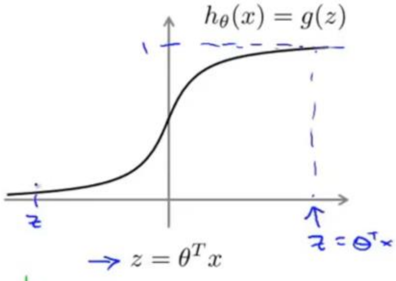
Support Vector Machines

1 Optimization objective

Alternative view of logistic regression

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



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

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

Alternative view of logistic regression

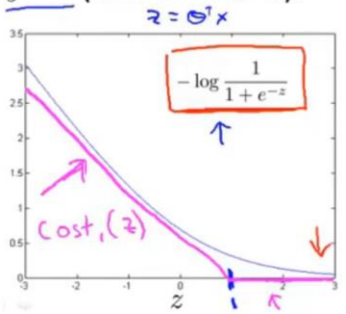
(x, y)

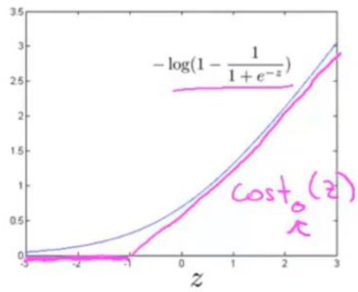
Cost of example: $-(y \log h_\theta(x) + (1-y)\log(1-h_\theta(x)))$

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

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

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





Support vector machine

Logistic regression:

$$\underbrace{\min_\theta \frac{1}{m}\left[\sum_{i=1}^{m} y^{(i)}\underbrace{\left(-\log h_\theta(x^{(i)})\right)}_{cost_1(\theta^T x^{(i)})} + (1-y^{(i)})\underbrace{\left((-\log(1-h_\theta(x^{(i)}))\right)}_{cost_0(\theta^T x^{(i)})}\right]}_{A} + \underbrace{\frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2}_{B}$$

Support vector machine:

$$\min_\theta \cancel{\frac{1}{m}}\, C \sum_{i=1}^{m} y^{(i)} cost_1(\theta^T x^{(i)}) + (1-y^{(i)}) cost_0(\theta^T x^{(i)}) + \frac{1}{2\cancel{m}}\sum_{i=0}^{n}\theta_j^2$$

$\min_u ((u-5)^2+1) \rightarrow u=5$ $\times 10$

$\min_u 10(u-5)^2+10 \rightarrow u=5$

$A + \lambda B$

$C A + B$

$C = \frac{1}{\lambda}$

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

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SVM hypothesis

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

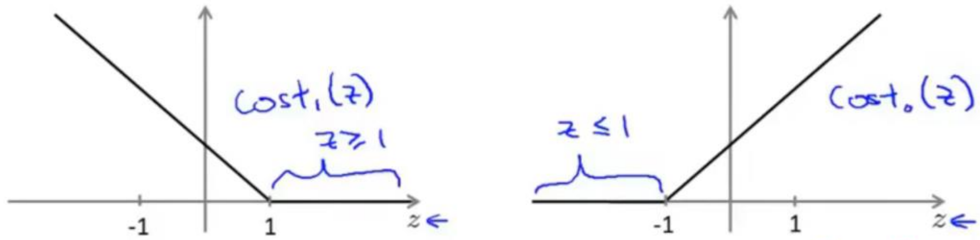
Hypothesis:

$$h_\theta(x) \begin{cases} 1 & \text{if } \theta^T x \geqslant 0 \\ 0 & \text{otherwise} \end{cases}$$

2 Large Margin Intuition

Support Vector Machine

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



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

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

$C = 100{,}000$

SVM Decision Boundary

$$\min_{\theta} C \underbrace{\boxed{\sum_{i=1}^{m} \left[y^{(i)} cost_1(\theta^T x^{(i)}) + (1 - y^{(i)}) cost_0(\theta^T x^{(i)}) \right]}}_{=0} + \frac{1}{2} \sum_{i=1}^{n} \theta_j^2$$

Whenever $y^{(i)} = 1$:

$\theta^T x^{(i)} \geq 1$

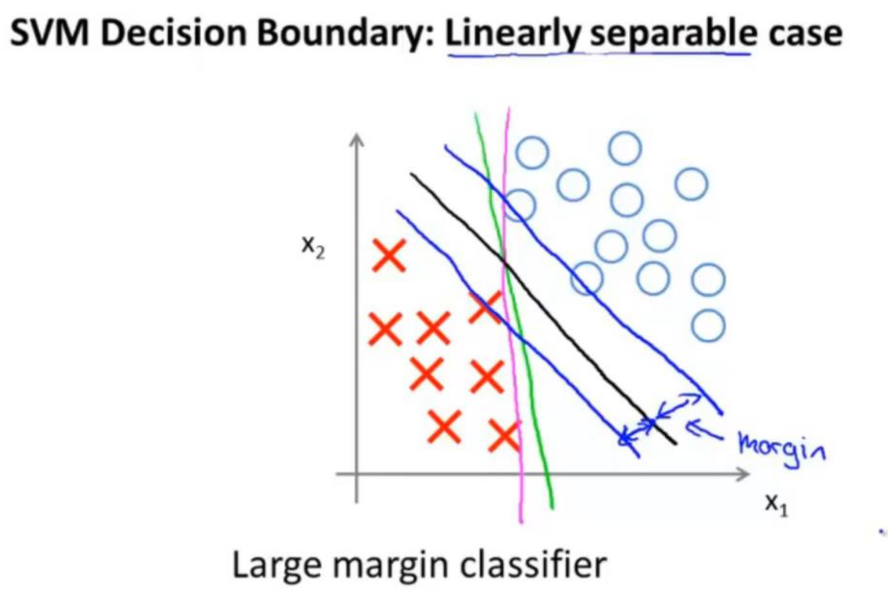
$$\min_{\theta} \cancel{C \times 0} + \frac{1}{2} \sum_{i=1}^{n} \theta_j^2$$

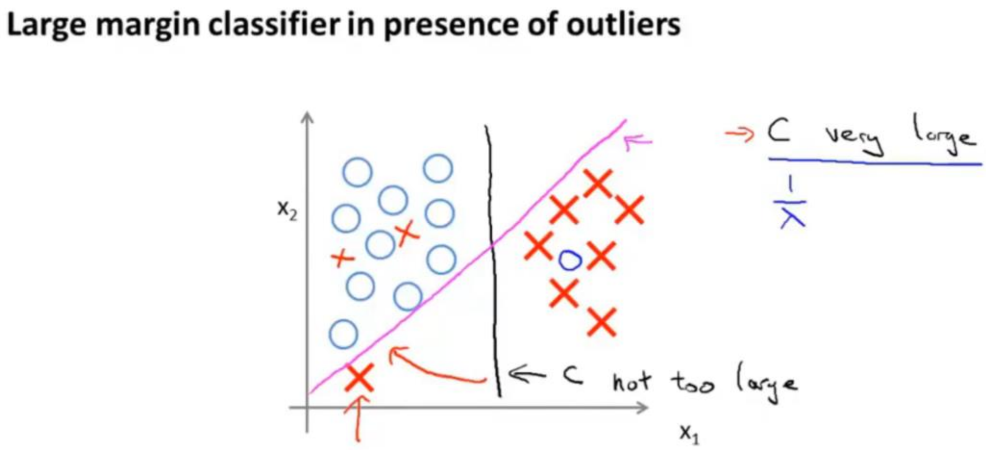
s.t. $\theta^T x^{(i)} \geq 1 \quad$ if $y^{(i)} = 1$

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

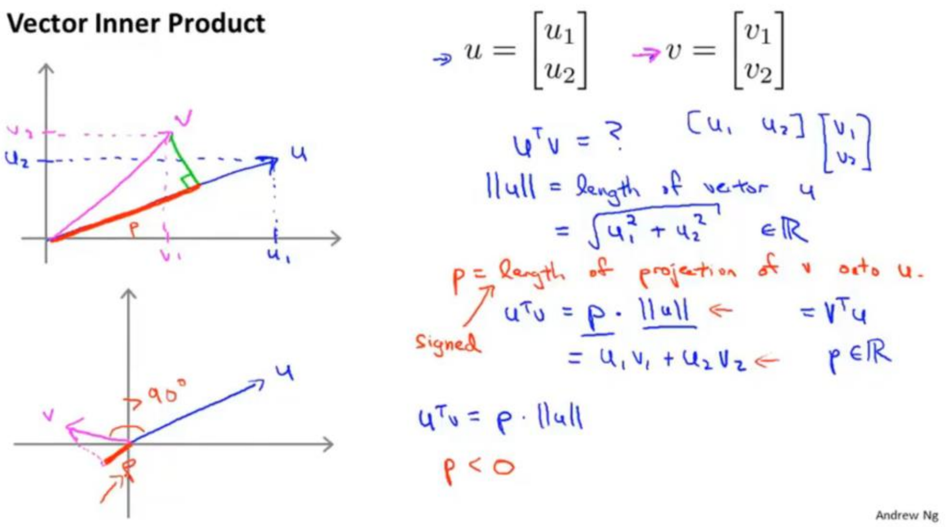
Whenever $y^{(i)} = 0$:

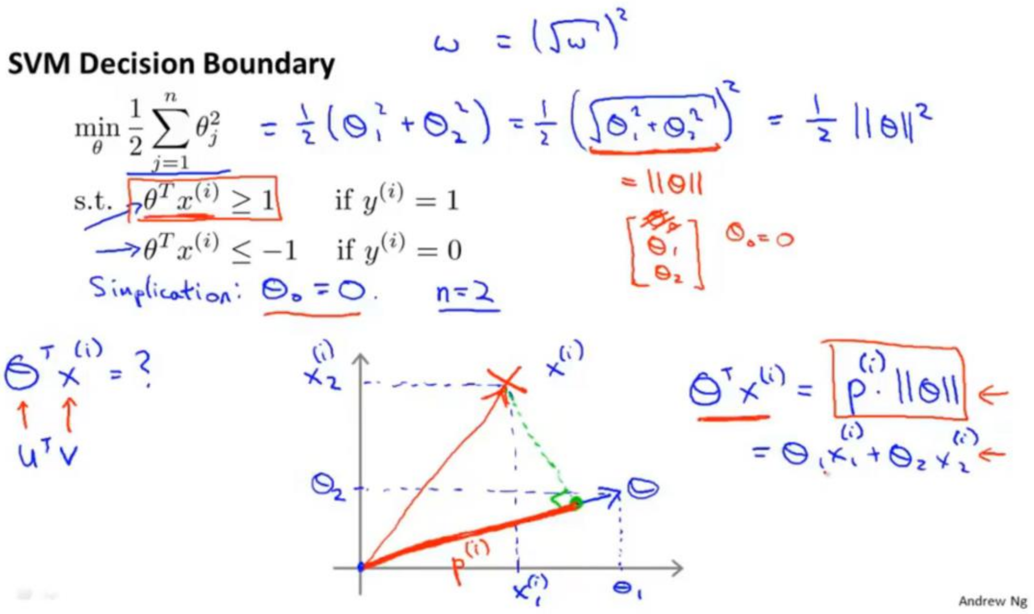
$\theta^T x^{(i)} \leq -1$





3 The mathematics behind large margin classification




SVM Decision Boundary
$\omega = (\sqrt{\omega})^2$
$\min_\theta \frac{1}{2}\sum_{j=1}^{n}\theta_j^2 = \frac{1}{2}(\theta_1^2+\theta_2^2) = \frac{1}{2}\left(\sqrt{\theta_1^2+\theta_2^2}\right)^2 = \frac{1}{2}\|\theta\|^2$
$= \|\theta\|$
s.t. $\theta^T x^{(i)} \geq 1$ if $y^{(i)} = 1$
$\theta^T x^{(i)} \leq -1$ if $y^{(i)} = 0$
Simplication: $\theta_0 = 0$. $n=2$
$\theta_0 = 0$
$\theta^T x^{(i)} = ?$
$u^T v$
$\theta^T x^{(i)} = p^{(i)} \cdot \|\theta\|$
$= \theta_1 x_1^{(i)} + \theta_2 x_2^{(i)}$
$x^{(i)}$
$x_2^{(i)}$
θ_2
θ
$p^{(i)}$
$x_1^{(i)}$
θ_1
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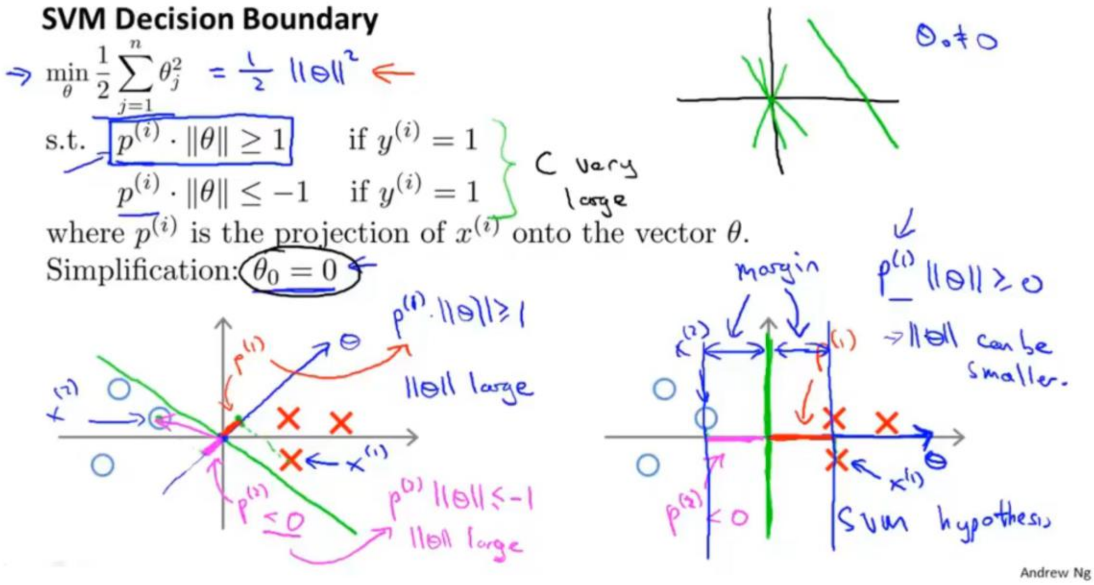
SVM Decision Boundary
$\min_\theta \frac{1}{2}\sum_{j=1}^{n}\theta_j^2 = \frac{1}{2}\|\theta\|^2$
s.t. $p^{(i)} \cdot \|\theta\| \geq 1$ if $y^{(i)} = 1$
