Linear Classification

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CPS 570

With content adapted from Andrew Ng, Lise Getoor, and Tom Dietterich
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Classification

- Supervised learning framework
- Features can be anything
- Targets are discrete classes:
  - Safe mushrooms vs. poisonous
  - Malignant vs. benign
  - Good credit risk vs. bad
- Can we treat classes as numbers?
  - Single class?
  - Multi class?

Representing Classes

- Interpret $t^{(i)}$ as the probability that the i^{th} element is in a particular class
- Classes usually disjoint
- For multiclass, $\mathbf{t}^{(i)}$ may be a vector
- $\mathbf{t}^{(i)}[j]=\mathbf{t}^{(i)}_j=1$ if i^{th} element is in class j, 0 OTW

- Notation: For convenience, we will sometimes refer to the "raw" variables $\mathbf{x}$, rather than the features as seen through the lens of our features, ϕ

What is a Linear Disciminant?

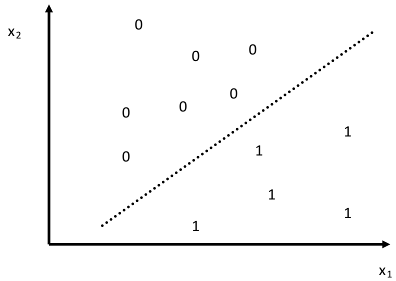
- Simplest kind of classifier, a **linear threshold unit (LTU):**

$$y(\mathbf{x}) = \begin{cases} 1 & \textit{if } w_1x_1 + \cdots + w_nx_n \geq w_0 \\ 0 & \textit{otherwise} \end{cases}$$

- A linear discriminant is an n-1 dimensional hyperplane
- $\mathbf{w}$ is orthogonal to this
- Four algorithms for linear decision boundaries:
  - Directly learn the LTU: Using Least Mean Square (LMS) algorithm
  - Learn the conditional distribution: Logistic regression
  - Learn the joint distribution:
    - Naïve Bayes
    - Linear discriminant analysis (LDA)

Decision Boundaries

- A classifier can be viewed as partitioning the input space or feature space X into decision regions

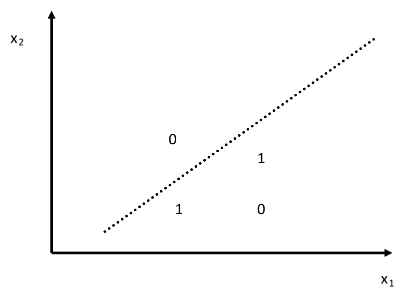


- A linear threshold unit always produces a linear decision boundary. A set of points that can be separated by a linear decision boundary is **linearly separable**.

What can be expressed?

- Examples of things that can be expressed (Assume n Boolean (0/1 features)
  - Conjunctions:
    - $x_1 \wedge x_3 \wedge x_4$: $1 \cdot x_1 + 0 \cdot x_2 + 1 \cdot x_3 + 1 \cdot x_4 \geq 3$
    - $x_1 \wedge \neg x_3 \wedge x_4$: $1 \cdot x_1 + 0 \cdot x_2 + -1 \cdot x_3 + 1 \cdot x_4 \geq 2$
  - at-least-m-of-n
    - at-least-2-of(x_1,x_2,x_4)
    - $1 \cdot x_1 + 1 \cdot x_2 + 0 \cdot x_3 + 1 \cdot x_4 \geq 2$
- Examples of things that cannot be expressed:
  - Non-trivial disjunctions:
    - $(x_1 \wedge x_3) + (x_3 \wedge x_4)$
  - Exclusive-Or
    - $(x_1 \wedge \neg x_2) + (\neg x_1 \wedge x_2)$

Non-linearly separable example

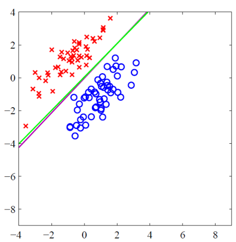


Multiclass

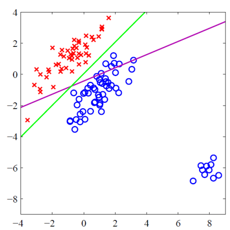
- k classes
- $O(k^2)$ one vs. one classifiers
  - Expensive
  - May not be consistent
- k-1 one vs. rest classifiers
  - Less expensive
  - Still may not be consistent
- K linear functions
  - Assign x to class j if $\mathbf{w}_j^T\mathbf{x} > \mathbf{w}_i^T\mathbf{x}$ for all i
  - Gives convex, singly connected decision regions
  - How to pick the linear functions?

