Recommended approach

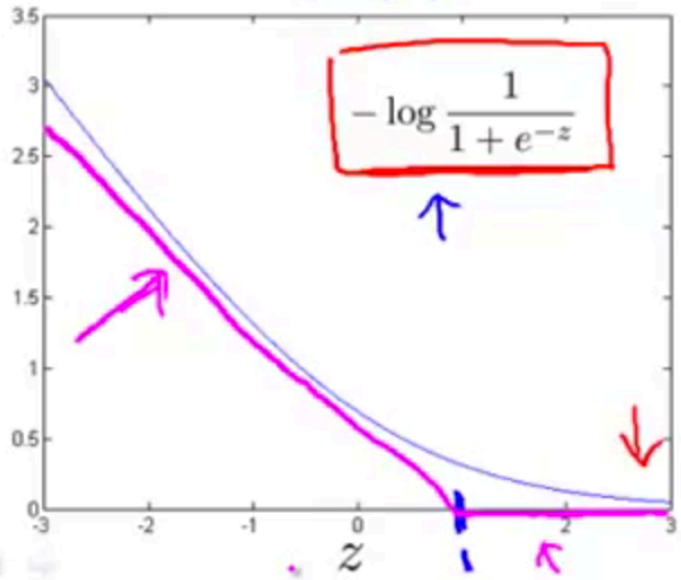
- Start with a simple algorithm that you can implement quickly. Implement it and test it on your cross-validation data.
- Plot learning curves to decide if more data, more features, etc. are likely to help.
- Error analysis: Manually examine the examples (in cross validation set) that your algorithm made errors on. See if you spot any systematic trend in what type of examples it is making errors on.

Alternative view of logistic regression

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

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

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



Alternative view of logistic regression

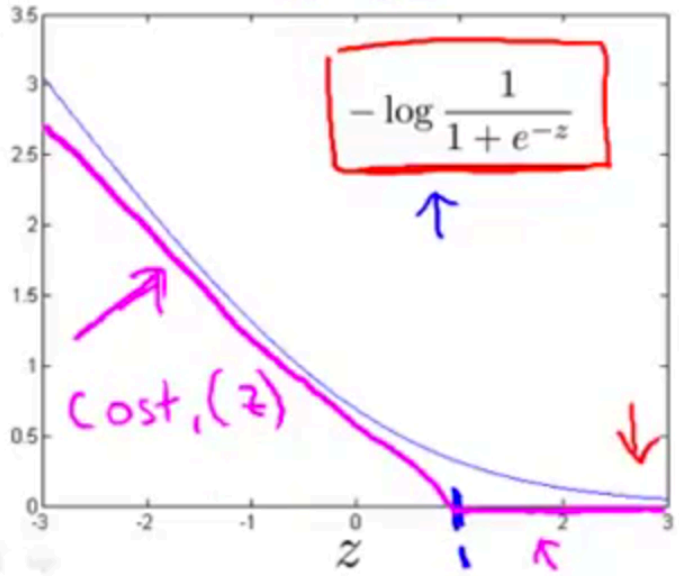
(x, y)

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

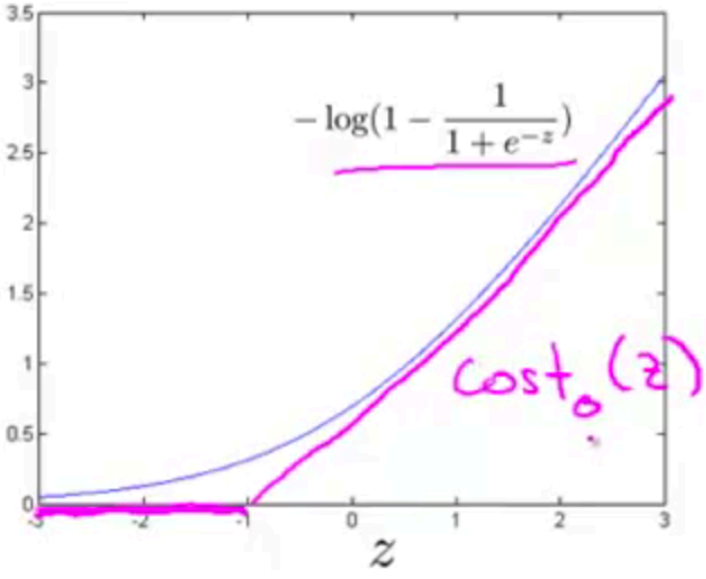
$$= -y \log \frac{1}{1+e^{-\theta^T x}} - (1-y)\log\left(1 - \frac{1}{1+e^{-\theta^T x}}\right)$$

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:

$$\min_\theta \frac{1}{m}\left[\sum_{i=1}^{m} y^{(i)}\underbrace{\left(-\log h_\theta(x^{(i)})\right)}_{\text{cost}_1(\theta^T x^{(i)})} + (1-y^{(i)})\underbrace{\left(-\log(1-h_\theta(x^{(i)}))\right)}_{\text{cost}_0(\theta^T x^{(i)})}\right] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

