Review: MLE and GLM

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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

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

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 $\left\{\mathcal{N}(\mu, \sigma^2) \mid \mu \in \mathbf{R}, \sigma^2 > 0\right\}$
- We have a single observation y.
- Is there an MLE?
- Taking $\mu = y$ and $\sigma^2 \to 0$ 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

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

• 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

$$0 = \frac{\partial}{\partial \lambda} [\log \rho(\mathcal{D}, \lambda)] = \sum_{i=1}^{n} \left[\frac{k_i}{\lambda} - 1 \right]$$

$$\implies \lambda = \frac{1}{n} \sum_{i=1}^{n} k_i$$

• 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}\}\$
 - $\mathcal{F} = \{\text{Histogram with bin for every } y \in \mathcal{Y}\}\ [\text{will likely overfit for continuous data}]$
- How to judge which model works the best?
- Choose the model with the highest likelihood on validation set.



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]:

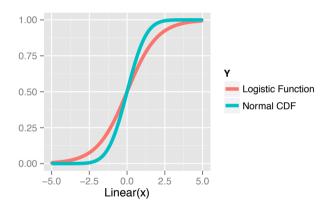
$$\underbrace{x}_{\in \mathbf{R}^d} \mapsto \underbrace{w^T x}_{\in \mathbf{R}} \mapsto \underbrace{f(w^T x)}_{\in [0,1]} = \theta$$

where $f : \mathbb{R} \to [0,1]$. 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: $f(\eta) = \frac{1}{1+e^{-\eta}} \implies \text{Logistic Regression}$
- Normal CDF $f(\eta) = \int_{-\infty}^{\eta} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \Longrightarrow$ Probit Regression

Learning

- Input space $\mathfrak{X} = \mathbf{R}^d$
- Outcome space $\mathcal{Y} = \{0, 1\}$
- Action space 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...

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} : $(x_1, y_1), \dots, (x_n, y_n) \in \mathbb{R}^d \times \{0, 1\}$.
- 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 SGD.
 - What guarantees us to find the global minima of J(w) by SGD?
 - Convexity of J(w)!



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

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

Poisson Regression: MLE

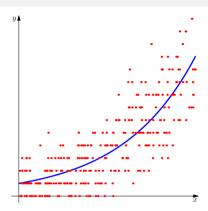
• To get MLE, need to maximize

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

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

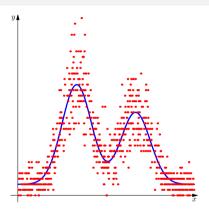
• No closed form for optimum, but it's concave, so easy to optimize.

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 $\mathfrak{X} = \mathbf{R}^d$, Output space $\mathfrak{Y} = \mathbf{R}$
- 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 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 $\mathcal{D} = \{(x_1, y_1), ..., (x_n, y_n)\}.$
- Compute the model likelihood for \mathfrak{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:

$$\sum_{i=1}^{n} \log p(y_i \mid x_i; w)$$

$$= \sum_{i=1}^{n} \log \left[\frac{1}{\sigma \sqrt{2\pi}} \exp \left(-\frac{(y_i - w^T x_i)^2}{2\sigma^2} \right) \right]$$

$$= \sum_{i=1}^{n} \log \left[\frac{1}{\sigma \sqrt{2\pi}} \right] + \sum_{i=1}^{n} \left(-\frac{(y_i - w^T x_i)^2}{2\sigma^2} \right)$$
independent of w

- 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

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

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

- 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:

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

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

- 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

$$\theta_i > 0 \qquad i = 1, \dots, k$$

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

- 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 $w_1, \ldots, w_k \in \mathbb{R}^d$.
- 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 $\mathcal{A} = \{p(y) \mid p \text{ is a probability density or mass function on } \mathcal{Y}\}.$
- Hypothesis space \mathcal{F} contains decision functions $f: \mathcal{X} \to \mathcal{A}$.
- Maximum likelihood estimation for dataset $\mathcal{D} = ((x_1, y_1), \dots, (x_n, y_n))$ is

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

Conditional Probability Modeling as Statistical Learning

• Take loss $\ell: \mathcal{A} \times \mathcal{Y} \to \mathbf{R}$ 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

Review Questions

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

• Suppose we have samples x_1, \ldots, x_n i.i.d drawn from 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:

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

• 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?

• Suppose we have samples x_1, \ldots, 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 $x_{(1)}, \ldots, x_{(n)}$ 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.

- We want to fit a regression model where $Y|X=x\sim \mathcal{U}([0,e^{w^Tx}])$ for some $w\in \mathbb{R}^d$. Given i.i.d. data points $(X_1,Y_1),\ldots,(X_n,Y_n)\in \mathbb{R}^d\times \mathbb{R}$, give a convex optimization problem that finds the MLE for w.
- ② Suppose we have input-output pairs $\{(x_1, y_1), \ldots, (x_n, y_n)\}$, where $x_i \in \mathbb{R}^p$ and $y_i \in N = \{0, 1, 2, 3, \ldots\}$ for $i = 1, \ldots, n$. 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?

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

Solution: The likelihood *L* is given by

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

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

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

subject to $\log(y_i) \leq w^T x_i$ for i = 1, ..., n.

- Suppose we have input-output pairs $\{(x_1, y_1), \ldots, (x_n, y_n)\}$, where $x_i \in \mathbb{R}^p$ and $y_i \in N = \{0, 1, 2, 3, \ldots\}$ for $i = 1, \ldots, n$. 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 ℓ₂ regularized Poisson GLM make on the test point?
 Solution: ℓ₂ penalized Poisson regression objective:

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

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

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

- Suppose we have input-output pairs $\{(x_1, y_1), \ldots, (x_n, y_n)\}$, where $x_i \in \mathbb{R}R^p$ and $y_i \in \mathbb{N} = \{0, 1, 2, 3, \ldots\}$ for i = 1, ..., 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