Why not use regression?

- Regression minimizes sum of squared errors on target function
- Gives strong influence to outliers



Note: Class labels are in Z dimension



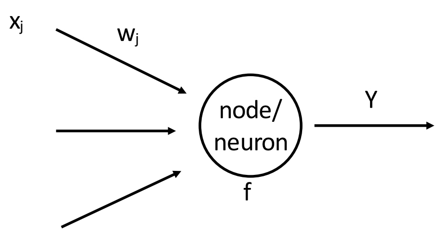
Magenta = linear regression

The "Neural" Story (Part I)

- Nice to justify machine learning w/nature
- Naïve introspection works badly
- Neural model biologically plausible

- Single neuron, linear threshold unit = perceptron
- (Longer rant on this later…)

Perceptron



f is a simple step function (sgn)

$$y = \mathrm{sgn}(\mathbf{w}^T\mathbf{x})$$

Perceptron Learning

- We are given a set of inputs $\mathbf{x}^{(1)} \ldots \mathbf{x}^{(n)}$
- $t^{(1)} \ldots t^{(n)}$ is a set of target outputs (Boolean) {-1,1}
- **w** is our set of weights
- output of perceptron = $\mathrm{sgn}(\mathbf{w}^T\mathbf{x})$
- Perceptron_error($\mathbf{x}^{(i)}$, w) = $-\mathrm{sgn}(\mathbf{w}^T\mathbf{x}) * t^{(i)}$
  - +1 when perceptron is incorrect
  - -1 when perceptron is correct
- Goal: Pick w to optimize:

$$\min_{\mathbf{w}} \sum_{i \in \text{misclassified}} perceptron\_error(\mathbf{x}^{(i)}, \mathbf{w})$$

Update Rule

Repeat until convergence:

$$\forall_{i \in \text{misclassified}} \forall_j : w_j \leftarrow w_j + \alpha x_j^{(i)} t^{(i)}$$

"Learning Rate"
(can be any constant)

- i iterates over samples
- j iterates over weights

Perceptron Learning Properties (LTU Properties)

- Good news:
  - If there exists a set of weights that will correctly classify every example, the perceptron learning rule will find it
  - Does not depend on step size!
- Bad news:
  - Perceptrons can represent only a small class of functions, "linearly separable," functions
  - May oscillate if not separable
  - No obvious generalization for multiclass

Logistic Regression

- In logistic regression, we learn the conditional distribution P(t|**x**)
- Let p_t(**x**; **W**) be our estimate of P(t|**x**), where **W** is a vector of adjustable parameters.
- Assume there are two classes, t = 0 and t = 1 and

$$p_1(\mathbf{x};\mathbf{w}) = \frac{e^{\mathbf{w}^T\mathbf{x}}}{1+e^{\mathbf{w}^T\mathbf{x}}} = \frac{1}{1+e^{-\mathbf{w}^T\mathbf{x}}}$$

$$p_0(\mathbf{x};\mathbf{w}) = 1 - p_1(\mathbf{x};\mathbf{w}) = \frac{e^{-\mathbf{w}^T\mathbf{x}}}{1+e^{-\mathbf{w}^T\mathbf{x}}} = \frac{1}{1+e^{\mathbf{w}^T\mathbf{x}}}$$

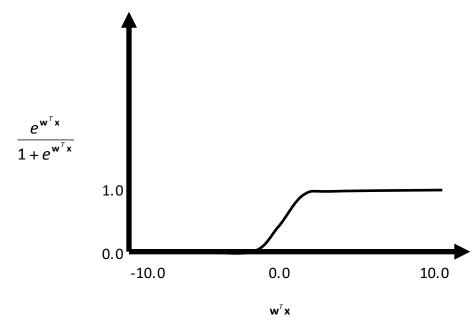
- This is equivalent to

$$\log \frac{p_1(\mathbf{x};\mathbf{w})}{p_0(\mathbf{x};\mathbf{w})} = \mathbf{w}^T\mathbf{x}$$

- IOW, the log odds of class 1 is a linear function of **x**

Why this form?

