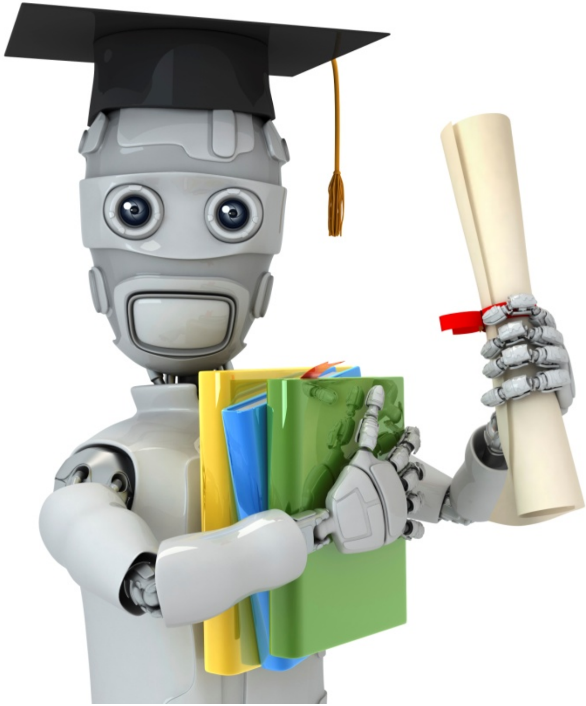


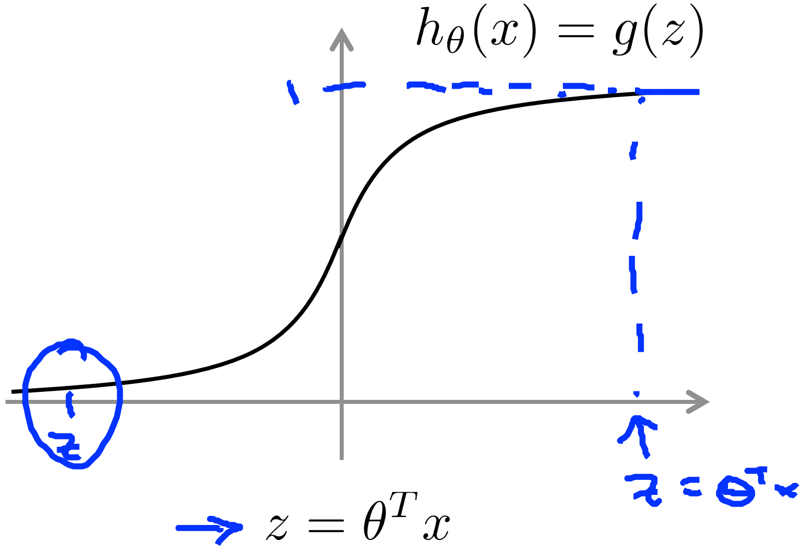
Machine Learning

Support Vector Machines

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 $h_\theta(x) \approx 0$, $\theta^T x \ll 0$

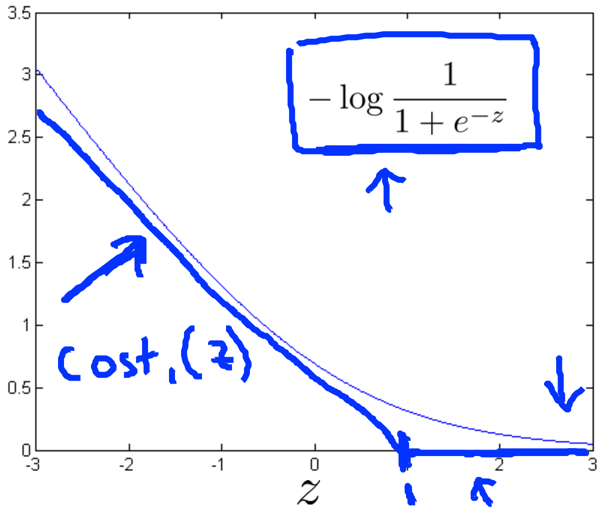
Alternative view of logistic regression

(x, y)

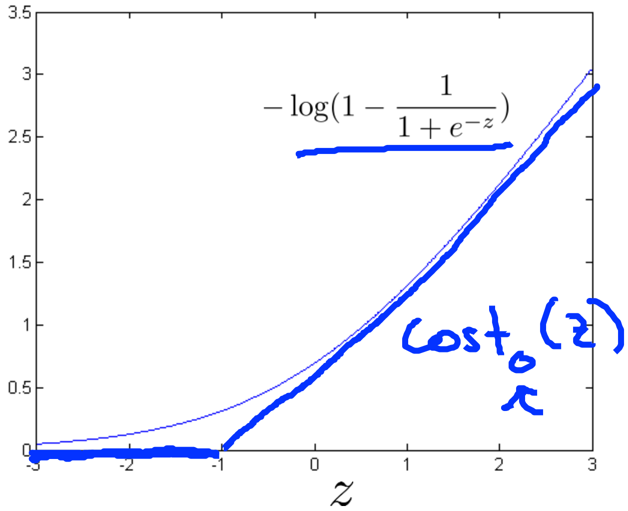
Cost of example: $-(y \log h_\theta(x) + (1-y)\log(1-h_\theta(x)))$