$p^{(i)} \cdot \|\theta\| \leq -1$ if $y^{(i)} = 1$
C very large
where $p^{(i)}$ is the projection of $x^{(i)}$ onto the vector θ.
Simplification: $\theta_0 = 0$
$\theta_0 \neq 0$
$p^{(1)} \cdot \|\theta\| \geq 1$
$\|\theta\|$ large
$p^{(2)} \|\theta\| \leq -1$
$\|\theta\|$ large
$x^{(1)}$
$x^{(2)}$
$p^{(1)}$
$p^{(2)} \leq 0$
margin
$p^{(i)} \|\theta\| \geq 0$
$\rightarrow \|\theta\|$ can be smaller.
$p^{(2)} < 0$
SVM hypothesis
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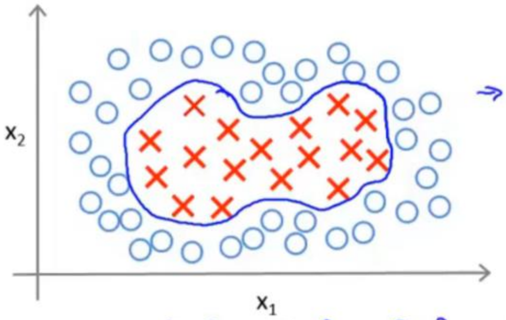
4 Kernels I

Non-linear Decision Boundary



Predict $y = 1$ if

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

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

$$\theta_0 + \theta_1 f_1 + \theta_2 f_2 + \theta_3 f_3 + \dots$$

$$f_1 = x_1, \quad f_2 = x_2, \quad f_3 = x_1 x_2, \quad f_4 = x_1^2, \quad f_5 = x_2^2, \dots$$

Is there a different / better choice of the features $f_1, f_2, f_3, \ldots$?