- One reason: transforms a linear function in the range (-∞,+∞) to be positive and sum to 1 so that it can represent a probability



Constructing a Learning Algorithm

- Find the probability distribution h that is most likely, given the data.

$$\begin{aligned}
\arg\max_{h_w} P(h_w \mid X) &= \arg\max_{h_w} \frac{P(X \mid h_w)P(h_w)}{P(X)} && \text{by Bayes' Rule} \\
&= \arg\max_{h_w} P(X \mid h_w)P(h_w) && \text{because P(X) doesn't depend on h} \\
&= \arg\max_{h_w} P(X \mid h_w) && \text{if we assume P(h) is uniform} \\
&= \arg\max_{h_w} \log P(X \mid h_w) && \text{because log is monotone}
\end{aligned}$$

- The **likelihood function** views $P(X|h_w)$ as a function of the parameters in the model. In this case, our parameters are the weights, **w.**
- The log likelihood is a commonly used objective function for learning algorithms. It is denoted L(w;X)
- The w that maximizes the likelihood of the training data is called the **maximum likelihood estimator**

Log Likelihood for Conditional Probability Estimators

- We can express the log likelihood in a compact from
- Take an example ($\mathbf{x}^{(i)}$, $t^{(i)}$)
  - if $y^{(i)} = 0$, the log likelihood is $\log(1-p_1(\mathbf{x};\ w))$
  - if $y^{(i)} = 1$, the log likelihood is $\log\ p_1(\mathbf{x};\ w)$
- These two are mutually exclusive, so we can combine them to get:

$$L(\mathbf{w};\mathbf{x}^{(i)},t) = \log P(t^{(i)} \mid \mathbf{x}^{(i)},\mathbf{w}) = (1-t^{(i)})\log\left[1-p_1(\mathbf{x}^{(i)};\mathbf{w})\right] + t^{(i)}\log p_1(\mathbf{x}^{(i)};\mathbf{w})$$

- The goal of our learning algorithm will be to find w to maximize:

$$L(\mathbf{w};\mathbf{X},\mathbf{t})$$

Computing the Gradient

$$\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}_j} = \sum_i \frac{\partial}{\partial \mathbf{w}_j} L(w;t^{(i)},\mathbf{x}^{(i)})$$

$$\begin{aligned}
\frac{\partial}{\partial \mathbf{w}_j} L(\mathbf{w};t^{(i)};\mathbf{x}^{(i)}) &= \frac{\partial}{\partial \mathbf{w}_j}\left((1-t^{(i)})\log\left[1-p_1(\mathbf{x}^{(i)};\mathbf{w})\right] + t^{(i)}\log p_1(\mathbf{x}^{(i)};\mathbf{w})\right) \\
&= (1-t^{(i)})\frac{1}{1-p_1(\mathbf{x}^{(i)};\mathbf{w})}\left(-\frac{\partial p_1(\mathbf{x}^{(i)};\mathbf{w})}{\partial \mathbf{w}_j}\right) + t^{(i)}\frac{1}{p_1(\mathbf{x}^{(i)};\mathbf{w})}\left(\frac{\partial p_1(\mathbf{x}^{(i)};\mathbf{w})}{\partial \mathbf{w}_j}\right) \\
&= \left[\frac{t^{(i)}}{p_1(\mathbf{x}^{(i)};\mathbf{w})} - \frac{(1-t^{(i)})}{1-p_1(\mathbf{x}^{(i)};\mathbf{w})}\right]\left(\frac{\partial p_1(\mathbf{x}^{(i)};\mathbf{w})}{\partial \mathbf{w}_j}\right) \\
&= \left[\frac{t^{(i)}(1-p_1(\mathbf{x}^{(i)};\mathbf{w})) - (1-t^{(i)})p_1(\mathbf{x}^{(i)};\mathbf{w})}{p_1(\mathbf{x}^{(i)};\mathbf{w})(1-p_1(\mathbf{x}^{(i)};\mathbf{w}))}\right]\left(\frac{\partial p_1(\mathbf{x}^{(i)};\mathbf{w})}{\partial \mathbf{w}_j}\right) \\
&= \left[\frac{t^{(i)} - p_1(\mathbf{x}^{(i)};\mathbf{w})}{p_1(\mathbf{x}^{(i)};\mathbf{w})(1-p_1(\mathbf{x}^{(i)};\mathbf{w}))}\right]\left(\frac{\partial p_1(\mathbf{x}^{(i)};\mathbf{w})}{\partial \mathbf{w}_j}\right)
\end{aligned}$$

Gradient cont.

