

Review: MLE and Conditional Probability Models

Xintian Han & David S. Rosenberg

CDS, NYU

March 5, 2019

Contents

- 1 Maximum Likelihood
- 2 Bernoulli Regression
- 3 Poisson Regression
- 4 Conditional Gaussian Regression
- 5 Multinomial Logistic Regression
- 6 Maximum Likelihood as ERM
- 7 Review Questions

Maximum Likelihood

Maximum Likelihood Estimation

- Suppose $\mathcal{D} = (y_1, \dots, y_n)$ is an i.i.d. sample from some distribution.

Definition

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

$$\begin{aligned}\hat{\theta} &\in \arg \max_{\theta \in \Theta} \log p(\mathcal{D}, \theta) \\ &= \arg \max_{\theta \in \Theta} \sum_{i=1}^n \log p(y_i; \theta).\end{aligned}$$

Maximum Likelihood Estimation

- Finding the MLE is an **optimization problem**.
- For some model families, calculus gives a closed form for the MLE.
- Can also use numerical methods we know (e.g. SGD).

MLE Existence

- In certain situations, the MLE may not exist.
- But there is usually a good reason for this.
- e.g. Gaussian family $\{\mathcal{N}(\mu, \sigma^2) \mid \mu \in \mathbf{R}, \sigma^2 > 0\}$
- We have a single observation y .
- Is there an MLE?
- Taking $\mu = y$ and $\sigma^2 \rightarrow 0$ drives likelihood to infinity.
- MLE doesn't exist.

Example: MLE for Poisson

- Observed counts $\mathcal{D} = (k_1, \dots, k_n)$ for taxi cab pickups over n weeks.
 - k_i is number of pickups at Penn Station Mon, 7-8pm, for week i .
- We want to fit a Poisson distribution to this data.
- The Poisson log-likelihood for a single count is

$$\begin{aligned}\log[p(k; \lambda)] &= \log \left[\frac{\lambda^k e^{-\lambda}}{k!} \right] \\ &= k \log \lambda - \lambda - \log(k!)\end{aligned}$$

- The full log-likelihood is

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

Example: MLE for Poisson

- The full log-likelihood is

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

- First order condition gives

$$\begin{aligned} 0 = \frac{\partial}{\partial \lambda} [\log p(\mathcal{D}, \lambda)] &= \sum_{i=1}^n \left[\frac{k_i}{\lambda} - 1 \right] \\ \implies \lambda &= \frac{1}{n} \sum_{i=1}^n k_i \end{aligned}$$

- So MLE $\hat{\lambda}$ is just the mean of the counts.

Estimating Distributions, Overfitting, and Hypothesis Spaces

- Just as in classification and regression, MLE can overfit!
- Example Probability Models:
 - $\mathcal{F} = \{\text{Poisson distributions}\}$.
 - $\mathcal{F} = \{\text{Negative binomial distributions}\}$.
 - $\mathcal{F} = \{\text{Histogram with 10 bins}\}$
 - $\mathcal{F} = \{\text{Histogram with bin for every } y \in \mathcal{Y}\}$ [will likely overfit for continuous data]
- How to judge which model works the best?
- Choose the model with the **highest likelihood on validation set**.

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 $[0, 1]$:

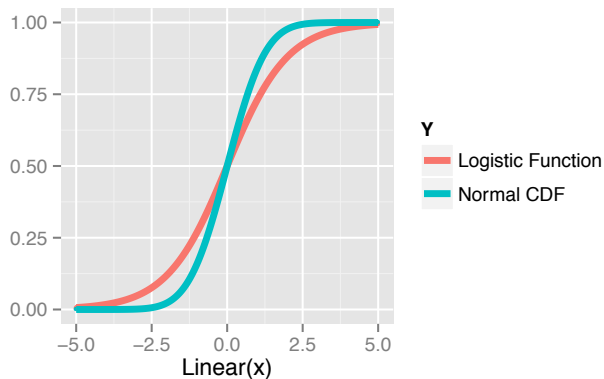
$$\underbrace{x}_{\in \mathbf{R}^d} \mapsto \underbrace{w^T x}_{\in \mathbf{R}} \mapsto \underbrace{f(w^T x)}_{\in [0,1]} = \theta,$$

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

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

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

- 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 $\mathcal{F} = \{x \mapsto f(w^T x) \mid w \in \mathbf{R}^d\}$
- Parameter space \mathbf{R}^d (Each prediction function represented by $w \in \mathbf{R}^d$.)
- We can choose w using maximum likelihood...

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

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

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

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

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

- 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

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

- For differentiable f ,
 - $J(w)$ is differentiable, and we can use SGD.
 - What guarantees us to find the global minima of $J(w)$ by SGD?
 - Convexity of $J(w)$!