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

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



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



Andrew Ng

Support vector machine

Logistic regression:

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

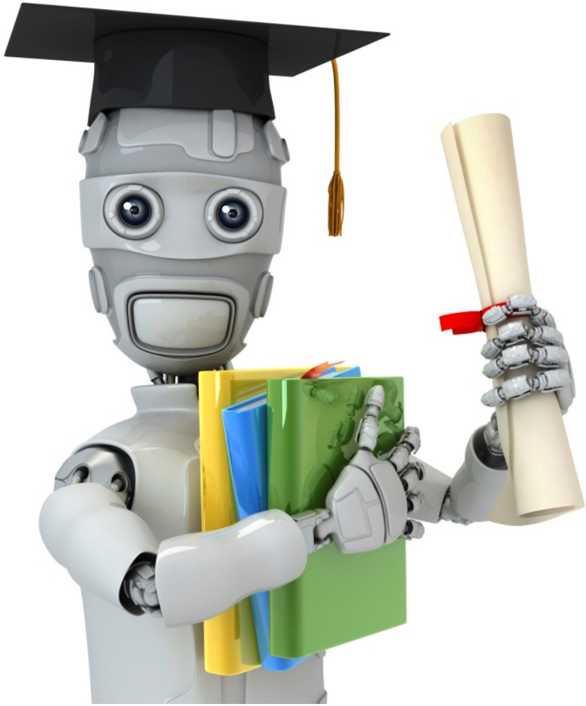
Support vector machine:

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

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:



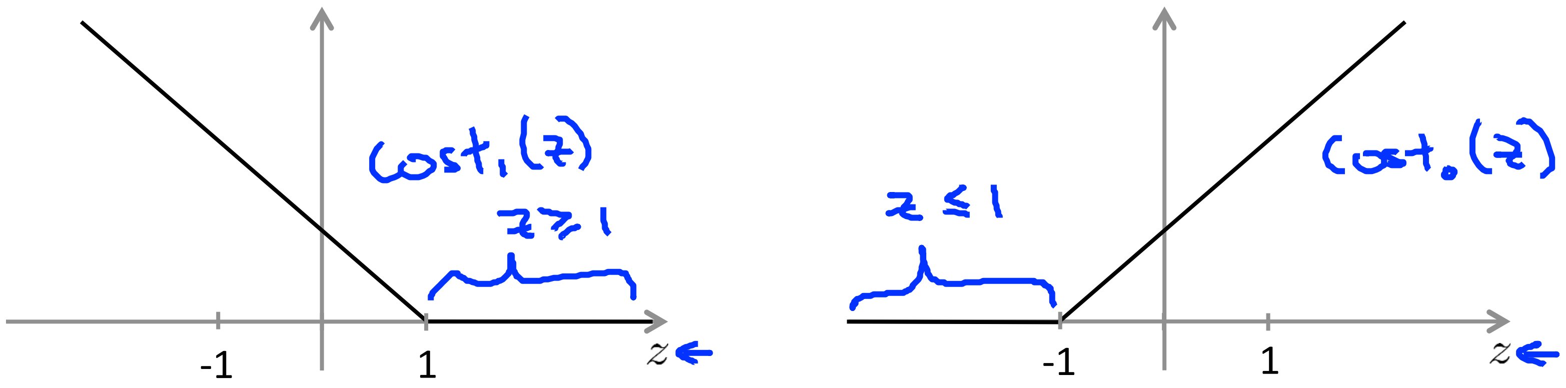
Support Vector Machines

Large Margin Intuition

Machine Learning

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

$C = 100{,}000$

SVM Decision Boundary

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

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

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

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

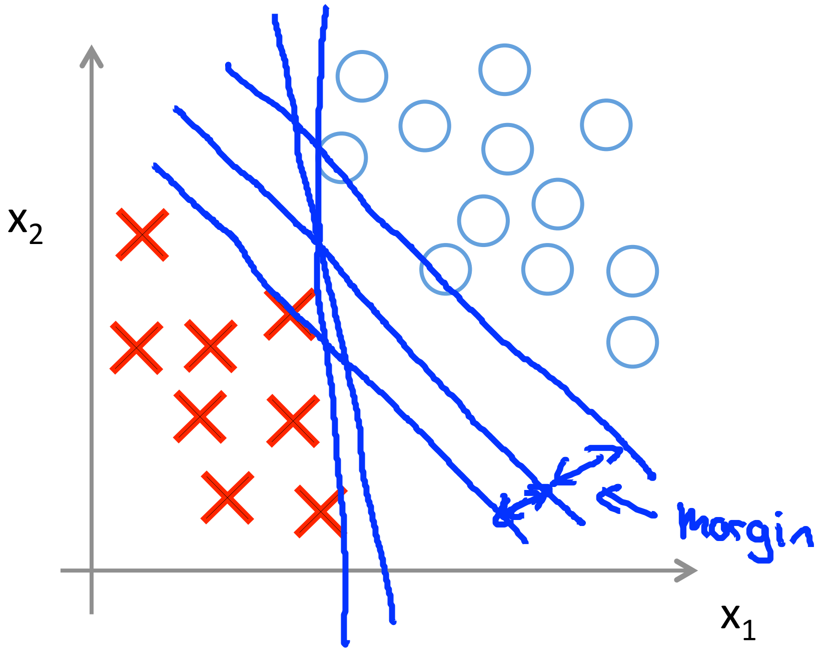
s.t. $\theta^T x^{(i)} \geq 1$ if $y^{(i)} = 1$

