Conditional Probability Models

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Contents

Overview and Disclaimer

Linear Probabilistic Models vs GLMs

- Today we'll be talking about **linear probabilistic models**.
- Most books and software libraries related to this topic are actually about
  - **generalized linear models** (GLMs).
- GLMs are a special case of what we're talking about today.
- They're "special" because
  - they're a restriction of our setting
  - there are theorems for GLMs that we don't have in our more general setting
- However, a full development of GLMs requires a fair bit of additional machinery.
  - In particular, **exponential families** – a topic from intermediate statistics courses.
- Exponential families are wonderful, but I don't believe they're worth the payoff at this level.
- For practical purposes, our development will be more than sufficient (and simpler).

Modeling Conditional Distributions

Conditional Distribution Estimation (Generalized Regression)

- Given x, predict *probability distribution* $p(y)$
- How do we represent the probability distribution?
- We'll consider *parametric families* of distributions.
  - distribution represented by parameter vector
- Examples:
  1. Logistic regression (Bernoulli distribution)
  2. Probit regression (Bernoulli distribution)
  3. Poisson regression (Poisson distribution)
  4. Linear regression (Normal distribution, fixed variance)
  5. Generalized Linear Models (GLM) (encompasses all of the above)
  6. Generalized Additive Models (GAM) (popular in statistics community)
  7. Gradient Boosting Machines (GBM) / AnyBoost [in a few weeks]
  8. Almost all neural network models used in practice (though this is not their essential feature)

Bernoulli Regression

Probabilistic Binary Classifiers

- Setting: $\mathcal{X} = \mathbf{R}^d$, $\mathcal{Y} = \{0,1\}$
- For each x, need to predict a distribution on $\mathcal{Y} = \{0,1\}$.
- How can we define a distribution supported on $\{0,1\}$?
- Sufficient to specify the **Bernoulli parameter** $\theta = p(y=1)$.
- We can refer to this distribution as $\text{Bernoulli}(\theta)$.

Linear Probabilistic Classifiers

- Setting: $\mathcal{X} = \mathbf{R}^d$, $\mathcal{Y} = \{0, 1\}$
- Want prediction function to map each $x \in \mathbf{R}^d$ to $\theta \in [0, 1]$.
- We first **extract information** from $x \in \mathbf{R}^d$ and summarize in a single number.
    - That number is analogous to the **score** in classification.
- For a **linear method**, this extraction is done with a linear function:

$$\underbrace{x}_{\in \mathbf{R}^d} \mapsto \underbrace{w^T x}_{\in \mathbf{R}}$$

- As usual, $x \mapsto w^T x$ will include affine functions if we include a constant feature in x.
- $w^T x$ is called the **linear predictor.**
- Still need to map this to $[0, 1]$.

The Transfer Function

- Need a function to map the linear predictor in $\mathbf{R}$ to $[0,1]$:

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

  where $f : \mathbf{R} \to [0,1]$. We'll call f the **transfer** function.

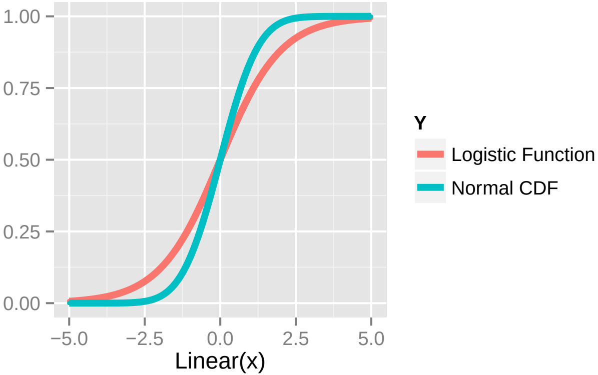
- So prediction function is $x \mapsto f(w^T x)$.

Terminology Alert

In generalized linear models (GLMs), if θ is the distribution mean, then f is called the **response function** or **inverse link** function. We avoid that terminology, since we do not require θ to be the distribution mean.

