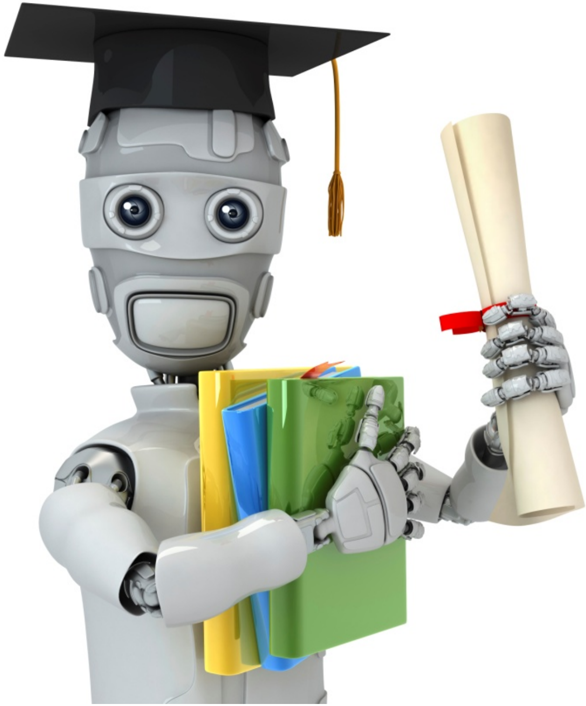


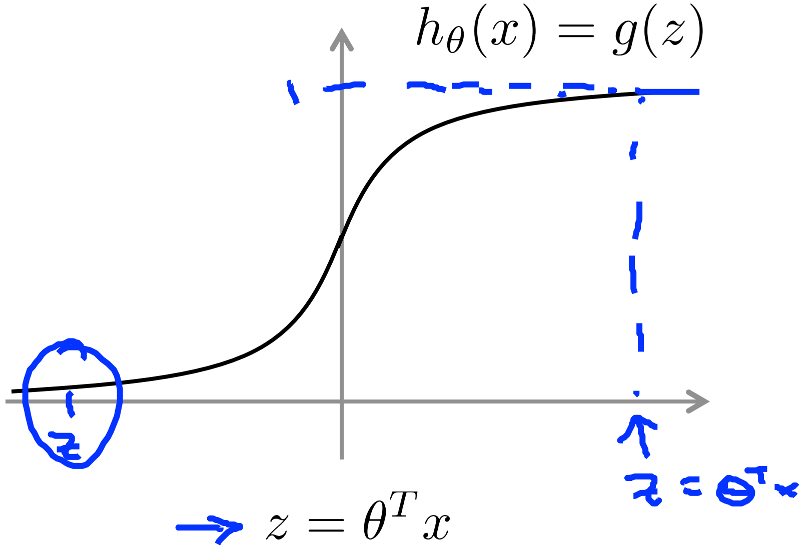
Machine Learning

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

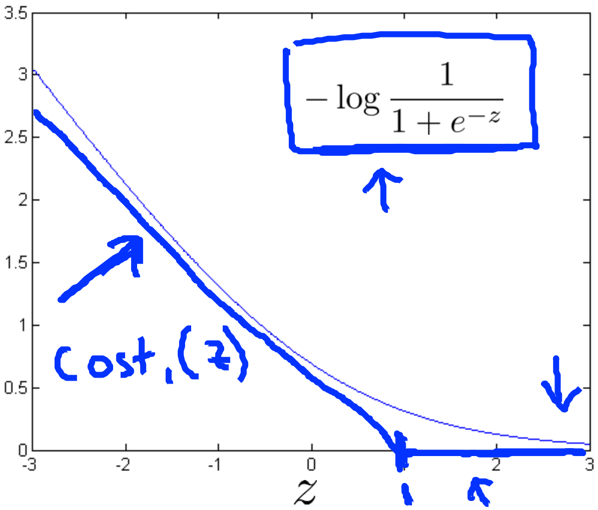
(x, y)

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

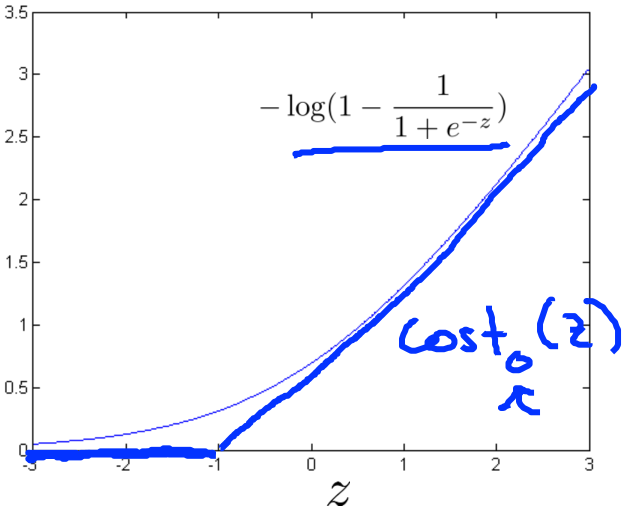
$$= \boxed{-y \log \frac{1}{1+e^{-\theta^T x}}} - \boxed{(1-y)\log\left(1-\frac{1}{1+e^{-\theta^T x}}\right)}$$