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

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

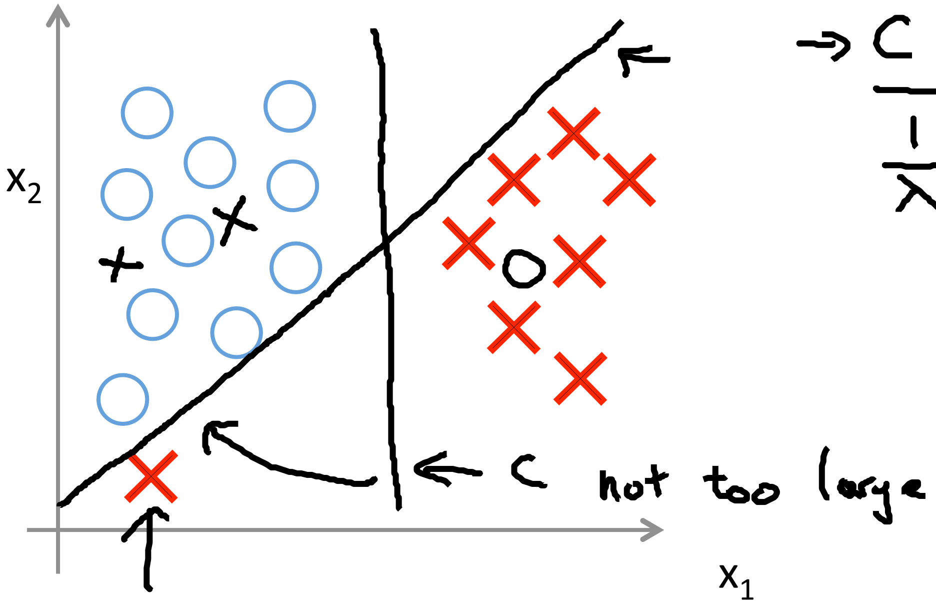
$\theta^T x^{(i)} \leq -1$

SVM Decision Boundary: Linearly separable case



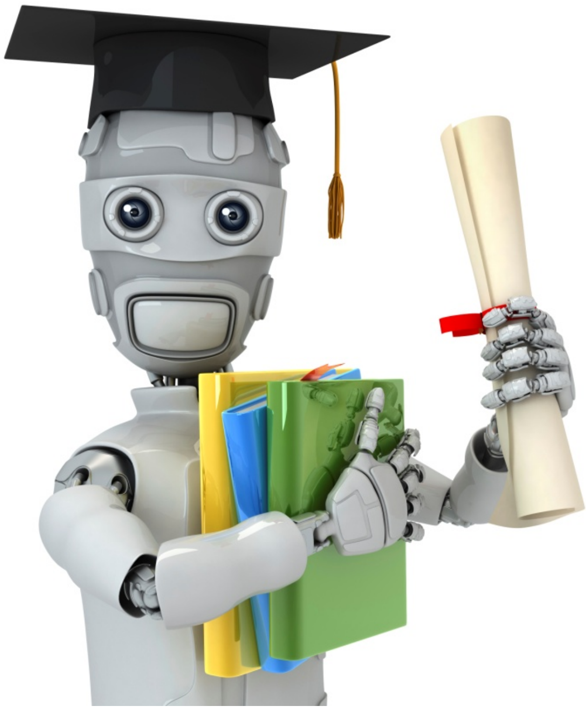
Large margin classifier

Large margin classifier in presence of outliers



$\rightarrow$ C very large

$\frac{1}{\lambda}$

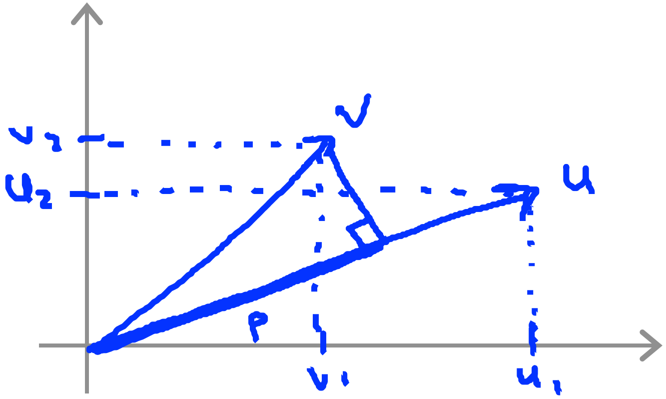


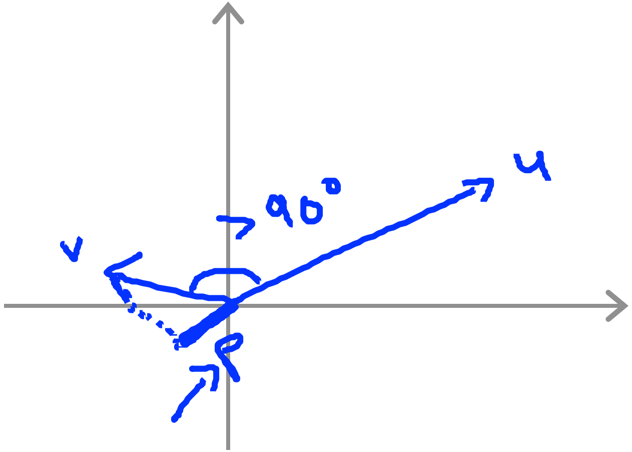
Machine Learning

Support Vector Machines

The mathematics behind large margin classification (optional)

Vector Inner Product





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

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

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

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

p = length of projection of v onto u.

signed

$u^T v = \underline{p} \cdot \underline{\|u\|} \leftarrow \quad = v^T u$

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

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

$p < 0$

$$w = (\sqrt{w})^2$$

SVM Decision Boundary

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

$$= \|\theta\|$$

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

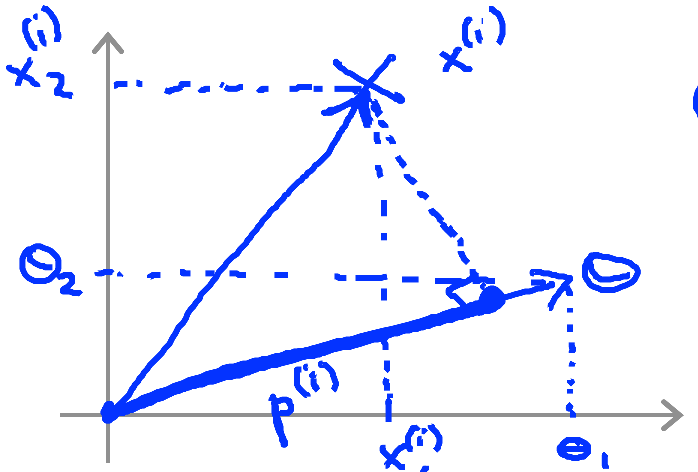
$\theta^T x^{(i)} \leq -1$ if $y^{(i)} = 0$

Simplification: $\theta_0 = 0$. $n = 2$

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

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

$$u^T v$$



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

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

SVM Decision Boundary

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

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

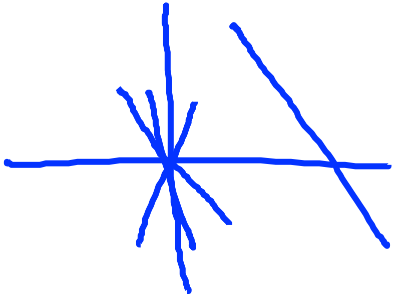
$$p^{(i)} \cdot \|\theta\| \leq -1 \quad \text{if } y^{(i)} = 1$$

