Lecture 6: Generalized Linear Models

Tao LIN

SoE, Westlake University

October 21, 2025

1. Review of Last Week

2. Exponential Families and Generalized Linear Models
    - Motivation
    - Exponential family
    - Application in ML (Generalized Linear Models)

Reading materials & Reference

Reading materials:

- Chapter 3, Stanford CS 229 Lecture Notes, `https://cs229.stanford.edu/notes2022fall/main_notes.pdf`
- Lecture 4, Stanford CS 231n, `http://cs231n.stanford.edu/schedule.html`

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This classifier is also called the *Bayes classifier*: $f^\star = \arg\min_f L_{\mathcal{D}}(f)$, where

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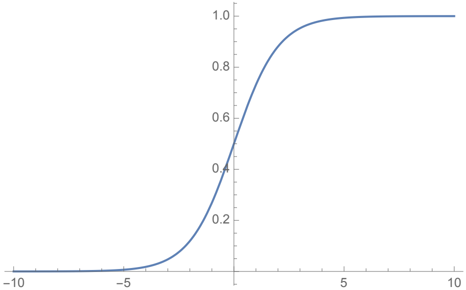
- In practice, we do not know the joint distribution $p(\mathbf{x}, y)$
  $\Rightarrow$ Bayes classifier is an unattainable gold standard.
  But we can use the data to learn the distribution (by assuming the data distribution)

The logistic function

Consider first of all the case of two classes.
The posterior probability for class $\mathcal{C}_1$:

$$p(\mathcal{C}_1|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1) + p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)} \quad (3)$$

$$= \frac{1}{1+\exp(-\eta)} = \sigma(\eta) \quad (4)$$



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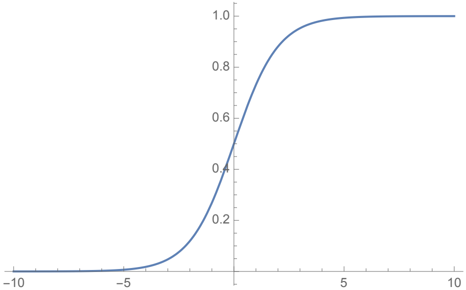
where we have defined

$$\eta = \ln \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)} \text{ and } \sigma(\eta) := \frac{e^\eta}{1+e^\eta} \quad (5)$$



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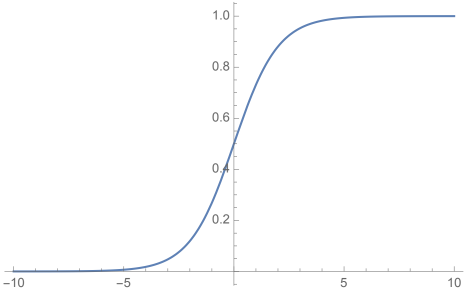
For the case of $K > 2$ classes, we have

$$p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{\sum_j p(\mathbf{x}|\mathcal{C}_j)p(\mathcal{C}_j)} = \frac{\exp(\eta_k)}{\sum_j \exp(\eta_j)} \tag{6}$$



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Logistic Regression

Given a “new” feature vector $\mathbf{x}$, we predict the (posterior) probability of the two class labels given $\mathbf{x}$ by means of

$$p(1|\mathbf{x}) := \Pr\left[Y = 1|\mathbf{X} = \mathbf{x}\right] = \sigma\left(\mathbf{x}^\top \mathbf{w} + w_0\right) \tag{7}$$

$$p(0|\mathbf{x}) := \Pr\left[Y = 0|\mathbf{X} = \mathbf{x}\right] = 1 - \sigma\left(\mathbf{x}^\top \mathbf{w} + w_0\right) \ , \tag{8}$$

where we predict a real value (a probability) and not a label.