Poisson Regression

Poisson Regression: Setup

- Input space $\mathcal{X} = \mathbf{R}^d$, Output space $\mathcal{Y} = \{0, 1, 2, 3, 4, \dots\}$
- In Poisson regression, prediction functions produce a Poisson distribution.
 - Represent $\text{Poisson}(\lambda)$ 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 $f : \mathbf{R} \rightarrow (0, \infty)$?

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 $f(w^T x) \in (0, \infty)$, (appropriate for the Poisson parameter).

Poisson Regression: Likelihood Scoring

- Suppose we have data $\mathcal{D} = \{(x_1, y_1), \dots, (x_n, y_n)\}$.
- 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

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

Poisson Regression: MLE

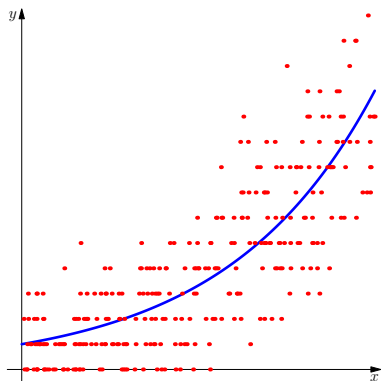
- To get MLE, need to maximize

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

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

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

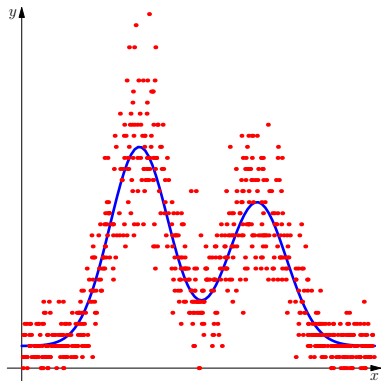
Poisson Regression Example



- Example application: Phone call counts per day for a startup company, over 300 days.
- Blue line is mean $\mu(x) = \exp(wx)$, some $w \in \mathbf{R}$. (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 $\mathcal{D} = \{(x_1, y_1), \dots, (x_n, y_n)\}$.
- Compute the model likelihood for \mathcal{D} :

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

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

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

- Let's start solving this!

Gaussian Regression: MLE

- The conditional log-likelihood is:

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

- 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.

- The MLE is

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

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

Multinomial Logistic Regression

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

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

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

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

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

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

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

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:

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

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

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

Multinomial Logistic Regression

- 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 $w_1, \dots, w_k \in \mathbf{R}^d$.
- 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 $f : \mathcal{X} \rightarrow \mathcal{A}$.
- Maximum likelihood estimation for dataset $\mathcal{D} = ((x_1, y_1), \dots, (x_n, y_n))$ is

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

Conditional Probability Modeling as Statistical Learning

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

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

- The risk of decision function $f : \mathcal{X} \rightarrow \mathcal{A}$ 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 $\mathcal{D} = \{y_1, \dots, y_n\} \in \mathcal{Y}$ 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

Review Questions

Maximum Likelihood

- 1 Suppose we have samples x_1, \dots, x_n i.i.d drawn from Bernoulli(p). Find the maximum likelihood estimator of p .
- 2 Suppose we have samples x_1, \dots, x_n i.i.d drawn from uniform distribution $\mathcal{U}(a, b)$. Find the maximum likelihood estimator of a and b .

Maximum Likelihood

- Suppose we have samples x_1, \dots, x_n i.i.d drawn from $\text{Bernoulli}(p)$. Find the maximum likelihood estimator of p .

Solution:

- The likelihood is:

$$L(p) = \prod_{i=1}^n p^{x_i} (1-p)^{(1-x_i)}.$$

- The log-likelihood is:

$$\ell(p) = \log p \sum_{i=1}^n x_i + \log(1-p) \sum_{i=1}^n (1-x_i).$$

- Set the derivative of log-likelihood w.r.t. p to zero:

$$\frac{\partial \ell(p)}{\partial p} = \frac{\sum_{i=1}^n x_i}{p} - \frac{\sum_{i=1}^n (1-x_i)}{1-p} = 0.$$

Maximum Likelihood

- Solving the equation above, we have:

$$p = \frac{1}{n} \sum_{i=1}^n x_i.$$

- The second derivative of log-likelihood w.r.t. p is

$$\frac{\partial^2 \ell(p)}{\partial p^2} = \frac{-\sum_{i=1}^n x_i}{p^2} - \frac{\sum_{i=1}^n (1-x_i)}{(1-p)^2}.$$

- Since $p \in [0, 1]$ and $x_i \in \{0, 1\}$, the second derivative is always negative. The log-likelihood is concave. Therefore, $p = \frac{1}{n} \sum_{i=1}^n x_i$ gives us the MLE.
- A twice differentiable function of one variable is concave on an interval if and only if its second derivative is non-positive there!
- Why cannot we have the same closed form solution for logistic regression?

