Generalised linear models

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Outline

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Generalised linear models

Iteratively reweighted least squares (IRLS)

Generalised linear models in Spark ML

Introduction

- You are probably familiar by now with different types of probability distributions: the Gaussian, the Bernoulli, the Poisson, the Gamma, etc.

- It turns out that most of these are members of a broader class of distributions known as the exponential family.

Why the exponential family is important?

- It can be shown that the exponential family is the only family of distributions with finite-sized sufficient statistics.
- The exponential family is the only family of distributions for which conjugate priors exist.
- The exponential family can be shown to be the family of distributions that makes the least set of assumptions subject to some user-chosen constraints.
- The exponential family is at the core of generalised linear models.

Definition

- It is said that a pdf or a pmf $p(\mathbf{x}|\boldsymbol{\theta})$, with $\mathbf{x} \in \mathbb{R}^p$ and $\boldsymbol{\theta} \in \mathbb{R}^d$, is in the **exponential family** if it is of the form

$$p(\mathbf{x}|\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} h(\mathbf{x}) \exp\left[\boldsymbol{\theta}^\top \phi(\mathbf{x})\right],$$

  where

$$Z(\boldsymbol{\theta}) = \int h(\mathbf{x}) \exp\left[\boldsymbol{\theta}^\top \phi(\mathbf{x})\right] d\mathbf{x}.$$

- $\boldsymbol{\theta}$ are known as the **natural parameters** or **canonical parameters**.
- $\phi(\mathbf{x}) \in \mathbb{R}^d$ is called a vector of **sufficient statistics**.
- $Z(\boldsymbol{\theta})$ is known as the **partition function**.
- $h(\mathbf{x})$ is a scaling constant, often 1.

Definition

- Distributions in the exponential family can also be expressed as

$$p(\mathbf{x}|\boldsymbol{\theta}) = h(\mathbf{x}) \exp\left[\boldsymbol{\theta}^\top \phi(\mathbf{x}) - A(\boldsymbol{\theta})\right],$$

  where

$$A(\boldsymbol{\theta}) = \log Z(\boldsymbol{\theta}).$$

- $A(\boldsymbol{\theta})$ is called the **log partition function** or **cumulant function**.

- If $\phi(\mathbf{x}) = \mathbf{x}$, we say it is a **natural exponential family**.

Example: Bernoulli (I)

- For the Bernoulli distribution, $x \in \{0, 1\}$, and we have

$$p(x|\mu) = \mathrm{Bern}(x|\mu) = \mu^x(1-\mu)^{1-x},$$

  where $\mu = p(x = 1)$.

- The distribution above can be written as

$$\begin{aligned} p(x|\mu) &= \exp\{x \log \mu + (1-x)\log(1-\mu)\}, \\ &= (1-\mu)\exp\left\{\log\left(\frac{\mu}{1-\mu}\right)x\right\} \end{aligned}$$

Example: Bernoulli (II)

- Comparing terms with the general expression for the exponential family, we observe that

$$\theta = \log\left(\frac{\mu}{1-\mu}\right), \quad Z(\theta) = \frac{1}{\sigma(-\theta)}.$$

- The Bernoulli distribution can be written as $p(x|\theta) = \sigma(-\theta)\exp(\theta x)$.

- The term $\theta = \log\left(\frac{\mu}{1-\mu}\right)$ is known as the **log-odds ratio**.

- Recall that the expected value of x is equal to $\mathbb{E}[x] = \mu$.

- Then, the mean parameter μ can be recovered from the canonical parameter using

$$\mu = \sigma(\theta) = \frac{1}{1+\exp(-\theta)}.$$

Example: univariate Gaussiana distribution

- The univariate Gaussian can be written in exponential family form as

$$
\begin{aligned}
\mathcal{N}(x|\mu,\sigma^2) &= \frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}} \exp\left[-\frac{1}{2\sigma^2}(x-\mu)^2\right] \\
&= \frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}} \exp\left[-\frac{1}{2\sigma^2}x^2 + \frac{\mu}{\sigma^2}x - \frac{1}{2\sigma^2}\mu^2\right] \\
&= \frac{1}{Z(\boldsymbol{\theta})} \exp\left(\boldsymbol{\theta}^\top \phi(x)\right),
\end{aligned}
$$

where

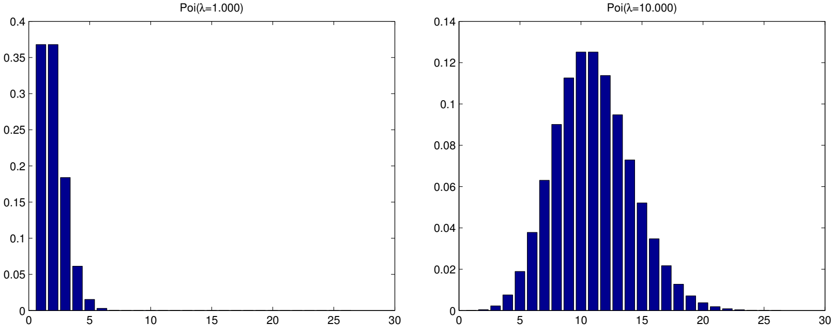
$$
\begin{aligned}
\boldsymbol{\theta} &= \begin{bmatrix} \mu/\sigma^2 \\ -\frac{1}{2\sigma^2} \end{bmatrix}, \qquad \phi(x) = \begin{bmatrix} x \\ x^2 \end{bmatrix}, \\
Z(\boldsymbol{\theta}) &= \sqrt{2\pi}\sigma \exp\left\{\frac{\mu^2}{2\sigma^2}\right\}, \\
A(\boldsymbol{\theta}) &= -\frac{\theta_1^2}{4\theta_2} - \frac{1}{2}\log(-2\theta_2) - \frac{1}{2}\log(2\pi).
\end{aligned}
$$

Example: Poisson distribution (I)

- The Poisson distribution follows as

$$\mathrm{Poi}(x|\lambda) = \exp(-\lambda)\frac{\lambda^x}{x!},$$

where $\lambda > 0$, and $x \in \{0, 1, 2, \ldots\}$.



