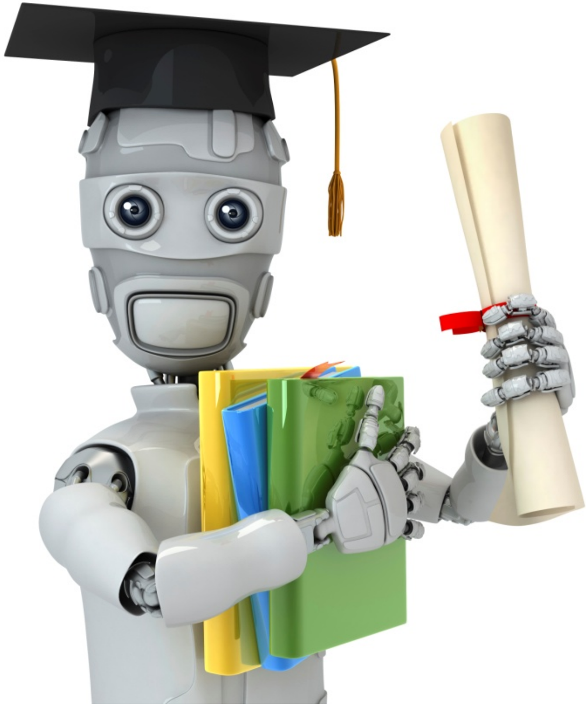


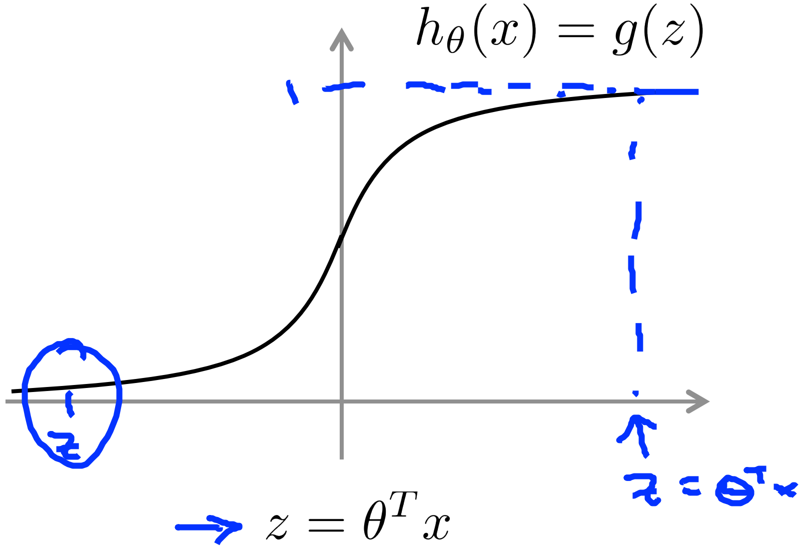
Machine Learning

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

(x, y)

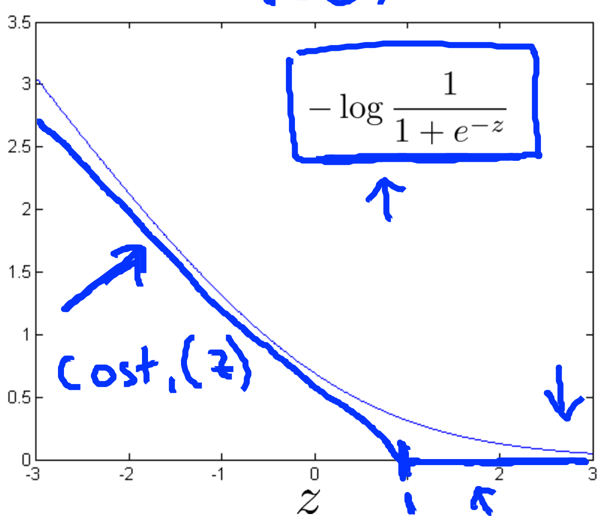
Alternative view of logistic regression

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

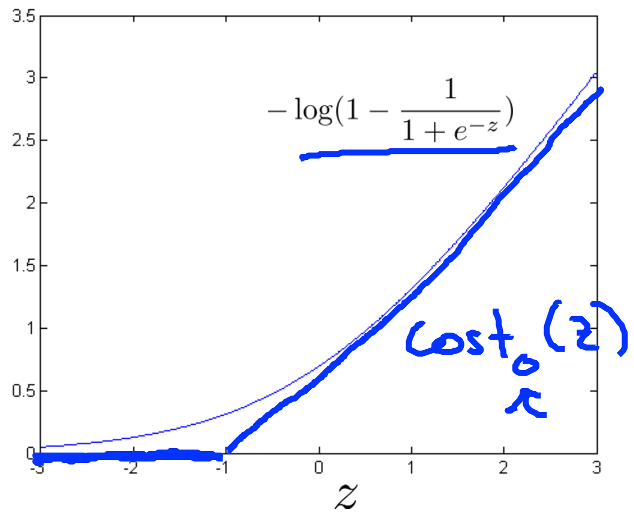
$$= \boxed{-y \log \frac{1}{\underline{1+e^{-\theta^T x}}}} \boxed{- \underline{(1-y)} \log\left(1 - \frac{1}{\underline{1+e^{-\theta^T x}}}\right)}$$

