Conditional Probability Models

David S. Rosenberg

New York University

February 27, 2018

Contents

- Overview and Disclaimer
- Modeling Conditional Distributions
- Bernoulli Regression
- Poisson Regression
- Conditional Gaussian Regression
- Multinomial Logistic Regression
- Maximum Likelihood as ERM

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:
 - Logistic regression (Bernoulli distribution)
 - 2 Probit regression (Bernoulli distribution)
 - 3 Poisson regression (Poisson distribution)
 - Linear regression (Normal distribution, fixed variance)
 - Generalized Linear Models (GLM) (encompasses all of the above)
 - Generalized Additive Models (GAM) (popular in statistics community)
 - Gradient Boosting Machines (GBM) / AnyBoost [in a few weeks]
 - 4 Almost all neural network models used in practice (though this is not their essential feature)

Bernoulli Regression

Probabilistic Binary Classifiers

- Setting: $X = \mathbb{R}^d$, $\mathcal{Y} = \{0, 1\}$
- 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 Bernoulli(θ).

Linear Probabilistic Classifiers

- Setting: $X = \mathbb{R}^d$, $y = \{0, 1\}$
- Want prediction function to map each $x \in \mathbb{R}^d$ to $\theta \in [0,1]$.
- We first extract information from $x \in \mathbb{R}^d$ 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 R to [0, 1]:

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

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

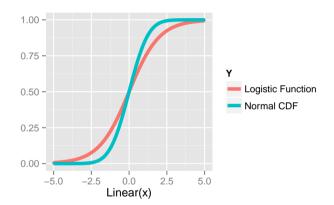
• So prediction function is $x \mapsto f(w^T x)$.

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

Learning

- Input space $\mathfrak{X} = \mathbf{R}^d$
- Outcome space $\mathcal{Y} = \{0, 1\}$
- Action space $\mathcal{A} = [0,1]$ (Representing Bernoulli(θ) distributions by $\theta \in [0,1]$)
- Hypothesis space $\mathcal{F} = \{x \mapsto f(w^T x) \mid w \in \mathbb{R}^d\}$
- Parameter space \mathbb{R}^d (Each prediction function represented by $w \in \mathbb{R}^d$.)
- 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 $w \in \mathbb{R}$.
- Compute the likelihood for each observation:

X	у	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	2 <i>w</i>	f(2w)	1-f(2w)

• The likelihood of w for the data \mathfrak{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 $x, w \in \mathbb{R}^d$ 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

$$p(y | x; w) = [f(w^T x)]^y [1 - f(w^T x)]^{1-y},$$

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

Bernoulli Regression: Likelihood Scoring

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

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

• Easier to work with the log-likelihood:

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

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 $\mathfrak{X} = \mathbb{R}^d$, Output space $\mathfrak{Y} = \{0, 1, 2, 3, 4, \dots\}$
- In Poisson regression, prediction functions produce a Poisson distribution.
 - Represent Poisson(λ) distribution by the mean parameter $\lambda \in (0, \infty)$.
- Action space $A = (0, \infty)$
- In Poisson regression, x enters **linearly**: $x \mapsto \underbrace{w^T x}_{R} \mapsto \lambda = \underbrace{f(w^T x)}_{(0,\infty)}$.
- 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

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

• Note that range of $f(w^Tx) \in (0, \infty)$, (appropriate for the Poisson parameter).

Poisson Regression: Likelihood Scoring

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

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

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

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

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

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

Poisson Regression: MLE

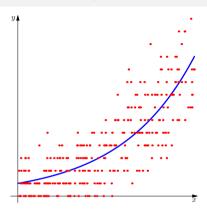
• To get MLE, need to maximize

$$J(w) = \log p(\mathcal{D}; w) = \sum_{i=1}^{n} [y_{i} w^{T} x_{i} - \exp(w^{T} x_{i}) - \log(y_{i}!)]$$

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

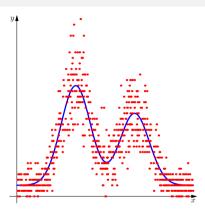
• No closed form for optimum, but it's concave, so easy to optimize.

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 $w \in \mathbb{R}$. (Only linear part $x \mapsto wx$ is learned.)
- Samples are $y_i \sim \text{Poisson}(wx_i)$.

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.

Conditional Gaussian Regression

Gaussian Linear Regression

- Input space $\mathfrak{X} = \mathsf{R}^d$, Output space $\mathfrak{Y} = \mathsf{R}$
- 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 A = 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 $\mu \in \mathbb{R}$, we can take the identity transfer function: $f(w^Tx) = w^Tx$.

Gaussian Regression: Likelihood Scoring

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

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

Let's start solving this!

Gaussian Regression: MLE

• The conditional log-likelihood is:

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

- 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

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

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

- Setting: $X = \mathbb{R}^d$, $\mathcal{Y} = \{1, \dots, k\}$
- \bullet 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 $\theta = (\theta_1, \dots, \theta_k) \in \mathbb{R}^k$:
 - $\sum_{i=1}^k \theta_i = 1$ and $\theta_i \geqslant 0$ for i = 1, ..., k (i.e. θ represents a **distribution**) and
- So $\forall y \in \{1, \ldots, k\}, \ p(y) = \theta_y$.

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

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

where we've introduced parameter vectors $w_1, \ldots, w_k \in \mathbb{R}^d$.

- ullet We need to map this \mathbf{R}^k vector of scores into a probability vector.
- Consider the softmax function:

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

• Note that $\theta \in \mathbb{R}^k$ and

$$\theta_i > 0 \quad i = 1, ..., k$$

$$\sum_{i=1}^k \theta_i = 1$$

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

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

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

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

Putting this together, we write multinomial logistic regression as

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

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

Maximum Likelihood as ERM

Conditional Probability Modeling as Statistical Learning

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

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

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

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

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 $\mathfrak{D} = \{y_1, \dots, y_n\} \in \mathcal{Y}$ is

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

This is called the negative conditional log-likelihood.

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