Transfer Functions for Bernoulli

- Two commonly used transfer functions to map from $w^T x$ to θ:



- Logistic function: $f(\eta) = \frac{1}{1+e^{-\eta}} \implies$ Logistic Regression
- Normal CDF $f(\eta) = \int_{-\infty}^{\eta} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \implies$ Probit Regression

Learning

- Input space $\mathcal{X} = \mathbf{R}^d$
- Outcome space $\mathcal{Y} = \{0, 1\}$
- Action space $\mathcal{A} = [0, 1]$ (Representing Bernoulli(θ) distributions by $\theta \in [0, 1]$)
- Hypothesis space $\mathcal{F} = \left\{x \mapsto f(w^T x) \mid w \in \mathbf{R}^d\right\}$
- Parameter space $\mathbf{R}^d$ (Each prediction function represented by $w \in \mathbf{R}^d$.)
- We can choose w using maximum likelihood...

Bernoulli Regression: Likelihood Scoring Example

- Suppose we have $\mathcal{X} = \mathbf{R}$ and data $\mathcal{D}$: $(-3,0),(0,0),(1,1),(2,0) \in \mathbf{R} \times \{0,1\}$
- Our model is $p(y=1 \mid x) = f(wx)$, for some parameter $w \in \mathbf{R}$.
- Compute the likelihood for each observation:

x	y	wx	$\theta = f(wx)$	$\hat{p}(y)$
-3	0	$-3w$	$f(-3w)$	$1-f(-3w)$
0	0	0	$f(0)$	$1-f(0)$
1	1	w	$f(w)$	$f(w)$
2	0	$2w$	$f(2w)$	$1-f(2w)$

- The likelihood of w for the data $\mathcal{D}$ is

$$p(\mathcal{D};w) = [1-f(-3w)] \cdot [1-f(0)] \cdot [f(w)] \cdot [1-f(2w)]$$

- The MLE $\hat{w}$ is the $w \in \mathbf{R}$ maximizing $p(\mathcal{D};w)$ for the given $\mathcal{D}$.

A Clever Way To Write $\hat{p}(y \mid x; w)$

- For a given $x, w \in \mathbf{R}^d$ and $y \in \{0,1\}$, the likelihood of w for (x,y) is

$$p(y \mid x; w) = \begin{cases} f(w^T x) & y = 1 \\ 1 - f(w^T x) & y = 0 \end{cases}$$

- It will be convenient to write this as

$$p(y \mid x; w) = \left[f(w^T x)\right]^y \left[1 - f(w^T x)\right]^{1-y},$$

which is obvious as long as you remember $y \in \{0,1\}$.

Bernoulli Regression: Likelihood Scoring

- Suppose we have data $\mathcal{D}: (x_1, y_1), \ldots, (x_n, y_n) \in \mathbf{R}^d \times \{0,1\}$.
- The likelihood of $w \in \mathbf{R}^d$ for data $\mathcal{D}$ is

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

- Easier to work with the log-likelihood:

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

Bernoulli Regression: MLE

- Maximum Likelihood Estimation (MLE) finds w maximizing $\log p(\mathcal{D}; w)$.
- Equivalently, minimize the **negative log-likelihood** 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.
- Possible Homework: Derive the SGD step directions for logistic regression and [harder] probit regression.

Poisson Regression

Poisson Regression: Setup

- Input space $\mathcal{X} = \mathbf{R}^d$, Output space $\mathcal{Y} = \{0, 1, 2, 3, 4, \ldots\}$
- In Poisson regression, prediction functions produce a Poisson distribution.
  - Represent Poisson(λ) distribution by the mean parameter $\lambda \in (0, \infty)$.
- Action space $\mathcal{A} = (0, \infty)$
- In Poisson regression, x enters **linearly:** $x \mapsto \underbrace{w^T x}_{\mathbf{R}} \mapsto \lambda = \underbrace{f(w^T x)}_{(0,\infty)}$.
- What can we use as the transfer function $f : \mathbf{R} \to (0, \infty)$?

Poisson Regression: Transfer Function

- In Poisson regression, x enters **linearly:**

$$x \mapsto \underbrace{w^T x}_{\mathbf{R}} \mapsto \lambda = \underbrace{f(w^T x)}_{(0,\infty)}.$$

- Standard approach is to take

$$f(w^T x) = \exp\left(w^T x\right).$$

- Note that range of $f(w^T x) \in (0, \infty)$, (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 parameter λ_i on observation y_i is:

$$\log p(y_i; \lambda_i) \quad = \quad [y_i \log \lambda_i - \lambda_i - \log(y_i!)]$$