- Recall the form of p_1:

$$p_1(\mathbf{x}^{(i)};\mathbf{w}) = \frac{e^{\mathbf{w}^T\mathbf{x}^{(i)}}}{1+e^{\mathbf{w}^T\mathbf{x}^{(i)}}} = \frac{1}{1+e^{-\mathbf{w}^T\mathbf{x}^{(i)}}}$$

- So we get:

$$\begin{aligned}
\frac{\partial p_1(\mathbf{x}^{(i)};\mathbf{w})}{\partial \mathbf{w}_j} &= \frac{-1}{(1+e^{-\mathbf{w}^T\mathbf{x}^{(i)}})^2}\frac{\partial}{\partial \mathbf{w}_j}(1+e^{-\mathbf{w}^T\mathbf{x}^{(i)}}) \\
&= \frac{1}{(1+e^{-\mathbf{w}^T\mathbf{x}^{(i)}})^2} e^{-\mathbf{w}^T\mathbf{x}^{(i)}} \frac{\partial}{\partial \mathbf{w}_j}(\mathbf{w}^T\mathbf{x}^{(i)}) \\
&= \frac{1}{(1+e^{-\mathbf{w}^T\mathbf{x}^{(i)}})^2} e^{-\mathbf{w}^T\mathbf{x}^{(i)}} (x^{(i)}{}_j) \\
&= p_1(\mathbf{x}^{(i)};\mathbf{w})(1-p_1(\mathbf{x}^{(i)};\mathbf{w}))x^{(i)}{}_j
\end{aligned}$$

Recall: $p_0(\mathbf{x};\mathbf{w}) = 1 - p_1(\mathbf{x};\mathbf{w}) = \frac{e^{-\mathbf{w}^T\mathbf{x}}}{1+e^{-\mathbf{w}^T\mathbf{x}}} = \frac{1}{1+e^{\mathbf{w}^T\mathbf{x}}}$

Gradient cont.

- The gradient of the log likelihood for a single point is thus:

$$\frac{\partial}{\partial \mathbf{w}_j} L(\mathbf{w};\mathbf{x}^{(i)},t^{(i)}) = \left[\frac{t^{(i)} - p_1(\mathbf{x}^{(i)};\mathbf{w})}{p_1(\mathbf{x}^{(i)};\mathbf{w})(1-p_1(\mathbf{x}^{(i)};\mathbf{w}))}\right]\left(\frac{\partial p_1(\mathbf{x}^{(i)};\mathbf{w})}{\partial \mathbf{w}_j}\right)$$

$$= \left[\frac{t^{(i)} - p_1(\mathbf{x}^{(i)};\mathbf{w})}{p_1(\mathbf{x}^{(i)};\mathbf{w})(1-p_1(\mathbf{x}^{(i)};\mathbf{w}))}\right] p_1(\mathbf{x}^{(i)};\mathbf{w})(1-p_1(\mathbf{x}^{(i)};\mathbf{w}))x^{(i)}{}_j$$

$$= (t^{(i)} - p_1(\mathbf{x}^{(i)};\mathbf{w}))x^{(i)}{}_j$$

- The overall gradient is:

$$\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}_j} = \sum_i (t^{(i)} - p_1(\mathbf{x}^i;\mathbf{w}))x^{(i)}{}_j$$

Compare w/percepton rule!

Batch Ascent/Descent

- Logistic regression w/training set $\{\langle \mathbf{x}^{(i)}, t^{(i)}\rangle\}$, i = 1..N

Repeat until convergence {

for every j

$$w_j^{(t+1)} = w_j + \alpha \sum_{i=1}^{N}\left(t^{(i)} - p(x^{(i)};w^{(t)})\right)x_j^{(i)}$$

t++}

- Perceptron:

Repeat until convergence {for every j

$$w_j^{(t+1)} = w_j^{(t)} + \alpha \sum_{i \in \text{misclassified}} t^{(i)} x_j^{(i)}$$

t++}

NB: t is a time index, which indicates that updates are done *synchronously*, i.e., all weights on the RHS are frozen until all updates are computed, then all weights are simultaneously updated together