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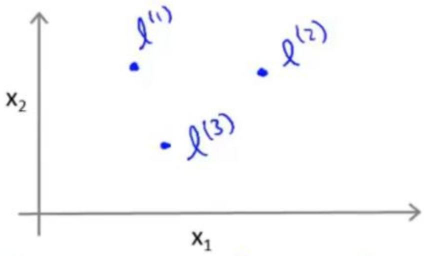
Kernel



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

$\|w\|$

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

Given x:

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

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

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

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

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Kernels and Similarity

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

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

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

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

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

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

x

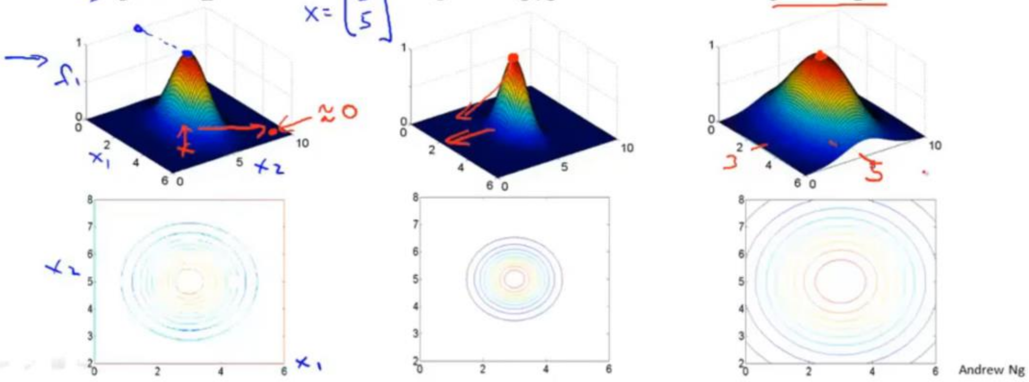
If x if far from $l^{(1)}$:

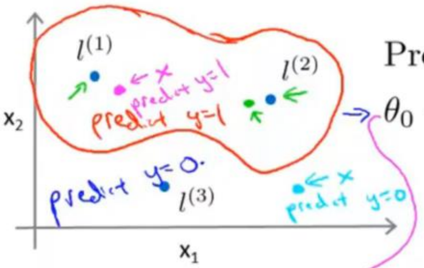
$$f_1 = \exp\left(-\frac{(\text{large number})^2}{2\sigma^2}\right) \approx 0.$$

Example:

$\rightarrow l^{(1)} = \boxed{\begin{bmatrix}3\\5\end{bmatrix}}$, $\quad f_1 = \exp\left(-\frac{\|x-l^{(1)}\|^2}{2\boxed{\sigma^2}}\right)$

$\rightarrow \sigma^2 = 1$ $\quad x = \begin{bmatrix}3\\5\end{bmatrix}$ $\quad \sigma^2 = 0.5$ $\quad \sigma^2 = 3$





Predict "1" when

$\rightarrow \theta_0 + \theta_1 f_1 + \theta_2 f_2 + \theta_3 f_3 \geq 0$

x

$\theta_0 = -0.5, \quad \theta_1 = 1, \quad \theta_2 = 1, \quad \theta_3 = 0$

$f_1 \approx 1, \quad f_2 \approx 0, \; f_3 \approx 0.$

$\rightarrow \theta_0 + \theta_1 \times 1 + \theta_2 \times 0 + \theta_3 \times 0$

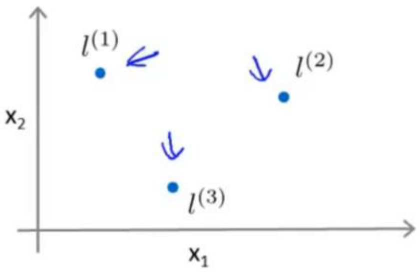
$= -0.5 + 1 = 0.5 \geq 0$

$f_1, f_2, f_3 \approx 0$

$\rightarrow \theta_0 + \theta_1 f_1 + \dots \approx -0.5 < 0$

5 Kernels II

Choosing the landmarks



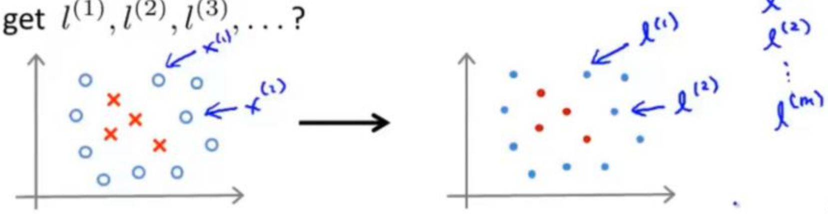
Given x:

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

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

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

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



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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 $\underline{x}$:

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

→ f_1 = similarity$(x, l^{(1)})$ $x^{(i)}$

→ f_2 = similarity$(x, l^{(2)})$

...

