Lecture 6: Generalized Linear Models

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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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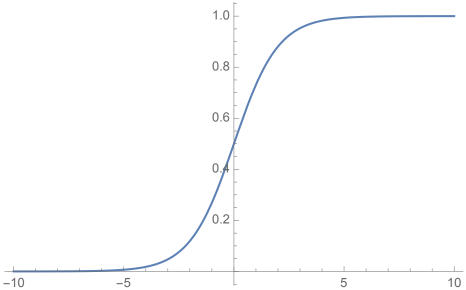
The logistic function

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

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

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



Properties of the logistic function:

- $1 - \sigma(\eta) = \sigma(-\eta)$
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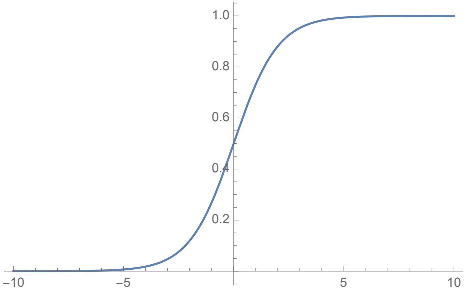
where we have defined

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



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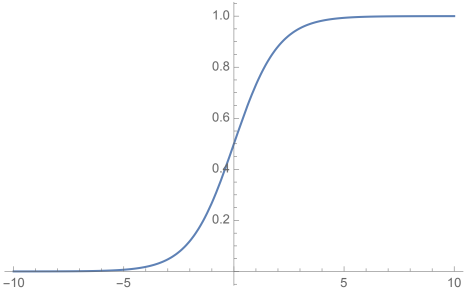
For the case of $K > 2$ classes, we have

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



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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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$$p(\mathbf{y}|\mathbf{X},\mathbf{w}) = \prod_{n=1}^{N} p(y_n|\mathbf{x}_n) = \prod_{n:y_n=1} p(y_n = 1|\mathbf{x}_n) \prod_{n:y_n=0} p(y_n = 0|\mathbf{x}_n) \tag{11}$$

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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:

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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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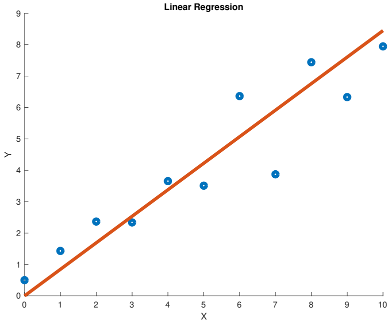

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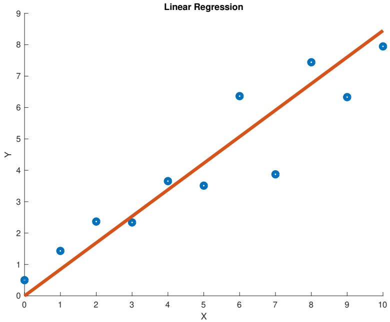

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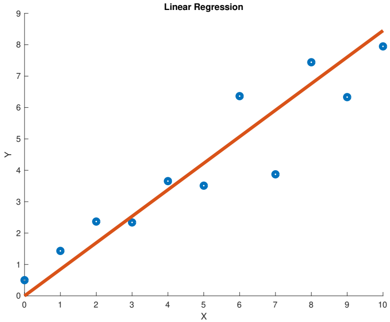

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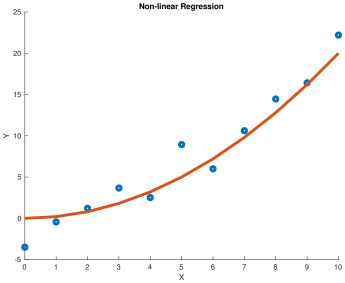
- **Features augmentations:**
  add non-linear features $(\mathbf{x}, \mathbf{x}^2, \mathbf{x}^3, \ldots)$



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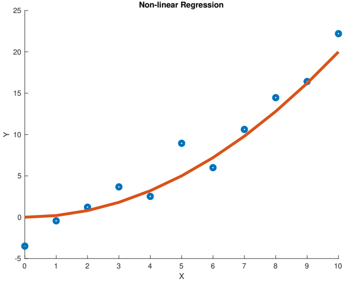

