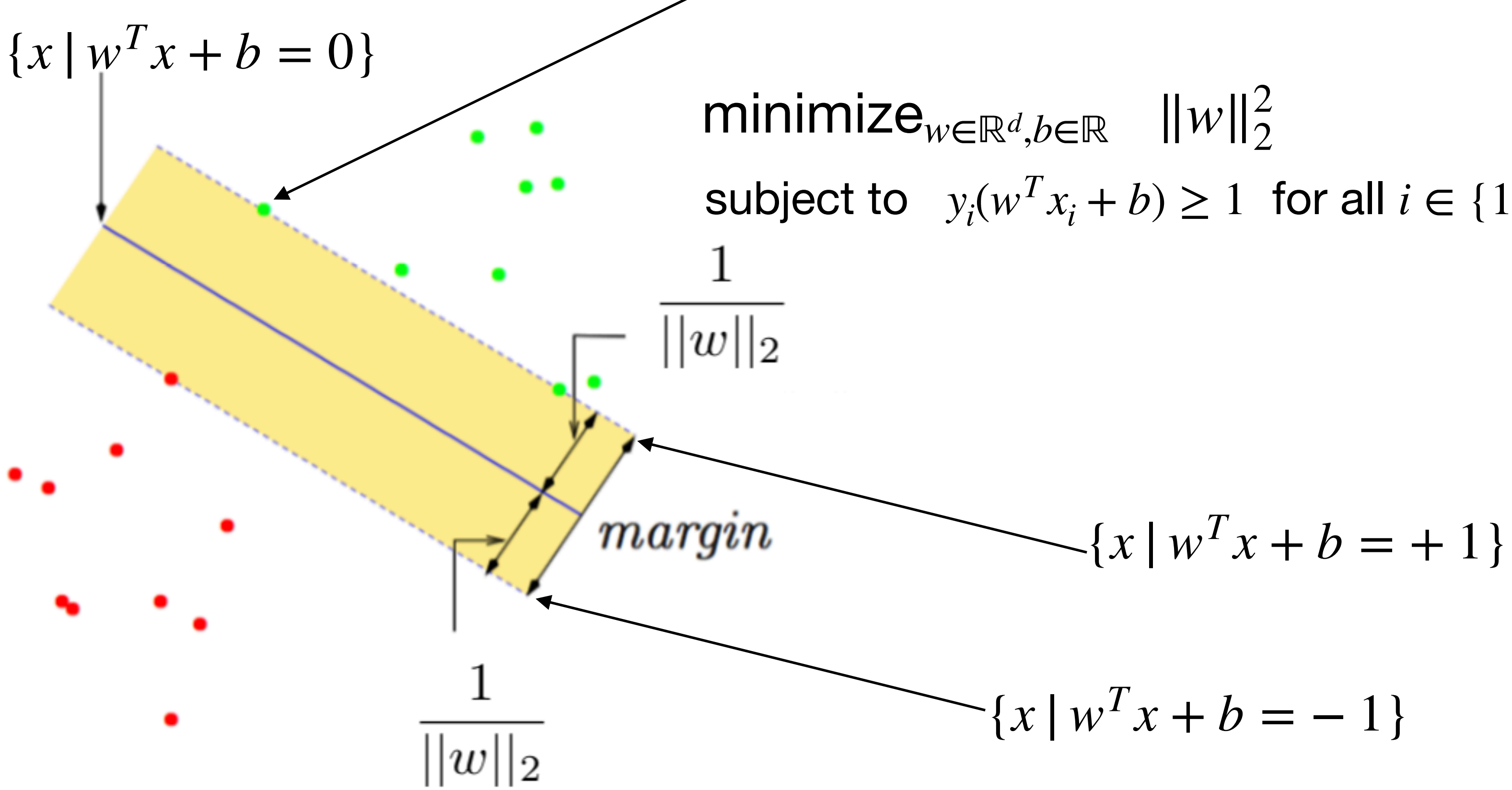

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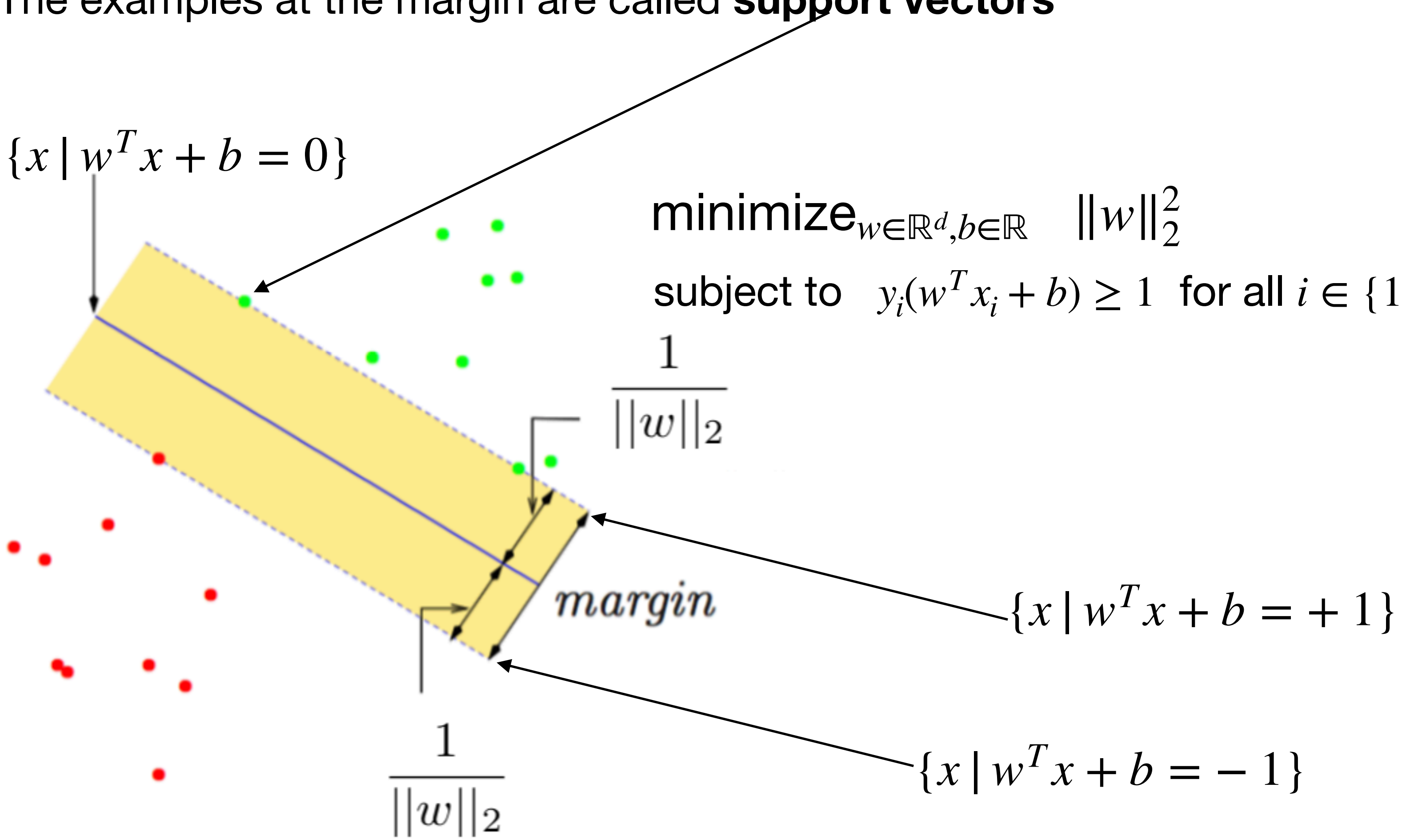

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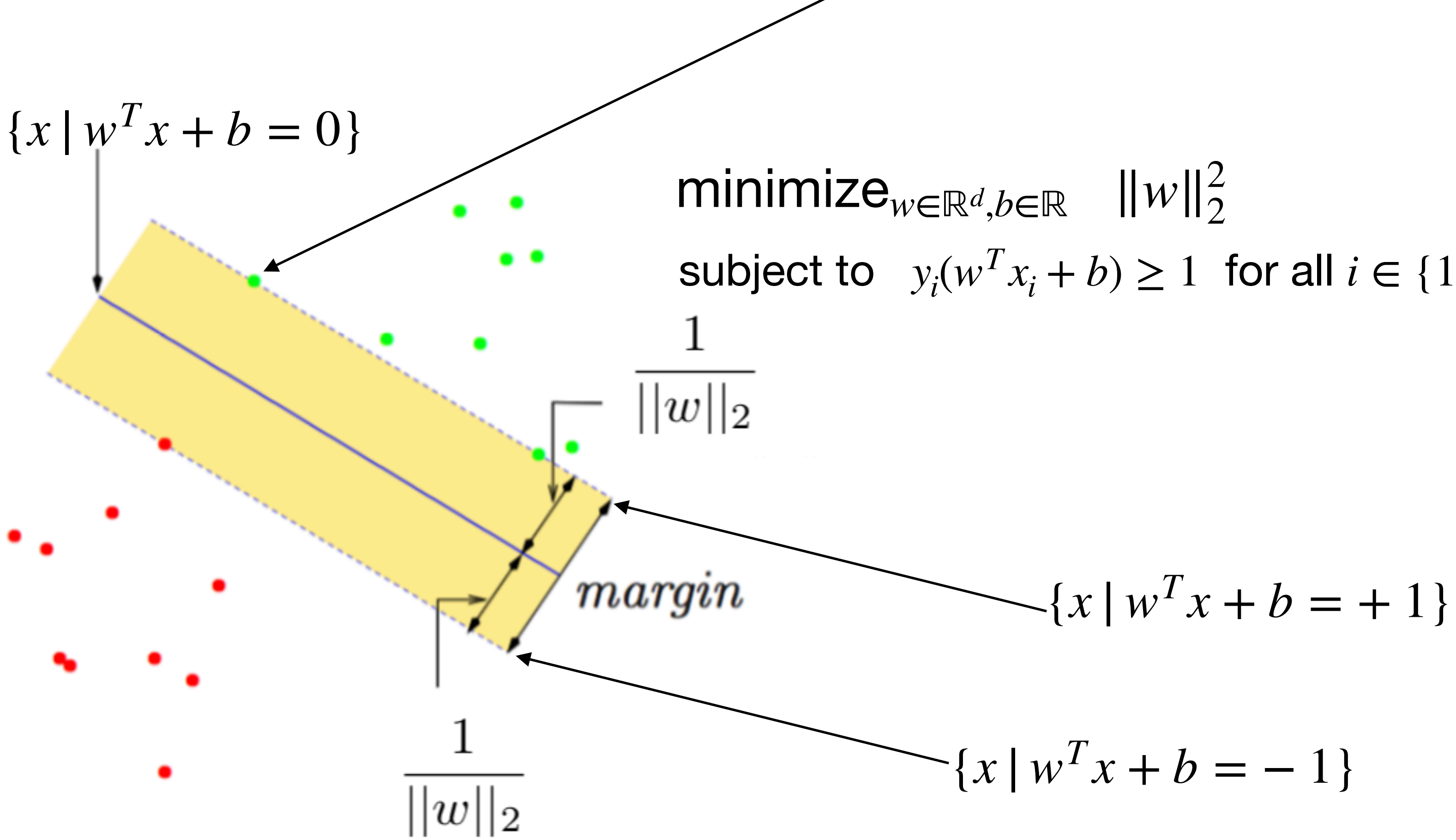


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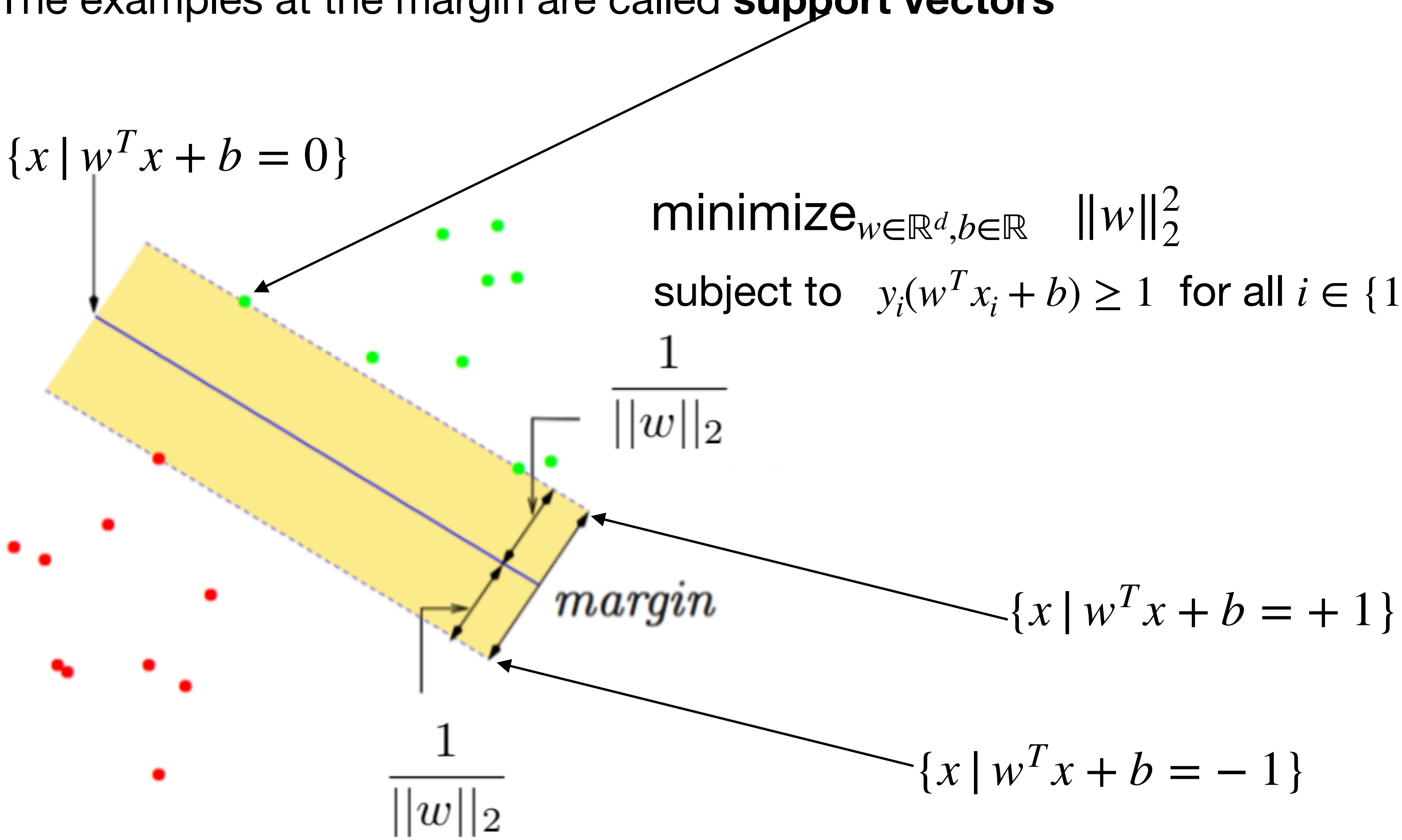