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:

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

Support vector machine:

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

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

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

$$A + \lambda B$$

$$C\,A + B$$

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

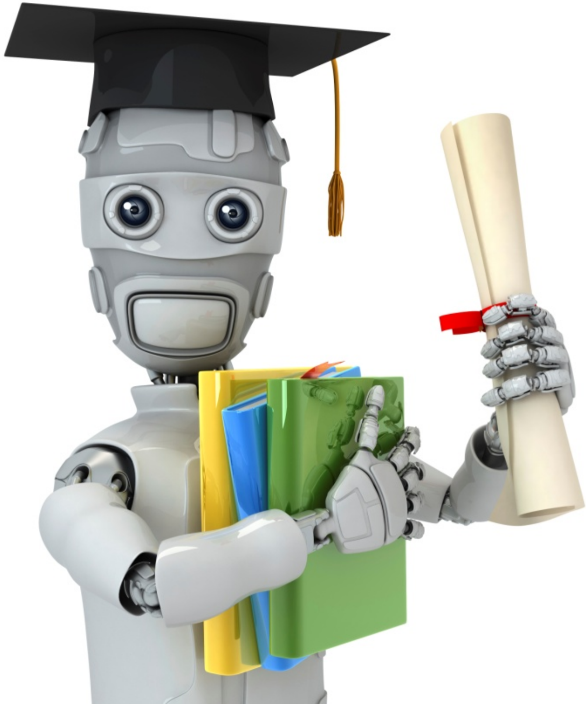
$$\min_\theta C\sum_{i=1}^m \left[y^{(i)} cost_1(\theta^T x^{(i)}) + (1-y^{(i)}) cost_0(\theta^T x^{(i)})\right] + \frac{1}{2}\sum_{i=1}^n \theta_j^2$$

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:

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



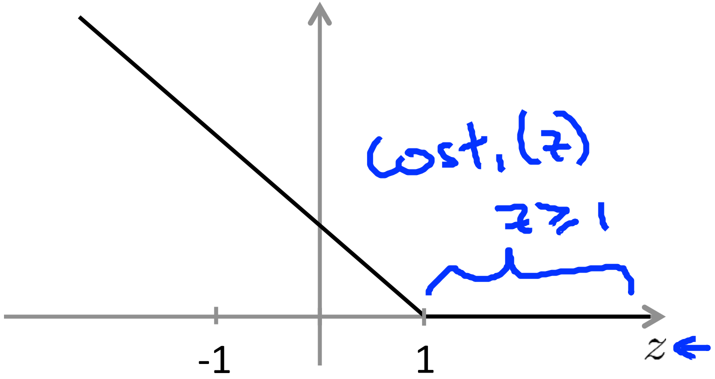
Machine Learning

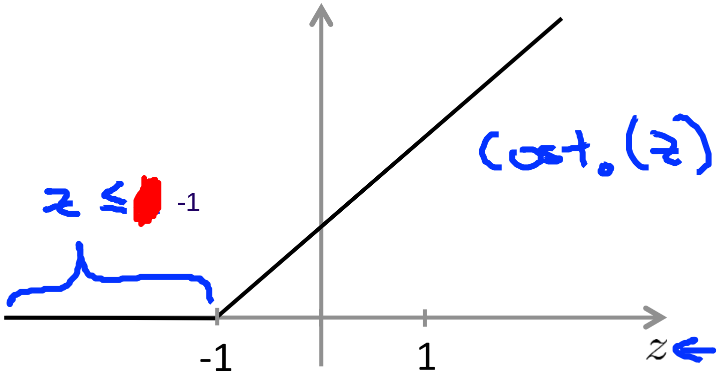
Support Vector Machines

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 $y = 1$, 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

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

$= 0$

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

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

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

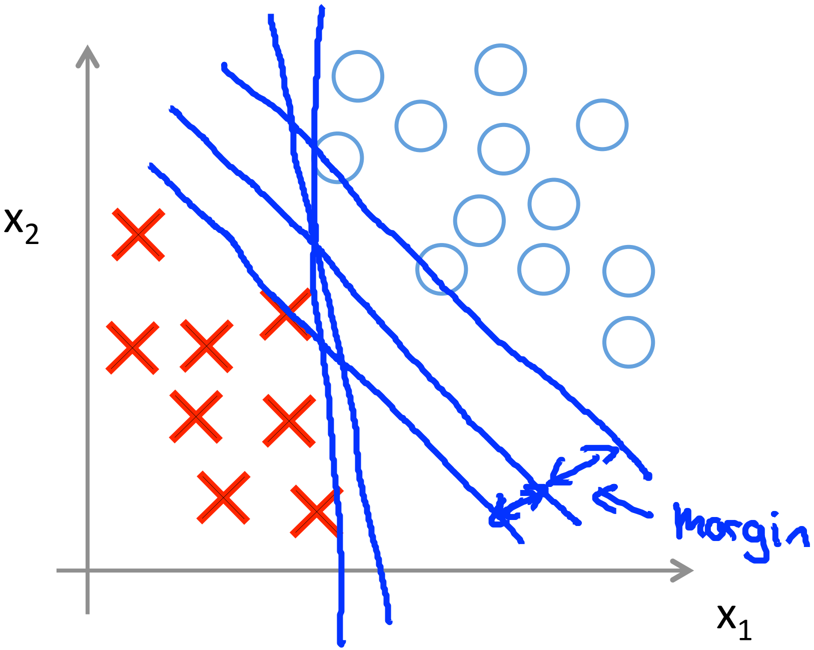
s.t. $\theta^T x^{(i)} \geq 1$ if $y^{(i)} = 1$