Maximum Likelihood

- Suppose we have samples x_1, \dots, x_n i.i.d drawn from uniform distribution $\mathcal{U}(a, b)$. Find the maximum likelihood estimator of a and b .

Solution:

- The likelihood is:

$$L(a, b) = \prod_{i=1}^n \left(\frac{1}{b-a} \mathbb{1}_{[a,b]}(x_i) \right)$$

- Let $x_{(1)}, \dots, x_{(n)}$ be the order statistics.
- The likelihood is greater than zero if and only $a < x_{(1)}$ and $b > x_{(n)}$.
- When $a < x_{(1)}$ and $b > x_{(n)}$, the likelihood is a monotonically decreasing function of $(b-a)$.
- And the smallest $(b-a)$ will be attained when $b = x_{(n)}$ and $a = x_{(1)}$.
- Therefore, $b = x_{(n)}$ and $a = x_{(1)}$ give us the MLE.

Maximum Likelihood

- 1 We want to fit a regression model where $Y|X = x \sim \mathcal{U}([0, e^{w^T x}])$ for some $w \in \mathbf{R}^d$. Given i.i.d. data points $(X_1, Y_1), \dots, (X_n, Y_n) \in \mathbf{R}^d \times \mathbf{R}$, give a convex optimization problem that finds the MLE for w .
- 2 Suppose we have input-output pairs $\{(x_1, y_1), \dots, (x_n, y_n)\}$, where $x_i \in \mathbb{R}^p$ and $y_i \in N = \{0, 1, 2, 3, \dots\}$ for $i = 1, \dots, n$. Our task is to train a Poisson regression to model the data. Assume the linear coefficients in the model is w .
 - 1 Suppose a test point x^* is orthogonal to the space generated by the training data. What is the prediction ℓ_2 regularized Poisson GLM make on the test point?
 - 2 Will the solution of the parameters \hat{w} still be sparse when we use ℓ_1 regularization?

Maximum Likelihood

- We want to fit a regression model where $Y|X = x \sim \mathcal{U}([0, e^{w^T x}])$ for some $w \in \mathbf{R}^d$. Given i.i.d. data points $(X_1, Y_1), \dots, (X_n, Y_n) \in \mathbf{R}^d \times \mathbf{R}$, give a convex optimization problem that finds the MLE for w .

Solution: The likelihood L is given by

$$L(w; x_1, y_1, \dots, x_n, y_n) = \prod_{i=1}^n \frac{\mathbb{1}(y_i \leq e^{w^T x_i})}{e^{w^T x_i}}.$$

Taking logs we get

$$-\sum_{i=1}^n w^T x_i = -w^T \left(\sum_{i=1}^n x_i \right)$$

if $y_i \leq \exp(w^T x_i)$ for all i , or $-\infty$ otherwise. Thus we obtain the linear program

$$\begin{aligned} & \text{minimize} && w^T \left(\sum_{i=1}^n x_i \right) \\ & \text{subject to} && \log(y_i) \leq w^T x_i \quad \text{for } i = 1, \dots, n. \end{aligned}$$

Maximum Likelihood

- Suppose we have input-output pairs $\{(x_1, y_1), \dots, (x_n, y_n)\}$, where $x_i \in \mathbb{R}^p$ and $y_i \in N = \{0, 1, 2, 3, \dots\}$ for $i = 1, \dots, n$. Our task is to train a Poisson regression to model the data. Assume the linear coefficients in the model is w .
- Suppose a test point x^* is orthogonal to the space generated by the training data. What is the prediction ℓ_2 regularized Poisson GLM make on the test point?

Solution: ℓ_2 penalized Poisson regression objective:

$$\hat{J}(w) = - \sum_{i=1}^n \left[y_i w^T x_i - \exp(w^T x_i) - \log(y_i!) \right] + \lambda \|w\|_2^2$$

From Representer Theorem, the minimizer $\hat{w} = \sum_{i=1}^n \alpha_i x_i$. The prediction is

$$\exp(w^T x^*) = \exp\left(\sum_{i=1}^n \alpha_i x_i^T x^*\right) = \exp(0) = 1$$

- Suppose we have input-output pairs $\{(x_1, y_1), \dots, (x_n, y_n)\}$, where $x_i \in \mathbb{R}^p$ and $y_i \in N = \{0, 1, 2, 3, \dots\}$ for $i = 1, \dots, n$. Our task is to train a Poisson regression to model the data. Assume the linear coefficients in the model is w .
 - Will the solution of the parameters \hat{w} still be sparse when we use ℓ_1 regularization?
Solution: Negative log-likelihood of Poisson regression is a convex function. The sublevel set is a convex set. The level set is the boundary of the sublevel set. When the level set approaches the diamond (level set of the ℓ_1 norm), it is still likely to hit the corner of the diamond.