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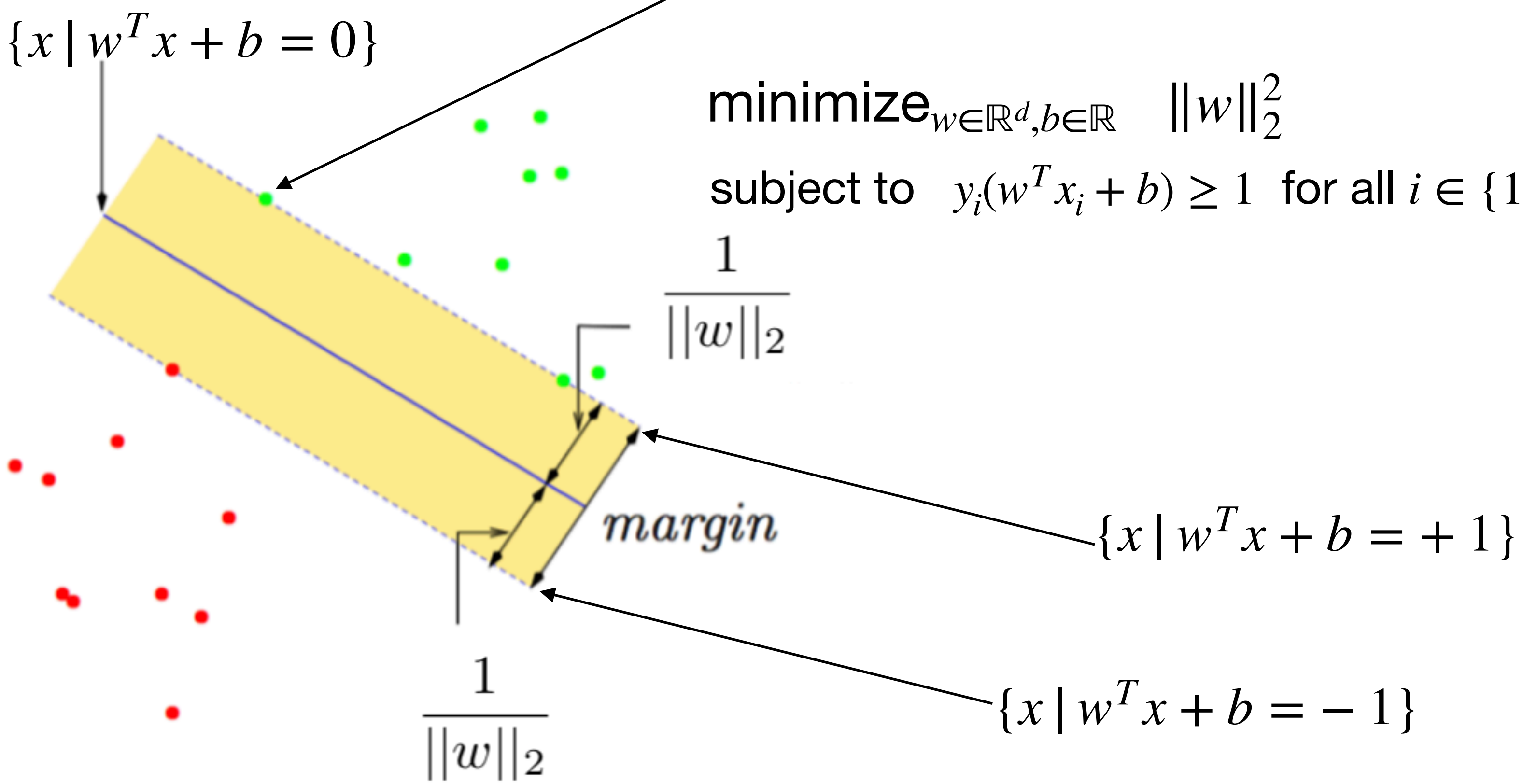

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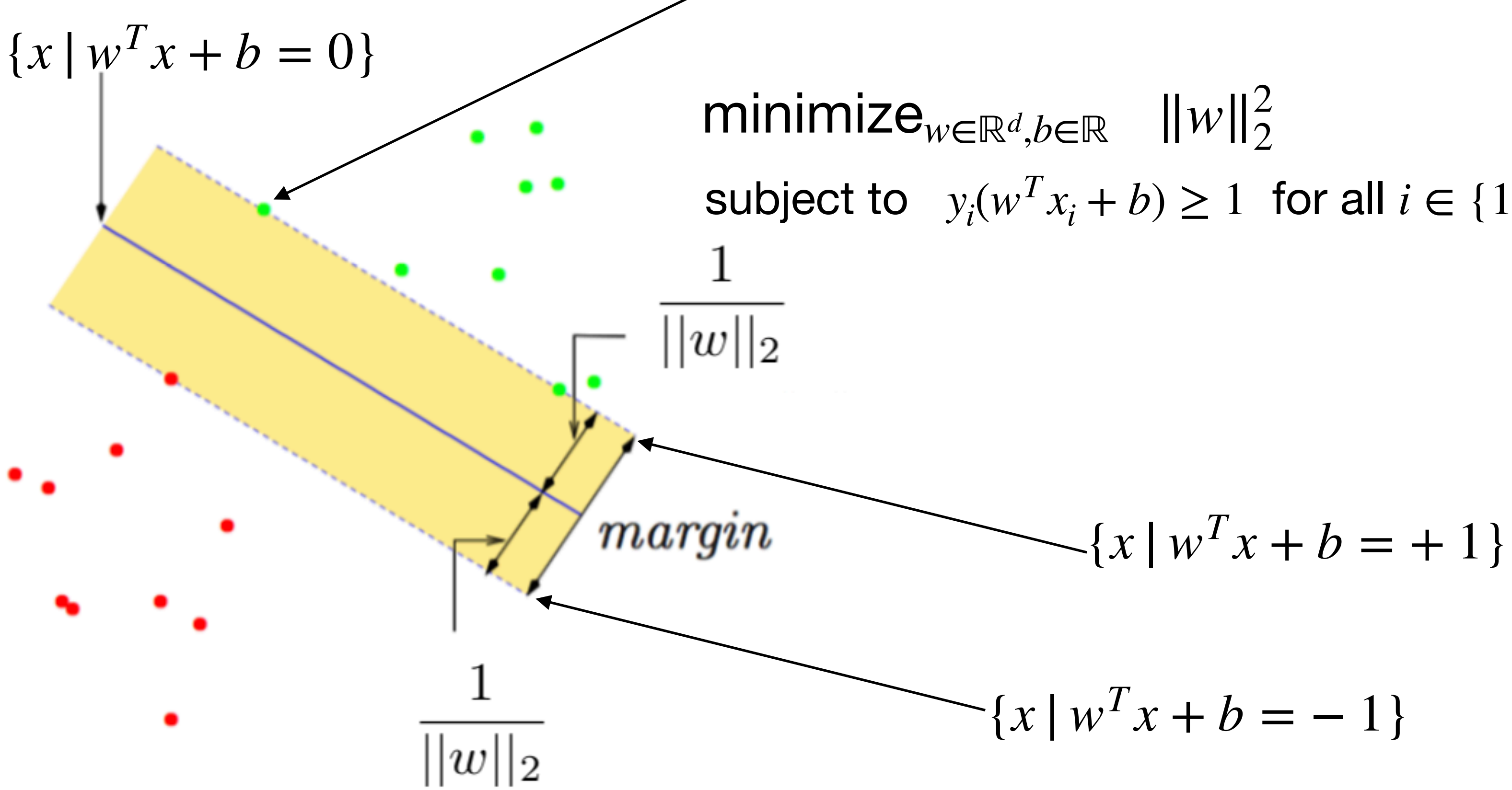


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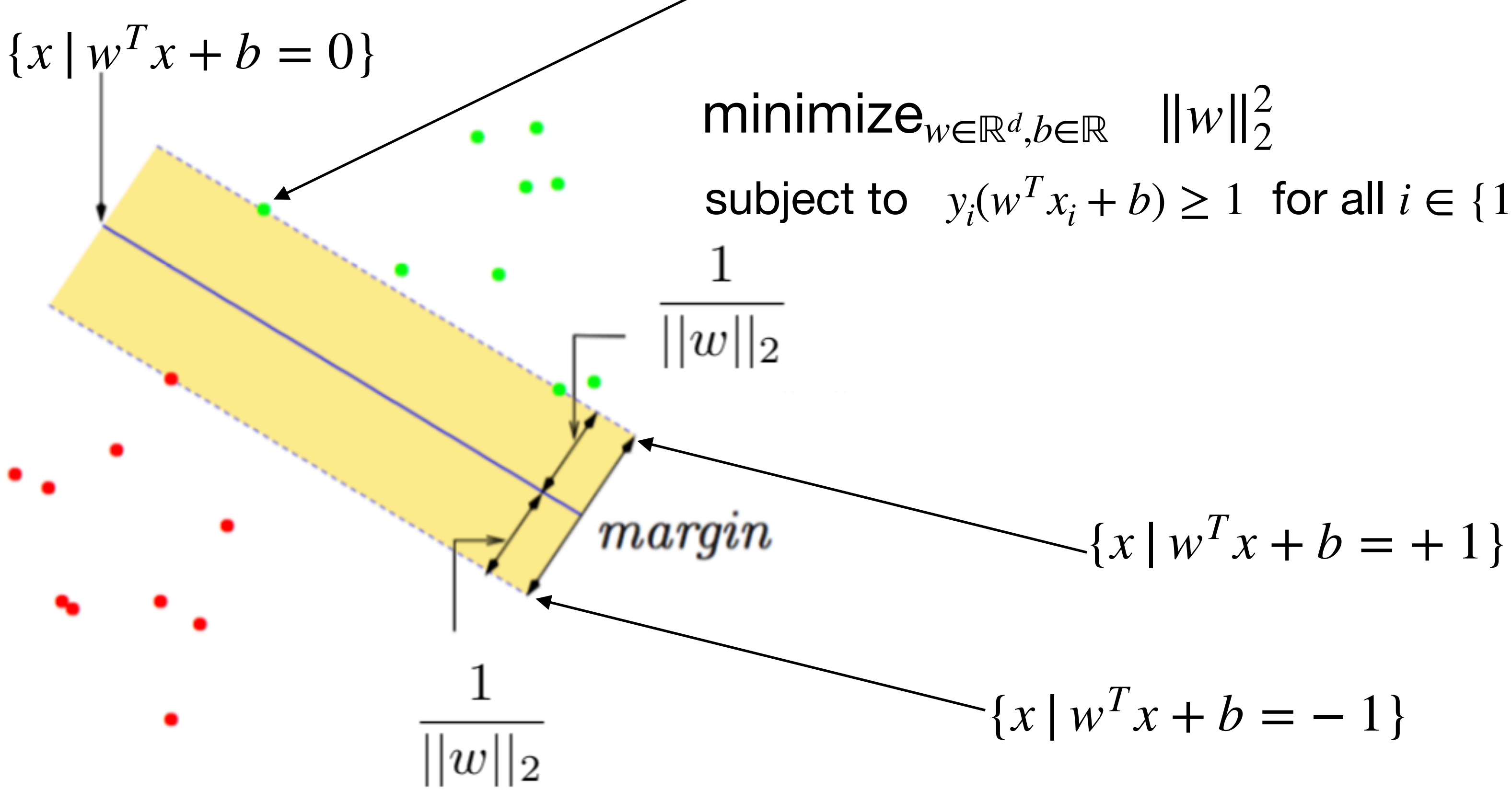
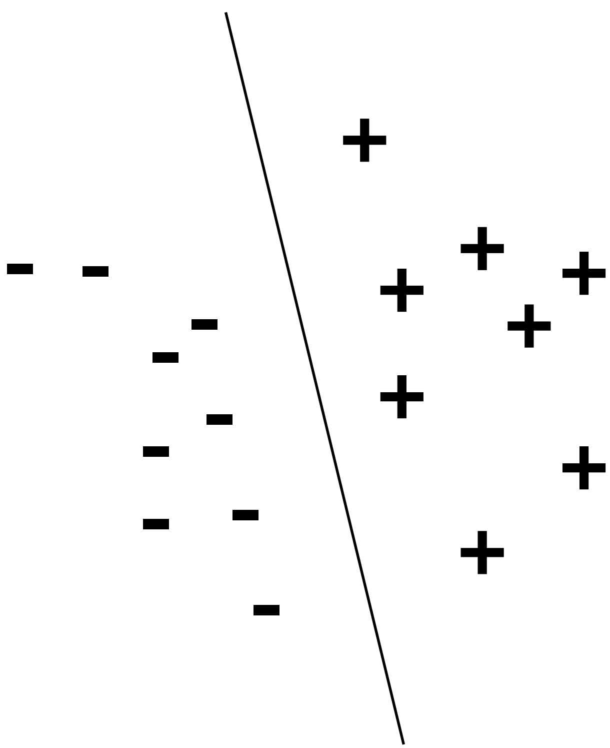
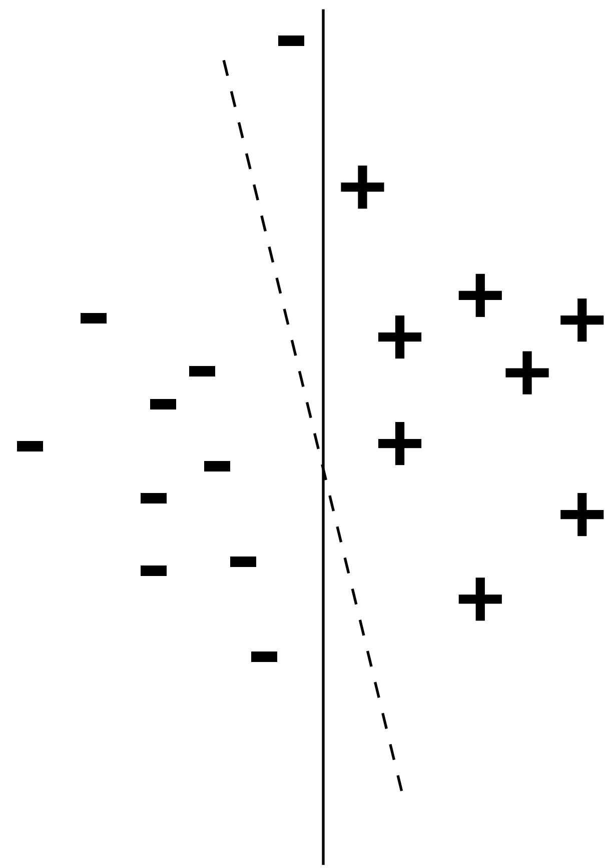


# Two issues

- it does not generalize to non-separable datasets
- max-margin formulation we proposed is sensitive to outliers