If $\underline{y=1}$ (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:

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

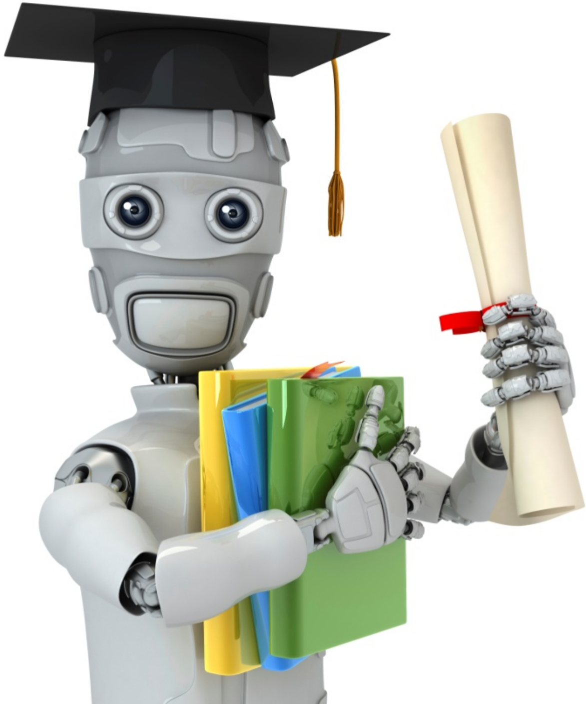
Support vector machine:

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

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:



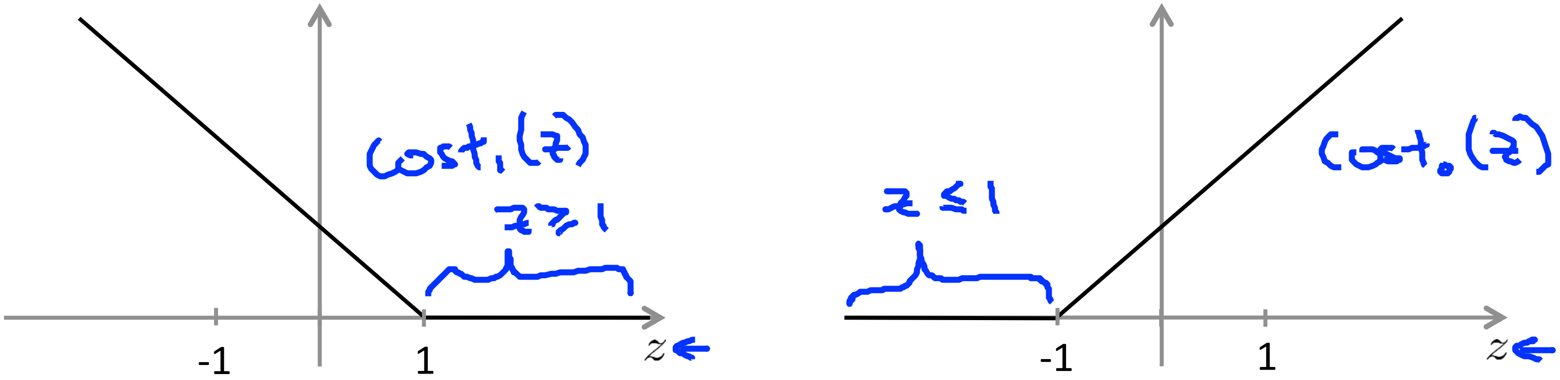
Machine Learning

Support Vector Machines

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 $\underline{y = 1}$, 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 $y^{(i)} = 1$:

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

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

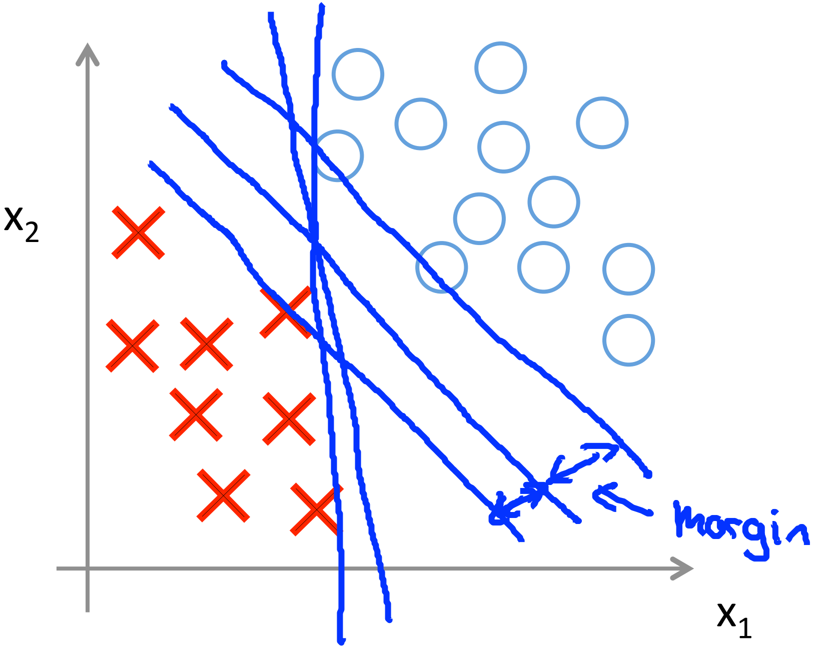
s.t. $\theta^T x^{(i)} \geq 1$ if $y^{(i)} = 1$