MLE is a method of estimating the parameters of a statistical model

The MLE finds the parameters $\mathbf{w}^\star$ under which $\{\mathbf{y}, \mathbf{X}\}$ are the most likely:

$$\mathbf{w}^\star = \arg\max_{\mathbf{w}} \left(\mathcal{L}(\mathbf{w}) := \prod_{n=1}^{N} p(\{\mathbf{x}_n, y_n\} | \mathbf{w}) \right) = \arg\min_{\mathbf{w}} \left[-\log \mathcal{L}(\mathbf{w}) \right] . \tag{9}$$

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The likelihood of the data $\{\mathbf{y}, \mathbf{X}\}$ given the parameter $\mathbf{w}$, i.e., $p(\mathbf{y}, \mathbf{X}|\mathbf{w})$.

$$p(\mathbf{y}, \mathbf{X}|\mathbf{w}) = p(\mathbf{X}|\mathbf{w})p(\mathbf{y}|\mathbf{X}, \mathbf{w}) = p(\mathbf{X})p(\mathbf{y}|\mathbf{X}, \mathbf{w}) , \tag{10}$$

where $\mathbf{X}$ does not depend on $\mathbf{w}$.

MLE for Logistic Regression

For Logistic Regression, we have:

$$p(\mathbf{y}|\mathbf{X}, \mathbf{w}) = \prod_{n=1}^{N} p(y_n|\mathbf{x}_n) \tag{12}$$

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Minimizing $\mathcal{L}(\mathbf{w})$ through the property of stationary points.

$$\nabla \mathcal{L}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_n \left(\sigma(\mathbf{x}_n^\top \mathbf{w}) - y_n\right) = \frac{1}{N} \mathbf{X}^\top \left[\sigma(\mathbf{X}\mathbf{w}) - \mathbf{y}\right] , \tag{13}$$

where $\mathbf{X} \in \mathbb{R}^{N\times d}$.

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where $\mathbf{X} \in \mathbb{R}^{N \times d}$. It has no closed-form solution to $\nabla \mathcal{L}(\mathbf{w}) = 0$.

Last lecture:

- Logistic Regression

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This lecture:

- Exponential Families
- Generalized Linear Models

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- **Geometric way:**
  Minimizing the sum of the squares of the residuals:

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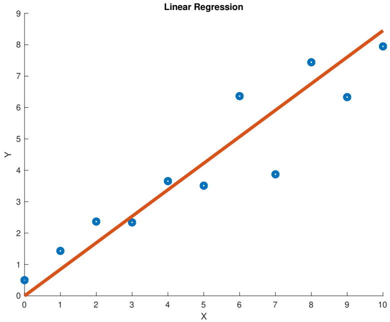

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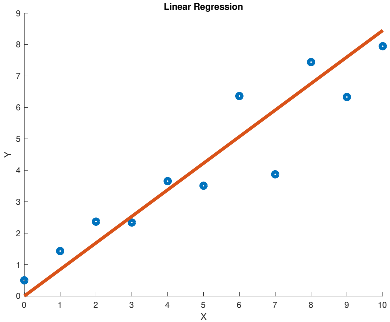

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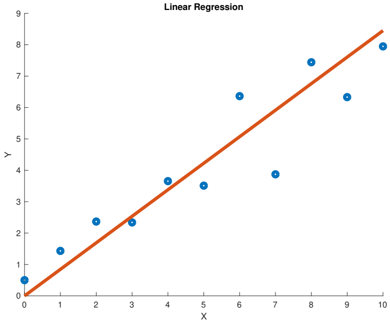

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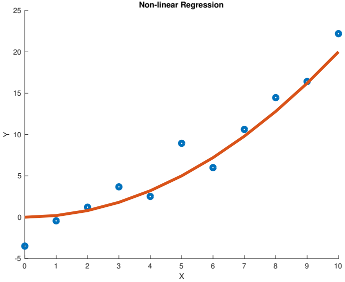
  add non-linear features $(\mathbf{x}, \mathbf{x}^2, \mathbf{x}^3, \ldots)$



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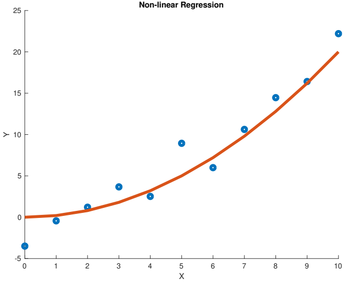