A B

Support vector machine:

$$\min_\theta \cancel{\frac{1}{m}} C \sum_{i=1}^{m} y^{(i)}\text{cost}_1(\theta^T x^{(i)}) + (1-y^{(i)})\text{cost}_0(\theta^T x^{(i)}) + \cancel{\frac{1}{2m}}\sum_{i=0}^{n}\theta_j^2$$

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

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

$A + \lambda B$

$C\,A + B$

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

$$\rightarrow \min_\theta C\sum_{i=1}^{m}\left[y^{(i)}\text{cost}_1(\theta^T x^{(i)}) + (1-y^{(i)})\text{cost}_0(\theta^T x^{(i)})\right] + \frac{1}{2}\sum_{i=1}^{n}\theta_j^2$$

SVM hypothesis

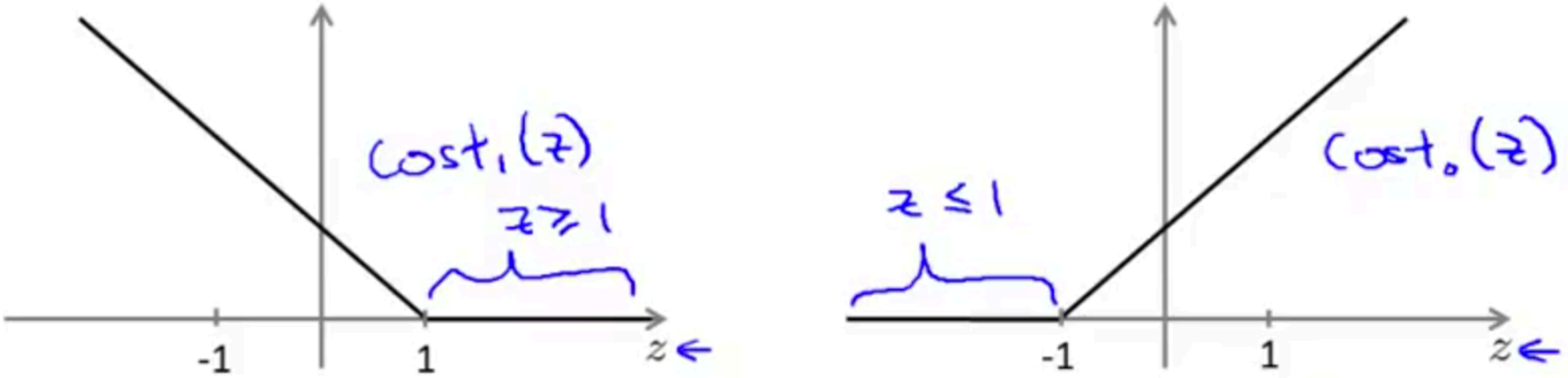
$$\min_{\theta} C \sum_{i=1}^{m} \left[y^{(i)} cost_1(\theta^T x^{(i)}) + (1 - y^{(i)}) cost_0(\theta^T x^{(i)}) \right] + \frac{1}{2} \sum_{i=1}^{n} \theta_j^2$$

Hypothesis:

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

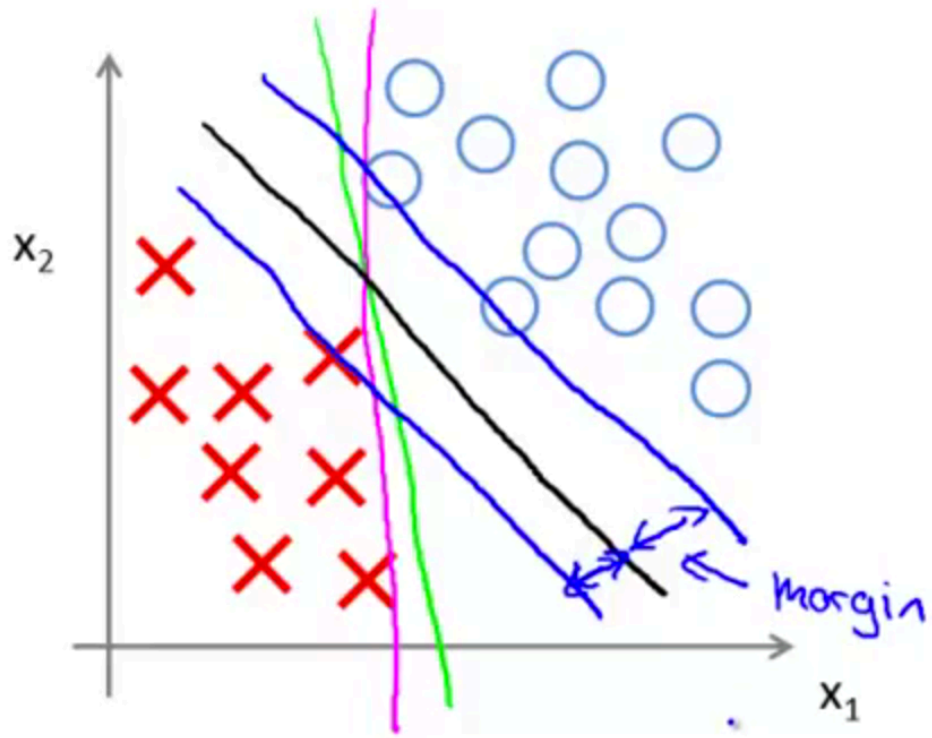
Support Vector Machine

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



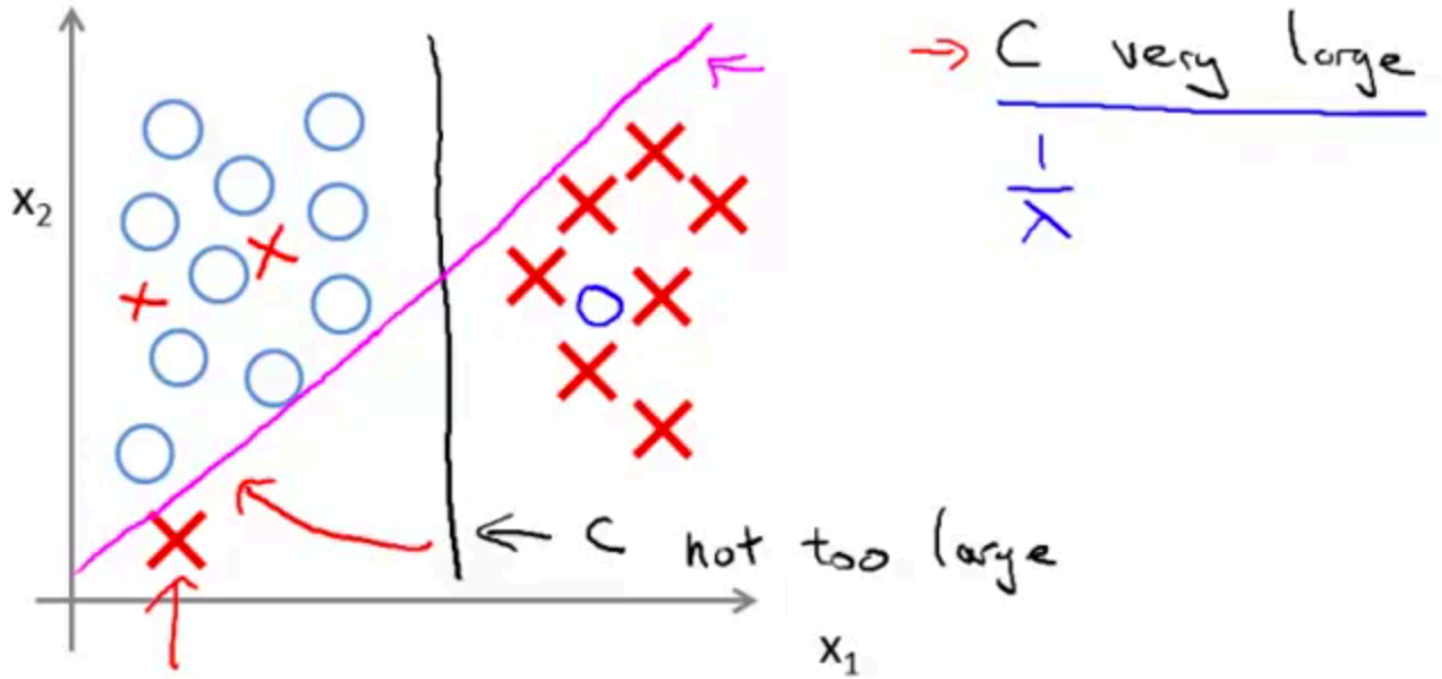
- If $y = 1$, we want $\theta^T x \geq 1$ (not just ≥ 0)
- If $y = 0$, we want $\theta^T x \leq -1$ (not just < 0)