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

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

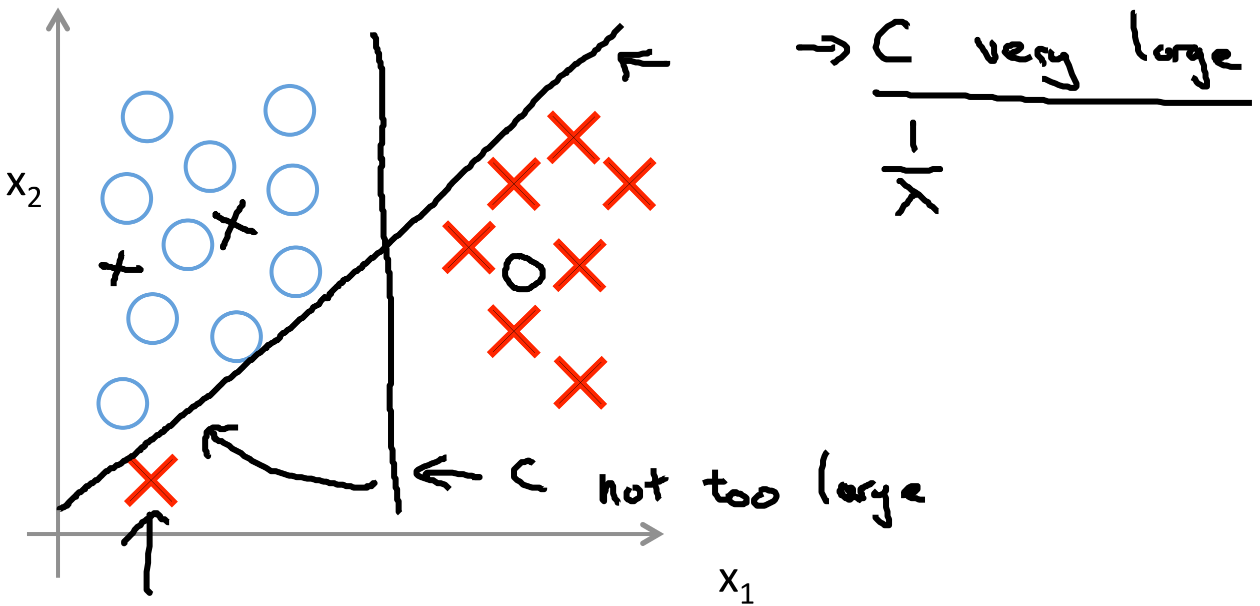
$\theta^T x^{(i)} \leq -1$

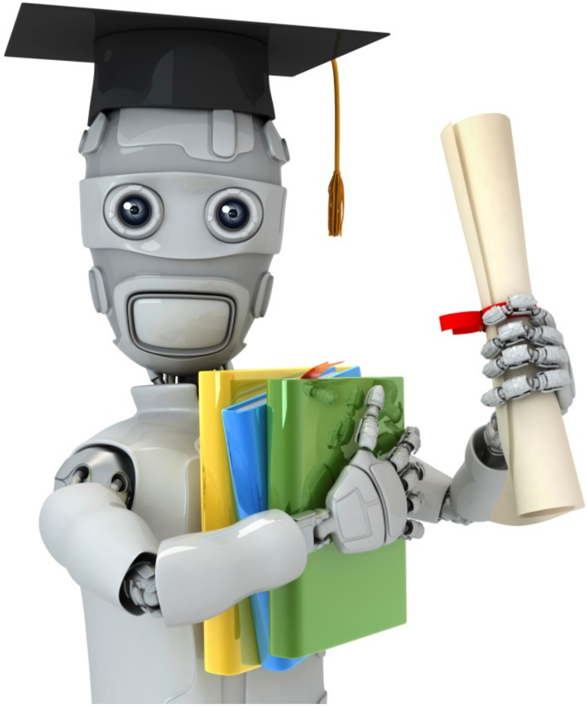
SVM Decision Boundary: Linearly separable case



Large margin classifier

Large margin classifier in presence of outliers



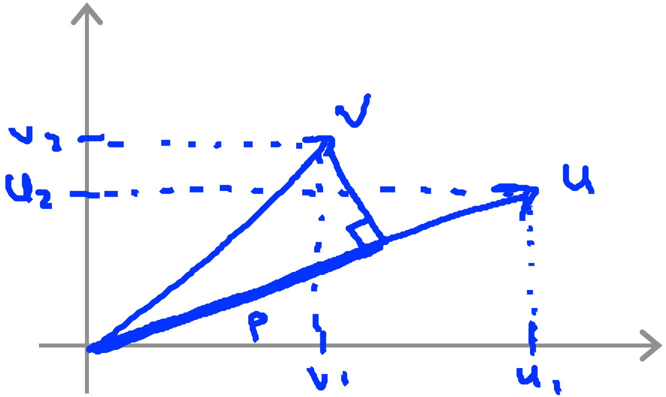


Machine Learning

Support Vector Machines

The mathematics behind large margin classification (optional)

