SEMANA 7 - MÁQUINAS DE VECTORES DE SOPORTE

Clasificación de margen grande

- Objetivo de optimización

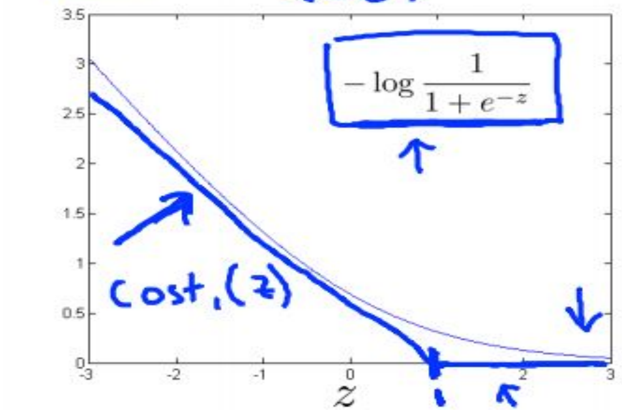
Alternative view of logistic regression

Cost of example: $-(y \log h_\theta(x) + (1-y)\log(1-h_\theta(x)))$

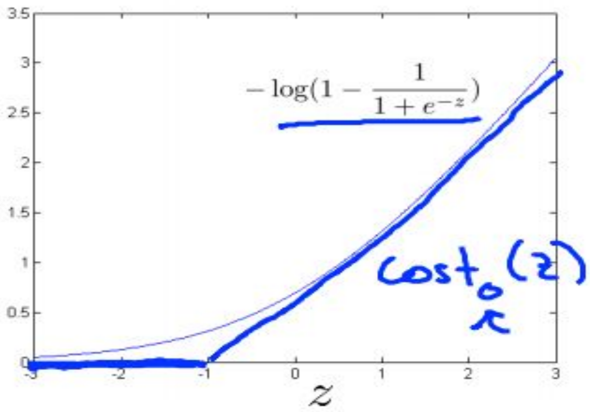
$$= \boxed{-y \log \frac{1}{1+e^{-\theta^T x}}} - \boxed{(1-y)\log\left(1-\frac{1}{1+e^{-\theta^T x}}\right)}$$

If $y=1$ (want $\theta^T x \gg 0$):

$z = \theta^T x$



If $y=0$ (want $\theta^T x \ll 0$):



