25: Logistic Regression

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Updated CS109 logistics and policies

We are implementing several changes to CS109 logistics and policies in response to growing concern about Covid-19. These changes affect lectures, section, office hours and the final exam.

Read the new policies in the announcements on the course webpage: <http://web.stanford.edu/class/cs109/>

We welcome your questions on piazza

Autograded Coding Problems

Run your code in the command line or install Pycharm following directions on Pset 6 webpage

Late Day Reminder

No late days permitted past last day of the quarter, 3/13

Today's plan

Logistic Regression

- Chapter O: Background
- Chapter 1: Big Picture
- Chapter 2: Details
- Chapter 3: Philosophy

Background: Weighted sum

If
$$
X = (X_1, X_2, ..., X_m)
$$
:
\n
$$
z = \theta^T X = \sum_{j=1}^m \theta_j X_j
$$
\nWeighted sum
\n
$$
= \theta_1 X_1 + \theta_2 X_2 + \dots + \theta_m X_m
$$
\nWeighted sum

Weighted sum with an intercept term:

$$
z = \theta_0 + \sum_{j=1}^{m} \theta_j X_j
$$

= $\theta_0 X_0 + \theta_1 X_1 + \theta_2 X_2 + \dots + \theta_m X_m$ Define $X_0 = 1$
= $\theta^T X$ New $X = (1, X_1, X_2, \dots, X_m)$

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Background: Sigmoid function $\sigma(z)$

• The sigmoid function:

 $\sigma(z) =$ 1 $1 + e^{-z}$

• Sigmoid squashes z to a number between 0 and 1.

• Recall definition of probability: A number between 0 and 1

 $\sigma(z)$ can represent a probability.

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Background: Chain Rule

 $f(x) = f(z(x))$

 $df(x)$ \boldsymbol{d} = $df(Z)$ $\overline{C}Z$ $\overline{C}Z$ \boldsymbol{d}

Calculus Chain Rule

Today's plan

Logistic Regression

- Chapter 0: Background
- Chapter 1: Big Picture
	- Chapter 2: Details
	- Chapter 3: Philosophy

From Naïve Bayes to Logistic Regression

Classification goal: Model $P(Y | X)$

$$
\widehat{Y} = \arg\max_{y=\{0,1\}} P(Y \mid \boldsymbol{X})
$$

Predict the Y that is most likely given our observation X

Naïve Bayes Classifier:

- Estimate $P(X | Y)$ and $P(Y)$ because $\arg \max_{y=\{0,1\}} P(Y | X) = \arg \max_{y=\{0,1\}} P(X|Y)P(Y)$ $v = \{0,1\}$ $v = \{0,1\}$
- Actually modeling $P(X, Y)$
- Assume $P(X|Y) = P(X_1, X_2, ..., X_n|Y) = \prod_{i=1}^{m} P(X_i|Y)$

Can we model $P(Y | X)$ directly?

• Welcome our friend: Logistic Regression!

Logistic Regression

 \hat{Y} = arg max $y=\{0,1\}$

Predict the Y that is most likely given our observation X

Logistic Regression Model

$$
P(Y = 1 | X = x) = \sigma \left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)
$$

models $P(Y | X)$ directly

Logistic Regression

input features

$$
P(Y = 1 | \mathbf{X} = x) = \sigma \left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j \right)
$$

Stanford University 11 Slides courtesy of Chris Piech

Logistic Regression Cartoon

θ parameter

Logistic Regression cartoon

Logistic Regression input/output

Different predictions for different inputs

Different predictions for different inputs

Parameters affect prediction

Parameters affect prediction

Logistic Regression Model

 $\hat{Y} = \arg \max_{\alpha \in \mathbb{R}^n} P(Y | X)$ where $P(Y = 1 | X = x) = \sigma \left(\theta_0 + \right)$ $y = \{0,1\}$

where
$$
P(Y = 1 | X = x) = \sigma \left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j \right)
$$

