Conditional Probability Models

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Maximum Likelihood Recap

Maximum Likelihood Estimation

Suppose we have a parametric model $\{p(y;\theta) \mid \theta \in \Theta\}$ and a sample $\mathcal{D} = \{y_1, \ldots, y_n\}$.

Definition

The maximum likelihood estimator (MLE) for θ in the model $\{p(y,\theta) \mid \theta \in \Theta\}$ is

$$\hat{\theta} = \underset{\theta \in \Theta}{\arg\max}\, L_{\mathcal{D}}(\theta) = \underset{\theta \in \Theta}{\arg\max} \prod_{i=1}^{n} p(y_i;\theta).$$

In practice, we prefer to work with the **log likelihood**. Same maximum but

$$\log p(\mathcal{D};\theta) = \sum_{i=1}^{n} \log p(y_i;\theta),$$

and sums are easier to work with than products.

Maximum Likelihood Estimation

- Finding the MLE is an optimization problem.
- For some model families, calculus gives closed form for MLE.
- Can also use numerical methods we know (e.g. SGD).
- Note: In certain situations, the MLE may not exist.
  - But there is usually a good reason for this.
- e.g. Gaussian family $\left\{\mathcal{N}(\mu, \sigma^2 \mid \mu \in \mathbf{R}, \sigma^2 > 0\right\}$, Single observation y.
  - Take $\mu = y$ and $\sigma^2 \to 0$ drives likelihood to infinity. MLE doesn't exist.

Bernoulli Regression

Probabilistic Binary Classifiers

- Setting: $\mathcal{X} = \mathbf{R}^d$, $\mathcal{Y} = \{0,1\}$
- For each x, need to predict a distribution on $\mathcal{Y} = \{0,1\}$.
- What kind of parametric distribution could be supported on $\{0,1\}$?
- Not a lot of choices....
- Bernoulli!
- For each x,
    - predict the Bernoulli parameter $\theta = p(y = 1 \mid x)$.

Linear Probabilistic Classifiers

- Setting: $\mathcal{X} = \mathbf{R}^d$, $\mathcal{Y} = \{0, 1\}$
- Want prediction function $x \mapsto \theta = p(y = 1 \mid x)$.
- We need $\theta \in [0, 1]$.
- For a "linear method", we can write this in two steps:

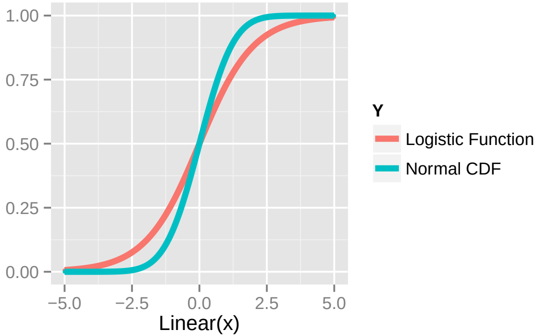
$$\underbrace{x}_{\in \mathbf{R}^D} \mapsto \underbrace{w^T x}_{\in \mathbf{R}} \mapsto \underbrace{f(w^T x)}_{\in [0,1]},$$

  where $f : \mathbf{R} \to [0, 1]$ is called the **transfer** or **inverse link** function.
- Probability model is then

$$p(y = 1 \mid x) = f(w^T x)$$

Inverse Link Functions

- Two commonly used "inverse link" functions to map from $w^T x$ to θ:



- Logistic function $\Longrightarrow$ Logistic Regression
- Normal CDF $\Longrightarrow$ Probit Regression

Learning

- $\mathcal{X} = \mathbf{R}^d$
- $\mathcal{Y} = \{0, 1\}$
- $\mathcal{A} =, 1$ (Representing Bernoulli(θ) distributions by $\theta \in [0, 1]$)
- $\mathcal{H} = \left\{ x \mapsto f\left(w^T x\right) \mid w \in \mathbf{R}^d \right\}$
- We can choose w using maximum likelihood...

Bernoulli Regression: Likelihood Scoring

- Suppose we have data $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$, iid.
- Compute the model likelihood for $\mathcal{D}$:

$$
\begin{aligned}
p_w(\mathcal{D}) &= \prod_{i=1}^{n} p_w(y_i \mid x_i) \text{ [by independence]} \\
&= \prod_{i=1}^{n} \left[f(w^T x_i) \right]^{y_i} \left[1 - f(w^T x_i) \right]^{1-y_i}.
\end{aligned}
$$

- Huh? Remember $y_i \in \{0, 1\}$.
- Easier to work with the log-likelihood:

$$
\log p_w(\mathcal{D}) = \sum_{i=1}^{n} y_i \log f(w^T x_i) + (1 - y_i) \log \left[1 - f(w^T x_i) \right]
$$

Bernoulli Regression: MLE

- Maximum Likelihood Estimation (MLE) finds w maximizing $\log p_w(\mathcal{D})$.
- Equivalently, minimize the objective function

$$J(w) = -\left[\sum_{i=1}^{n} y_i \log f(w^T x_i) + (1-y_i)\log\left[1-f(w^T x_i)\right]\right]$$

- For differentiable f,
  - $J(w)$ is differentiable, and we can use our standard tools.
- Homework: Derive the SGD step directions for logistic regression.

