25: Logistic Regression

David Varodayan March 6, 2020 Adapted from slides by Lisa Yan

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

<u>Problem Set 6</u>		<u>Regrades</u>
Due:	Wednesday 3/11	Pset 1 to 5 and
Covers:	Up to Lecture 25	Midterm regrades to
Extra Python Office Hours:	Saturday 3/7, 3-5PM	close on 3/11 at 1pm

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

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:

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

 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

 $f(x) = f\big(z(x)\big)$

 $\frac{\partial f(x)}{\partial x} = \frac{\partial f(z)}{\partial z} \frac{\partial z}{\partial x}$

Calculus Chain Rule

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Logistic Regression

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From Naïve Bayes to Logistic Regression

Classification goal: Model $P(Y \mid X)$

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

Predict the *Y* that is most likely given our observation *X*

Naïve Bayes Classifier:

- Estimate P(X | Y) and P(Y) because $\underset{v=\{0,1\}}{\arg \max} P(Y | X) = \underset{v=\{0,1\}}{\arg \max} P(X | Y) P(Y)$
- 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 $P(Y \mid X)$ directly?

• Welcome our friend: Logistic Regression!

Logistic Regression

 $\widehat{Y} = \underset{y = \{0,1\}}{\operatorname{arg\,max}} P(Y \mid X)$

Predict the *Y* that is most likely given our observation *X*

Logistic Regression Model

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

models $P(Y \mid X)$ directly

Logistic Regression



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

Slides courtesy of Chris Piech Stanford University 11

Logistic Regression Cartoon



θ parameter

Logistic Regression cartoon



Slides courtesy of Chris Piech Stanford University 13

Logistic Regression input/output





Slides courtesy of Chris Piech Stanford University 15



Slides courtesy of Chris Piech Stanford University 16





Slides courtesy of Chris Piech Stanford University 18

Different predictions for different inputs



Slides courtesy of Chris Piech Stanford University 19

Different predictions for different inputs



Slides courtesy of Chris Piech Stanford University 20

Parameters affect prediction



Slides courtesy of Chris Piech Stanford University 21

Parameters affect prediction



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Logistic Regression Model

$$\widehat{Y} = \underset{y \in \{0,1\}}{\operatorname{arg\,max}} P(Y \mid X)$$
 where

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

Predict the Y that is most likely given our observation X

models $P(Y \mid X)$ 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: $P(Y = 0 | \mathbf{X} = \mathbf{x}) = 1 - \sigma(\theta^T \mathbf{x})$

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Classifying using the sigmoid function

Logistic Regression Model $\hat{Y} = \underset{y=\{0,1\}}{\operatorname{arg max}} P(Y \mid X)$ where $P(Y = 1 \mid X = x) = \sigma \left(\theta_0 + \sum_{j=1}^m \theta_j x_j \right)$



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

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



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

- A. If $\sigma(\theta^T \mathbf{x}) > 1 \sigma(\theta^T \mathbf{x})$
- 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 $\theta = (\theta_0, \theta_1, \dots, \theta_m)$.

- 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:

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

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

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

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

Training: Learning the parameters via MLE

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

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

2. Compute log-likelihood $LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \sigma(\theta^T x^{(i)}) + (1 - y^{(i)}) \log (1 - \sigma(\theta^T x^{(i)}))$ of training data:

3. Compute derivative of log-likelihood with respect to each θ_j , j = 0, 1, ..., m:

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

Gradient Ascent

Review

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





Logistic regression $LL(\theta)$ is convex

Training: Gradient ascent step

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

Repeat many times:

For all thetas:

$$\theta_{j}^{\text{new}} = \theta_{j}^{\text{old}} + \eta \cdot \frac{\partial LL(\theta^{\text{old}})}{\partial \theta_{j}^{\text{old}}}$$

$$= \theta_{j}^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \left[y^{(i)} - \sigma \left(\theta^{\text{old}^{T}} \boldsymbol{x}^{(i)} \right) \right] x_{j}^{(i)}$$

What does this look like in code?