Predict the Y that is most likely given our observation \boldsymbol{X} models $P(Y | X)$ directly

- $\sigma(z) = \frac{1}{1+e^{-z}}$, the sigmoid function
- For simplicity, define $x_0 = 1$: $P(Y = 1 | X = x) = \sigma(\theta^T x)$
- Since $P(Y = 1 | X = x) + P(Y = 0 | X = x) = 1$: $P(Y = 0 | X = x) = 1 - \sigma(\theta^T x)$

 \mathbf{A}

Classifying using the sigmoid function

 \dot{Y} = arg max $y = 0,1$ $P(Y | X)$ where $P(Y = 1 | X = x) = \sigma \left(\theta_0 + \sum_{i=1}^{n} A_i \right)$ $J=1$ $\frac{m}{2}$ where $P(Y = 1 | X = x) = \sigma \left(\theta_0 + \sum \theta_j x_j \right)$ Logistic Regression Model

Logistic Regression uses the sigmoid function to try and distinguish $y = 1$ (blue) points from $y = 0$ (red) points.

Classifying using the sigmoid function

Logistic Regression Model

$$
\widehat{Y} = \underset{y=\{0,1\}}{\arg \max} P(Y \mid \boldsymbol{X}) \quad \text{where} \quad P(Y=1|\boldsymbol{X}=\boldsymbol{x}) = \sigma \left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)
$$

When do we predict $\dot{Y} = 1$?

- A. If $\sigma(\theta^T x) > 1 \sigma(\theta^T x)$
- B. If $\sigma(\theta^T x) > 0.5$
- C. If $\theta^T x > 0$
- D. All are valid, but C is easiest
- E. None/Other

Naming algorithms

Regression Algorithms

Linear Regression

Classification Algorithms

Training: Learning the parameters

Logistic regression gets its intelligence from its parameters $\theta =$ $(\theta_0, \theta_1, ..., \theta_m)$.

- Logistic Regression Model:
- Want to predict training data as correctly as possible:
- Therefore, choose θ that maximizes the conditional likelihood of observing i.i.d. training data:

$$
P(Y = 1 | X = x) = \sigma(\theta^T x)
$$

$$
\arg \max_{y=\{0,1\}} P(Y|X=x^{(i)}) = y^{(i)} \text{ as often}
$$
\n
$$
\arg \max_{y=\{0,1\}} P(Y|X=x^{(i)}) = y^{(i)} \text{ as possible}
$$

$$
L(\theta) = \prod_{i=1}^{n} P(Y = y^{(i)} | X = x^{(i)}, \theta)
$$

During training, find the θ that maximizes log-conditional likelihood of the training data. Use MLE!

Training: Learning the parameters via MLE

- **0.** Add $x_0^{(l)} = 1$ to each $x^{(l)}$
- 1. Logistic Regression model:

$$
P(Y=1|X=x)=\sigma(\theta^Tx)
$$

- 2. Compute log-likelihood of training data: $LL(\theta) = \sum$ $l=1$ $\frac{n}{2}$ $(y^{(l)}\log\sigma\big(\theta^T\pmb{x^{(l)}}\big) + \big(1-y^{(l)}\big)\log\big(\mathbb{1}-\sigma\big(\theta^T\pmb{x^{(l)}}\big)$
- 3. Compute derivative of log-likelihood with respect to each θ_i , $j = 0, 1, ..., m$:

$$
\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^n \left[y^{(i)} - \sigma \left(\theta^T \mathbf{x}^{(i)} \right) \right] x_j^{(i)}
$$

Gradient Ascent

Review

Walk uphill and you will find a local maxima (if your step is small enough).

is convex

Training: Gradient ascent step

4. Optimize.
$$
\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^n [y^{(i)} - \sigma(\theta^T x^{(i)})] x_j^{(i)}
$$

Repeat many times:

For all theta:
\n
$$
\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \frac{\partial LL(\theta^{\text{old}})}{\partial \theta_j^{\text{old}}}
$$
\n
$$
= \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \left[y^{(i)} - \sigma \left(\theta^{\text{old}}^T x^{(i)} \right) \right] x_j^{(i)}
$$

What does this look like in code?