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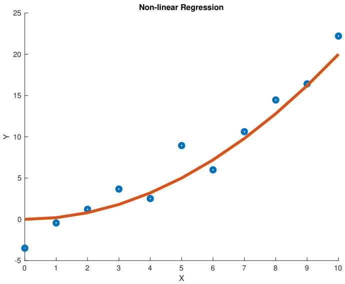

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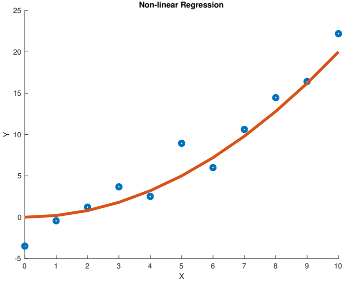

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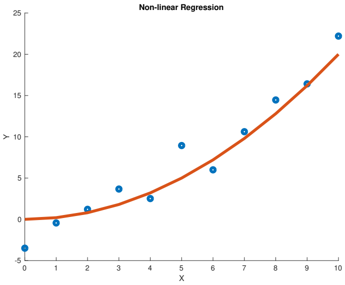

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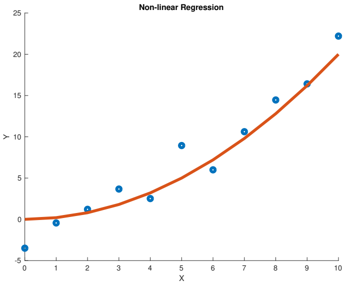

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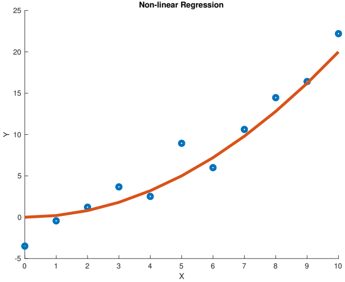

> $\Longrightarrow$ Generalized linear model
> $\Longrightarrow$ Exponential family

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- The relation between
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  makes possible to use linear model in this context.

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- The linear model predicts $\sigma(\eta)$ which is not the mean of the distribution.
- Rather η is related to the mean μ by the non-linear relation $\eta = \ln \frac{\mu}{1-\mu}$ or $\mu = \sigma(\eta)$.
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  makes possible to use linear model in this context.

Recall the definition of Logistic Regression

Logistic Regression models the probability of the two classes $\{0, 1\}$ by

$$p(1|\eta) = \sigma(\eta) \text{ and } p(0|\eta) = 1 - \sigma(\eta)\,, \tag{16}$$

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It is called the **link function**.

A unified framework: exponential family

The distribution used in Logistic Regression can be written in a very specific form:

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Goals: a unified framework to generalize other forms of distributions.

- The discussion on a class of distributions, known as *exponential families*.
- Many distributions (but not all) fit into this framework and that distributions in this family have many nice properties.

Table of Contents

Exponential family — definition

A distribution belongs to the exponential family if it can be written in the form

$$p(y|\boldsymbol{\eta}) = \underbrace{h(y)}_{\geq 0} \exp\left[\boldsymbol{\eta}^\top \boldsymbol{\phi}(y) - A(\boldsymbol{\eta})\right] \tag{19}$$

- y: our observed data, or the random variable.

[1] Assume that we are given independent samples from this distribution. We do know $\boldsymbol{\phi}(y)$ and $h(y)$ but not $\boldsymbol{\eta}$. In order to optimally estimate $\boldsymbol{\eta}$ given these samples, all we need is the empirical average of the $\boldsymbol{\phi}(y)$.

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> We will exclude such parameters by only looking at the set of parameters
>
> $$\text{Natural parameter space } M := \left\{\boldsymbol{\eta} : \int_y h(y)\exp\left[\boldsymbol{\eta}^\top \boldsymbol{\phi}(y)\right] dy < \infty\right\} \tag{23}$$

Why?