- Now we want to predict a different λ_i for every x_i with the model

$$\lambda_i = f(w^T x_i) = \exp\left(w^T x_i\right).$$

- The likelihood for w on the full dataset $\mathcal{D}$ is

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

Poisson Regression: MLE

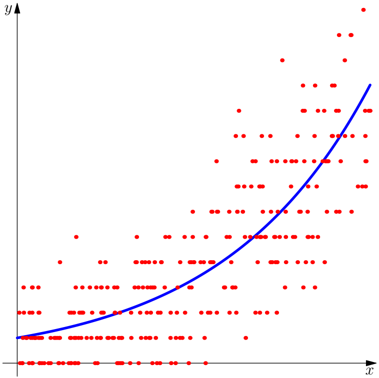
- To get MLE, need to maximize

$$J(w)=\log p(\mathcal{D};w)=\sum_{i=1}^{n}\left[y_iw^Tx_i-\exp\left(w^Tx_i\right)-\log\left(y_i!\right)\right]$$

over $w\in\mathbf{R}^d$.

- No closed form for optimum, but it's concave, so easy to optimize.

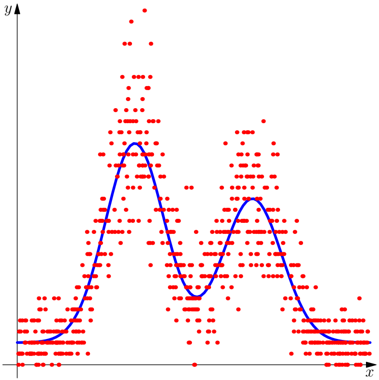
Poisson Regression Example



- Example application: Phone call counts per day for a startup company, over 300 days.
- Blue line is mean $\mu(x) = \exp(wx)$, some $w \in \mathbf{R}$. (Only linear part $x \mapsto wx$ is learned.)
- Samples are $y_i \sim \text{Poisson}(wx_i)$.

Plot courtesy of Brett Bernstein.

Nonlinear Score Function: Sneak Preview



- Blue line is mean $\mu(x) = \exp(f(x))$, for some nonlinear f learned from data.
- Samples are $y_i \sim \text{Poisson}(\exp(f(x_i)))$.
- We can do this with gradient boosting and neural networks, coming up in a few weeks.

Plot courtesy of Brett Bernstein.

Conditional Gaussian Regression

Gaussian Linear Regression

- Input space $\mathcal{X} = \mathbf{R}^d$, Output space $\mathcal{Y} = \mathbf{R}$
- In Gaussian regression, prediction functions produce a distribution $\mathcal{N}(\mu, \sigma^2)$.
  - Assume σ^2 is known.
- Represent $\mathcal{N}(\mu, \sigma^2)$ by the mean parameter $\mu \in \mathbf{R}$.
- Action space $\mathcal{A} = \mathbf{R}$
- In Gaussian linear regression, x enters **linearly:** $x \mapsto \underbrace{w^T x}_{\mathbf{R}} \mapsto \mu = \underbrace{f(w^T x)}_{\mathbf{R}}$.
- Since $\mu \in \mathbf{R}$, we can take the identity transfer function: $f(w^T x) = w^T x$.

Gaussian Regression: Likelihood Scoring

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

$$p(\mathcal{D}; w) = \prod_{i=1}^{n} p(y_i \mid x_i; w) \text{ [by independence]}$$

- Maximum Likelihood Estimation (MLE) finds w maximizing $\hat{p}(\mathcal{D}; w)$.
- Equivalently, maximize the data log-likelihood:

$$w^* = \underset{w \in \mathbf{R}^d}{\arg\max} \sum_{i=1}^{n} \log p(y_i \mid x_i; w)$$

- Let's start solving this!

Gaussian Regression: MLE

- The conditional log-likelihood is:

$$\begin{aligned}
& \sum_{i=1}^{n} \log p(y_i \mid x_i; w) \\
= \quad & \sum_{i=1}^{n} \log \left[\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(y_i - w^T x_i)^2}{2\sigma^2} \right) \right] \\
= \quad & \underbrace{\sum_{i=1}^{n} \log \left[\frac{1}{\sigma\sqrt{2\pi}} \right]}_{\text{independent of } w} + \sum_{i=1}^{n} \left(-\frac{(y_i - w^T x_i)^2}{2\sigma^2} \right)
\end{aligned}$$

- MLE is the w where this is maximized.
- Note that σ^2 is irrelevant to finding the maximizing w.
- Can drop the negative sign and make it a minimization problem.