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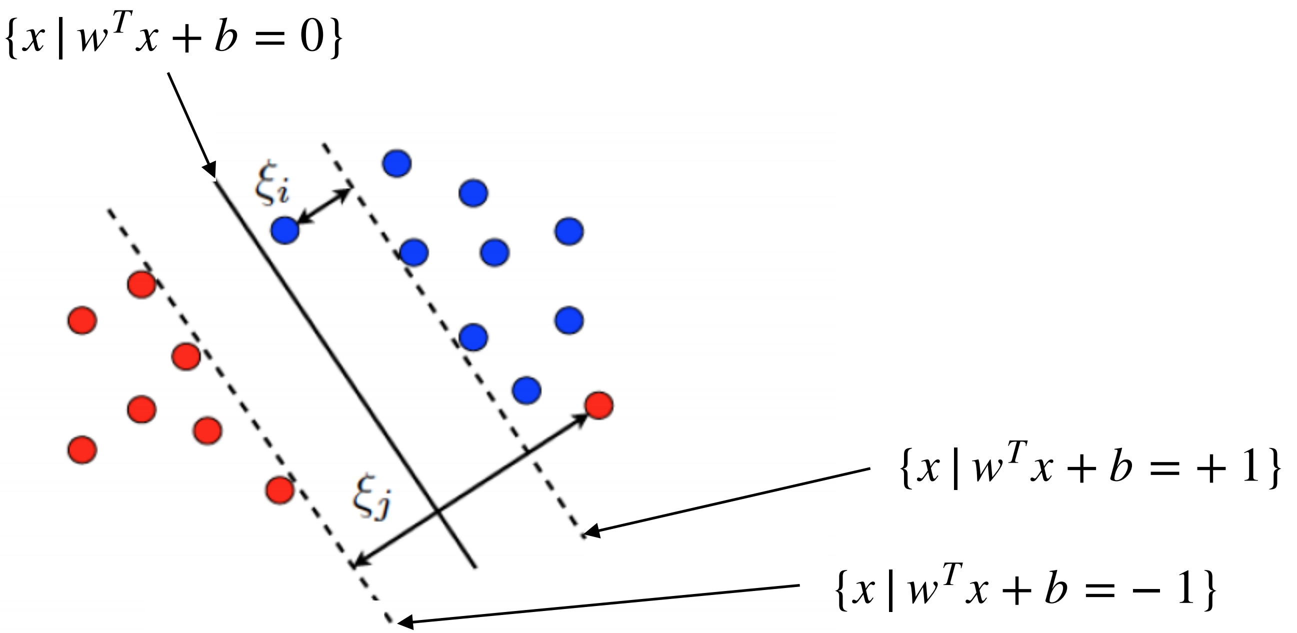

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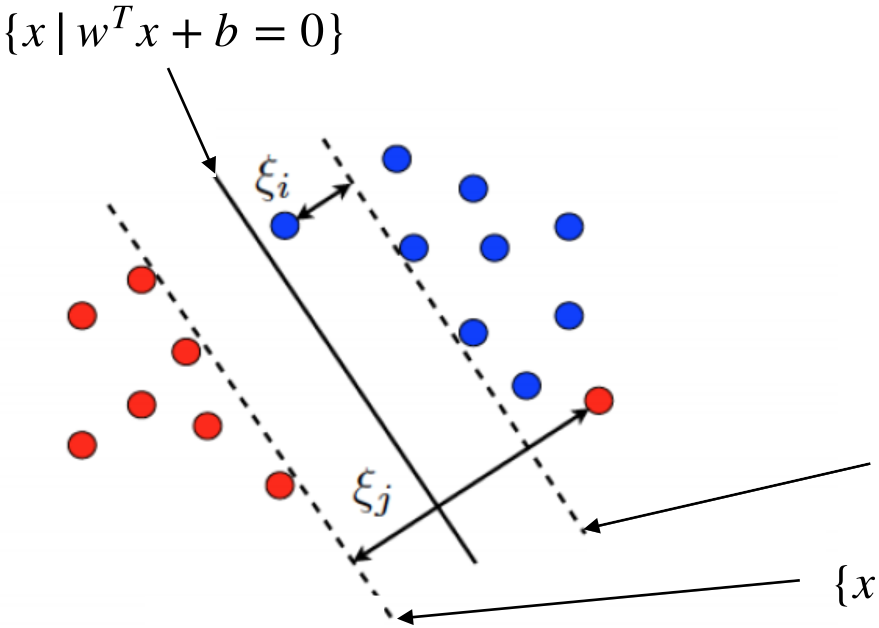


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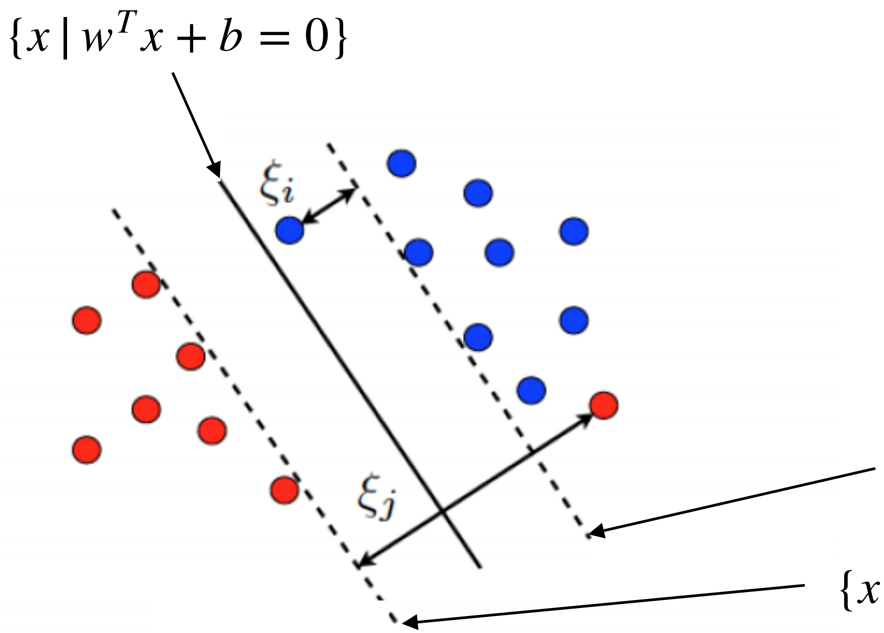


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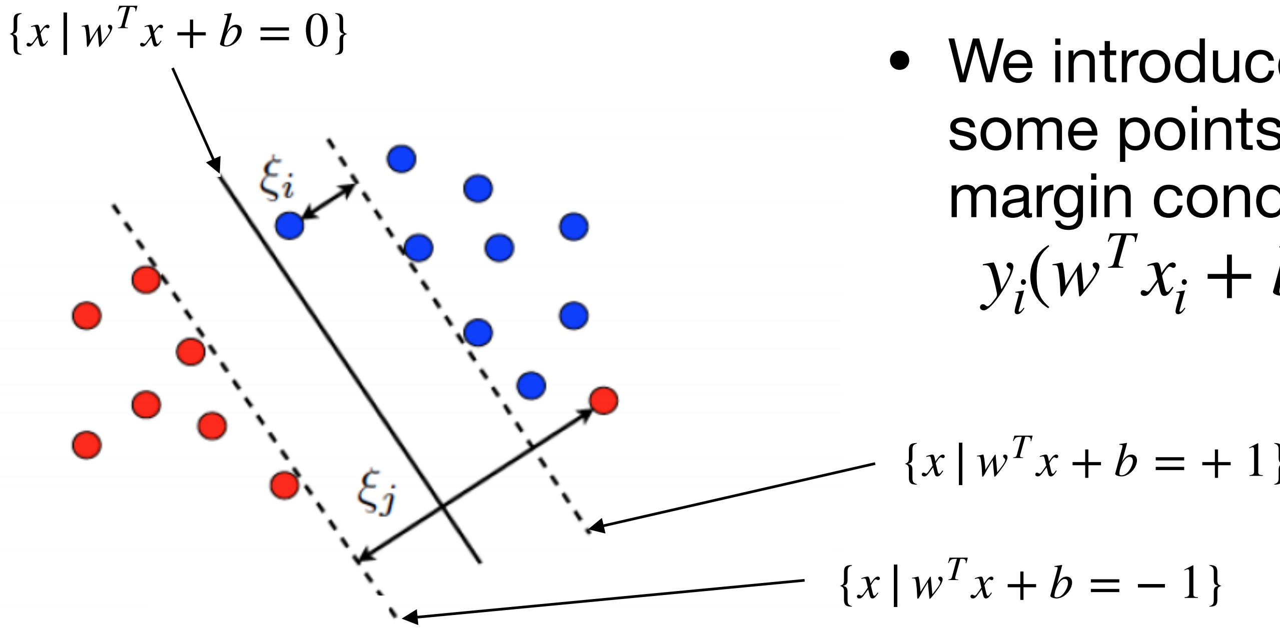


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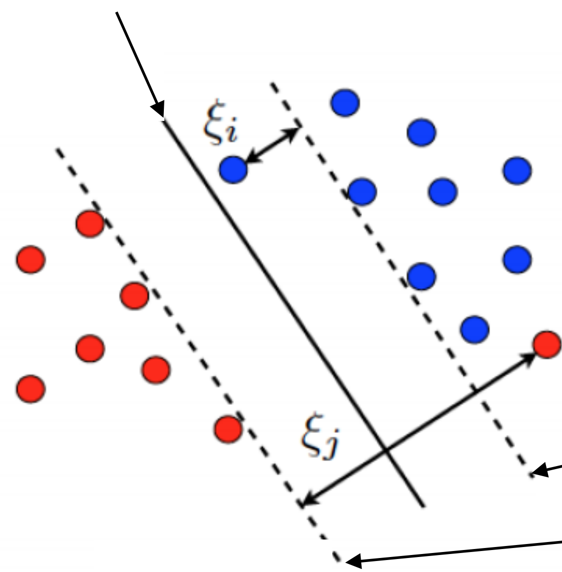


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the (re-scaled) margin (for each sample) is allowed to be less than one,
but you pay $c\xi_i$ in the cost, and $c$ balances the two goals:
maximizing the margin for most examples vs. having small number of violations

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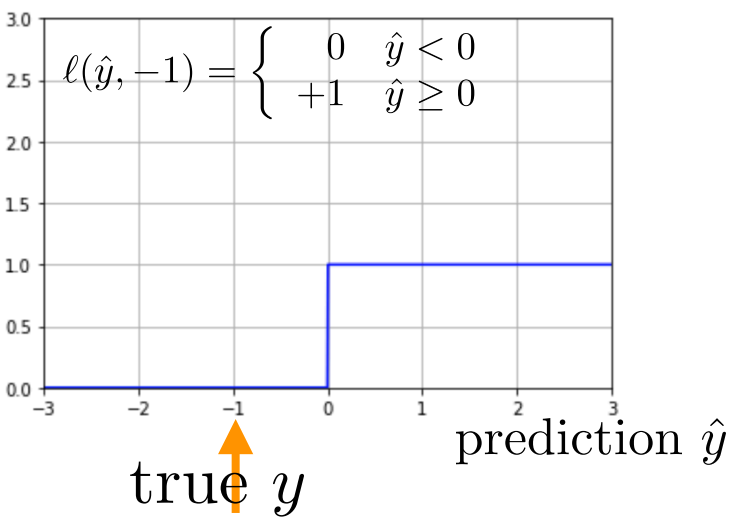
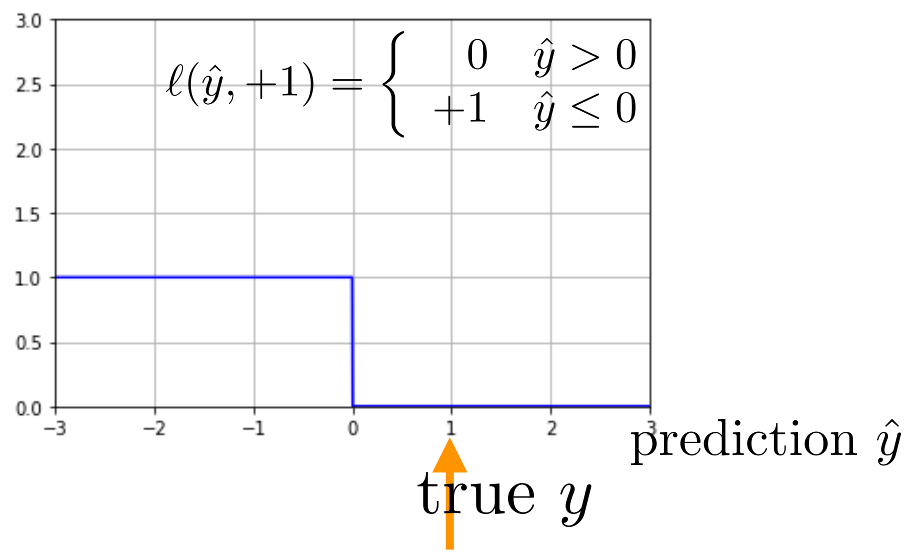
# Recall: we were looking for a loss function

- We want a loss function that
  - approximates (captures the flavor of) the 0-1 loss
  - can be easily optimized (e.g. convex and/or non-zero derivatives)
- More formally, we want a **loss function**
  - with $\ell(\hat{y}, -1)$ small when $\hat{y} < 0$ and larger when $\hat{y} > 0$
  - with $\ell(\hat{y}, 1)$ small when $\hat{y} > 0$ and larger when $\hat{y} < 0$
  - which has other nice characteristics, e.g., differentiable or convex
- We now have a new loss function from the SVM optimization problem:

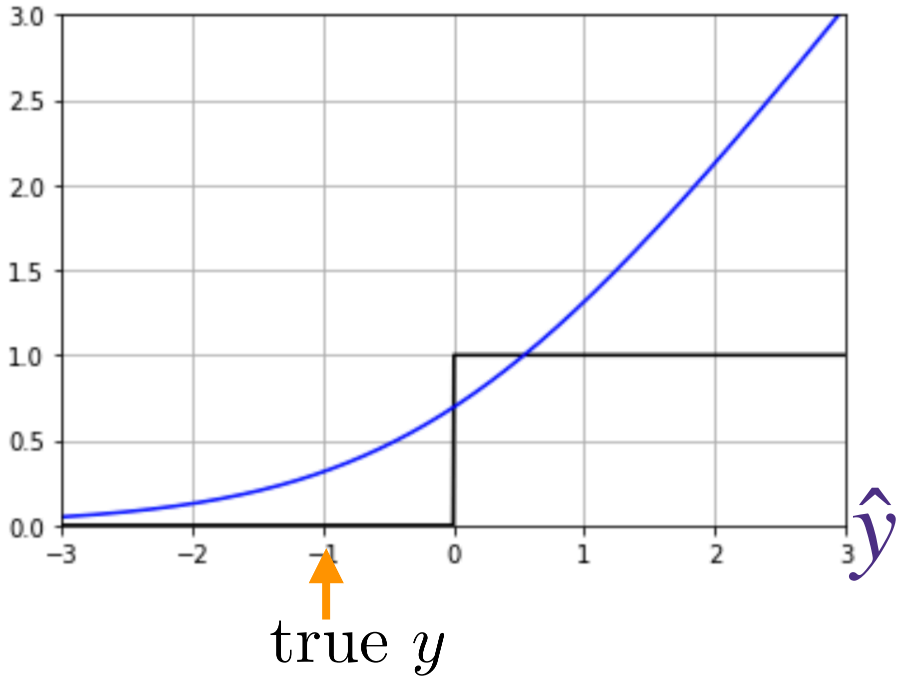
$$\text{minimize}_{w \in \mathbb{R}^d, b \in \mathbb{R}} \quad \frac{1}{c}\|w\|_2^2 + \sum_{i=1}^{n} \max\{0, 1 - y_i(w^T x_i + b)\}$$