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

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

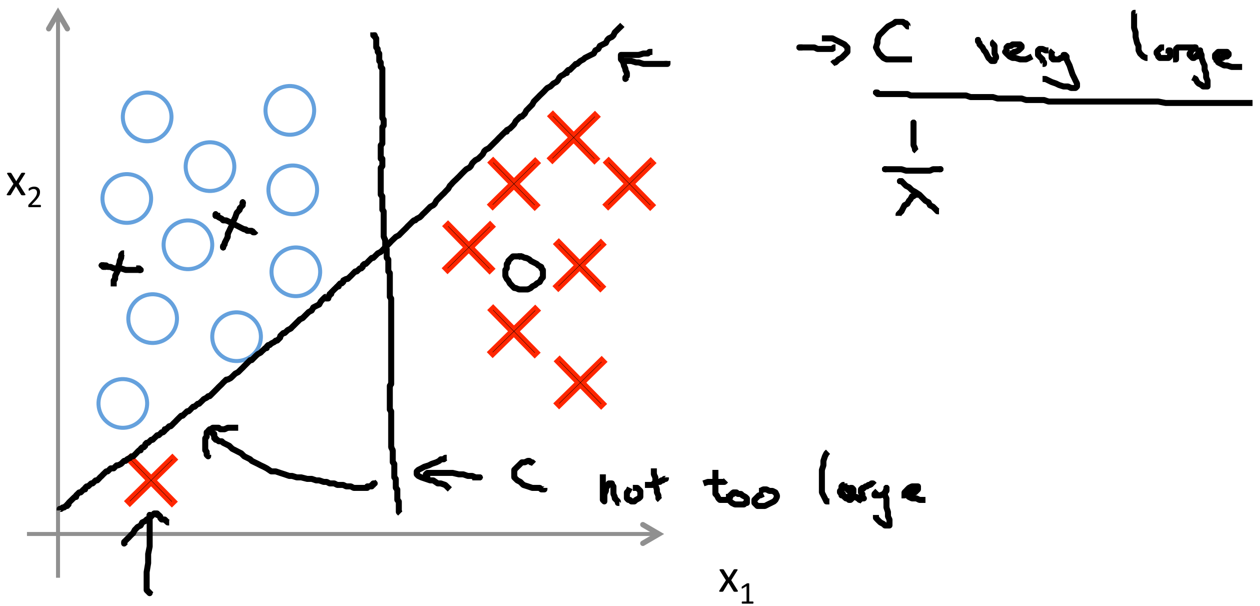
$\theta^T x^{(i)} \leq -1$

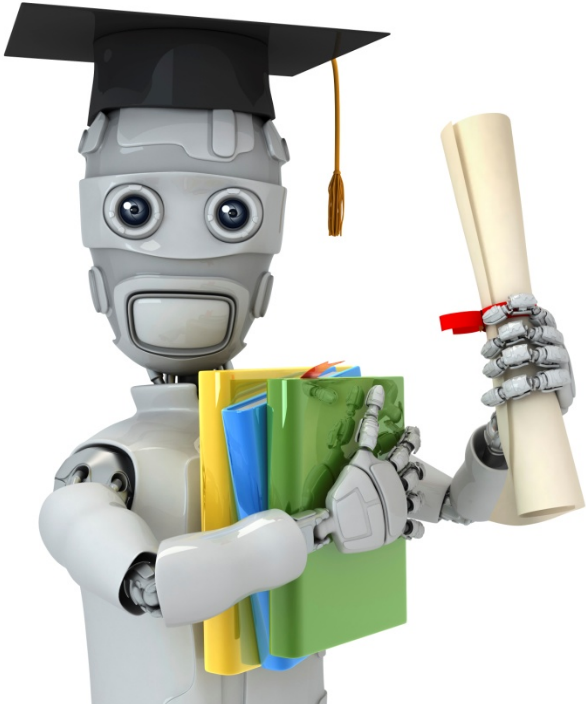
SVM Decision Boundary: Linearly separable case