SVM Decision Boundary: Linearly separable case

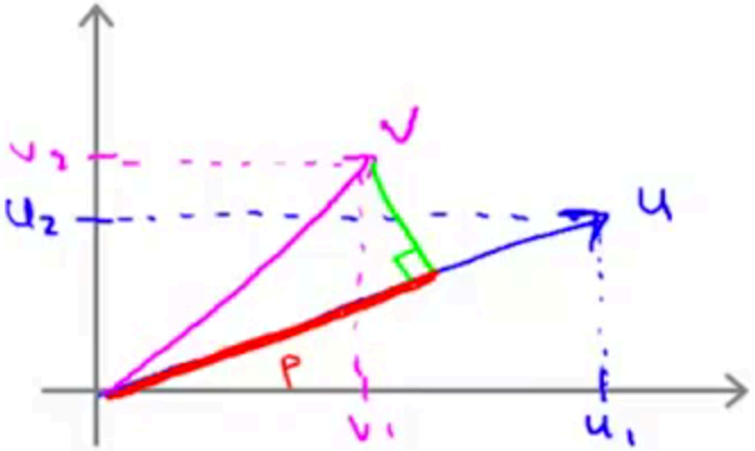


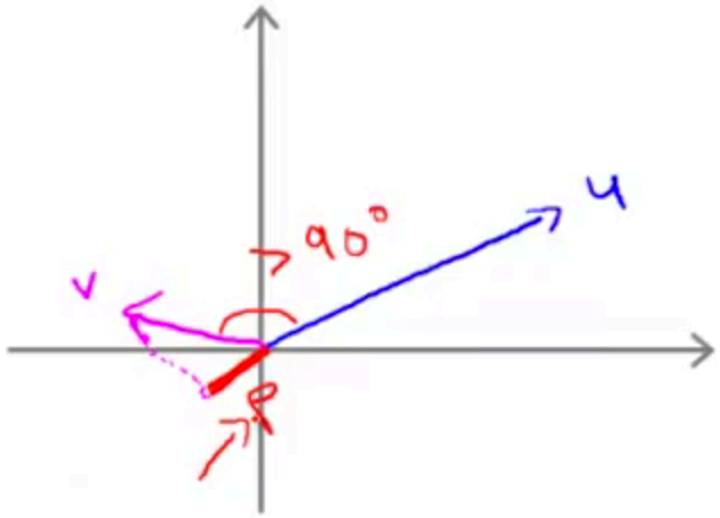
Large margin classifier

Large margin classifier in presence of outliers



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

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

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

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

$p < 0$

SVM Decision Boundary

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

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

$$= \|\theta\|$$

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

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

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

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

SVM Decision Boundary

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

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

$$= \|\theta\|$$

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

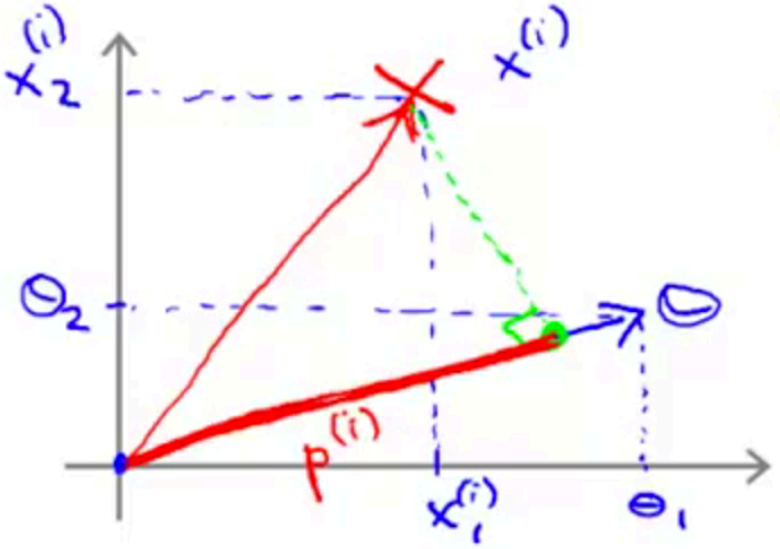
$$\theta^T x^{(i)} \leq -1 \quad \text{if } y^{(i)} = 0$$

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

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

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

$u^T v$



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

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

SVM Decision Boundary

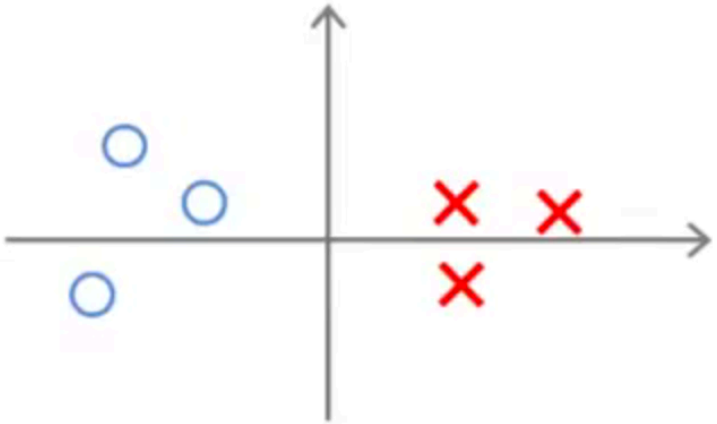
$$\min_{\theta} \frac{1}{2} \sum_{j=1}^{n} \theta_j^2$$

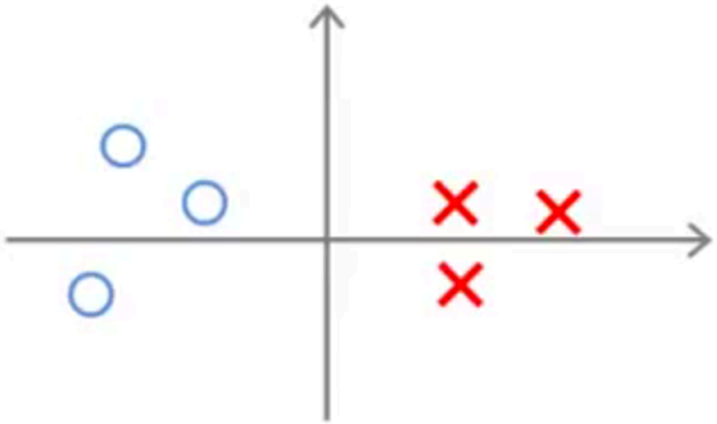
s.t. $p^{(i)} \cdot \|\theta\| \geq 1 \quad$ if $y^{(i)} = 1$