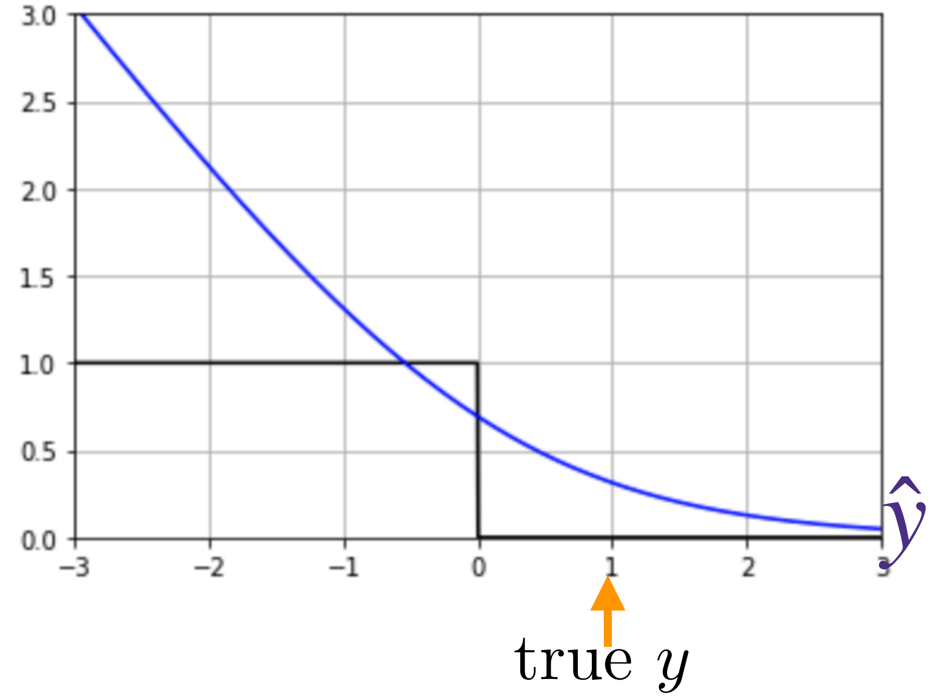


# Logistic loss $\ell(\hat{y}, y) = \log(1 + e^{-y\hat{y}})$

$$\ell(\hat{y}, -1) = \log(1 + e^{\hat{y}}) \qquad \ell(\hat{y}, +1) = \log(1 + e^{-\hat{y}})$$




- Differentiable and convex in $\hat{y}$
- Approximation of 0-1 loss
- Most popular choice of a loss function for classification problems

# Sub-gradient descent for SVM

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- SVM is the solution of

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- which is exactly the same as gradient descent, except when we are at a non-differentiable point, we take one of the sub-gradients instead of the gradient (recall sub-gradient is a set)
- this means that we can take (a generic form derived from previous page)

$$\partial_w \ell(w^T x_i + b, y_i) \;=\; \mathbf{I}\{y_i(w^T x_i + b) \le 1\}(-y_i x_i)$$

and apply

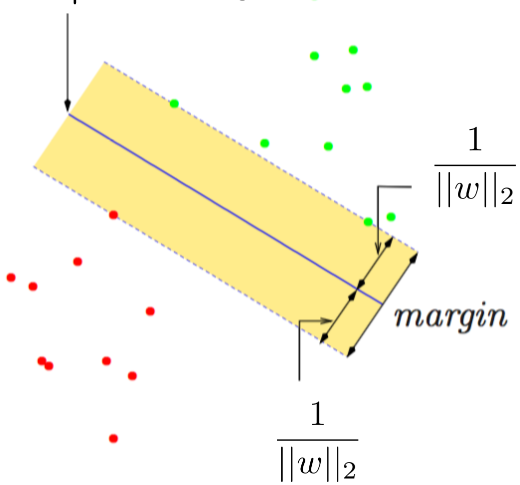
$$w^{(t+1)} \;\leftarrow\; w^{(t)} - \eta \left( \sum_{i=1}^{n} \mathbf{I}\{y_i((w^{(t)})^T x_i + b^{(t)}) \le 1\}(-y_i x_i) \;+\; \frac{2}{c} w^{(t)} \right)$$

$$b^{(t+1)} \;\leftarrow\; b^{(t)} - \eta \sum_{i=1}^{n} \mathbf{I}\{y_i((w^{(t)})^T x_i + b^{(t)}) \le 1)\}(-y_i)$$

# Kernels

# What if the data is not linearly separable?

- $x^T w + b = 0$




Some points do not satisfy margin constraint:

$$\min_{w,b} ||w||_2^2$$

$$y_i(x_i^T w + b) \geq 1 \quad \forall i$$

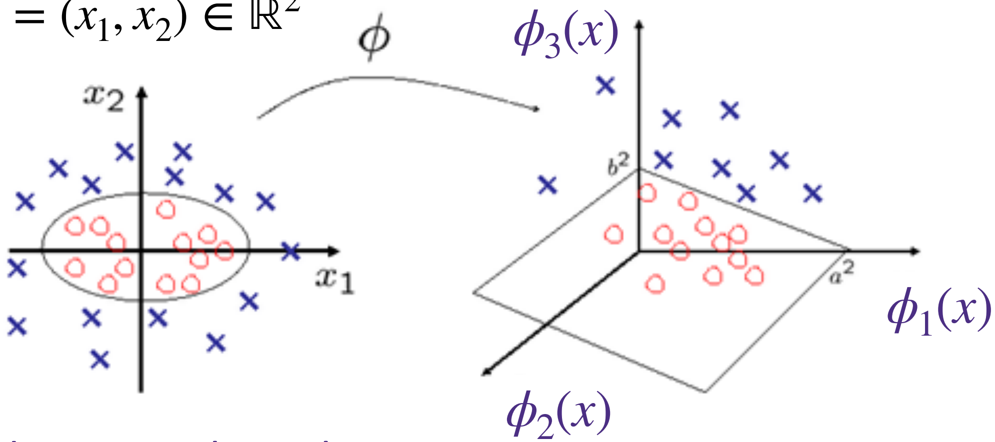
Two options:

1. Introduce slack to this optimization problem (Support Vector Machine)
2. **Lift to higher dimensional space (Kernels)**

# What if the data is not linearly separable?

- Use features, for example,

$x = (x_1, x_2) \in \mathbb{R}^2$

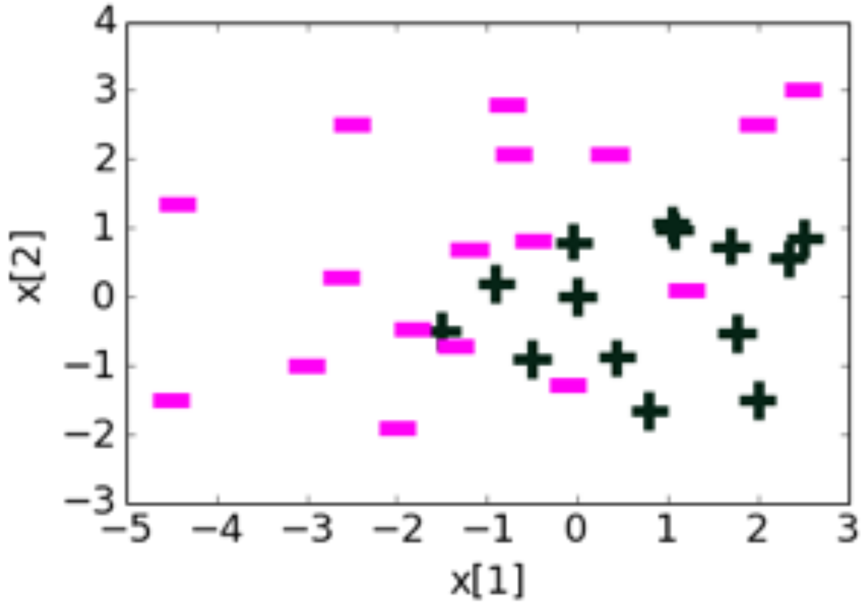



This data is not linearly separable

Can you suggest some features $\phi_1(x_1, x_2), \phi_2(x_1, x_2), \phi_3(x_1, x_2)$ such that this data is linearly separable in this 3-dimensional space?

- Generally, in high dimensional feature space, it is easier to linearly separate different classes
- However, it is hard to know which feature map will work for given data
- So the rule of thumb is to use high-dimensional features and hope that the algorithm will automatically pick the right set of features

# Example: adding more polynomial features



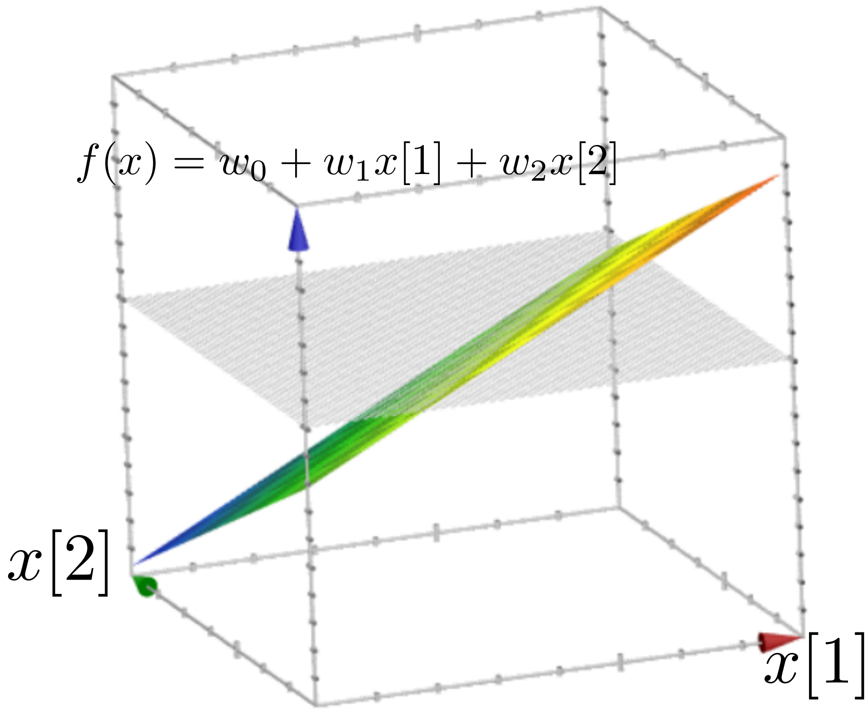

Polynomial

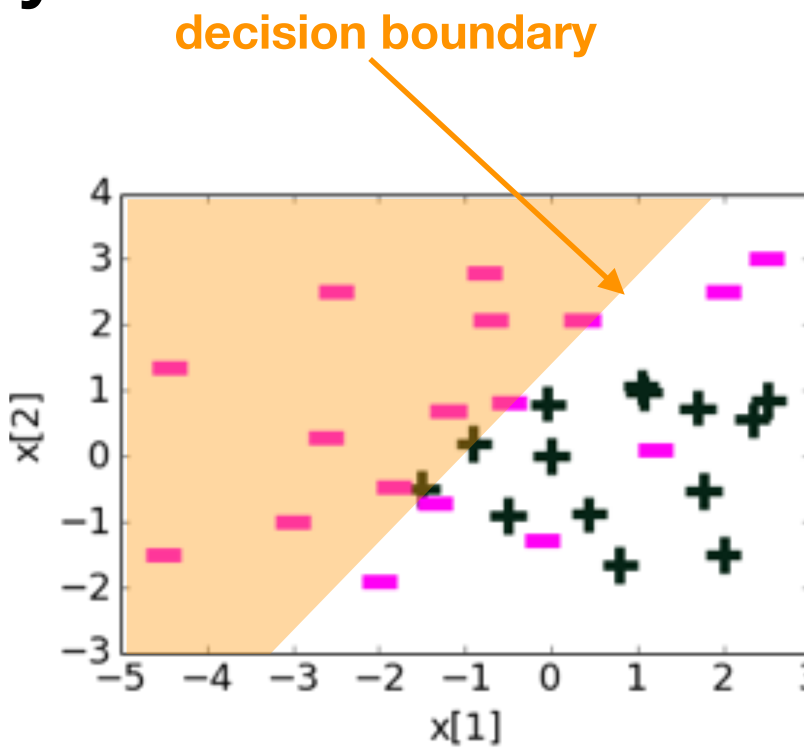
features

$$\begin{bmatrix} h_0(x) = 1 \\ h_1(x) = x[1] \\ h_2(x) = x[2] \\ h_3(x) = x[1]^2 \\ h_4(x) = x[2]^2 \\ \vdots \end{bmatrix}$$

- data: ***x*** in 2-dimensions, ***y*** in {+1,-1}
- features: polynomials
- model: linear on polynomial features
- $$f(x) \;=\; w_0 h_0(x) + w_1 h_1(x) + w_2 h_2(x) + \cdots$$

# Learned decision boundary




| Feature | Value | Coefficient |
|---|---|---|
| $h_0(x)$ | 1 | 0.23 |
| $h_1(x)$ | x[1] | 1.12 |
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- Simple **regression** models had **smooth** predictors
- Simple **classifier** models have **smooth** decision boundaries

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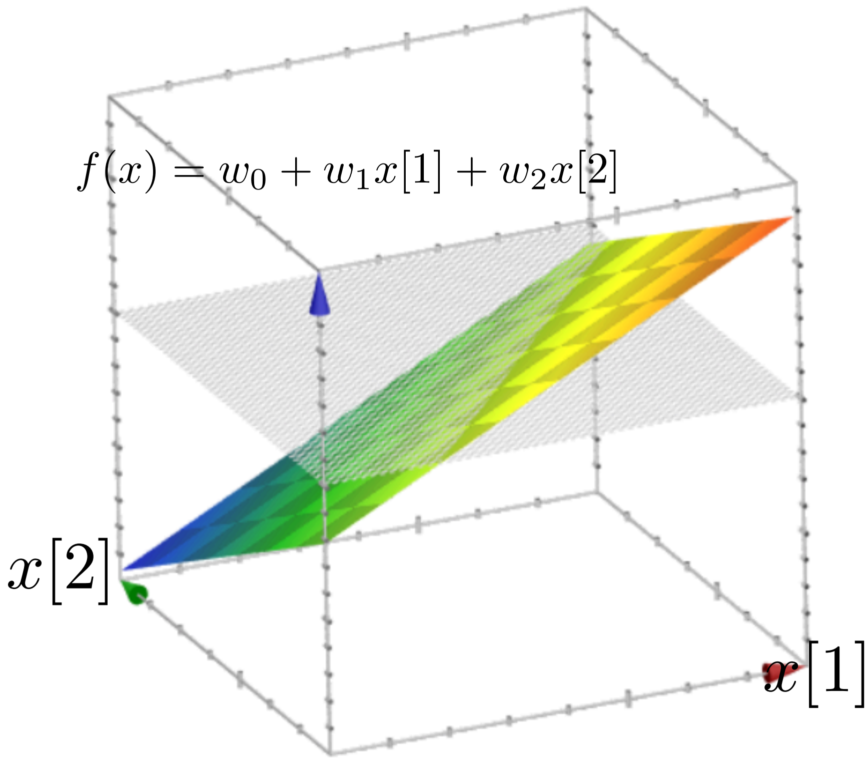


