Lecture 7: Generating Learning Algorithm

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WESTLAKE UNIVERSITY | SCHOOL OF ENGINEERING

1. Review of Last Week
   - Exponential Families
   - Generalized Linear Models

2. Generative Learning Algorithms
   - Discriminative vs. Generative Learning Algorithms
   - Gaussian Discriminant Analysis (GDA)
   - Linear Discriminant Analysis (LDA)
   - LDA and Logistic Regression
   - MLE for GDA
   - Naïve Bayes

Reading materials & Reference

Reading materials:

- Chapter 4, Stanford CS 229 Lecture Notes,
  `https://cs229.stanford.edu/notes2022fall/main_notes.pdf`
- Chapter 9, Probabilistic Machine Learning: an introduction.
- Learning From Data Lecture 4: Generative Learning Algorithms,
  `http://yangli-feasibility.com/`

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Logistic Regression and Exponential Families

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It is called the **link function**.

Exponential family — definition

A distribution belongs to the exponential family if it can be written in the form

$$p(y|\boldsymbol{\eta}) = \underbrace{h(y)}_{\geq 0} \exp\left[\boldsymbol{\eta}^\top \boldsymbol{\phi}(y) - A(\boldsymbol{\eta})\right] \tag{3}$$

[1] Assume that we are given independent samples from this distribution. We do know $\boldsymbol{\phi}(y)$ and $h(y)$ but not $\boldsymbol{\eta}$. In order to optimally estimate $\boldsymbol{\eta}$ given these samples, all we need is the empirical average of the $\boldsymbol{\phi}(y)$.

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$$\text{(we need)} \int p(y|\boldsymbol{\eta})dy = \int h(y) \exp\left[\boldsymbol{\eta}^\top \boldsymbol{\phi}(y) - A(\boldsymbol{\eta})\right] dy = 1 \tag{4}$$

$$\Longrightarrow \int h(y) \exp\left[\boldsymbol{\eta}^\top \boldsymbol{\phi}(y)\right] dy = \int h(y) \exp\left[A(\boldsymbol{\eta})\right] dy = \exp\left[A(\boldsymbol{\eta})\right] \tag{5}$$

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$$\boldsymbol{\eta} = \mathbf{g}\left(\boldsymbol{\mu} := \mathbb{E}\left[\phi(y)\right]\right) \iff \boldsymbol{\mu} = \mathbf{g}^{-1}(\boldsymbol{\eta}) = \nabla A(\boldsymbol{\eta}) \tag{6}$$

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- The GLM framework extends these ideas to the general exponential family.

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The condition probability is thus modeled as:

$$p(y|\mathbf{x};\mathbf{w}) = h(y_n)\exp\left(\eta\phi(y) - A(\eta)\right) \qquad \text{for} \quad \eta = g \circ f(\mathbf{x}^\top \mathbf{w}) \tag{7}$$

Negative log-likelihood estimation

Note that:

$$\mathcal{L}(\mathbf{w}) = -\frac{1}{N}\sum_{n=1}^{N} \ln p(y_n|\mathbf{x}_n^\top \mathbf{w}) = -\frac{1}{N}\sum_{n=1}^{N} (\ln(h(y_n)) + \eta_n \phi(y_n) - A(\eta_n)) \tag{8}$$

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In the case of Logistic Regression:

$$\nabla_{\mathbf{w}}\mathcal{L}(\mathbf{w}) = \frac{1}{N}\mathbf{X}^\top \left[\sigma(\mathbf{X}\mathbf{w}) - \mathbf{y}\right] \tag{12}$$

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This lecture:

- Discriminative vs. Generative learning algorithms
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Recap

Classification: we observe some data $\mathcal{S} = \{\mathbf{x}_n, y_n\}_{n=1}^{N} \in \mathcal{X} \times \underbrace{\mathcal{Y}}_{\text{Discrete set}}$

Goal: given a new observation $\mathbf{x}$, we want to predict its label y

How: relates input to a categorical variable

Recap

In previous lectures, we assume that we know the joint distribution $p(\mathbf{x}, y)$.