Vector Inner Product



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

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

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

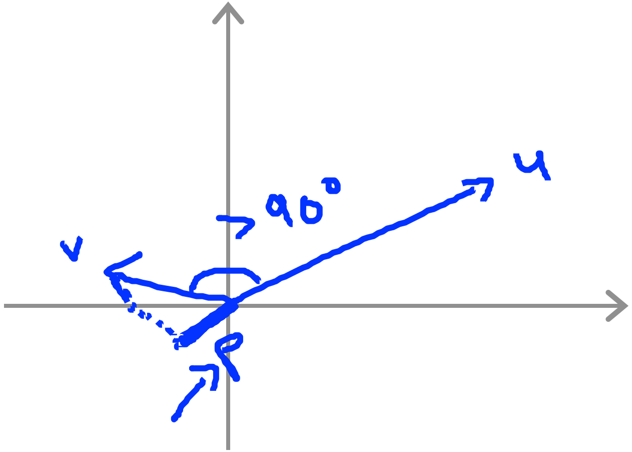
$= \sqrt{u_1^2 + u_2^2} \quad \in \mathbb{R}$

p = length of projection of v onto u.

signed

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

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



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

$p < 0$

Andrew Ng

SVM Decision Boundary

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

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

$$\sqrt{\theta_1^2+\theta_2^2} = \|\theta\|$$

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

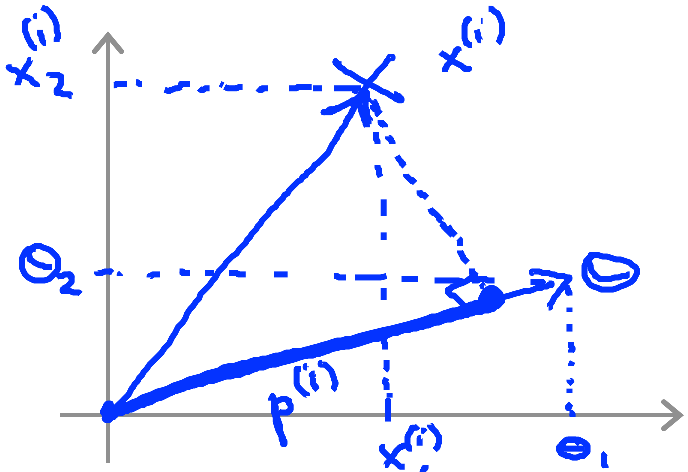
s.t. $\boxed{\theta^T x^{(i)} \geq 1}$ if $y^{(i)} = 1$

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

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

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

$$u^T v$$



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

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

Andrew Ng

SVM Decision Boundary

The theta vector is always perpendicular to the line of decision of boundary (θ^tX =0). This is because θ^tX = θ dot X = θX cos(alpha) = 0, where alpha has to be 90 degrees.

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

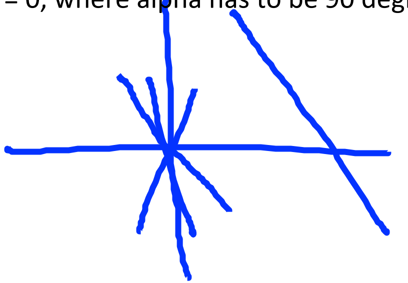
$$\text{s.t.}\quad \boxed{p^{(i)}\cdot\|\theta\| \geq 1} \quad \text{if } y^{(i)} = 1$$
$$p^{(i)}\cdot\|\theta\| \leq -1 \quad \text{if } y^{(i)} = 1$$

C very large

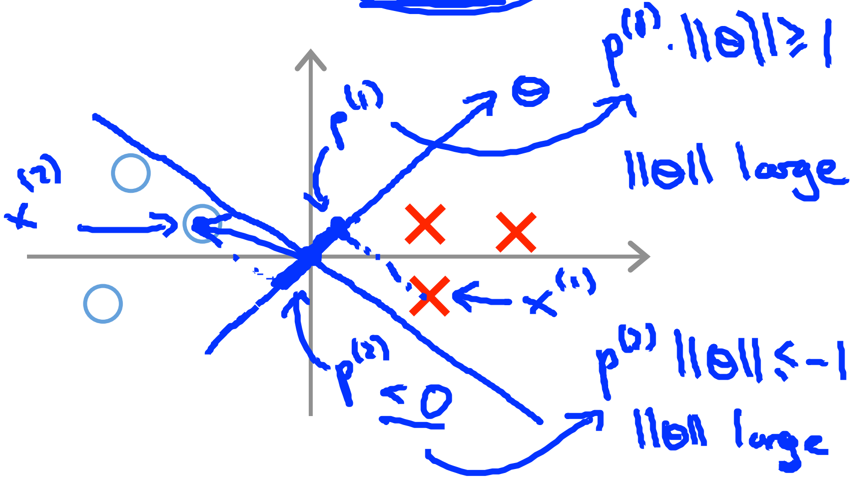
where $p^{(i)}$ is the projection of $x^{(i)}$ onto the vector θ.

