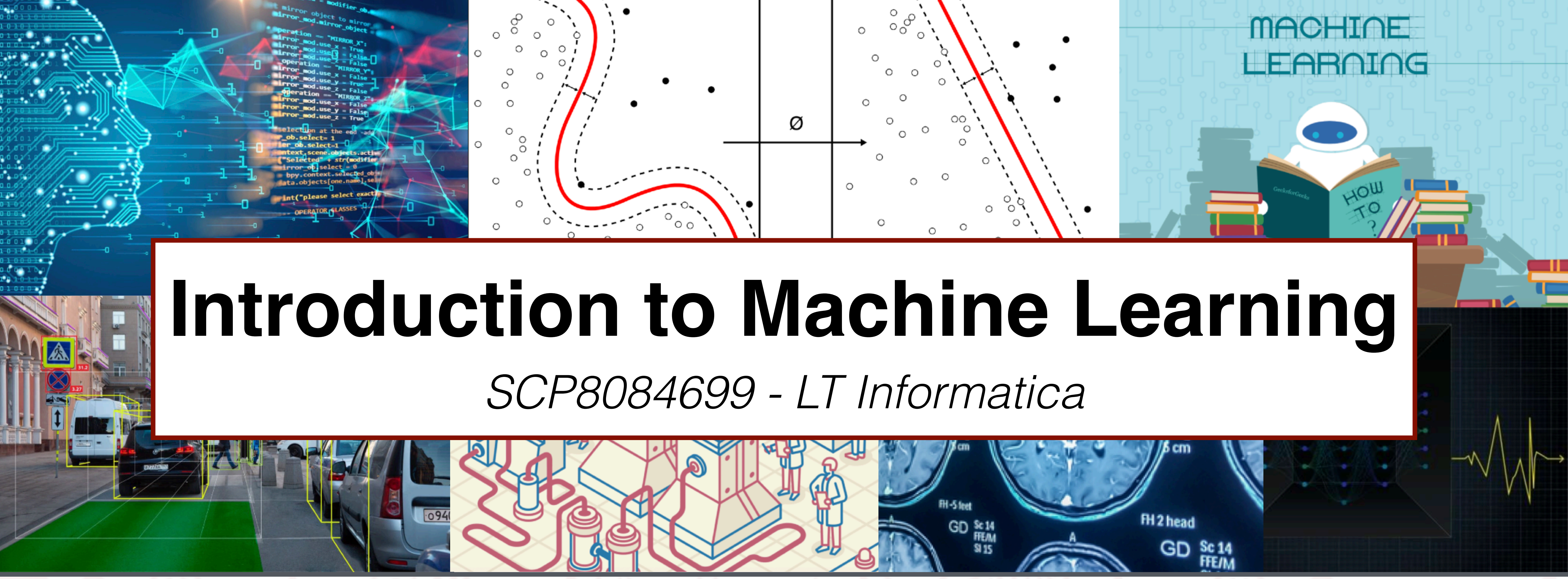

Introduction to Machine Learning

SCP8084699 - LT Informatica

Support Vector Machines: loss function

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University of Padova, A.Y. 2021/22 April 26, 2022

DIPARTIMENTO MATEMATICA
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What we learned until now

(a brief summary)

- By now you have seen a range of different machine learning algorithms
  - Linear regression / classification
  - Logistic regression
  - Artificial Neural Networks

Parametric models

Goal: $h_{\theta}(\mathbf{x})$, $\boldsymbol{\theta}$

- Regularization, bias-variance tradeoff, evaluation and diagnosing machine learning systems

Support Vector Machines (SVM)

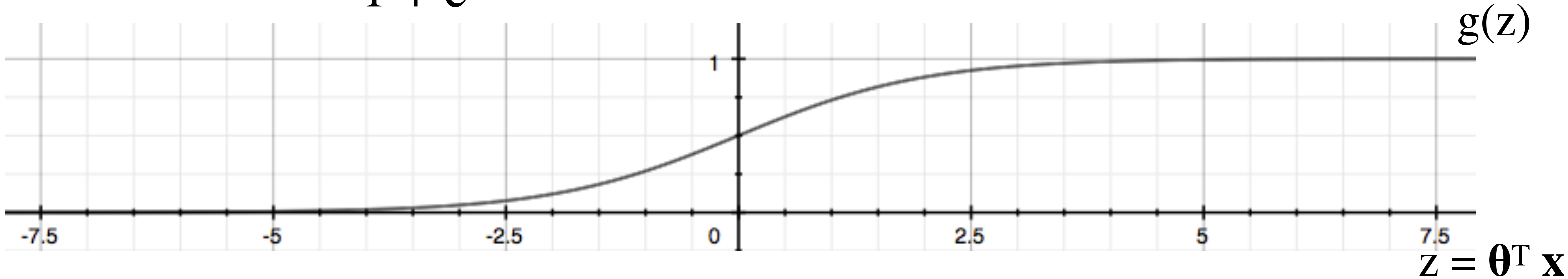
- SVM is a very powerful and popular algorithm
  - It is a <u>supervised learning</u> algorithm usually used for classification (but can be used also for regression)
  - It is a <u>non-probabilistic</u> (binary) classifier, although there are methods such as Platt scaling to give a probabilistic interpretation of the SVM output
  - It is a <u>linear classification</u> model but SVM can efficiently perform non-linear classification using the *kernel trick*

Another view on Logistic Regression

- Hypothesis representation:

$$h_\theta(\mathbf{x}) = g(\boldsymbol{\theta}^T \mathbf{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^T \mathbf{x}}}$$

where $g(z) = \dfrac{1}{1 + e^{-z}}$ (*Sigmoid* or *Logistic* function)



- Interpretation (i.e. what we'd like logistic regression to do):

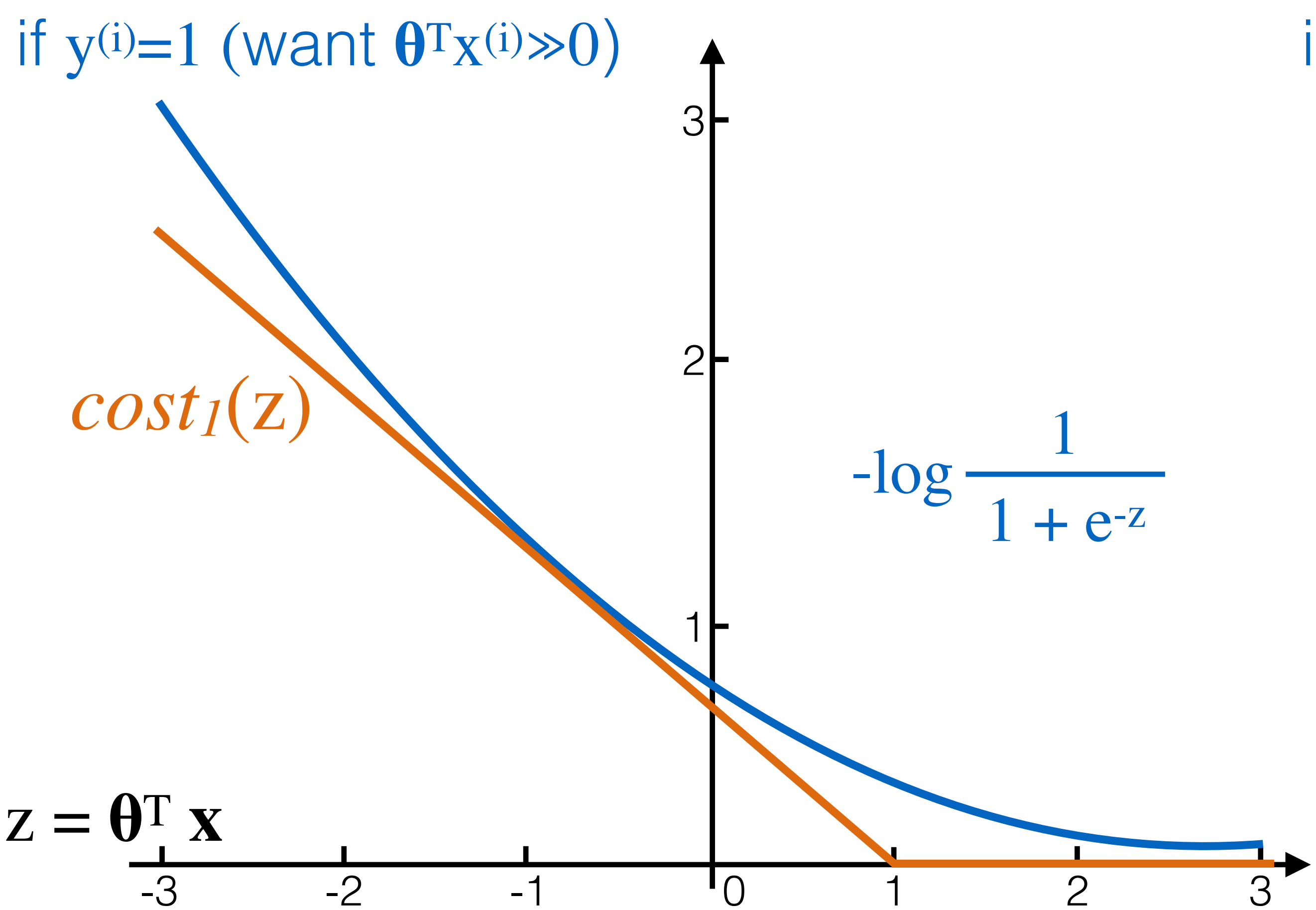
If $y = 1$, we want $h_\theta(\mathbf{x}) \approx 1$, $\boldsymbol{\theta}^T \mathbf{x} \gg 0$