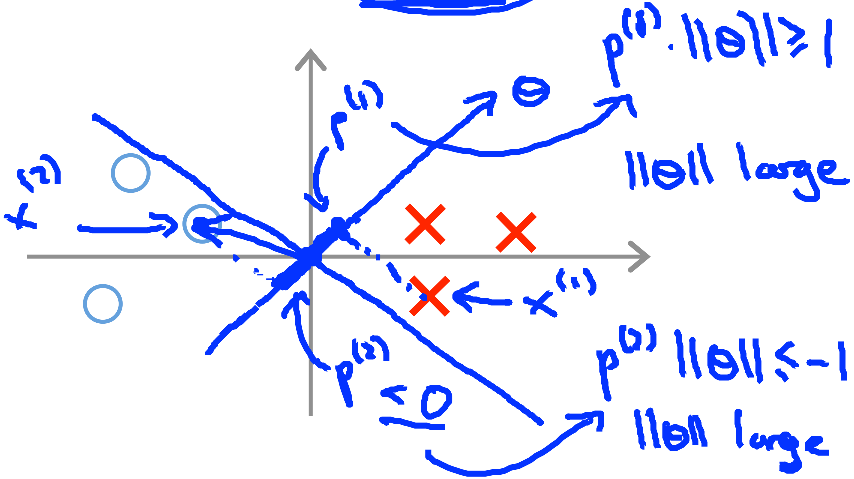
C very large

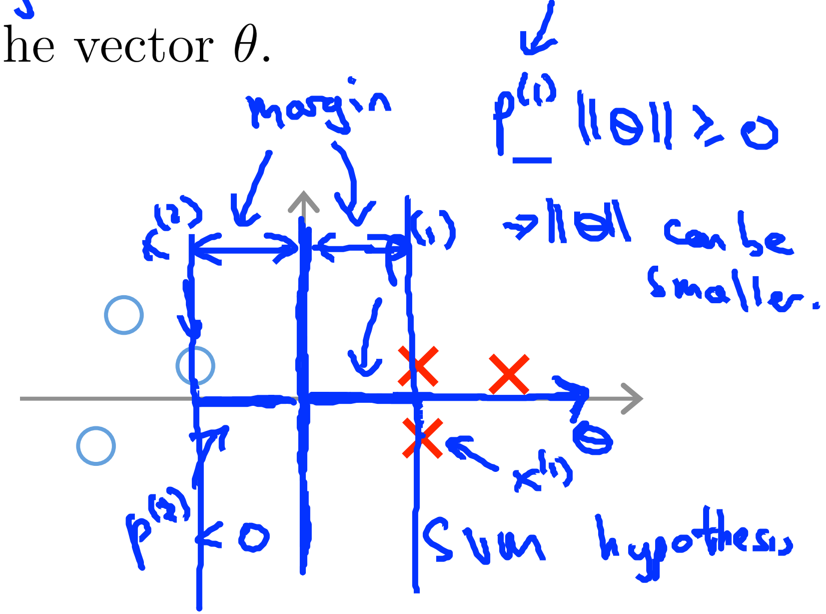
where $p^{(i)}$ is the projection of $x^{(i)}$ onto the vector θ.

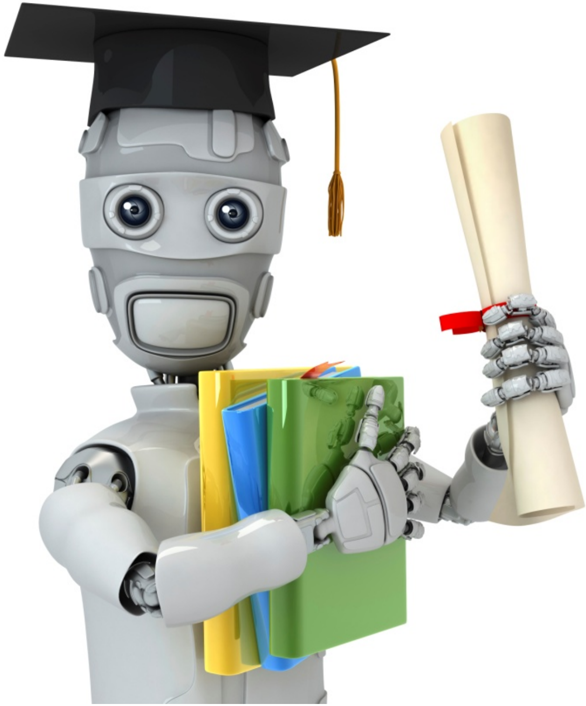
Simplification: $\theta_0 = 0$ ←

$\theta_0 \neq 0$







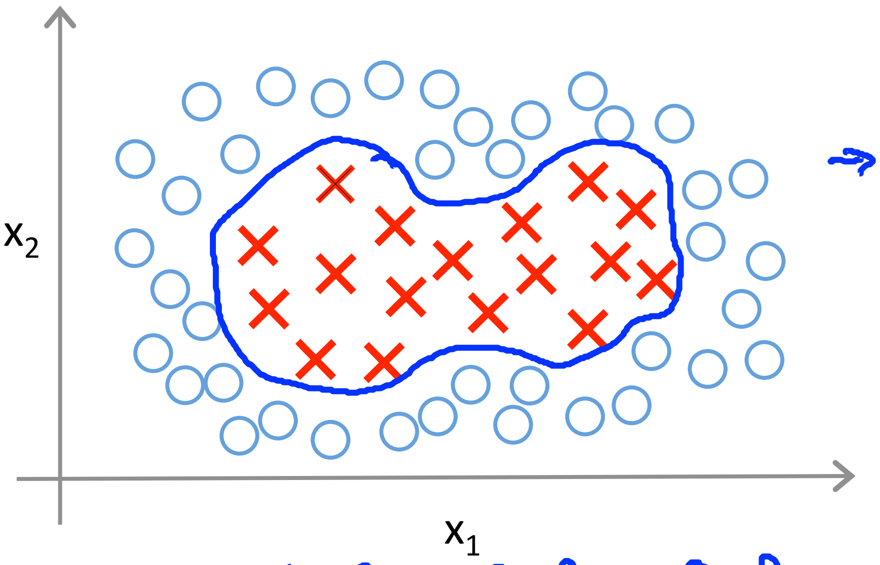