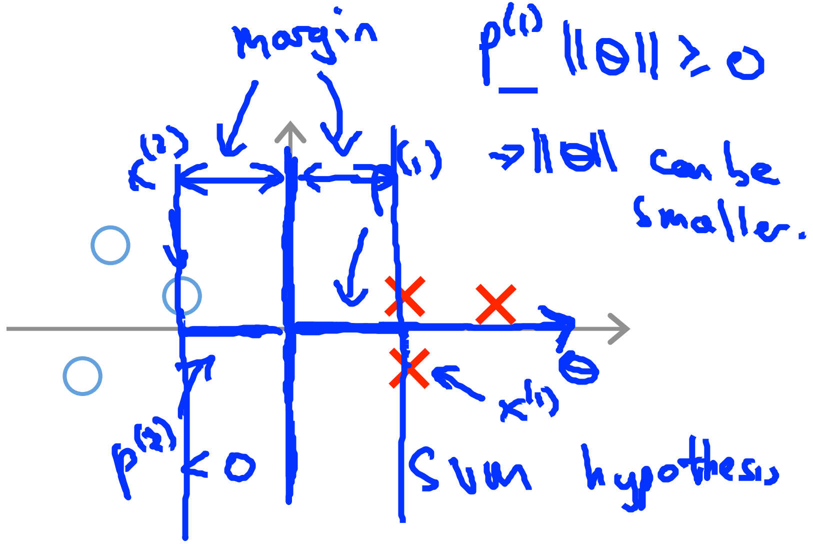
Simplification: $\theta_0 = 0$

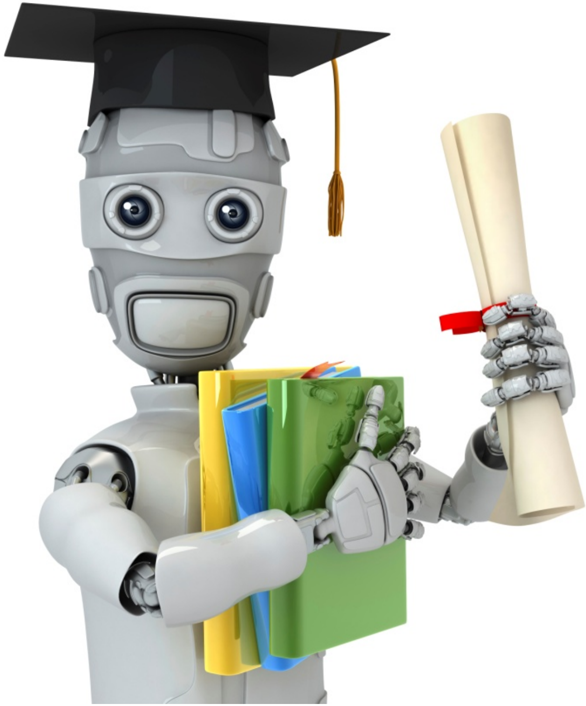
$\theta_0 \neq 0$



$p^{(i)}\|\theta\| \geq 0$







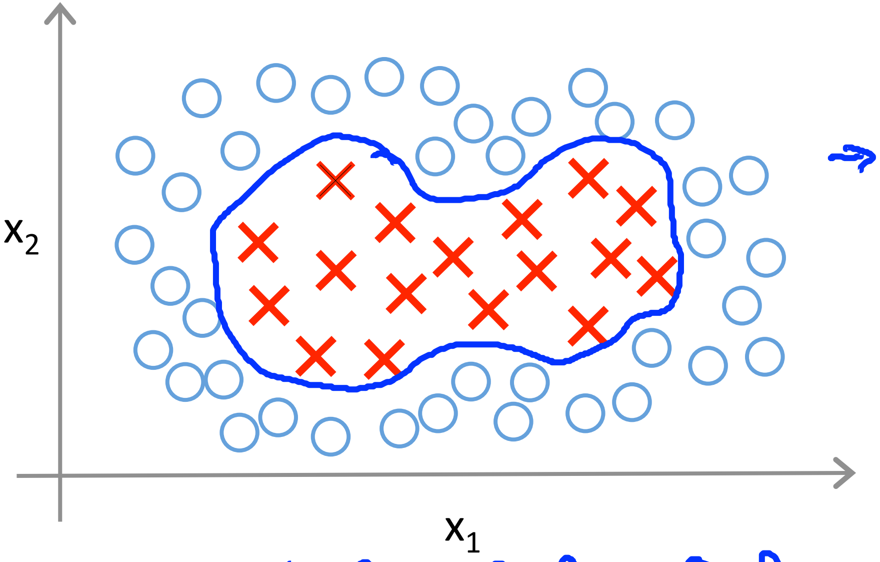
Support Vector Machines

Kernels I

Machine Learning

This is because of the definition of hypothesis

Non-linear Decision Boundary



Predict $y = 1$ if

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

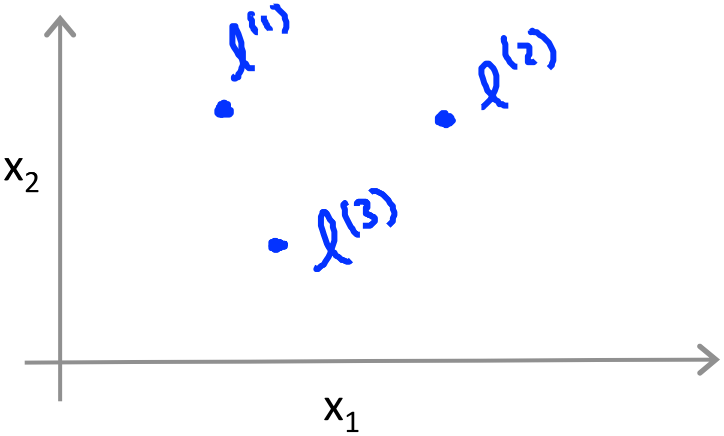
$$h_\theta(x) = \begin{cases} 1 & \text{if } \theta_0 + \theta_1 x_1 + \cdots \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