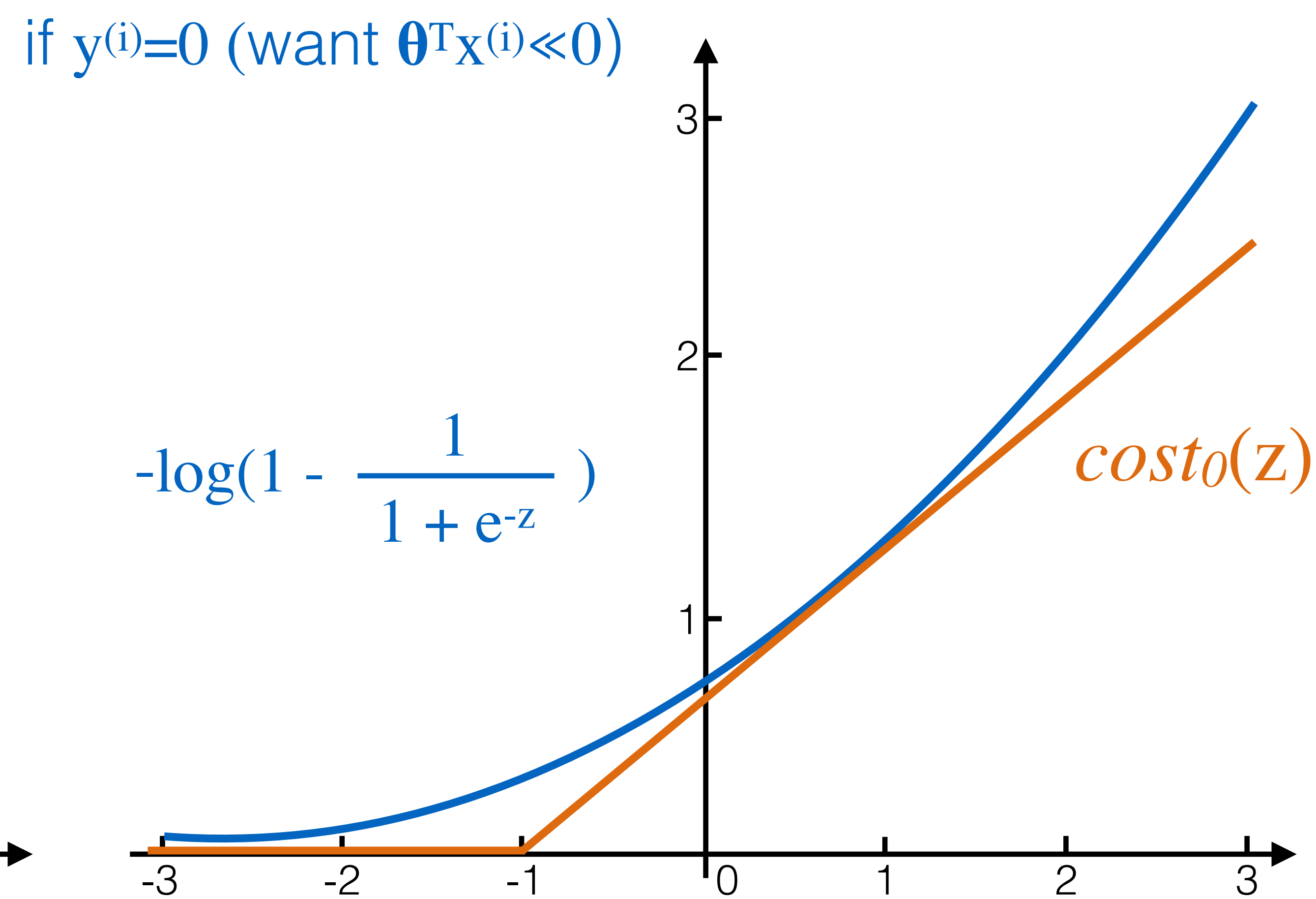
If $y = 0$, we want $h_\theta(\mathbf{x}) \approx 0$, $\boldsymbol{\theta}^T \mathbf{x} \ll 0$

Another view on Logistic Regression

- Loss function: $J(\boldsymbol{\theta}) = \frac{1}{m}\sum_{i=1}^{m} cost(h_\theta(x^{(i)}), y^{(i)})$ *where:*
    - If we take the definition for $h_\theta(\mathbf{x})$ and plug it in, we get:

$$cost(\cdot) = \boxed{-y^{(i)} \cdot \log\left(\frac{1}{1 + e^{-\boldsymbol{\theta}^T x^{(i)}}}\right)}\boxed{- (1 - y^{(i)}) \cdot \log\left(1 - \frac{1}{1 + e^{-\boldsymbol{\theta}^T x^{(i)}}}\right)}$$





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SVM: optimization objective

- (Regularized) Logistic Regression:

$$\min_{\theta} \frac{1}{m}\left[\sum_{i=1}^{m} -y^{(i)} \cdot \log(h_\theta(x^{(i)})) - (1 - y^{(i)}) \cdot \log(1 - h_\theta(x^{(i)}))\right] + \frac{\lambda}{2m}\sum_{j=1}^{n} \theta_j^2$$

- Support Vector Machine:

$$\min_{\theta} \frac{1}{\cancel{m}}\boxed{\left[\sum_{i=1}^{m} y^{(i)} \cdot cost_1(\boldsymbol{\theta}^T x^{(i)}) + (1-y^{(i)}) \cdot cost_0(\boldsymbol{\theta}^T x^{(i)})\right]} + \boxed{\frac{1\cancel{\lambda}}{2\cancel{m}}\sum_{j=1}^{n} \theta_j^2}$$

$$C\,A + B \quad , \quad C = \frac{1}{\lambda}$$

$$\Rightarrow \min_{\theta} C \sum_{i=1}^{m}\left[y^{(i)} \cdot (cost_1(\boldsymbol{\theta}^T x^{(i)})) + (1-y^{(i)}) \cdot (cost_0(\boldsymbol{\theta}^T x^{(i)}))\right] + \frac{1}{2}\sum_{j=1}^{n} \theta_j^2$$

SVM: large margin intuition

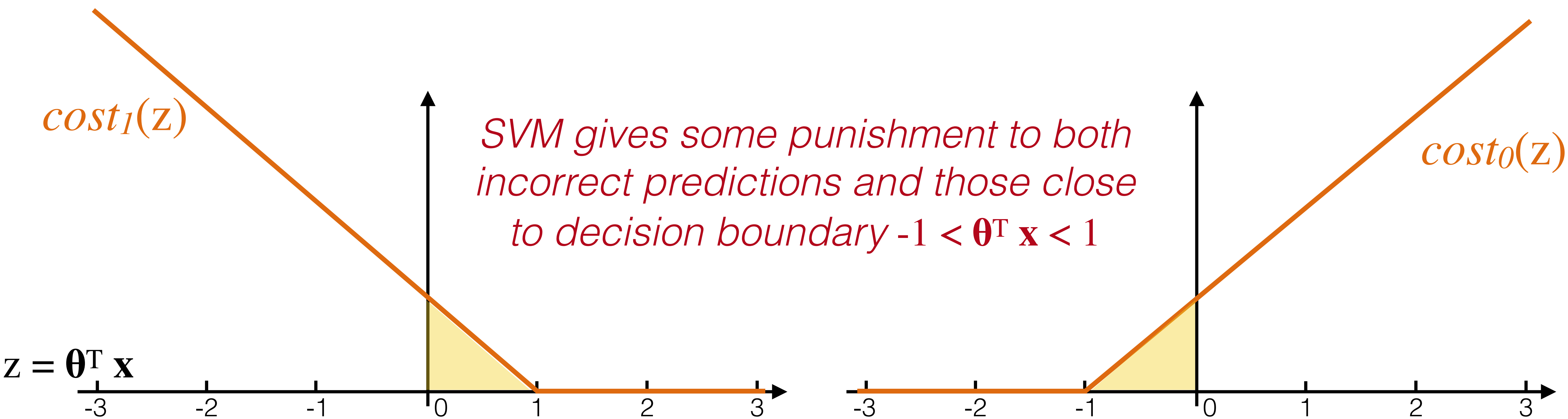
- Optimization objective:

$$\min_{\boldsymbol{\theta}} \; C \sum_{i=1}^{m} \left[y^{(i)} \cdot (cost_1(\boldsymbol{\theta}^T x^{(i)})) + (1-y^{(i)}) \cdot (cost_0(\boldsymbol{\theta}^T x^{(i)})) \right] + \frac{1}{2} \sum_{j=1}^{n} \theta_j^2$$

  - Interpretation (i.e. what we'd like SVM to do):

    If $y^{(i)} = 1$, we want $\boldsymbol{\theta}^T x^{(i)} \geq 1$ (not just ≥ 0)

    If $y^{(i)} = 0$, we want $\boldsymbol{\theta}^T x^{(i)} \leq -1$ (not just < 0)