Large margin classifier

Large margin classifier in presence of outliers





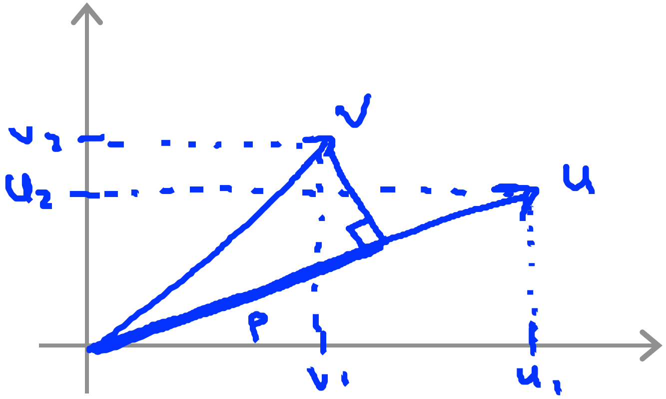
Machine Learning

Support Vector Machines

The mathematics behind large margin classification (optional)

Vector Inner Product

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



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

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

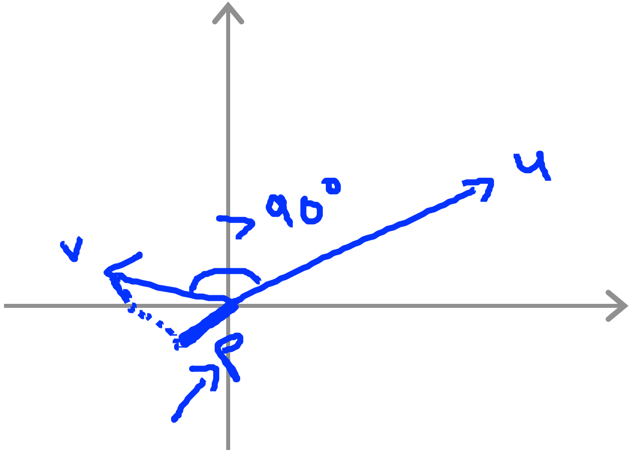
$= \sqrt{u_1^2 + u_2^2} \in \mathbb{R}$

p = length of projection of v onto u.

Signed

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

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



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

$p < 0$

SVM Decision Boundary

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

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

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

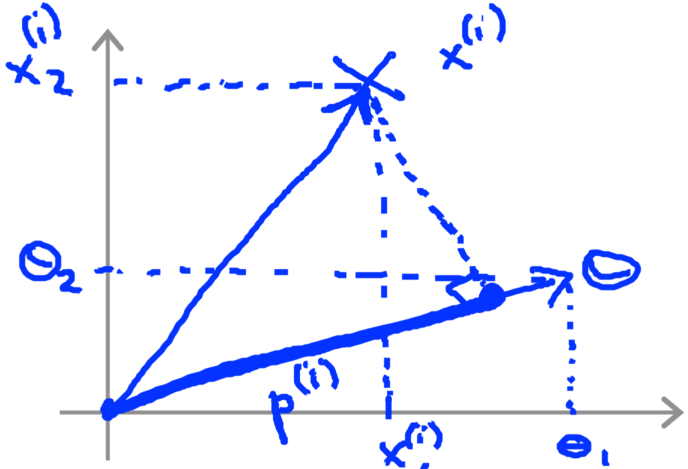
$$\text{s.t.} \quad \boxed{\theta^T x^{(i)} \geq 1} \qquad \text{if } y^{(i)} = 1$$

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

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

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

$$u^T v$$



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

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

SVM Decision Boundary

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

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

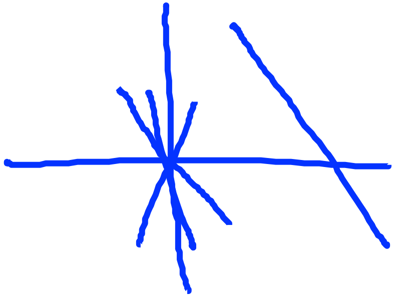
$p^{(i)} \cdot \|\theta\| \le -1$ if $y^{(i)} = 1$

