Probabilistic models
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Conditional Probability Models

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06c from David Rosenberg's course materials
(https://github.com/davidrosenberg/mlcourse)

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Contents

Table of Contents

Conditional Distribution Estimation (Generalized Regression)

- Task: Given x, predict probability distribution $p(y|x)$
- Method:
  1. Represent $p(y|x)$ with *parametric families* of distributions: $p(y;\theta(x))$ with parameters θ.
  2. Maximize likelihood of training data: $\hat{\theta} \in \arg\max_{\theta} \log p(\mathcal{D}, \hat{\theta})$
- Examples:
  1. Logistic regression (Bernoulli distribution)
  2. Poisson regression (Poisson distribution)
  3. Linear regression (Normal distribution, fixed variance)
  4. Gradient Boosting Machines (GBM) [in a few weeks]
  5. Many neural network models used in practice (though this is not their essential feature)

Linear Probabilistic Classifiers

- Setting: $\mathcal{X} = \mathbf{R}^d$, $\mathcal{Y}$ arbitrary for now
- Want prediction function to map each $x \in \mathbf{R}^d$ to $\theta \in \Theta$ for $p(y; \theta(x))$.
- For a **linear method**, we first **extract information** from $x \in \mathbf{R}^d$ and summarize in a single number with a linear function:

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

  (That number is analogous to the **score** in classification.)
- 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 Θ.

The Transfer Function

- Need a function to map the linear predictor in $\mathbf{R}$ to Θ:

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

  where $f : \mathbf{R} \to \Theta$. We'll call f the **transfer** function.

- So prediction function is $x \mapsto f(w^T x)$.
- The prediction function gives us the parameter for $p(y; \theta(x))$ used to estimate $p(y|x)$.
- Later in the course we will use some non linear predictors, but not today.

Contents

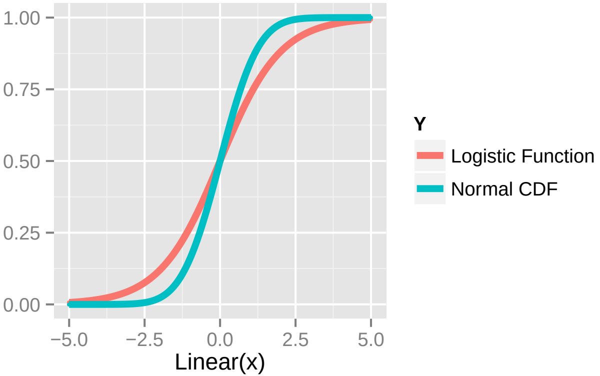
Table of Contents

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 $\text{Bernoulli}(\theta)$.

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 $\mathcal{A} = \Theta = [0, 1]$ (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.
  - In labs, already derived the SGD step directions for logistic regression.
  - Possible [harder] homework: derived the SGD step directions for probit regression.

Table of Contents

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:

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

- 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

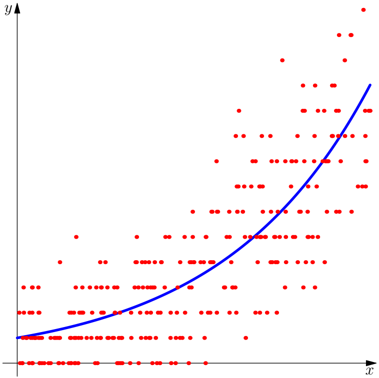
- To get MLE, need to maximize

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

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

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

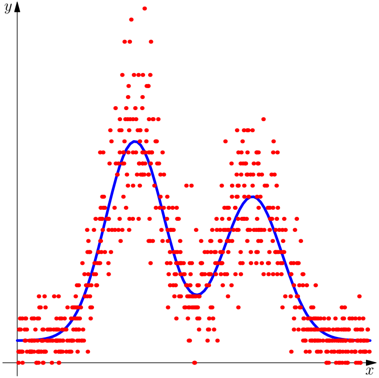
Poisson Regression Example



- 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.

Table of Contents

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:

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

  - 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.
- We provided a probabilistic interpretation of the least square objective.
- From here, can use usual approaches to solve for w^* (SGD, linear algebra, calculus, etc.)

Table of Contents

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 **discrete distribution**)
- 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 $w_1, \ldots, w_k \in \mathbf{R}^d$.
- Find parameter settings maximizing the log-likelihood of data $\mathcal{D}$.
- This objective function is concave in w's and straightforward to optimize.

Table of Contents

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

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

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

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