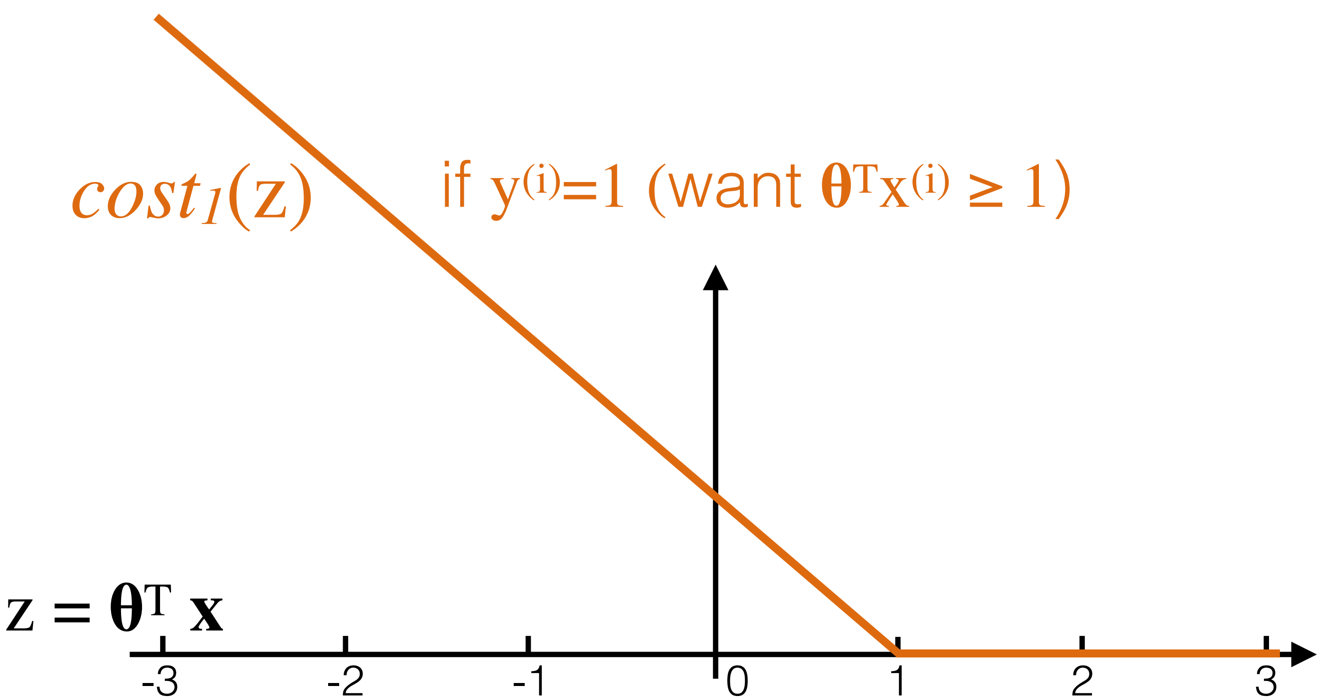


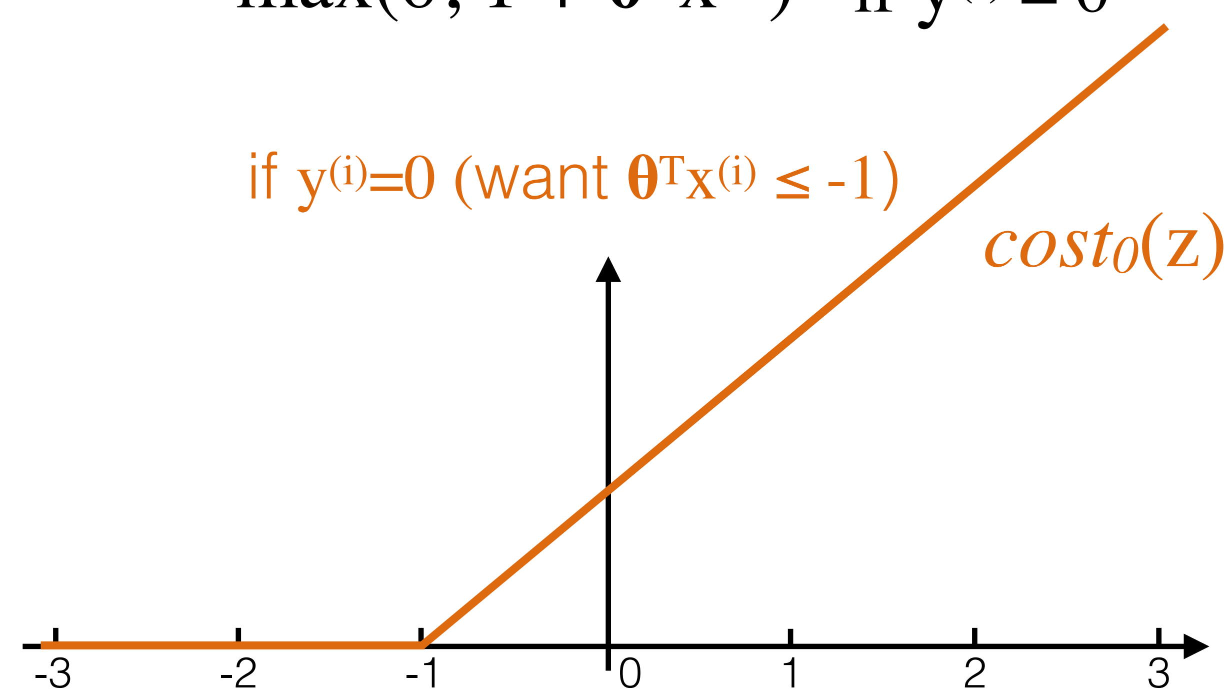
SVM: hypothesis and loss function

- Optimization objective:

$$\min_{\boldsymbol{\theta}} C \sum_{i=1}^{m} \left[y^{(i)} \cdot \left(cost_1(\boldsymbol{\theta}^T x^{(i)})\right) + (1-y^{(i)}) \cdot \left(cost_0(\boldsymbol{\theta}^T x^{(i)})\right) \right] + \frac{1}{2} \sum_{j=1}^{n} \theta_j^2$$

- Let's write the SVM's loss: $J(\boldsymbol{\theta}) = \sum_{i=1}^{m} cost(h_\theta(x^{(i)}), y^{(i)})$
  - Hinge loss: $cost(h_\theta(x^{(i)}), y^{(i)}) = \begin{cases} \max(0, 1 - \boldsymbol{\theta}^T x^{(i)}) & \text{if } y^{(i)} = 1 \\ \max(0, 1 + \boldsymbol{\theta}^T x^{(i)}) & \text{if } y^{(i)} = 0 \end{cases}$

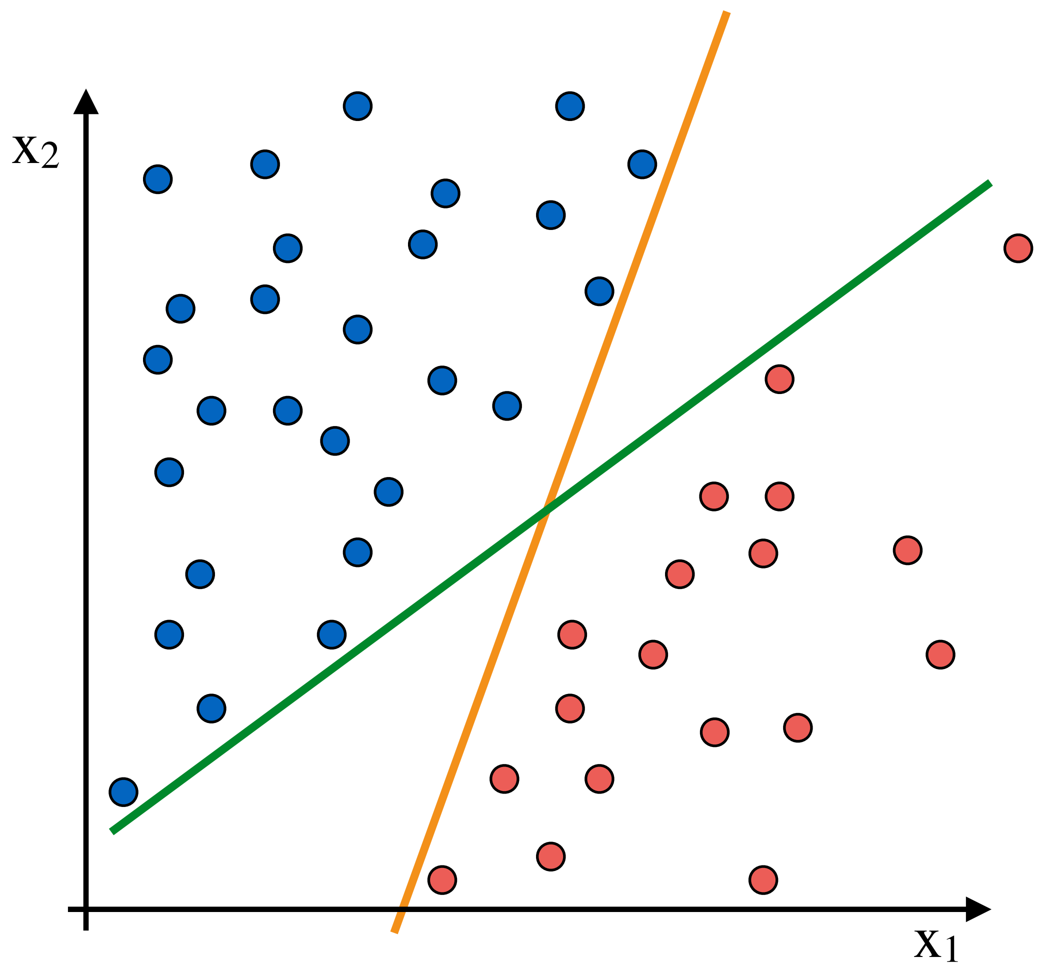




SVM: decision boundary

- Large margin intuition:

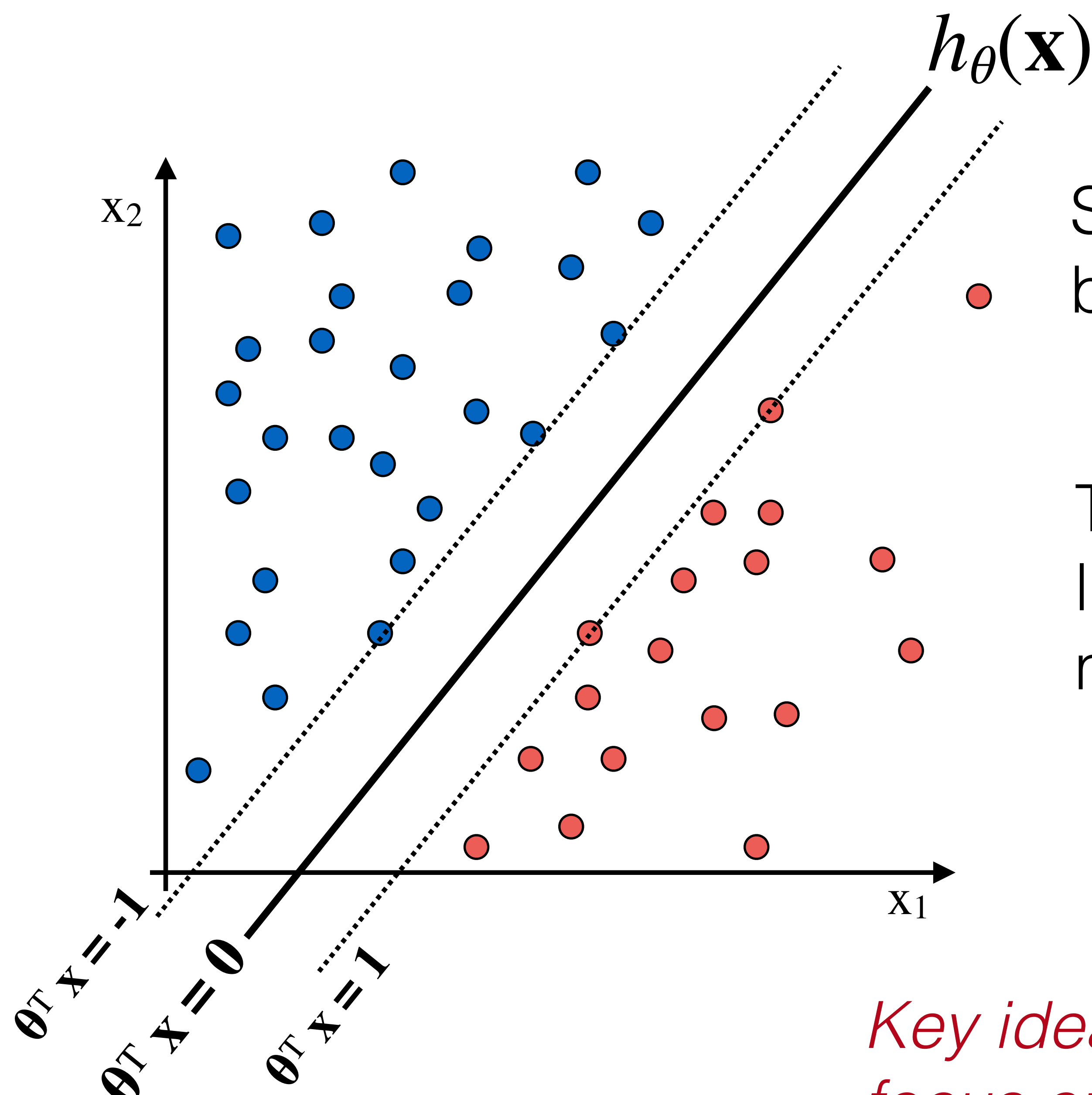
(Linearly separable case)



Let's start with two possible lines…

SVM: decision boundary

- Large margin intuition:



SVM will instead pick a decision boundary such as this one

This decision boundary has a larger min distance from any of my training samples

Key idea: instead of fitting all the points focus on boundary points

SVM: decision boundary

- Optimization objective:

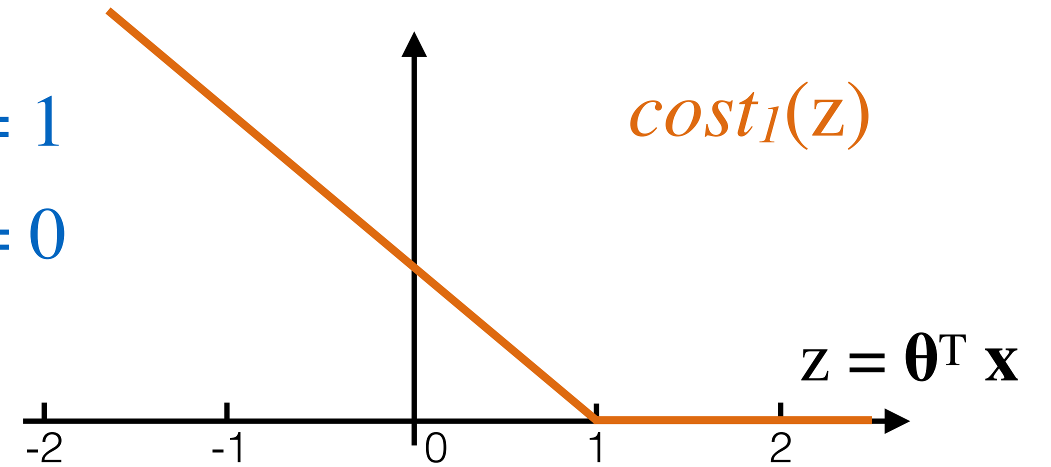
$$\min_{\boldsymbol{\theta}} \; C \boxed{\sum_{i=1}^{m} \left[y^{(i)} \cdot \left(cost_1(\boldsymbol{\theta}^T x^{(i)})\right) + (1-y^{(i)}) \cdot \left(cost_0(\boldsymbol{\theta}^T x^{(i)})\right) \right]} + \frac{1}{2} \sum_{j=1}^{n} \theta_j^2$$

e.g. $C \approx 10^5$ $\qquad\qquad\qquad\qquad \approx 0$

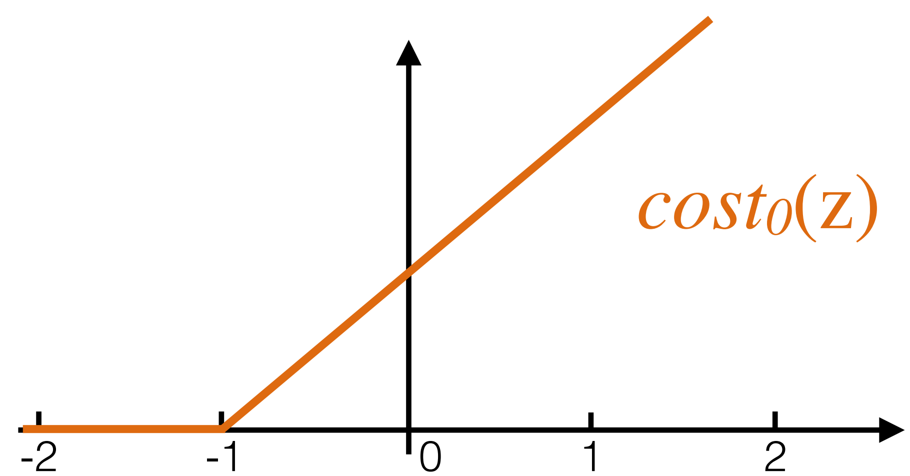
$$\min_{\boldsymbol{\theta}} \; \frac{1}{2} \sum_{j=1}^{n} \theta_j^2 \quad \text{s.t.} \quad \boldsymbol{\theta}^T \mathbf{x}^{(i)} \geq 1 \text{ if } y^{(i)} = 1$$

$$\boldsymbol{\theta}^T \mathbf{x}^{(i)} \leq -1 \text{ if } y^{(i)} = 0$$

Whenever $y^{(i)} = 1$: $\quad \boldsymbol{\theta}^T x^{(i)} \geq 1$



Whenever $y^{(i)} = 0$: $\quad \boldsymbol{\theta}^T x^{(i)} \leq -1$

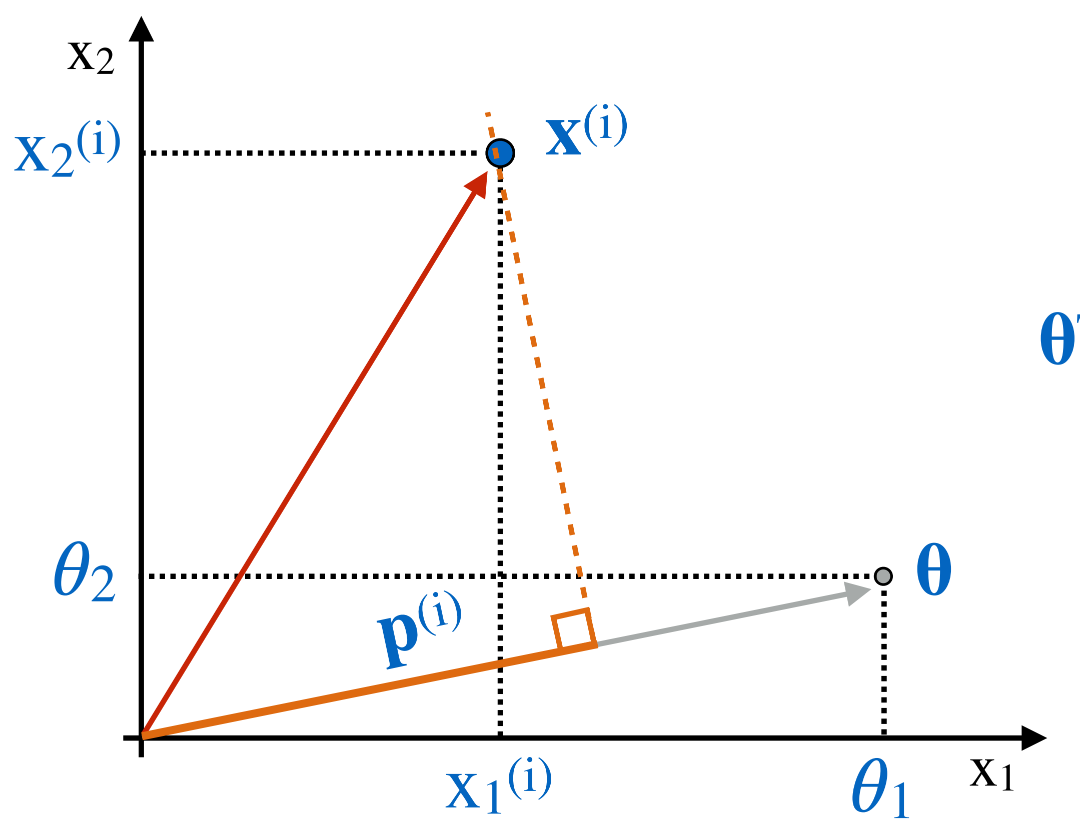


SVM: decision boundary

- Optimization objective:

$$\min_{\boldsymbol{\theta}} \frac{1}{2}\sum_{j=1}^{n}\theta_j^2 = \frac{1}{2}(\theta_1^2+\theta_2^2) = \frac{1}{2}\sqrt{(\theta_1^2+\theta_2^2)} = \frac{1}{2}\|\boldsymbol{\theta}\|^2$$

s.t. $\boxed{\begin{array}{l}\boldsymbol{\theta}^T \mathbf{x}^{(i)} \geq 1 \\ \boldsymbol{\theta}^T \mathbf{x}^{(i)} \leq -1\end{array}}$ $\begin{array}{l}\text{if } y^{(i)} = 1 \\ \text{if } y^{(i)} = 0\end{array}$ $\Rightarrow$ s.t. $\begin{array}{ll}\mathbf{p}^{(i)}\|\boldsymbol{\theta}\| \geq 1 & \text{if } y^{(i)} = 1 \\ \mathbf{p}^{(i)}\|\boldsymbol{\theta}\| \leq -1 & \text{if } y^{(i)} = 0\end{array}$



$$\boldsymbol{\theta}^T \mathbf{x}^{(i)} = \boxed{\mathbf{p}^{(i)}\|\boldsymbol{\theta}\|}$$

Thus we can write our optimization objective w.r.t. $\mathbf{p}^{(i)}$

SVM: decision boundary

- Optimization objective:

$$\min_{\boldsymbol{\theta}} \frac{1}{2} \sum_{j=1}^{n} \theta_j^2 = \frac{1}{2} \|\boldsymbol{\theta}\|^2$$

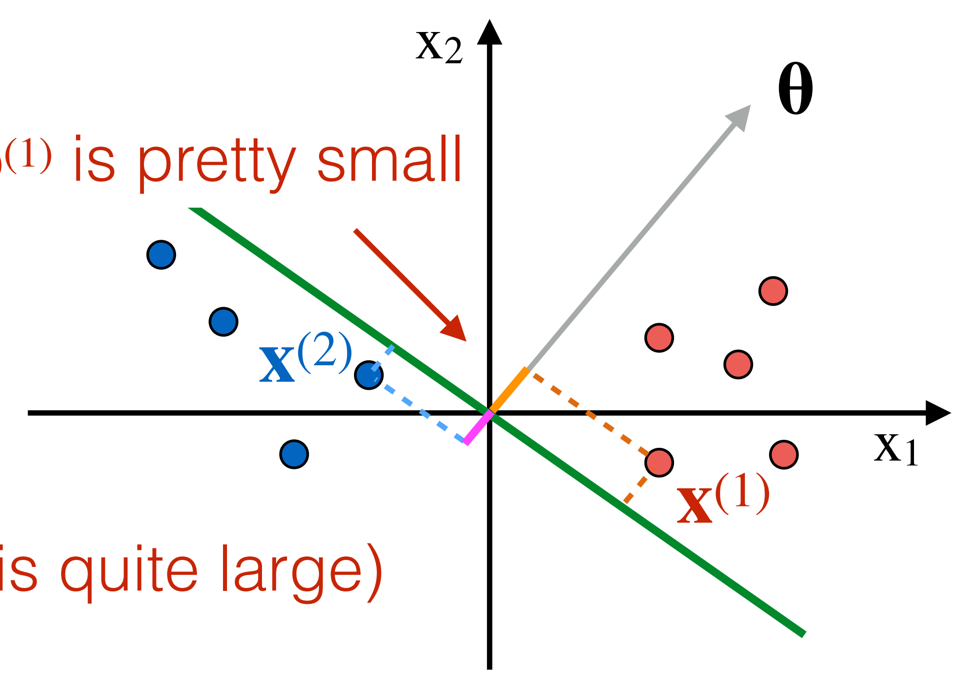
s.t. $\mathbf{p}^{(i)} \|\boldsymbol{\theta}\| \geq 1$ if $y^{(i)} = 1$

$\mathbf{p}^{(i)} \|\boldsymbol{\theta}\| \leq -1$ if $y^{(i)} = 0$

Where $\mathbf{p}^{(i)}$ is the projection of $\mathbf{x}^{(i)}$ onto the vector $\boldsymbol{\theta}$

- An example:

$\mathbf{p}^{(1)}$ is pretty small



(therefore $\|\boldsymbol{\theta}\|$ is quite large)

Adapted from slide by A. Ng

SVM: decision boundary

- Optimization objective:

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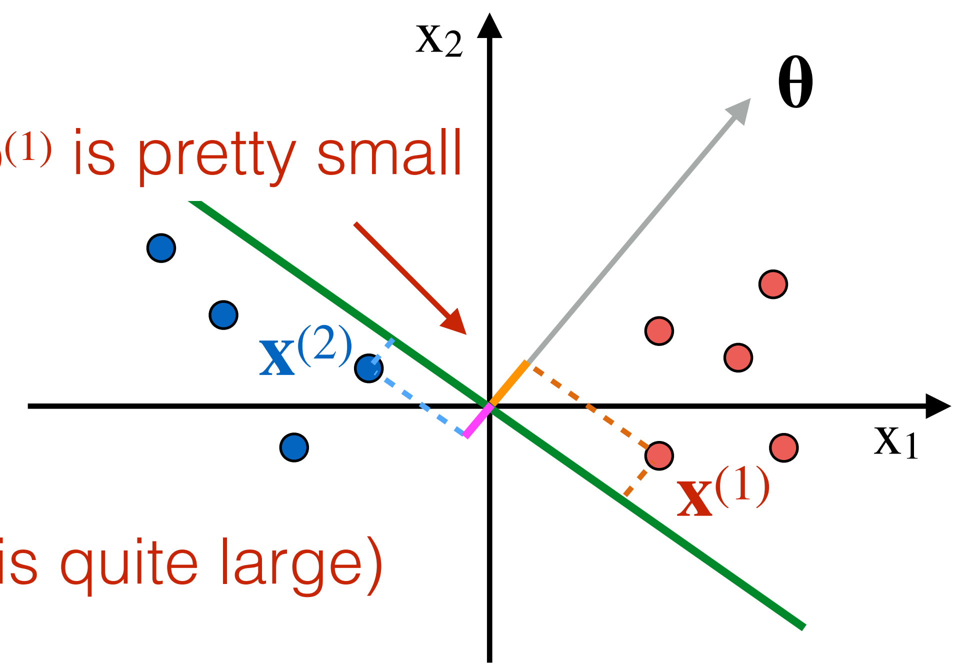

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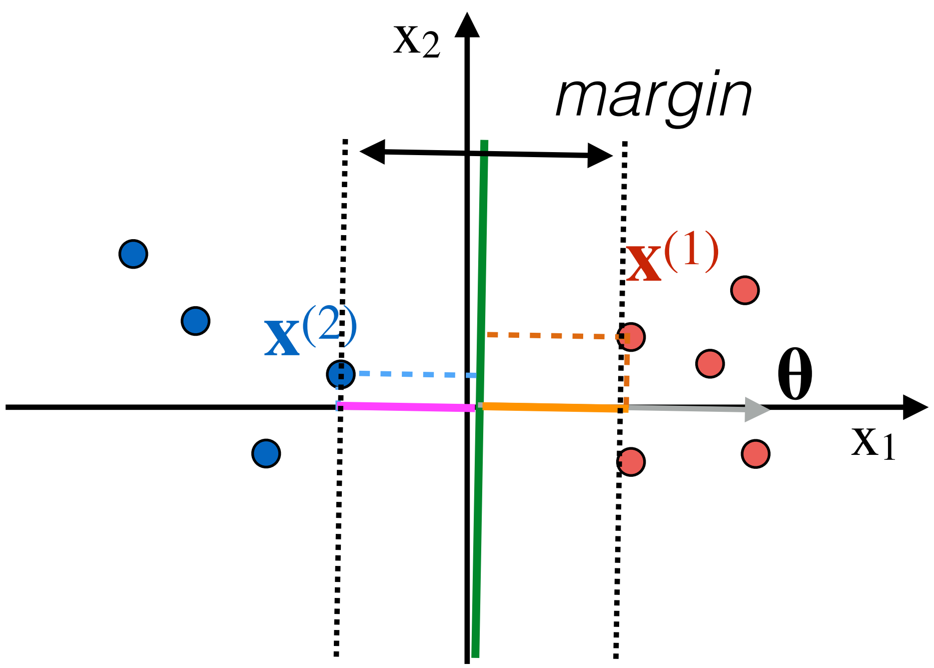
SVM hypothesis



SVM: decision boundary

- Optimization objective:

$$\min_{\boldsymbol{\theta}} \frac{1}{2} \sum_{j=1}^{n} \theta_j^2 = \frac{1}{2} \|\boldsymbol{\theta}\|^2$$

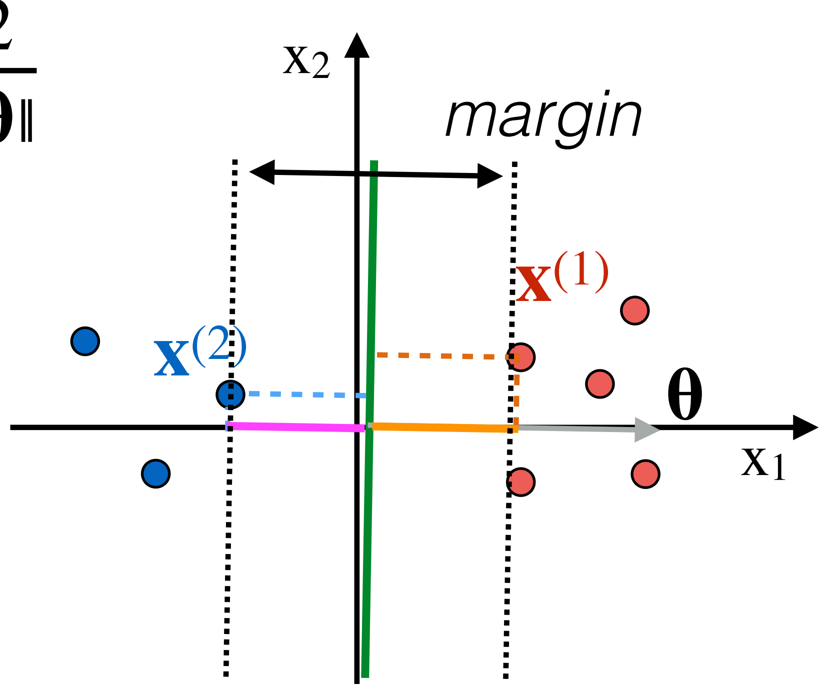
s.t. $\mathbf{p}^{(i)} \|\boldsymbol{\theta}\| \geq 1$ if $y^{(i)} = 1$

$\mathbf{p}^{(i)} \|\boldsymbol{\theta}\| \leq -1$ if $y^{(i)} = 0$

Where $\mathbf{p}^{(i)}$ is the projection of $\mathbf{x}^{(i)}$ onto the vector $\boldsymbol{\theta}$

- Large-margin classification:
  - Geometrically, the margin is: $M = \frac{2}{\|\boldsymbol{\theta}\|}$
  - A key consequence is that the max-margin hyperplane is defined by those $\mathbf{x}^{(i)}$ that lie nearest to it *(support vectors)*

SVM hypothesis



SVM: decision boundary

- Optimization objective:

$$\min_{\boldsymbol{\theta}} \frac{1}{2} \sum_{j=1}^{n} \theta_j^2 = \frac{1}{2} \|\boldsymbol{\theta}\|^2$$

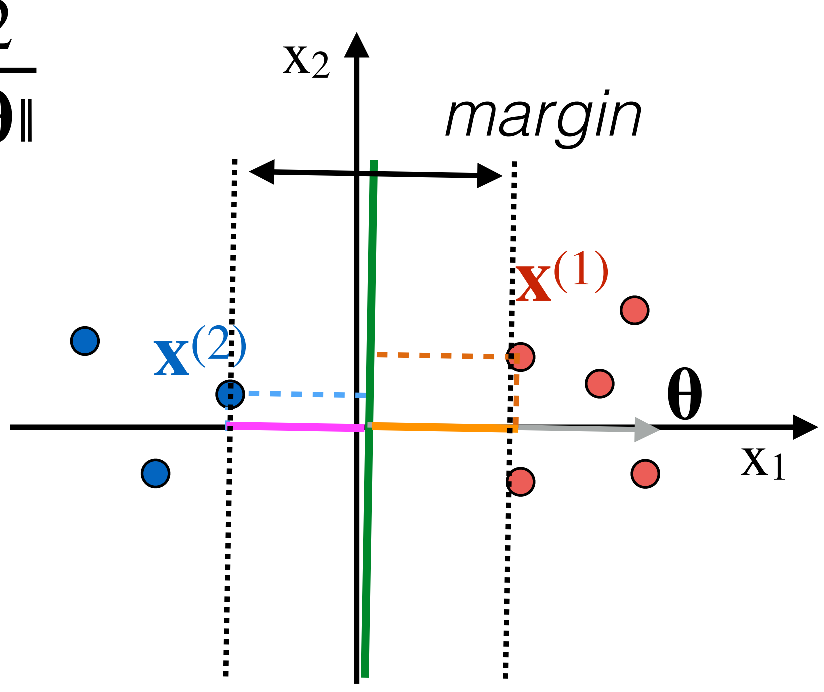
s.t. $\mathbf{p}^{(i)} \|\boldsymbol{\theta}\| \geq 1$ if $y^{(i)} = 1$

$\mathbf{p}^{(i)} \|\boldsymbol{\theta}\| \leq -1$ if $y^{(i)} = -1$

In SVM usually we use a different notation

- Large-margin classification:
  - Geometrically, the margin is: $M = \dfrac{2}{\|\boldsymbol{\theta}\|}$
  - A key consequence is that the max-margin hyperplane is defined by those $\mathbf{x}^{(i)}$ that lie nearest to it *(support vectors)*

SVM hypothesis



SVM: decision boundary

- Optimization objective:

$$\min_{\boldsymbol{\theta}} \frac{1}{2} \sum_{j=1}^{n} \theta_j^2 = \frac{1}{2} \|\boldsymbol{\theta}\|^2$$

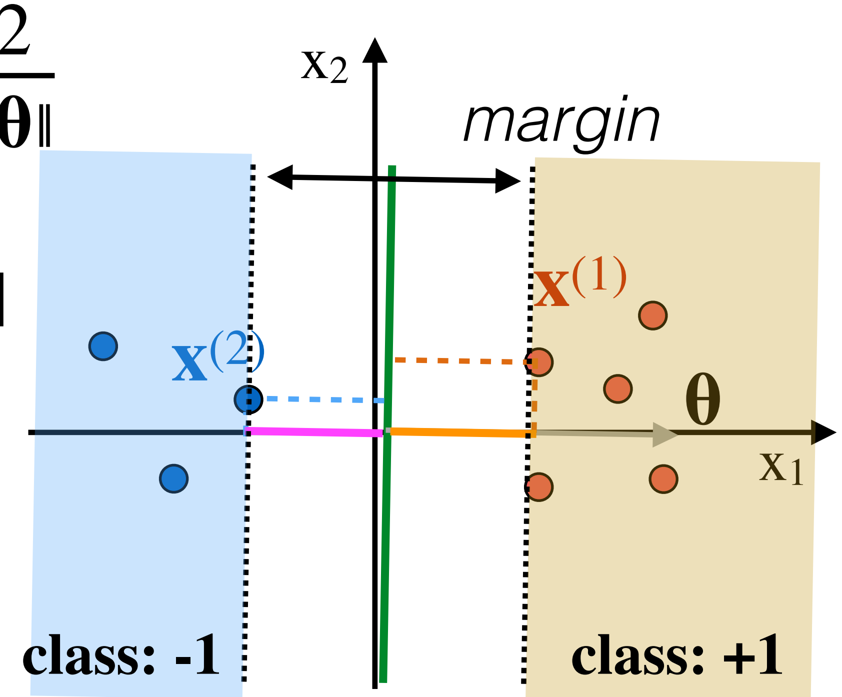
s.t. $y^{(i)} (\mathbf{p}^{(i)} \|\boldsymbol{\theta}\|) \geq 1$