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Gradient
Ascent Step
$$
\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \left[y^{(i)} - \sigma \left(\theta^{\text{old}^T} x^{(i)} \right) \right] x_j^{(i)}
$$

gradient[j] = 0 for $0 \le j \le m$

// compute all gradient[j]'s // based on n training examples

 θ_j += η * gradient[j] for all 0 \leq j \leq m

Gradient
$$
\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \left[y^{(i)} - \sigma \left(\theta^{\text{old}}^T x^{(i)} \right) \right] x_j^{(i)}
$$

```
gradient[j] = 0 for 0 \le j \le m
```
for each training example (x, y):

```
for each 0 \le j \le m:
```
// update gradient[j] for // current (x,y) example

 θ_i += η * gradient[j] for all 0 \leq j \leq m

Gradient
Ascent Step
$$
\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \left[y^{(i)} - \sigma \left(\theta^{\text{old}^T} x^{(i)} \right) \right] x_j^{(i)}
$$

 $gradient[j] = 0$ for $0 \le j \le m$

for each training example (x, y):

for each $0 \le j \le m$:

gradient[j] +=
$$
\left[y - \frac{1}{1 + e^{-\theta^{T} x}} \right] x_{j}
$$

 θ_i += η * gradient[j] for all 0 ≤ j ≤ m

What are important implementation details?

Gradient
Ascent Step
$$
\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \left[y^{(i)} - \sigma \left(\theta^{\text{old}}^T x^{(i)} \right) \right] x_j^{(i)}
$$

 $gradient[j] = 0$ for $0 \le j \le m$

for each training example (x, y):

for each $0 \le j \le m$:

 $gradient[j] +=$

$$
\left[y - \frac{1}{1 + e^{-\theta^T x}} \right] \left[x_j \right]
$$

 \wedge

 θ_i += η * gradient[j] for all 0 ≤ j ≤ m

 x_j is *j*-th feature of input var $x = (x_1, ..., x_m)$

Training: Gradient Ascent

Gradient
Ascent Step
$$
\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \left[y^{(i)} - \sigma \left(\theta^{\text{old}}^T x^{(i)} \right) \right] x_j^{(i)}
$$

initialize $\theta_j = 0$ for $0 \le j \le m$ repeat many times:

gradient[j] = 0 for $0 \le j \le m$

for each training example (x, y):

for each $0 \le j \le m$:

gradient[j] +=
$$
\left[y - \frac{1}{1 + e^{-\theta^T x}} \right] x_j
$$

 θ_i += η * gradient[j] for all 0 ≤ j ≤ m

- x_j is *j*-th feature of input var $x = (x_1, ..., x_m)$
- Insert $x_0 = 1$ before training

 $\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{j}$ $l=1$ $\frac{n}{2}$ $y^{(i)} - \sigma\left(\theta^{\,\text{old}^T} x^{(i)}\right) \big] \; x^{\text{(i)}}_j$ Gradient $\theta_{\text{new}} = \theta_{\text{old}} + n \sum_{i=1}^{n} [N_{i}(i) - \sigma(\theta_{\text{old}}^T \mathbf{v}(i))] \mathbf{v}^{(i)}$ Ascent Step

initialize $\theta_j = 0$ for $0 \le j \le m$ repeat many times:

gradient[j] = 0 for $0 \le j \le m$

for each training example (x, y):

for each $0 \le j \le m$:

 $gradient[j] +=$

$$
\left[y - \frac{1}{1 + e^{-\theta^T x}}\right] x_j
$$

 θ_i += η * gradient[j] for all 0 \leq j \leq m

- x_j is *j*-th feature of input var $x = (x_1, ..., x_m)$
- Insert $x_0 = 1$ before training
- Finish computing gradient before updating any part of θ