Multinomial Logistic Regression

Multinomial Logistic Regression

- Setting: $\mathcal{X} = \mathbf{R}^d$, $\mathcal{Y} = \{1, \ldots, k\}$
- The numbers $(\theta_1, \ldots, \theta_k)$ where $\sum_{c=1}^{k} \theta_c = 1$ represent a
  - "**multinoulli**" or "**categorical**" distribution.
- For each x, we want to produce a distribution on the k classes.
- That is, for each x and each $y \in \{1, \ldots, y\}$, we want to produce a probability

$$p(y \mid x) = \theta_y,$$

where $\sum_{y=1}^{K} \theta_y = 1$.

Multinomial Logistic Regression: Classic Setup

- From each x, we compute a linear score function for each class:

$$x \mapsto (\langle w_1, x\rangle, \ldots, \langle w_k, x\rangle) \in \mathbf{R}^k$$

- We need to map this $\mathbf{R}^k$ vector into a probability vector.
- Use the **softmax function:**

$$(\langle w_1, x\rangle, \ldots, \langle w_k, x\rangle) \mapsto \left(\frac{\exp\left(w_1^T x\right)}{\sum_{c=1}^K \exp\left(w_c^T x\right)}, \ldots, \frac{\exp\left(w_k^T x\right)}{\sum_{c=1}^K \exp\left(w_c^T x\right)} \right)$$

- If $\theta \in \mathbf{R}^k$ is the output of the softmax, note that

$$\begin{aligned} \theta_i &> 0 \\ \sum_{i=1}^k \theta_i &= 1 \end{aligned}$$

Multinomial Logistic Regression: Classic Setup

- Putting this together, we write multinomial logistic regression as

$$p(y \mid x) = \frac{\exp\left(w_y^T x\right)}{\sum_{c=1}^{K} \exp\left(w_c^T x\right)},$$

  where we've introduced parameter vectors $w_1, \ldots, w_k \in \mathbf{R}^d$.
- Can view $x \mapsto w_y^T x$ as the score for class y, for $y \in \{1, \ldots, k\}$.
- We can also "flatten" this as we did for multiclass classification.
  - Introduce a class-sensitive feature vector $\Psi(x, y) \in \mathbf{R}^{dk}$
  - Parameter vector $w \in \mathbf{R}^{dk}$.
- The log of this likelihood is concave and straightforward to optimize.

Poisson Regression

Poisson Regression: Setup

- Input space $\mathcal{X} = \mathbf{R}^d$, Output space $\mathcal{Y} = \{0,1,2,3,4,\ldots\}$
- Hypothesis space consists of functions $f : x \mapsto \text{Poisson}\left(\lambda(x)\right)$.
  - That is, for each x, $f(x)$ returns a Poisson with mean $\lambda(x) \in (0,\infty)$.
  - What function?
- Recall $\lambda > 0$.
- In Poisson regression, x enters **linearly:** $x \mapsto w^T x \mapsto \lambda = f(w^T x)$.
- Standard approach is to take
$$\lambda(x) = \exp\left(w^T x\right),$$
  for some parameter vector w.
- Note that range of $\lambda(x) = (0,\infty)$, (appropriate for the Poisson parameter).

Poisson Regression: Likelihood Scoring

- Suppose we have data $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$.
- Recall the log-likelihood for Poisson is:

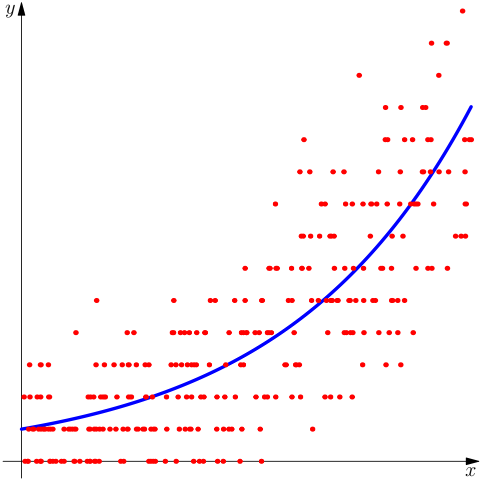
$$\log p(\mathcal{D}, \lambda) = \sum_{i=1}^{n} \left[y_i \log \lambda - \lambda - \log (y_i!) \right]$$

- Plugging in $\lambda(x) = \exp\left(w^T x\right)$, we get

$$\begin{aligned} \log p(\mathcal{D}, \lambda) &= \sum_{i=1}^{n} \left[y_i \log \left[\exp\left(w^T x_i\right) \right] - \exp\left(w^T x_i\right) - \log (y_i!) \right] \\ &= \sum_{i=1}^{n} \left[y_i w^T x_i - \exp\left(w^T x_i\right) - \log (y_i!) \right] \end{aligned}$$

- Maximize this w.r.t. w to find the Poisson regression.
- No closed form for optimum, but it's concave, so easy to optimize.