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Support vector machine

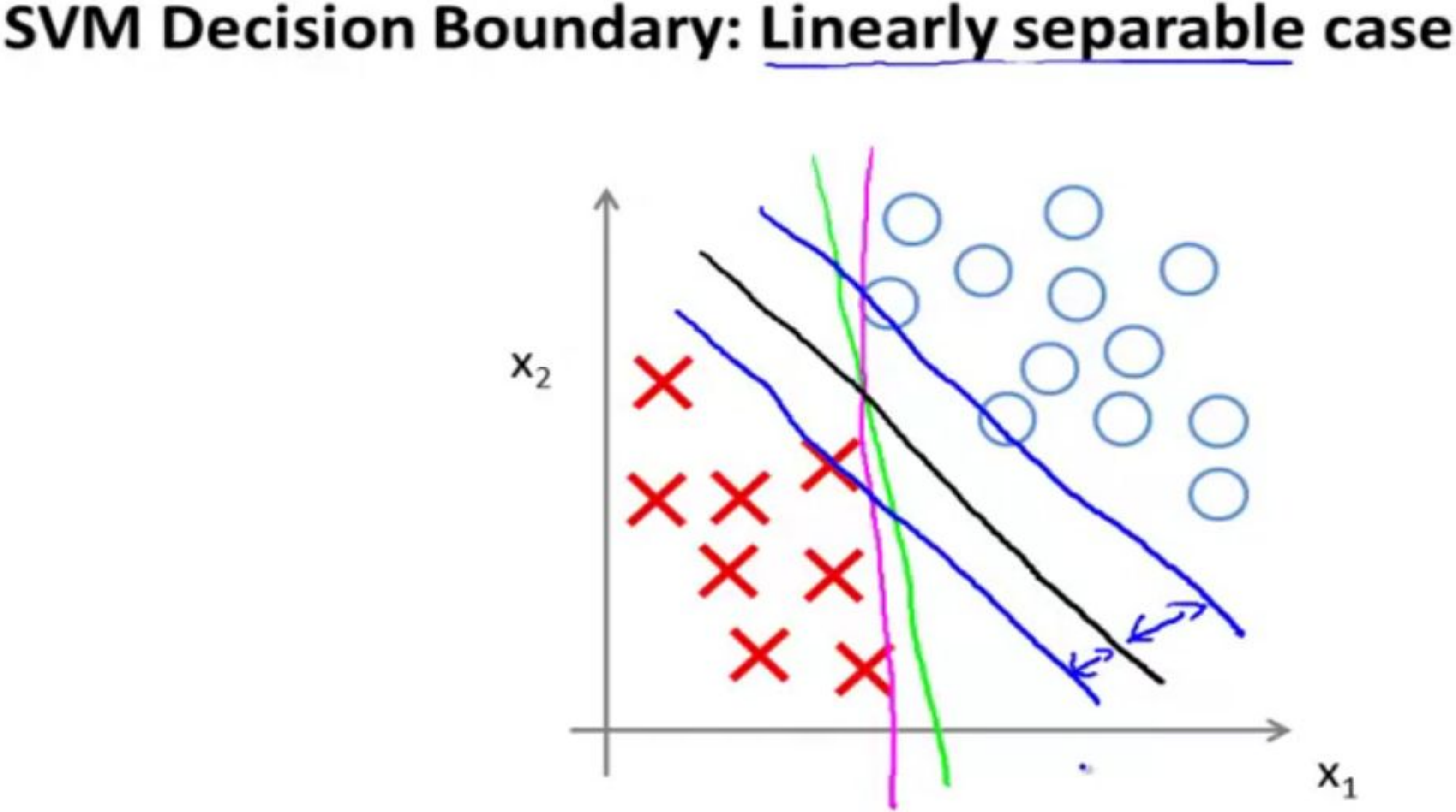
Logistic regression:

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

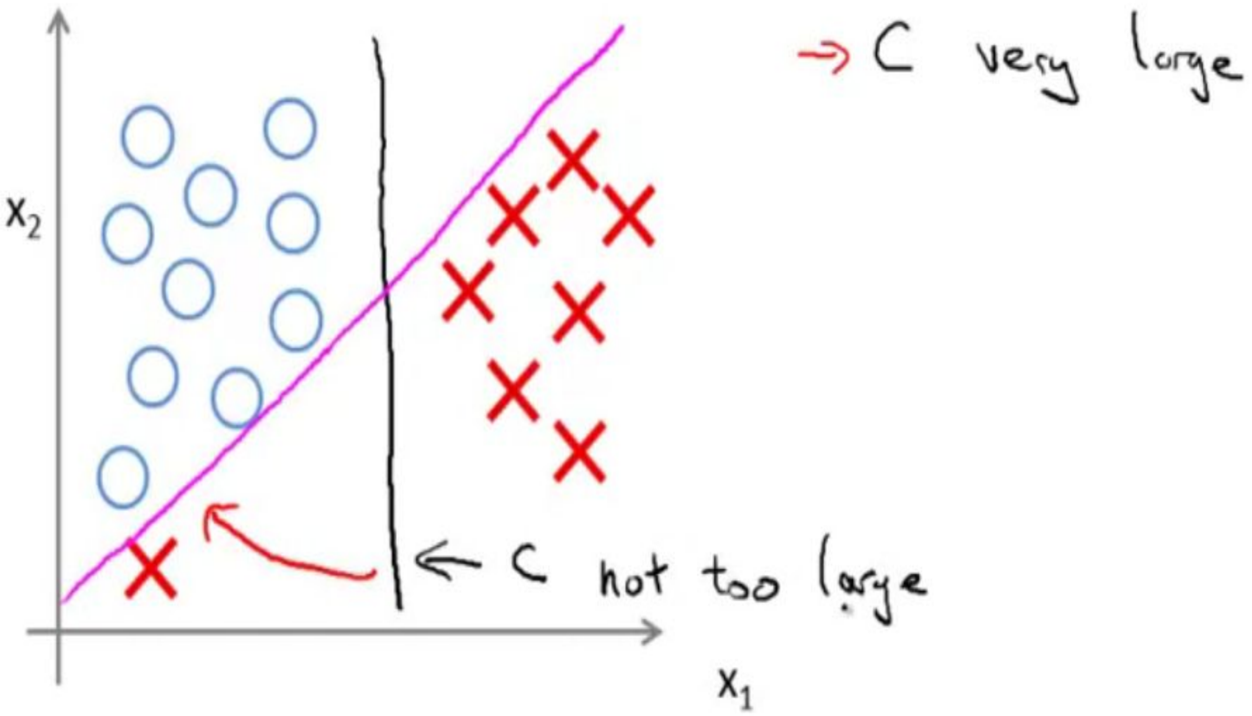
Support vector machine:

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

- Intuición de gran marge

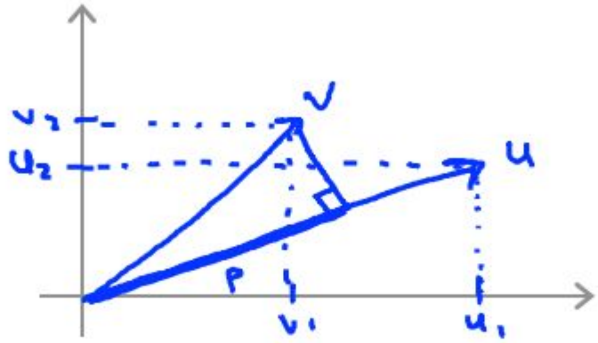


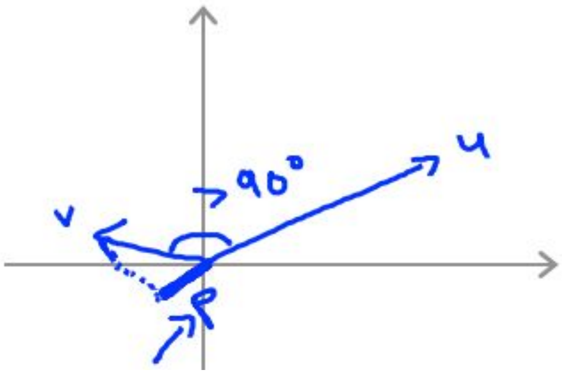
Large margin classifier in presence of outliers



❑ Matemáticas detrás de la clasificación

Vector Inner Product





$$u = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \qquad v = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

$$u^T v = ? \qquad [u_1 \;\; u_2] \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

$\|u\|$ = length of vector u

$$= \sqrt{u_1^2 + u_2^2} \in \mathbb{R}$$

p = length of projection of v onto u.

Signed

$$u^T v = p \cdot \|u\| \qquad = v^T u$$

$$= u_1 v_1 + u_2 v_2 \qquad p \in \mathbb{R}$$

$$u^T v = p \cdot \|u\|$$

$$p < 0$$

SVM Decision Boundary

$$\omega = \left(\sqrt{\omega}\right)^2$$

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

$$\text{s.t.}\quad \boxed{\theta^T x^{(i)} \geq 1} \quad \text{if } y^{(i)} = 1$$