This is called the *primal formulation* of Support Vector Machines

In SVM usually we use a different notation (this simplify a little bit our formulation)

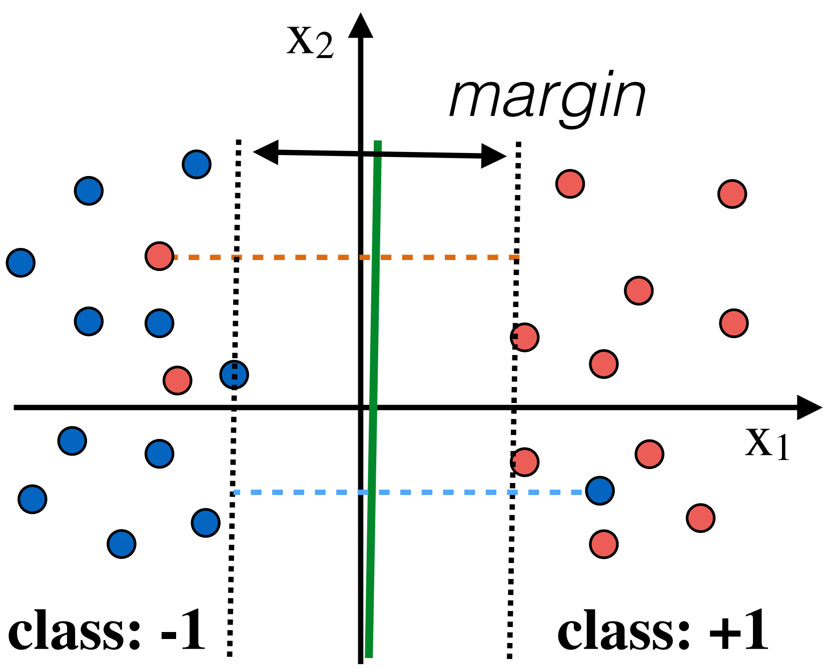
- Large-margin classification:
  - Geometrically, the margin is: $M = \frac{2}{\|\boldsymbol{\theta}\|}$
  - A key consequence is that the max-margin hyperplane is defined by those $\mathbf{x}^{(i)}$ that lie nearest to it *(support vectors)*

SVM hypothesis



What if data is not linearly separable?

- What we have seen until know is called *hard-margin*
- What about examples that lies on the wrong side?



α trades off training error vs model complexity

- Introduce the slack variable $\xi^{(i)}$
- New optimization objective:

$$\min_{\boldsymbol{\theta}} \frac{1}{2} \|\boldsymbol{\theta}\|^2 + \alpha \sum_{i=1}^{m} \xi^{(i)}$$

$$\text{s.t.} \quad \xi^{(i)} \geq 0 \,, \forall i: \; y^{(i)}(\mathbf{p}^{(i)} \|\boldsymbol{\theta}\|) \geq 1 - \xi^{(i)}$$

- $\sum_{i=1}^{m} \xi^{(i)}$ bounds num. of training errors
- This is called *soft-margin* extension

Hinge Loss and soft-margins

- The soft-margin extension leads to the definition of the hinge loss (that we have previously seen)
  - Hinge loss: $\ell(h_\theta(\mathbf{x}^{(i)}), y^{(i)}) = \max(0, 1 - y^{(i)} (\boldsymbol{\theta}^T \mathbf{x}^{(i)})$

    where $\boldsymbol{\theta}^T \mathbf{x}^{(i)} = \mathbf{p}^{(i)} \|\boldsymbol{\theta}\|$, *i.e.* $\mathbf{p}^{(i)}$ *is the projection of* $\mathbf{x}^{(i)}$ *onto the vector* $\boldsymbol{\theta}$
  - The hinge loss $\ell(\cdot)$, is a convex function and can be optimized using gradient descent
  - Interpretation:
    - When $y^{(i)}$ and $\mathbf{p}^{(i)}$ have the same sign and $|y^{(i)}| \geq 1$, $\ell(\cdot)=0$
    - When they have opposite sign, ℓ increases linearly with $y^{(i)}$
    - Similarly, if $|y^{(i)}| < 1$ (it has the same sign: correct prediction but not by enough margin) ℓ increases linearly with $y^{(i)}$

Non-linear Classification

- The *soft-margin* extension is great, but SVM is still a linear classification model

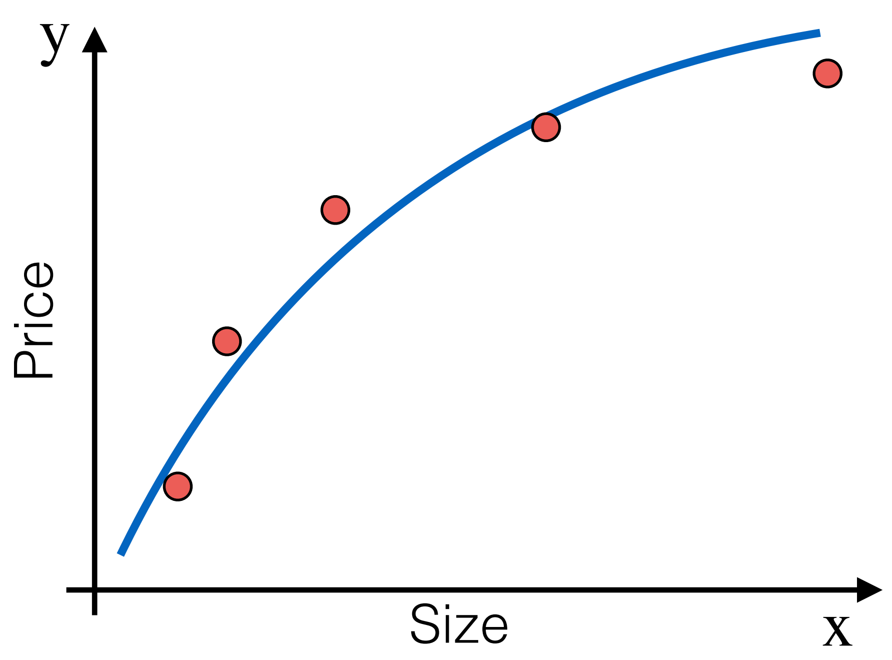
- However, SVM can efficiently perform non-linear classification using the so-called "kernel trick"

  - SVM is the most popular example of a class of methods / algorithms called **kernel machines** (or kernel methods)

  - Kernel methods use kernel functions (i.e. similarity functions over pairs of data samples) which enable them to operate in high-dimensional "implicit" feature spaces

Non-linear Classification

- From feature combination to kernels:
  - If you remember, we already introduced a trick to "extend" linear models by introducing feature transformations



Features and Polynomial Regression

$$h_\theta(\mathrm{x}) = \theta_0 + \theta_1\, \mathrm{x} + \theta_2\, \mathrm{x}^2$$

How to get this $h_\theta(\mathrm{x})$ from our linear regression model $\boldsymbol{\theta}^T \mathbf{x}$?

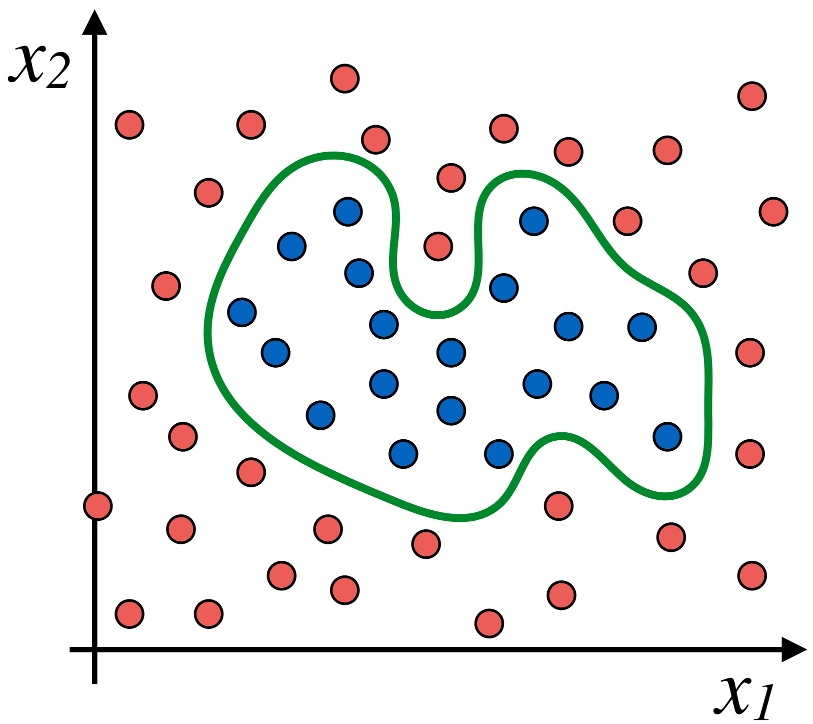
$$\Rightarrow \quad h_\theta(\mathrm{x}) = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix}^T \begin{bmatrix} \mathrm{x}_0 \\ \mathrm{x}_1 \\ \mathrm{x}_2 \end{bmatrix} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix}^T \begin{bmatrix} 1 \\ \mathrm{x} \\ \mathrm{x}^2 \end{bmatrix}$$

x_1: size of house

x_2: (size of house)^2

Non-linear Classification

- We introduce a trick to adapt linear regression (or classification) models to non-linear data:



- Negative class
- Positive class

Predict $y = 1$ if:

$$\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1 x_2 + \theta_4 x_1^2 + \theta_5 x_2^2 + \ldots \geq 0$$

$$h_\theta(x) = \begin{cases} 1 & \text{if } \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

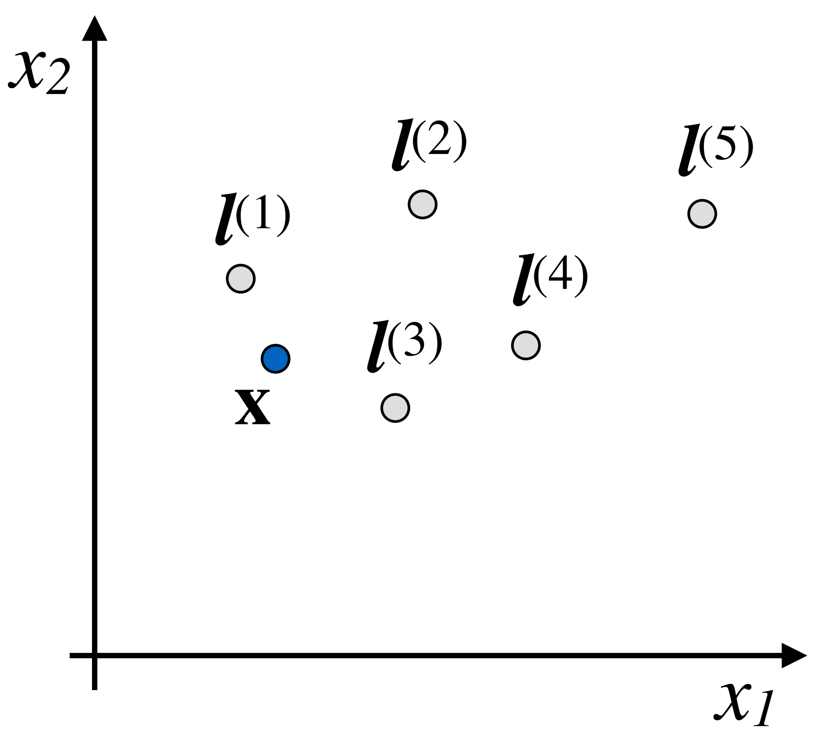
$$\theta_0 + \theta_1 f_1 + \theta_2 f_2 + \theta_3 f_3 + \theta_4 f_4 + \theta_5 f_5 + \ldots$$

where $f_1 = x_1$, $f_2 = x_2$, $f_3 = x_1 x_2$, $f_4 = x_1^2$, $f_5 = x_2^2$, …

How to choose features f_1, f_2, … ?