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

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

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

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)

$k(x, l^{(i)})$

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 $l^{(1)}$:

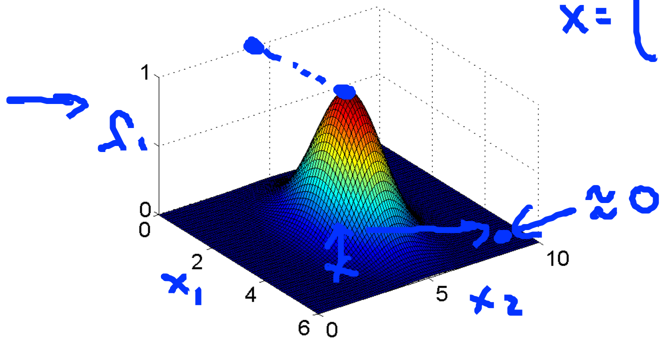
$$f_1 = \exp\left(-\frac{(\text{large number})^2}{2\sigma^2}\right) \approx 0.$$

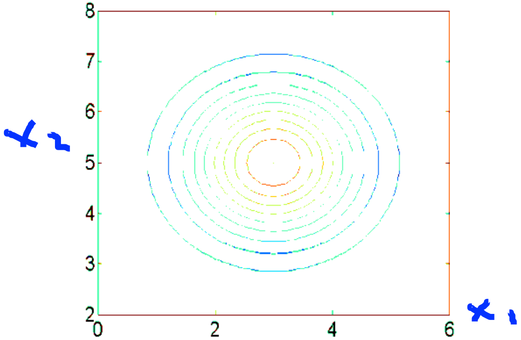
Example:

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

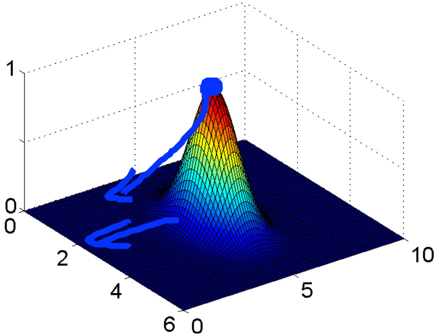
$\sigma^2 = 1$

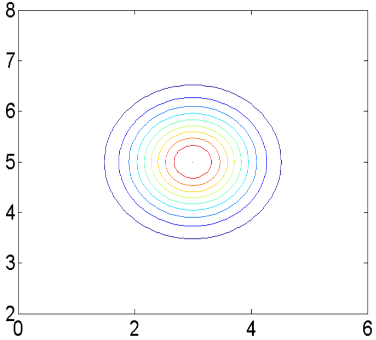
$x = \begin{bmatrix}3\\5\end{bmatrix}$



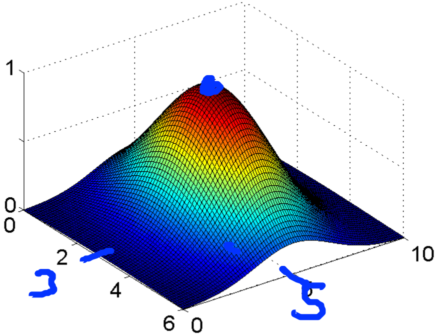


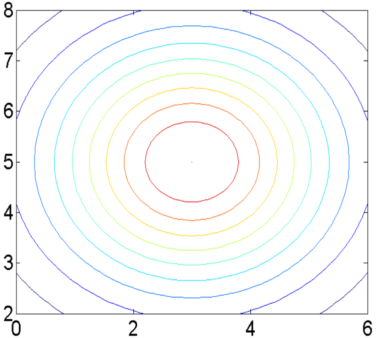
$\sigma^2 = 0.5$



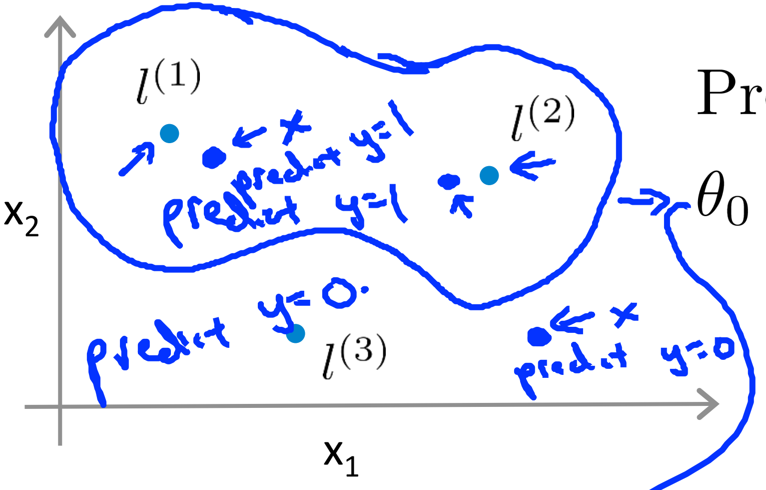


$\sigma^2 = 3$





With kernels, the definition of the hypothesis changes



Predict "1" when

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

x

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

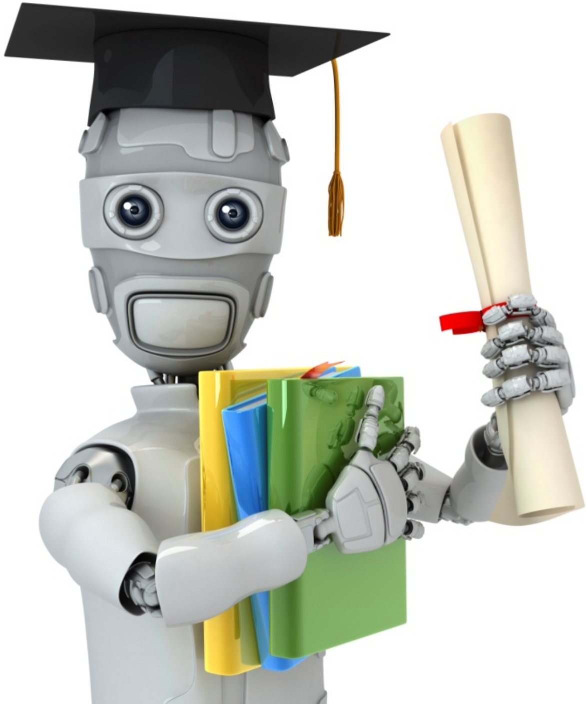
$f_1 \approx 1, \quad f_2 \approx 0, \quad f_3 \approx 0.$

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

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

$f_1, f_2, f_3 \approx 0$

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

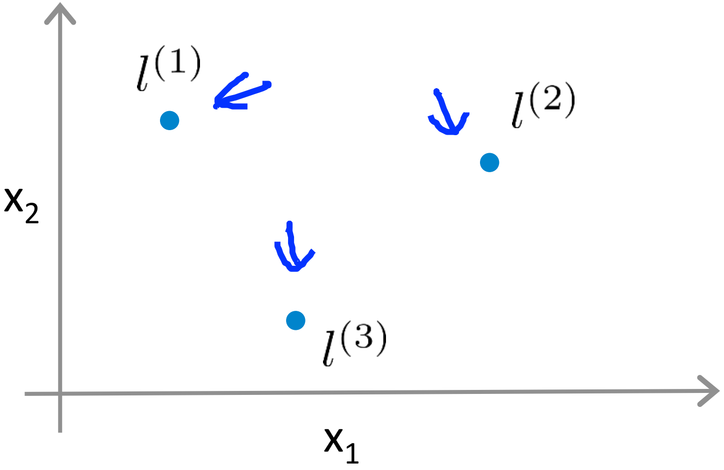


Machine Learning

Support Vector Machines

Kernels II

Choosing the landmarks

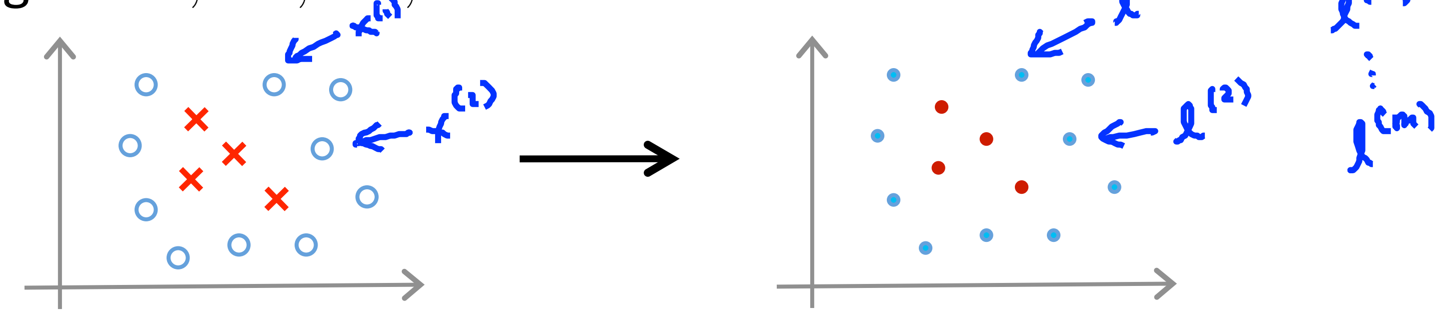


Given x:

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

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 $\underline{x}$:

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

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

$\ldots$

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

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

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

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

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

$\vdots$

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

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

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

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

Andrew Ng

SVM with Kernels

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

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

Training:

$n = m$

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

$\cancel{\theta^T x^{(i)}}$ $\theta^T f^{(i)}$ → θ_0

$$\sum_j \theta_j^2 = \theta^T \theta \leftarrow \theta = \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_m \end{bmatrix} \quad \text{(ignoring } \theta_0\text{)}$$

$\|\theta\|^2$

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

$m = 10{,}000$

How does SVM with Regularization and Kernels work?