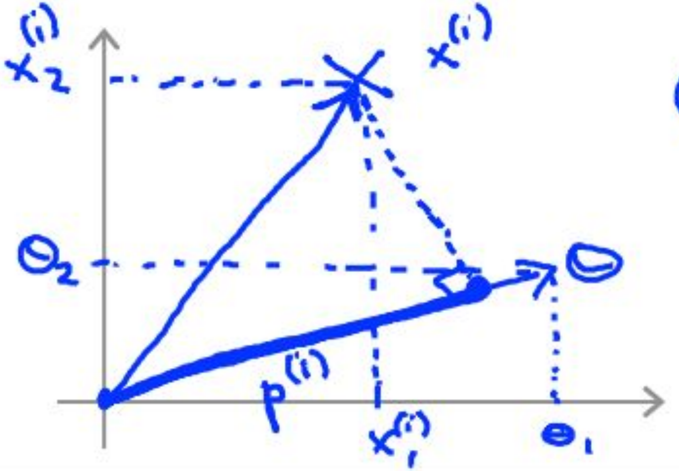
$$\theta^T x^{(i)} \leq -1 \quad \text{if } y^{(i)} = 0$$

$$\begin{bmatrix} \cancel{\theta_0} \\ \theta_1 \\ \theta_2 \end{bmatrix} \quad \theta_0 = 0$$

Simplication: $\theta_0 = 0$ $n=2$

$$\theta^T x^{(i)} = ?$$

$$u^T v$$



$$\theta^T x^{(i)} = \boxed{p^{(i)} \cdot \|\theta\|} \leftarrow$$

$$= \theta_1 x_1^{(i)} + \theta_2 x_2^{(i)} \leftarrow$$

SVM Decision Boundary

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

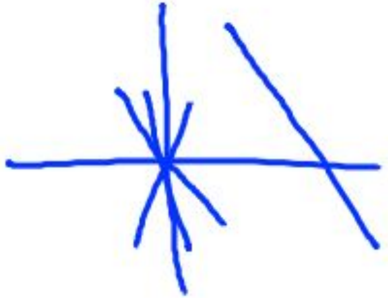
s.t. $\boxed{p^{(i)} \cdot \|\theta\| \geq 1}$ if $y^{(i)} = 1$