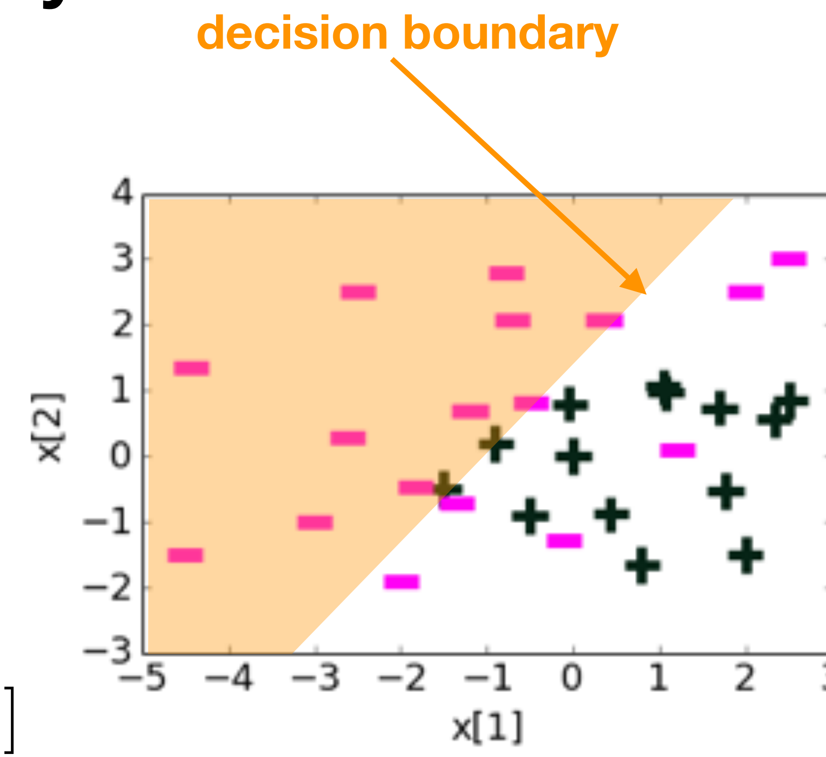


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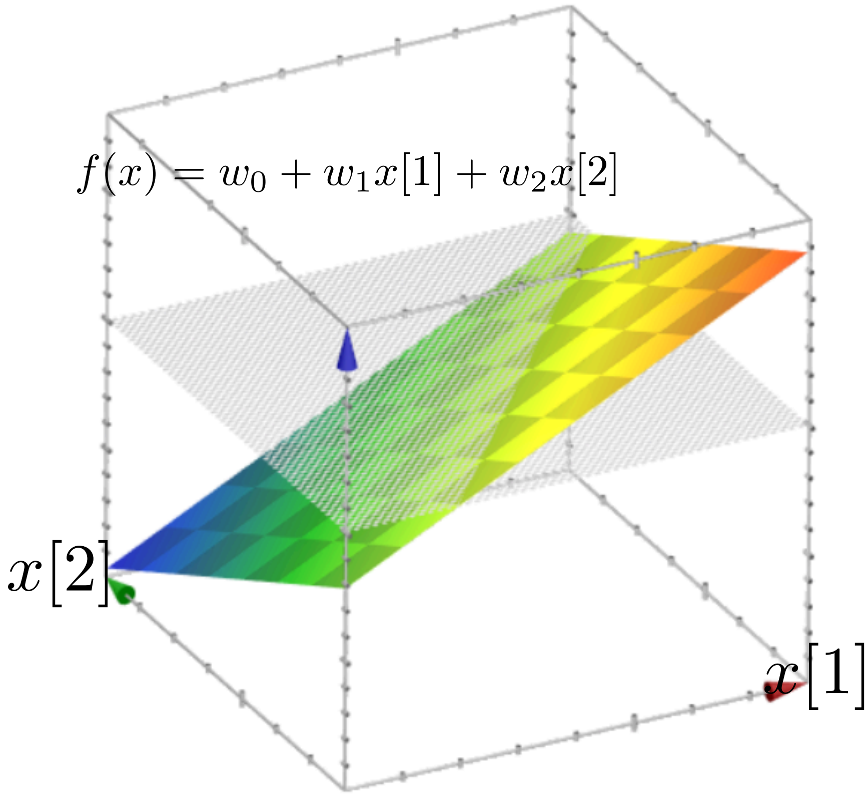


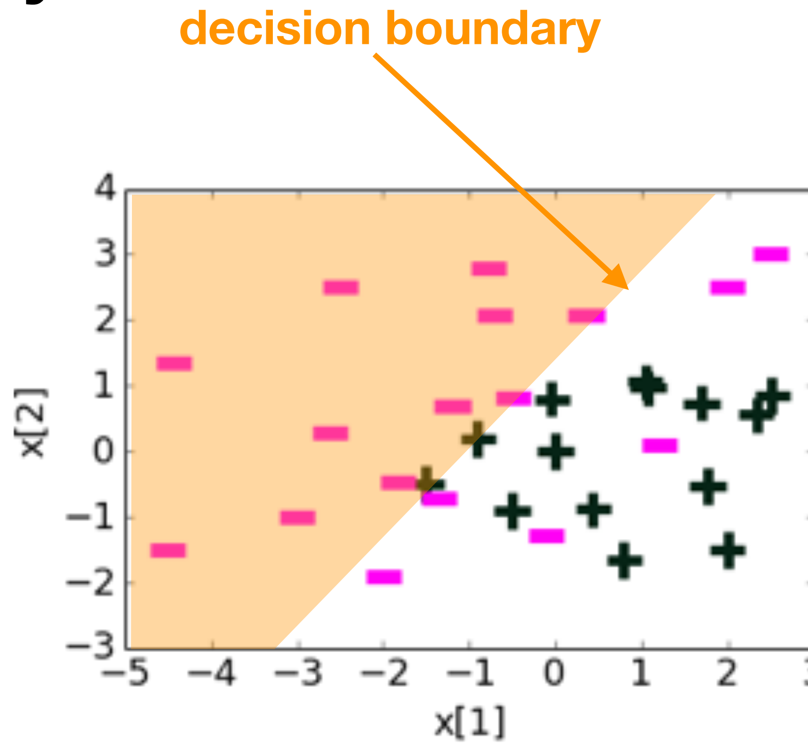


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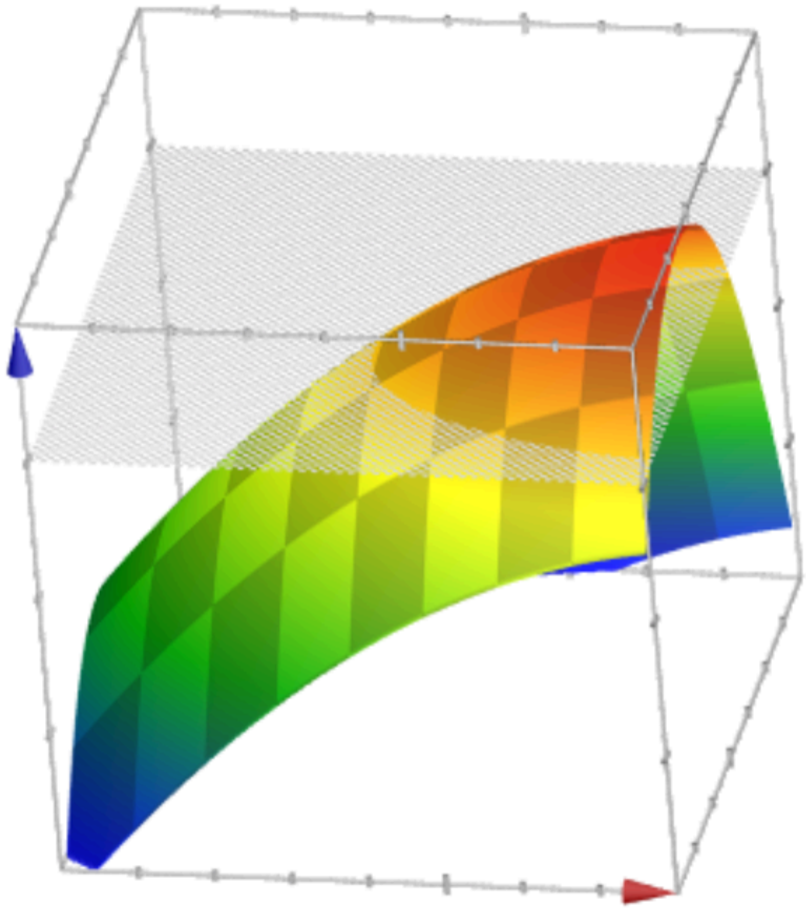
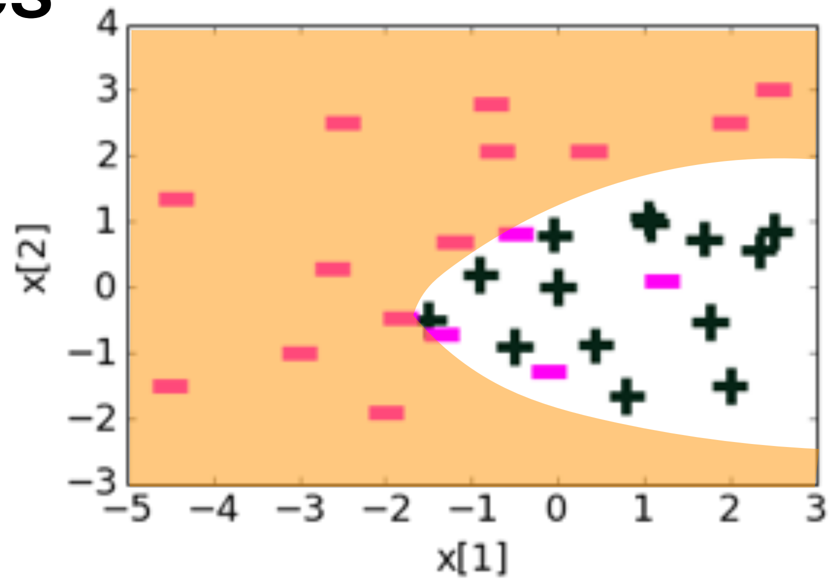
# Adding quadratic features



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| $h_3(x)$ | $(x[1])^2$ | -0.17 |
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- Adding more features gives more complex models
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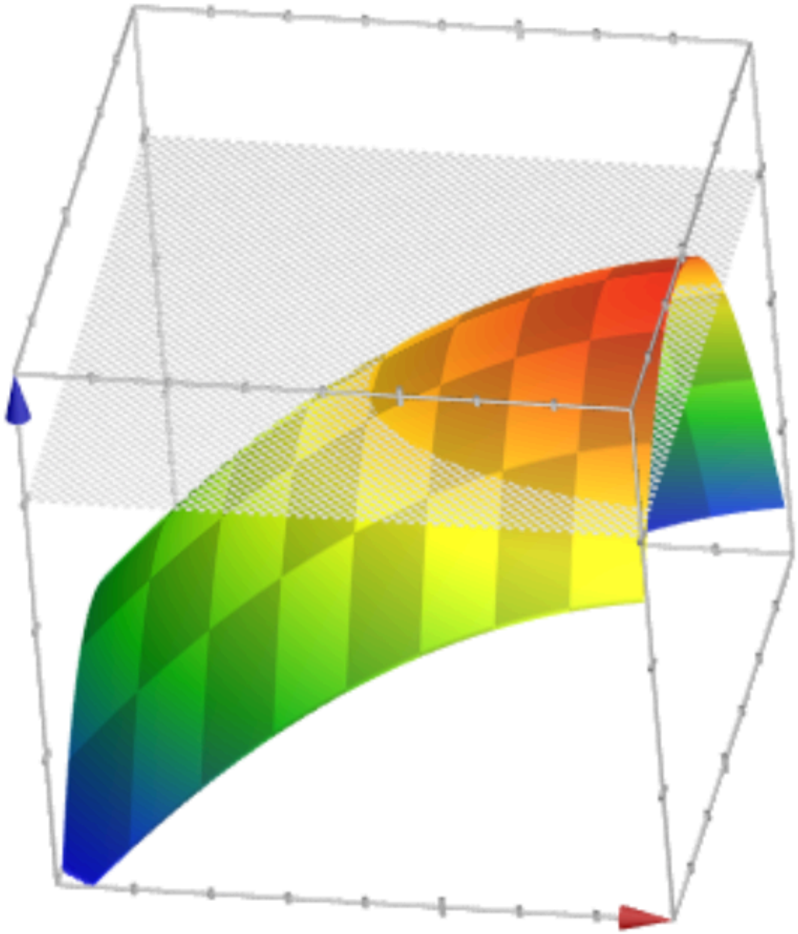

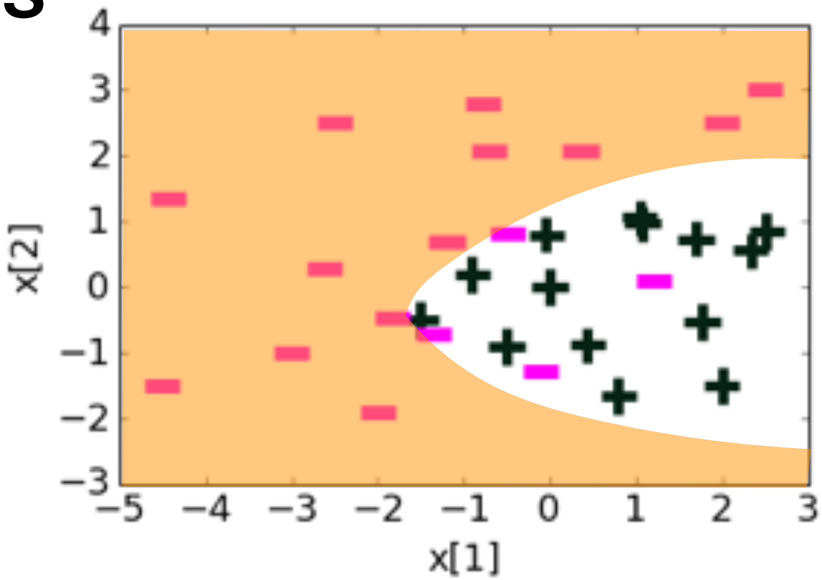


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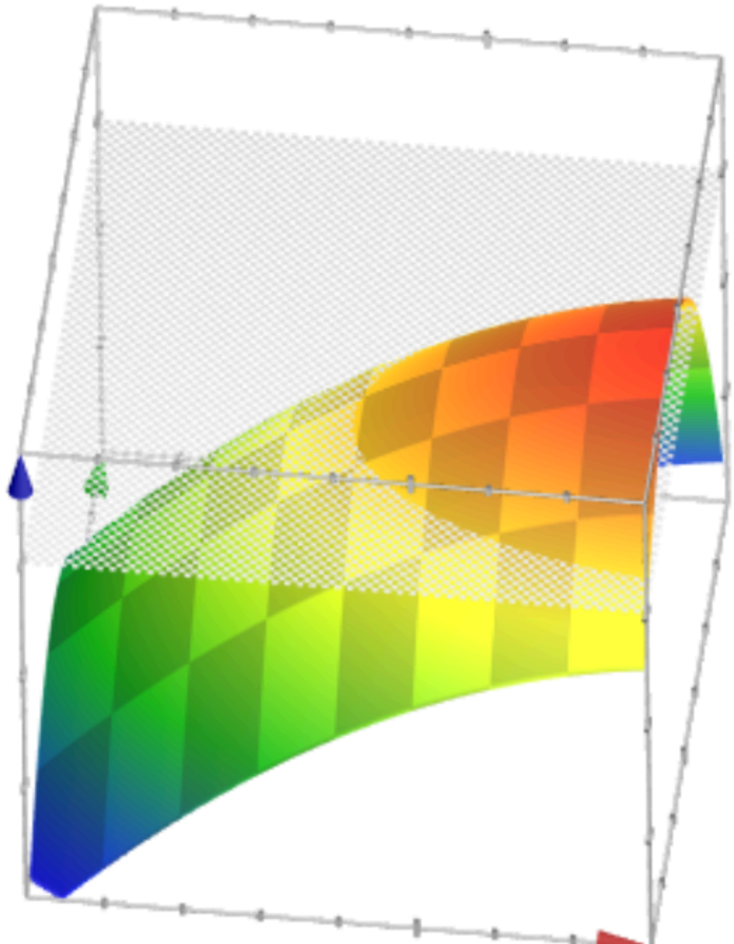