 $\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{j}$ $l=1$ $\frac{n}{2}$ $y^{(i)} - \sigma\left(\theta^{\,\text{old}^T} x^{(i)}\right) \big] \; x^{\text{(i)}}_j$ Gradient $\theta_{\text{new}} = \theta_{\text{old}} + n \sum_{i=1}^{n} [N_{i}(i) - \sigma(\theta_{\text{old}}^T \mathbf{v}(i))] \mathbf{v}^{(i)}$ Ascent Step

initialize $\theta_j = 0$ for $0 \le j \le m$ repeat many times:

gradient[j] = 0 for $0 \le j \le m$

for each training example (x, y):

for each $0 \le j \le m$:

gradient[j] +=
$$
\left[y - \frac{1}{1 + e^{-\theta^T x}} \right] x_j
$$

 θ_i += η r gradient[j] for all 0 \leq j \leq m

- x_j is *j*-th feature of input var $x = (x_1, ..., x_m)$
- Insert $x_0 = 1$ before training
- Finish computing gradient before updating any part of θ
- Learning rate η is a constant you set before training

 $\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{j}$ $l=1$ $\frac{n}{2}$ $y^{(i)} - \sigma\left(\theta^{\,\text{old}^T} x^{(i)}\right) \big] \; x^{\text{(i)}}_j$ Gradient $\theta_{\text{new}} = \theta_{\text{old}} + n \sum_{i=1}^{n} [N_{i}(i) - \sigma(\theta_{\text{old}}^T \mathbf{v}(i))] \mathbf{v}^{(i)}$ Ascent Step

initialize $\theta_j = 0$ for $0 \le j \le m$ repeat many times:

gradient[j] = 0 for $0 \le j \le m$

for each training example (x, y):

for each $0 \le j \le m$:

 $gradient[j] +=$

$$
\left[y - \frac{1}{1 + e^{-\theta^T x}}\right] x_j
$$

 θ_i += η * gradient[j] for all 0 \leq j \leq m

- x_j is *j*-th feature of input var $x = (x_1, ..., x_m)$
- Insert $x_0 = 1$ before training
- Finish computing gradient before updating any part of θ
- Learning rate η is a constant you set before training

Testing: Classification with Logistic Regression

Training

Learn parameters
$$
θ = (θ_0, θ_1, ..., θ_m)
$$

via gradient
assert: $θ_j^{new} = θ_j^{old} + η \cdot \sum_{i=1}^{n} [y^{(i)} - σ(e^{old^T} x^{(i)})] x_j^{(i)}$

• Compute $\hat{y} = P(Y = 1 | X = x) = \sigma(\theta^T x) =$ • Classify instance as:

Testing

 $\begin{cases} 1 & \hat{y} > 0.5, \text{ equivalently } \theta^T x > 0 \\ 0 & \text{otherwise} \end{cases}$ 0 otherwise

Parameters θ_i are not updated during testing phase

1

 $1 + e^{-\theta^T x}$

Today's plan

Logistic Regression

- Chapter O: Background
- Chapter 1: Big Picture
- Chapter 2: Details
	- Chapter 3: Philosophy

Introducing notation \hat{y}

Logistic Regression

$$
\hat{y} = P(Y = 1 | \mathbf{X} = \mathbf{x}) = \sigma(\theta^T \mathbf{x})
$$

model:
$$
P(Y = y | X = x) = \begin{cases} \hat{y} & \text{if } y = 1 \\ 1 - \hat{y} & \text{if } y = 0 \end{cases}
$$

Prediction:

$$
\hat{Y} = \underset{y=\{0,1\}}{\arg \max} P(Y | \mathbf{X} = \mathbf{x}) = \begin{cases} 1 & \text{if } \hat{y} > 0.5 \\ 0 & \text{otherwise} \end{cases}
$$