Logistic Regression for K > 2

(Not Presented, but for reference)

- To handle K >2 classes, we make one class the 'reference' class. Suppose it is class K. Then we represent each of the other classes as a logistic function of the odds of class k versus class K:

$$\log\frac{P(y=1\mid\mathbf{x})}{P(y=K\mid\mathbf{x})} = \theta_1\cdot\mathbf{x}$$

$$\log\frac{P(y=2\mid\mathbf{x})}{P(y=K\mid\mathbf{x})} = \theta_2\cdot\mathbf{x}$$

$$\vdots$$

$$\log\frac{P(y=k-1\mid\mathbf{x})}{P(y=K\mid\mathbf{x})} = \theta_{k-1}\cdot\mathbf{x}$$

- The conditional probability for class k ≠ K is

$$P(y=k\mid x) = \frac{e^{\theta_k\cdot\mathbf{x}}}{1+\sum_{j=1}^{K-1} e^{\theta_j\cdot\mathbf{x}}}$$

- and for class k = K:

$$P(y=K\mid x) = \frac{1}{1+\sum_{j=1}^{K-1} e^{\theta_j\cdot\mathbf{x}}}$$

Summary of Logistic Regression

- Learns the **Conditional Probability Distribution** P(t|**x**)
- No closed form solution
- Very simple expression for gradient permits local search
  - Begin with initial weight vector.
  - Gradient ascent to maximize objective function.
  - Objective function is the **log likelihood** of the data
  - Algorithm seeks the probability distribution P(t|**x**) that is most likely given the data.
- May be done online or in batch
- Can be used with acceleration methods (Newton-Raphson, etc.)

What We Already Know

- Linear Threshold Unit (LTU)
  - Tries to discover a linear function (in feature space) that separates positive and negative examples
  - Example: Perceptron
- Logistic Regression
  - Maximizes log likelihood

$$\log \frac{p_1(\mathbf{x};\mathbf{w})}{p_0(\mathbf{x};\mathbf{w})} = \mathbf{w}^T\mathbf{x}$$

Naïve Bayes is a linear method!

- Choose class 1 when:

$$P(x_1 \ldots x_n \mid t_1)P(t_1) > P(x_1 \ldots x_n \mid t_0)P(t_1)$$

$$P(t_1)\prod_{i=1}^{n} P(x_i \mid t_1) > P(t_0)\prod_{i=1}^{n} P(x_i \mid t_0)$$

$$\log(P(t_1)) + \sum_{i=1}^{n} \log(P(x_i \mid t_1)) > \log(P(t_0)) + \sum_{i=1}^{n} \log(P(x_i \mid t_0))$$

- Fundamentally same expressive power as other linear methods

Linear Discriminant Analysis

- In LDA, we learn the distribution P(**x**|t)
- We assume that **x** is continuous
- We assume P(**x**|t) is distributed according to a multivariate normal distribution and P(t) is a discrete distribution
- Nota bene: LDA can also mean "Latent Dirichlet Allocation", which is something different

Estimating the MVG parameters

- Given a set of data points {$\mathbf{x}^1$,..., $\mathbf{x}^N$}, the maximum likelihood estimates for the parameters of the MVG are:

$$\hat{\mu} = \frac{1}{N}\sum_i \mathbf{x}^{(i)}$$

$$\hat{\Sigma} = \frac{1}{N-1}\sum_i (\mathrm{x}^{(i)} - \hat{\mu})(\mathrm{x}^{(i)} - \hat{\mu})^T$$

Putting it all together in LDA

- Also called Gaussian Discriminant Analysis
- Here
  - t ~ Bernoulli(**w**)
  - **x**|t=0 ~ N(μ_0, Σ)
  - **x**|t=1 ~ N(μ_1, Σ)
- Writing this out, we get:

$$p(x \mid t=0) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left[-\frac{1}{2}(x-\mu_0)^T \Sigma^{-1} (x-\mu_0)\right]$$

$$p(x \mid t=1) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left[-\frac{1}{2}(x-\mu_1)^T \Sigma^{-1} (x-\mu_1)\right]$$

Called the *Class Conditional* densities

Picking A Class

- We again use Bayes rule:

MVG conditional feature probability

Prior class probability

$$P(t \mid X) = \frac{P(X \mid t)P(t)}{P(X)}$$

Posterior label probability

Prior feature probability (ignored)

The Beauty of Homoscedasticity

- Recall we assumed Σ same for all classes
- When is P(t0|x)>P(t1|x)???