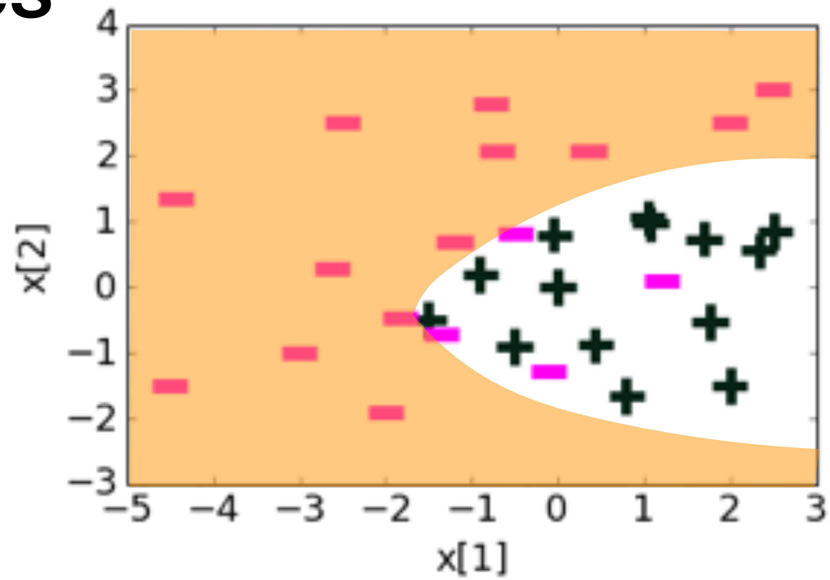


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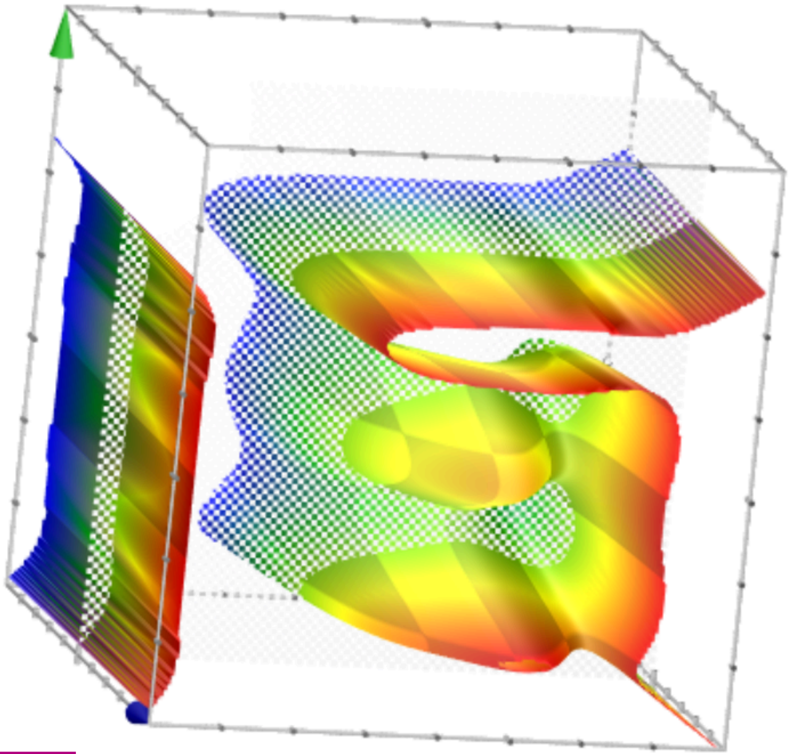
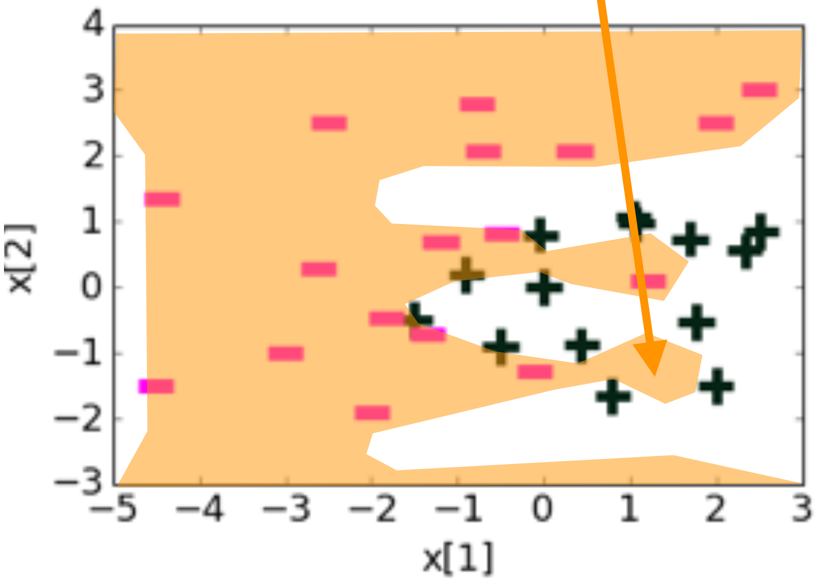


Overfitting leads to non-generalization




| Feature | Value | Coefficient learned |
|---|---|---|
| $h_0(x)$ | 1 | 21.6 |
| $h_1(x)$ | x[1] | 5.3 |
| $h_2(x)$ | x[2] | -42.7 |
| $h_3(x)$ | $(x[1])^2$ | -15.9 |
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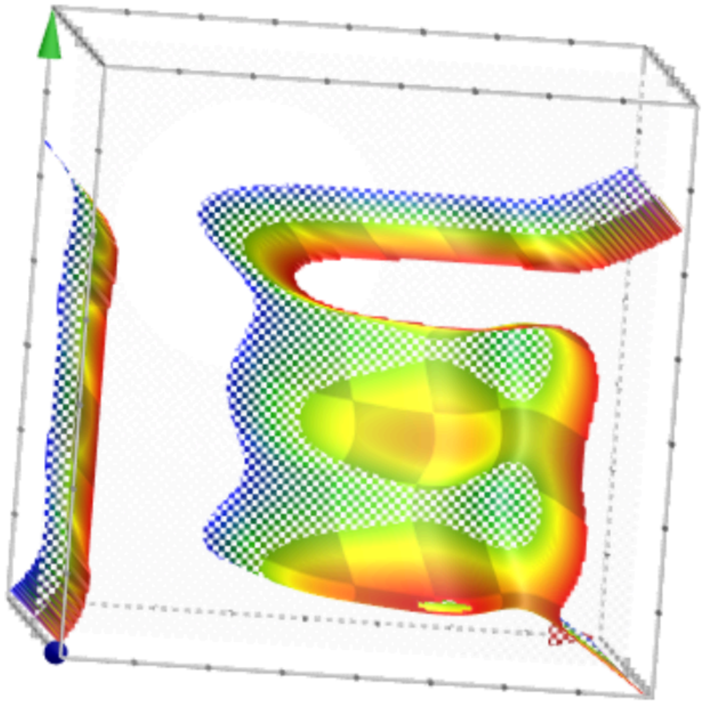

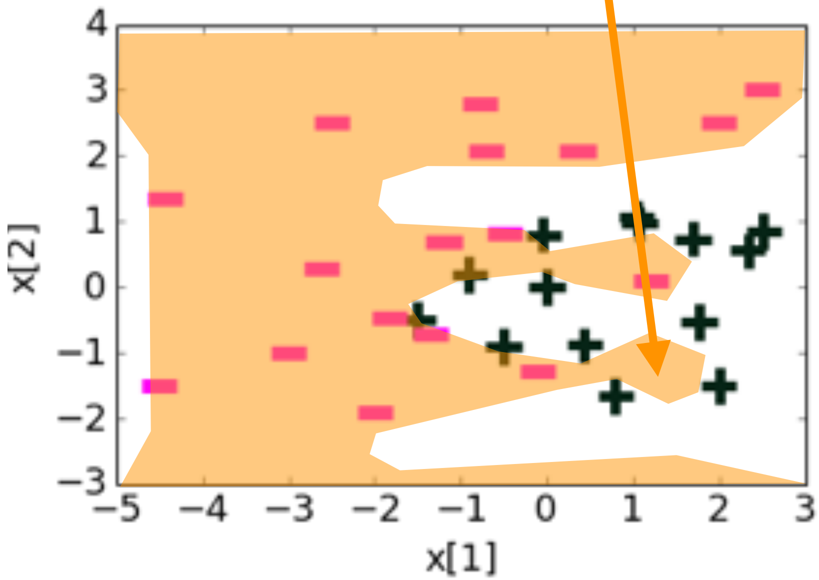


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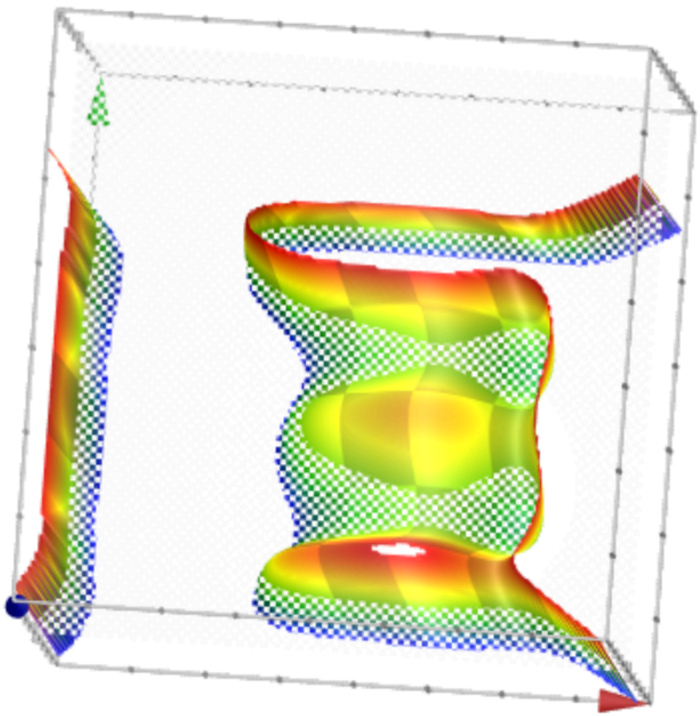

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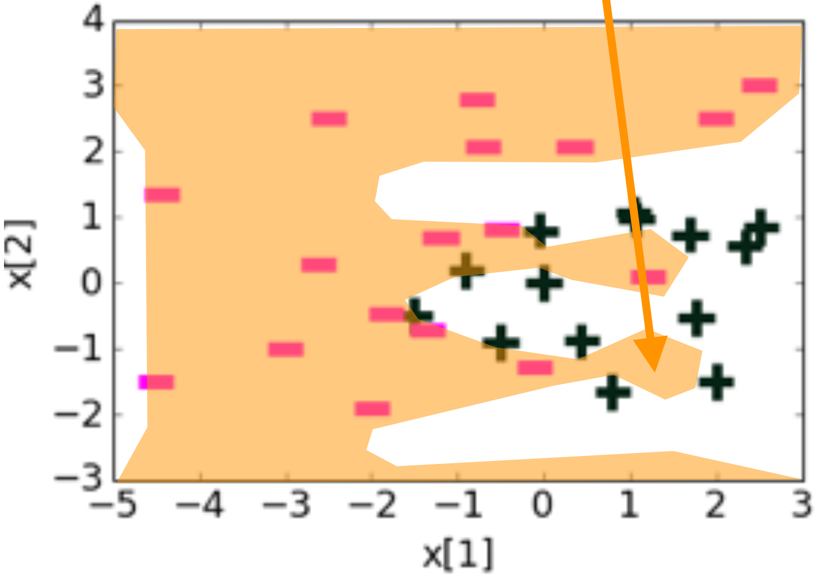


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# Creating Features

- Feature mapping $\phi : \mathbb{R}^d \rightarrow \mathbb{R}^p$ maps original data into a rich and high-dimensional feature space (usually $d \ll p$)

For example, in d=1, one can use

$$\phi(x) = \begin{bmatrix} \phi_1(x) \\ \phi_2(x) \\ \vdots \\ \phi_k(x) \end{bmatrix} = \begin{bmatrix} x \\ x^2 \\ \vdots \\ x^k \end{bmatrix}$$

For example, for d>1,
one can generate vectors

and define features:

$$\phi_j(x) = \cos(u_j^T x)$$

$$\phi_j(x) = (u_j^T x)^2$$

$$\phi_j(x) = \frac{1}{1 + \exp(u_j^T x)}$$

- Feature space can get really large really quickly!
- How many coefficients/parameters are there for degree-$k$ polynomials for $x = (x_1, \ldots, x_d) \in \mathbb{R}^d$ ?
- At a first glance, it seems inevitable that we need memory (to store the features $\{\phi(x_i) \in \mathbb{R}^p\}_{i=1}^n$) and run-time that increases with $p$ where $d < n \ll p$

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# How do we deal with high-dimensional lifts/data?

## A fundamental trick in ML: use kernels

A function $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a *kernel* for a map $\phi$ if $K(x, x') = \phi(x) \cdot \phi(x')$ for all $x, x'$.