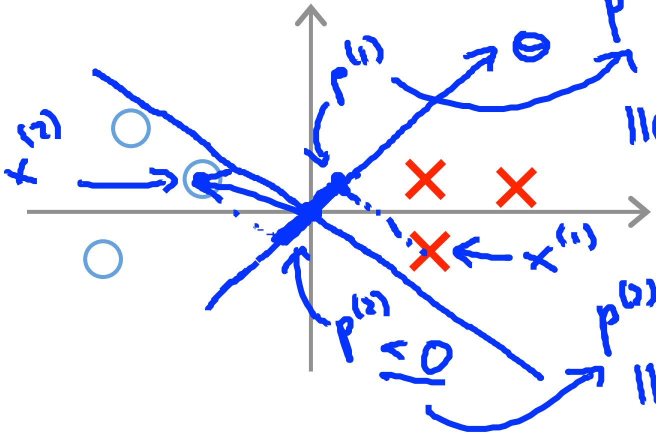
C very large

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

Simplification: $\theta_0 = 0$

$\theta_0 \neq 0$





$p^{(1)} \cdot \|\theta\| \ge 1$

$\|\theta\|$ large

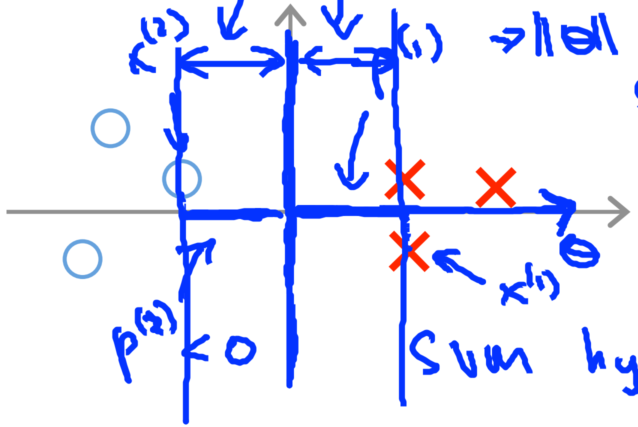
$p^{(2)} \|\theta\| \le -1$

$\|\theta\|$ large

margin

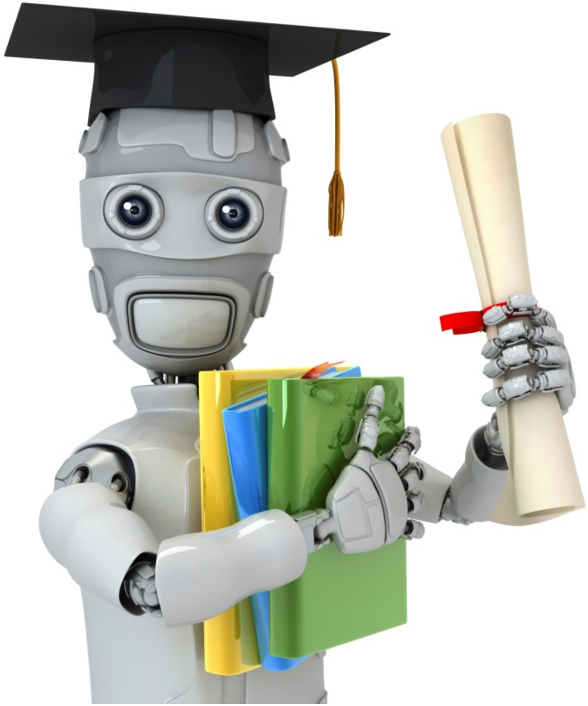
$p^{(1)} \|\theta\| \ge 0$

$\rightarrow \|\theta\|$ can be smaller.



SVM hypothesis

https://towardsdatascience.com/optimization-loss-function-under-the-hood-part-iii-5dff33fa015d

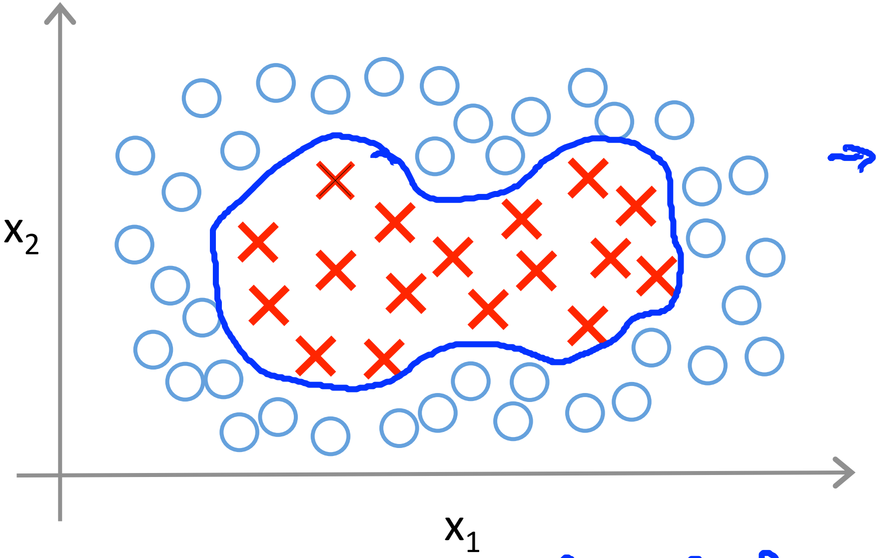


Support Vector Machines

Kernels I

Machine Learning

Non-linear Decision Boundary



Predict $y = 1$ if

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

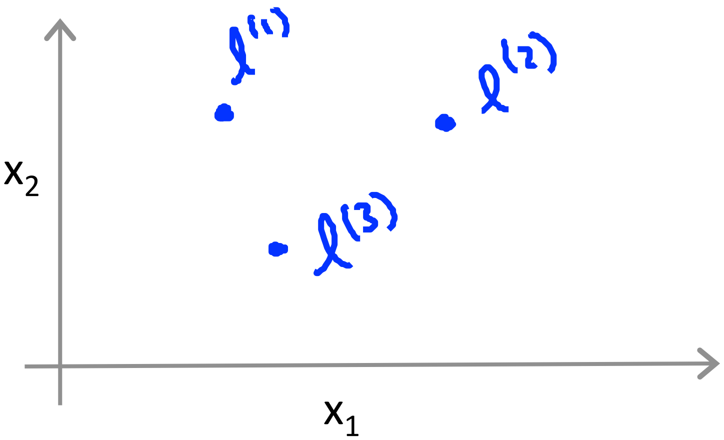
$$h_\theta(x) = \begin{cases} 1 & \text{if } \theta_0 + \theta_1 x_1 + \cdots \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