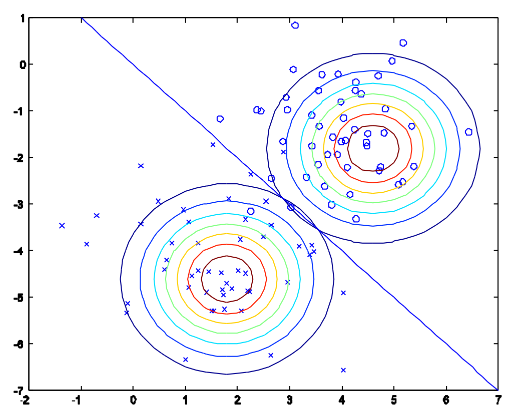
$$\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left[-\frac{1}{2}(x-\mu_0)^T \Sigma^{-1} (x-\mu_0)\right] p(t0) >$$

$$\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left[-\frac{1}{2}(x-\mu_1)^T \Sigma^{-1} (x-\mu_1)\right] p(t1)$$

$$-(x-\mu_0)^T \Sigma^{-1} (x-\mu_0) + k_a > -(x-\mu_1)^T \Sigma^{-1} (x-\mu_1) + k_b$$

Linear!!!

Example



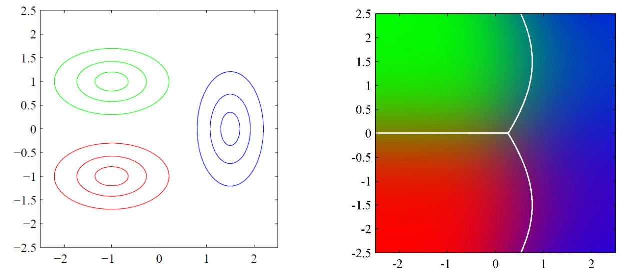
The decision boundary is at p(y=1|x) = 0.5

Homoscedastic LDA Discussion

- For multiclass, this gives convex decision boundaries
- This is nice because it makes classification easy (easy to use geometric data structures)

- How realistic is this?
- What do we give up?

Heteroscedastic Distributions



(assuming uniform class priors, in this example)

Comparing LTU, LR, LDA

- Big debate about the relative merits of
  - direct classifiers (like LTU) versus
  - conditional models (like LR) versus
  - generative models (like LDA, NB)

LDA vs LR

- What is the relationship?
  - In LDA, it turns out the p(t|**x**) can be expressed as a logistic function where the weights are some function of μ_1, μ_2, and Σ!
  - But, the converse is NOT true. If p(t|x) is a logistic function, that does not imply p(**x**|t) is MVG
- LDA makes stronger modeling assumptions than LR
  - when these modeling assumptions are correct, LDA will perform better
    - LDA is asymptotically efficient: in the limit of very large training sets, there is no algorithm that is strictly better than LDA
  - however, when these assumptions are incorrect, LR is more robust
    - weaker assumptions, more robust to deviations from modeling assumptions
    - if the data are non-Gaussian, then in the limit, logistic outperforms LDA
    - For this reason, LR is a more commonly used algorithm

Issues

- **Statistical efficiency:** if the generative model is correct, then it usually gives better accuracy, especially for small training sets.
- **Computational efficiency:** generative models typically are the easiest to compute. In LDA, we estimated the parameters directly, no need for gradient ascent
- **Robustness to changing loss function:** Both generative and conditional models allow the loss function to change without re-estimating the model. This is not true for direct LTU methods
- **Robustness to model assumptions:** The generative model usually performs poorly when the assumptions are violated.
- **Robustness to missing values and noise:** In many applications, some of the features $x^{(i)}_j$ may be missing or corrupted for some training examples. Generative models provide better ways of handling this than non-generative models.

Conclusions

- Four linear methods
  - Perceptron
  - Logistic regression
  - Naïve Bayes
  - Linear Discriminant Analysis
- Perceptrons are fast
- LR, NB gives probabilities, are more robust
- LDA models the data