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

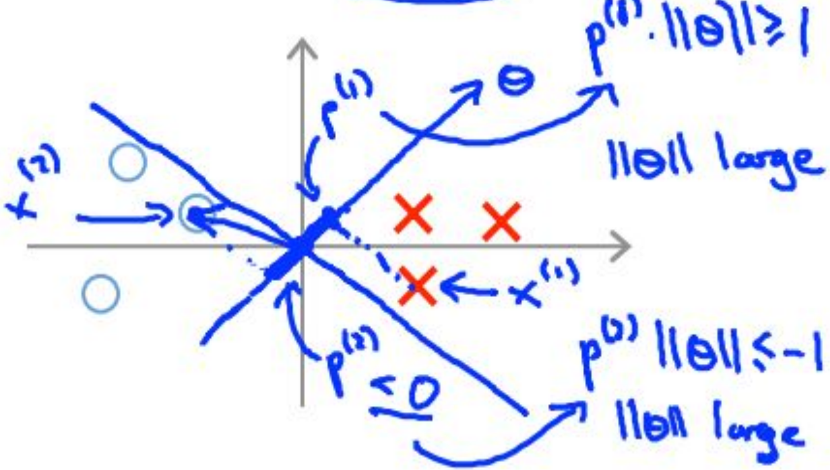
C very large

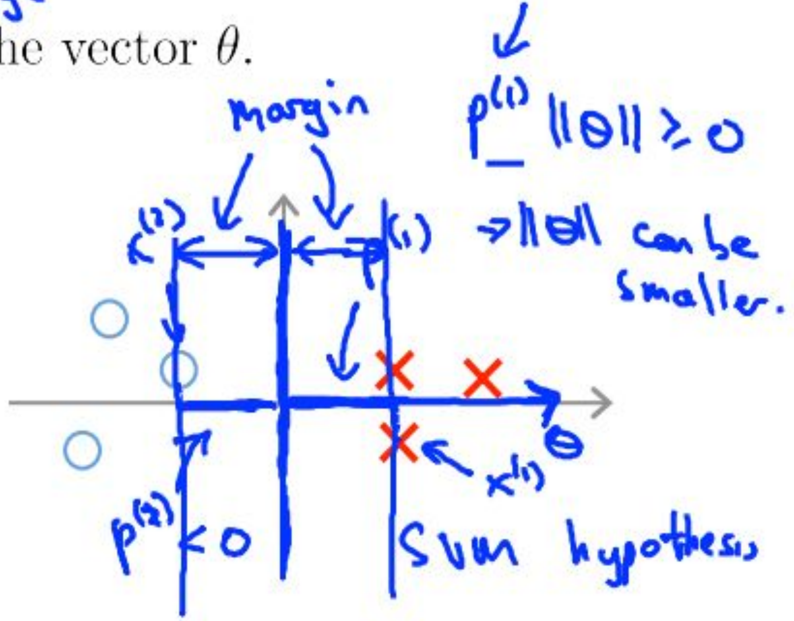
where $p^{(i)}$ is the projection of $x^{(i)}$ onto the vector θ.

Simplification: $\theta_0 = 0$



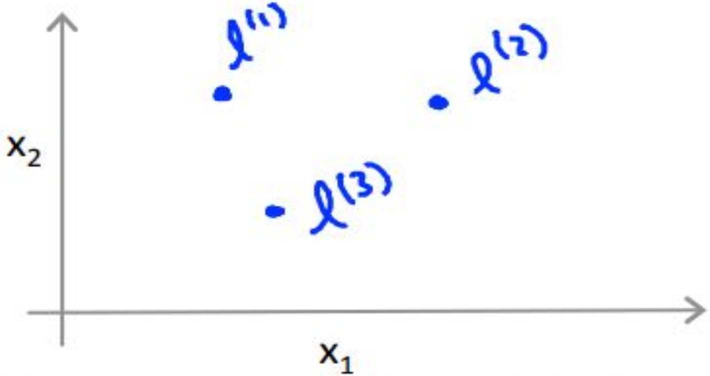
$\theta_0 \neq 0$





Kernel I

Kernel



Given x, compute new feature depending on proximity to landmarks $l^{(1)}, l^{(2)}, l^{(3)}$

$\|w\|$

$\|x - \ell^{(1)}\|^2$

Given x:

$$f_1 = \text{similarity}(x, \ell^{(1)}) = \exp\left(-\frac{\|x - \ell^{(1)}\|^2}{2\sigma^2}\right)$$

$$f_2 = \text{similarity}(x, \ell^{(1)}) = \exp\left(-\frac{\|x - \ell^{(2)}\|^2}{2\sigma^2}\right)$$

$$f_3 = \text{similarity}(x, \ell^{(3)}) = \exp(\ldots)$$

Kernel (Gaussian kernels) $\quad k(x, \ell^{(i)})$

Kernels and Similarity

$$f_1 = \text{similarity}(x, l^{(1)}) = \exp\left(-\frac{\boxed{\|x - l^{(1)}\|^2}}{2\sigma^2}\right)$$

If $x \approx l^{(1)}$:

$$f_1 \approx \exp\left(-\frac{0^2}{2\sigma^2}\right) \approx 1$$

$l^{(1)} \rightarrow f_1$

$l^{(2)} \rightarrow f_2$

$l^{(3)} \rightarrow f_3$.

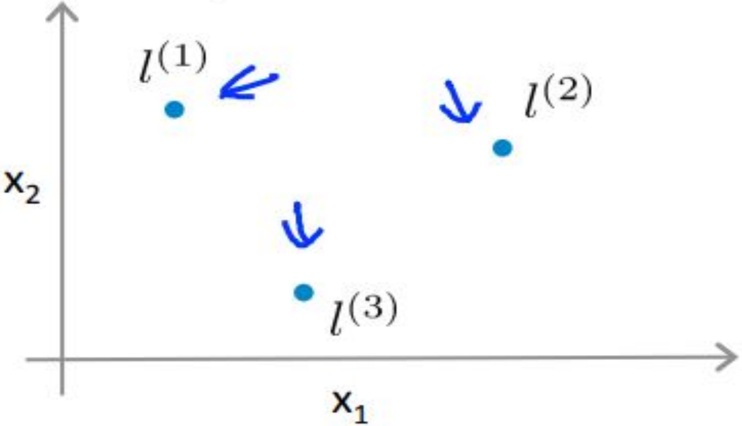
x

If x if far from $l^{(1)}$:

$$f_1 = \exp\left(-\frac{(\text{large number})^2}{2\sigma^2}\right) \approx 0.$$

Kernels II

Choosing the landmarks



Given x:

$$f_i = \text{similarity}(x, l^{(i)})$$

$$= \exp\left(-\frac{||x - l^{(i)}||^2}{2\sigma^2}\right)$$

Predict $y = 1$ if $\theta_0 + \theta_1 f_1 + \theta_2 f_2 + \theta_3 f_3 \geq 0$

Where to get $l^{(1)}, l^{(2)}, l^{(3)}, \ldots$?

SVM with Kernels

- Given $(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})$,
- choose $l^{(1)} = x^{(1)}, l^{(2)} = x^{(2)}, \ldots, l^{(m)} = x^{(m)}$.

Given example x:

$$\boxed{\begin{array}{l} f_1 = \text{similarity}(x, l^{(1)}) \\ f_2 = \text{similarity}(x, l^{(2)}) \\ \ldots \end{array}}$$

$x^{(1)}$

$$f = \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_m \end{bmatrix} \qquad f_0 = 1$$

For training example $(x^{(i)}, y^{(i)})$:

$$x^{(i)} \rightarrow \begin{array}{l} f_1^{(i)} = \text{sim}(x^{(i)}, l^{(1)}) \\ f_2^{(i)} = \text{sim}(x^{(i)}, l^{(2)}) \\ \vdots \\ f_i^{(i)} = \text{sim}(x^{(i)}, l^{(i)}) = \exp\left(-\frac{0}{2\sigma^2}\right) = 1 \\ f_m^{(i)} = \text{sim}(x^{(i)}, l^{(m)}) \end{array}$$

$x^{(i)}$

$x^{(i)} \in \mathbb{R}^{n+1}$ (or $\mathbb{R}^n$)

$$f^{(i)} = \begin{bmatrix} f_0^{(i)} \\ f_1^{(i)} \\ \vdots \\ f_m^{(i)} \end{bmatrix}$$

$f_0^{(i)} = 1$

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SVM with Kernels

Hypothesis: Given x, compute features $f \in \mathbb{R}^{m+1}$ $\quad \theta \in \mathbb{R}^{m+1}$

→ Predict "y=1" if $\theta^T f \geq 0$ $\quad \theta_0 f_0 + \theta_1 f_1 + \cdots + \theta_m f_m$

Training:

$n = m$

$$\min_\theta C \sum_{i=1}^{m} y^{(i)} cost_1(\theta^T f^{(i)}) + (1 - y^{(i)}) cost_0(\theta^T f^{(i)}) + \boxed{\frac{1}{2} \sum_{j=1}^{\cancel{n} = m} \theta_j^2}$$

$\cancel{\theta^T x^{(i)}}$ $\quad \theta^T f^{(i)}$

$\to \theta_0$

$\sum_j \theta_j^2 = \theta^T \theta \leftarrow \theta = \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_m \end{bmatrix}$ (ignore θ_0)

$\|\theta\|^2$

$\theta^T M \theta$

$m = 10{,}000$

SVM parameters:

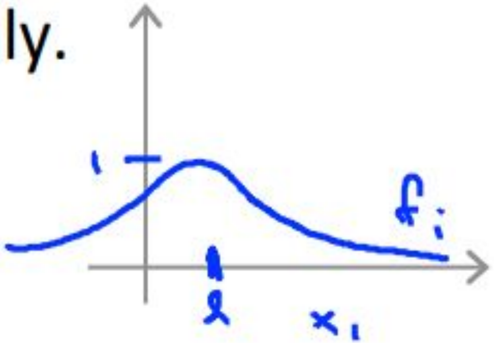
C ($= \frac{1}{\lambda}$). → Large C: Lower bias, high variance. (small λ)

→ Small C: Higher bias, low variance. (large λ)

σ^2 Large σ^2: Features f_i vary more smoothly.

