INTRODUCTION TO GENERATIVE SUPERVISED LEARNING MODELS

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OVERVIEW OF DISCRIMINATIVE VS. GENERATIVE MODELS

Discriminative Learning

- Models that directly aim at learning (or approximating) the **posterior probability distribution** $\mathbb{P}(Y|X)$.
- The posterior distribution $\mathbb{P}(Y|X)$ is the distribution of the target variable Y conditioned on observing a set of data features X.
- This distribution is given the name "**posterior**" distribution in reference to the probability of the target variable Y "**post**" (or after) observing the data X.
- Alternatively, we refer to $\mathbb{P}(Y)$ as the **prior distribution** since it is meant to represent our knowledge or belief in an outcome of interest Y before observing any data X, hence the name "**prior**".

Generative Learning

- Models that *still* predict posterior probabilities, but instead of learning the posterior distribution directly, generative models focus on learning the **underlying joint probability distribution** $\mathbb{P}(X,Y)$, after which **Baye's Theorem** can be applied to "**generate**" probabilities from the posterior distribution.
- Once the joint probability distribution $\mathbb{P}(X,Y)$ is learned, using **Baye's Theorem**, posterior probabilities are generated according to the equation

$$\mathbb{P}(Y|X) = \frac{\mathbb{P}(Y)\mathbb{P}(X|Y)}{\mathbb{P}(X)}.$$

GENERATIVE MODELS & BAYES' THEOREM

- As stated, the difference between discriminative models and generative models in supervised learning is that discriminative models aim at learning the posterior distribution $\mathbb{P}(y|x)$ directly whereas generative models aim at learning the joint distribution $\mathbb{P}(x,y)$ from which one can generate posterior probabilities via Bayes' Theorem.
- Recall from the *Probability & Statistics Slides* that conditional probability is defined as

$$\mathbb{P}(y|x) = \frac{\mathbb{P}(x,y)}{\mathbb{P}(x)}.$$

- However, in machine learning problems, we do not typically have access to "exact" information of the joint probability distribution $\mathbb{P}(x,y)$ (recall from the *Linear Regression Slides* that this is a direct approximation of the true underlying distribution that the data is drawn from, denoted by $\mathcal{P}(x,y)$).
- On the other hand, we do typically have information of the marginal "**prior**" $\mathbb{P}(y)$, the marginal $\mathbb{P}(x)$, and the conditional distribution $\mathbb{P}(x|y)$, which can be modeled by again using the definition of conditional probability as

$$\mathbb{P}(x|y) = \frac{\mathbb{P}(x,y)}{\mathbb{P}(y)}.$$

- Using this, we can solve for the joint distribution in terms of quantities that we do know

$$\mathbb{P}(x,y) = \mathbb{P}(y)\mathbb{P}(x|y).$$

- Lastly, substituting this into the equation for the posterior distribution above, we obtain Bayes' Theorem

$$\mathbb{P}(y|x) = \frac{\mathbb{P}(y)\mathbb{P}(x|y)}{\mathbb{P}(x)}.$$

Therefore, **if one can <u>correctly model</u>** the probability distributions $\mathbb{P}(y)$ and $\mathbb{P}(x|y)$, then one can generate posterior probabilities $\mathbb{P}(y|x)$ via Bayes' Theorem. **This is the idea behind Generative Models**.

WHAT MAKES GENERATIVE MODELS USEFUL?

- Although generative models "can" be used to predict a target variable y in a supervised learning context, they are typically only used for this purpose in scenarios when there is **not much data available** to train on.

- If relatively large amounts of data are available, then one would typically use a discriminative model which will almost always have higher predictive power.

So, then what are generative models used for?

- The reason that these models are given the moniker "**generative**" is because they are very useful for **generating synthetic data that mimics the original "true" distribution** $\mathcal{P}(x, y)$ (with the approximation obtained by $\mathbb{P}(x, y) = \mathbb{P}(y)\mathbb{P}(x|y)$).

- As a result, once the approximate joint distribution $\mathbb{P}(x, y)$ has been learned, one can **sample new synthetic data from that distribution**.

- This can be very useful for a variety of problems, such as **class-imbalance problems** (i.e., artificially increasing the number of instances for an underrepresented class), **data cleaning** (i.e., replacing missing data), and others.

GAUSSIAN DISCRIMINANT ANALYSIS

The first generative model that we will introduce is the **Gaussian Discriminant Analysis** model. This model (and all other generative models for that matter) assumes that the features and target variable of a dataset follow certain distributions, from which we can model relatively well.