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

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

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 $l^{(1)}, l^{(2)}, l^{(3)}$

$\|w\|$

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

Given x:

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

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

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

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 $l^{(1)}$:

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

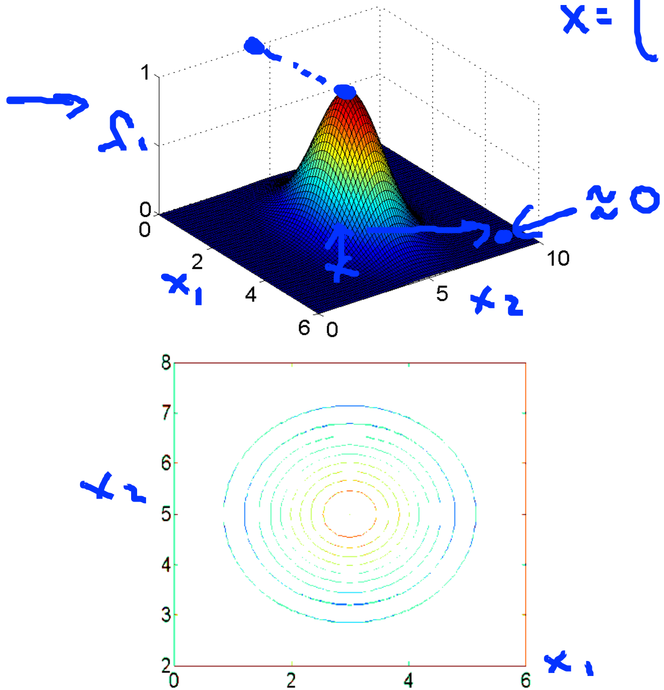
Using the values of x1, x2 and plotting f using Gaussian's kernel.

Example:

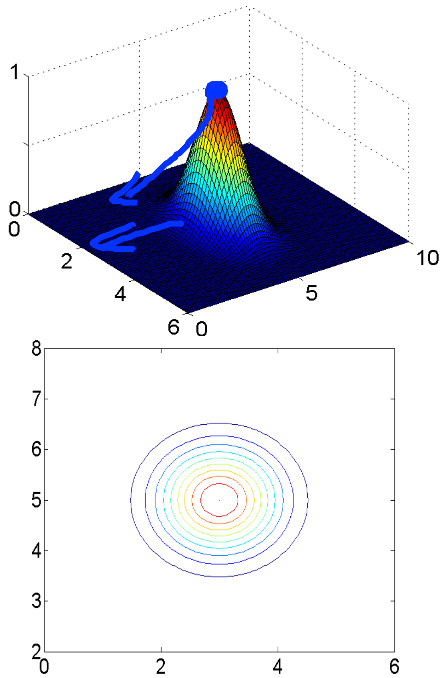
$$l^{(1)} = \boxed{\begin{bmatrix}3\\5\end{bmatrix}}, \qquad f_1 = \exp\left(-\frac{\|x-l^{(1)}\|^2}{2\boxed{\sigma^2}}\right)$$

