Conditional Probability Models

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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, but more importantly
  - we can state theorems for GLMs, and
  - all GLMs can be implemented in essentially the same way.
- However, a full development of GLMs requires a fair bit of additional machinery.
- I don't believe the machinery is worth the payoff at this level.

Generalized Regression

Generalized Regression / Conditional Distribution Estimation

- Given x, predict *probability distribution* $p(y \mid x)$
- 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)
    7. Gradient Boosting Machines (GBM) / AnyBoost [in a few weeks]

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** $\theta = p(y = 1 \mid x)$.
- 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 the right $\theta \in [0, 1]$.
- 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.

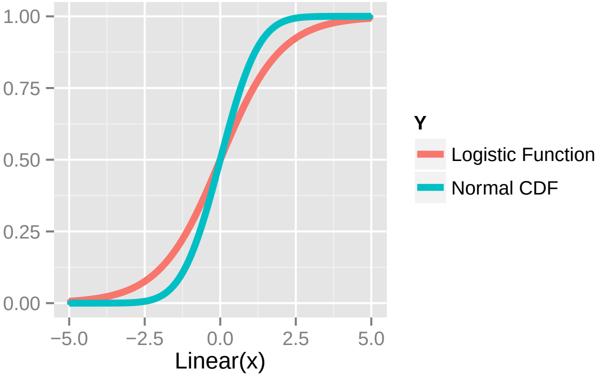
- So prediction function is $x \mapsto f(w^T x)$, which gives value for $\theta = p(y = 1 \mid x)$.

Terminology Alert

In generalized linear models (GLMs), if θ is the distribution mean, then f is called the **response function** or **inverse link** function. **Transfer function is not standard terminology**, but we're avoiding the heavy set of definitions needed for a full development of GLMs, which is actually more restrictive than our current framework.

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

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

Bernoulli Regression: Likelihood Scoring

- Suppose we have data $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$.
- 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 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 $f : \mathbf{R} \to (0, \infty)$?

- 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 is:

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

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

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

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

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 link 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 $\mathcal{D}$:

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

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

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

- Let's start solving this!

Gaussian Regression: MLE

- The conditional log-likelihood is:

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

  - 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:

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

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

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

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

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

- Putting this together, we write multinomial logistic regression as

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

  where we've introduced parameter vectors $w_1, \ldots, w_k \in \mathbf{R}^d$.
- Do we still see score functions in here?
- Can view $x \mapsto w_y^T x$ as the score for class y, for $y \in \{1, \ldots, k\}$.
- How do we do learning here? What parameters are we estimatimg?
- Our model is specified once we have $w_1, \ldots, w_k \in \mathbf{R}^d$.
- 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

Generalized Regression 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 $\mathcal{H}$ contains decision functions $f : \mathcal{X} \to \mathcal{A}$.
  - Given an $x \in \mathcal{X}$, predict a probability distribution $p(y)$ on $\mathcal{Y}$.
- Maximum likelihood estimation for dataset $\mathcal{D} = ((x_1, y_1), \ldots, (x_n, y_n))$ is

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

Exercise

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

Generalized Regression 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.

Generalized Regression 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