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

$x^{(i)} \to$

$f_1^{(i)} = sim(x^{(i)}, l^{(1)})$

$f_2^{(i)} = sim(x^{(i)}, l^{(2)})$

$\vdots$

$f_i^{(i)} = sim(x^{(i)}, l^{(i)}) = \exp(-\frac{0}{2\sigma^2}) = 1$ $x^{(i)}$

$f_m^{(i)} = sim(x^{(i)}, l^{(m)})$

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

$$f^{(i)} = \begin{bmatrix} f_0^{(i)} \\ f_1^{(i)} \\ \vdots \\ f_m^{(i)} \end{bmatrix} \qquad f_0^{(i)} = 1$$

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SVM with Kernels

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

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

Training: $n = m$

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

$\cancel{\theta^T x^{(i)}}$ $\theta^T f^{(i)}$ $\to \theta_0$

- $\sum_j \theta_j^2 = \theta^T \theta$ $\|\theta\|^2$ $\theta = \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_m \end{bmatrix}$ (ignoring θ_0)
- $\underline{\theta^T M \theta}$ $m = 10{,}000$

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SVM parameters:

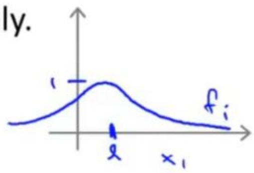
C ($= \frac{1}{\lambda}$). → Large C: Lower bias, high variance.   (small λ)

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

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

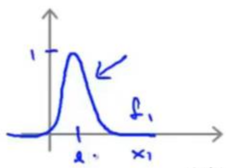
→ Higher bias, lower variance.

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



Small σ^2: Features f_i vary less smoothly.

Lower bias, higher variance.



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6 Using an SVM

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 $\theta^T x \geq 0$

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

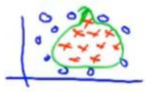
→ n large, m small $x \in \mathbb{R}^{n+1}$

Gaussian kernel:

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

$x \in \mathbb{R}^n$, n small and/or m large

Need to choose σ^2.



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Kernel (similarity) functions:

$x^{(i)}$ $l^{(j)} = x^{(j)}$ f_i

```
function f = kernel(x1,x2)
```

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

```
return
```

$x \to f_1, f_2, \ldots, f_m$

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

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

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

$v = x - l$

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

$= (x_1 - l_1)^2 + (x_2 - l_2)^2 + \cdots + (x_n - l_n)^2$.

1000 feet^2 1-5 bedrooms

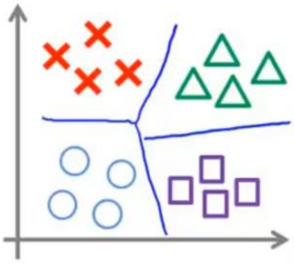
Other choices of kernel

Note: Not all similarity functions 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: $k(x, l) = (x^T l)^2$ $(x^T l + \text{constant})^{\text{degree}}$
  $(x^T l)^3$, $(x^T l + 1)^3$, $(x^T l + 5)^4$
- More esoteric: String kernel, chi-square kernel, histogram intersection kernel, ...
  $\text{sim}(x, l)$

Multi-class classification



$y \in \{1, 2, 3, \ldots, K\}$

Many SVM packages already have built-in multi-class classification functionality.

→ Otherwise, use one-vs.-all method. (Train K SVMs, one to distinguish $y = i$ from the rest, for $i = 1, 2, \ldots, K$), get $\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(K)}$

Pick class i with largest $(\theta^{(i)})^T x$

$y=1$ $y=2$ .... $\theta = K$

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Logistic regression vs. SVMs

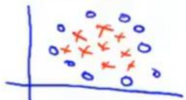
$n =$ number of features ($x \in \mathbb{R}^{n+1}$), $m =$ number of training examples

→ If n is large (relative to m): (E.g. $n \geq m$, $n = 10{,}000$, $m = 10 \ldots 1000$)

→ 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.