Support Vector Machines

Kernels I

Machine Learning

Non-linear Decision Boundary



Predict $y = 1$ if

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

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

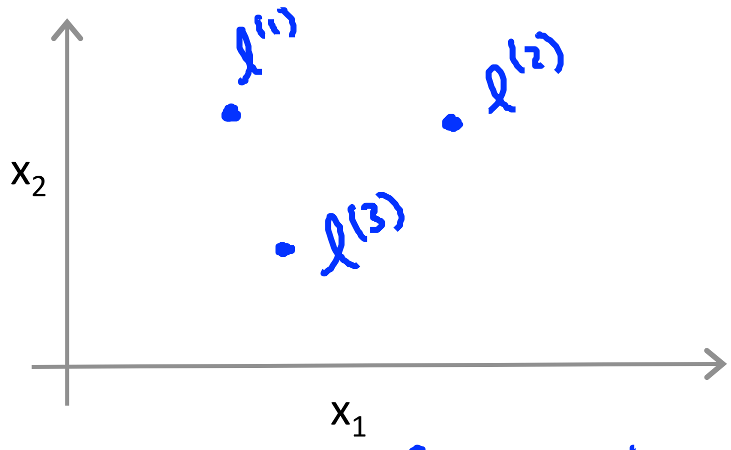
$$\theta_0 + \theta_1 f_1 + \theta_2 f_2 + \theta_3 f_3 + \cdots$$