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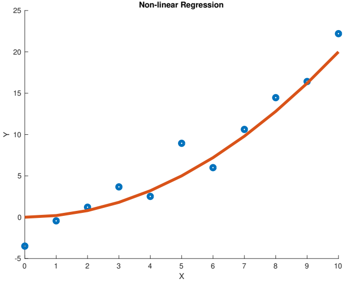

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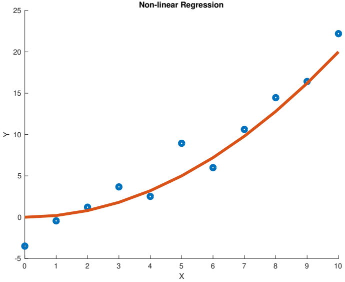

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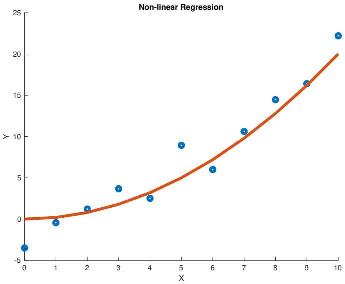

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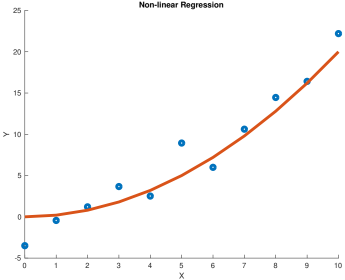

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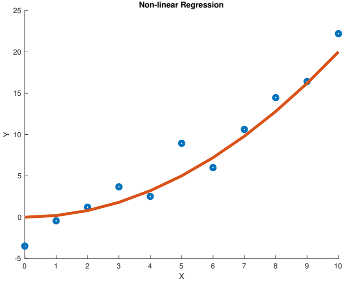

> $\Longrightarrow$ Generalized linear model
> $\Longrightarrow$ Exponential family

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  makes possible to use linear model in this context.

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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

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

where $\eta = \mathbf{x}^\top \mathbf{w}$. This can be compactly written as (exercise: express it as the format of $\exp(\ldots)$)

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- The linear model predicts $\sigma(\eta)$ which is not the mean of the distribution.
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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

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

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

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Poisson distributions belong to the exponential family

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

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

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):

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

Link function (exercise):

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

Basic properties

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

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$$\boldsymbol{\eta} = \mathbf{g}\left(\boldsymbol{\mu} := \mathbb{E}\left[\phi(y)\right]\right) \Longleftrightarrow \boldsymbol{\mu} = \mathbf{g}^{-1}(\boldsymbol{\eta}) = \nabla A(\boldsymbol{\eta}) \tag{37}$$

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.

Proof: convexity

- 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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- Note that

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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

$$
\begin{aligned}
\exp A(\boldsymbol{\eta}) &= \int h(y) \exp\left(\boldsymbol{\eta}^\top \boldsymbol{\phi}(y)\right) dy && (48)\\
&= \int h(y) \exp\left(\left(\lambda \boldsymbol{\eta}_1 + (1-\lambda)\boldsymbol{\eta}_2\right)^\top \boldsymbol{\phi}(y)\right) dy && (49)\\
&= \int \underbrace{\left[h(y)^\lambda \exp\left(\lambda \boldsymbol{\eta}_1^\top \boldsymbol{\phi}(y)\right)\right]}_{f(y)} \cdot \underbrace{\left[h(y)^{1-\lambda} \exp\left((1-\lambda)\boldsymbol{\eta}_2^\top \boldsymbol{\phi}(y)\right)\right]}_{g(y)} dy && (50)\\
&\le \left(\int h(y) \exp\left(\boldsymbol{\eta}_1^\top \boldsymbol{\phi}(y)\right) dy\right)^\lambda \left(\int h(y) \exp\left(\boldsymbol{\eta}_2^\top \boldsymbol{\phi}(y)\right) dy\right)^{1-\lambda} && (51)\\
&= \exp\left(\lambda A(\boldsymbol{\eta}_1)\right) \exp\left((1-\lambda) A(\boldsymbol{\eta}_2)\right) && (52)
\end{aligned}
$$

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

- Bernoulli distribution:

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

$$A''(\boldsymbol{\eta}) = \frac{d}{\boldsymbol{\eta}}\sigma(\boldsymbol{\eta}) = \sigma(\boldsymbol{\eta})\,(1 - \sigma(\boldsymbol{\eta})) = \mu(1 - \mu) \tag{54}$$