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

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

Simplification: $\theta_0 = 0$





SVM Decision Boundary

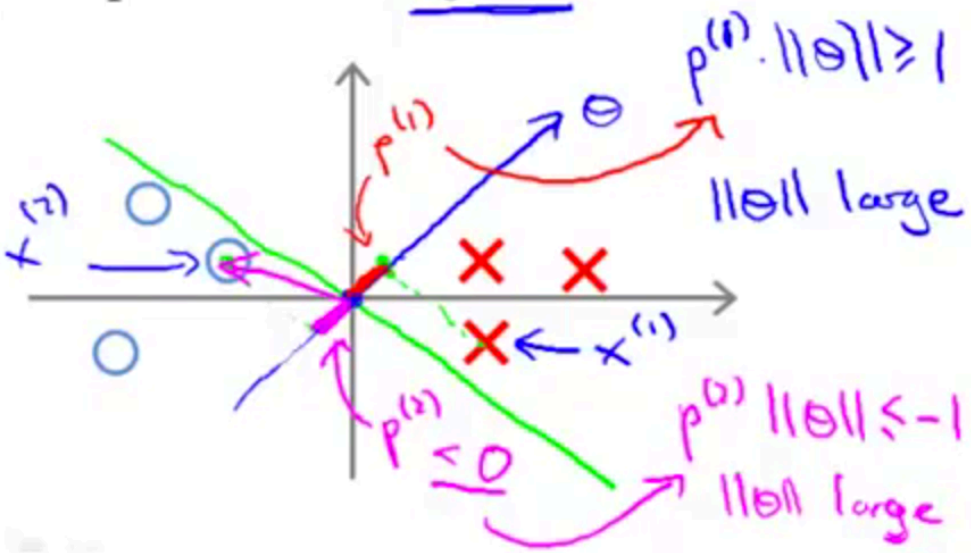
$$\min_{\theta} \frac{1}{2}\sum_{j=1}^{n}\theta_j^2 = \frac{1}{2}\|\theta\|^2$$

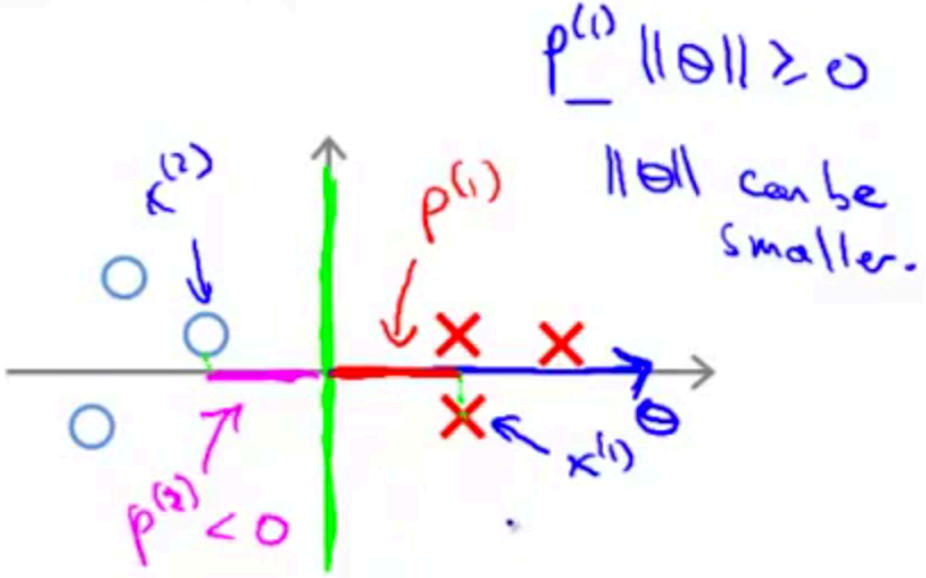
s.t. $p^{(i)} \cdot \|\theta\| \geq 1$ if $y^{(i)} = 1$

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

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

Simplification: $\theta_0 = 0$





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 $y^{(i)} = 1$

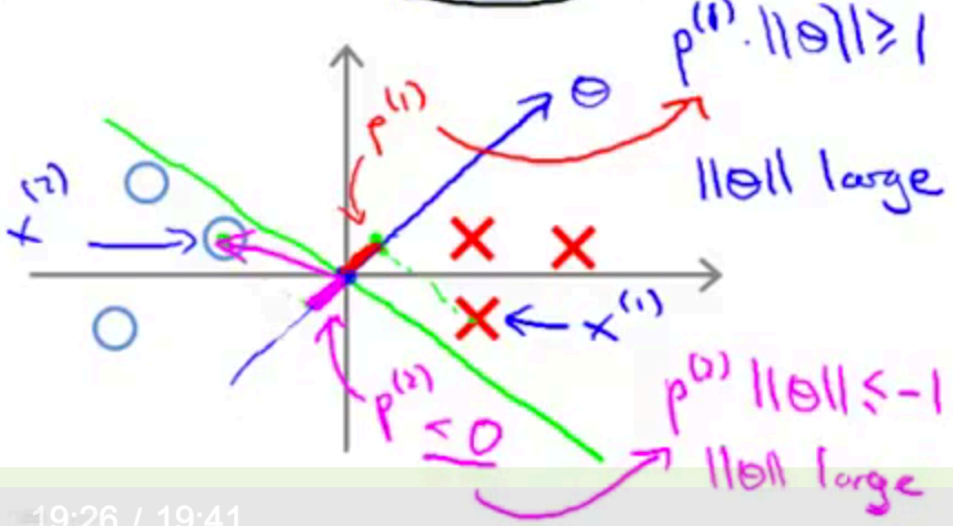
$p^{(i)} \cdot \|\theta\| \leq -1$ if $y^{(i)} = 1$