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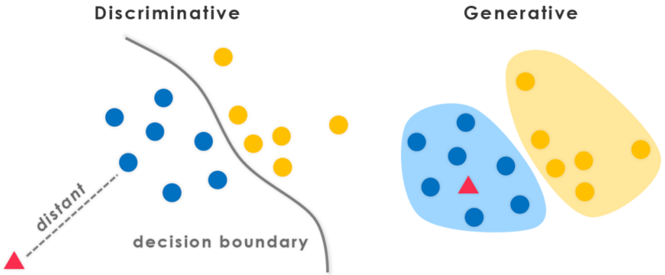
Discriminative v/s Generative Learning Algorithms



Discriminative Learning Algorithm:

Generative Learning Algorithm:

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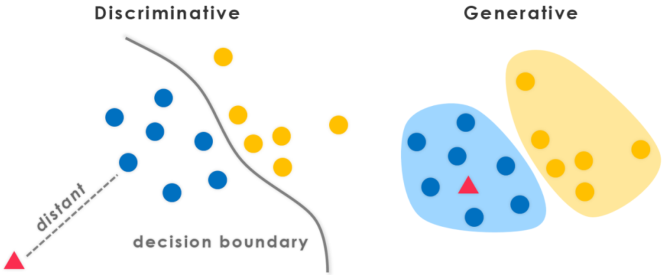

Discriminative Learning Algorithm:
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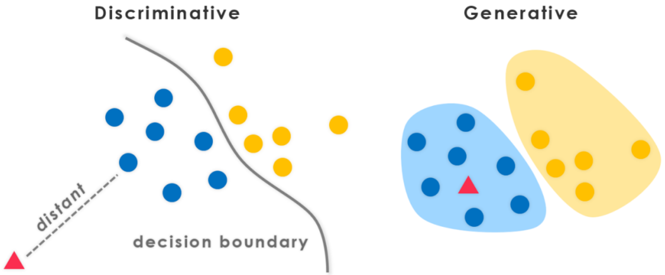

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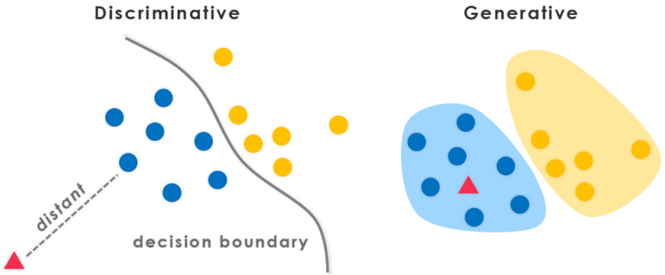

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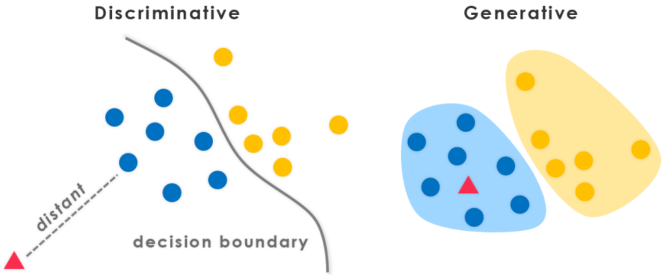

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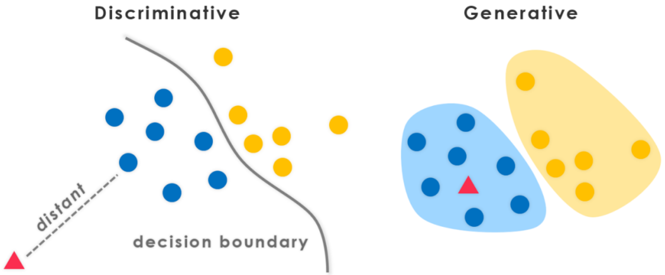

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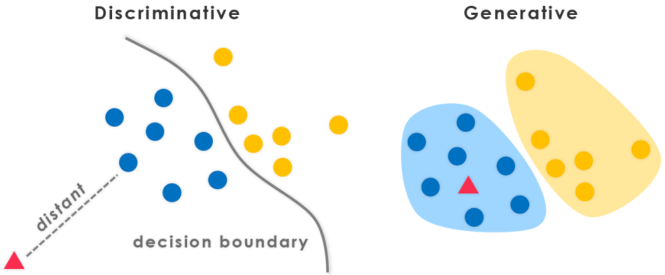

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- learned models are transformed to $p(y|\mathbf{x}, \mathbf{w})$ later to classify data using Bayes' rule: $p(y|\mathbf{x}) = \frac{p(\mathbf{x}|y)p(y)}{p(\mathbf{x})}$