Gaussian Regression: MLE

- The MLE is

$$w^* = \underset{w \in \mathbf{R}^d}{\arg\min} \sum_{i=1}^{n} (y_i - w^T x_i)^2$$

- This is exactly the objective function for least squares.
- From here, can use usual approaches to solve for w^* (SGD, linear algebra, calculus, etc.)

Multinomial Logistic Regression

Multinomial Logistic Regression

- Setting: $\mathcal{X} = \mathbf{R}^d$, $\mathcal{Y} = \{1, \ldots, k\}$
- For each x, we want to produce a distribution on k classes.
- Such a distribution is called a "**multinoulli**" or "**categorical**" distribution.
- Represent categorical distribution by probability vector $\theta = (\theta_1, \ldots, \theta_k) \in \mathbf{R}^k$:
  - $\sum_{i=1}^{k} \theta_i = 1$ and $\theta_i \geqslant 0$ for $i = 1, \ldots, k$ (i.e. θ represents a **distribution**) and
- So $\forall y \in \{1, \ldots, k\}$, $p(y) = \theta_y$.

Multinomial Logistic Regression

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

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

  where we've introduced parameter vectors $w_1, \ldots, w_k \in \mathbf{R}^d$.
- We need to map this $\mathbf{R}^k$ vector of scores into a probability vector.
- Consider the **softmax function**:

$$(s_1, \ldots, s_k) \mapsto \theta = \left(\frac{e^{s_1}}{\sum_{i=1}^k e^{s_i}}, \ldots, \frac{e^{s_k}}{\sum_{i=1}^k e^{s_i}} \right).$$

- Note that $\theta \in \mathbf{R}^k$ and

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

Multinomial Logistic Regression

- Say we want to get the predicted categorical distribution for a given $x \in \mathbf{R}^d$.
- First compute the scores ($\in \mathbf{R}^k$) and then their softmax:

$$x \mapsto (\langle w_1, x \rangle, \ldots, \langle w_k, x \rangle) \mapsto \theta = \left(\frac{\exp\left(w_1^T x\right)}{\sum_{i=1}^k \exp\left(w_i^T x\right)}, \ldots, \frac{\exp\left(w_k^T x\right)}{\sum_{i=1}^k \exp\left(w_i^T x\right)} \right)$$

- We can write the conditional probability for any $y \in \{1, \ldots, k\}$ as

$$p(y \mid x; w) = \frac{\exp\left(w_y^T x\right)}{\sum_{i=1}^k \exp\left(w_i^T x\right)}.$$

Multinomial Logistic Regression

- Putting this together, we write multinomial logistic regression as

$$p(y \mid x; w) = \frac{\exp\left(w_y^T x\right)}{\sum_{i=1}^k \exp\left(w_i^T x\right)}.$$

- How do we do learning here? What parameters are we estimating?
- Our model is specified once we have $w_1, \dots, w_k \in \mathbf{R}^d$.
- Find parameter settings maximizing the log-likelihood of data $\mathcal{D}$.
- This objective function is concave in w's and straightforward to optimize.

Maximum Likelihood as ERM

Conditional Probability Modeling as Statistical Learning

- Input space $\mathcal{X}$
- Outcome space $\mathcal{Y}$
- All pairs (x, y) are independent with distribution $P_{\mathcal{X}\times\mathcal{Y}}$.
- **Action space** $\mathcal{A} = \{p(y) \mid p \text{ is a probability density or mass function on } \mathcal{Y}\}$.
- Hypothesis space $\mathcal{F}$ contains decision functions $f : \mathcal{X} \to \mathcal{A}$.
- Maximum likelihood estimation for dataset $\mathcal{D} = ((x_1, y_1), \ldots, (x_n, y_n))$ is

$$\hat{f}_{\text{MLE}} \in \underset{f \in \mathcal{F}}{\arg\max} \sum_{i=1}^{n} \log\left[f(x_i)(y_i)\right]$$

Exercise

Write the MLE optimization as empirical risk minimization. What's the loss?

Conditional Probability Modeling as Statistical Learning

- Take loss $\ell : \mathcal{A} \times \mathcal{Y} \to \mathbf{R}$ for a predicted PDF or PMF $p(y)$ and outcome y to be

$$\ell(p, y) = -\log p(y)$$

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

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

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

Conditional Probability Modeling as Statistical Learning

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

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

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

- Thus for the negative log-likelihood loss, ERM and MLE are equivalent