Bernoulli distributions belong to the exponential family

Recall: A distribution belongs to the exponential family if it can be written in the form

$$p(y|\boldsymbol{\eta}) = h(y) \exp\left[\boldsymbol{\eta}^\top \boldsymbol{\phi}(y) - A(\boldsymbol{\eta})\right] \tag{24}$$

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$\implies \eta = g(\mu) = \ln \frac{\mu}{1-\mu} \Leftrightarrow \mu = g^{-1}(\eta) = \frac{e^\eta}{1+e^\eta}$. Link function $g(\mu)$ links the mean of $\phi(y)$ to $\boldsymbol{\eta}$.

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$$p(y|\mu) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-\mu)^2}{2\sigma^2}}, \qquad \mu \in \mathbb{R}, \sigma^2 \in \mathbb{R}^+ \tag{30}$$

$$= \exp\left[\left(\mu/\sigma^2, -1/(2\sigma^2)\right)(y, y^2)^\top - \frac{\mu^2}{2\sigma^2} - \frac{1}{2}\ln(2\pi\sigma^2)\right]. \tag{31}$$

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Link function: $\eta_1 = \frac{\mu}{\sigma^2}, \eta_2 = -\frac{1}{2\sigma^2} \iff \mu = -\frac{\eta_1}{2\eta_2}, \sigma^2 = -\frac{1}{2\eta_2}$.

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Claim: the Poisson distribution with mean μ belongs to the family: for $y \in \mathbb{N}$

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Link function (exercise):

$$\boldsymbol{\eta} = g(\mu) \tag{36}$$

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$$p(y|\boldsymbol{\eta}) = h(y) \exp\left[\boldsymbol{\eta}^\top \boldsymbol{\phi}(y) - A(\boldsymbol{\eta})\right] \tag{33}$$

Claim: the Poisson distribution with mean μ belongs to the family: for $y \in \mathbb{N}$

$$p(y|\mu) = \frac{\mu^y e^{-\mu}}{y!} = \frac{1}{y!} e^{y \ln(\mu) - \mu} = h(y) e^{\boldsymbol{\eta}\boldsymbol{\phi}(y) - A(\boldsymbol{\eta})} \tag{34}$$

We can identify (exercise):

$$h(y) = \frac{1}{y!}\,, \ \phi(y) = y\,, \ \text{ and } \eta = \ln(\mu) \tag{35}$$

Link function (exercise):

$$\boldsymbol{\eta} = g(\mu) = \ln(\mu) \tag{36}$$

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$$\boldsymbol{\eta} = g(\mu) = \ln(\mu) \iff \mu = g^{-1}(\boldsymbol{\eta}) = e^{\boldsymbol{\eta}} \tag{36}$$

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- $\nabla^2 A(\boldsymbol{\eta}) = \mathbb{E}\left[\boldsymbol{\phi}(y)\boldsymbol{\phi}(y)^\top\right] - \mathbb{E}\left[\boldsymbol{\phi}(y)\right]\mathbb{E}\left[\boldsymbol{\phi}(y)\right]^\top$
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Proof: convexity

- For $\boldsymbol{\eta}_1, \boldsymbol{\eta}_2$ two parameters, we define $\boldsymbol{\eta} = \lambda \boldsymbol{\eta}_1 + (1 - \lambda)\boldsymbol{\eta}_2$. We want to show

$$A(\boldsymbol{\eta}) \leq \lambda A(\boldsymbol{\eta}_1) + (1 - \lambda) A(\boldsymbol{\eta}_2) \tag{38}$$

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\end{aligned}$$
- We will continue the proof with the Hoelder's inequality.

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- We recall the **Hoelder's inequality:**

$$\|fg\|_1 \leq \|f\|_p \|g\|_q \tag{44}$$

for $p, q \in [1, +\infty]$ $s.t.$ $\frac{1}{p} + \frac{1}{q} = 1$, and $\|f\|_p = (\int |f(y)|^p \, dy)^{1/p}$.