1) Assign random theta values
2) Normalize all the features.
3) For each point in the dataset calculate the similarity from each landmark based on whatever kernel is chosen (and all of its associated parameters). Make a matrix of F storing the similarities of each point to other landmarks. This matrix will be similar to the X matrix storing features previously used.
4) Calculate the hypothesis based on the definition as given by SVM.
5) Choose a value for C based on whether you want to increase or decrease bias/ variance
6) Compare the hypothesis with the actual y values and calculate the cost (associated with that specific theta values).
7) Add the regularization term to the cost ($\theta^T M\theta$) based on the kernel specific matrix M.
8) Get better theta values by optimizing cost.
9) Once the theta values are found, we can construct the decision boundary by $\theta^T x = 0$, where x is x_0 , x_1, x_2, x_1^2....

Recall:

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

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

SVM parameters:

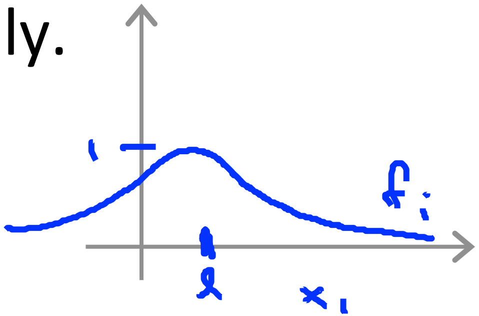
C ($= \frac{1}{\lambda}$). → Large C: Lower bias, high variance. (small λ)

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

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

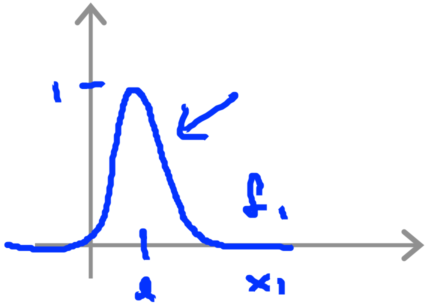
→ Higher bias, lower variance.

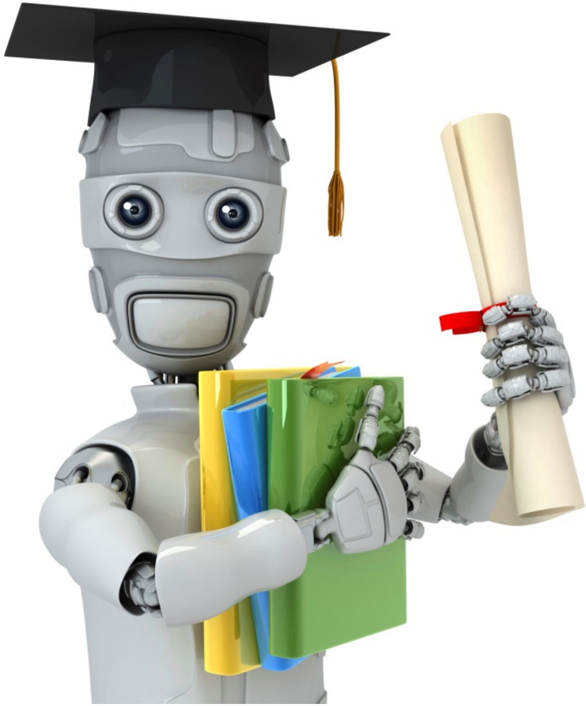
$\exp\left(-\frac{\|x - l^{(i)}\|^2}{2\sigma^2}\right)$



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):

linear kernel and logistic regression are basically the same thing. The only difference being we have to choose C instead of lamda as well as the M matrix

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

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

In some texts, the equation of linear kernel is defined as x*l or $x_1^T * x_2$

→ 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).

$(x^T l + \text{constant})^{\text{degree}}$

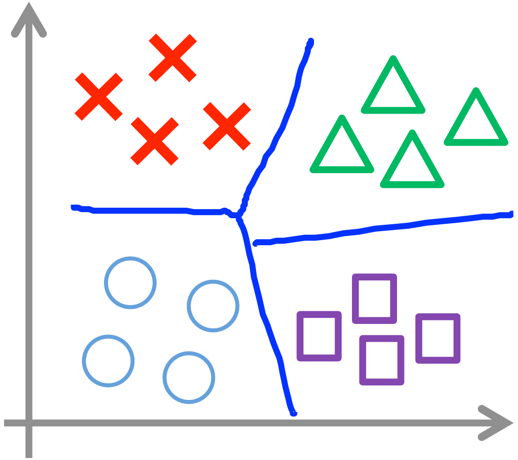
Many off-the-shelf kernels available:

- Polynomial kernel: $k(x, l) = (x^T l)^2$, $(x^T l)^3$, $(x^T l + 1)^3$, $(x^T l + 5)^4$

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

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

Logistic regression vs. SVMs

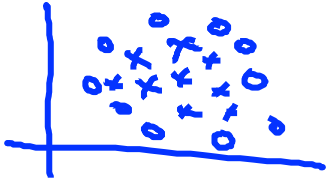
$n =$ number of features ($x \in \mathbb{R}^{n+1}$), $m =$ number of training examples

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.

If m is large and n is comparable to m, then we prefer to use logistic regression or linear kernel as it would still give accurate results and also will not be too taxing to the system.