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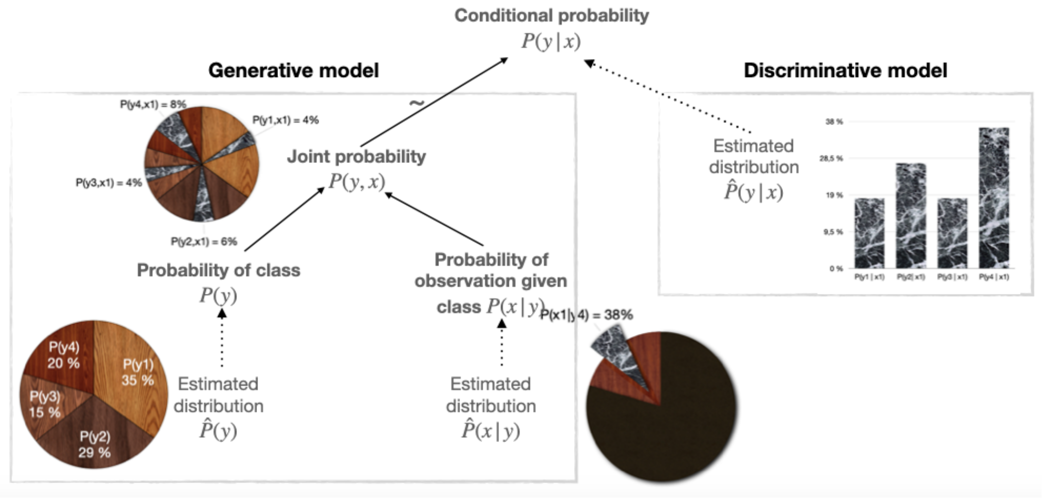
Make predictions in a generative model (exercise):

$$\arg\max_{y \in \mathcal{Y}} p(y|\mathbf{x}, \mathbf{w}) = \arg\max_{y \in \mathcal{Y}} \frac{p(\mathbf{x}|y, \mathbf{w})p(y|\mathbf{w})}{p(\mathbf{x}|\mathbf{w})} = \arg\max_{y \in \mathcal{Y}} p(\mathbf{x}|y, \mathbf{w})p(y|\mathbf{w})$$

Discriminative v/s Generative Learning Algorithms (an alternative view)



From https://towardsdatascience.com/introduction-to-generative-and-discriminative-models-9c9ef152b9af/

Discriminative Models v.s. Generative Models (an alternative view)

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- more powerful with lots of examples

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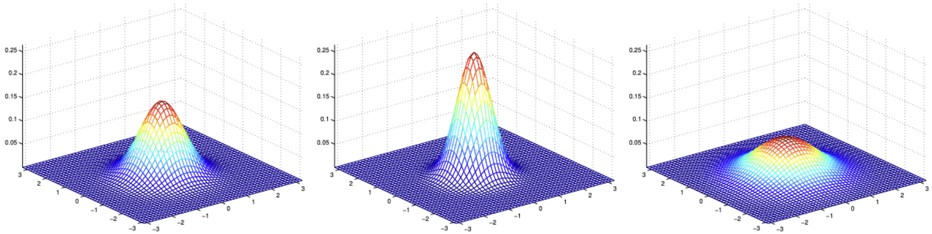
where $\boldsymbol{\Sigma}$ (exercise) is symmetric and positive semi-definite matrix.



(Left): $\mathbf{\Sigma} = \mathbf{I}$; (Middle): $\mathbf{\Sigma} = 0.6\mathbf{I}$; (Right): $\mathbf{\Sigma} = 2\mathbf{I}$.

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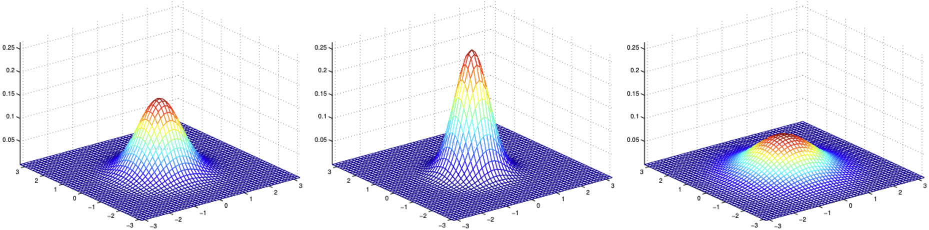

(Left): $\boldsymbol{\Sigma} = \mathbf{I}$; (Middle): $\boldsymbol{\Sigma} = 0.6\mathbf{I}$; (Right): $\boldsymbol{\Sigma} = 2\mathbf{I}$. We can see that as

- $\boldsymbol{\Sigma}$ becomes larger, the Gaussian becomes more "spread-out"
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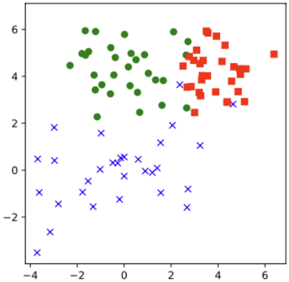

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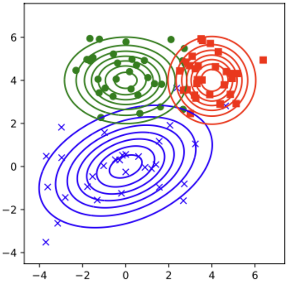

(b)

2d data from 3 different classes in (a), and we fit the full covariance Gaussian class-conditionals in (b).