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

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

Andrew Ng

Kernel



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

Given x:

$\|w\|$

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

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

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

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

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

Andrew Ng

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 $l^{(1)}$:

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

Example:

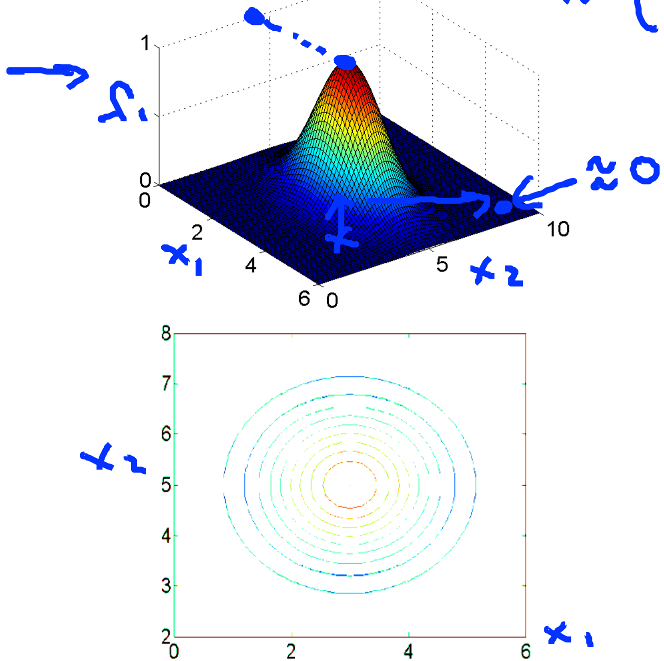
$l^{(1)} = \boxed{\begin{bmatrix}3\\5\end{bmatrix}}$, $\quad f_1 = \exp\left(-\frac{\|x-l^{(1)}\|^2}{2\boxed{\sigma^2}}\right)$

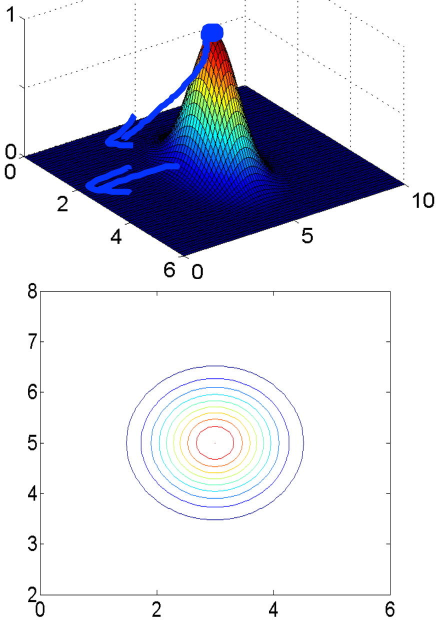
$\sigma^2 = 1$

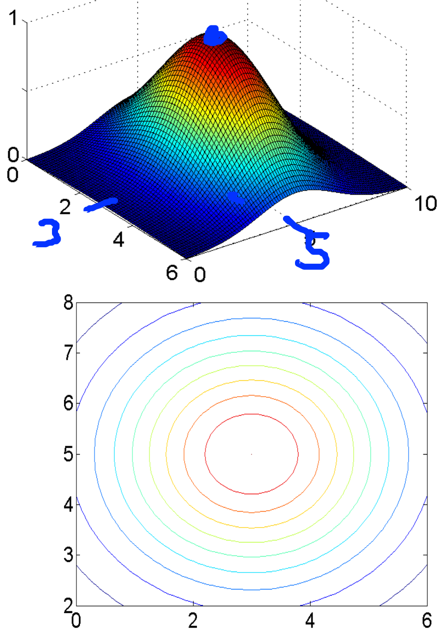
$x = \begin{bmatrix}3\\5\end{bmatrix}$

$\sigma^2 = 0.5$

$\sigma^2 = 3$







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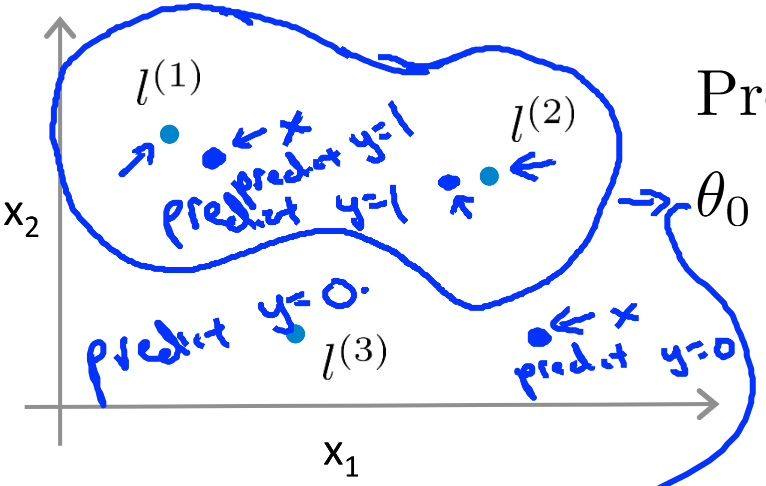