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

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

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

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

 $\theta_j += \eta * \text{gradient}[j] \text{ for all } 0 \le j \le m$

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

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:
```

// update gradient[j] for
// current (x,y) example

 $\theta_j += \eta * \text{gradient}[j] \text{ for all } 0 \le j \le m$

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

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

 $\theta_j += \eta * \text{gradient}[j] \text{ for all } 0 \le j \le m$

What are important implementation details?

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

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

 $\theta_j += \eta * \text{gradient}[j] \text{ for all } 0 \le j \le m$

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

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

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] +=
$$\begin{bmatrix} y - \frac{1}{1 + e^{-\theta^T x}} x_j \end{bmatrix}$$

 $\theta_j += \eta * \text{gradient}[j] \text{ for all } 0 \le j \le m$

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

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

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] +=

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

 $\theta_j += \eta * \text{gradient}[j] \text{ for all } 0 \le j \le m$

- 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

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

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

 $\theta_j += \eta$ gradient[j] for all $0 \le j \le m$

- 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

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

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

 $\theta_j += \eta * \text{gradient}[j] \text{ for all } 0 \le j \le m$

• 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
$$\theta = (\theta_0, \theta_1, ..., \theta_m)$$

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

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

Testing

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

Parameters θ_i are <u>not</u> updated during testing phase

Today's plan

Logistic Regression

- Chapter O: Background
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Introducing notation \hat{y}

Logistic Regression model:

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

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

Prediction:

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

Training: Learning the parameters via MLE

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

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

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

Log-likelihood of data

Logistic
Regression
model:
$$P(Y = y | X = x) = \begin{cases} \hat{y} & \text{if } y = 1 \\ 1 - \hat{y} & \text{if } y = 0 \end{cases}$$
where $\hat{y} = \sigma(\theta^T x)$ $= (\hat{y})^y (1 - \hat{y})^{1-y}$ (see Bernoulli
MLE PMF)

Likelihood
$$L(\theta) = 0$$
 of training data:

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

Notes:

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

Log-likelihood of data

Logistic
Regression
model:
$$P(Y = y | X = x) = \begin{cases} \hat{y} & \text{if } y = 1 \\ 1 - \hat{y} & \text{if } y = 0 \end{cases}$$
where $\hat{y} = \sigma(\theta^T x)$ $= (\hat{y})^y (1 - \hat{y})^{1-y}$ (see Bernoulli
MLE 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:
$$LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \hat{y}^{(i)} + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)})$$
$$= \sum_{i=1}^{n} y^{(i)} \log \sigma(\theta^T \boldsymbol{x}^{(i)}) + (1 - y^{(i)}) \log(1 - \sigma(\theta^T \boldsymbol{x}^{(i)}))$$
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Training: Learning the parameters via MLE

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

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

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

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

How did we get this gradient? Stanford University 45

Aside: Sigmoid has a beautiful derivative

Sigmoid function:

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

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

Derivative:

What is
$$\frac{\partial}{\partial \theta_j} \sigma(\theta^T \mathbf{x})$$
?
A. $\sigma(x_j) [1 - \sigma(x_j)] x_j$
B. $\sigma(\theta^T \mathbf{x}) [1 - \sigma(\theta^T \mathbf{x})] \mathbf{x}$
C. $\sigma(\theta^T \mathbf{x}) [1 - \sigma(\theta^T \mathbf{x})] x_j$
D. $\sigma(\theta^T \mathbf{x}) x_j [1 - \sigma(\theta^T \mathbf{x}) x_j]$
E. None/other

Aside: Sigmoid has a beautiful derivative



Compute gradient of log-conditional likelihood



Compute gradient of log-likelihood

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

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

(Chain Rule)

$$= \sum_{i=1}^{n} \left[y^{(i)} \frac{1}{\hat{y}^{(i)}} - (1 - y^{(i)}) \frac{1}{1 - \hat{y}^{(i)}} \right] \cdot \hat{y}^{(i)} (1 - \hat{y}^{(i)}) x_j^{(i)} \qquad \text{(calculus)}$$
$$= \sum_{i=1}^{n} \left[y^{(i)} - \hat{y}^{(i)} \right] x_j^{(i)} \qquad = \sum_{i=1}^{n} \left[y^{(i)} - \sigma(\theta^T \boldsymbol{x}^{(i)}) \right] x_j^{(i)} \qquad \text{(simplify)}$$

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Logistic Regression

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Logistic Regression Model

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

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



m

- We call such data (or functions generating the data <u>linearly separable</u>.
- 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

Generative or discriminative?

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

Naïve Bayes

 $P(\boldsymbol{X},\boldsymbol{Y})$

Continuous input features?

Discrete input features?

Needs parametric form (e.g., Gaussian) or discretized buckets (for multinomial features)

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

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

Yes, easily

Multi-valued discrete data hard(e.g., if $X_i \in \{A, B, C\}$, notnecessarily good to encode as $\{1, 2, 3\}$ Stanford University 53