Training: Learning the parameters via MLE

- 0. Add $x_0^{(l)} = 1$ to each $x^{(l)}$
- 1. Logistic Regression model:

$$
P(Y = 1 | \mathbf{X} = \mathbf{x}) = \hat{y}
$$

$$
\hat{y} = \sigma(\theta^T \mathbf{x})
$$

 $l=1$

- 2. Compute log-likelihood of training data: $LL(\theta) = \sum$ $l=1$ $\frac{n}{2}$ $(y^{(l)}\log\sigma\big(\theta^T\pmb{x^{(l)}}\big) + \big(1-y^{(l)}\big)\log\big(\mathbb{1}-\sigma\big(\theta^T\pmb{x^{(l)}}\big)$
- 3. Compute derivative of log-likelihood with respect to each θ_i , $j = 0, 1, ..., m$: $OLL(\theta)$ $\partial \theta_j$ $=$ \sum $\frac{n}{2}$ $y^{(i)} - \sigma(\theta^T x^{(i)})$ $x_j^{(i)}$ How did we get this log-likelihood function?

Log-likelihood of data

Logistic
\n*P(Y = y | X = x) =*

\n
$$
\begin{cases}\n\hat{y} & \text{if } y = 1 \\
1 - \hat{y} & \text{if } y = 0\n\end{cases}
$$
\nwhere $\hat{y} = \sigma(\theta^T x)$

\nmodel:

\n
$$
= (\hat{y})^y (1 - \hat{y})^{1-y}
$$
\n(see Bernoulli
\nMLE PMF)

Likelihood
of training data:
$$
L(\theta) = \prod_{i=1}^{n}
$$

$$
L(\theta) = \prod_{i=1}^n P(Y = y^{(i)} | X = x^{(i)}, \theta)
$$

Notes:

- Actually conditional likelihood
- Still correctly gets correct θ_{MLE} since X, θ independent
- See lecture notes

Log-likelihood of data

Logistic
\nRegression
\nmodel:
\n
$$
P(Y = y | X = x) = \begin{cases} \hat{y} & \text{if } y = 1 \\ 1 - \hat{y} & \text{if } y = 0 \end{cases}
$$
\nwhere $\hat{y} = \sigma(\theta^T x)$
\nmodel:
\n
$$
= (\hat{y})^y (1 - \hat{y})^{1-y}
$$
\n(see Bernoulli
\nMLE PMF)

Likelihood
of training data:
$$
L(\theta) = \prod_{i=1}^{n} P(Y = y^{(i)} | X = x^{(i)}, \theta) = \prod_{i=1}^{n} (\hat{y}^{(i)})^{y^{(i)}} (1 - \hat{y}^{(i)})^{1-y^{(i)}}
$$

Log-likelihood:
$$
LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \hat{y}^{(i)} + (1 - y^{(i)}) \log (1 - \hat{y}^{(i)})
$$

$$
= \sum_{i=1}^{n} y^{(i)} \log \sigma(\theta^T x^{(i)}) + (1 - y^{(i)}) \log (1 - \sigma(\theta^T x^{(i)}))
$$

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Training: Learning the parameters via MLE

- 0. Add $x_0^{(l)} = 1$ to each $x^{(l)}$
- 1. Logistic Regression model:

$$
P(Y=1|X=x)=\sigma(\theta^Tx)
$$

- 2. Compute log -likelihood $LL(\theta) = \sum_{k=1}^{n}$ of training data: $l=1$ $\frac{n}{2}$ $(y^{(l)}\log\sigma\big(\theta^T\pmb{x}^{(l)}\big) + \big(1-y^{(l)}\big)\log\big(\mathbb{1}-\sigma\big(\theta^T\pmb{x}^{(l)}\big)\big)$
- 3. Compute derivative of log-likelihood with respect to each θ_i , $j = 0, 1, ..., m$:

$$
\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^n \left[y^{(i)} - \sigma\left(\theta^T x^{(i)}\right) \right] x_j^{(i)}
$$

Stanford University 45 How did we get this gradient?