Predict "1" when

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

x

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

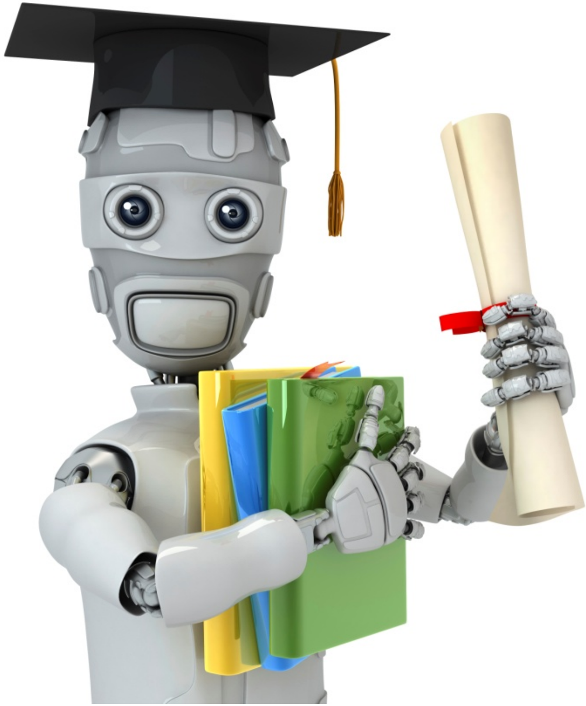
$f_1 \approx 1, \quad f_2 \approx 0, \quad f_3 \approx 0.$

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

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

$f_1, f_2, f_3 \approx 0$

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

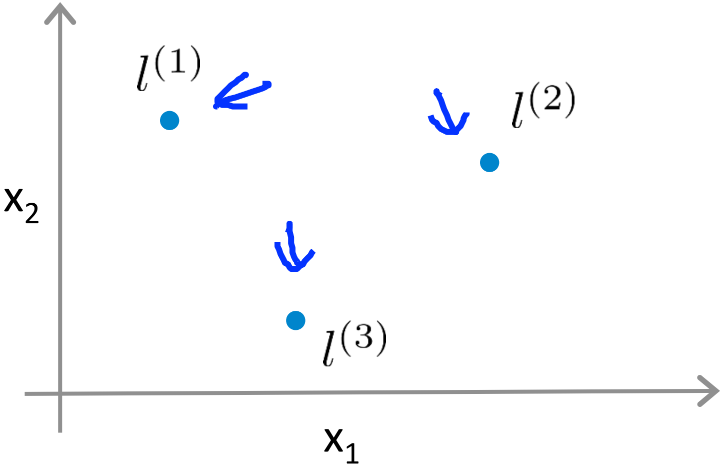


Machine Learning

Support Vector Machines

Kernels II

Choosing the landmarks

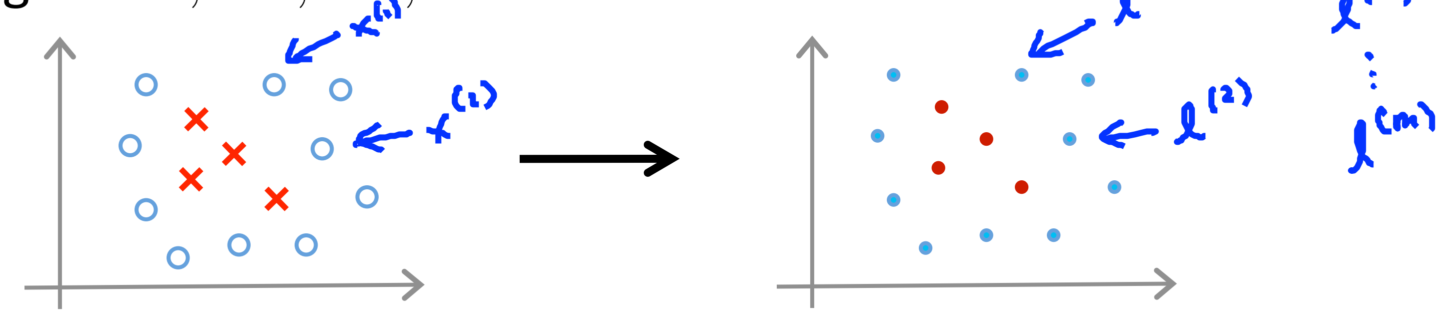


Given x:

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

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 $\underline{x}$:

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

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

$$\ldots$$

$x^{(1)}$

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

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

$\underline{x^{(i)}} \rightarrow$

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

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

$$\vdots$$

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

$x^{(i)}$

$$\vdots$$

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

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

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

$f_0^{(i)} = 1$

Andrew Ng

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:

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

$n = m$

$\cancel{n} = m$

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

→ θ_0

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

$\|\theta\|^2$

$\underline{\theta^T M \theta}$

$m = 10{,}000$

SVM parameters:

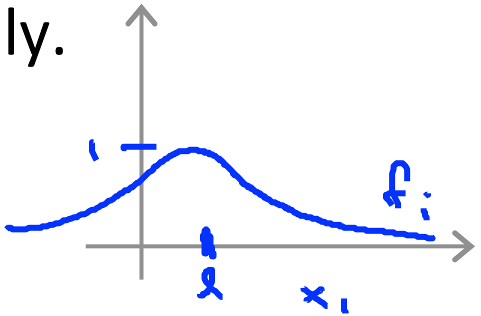
C ($= \frac{1}{\lambda}$). Large C: Lower bias, high variance. (small λ)

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

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

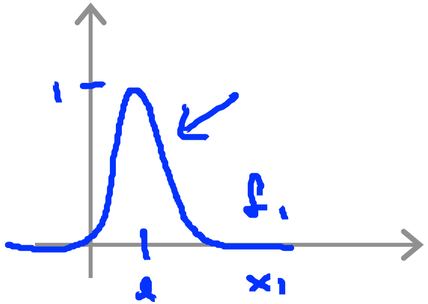
Higher bias, lower variance.

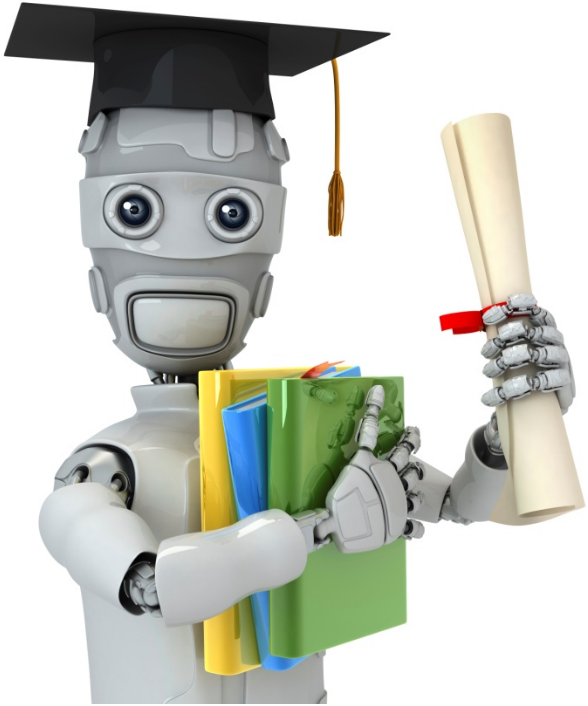
$\exp\left(-\frac{\|x-l^{(i)}\|^2}{2\sigma^2}\right)$



Small σ^2: Features f_i vary less smoothly.

Lower bias, higher variance.





Machine Learning

Support Vector Machines

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 $\theta^T x \geq 0$

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

n large, m small

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

To avoid overfitting.

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.

Kernel (similarity) functions:

$x^{(i)}$ $\quad l^{(j)} = x^{(j)}$

f_i

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

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

```
return
```

$x \rightarrow f_1, f_2, \vdots, f_m$

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: $k(x, l) = (x^T l)^2$, $+0$, $(x^T l + \text{constant})^{\text{degree}}$

$(x^T l)^3$, $(x^T l + 1)^3$, $(x^T l + 5)^4$

rarely used

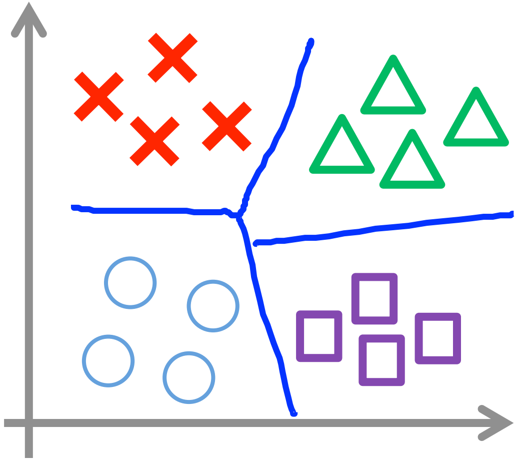
- More esoteric: String kernel, chi-square kernel, histogram intersection kernel, …

(known & understand by only small number of people)

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

Text classification.

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

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

Logistic regression vs. SVMs

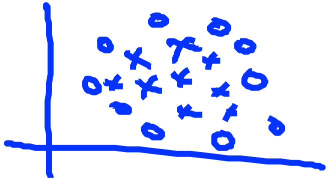
$n =$ number of features ($x \in \mathbb{R}^{n+1}$), $m =$ number of training examples

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.