Kernels - Intuition

- We introduce a trick to adapt linear regression (or classification) models to non-linear data:



- Negative class
- Positive class

Given $\mathbf{x}$, compute features $\mathbf{f}$ depending on proximity to landmarks $\boldsymbol{l}^{(1)}, \boldsymbol{l}^{(2)}, \ldots$

$$f_1 = \text{similarity}(\mathbf{x}, \boldsymbol{l}^{(1)})$$

$$f_2 = \text{similarity}(\mathbf{x}, \boldsymbol{l}^{(2)})$$

$$\vdots$$

Predict $y = 1$ if:

$$\theta_0 + \theta_1 f_1 + \theta_2 f_2 + \theta_3 f_3 + \theta_4 f_4 + \theta_5 f_5 + \ldots \geq 0$$

where $f_1 = x_1$, $f_2 = x_2$, $f_3 = x_1 x_2$, $f_4 = x_1^2$, $f_5 = x_2^2, \ldots$

Kernels - Intuition

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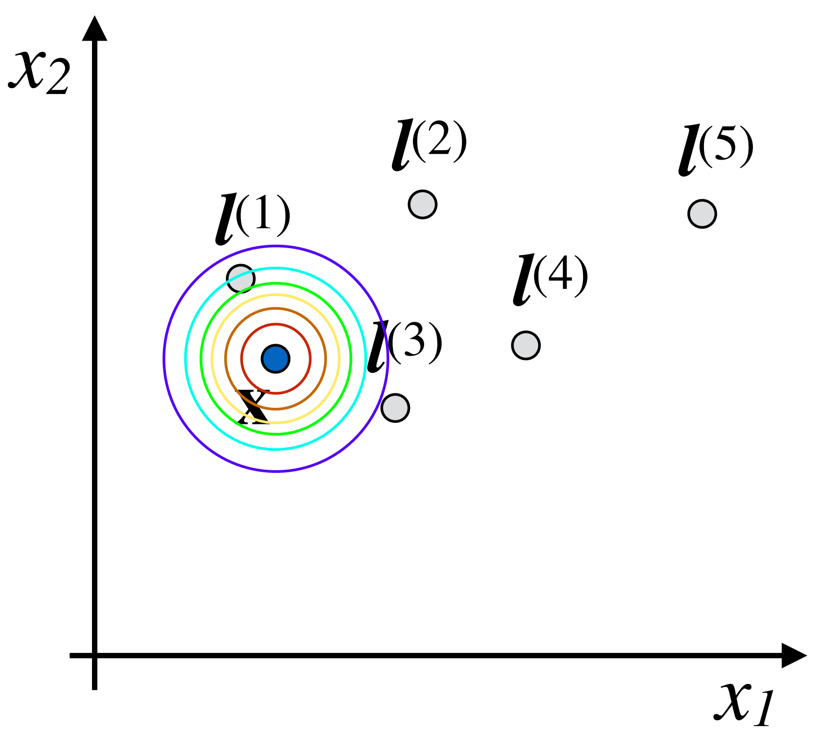


Given $\mathbf{x}$, compute features $\mathbf{f}$ depending on proximity to landmarks $\boldsymbol{l}^{(1)}, \boldsymbol{l}^{(2)}, \ldots$

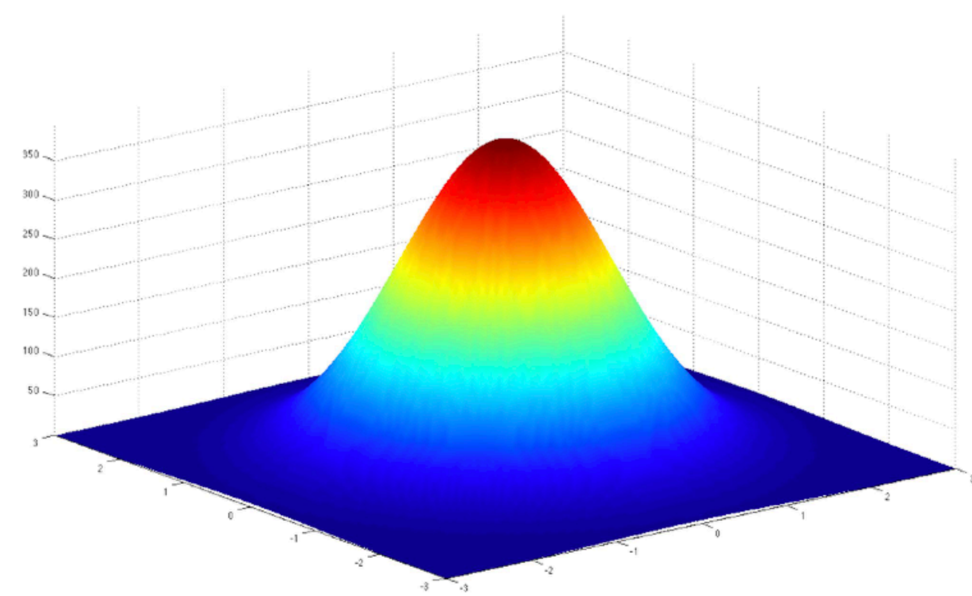
$$f_1 = k(\mathbf{x}, \boldsymbol{l}^{(1)})$$

$$f_2 = k(\mathbf{x}, \boldsymbol{l}^{(2)})$$

$$f_3 = k(\mathbf{x}, \boldsymbol{l}^{(3)})$$

$$f_4 = k(\mathbf{x}, \boldsymbol{l}^{(4)})$$

$$f_5 = k(\mathbf{x}, \boldsymbol{l}^{(5)})$$



if $\mathbf{x} \approx \boldsymbol{l}^{(i)}$: $f_1 = \exp(-\, 0^2/(2\sigma^2)) \approx 1$

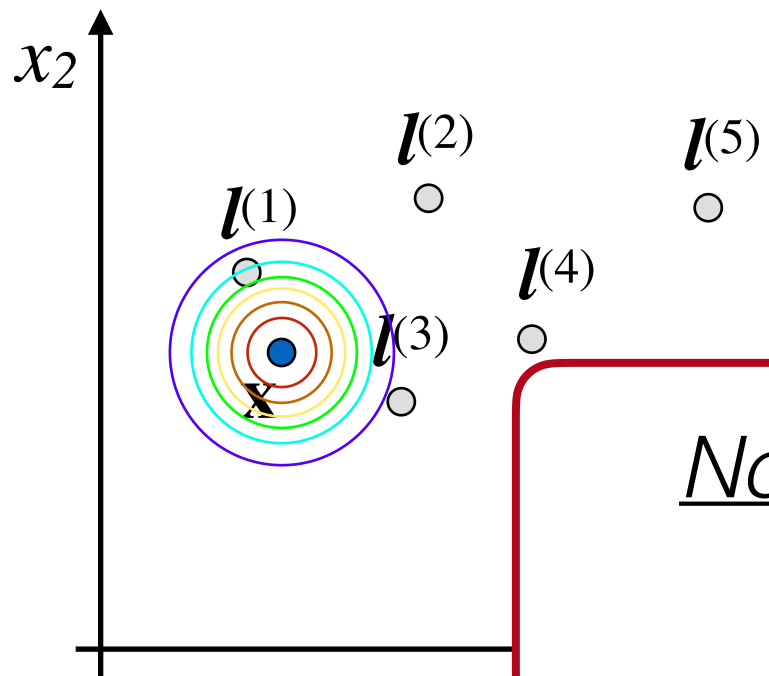
if $\mathbf{x}$ is far from $\boldsymbol{l}^{(i)}$: $f_1 \approx 0$

e.g. $k(\mathbf{x}, \boldsymbol{l}^{(i)}) = \exp\left(- \dfrac{\|\mathbf{x} - \boldsymbol{l}^{(i)}\|^2}{2\sigma^2}\right)$ *Gaussian Kernel*

Kernels - Intuition

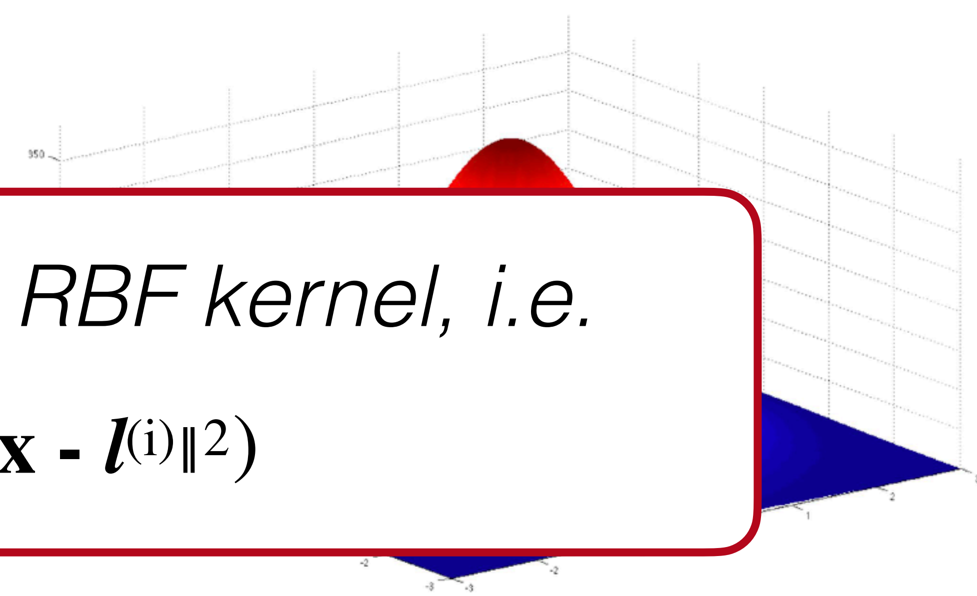
- We introduce a trick to adapt linear regression (or classification) models to non-linear data:

Given $\mathbf{x}$, compute features $\mathbf{f}$ depending on proximity to landmarks $\boldsymbol{l}^{(1)}, \boldsymbol{l}^{(2)}, \ldots$



$$f_1 = k(\mathbf{x}, \boldsymbol{l}^{(1)})$$

$$f_2 = k(\mathbf{x}, \boldsymbol{l}^{(2)})$$



<u>Note</u>: this is the popular RBF kernel, i.e.

$$k(\mathbf{x}, \boldsymbol{l}^{(i)}) = \exp(-\gamma \|\mathbf{x} - \boldsymbol{l}^{(i)}\|^2)$$

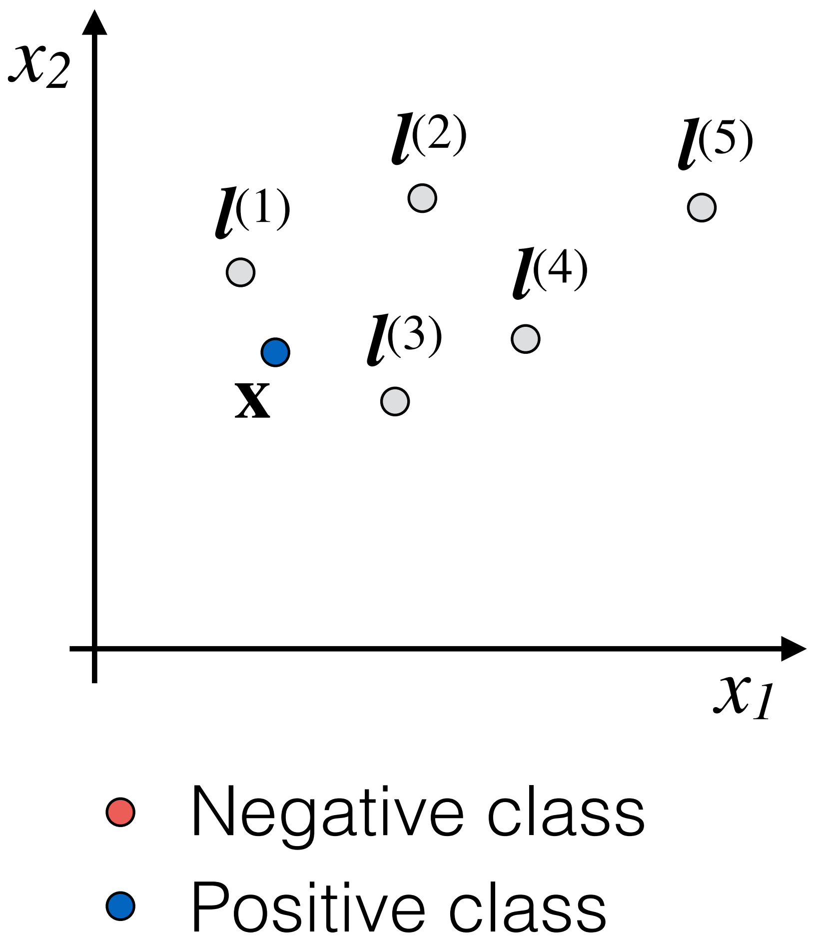
if $\mathbf{x} \approx \boldsymbol{l}^{(i)}$: $f_1 = \exp(-0^2/(2\sigma^2)) \approx 1$

if $\mathbf{x}$ is far from $\boldsymbol{l}^{(i)}$: $f_1 \approx 0$

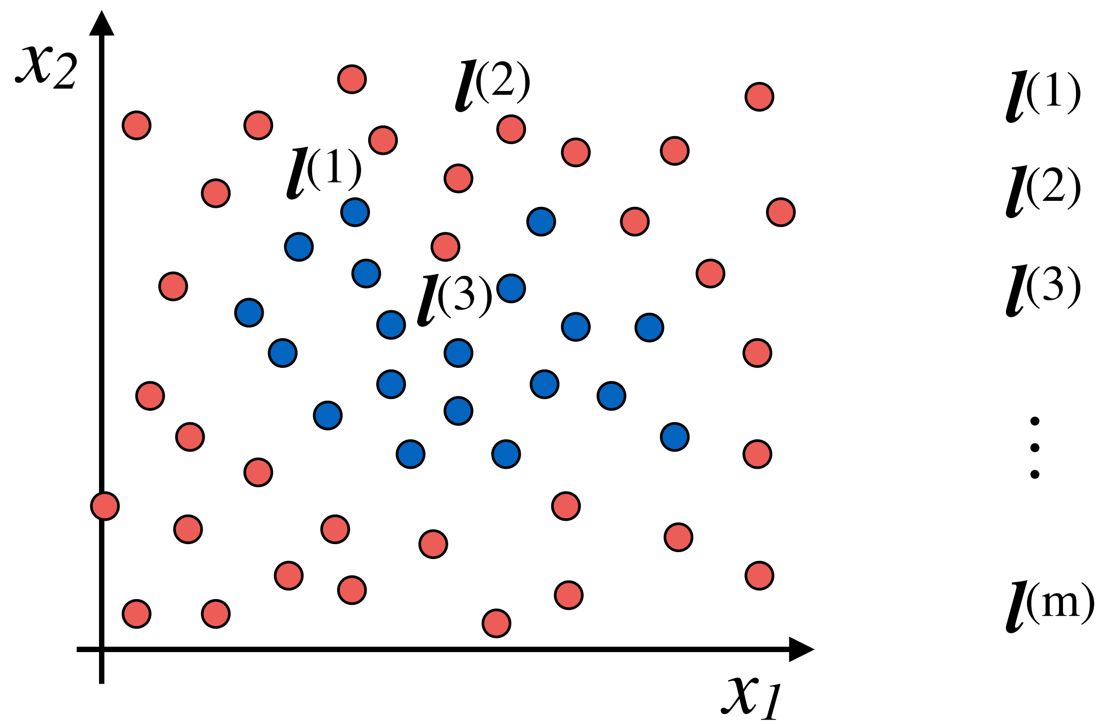
e.g. $k(\mathbf{x}, \boldsymbol{l}^{(i)}) = \exp(-\dfrac{\|\mathbf{x} - \boldsymbol{l}^{(i)}\|^2}{2\sigma^2})$ *Gaussian Kernel*

Kernels - Intuition

- We introduce a trick to adapt linear regression (or classification) models to non-linear data:

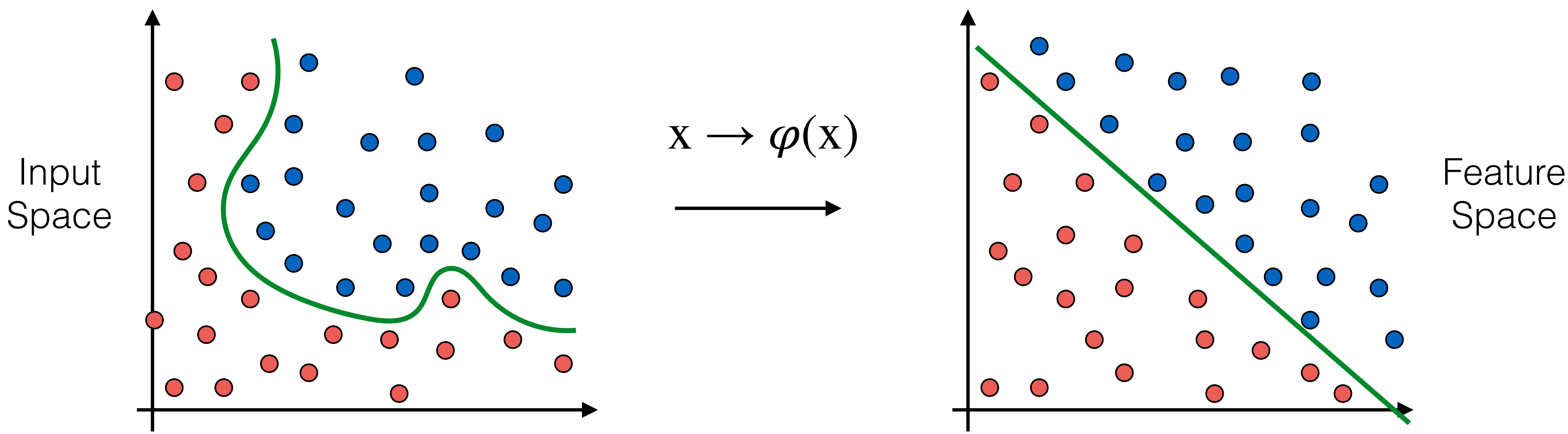


Where to get the landmarks $\boldsymbol{l}^{(1)}, \boldsymbol{l}^{(2)}, \ldots$?



Kernel Methods

- Goal: transform/map raw data into feature vectors
  - Instead of using explicit user-specified feature maps, rely on a *similarity function* (kernel) over pairs of data points
  - A kernel is a function $\varphi: \mathbb{R}^n \rightarrow \mathbb{R}^m$ which maps $x \rightarrow \varphi(x)$
  - Then, given this mapping, we try to find a linear decision boundary in the feature space



Kernel Methods

- Summarizing what we have seen till now:
    - A kernel is a function $\varphi\colon \mathbb{R}^n \rightarrow \mathbb{R}^m$ which maps our vectors in $\mathbb{R}^n$ to some (possibly very high dimensional) space $\mathbb{R}^m$
    - Kernels are sometimes called "generalized dot product":

$\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ $\quad k(\mathbf{x}, \mathbf{y}) = \varphi(\mathbf{x})^T\varphi(\mathbf{y})$ corresponds to a dot product in $\mathbb{R}^n$

Kernels give a way to compute dot products in some feature space without even knowing what this space is and what is φ

Kernel Methods

- Let's see an example (polynomial kernel):

$\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ $\quad k(\mathbf{x}, \mathbf{y}) = \varphi(\mathbf{x})^T \varphi(\mathbf{y})$ corresponds to a dot product in $\mathbb{R}^n$

$k(\mathbf{x}, \mathbf{y}) = (1 + \mathbf{x}^T \mathbf{y})^2$ assuming $\mathbf{x}, \mathbf{y} \in \mathbb{R}^2$, i.e. $\mathbf{x} = (x_1, x_2)$, $\mathbf{y} = (y_1, y_2)$

$$k(\mathbf{x}, \mathbf{y}) = (1 + x_1 y_1 + x_2 y_2)^2 = 1 + x_1^2 y_1^2 + x_2^2 y_2^2 + 2x_1 y_1 + 2x_2 y_2 + 2x_1 x_2 y_1 y_2$$

Note that this is nothing else but a dot product between vectors:

$$\varphi(\mathbf{x}) = (1, x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1 x_2) \text{ , } \varphi(\mathbf{y}) = (1, y_1^2, y_2^2, \sqrt{2}y_1, \sqrt{2}y_2, \sqrt{2}y_1 y_2)$$

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