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

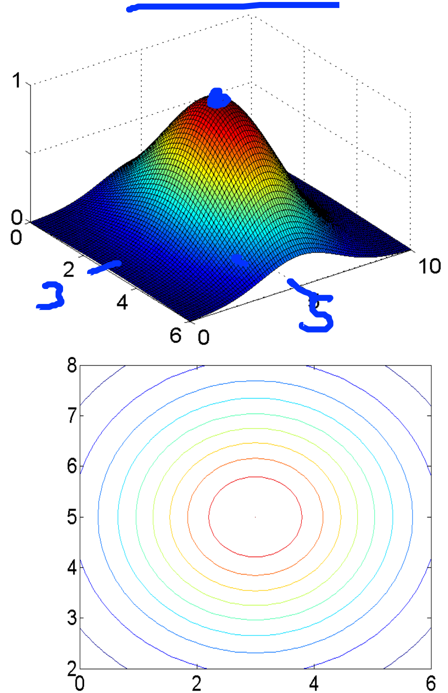
$\sigma^2 = 1$

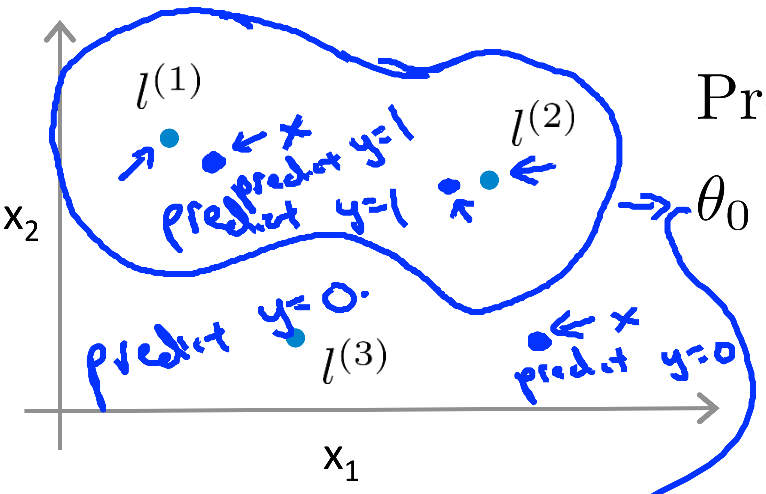


$\sigma^2 = 0.5$



$\sigma^2 = 3$





Predict "1" when

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

x

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

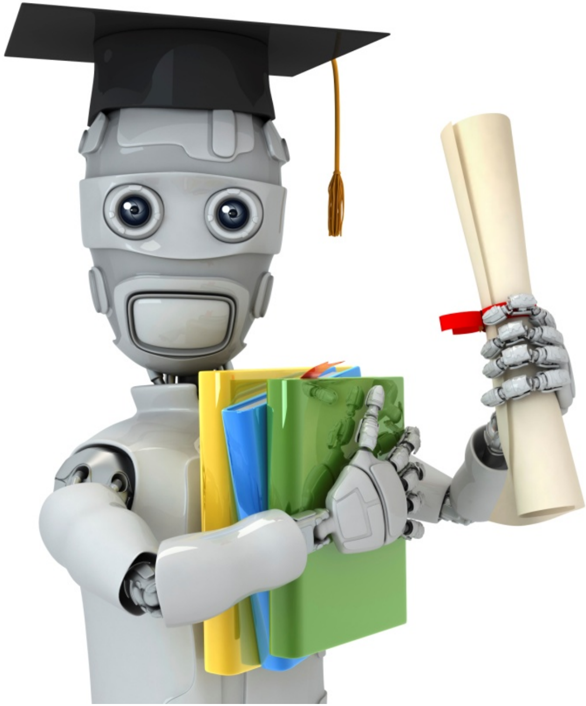
$$f_1 \approx 1, \quad f_2 \approx 0, \quad f_3 \approx 0.$$

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

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

$$f_1, f_2, f_3 \approx 0$$

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

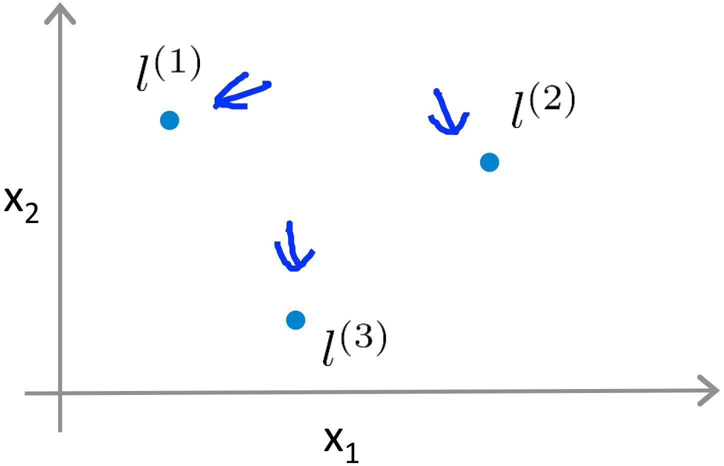


Machine Learning

Support Vector Machines

Kernels II

Choosing the landmarks

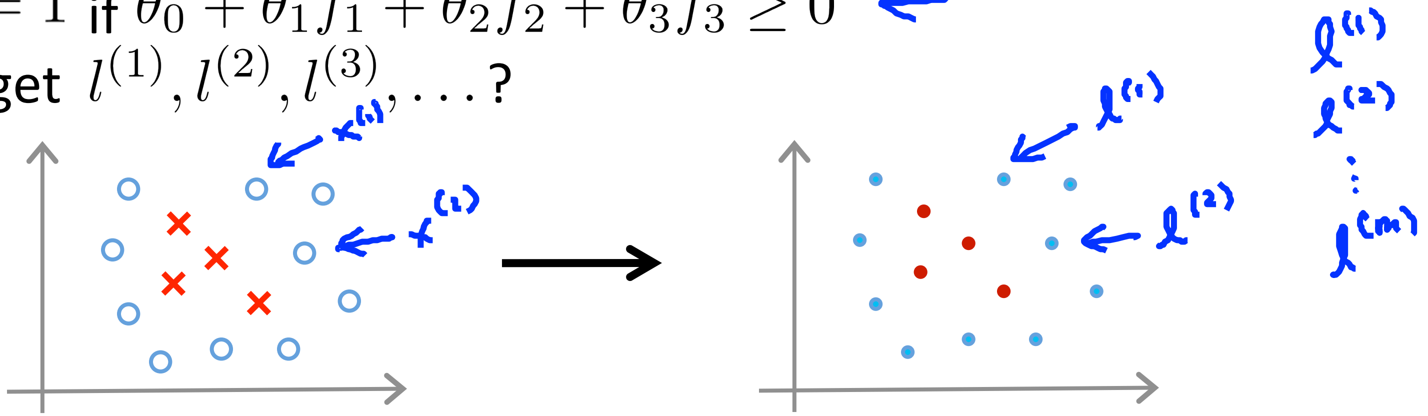


Given x:

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

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 x:

$x^{(1)}$

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

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

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

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

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

$x^{(i)}$

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

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:

$n = m$

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

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

Another way to calculate theta^2

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

$\|\theta\|^2$ $\quad m = 10{,}000$

$\theta^T M \theta$

The M here represents a Matrix, so instead of minimizing theta'*theta, we use theta'*M*theta for efficiency

SVM parameters:

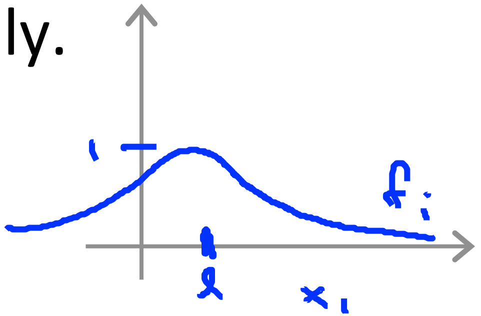
C ($= \frac{1}{\lambda}$). → Large C: Lower bias, high variance. (small λ)

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

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

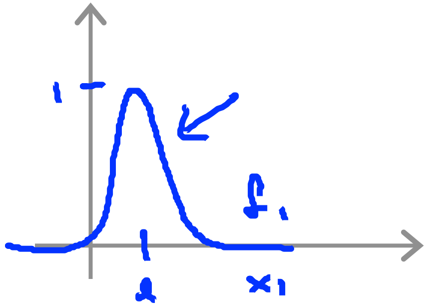
Will lead to → Higher bias, lower variance.

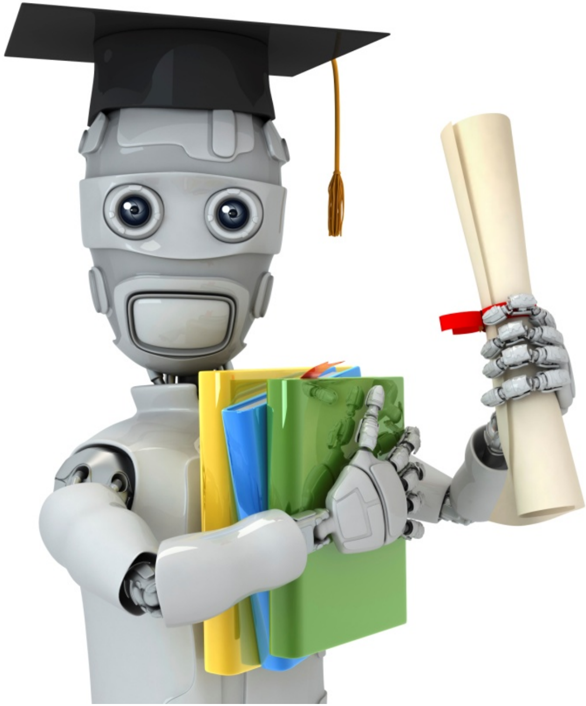
$\exp\left(-\frac{\|x-l^{(i)}\|^2}{2\sigma^2}\right)$



Small σ^2: Features f_i vary less smoothly.

Will lead to - 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 $\theta^T x \geq 0$

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

→ 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

Andrew Ng

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
```

$x \rightarrow \begin{matrix} f_1 \\ f_2 \\ \vdots \\ f_m \end{matrix}$

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:

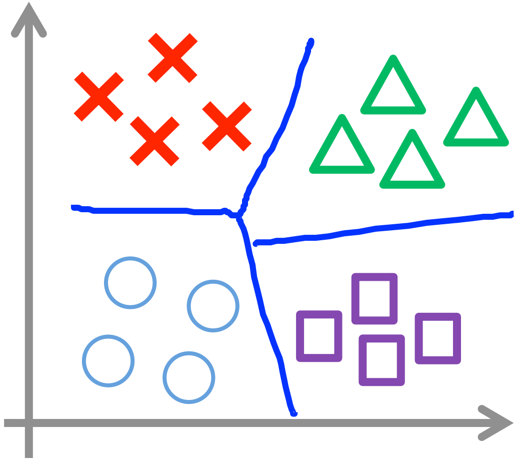
- Polynomial kernel: $k(x, l) = (x^T l)^2$, $+0$, $(x^T l)^3$, $(x^T l + 1)^3$, $(x^T l + 5)^4$

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

- 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 .... θ=K

Logistic regression vs. SVMs

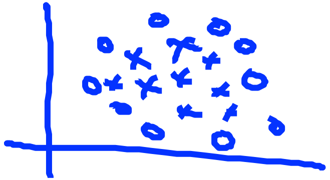
$n =$ number of features ($x \in \mathbb{R}^{n+1}$), $m =$ number of training examples

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.