The Gaussian Discriminant Analysis (GDA) Model

Consider some dataset $\mathcal{D} = \left\{\left(x^{(i)}, y^{(i)}\right)\right\}_{i=1}^{m}$, where $x^{(i)} \in \mathbb{R}^n$ and the target variable is **binary** $y \in \{0,1\}$.

- Therefore, the target variable y can be modeled as a **Bernoulli random variable** with probability parameter given by $\phi \in [0,1]$ such that $\mathbb{P}(y = 1) = \phi$.
- Further, this model assumes that each feature vector $x \in \mathbb{R}^n$comes from an **$\boldsymbol{n}$-dimensional multivariate Gaussian distribution when conditioned on $\boldsymbol{y}$**. More specifically, this means that given some mean vector $\mu_y \in \mathbb{R}^n$ and covariance matrix $\Sigma \in \mathbb{R}^{n\times n}$, then it follows that $\mathbb{P}(x|y) \sim \mathcal{N}\left(\mu_y, \Sigma_y\right)$ for $y \in \{0,1\}$. Thus, we have that

$$\mathbb{P}\left(x|y;\mu_y,\Sigma_y\right) = \frac{1}{(2\pi)^{n/2}\left|\Sigma_y\right|^{1/2}} e^{-\frac{1}{2}\left(x-\mu_y\right)^T \Sigma_y^{-1}\left(x-\mu_y\right)}.$$

Therefore, when trying to classify a new datapoint (x, y), the GDA model h_θ (where the parameters $\theta = [\mu_0, \mu_1, \Sigma_0, \Sigma_1]$) utilizes Bayes' Theorem and chooses the value of $y \in \{0,1\}$ that maximizes the posterior probability $\mathbb{P}(y|x)$, i.e.,

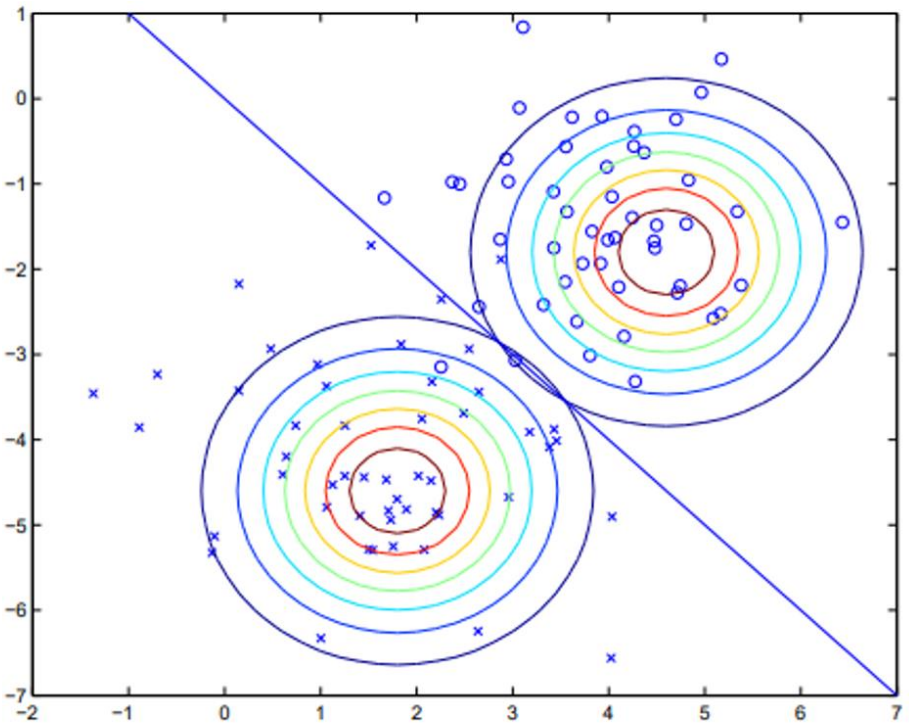
$$h_\theta(x) \coloneqq \underset{y\in\{0,1\}}{\operatorname{argmax}}\, \mathbb{P}(y|x) = \underset{y\in\{0,1\}}{\operatorname{argmax}} \frac{\mathbb{P}(y)\mathbb{P}(x|y)}{\mathbb{P}(x)} = \underset{y\in\{0,1\}}{\operatorname{argmax}}\, \mathbb{P}(y)\mathbb{P}(x|y)\,.$$

Since $\mathbb{P}(x)$ will only be a function in x and not y, we can omit it in the maximization over y.

- For the remainder of these slides, we will make the simplifying assumption that $\Sigma_0 = \Sigma_1 = \Sigma$ (i.e., equal covariances).

ILLUSTRATION OF GDA

This figure illustrates a **Gaussian Discriminative Analysis** (GDA) Model where the conditional distribution is a multivariate Gaussian distribution conditioned on a binary variable $Y \in \{0,1\}$, i.e., $f_{X|Y}(X|Y=y) \sim \mathcal{N}(\mu_y, \Sigma)$.