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then we can avoid explicitly computing and storing (high-dimensional) $\{\phi(x_i)\}_{i=1}^{n}$ and instead only work with the kernel matrix of the training data $\{K(x_i, x_j)\}_{i,j \in \{1,\ldots,n\}}$

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- Hence, to make prediction on any future data points, all we need to know is
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- Even if we run ridge linear regression on feature map $\phi(x) \in \mathbb{R}^p$, we only need to access the features via kernel $K(x_i, x_j)$ and $K(x_i, x_{\text{new}})$ and not the features $\phi(x_i)$

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  - The features are **implicit** and accessed only via kernels, making it efficient

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4. Make prediction with $\widehat{y}_{\text{new}} = \sum_{i=1}^n \alpha_i K(x_i, x_{\text{new}})$

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(Solve for $\widehat{\alpha}_{\text{kernel}}$)

Thus, $\widehat{\alpha}_{\text{kernel}} = (\mathbf{K} + \lambda \mathbf{I}_{n \times n})^{-1} \mathbf{y}$

# Examples of popular Kernels

- **Polynomials of degree exactly $k$**

$$K(x, x') = (x^T x')^k$$

- **Polynomials of degree up to $k$**

$$K(x, x') = (1 + x^T x')^k$$

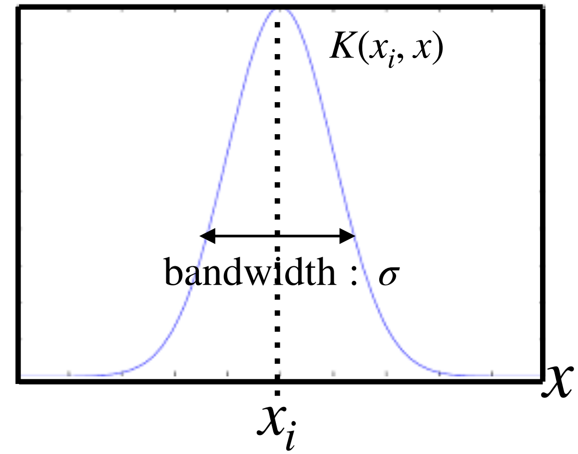
- **Gaussian (squared exponential) kernel**
  (a.k.a RBF kernel for Radial Basis Function)

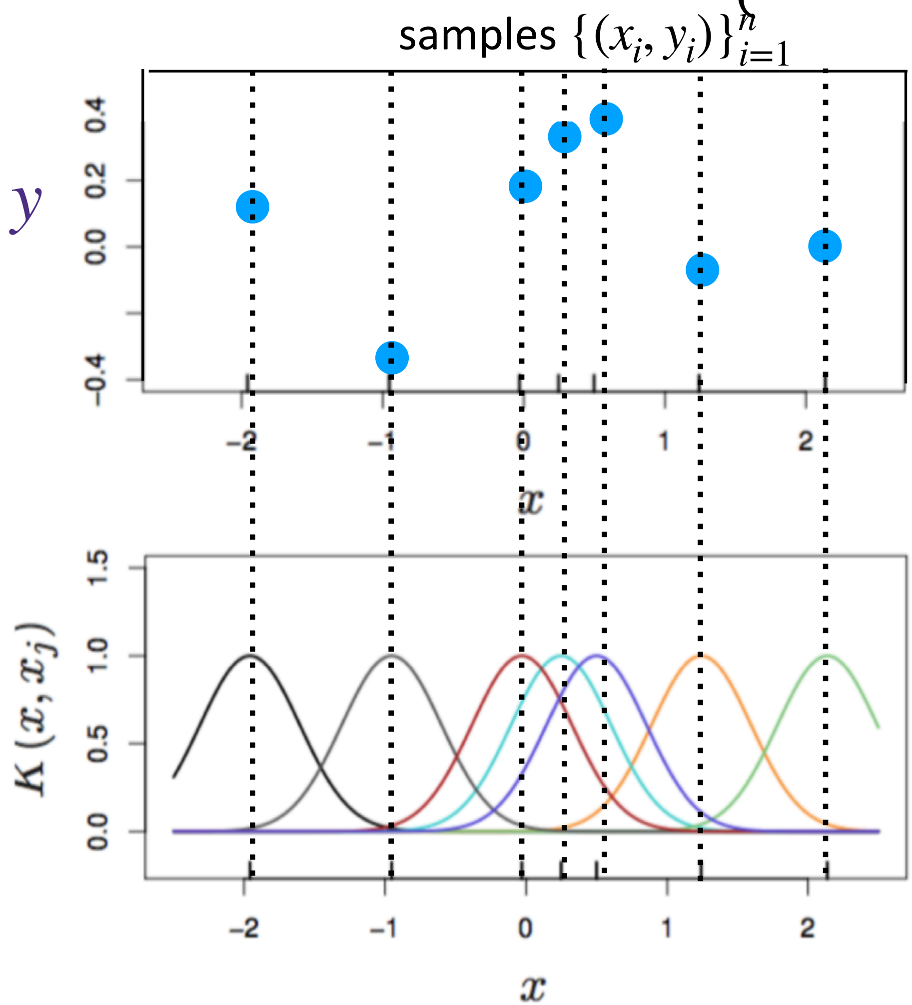
$$K(x, x') = \exp\Big( - \frac{\|x - x'\|_2^2}{2\sigma^2} \Big)$$

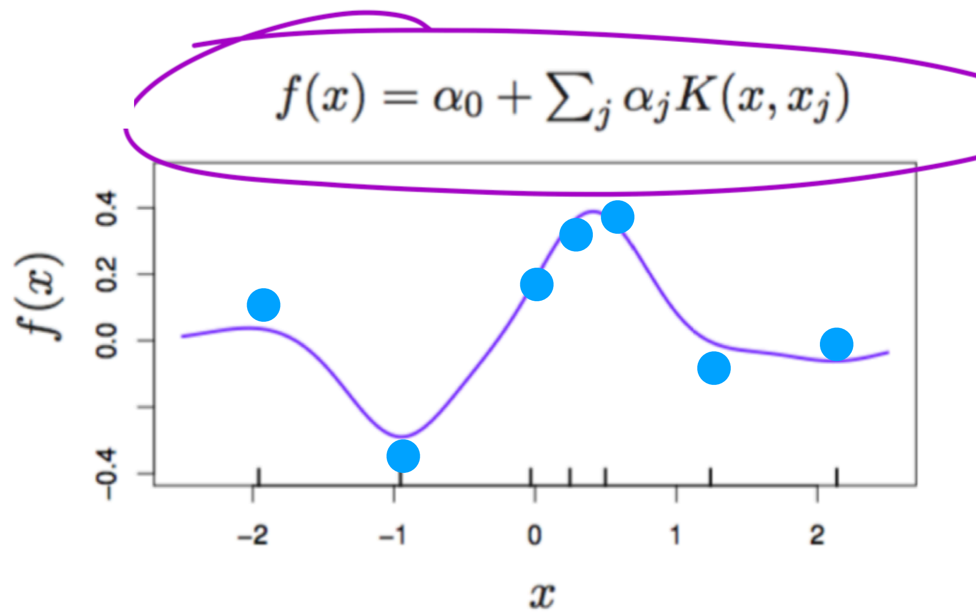
- **Sigmoid**

$$K(x, x') = \tanh(\gamma x^T x' + r)$$

RBF kernel $k(x_i, x) = \exp\left\{ -\frac{\|x_i - x\|_2^2}{2\sigma^2} \right\}$



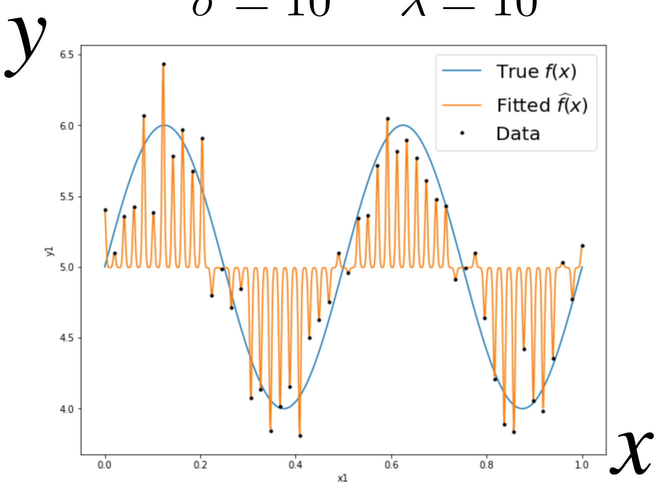




- predictor $f(x) = \sum_{i=1}^{n} \alpha_i K(x_i, x)$ is taking weighted sum of $n$ kernel functions centered at each sample points

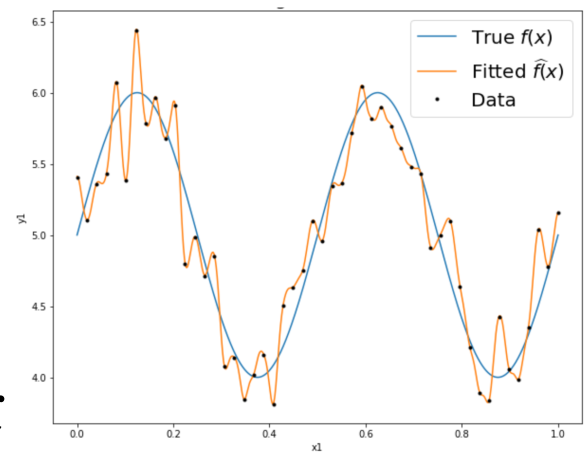
# RBF kernel $k(x_i, x) = \exp\left\{ -\frac{\|x_i - x\|_2^2}{2\sigma^2} \right\}$

- $\mathscr{L}(\alpha) \;=\; \|\mathbf{K}\alpha - \mathbf{y}\|_2^2 \;+\; \lambda \alpha^T K \alpha$
- The bandwidth $\sigma^2$ of the kernel regularizes the predictor, and the regularization coefficient $\lambda$ also regularizes the predictor

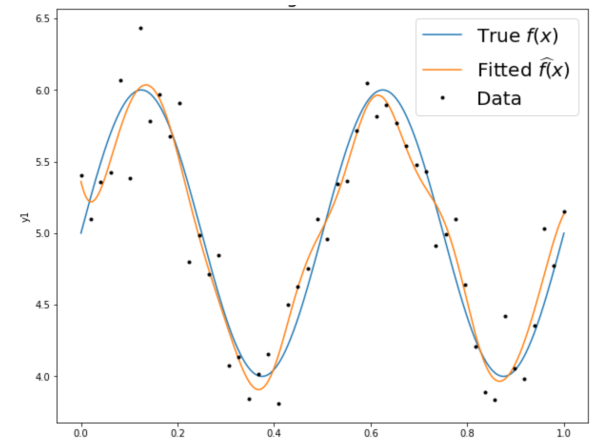
$\sigma = 10^{-3} \;\; \lambda = 10^{-4}$



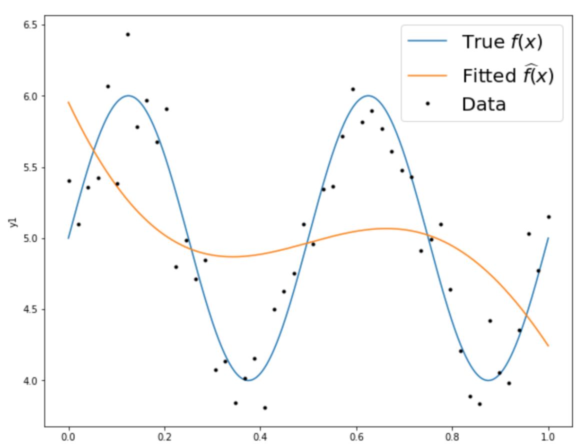

$\sigma = 10^{-2} \;\; \lambda = 10^{-4}$




$\sigma = 10^{-1} \;\; \lambda = 10^{-4}$

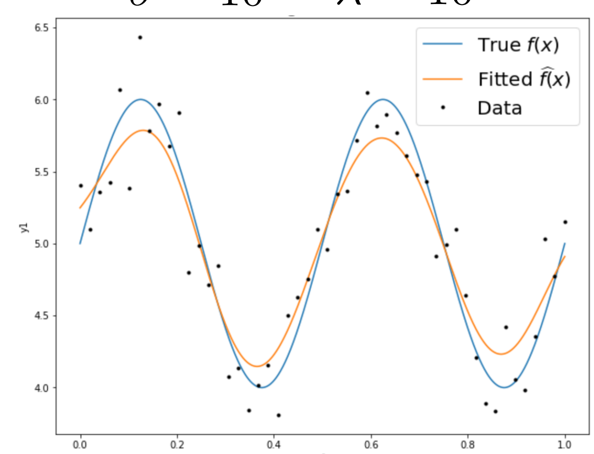



$\sigma = 10^{-0} \;\; \lambda = 10^{-4}$




$$\widehat{f}(x) = \sum_{i=1}^{n} \widehat{\alpha}_i K(x_i, x)$$

$\sigma = 10^{-1} \;\; \lambda = 10^{-0}$

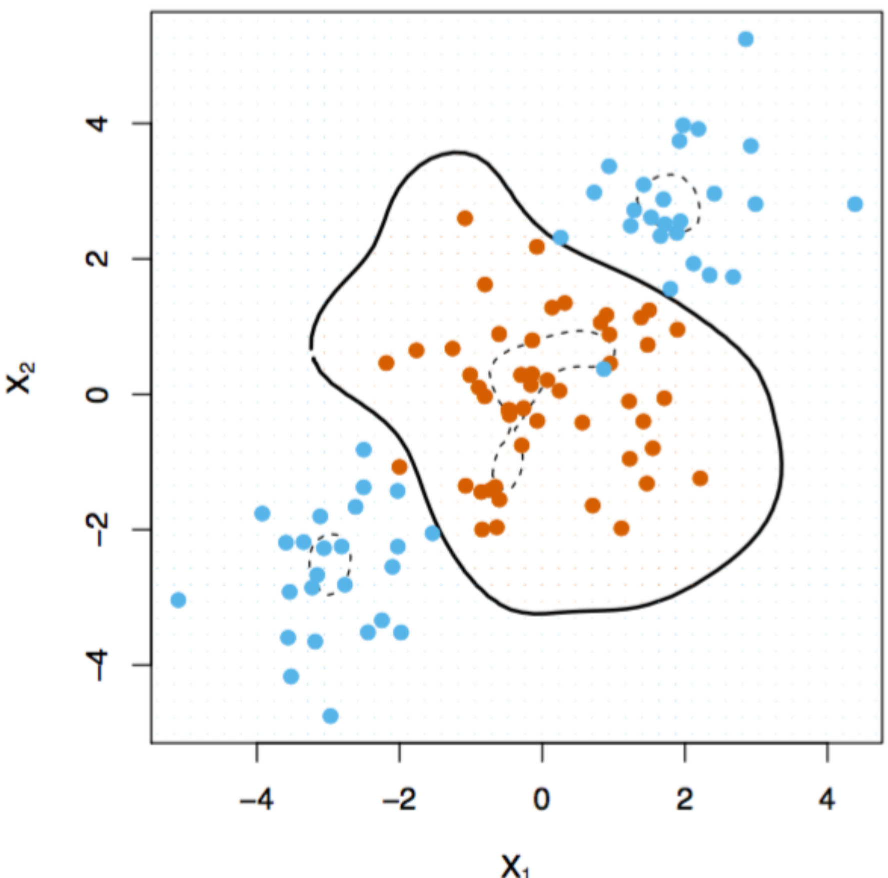


# RBF kernel for SVMs

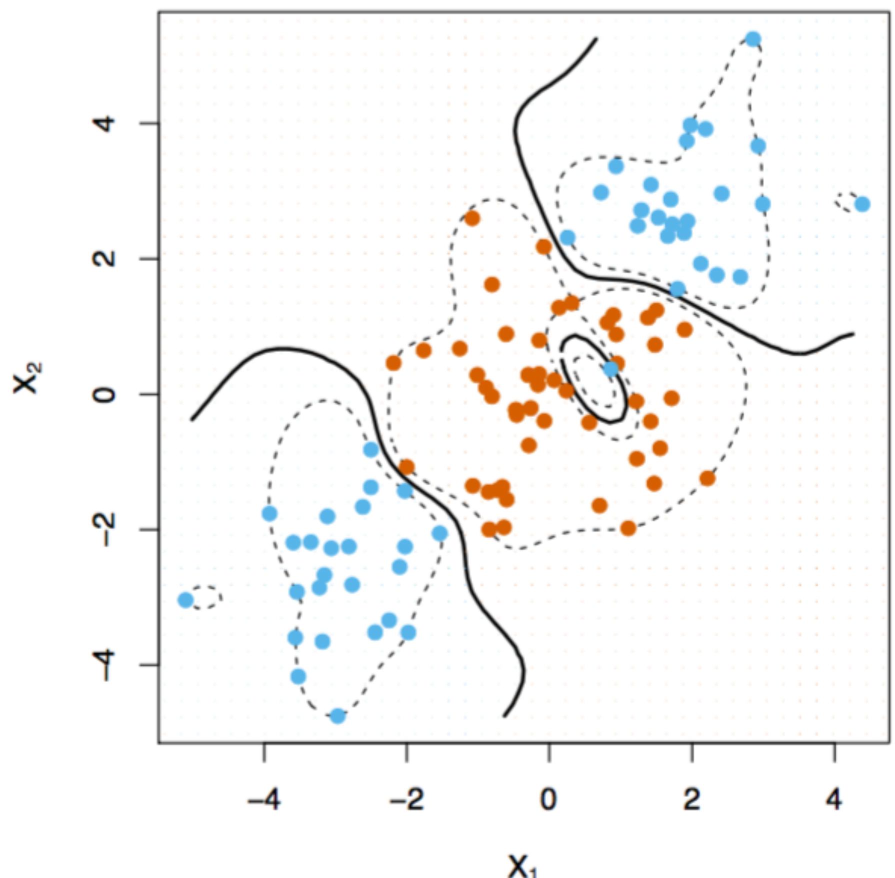
$$\widehat{w} = \arg\min_{w,b} \frac{1}{n}\sum_{i=1}^{n} \max\{0, 1 - y_i(b + w^T x_i)\} + \lambda \|w\|_2^2$$

$$\widehat{\alpha}, \widehat{b} = \arg\min_{\alpha \in \mathbb{R}^n, b} \frac{1}{n}\sum_{i=1}^{n} \max\{0, 1 - y_i(b + \sum_{j=1}^{n} \alpha_j K(x_j, x_i))\} + \lambda \sum_{i=1, j=1}^{n} \alpha_i \alpha_j K(x_i, x_j)$$