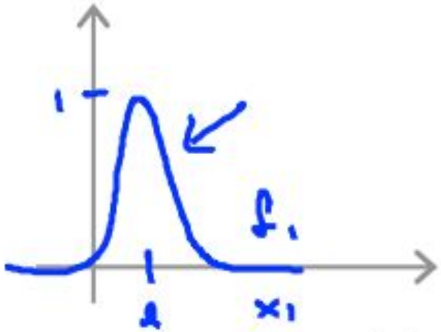
→ Higher bias, lower variance.

$\exp\left(-\frac{\|x-l^{(i)}\|^2}{2\sigma^2}\right)$



Small σ^2: Features f_i vary less smoothly.

Lower bias, higher variance.



SVM en la práctica

Use SVM software package (e.g. liblinear, libsvm, ...) to solve for parameters θ.

Need to specify:

→ Choice of parameter C.

Choice of kernel (similarity function):

E.g. No kernel ("linear kernel")

Predict "y = 1" if $\theta^T x \geq 0$

$\theta_0 + \theta_1 x_1 + \cdots + \theta_n x_n \geq 0$

→ n large, m small

$x \in \mathbb{R}^{n+1}$

→ Gaussian kernel:

$$f_i = \exp\left(-\frac{||x - l^{(i)}||^2}{2\sigma^2}\right), \text{ where } l^{(i)} = x^{(i)}.$$

Need to choose σ^2.

$x \in \mathbb{R}^n$, n small

and/or m large

Kernel (similarity) functions: $x^{(i)}$ $l^{(j)} = x^{(j)}$

f_i

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function f = kernel(x1,x2)
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$$f = \exp\left(-\frac{\| \mathbf{x1} - \mathbf{x2} \|^2}{2\sigma^2}\right)$$

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return
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$x \rightarrow f_1, f_2, \ldots, f_m$

→ Note: Do perform feature scaling before using the Gaussian kernel.

$x \in \mathbb{R}^n$

$\boxed{\|x - l\|^2}$

$v = x - l$

$\|v\|^2 = v_1^2 + v_2^2 + \cdots + v_n^2$

$= \underbrace{(x_1 - l_1)^2}_{1000 \text{ feet}^2} + \underbrace{(x_2 - l_2)^2}_{1\text{-}5 \text{ bedrooms}} + \cdots + (x_n - l_n)^2$

Other choices of kernel

Note: Not all similarity functions $\text{similarity}(x, l)$ make valid kernels.
(Need to satisfy technical condition called "Mercer's Theorem" to make sure SVM packages' optimizations run correctly, and do not diverge).

Many off-the-shelf kernels available:

- Polynomial kernel: $k(x, l) = (x^T l)^2$, $(x^T l)^3$, $(x^T l + 1)^3$, $(x^T l + 5)^4$ $\qquad (x^T l + \text{constant})^{\text{degree}}$

- More esoteric: String kernel, chi-square kernel, histogram intersection kernel, ...

$\text{sim}(x, l)$

Logistic regression vs. SVMs

$n =$ number of features ($x \in \mathbb{R}^{n+1}$), $m =$ number of training examples

If n is large (relative to m): (e.g. $n \geq m$, $n = 10,000$, $m = 10 \cdots 1000$)

Use logistic regression, or SVM without a kernel ("linear kernel")

If n is small, m is intermediate: ($n = 1 - 1000$, $m = 10 - 10,000$)

Use SVM with Gaussian kernel

If n is small, m is large: ($n = 1 - 1000$, $m = 50,000+$)

Create/add more features, then use logistic regression or SVM without a kernel

Neural network likely to work well for most of these settings, but may be slower to train.