Aside: Sigmoid has a beautiful derivative

Sigmoid function: Derivative:

$$
\sigma(z) = \frac{1}{1 + e^{-z}}
$$

$$
\frac{d}{dz}\sigma(z) = \sigma(z)[1 - \sigma(z)]
$$

What is
$$
\frac{\partial}{\partial \theta_j} \sigma(\theta^T x)
$$
?
\nA. $\sigma(x_j)[1 - \sigma(x_j)]x_j$
\nB. $\sigma(\theta^T x)[1 - \sigma(\theta^T x)]x$
\nC. $\sigma(\theta^T x)[1 - \sigma(\theta^T x)]x_j$
\nD. $\sigma(\theta^T x)x_j[1 - \sigma(\theta^T x)x_j$
\nE. None/other

Aside: Sigmoid has a beautiful derivative

Compute gradient of log-conditional likelihood

where

Log-conditional
Likelihood:
$$
LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \sigma(\theta^T x^{(i)}) + (1 - y^{(i)}) \log (1 - \sigma(\theta^T x^{(i)}))
$$

Compute gradient of log-likelihood

$$
\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^n \frac{\partial}{\partial \theta_j} \left[y^{(i)} \log(\hat{y}^{(i)}) + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)}) \right] \qquad \text{Let } \hat{y}^{(i)} = \sigma(\theta^T \mathbf{x}^{(i)})
$$

$$
= \sum_{i=1}^n \frac{\partial}{\partial \hat{y}^{(i)}} \left[y^{(i)} \log(\hat{y}^{(i)}) + \left(1 - y^{(i)} \right) \log(1 - \hat{y}^{(i)}) \right] \cdot \frac{\partial \hat{y}^{(i)}}{\partial \theta_j}
$$

(Chain Rule)

$$
= \sum_{i=1}^{n} \left[y^{(i)} \frac{1}{\hat{y}^{(i)}} - (1 - y^{(i)}) \frac{1}{1 - \hat{y}^{(i)}} \right] \cdot \hat{y}^{(i)} (1 - \hat{y}^{(i)}) x_j^{(i)}
$$
 (calculus)

$$
= \sum_{i=1}^{n} \left[y^{(i)} - \hat{y}^{(i)} \right] x_j^{(i)} = \sum_{i=1}^{n} \left[y^{(i)} - \sigma \left(\theta^T x^{(i)} \right) \right] x_j^{(i)}
$$
 (simply)

Today's plan

Logistic Regression

- Chapter O: Background
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Logistic Regression Model

$$
P(Y = 1 | X = x) = \sigma(\theta^T x) \quad \text{where} \quad \theta^T x = \sum_{j=0}^m \theta_j x_j
$$

Logistic Regression is trying to fit a line that separates data instances where $y = 1$ from those where $y = 0$:

 \boldsymbol{m}

- We call such data (or functions generating the data *linearly separable*.
- Naïve Bayes is linear too, because there is no interaction between different features.

Data is often not linearly separable

- Not possible to draw a line that successfully separates all the $y = 1$ points (green) from the $y = 0$ points (red)
- Despite this fact, Logistic Regression and Naive Bayes still often work well in practice

Many tradeoffs in choosing an algorithm

Modeling goal $P(X, Y)$ $P(Y|X)$

Generative or discriminative? Generative: could use joint distribution to generate new points (but you might not need this extra effort)

Continuous input

Discrete input features?

Example 2011, the continued of the continues of the continuity of the continui Needs parametric form (e.g., Gaussian) or multinomial features)

> Yes, multi-value discrete data = multinomial $P(X_i|Y)$

Naïve Bayes **Logistic Regression**

Discriminative: just tries to discriminate $y = 0$ vs $y = 1$ (Cannot generate new points b/c no $P(X, Y)$

Stanford University 53 Multi-valued discrete data hard (e.g., if $X_i \in \{A, B, C\}$, not necessarily good to encode as ${1, 2, 3}$