Recall from Homework Assignment 6 that a GDA model with the same covariance matrices (i.e., $\boldsymbol{\Sigma_0 = \Sigma_1 = \Sigma}$) describing each of the Gaussians is equivalent to a Logistic Regression model.

LIKELIHOOD FUNCTION OF GDA

As with all probabilistic models that we have seen, we can go about "training" the GDA model by choosing the set of parameters θ that maximize the likelihood function of observing the data that was observed.

Likelihood Function for GDA

Under the assumptions that the datapoints, given by the set $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^{m}$, are i.i.d. and the prior distribution $\mathbb{P}(y^{(i)})$ is given by the **Bernoulli distribution**

$$\mathbb{P}(y^{(i)}) = \phi^{y^{(i)}}(1-\phi)^{(1-y^{(i)})},$$

and the conditional distribution $\mathbb{P}(x^{(i)}|y^{(i)})$ is given by the **multivariate Gaussian distribution** $\mathcal{N}\left(\mu_{y^{(i)}}, \Sigma\right)$ written as

$$\mathbb{P}(x^{(i)}|y^{(i)}) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} e^{-\frac{1}{2}\left(x^{(i)}-\mu_{y^{(i)}}\right)^T \Sigma^{-1}\left(x^{(i)}-\mu_{y^{(i)}}\right)}.$$

Then, one can define the **likelihood** function of observing the data $\mathcal{D}$, given the set of model parameters $\theta \coloneqq [\mu_0, \mu_1, \Sigma]$, as

$$L\left(\theta; \{(x^{(i)}, y^{(i)})\}_{i=1}^{m}\right) = \prod_{i=1}^{m} \mathbb{P}(x^{(i)}, y^{(i)}) = \prod_{i=1}^{m} \mathbb{P}(y^{(i)})\mathbb{P}(x^{(i)}|y^{(i)}).$$

Similarly, the corresponding **log-likelihood** function is given by

$$\ell\left(\theta; \{(x^{(i)}, y^{(i)})\}_{i=1}^{m}\right) = \sum_{i=1}^{m}\left[\log \mathbb{P}(y^{(i)}) + \log \mathbb{P}(x^{(i)}|y^{(i)})\right].$$

MAXIMUM LIKELIHOOD ESTIMATES FOR GDA

Training the GDA model amounts to solving the optimization problem of maximizing the likelihood function, i.e.,

$$\theta^* = \underset{\theta}{\operatorname{argmax}}\, \ell\left(\theta; \left\{\left(x^{(i)}, y^{(i)}\right)\right\}_{i=1}^{m}\right).$$

After some algebra, the explicit form of the log-likelihood can be written as

$$\ell(\theta) = \sum_{i=1}^{m} \left[y^{(i)} \log \phi + \left(1 - y^{(i)}\right) \log(1-\phi) - \frac{1}{2}\left(x^{(i)} - \mu_{y^{(i)}}\right)^T \Sigma^{-1} \left(x^{(i)} - \mu_{y^{(i)}}\right)\right] - \frac{mn}{2} \log 2\pi - \frac{m}{2} \log|\Sigma|.$$

- **An important point**: this **log-likelihood function is not concave in general**… However, we can **still solve for closed-form analytical solutions** for the maximum-likelihood estimates (MLE) ϕ^*, μ_0^*, μ_1^*, and Σ^* because the partial derivatives with respect to each of these parameters reduces to solvable linear or quadratic equations, which do enable closed-form solutions. It can be shown that, by setting the partial derivatives of the parameters to zero, their optimal solutions can be derived as

$$\phi^* = \frac{1}{m} \sum_{i=1}^{m} y^{(i)} \qquad \textit{and} \qquad \mu_y^* = \frac{\sum_{i=1}^{m} \mathbb{I}\left[y^{(i)} = y\right] x^{(i)}}{\sum_{i=1}^{m} \mathbb{I}\left[y^{(i)} = y\right]},$$

$$\Sigma^* = \frac{1}{m} \sum_{i=1}^{m} \left[\left[y^{(i)} = 0\right] x^{(i)} \left(x^{(i)}\right)^T + \left[y^{(i)} = 1\right] x^{(i)} \left(x^{(i)}\right)^T \right].$$

- Lastly, if the covariance matrices are not equivalent (i.e., $\Sigma_0 \neq \Sigma_1$), the other MLEs of the other parameters are the same, but the solutions Σ_0^* and Σ_1^* will take on different forms; however, they can still be derived by setting the respective partial derivatives of the log-likelihood equal to 0 and solving.