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- We apply Hoelder's inequality to f and g for $p = 1/\lambda$ and $q = 1/(1-\lambda)$:

$$\|fg\|_1 \leq \|f\|_p \|g\|_q \quad \text{where} \quad 1/p + 1/q = \lambda + (1-\lambda) = 1 \tag{45}$$

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$$\|g\|_q = \left(\int g(y)^q dy \right)^{1/q} = \left(\int \left[h(y)^{1-\lambda} \exp\left((1-\lambda) \boldsymbol{\eta}_2^\top \boldsymbol{\phi}(y) \right) \right]^{\frac{1}{1-\lambda}} dy \right)^{1-\lambda} = \left(\int h(y) \exp\left(\boldsymbol{\eta}_2^\top \boldsymbol{\phi}(y) \right) dy \right)^{1-\lambda}$$

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- Therefore we have

$$\|f\|_p \|g\|_q = \left(\int h(y) \exp\left(\boldsymbol{\eta}_1^\top \boldsymbol{\phi}(y)\right) dy\right)^\lambda \left(\int h(y) \exp\left(\boldsymbol{\eta}_2^\top \boldsymbol{\phi}(y)\right) dy\right)^{1-\lambda} \tag{46}$$

$$= \exp\left(\lambda A(\boldsymbol{\eta}_1)\right) \exp\left((1-\lambda) A(\boldsymbol{\eta}_2)\right) \tag{47}$$

Summary of proof: convexity

We have

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\begin{aligned}
\exp A(\boldsymbol{\eta}) &= \int h(y) \exp\left(\boldsymbol{\eta}^\top \boldsymbol{\phi}(y)\right) dy && (48)\\
&= \int h(y) \exp\left(\left(\lambda \boldsymbol{\eta}_1 + (1-\lambda)\boldsymbol{\eta}_2\right)^\top \boldsymbol{\phi}(y)\right) dy && (49)\\
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&\le \left(\int h(y) \exp\left(\boldsymbol{\eta}_1^\top \boldsymbol{\phi}(y)\right) dy\right)^\lambda \left(\int h(y) \exp\left(\boldsymbol{\eta}_2^\top \boldsymbol{\phi}(y)\right) dy\right)^{1-\lambda} && (51)\\
&= \exp\left(\lambda A(\boldsymbol{\eta}_1)\right) \exp\left((1-\lambda) A(\boldsymbol{\eta}_2)\right) && (52)
\end{aligned}
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Derivate of $A(\boldsymbol{\eta})$ and moments: particular cases

- Bernoulli distribution:

$$A'(\boldsymbol{\eta}) = \frac{d}{d\boldsymbol{\eta}} \ln(1 + e^{\boldsymbol{\eta}}) = \frac{e^{\boldsymbol{\eta}}}{1 + e^{\boldsymbol{\eta}}} = \sigma(\boldsymbol{\eta}) = \mu \tag{53}$$

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- Gaussian distribution:

$$\frac{\partial}{\partial \eta_1} A(\boldsymbol{\eta}) = \frac{\partial}{\partial \eta_1}\left(-\frac{\eta_1^2}{4\eta_2} - \frac{1}{2}\ln\left(-\eta_2/\pi\right)\right) = -\frac{\eta_1}{2\eta_2} = \mu \quad (55)$$

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Derivate of $A(\boldsymbol{\eta})$ and moments: general cases

$$\nabla A(\boldsymbol{\eta}) = \nabla \left[\ln \left(\int h(y) \exp\left(\boldsymbol{\eta}^\top \boldsymbol{\phi}(y) \right) dy \right) \right] \tag{58}$$

(64)

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(64)

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$$\begin{aligned}
\nabla A(\boldsymbol{\eta}) &= \nabla \left[\ln \left(\int h(y) \exp \left(\boldsymbol{\eta}^\top \boldsymbol{\phi}(y) \right) dy \right) \right] && (58) \\
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&= \nabla \left[\left(\int h(y) \exp \left(\boldsymbol{\eta}^\top \boldsymbol{\phi}(y) \right) dy \right) \right] \cdot \exp\left(-A(\boldsymbol{\eta})\right) && (60) \\
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We are interested in establishing a relationship between

- our input variables $\mathbf{x}$
- the mean of our output variable $\boldsymbol{\mu} = \mathbb{E}\left[\phi(y)\right]$