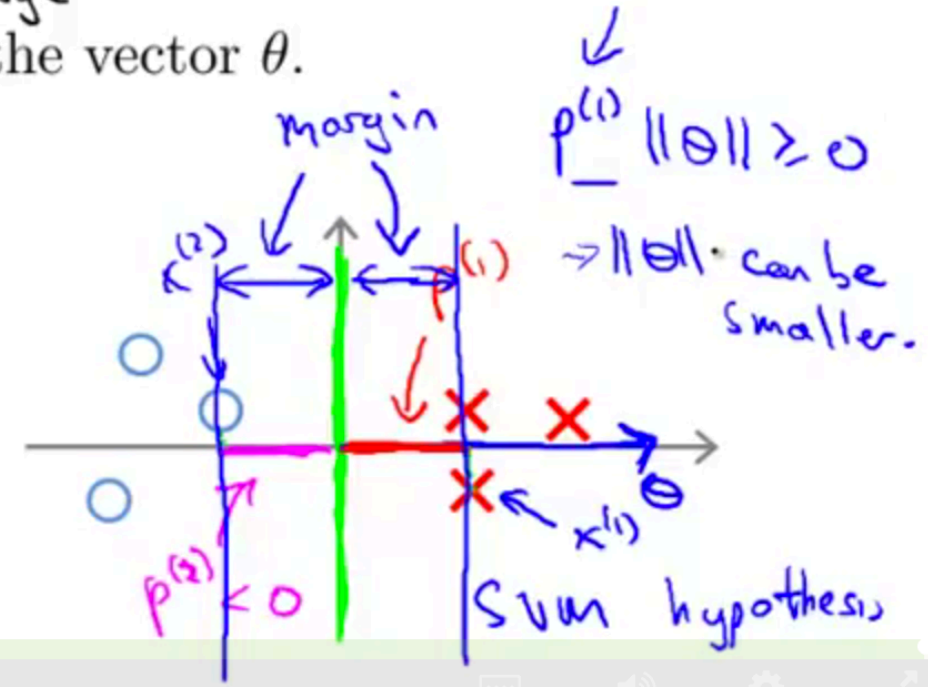
C very large

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

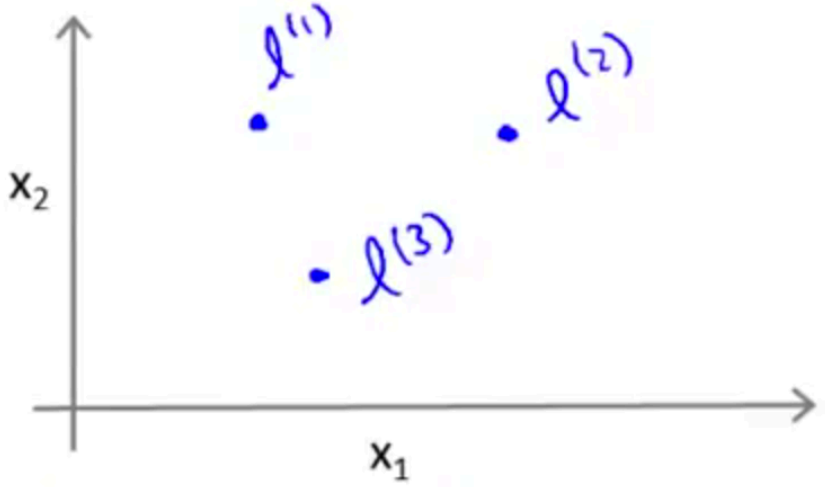
Simplification: $\theta_0 = 0$

$\theta_0 \neq 0$





Kernel



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

$\|w\|$

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

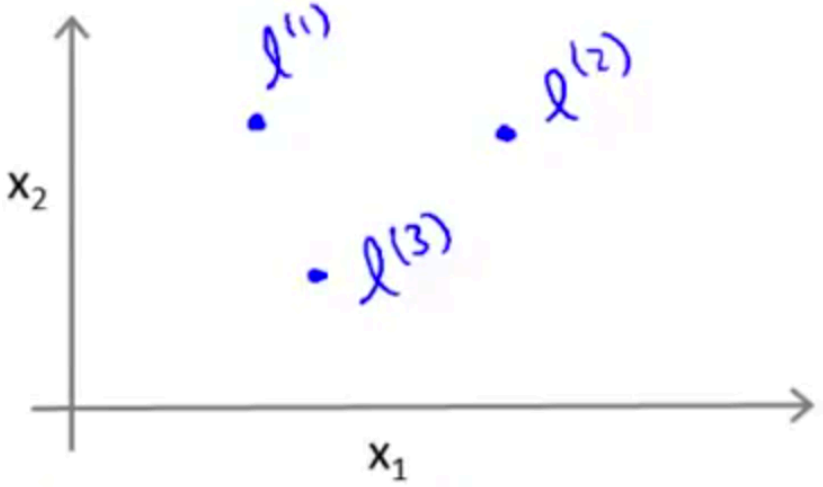
Given x:

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

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

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

Kernel



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

Given x:

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

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

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

$\|w\|$

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

Kernel (Gaussian kernels)

Kernels and Similarity

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

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

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

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

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

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

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

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

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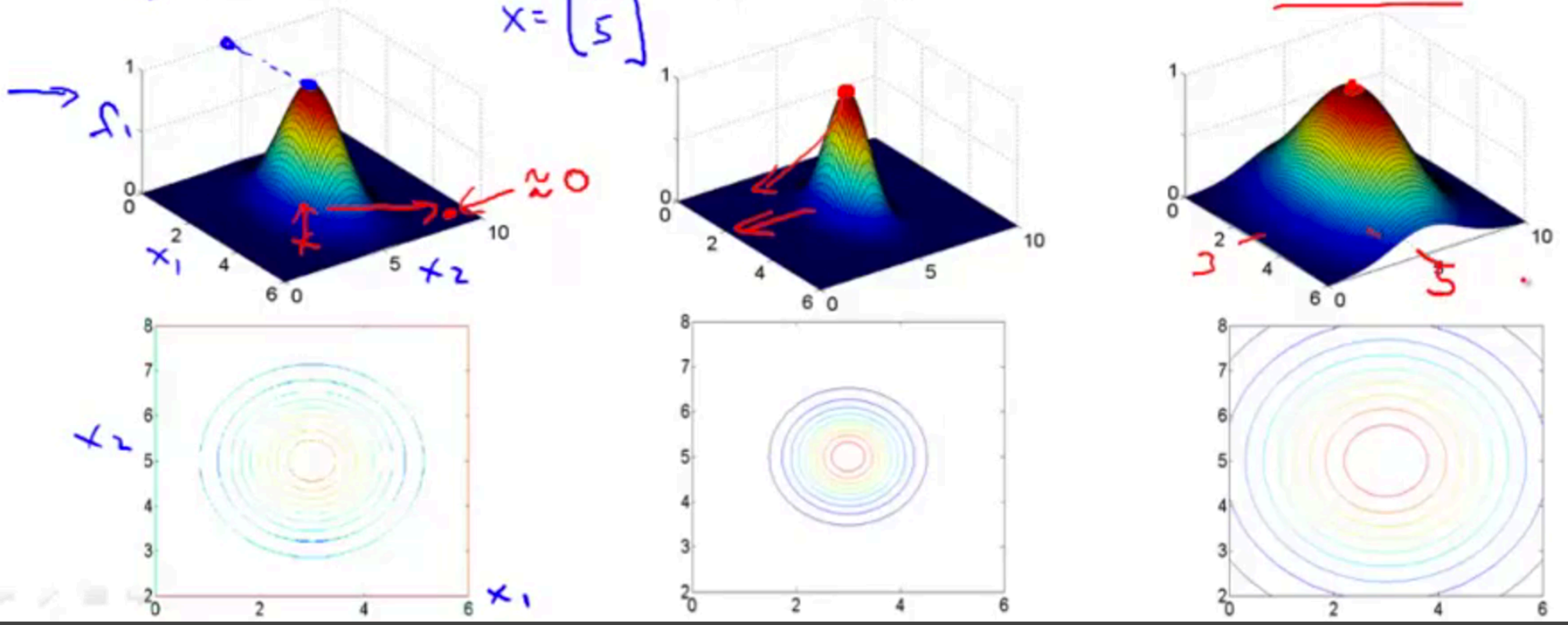
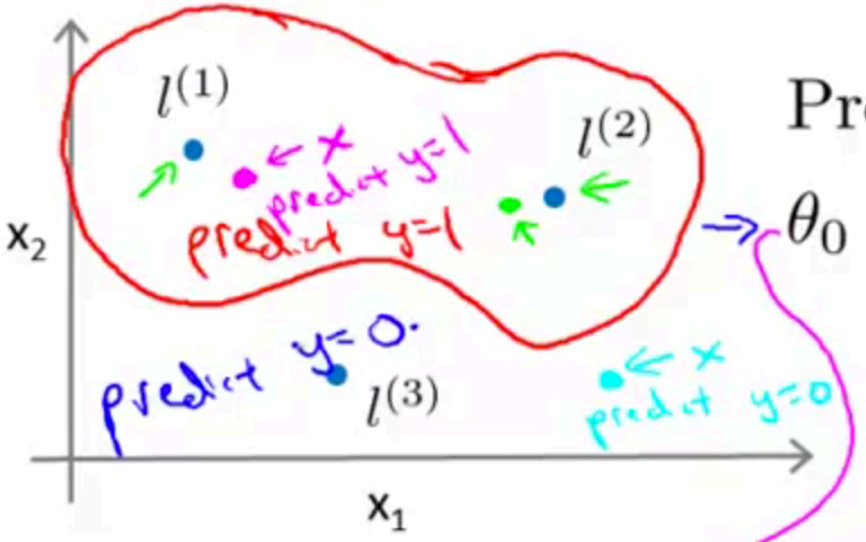
Example:

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

$\sigma^2 = 1$ $\quad$ $\sigma^2 = 0.5$ $\quad$ $\sigma^2 = 3$

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





Predict "1" when

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

x

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

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

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

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

$f_1, f_2, f_3 \approx 0$

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

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:

$x^{(i)}$

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

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

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

$x^{(i)} \rightarrow$

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

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

$\vdots$

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

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

$x^{(i)} \in \mathbb{R}^{n+1}$ (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 $f \in \mathbb{R}^{m+1}$ $\theta \in \mathbb{R}^{m+1}$

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

$\theta_0 f_0 + \theta_1 f_1 + \cdots + \theta_m f_m$

Training:

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

$n = m$

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

$\rightarrow \theta_0$

$$\sum_{j=1}^{m} \theta_j^2 = \theta^T \theta \leftarrow \theta = \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_m \end{bmatrix} \quad \text{(ignore } \theta_0\text{)}$$

$\leftarrow \|\theta\|^2$

$\rightarrow \theta^T M \theta$

$m = 10,000$

SVM parameters:

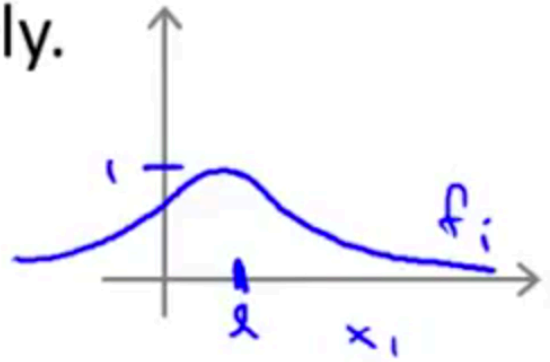
C ($= \frac{1}{\lambda}$). → Large C: Lower bias, high variance. (small λ)

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

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

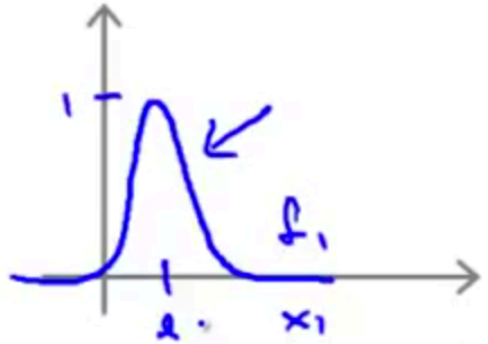
→ Higher bias, lower variance.

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



Small σ^2: Features f_i vary less smoothly.

Lower bias, higher variance.



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:

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

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

```
return
```

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

Other choices of kernel

Note: Not all similarity functions $\text{similarity}(x, l)$ make valid kernels.

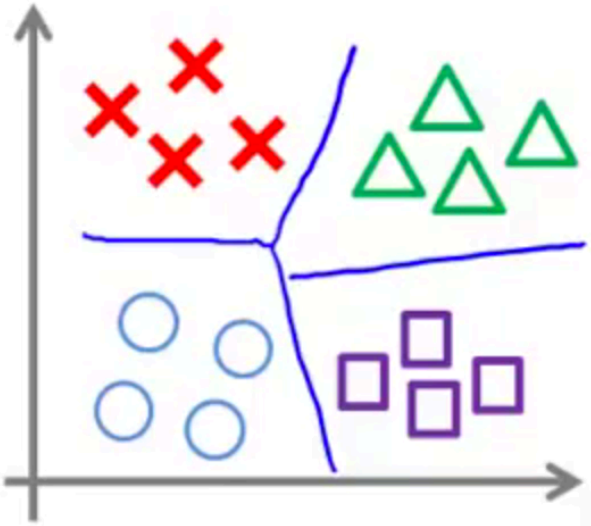
(Need to satisfy technical condition called "Mercer's Theorem" to make sure SVM packages' optimizations run correctly, and do not diverge).

Many off-the-shelf kernels available:

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

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

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

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

Logistic regression vs. SVMs

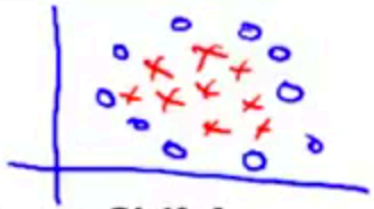
n = number of features ($x \in \mathbb{R}^{n+1}$), m = number of training examples

→ 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



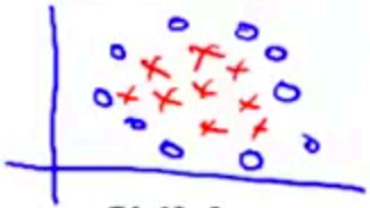
If n is small, m is large: ($n = 1 - 1000$, $m = 50{,}000+$)

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

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: ($n = 1\text{-}1000$, $m = 10\text{-}10{,}000$)
  - Use SVM with Gaussian kernel
- If n is small, m is large: ($n = 1\text{-}1000$, $m = 50{,}000+$)
  - 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.