Bandwidth $\sigma$ is large enough




Bandwidth $\sigma$ is small



# Bootstrap

# Confidence intervals

- Suppose you have training data $\{(x_i, y_i)\}_{i=1}^n$ drawn i.i.d. from some true distribution $P_{x,y}$
- We train a kernel ridge regressor, with some choice of a kernel $K : \mathbb{R}^{d\times d} \to \mathbb{R}$

$$\text{minmize}_\alpha \ \|\mathbf{K}\alpha - \mathbf{y}\|_2^2 + \lambda \alpha^T \mathbf{K}\alpha$$

- The resulting predictor is

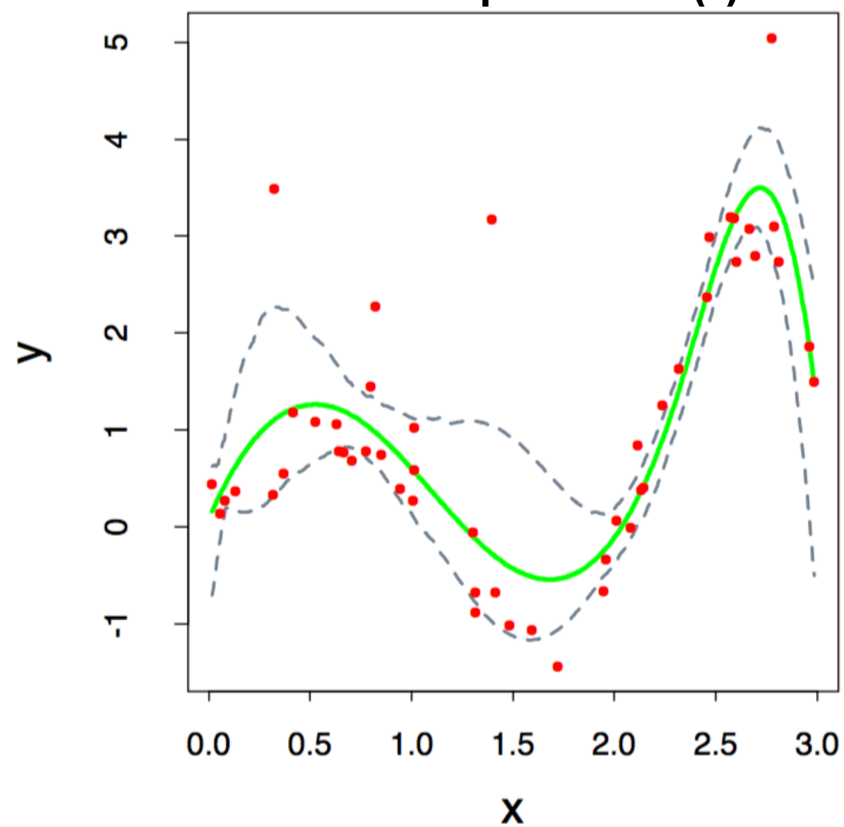
$$f(x) \ = \ \sum_{i=1}^n K(x_i, x)\hat{\alpha}_i,$$

where

$$\hat{\alpha} \ = \ (\mathbf{K} + \lambda \mathbf{I})^{-1}\mathbf{y} \quad \in \mathbb{R}^n$$

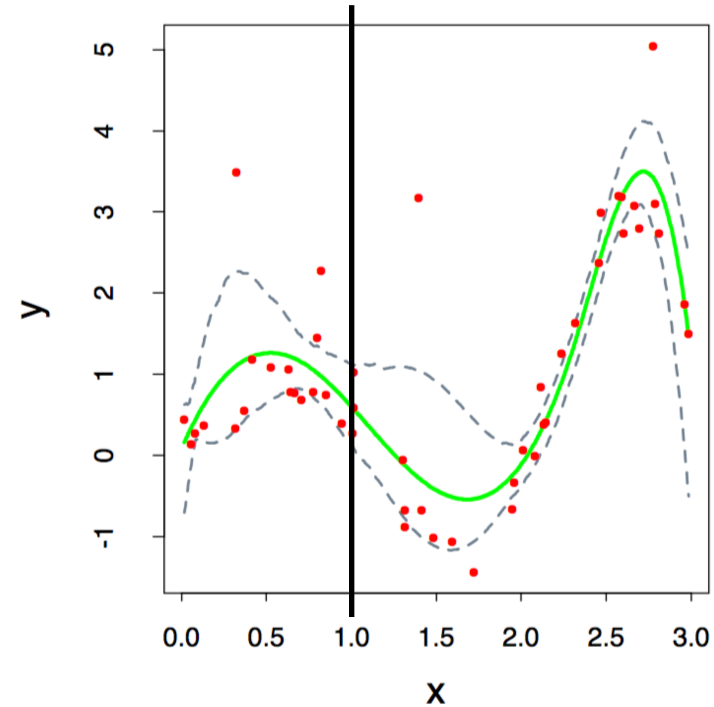
- We wish to build a confidence interval for our predictor $f(x)$, using 5% and 95% percentiles

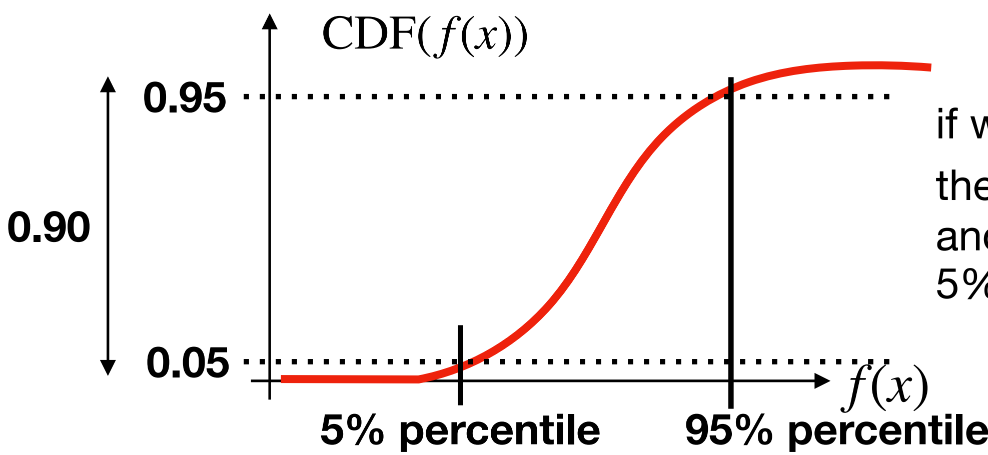
**Example of 5% and 95% percentile curves for predictor f(x)**



# Confidence intervals

- Let's focus on a single $x \in \mathbb{R}^d$
- Note that our predictor $f(x)$ is a random variable, whose randomness comes from the training data $S_{\text{train}} = \{(x_i, y_i)\}_{i=1}^n$
- If we know the statistics (in particular the CDF of the random variable $f(x)$) of the predictor, then the **confidence interval** with **confidence level 90%** is defined as



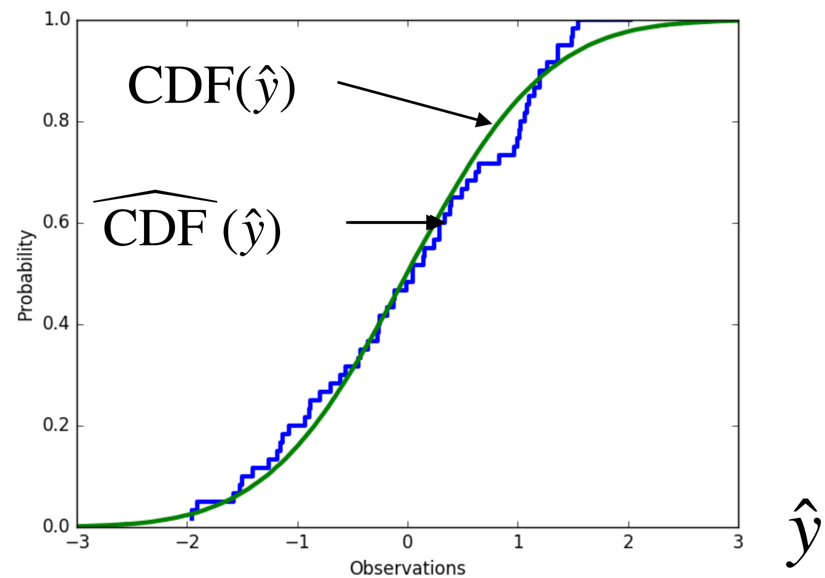

if we know the distribution of our predictor $f(x)$, the green line is the expectation $\mathbb{E}[f(x)]$ and the black dashed lines are the 5% and 95% percentiles in the figure above

- As we do not have the cumulative distribution function (CDF), we need to approximate them

# Confidence intervals

- Hypothetically, if we can sample as many times as we want, then we can train $B \in \mathbb{Z}^+$ i.i.d. predictors, each trained on $n$ fresh samples to get **empirical estimate of the CDF of** $\hat{y} \;=\; f(x)$

- For b=1,…,B
  - Draw $n$ fresh samples $\{(x_i^{(b)}, y_i^{(b)})\}_{i=1}^n$
  - Train a regularized kernel regression $\alpha^{*(b)}$
  - Predict $\hat{y}^{(b)} \;=\; \sum_{i=1}^{n} K(x_i^{(b)}, x)\alpha_i^{*(b)}$




- Let the empirical CDF of those B predictors $\{\hat{y}^{(b)}\}_{b=1}^B$ be $\widehat{\mathrm{CDF}}(\hat{y})$, defined as

$$\widehat{\mathrm{CDF}}(\hat{y}) \;=\; \frac{1}{B}\sum_{b=1}^{B} \mathbf{I}\{\,\hat{y}^{(b)} \le \hat{y}\,\}$$

- Compute the confidence interval using $\widehat{\mathrm{CDF}}(\hat{y})$

# Bootstrap

- As we cannot sample repeatedly (in typical cases), we use **bootstrap samples** instead
- Bootstrap is a general tool for assessing statistical accuracy
- We learn it in the context of confidence interval for trained models

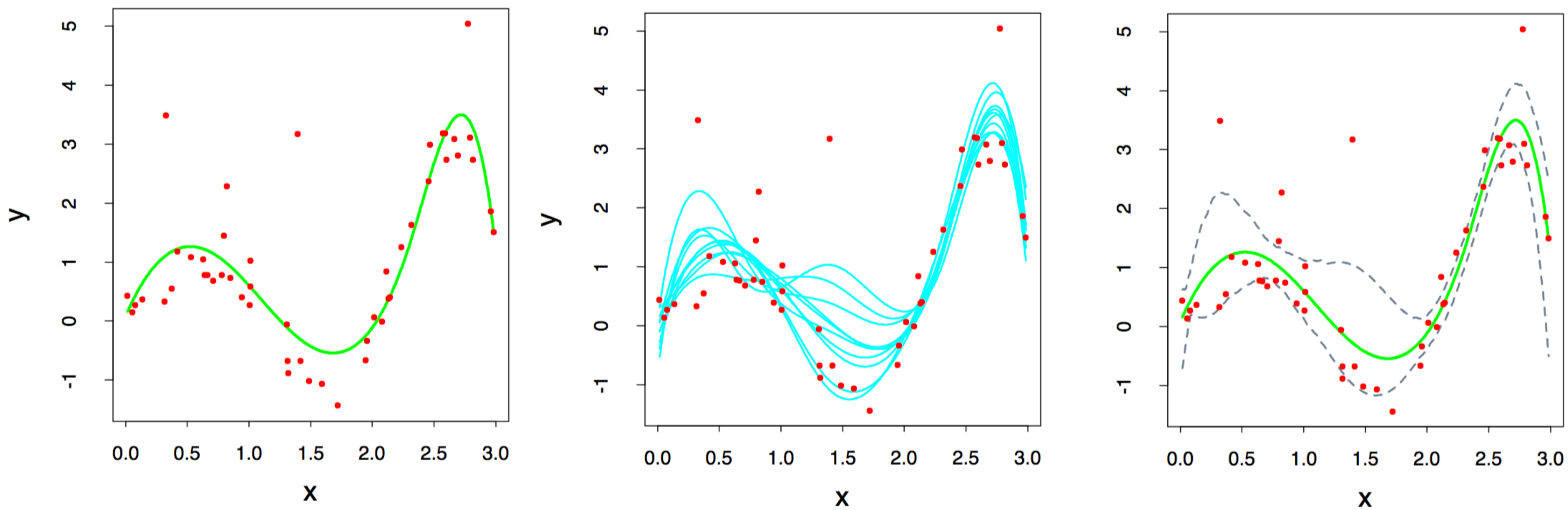
- A **bootstrap dataset** is created from the training dataset by taking $n$ (the same size as the training data) examples uniformly at random **with replacement** from the training data $\{(x_i, y_i)\}_{i=1}^n$

- For b=1,…,B
  - Create a bootstrap dataset $S_{\text{bootstrap}}^{(b)}$
  - Train a regularized kernel regression $\alpha^{*(b)}$
  - Predict $\hat{y}^{(b)} = \sum_{i=1}^{n} K(x_i^{(b)}, x)\alpha_i^{*(b)}$

- Compute the empirical CDF from the bootstrap datasets, and compute the confidence interval

# bootstrap

**training a single predictor** | **multiple bootstrapped predictors** | **90% confidence interval**




Figures from Hastie et al