Recall that there is a $1-1$ relationship between the "mean" $\boldsymbol{\mu} := \mathbb{E}\left[\phi(y)\right]$ and natural parameter $\boldsymbol{\eta}$, defined using a so-called *link function* $\mathbf{g}$:

$$\boldsymbol{\eta} = \mathbf{g}\left(\boldsymbol{\mu} := \mathbb{E}\left[\phi(y)\right]\right) \Longleftrightarrow \boldsymbol{\mu} = \mathbf{g}^{-1}(\boldsymbol{\eta}) = \nabla A(\boldsymbol{\eta}) \tag{65}$$

Namely,

- $\boldsymbol{\eta} = \mathbf{g}(\mu)$: The link function $\mathbf{g}$ maps the mean $\boldsymbol{\mu}$ to the natural parameter $\boldsymbol{\eta}$.
- $\boldsymbol{\mu} = \mathbf{g}^{-1}(\boldsymbol{\eta})$: we can use the inverse of $\mathbf{g}$ (also called the response function) to calculate the mean $\boldsymbol{\mu}$ from $\boldsymbol{\eta}$.
- $\boldsymbol{\mu} = \nabla A(\boldsymbol{\eta}) = \mathbb{E}\left[\phi(y)\right]$: It tells us that the mean $\boldsymbol{\mu}$, which we calculate via the inverse link function $\mathbf{g}^{-1}$, is exactly the same as the first derivative of $A(\boldsymbol{\eta})$.

Maximum Likelihood Estimation (MLE)

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$\Longrightarrow$ The cost function $\mathcal{L}$ is a convex function in $\boldsymbol{\eta}$ since $A(\boldsymbol{\eta})$ is convex.

Given the definition

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Closed-form: assume we have determined the link function $\mathbf{g}(\boldsymbol{\mu}) = \boldsymbol{\eta}$

$$\boldsymbol{\eta} = \mathbf{g}\left(\frac{1}{N}\sum_{n=1}^{N}\boldsymbol{\phi}(y_n)\right), \tag{70}$$

and justify why we called $\phi(y)$ a sufficient statistics.

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Generalized Linear Models (GLM)

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- The GLM framework extends these ideas to the general exponential family.

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We can apply a Generalized Linear Model (GLM)!

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- $g(\mu) = \eta$ (The link function g maps the mean μ to the linear predictor η)
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The condition probability is thus modeled as:

$$p(y|\mathbf{x};\mathbf{w}) = h(y_n)\exp\left(\eta\phi(y) - A(\eta)\right) \qquad \text{for} \quad \eta = g \circ f(\mathbf{x}^\top \mathbf{w}) \tag{71}$$

- Two choice points in the specification of a GLM:
  1. The choice of the exponential family distribution
     $\Longrightarrow$ Generally constrained by the nature of the data Y
  2. The choice of the response function f
     $\Longrightarrow$ Real degree of freedom!
     $\Longrightarrow$ Canonical response function: $f = g^{-1}$, uniquely associated with the given exponential family distribution.

- If we decide to use the canonical response function, the choice of the exponential family density completely determines the GLM:

$$p(y|\mathbf{x};\mathbf{w}) = h(y_n)\exp\left(\eta\phi(y) - A(\eta)\right) \qquad \text{for} \quad \eta = \mathbf{x}^\top \mathbf{w} \tag{72}$$

Negative log-likelihood estimation

Note that:

$$\mathcal{L}(\mathbf{w}) = -\frac{1}{N}\sum_{n=1}^{N} \ln p(y_n|\mathbf{x}_n^\top \mathbf{w}) = -\frac{1}{N}\sum_{n=1}^{N} (\ln(h(y_n)) + \eta_n \phi(y_n) - A(\eta_n)) \tag{73}$$

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(76)

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In the case of Logistic Regression:

$$\nabla_{\mathbf{w}}\mathcal{L}(\mathbf{w}) = \frac{1}{N}\mathbf{X}^\top\left[\sigma(\mathbf{X}\mathbf{w}) - \mathbf{y}\right] \tag{77}$$

Some examples

- Gaussian distribution Least Squares

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Some examples

• Gaussian distribution	Least Squares
• Bernoulli distribution	Logistic Regression
• Multi-nomial distribution	Softmax Regression

Last lecture:

- Logistic Regression

This lecture:

- Exponential Families
- Generalized Linear Models