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$\Longrightarrow$ in which models $p(\mathbf{x}|y, \mathbf{w})$ uses a multi-variate normal distribution:

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$$y \sim \text{Bernoulli}(\phi) \tag{17}$$

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The corresponding class posterior ((Gaussian Discriminant Analysis: GDA)) therefore has the form

$$p(y = c|\mathbf{x}, \mathbf{w}) \propto \pi_c \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)\ , \tag{20}$$

where $\pi_c = p(y = c|\mathbf{w})$.

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Write out the Probability Density Functions (PDFs):

$$p(y) = \phi^y (1-\phi)^{1-y} \tag{21}$$

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(a) (b)

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(a): GDA fits to data, where unconstrained covariances induce quadratic decision boundaries;
(b): LDA fits to data, where tied covariances induce linear decision boundaries.

What is LDA?

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Linear Discriminant Analysis (LDA)

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The connection between LDA and logistic regression

Recall that in LDA, we have

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Then,

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where $\mathbf{w}_c = [\gamma_c, \boldsymbol{\beta}_c]$.

The connection between LDA and logistic regression

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To gain further insights, let's consider the binary case.

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This has the same form as binary logistic regression, and the MAP decision rule is

$$\hat{y}(\mathbf{x}) = 1 \text{ iff } \mathbf{w}^\top \mathbf{x} > c\,, \text{ where } c = \mathbf{w}^\top \mathbf{x}_0$$

Geometry interpretation of LDA

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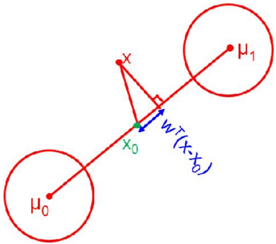

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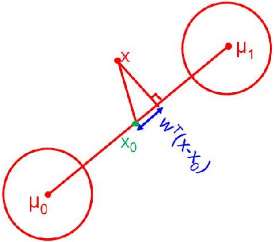
$\Longrightarrow$ we can classify a point by projecting it onto this line, and check its distance to $\boldsymbol{\mu}_0$ and $\boldsymbol{\mu}_1$.



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Some remarks

GDA

- maximizes the **joint likelihood** $\prod_{i=1}^{n} p(\mathbf{x}^{(i)}, y^{(i)})$
- modeling assumptions:
  $\mathbf{x}|y = b \sim \mathcal{N}(\boldsymbol{\mu}_b, \boldsymbol{\Sigma}), y \sim$ Bernoulli(ϕ)
- when modeling assumptions are correct, GDA is asymptotically efficient[a] and data efficient.

[a] in the limit of very large training sets (large n), there is no algorithm that is strictly better than GDA.

Logistic Regression

- maximizes the **conditional likelihood** $\prod_{i=1}^{n} p(y^{(i)}|\mathbf{x}^{(i)})$
- modeling assumptions:
  $p(y|\mathbf{x})$ is a logistic function; no restriction on $p(\mathbf{x})$
- more robust and less sensitive to incorrect modeling assumptions.

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Maximimum Likelihood Estimation for GDA

The likelihood function of a GDA model is as follows:

$$p(\mathcal{D}|\mathbf{w}) = \prod_{i=1}^{N} \mathrm{Cat}(y_i|\boldsymbol{\pi}) \prod_{c=1}^{C} \mathcal{N}(\mathbf{x}_i|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)^{1\{y_i=c\}}$$

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MLE estimation:

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- $\hat{\boldsymbol{\mu}}_c = \frac{1}{N_c} \sum_{i:y_i=c} \mathbf{x}_n$
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A different version of derivatives for MLE of LDA

Log-likelihood of the data:

$\ell(\phi, \boldsymbol{\mu}_0, \boldsymbol{\mu}_1, \boldsymbol{\Sigma})$

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By maximizing ℓ w.r.t. the parameters, the maximumn likelihood estimate of the parameters:

$$
\begin{aligned}
\phi &= \frac{1}{n} \sum_{i=1}^{n} 1\{y^{(i)} = 1\} \\
\boldsymbol{\mu}_b &= \frac{\sum_{i=1}^{n} 1\{y^{(i)} = b\}\mathbf{x}^{(i)}}{\sum_{i=1}^{n} 1\{y^{(i)} = b\}} \text{ for } b = 0, 1 \\
\boldsymbol{\Sigma} &= \frac{1}{n} \sum_{i=1}^{n} (\mathbf{x}^{(i)} - \boldsymbol{\mu}_{y^{(i)}})(\mathbf{x}^{(i)} - \boldsymbol{\mu}_{y^{(i)}})^\top
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$\Longrightarrow$ **Naïve Bayes**

Naïve Bayes: Motivating Example

Example 2 (Spam filter (document classification))

Classify email message $\mathbf{x}$ to spam $(y = 1)$ and non-spam $(y = 0)$ classes.

Hello [redacted]
We need to confirm your info...
(1) FINAL MESSAGE: Payout Verification - $3000 PAYOUT is ready to be addressed in your Name and we want to be sure it gets to the right place. Click below to start the confirmation process. The sooner you act, the sooner it can be in your hands!
Raging Bull Casino

A sample spam email

Example: Spam Filter

We would like to represent an email via a feature vector.

Binary text features: Given a dictionary of size n, represent a message composed of dictionary words as $\mathbf{x} \in \{0,1\}^n$:

$$x_i = \begin{cases} 1 & i\text{-th dictionary word is in message} \\ 0 & \text{otherwise} \end{cases}$$

$$x = \begin{array}{cl} \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} & \begin{array}{l} \text{a} \\ \text{aardvark} \\ \text{aardwolf} \\ \vdots \\ \text{buy} \\ \vdots \\ \text{zygmurgy} \end{array} \end{array}$$

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To build a generative model, we have to model $p(\mathbf{x}|y)$

Naïve Bayes assumption and Naïve Bayes classifier

Probability of observing email $x_1, \ldots, x_n$ given spam class y:

$$p(x_1, \ldots, x_n | y) = p(x_1 | y) p(x_2 | x_1, y), \ldots, p(x_n | x_1, \ldots x_{n-1}, y)$$

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To model $p(\mathbf{x}|y)$, we will therefore make a very strong assumption.

Assumption 1 (Naïve Bayes assumption)

x_i's are conditionally independent given y:

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As a result,

$$p(x_1, \ldots, x_n|y) = p(x_1|y)p(x_2|y) \ldots p(x_n|y) = \prod_{i=1}^{n} p(x_i|y)$$

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Model parameters:

- $\phi_y \in \mathbb{R}$
- $\phi_{i|y=1}, \phi_{i|y=0}$ for $i = 1, \ldots, n$

Naïve Bayes Parameter Learning

Likelihood of i.i.d. training data $(\mathbf{x}^{(1)}, y^{(1)}), \ldots, (\mathbf{x}^{(n)}, y^{(n)})$:

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Maximum likelihood estimation of parameters:

$$\phi_y = \frac{1}{n} \sum_{i=1}^{n} 1\{y^{(i)} = 1\} \qquad \text{(\% of spam emails)}$$

$$\phi_{i|y=b} = \frac{\sum_{i=1}^{n} 1\{x_j^{(i)} = 1, y^{(i)} = b\}}{\sum_{i=1}^{n} 1\{y^{(i)} = b\}} \quad \text{for } b = 1, 0$$

(% of spam (non-spam) emails containing j-th dictionary word)

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Choose label $y=1$ (spam) if $p(y=1|x) > T$, where $T \in [0,1]$ is a threshold, e.g., $T=0.5$.

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In case of taking the x_j value in $\{1,\ldots,k_j\}$,
we can model $p(x_j|y)$ as multi-nomial distribution, rather than as Bernoulli.

Laplace smoothing

Issue with Naïve Bayes prediction:

- Suppose word x_j hasn't been seen in the training data,

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- We cannot compute class posterior

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- Laplace smoothing can be used to eliminate this issue:

$$\phi_j = \frac{1 + \sum_{i=1}^{n} 1\{z^{(i)} = j\}}{k + n} \qquad \text{where}$$

  - $\phi_j \neq 0$ for all j
  - $\sum_{j=1}^{k} \phi_j = 1$

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- In practice we don't apply Laplace smoothing to $\phi_y = p(y = 1)$, which is greater than 0.

Last lecture:

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- Generalized Linear Models

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This lecture:

- Discriminative vs. Generative learning algorithms
- Gaussian Discriminant Analysis (GDA)
- Linear Discriminant Analysis (LDA)
- LDA and Logistic regression
- Naïve Bayes