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- Gaussian distribution:

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

$$\frac{\partial}{\partial \eta_2} A(\boldsymbol{\eta}) = \frac{\partial}{\partial \eta_2}\left(-\frac{\eta_1^2}{4\eta_2} - \frac{1}{2}\ln\left(-\eta_2/\pi\right)\right) = \frac{\eta_1^2}{4\eta_2^2} - \frac{1}{2\eta_2} = \mu^2 + \sigma^2 \tag{56}$$

$$\frac{\partial^2}{\partial \eta_1^2} A(\boldsymbol{\eta}) = \frac{\partial}{\partial \eta_1}\left(-\frac{\eta_1}{2\eta_2}\right) = -\frac{1}{2\eta_2} = \sigma^2 \tag{57}$$

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)

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

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

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$$= \nabla \left[\left(\int h(y) \exp\left(\boldsymbol{\eta}^\top \boldsymbol{\phi}(y)\right) dy \right) \right] \cdot \exp\left(-A(\boldsymbol{\eta})\right) \tag{60}$$

(64)

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

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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)\\
&= \int \nabla\left[h(y)\exp\left(\boldsymbol{\eta}^\top \boldsymbol{\phi}(y)\right)\right]dy\cdot\exp\left(-A(\boldsymbol{\eta})\right) && (61)
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$$= \int h(y) \exp\left(\boldsymbol{\eta}^\top \boldsymbol{\phi}(y)\right) \boldsymbol{\phi}(y) dy \cdot \exp\left(-A(\boldsymbol{\eta})\right) \tag{62}$$

(64)

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

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$$\tag{64}$$

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

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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) \\
&= \nabla \left[\left(\int h(y) \exp \left(\boldsymbol{\eta}^\top \boldsymbol{\phi}(y) \right) dy \right) \right] \cdot \left(\int h(y) \exp \left(\boldsymbol{\eta}^\top \boldsymbol{\phi}(y) \right) dy \right)^{-1} && (59) \\
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&= \int h(y) \exp \left(\boldsymbol{\eta}^\top \boldsymbol{\phi}(y) - A(\boldsymbol{\eta}) \right) \boldsymbol{\phi}(y) dy && (63) \\
&= \int p(y|\boldsymbol{\eta}) \boldsymbol{\phi}(y) dy && (64)
\end{aligned}
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Derivate of $A(\boldsymbol{\eta})$ and moments: general cases

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&= \int p(y|\boldsymbol{\eta}) \boldsymbol{\phi}(y) dy = \mathbb{E}\left[\phi(Y) \right] && (64)
\end{aligned}
$$

Table of Contents

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How: MLE for $p(y|\boldsymbol{\eta}) = h(y) \exp\left[\boldsymbol{\eta}^\top \boldsymbol{\phi}(y) - A(\boldsymbol{\eta})\right]$.

$$\mathcal{L}(\boldsymbol{\eta}) = -\frac{1}{N} \ln\left(p(y|\boldsymbol{\eta})\right) \tag{65}$$

$$= \frac{1}{N} \sum_{n=1}^{N} \left[-\ln\left(h(y_n)\right) - \boldsymbol{\eta}^\top \boldsymbol{\phi}(y_n) + A(\boldsymbol{\eta})\right] . \tag{66}$$

Maximum Likelihood Estimation (MLE)

Assume a set of iid samples $\{y_n\}_{n=1}^N$, sampled from a member of the exponential family with given $h(y)$, sufficient statistics $\phi(y)$, but unknown parameter $\boldsymbol{\eta}$.

Goal: Estimate the natural parameter $\boldsymbol{\eta}$.

How: MLE for $p(y|\boldsymbol{\eta}) = h(y)\exp\left[\boldsymbol{\eta}^\top \boldsymbol{\phi}(y) - A(\boldsymbol{\eta})\right]$.

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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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$$\nabla_{\boldsymbol{\eta}} \mathcal{L}(\boldsymbol{\eta}) = -\frac{1}{N} \sum_{n=1}^{N} \boldsymbol{\phi}(y_n) + \mathbb{E}\left[\boldsymbol{\phi}(y)\right] , \tag{68}$$

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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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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:

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

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If we rewrite this sum by using the matrix notation, we get (exercise:)

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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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- Bernoulli distribution — Logistic Regression

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