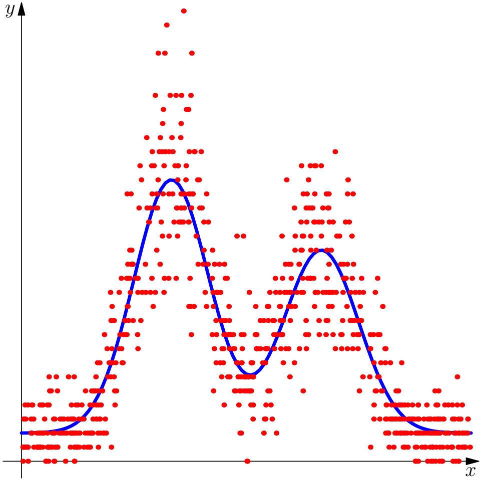
Poisson Regression Example



e.g. Phone call counts per day for a startup company, over 300 days.

What About Nonlinear Score Functions

Poisson Count Example



Let's Use Gradient Boosting

- Recall the log-likelihood for Poisson regression

$$\log p(\mathcal{D}, \lambda) \quad = \quad \sum_{i=1}^{n} \left[y_i w^T x_i - \exp\left(w^T x_i\right) - \log\left(y_i!\right) \right]$$

- Let's replace $w^T x$ by a general function $f(x)$:

$$J(f) = \sum_{i=1}^{n} \left[y_i f(x_i) - \exp\left(f(x_i)\right) - \log\left(y_i!\right) \right]$$

Generalized Regression

Generalized Regression as Statistical Learning

- Input space $\mathcal{X}$
- Output space $\mathcal{Y}$
- All pairs (x, y) are independent with distribution $P_{\mathcal{X}\times\mathcal{Y}}$.
- **Action space** $\mathcal{A} = \{p(y) \mid p$ is a probability density or mass function on $\mathcal{Y}\}$.
- Hypothesis spaces contain decision functions $f : \mathcal{X} \to \mathcal{A}$.
    - Given an $x \in \mathcal{X}$, predict a probability distribution $p(y)$ on $\mathcal{Y}$.

A Note on Notation

- Hypothesis spaces contain decision functions $f : \mathcal{X} \to \mathcal{A}$.
  - Given an $x \in \mathcal{X}$, predict a probability distribution $p(y)$ on $\mathcal{Y}$.
- Let f be a decision function.
  - In regression, $f(x) \in \mathbf{R}$
  - In hard classification, $f(x) \in \{-1, 1\}$
  - For generalized regression, $f(x) \in ?$
- $f(x)$ is a PDF or PMF on $\mathcal{Y}$.
- If $p = f(x)$, can evaluate $p(y)$ for predicted probability of y.
- Or just write $[f(x)](y)$ or even $f(x)(y)$.

Generalized Regression as Statistical Learning

- The risk of decision function $f : \mathcal{X} \to \mathcal{A}$

$$R(f) = -\mathbb{E}_{x,y} \log [f(x)](y),$$

where $f(x)$ is a PDF or PMF on $\mathcal{Y}$, and we're evaluating it on Y.

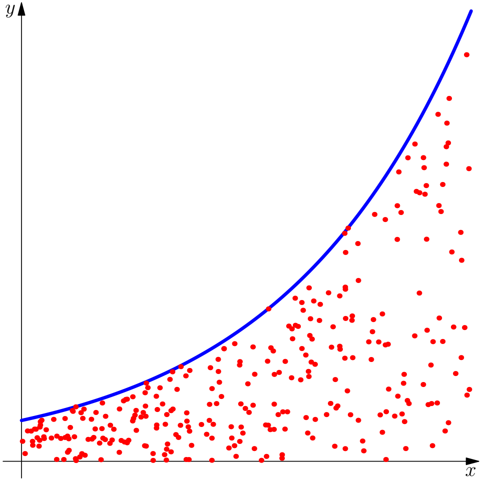
- The empirical risk of f for a sample $\mathcal{D} = \{y_1, \ldots, y_n\} \in \mathcal{Y}$ is

$$\hat{R}(f) = -\sum_{i=1}^{n} \log [f(x_i)](y_i).$$

This is called the negative **conditional log-likelihood**.

How General A Distribution Can We Use?

Uniform Example?



- Can't use it in GBM: likelihood not differentiable (not continuous)