$\lambda = 1$ $\qquad$ $\lambda = 10$

Example: Poisson distribution (II)

- As a member of the exponential family, it can be written as

$$\mathrm{Poi}(x|\lambda) = \frac{h(x)}{Z(\theta)} \exp(\theta x),$$

where $\theta = \log \lambda$, $h(x) = 1/x!$, and $Z(\theta) = \exp(\lambda)$. Also, $A(\theta) = \lambda$.

- Recall that the expected value of x is equal to $\mathbb{E}[x] = \lambda$.

- Then, the mean parameter λ can be recovered from the canonical parameter using

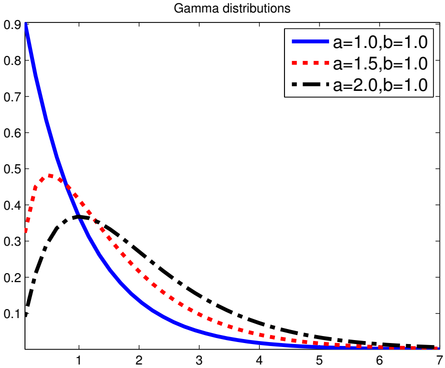
$$\lambda = \exp(\theta).$$

Example: Gamma distribution (I)

- The Gamma distribution follows as

$$\mathrm{Ga}(x|a,b) = \frac{b^a}{\Gamma(a)} x^{a-1} \exp(-bx),$$

where $a > 0$ (shape), and $b > 0$ (rate). $\Gamma(a) = \int_0^\infty u^{a-1} e^{-u} du$ is the Gamma function.



Example: Gamma distribution (II)

- As a member of the exponential family, it can be written as

$$\mathrm{Ga}(x|a,b) = \frac{1}{Z(\boldsymbol{\theta})}\exp(\boldsymbol{\theta}^\top \phi(x)),$$

where

$$\boldsymbol{\theta} = \begin{bmatrix} a-1 \\ -b \end{bmatrix}, \qquad \phi(x) = \begin{bmatrix} \log x \\ x \end{bmatrix},$$

$$Z(\boldsymbol{\theta}) = \frac{\Gamma(a)}{b^a}, \quad A(\boldsymbol{\theta}) = \log\Gamma(a) - a\log b.$$

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Definition

- Linear and logistic regression are examples of generalised linear models, or GLM.

- These are models in which the output density is in the exponential family.

- The mean parameters are a linear combination of the inputs, passed through a possibly nonlinear function, such as the logistic function.

General form (I)

- We want to model the relationship between a response variable y_i, and an input vector $\mathbf{x}_i$.

- Let us first consider the case of an unconditional distribution for the response variable

$$p(y_i|\theta, \sigma^2) = \exp\left[\frac{y_i\theta - A(\theta)}{\sigma^2} + c(y_i, \sigma^2)\right],$$

  where σ^2 is the **dispersion parameter**, θ is the natural parameter, A is the partition function, and c is the normalisation constant.

- Usually, $\sigma^2 = 1$.

- The expression for $p(y_i|\theta, \sigma^2)$ looks similar to the exponential family.

General form (II)

- For example, in logistic regression, θ is the log-odds ratio

$$\theta = \log\left(\frac{\mu}{1-\mu}\right),$$

where $\mu = \mathbb{E}[y] = P(y = 1)$ is the mean parameter.

- To convert from the mean parameter to the natural parameter, we can use a function ψ, $\theta = \psi(\mu)$.

- ψ is uniquely determined by the form of the exponential family distribution.

- The mapping is invertible, so that $\mu = \psi^{-1}(\theta)$.

General form (III)

- Now let us add inputs or covariates.
- We first define a linear function of the inputs $\eta_i = \mathbf{w}^\top \mathbf{x}_i$.
- We now make the mean of the distribution be some invertible monotonic function of this linear combination.
- By convention, this function, known as the **mean function**, is denoted by g^{-1}, so

$$\mu_i = g^{-1}(\eta_i) = g^{-1}(\mathbf{w}^\top \mathbf{x}_i).$$

- The inverse of the mean function, namely $g()$, is called the **link function**.

Relationships between functions

$$
\begin{tikzcd}
\boldsymbol{w} \arrow[dr] & & & \\
& \eta_i \arrow[r, shift left, "g^{-1}"] & \mu_i \arrow[l, shift left, "g"] \arrow[r, shift left, "\Psi"] & \theta_i \arrow[l, shift left, "\Psi^{-1}"] \\
\boldsymbol{x}_i \arrow[ur] & & &
\end{tikzcd}
$$

Link function

- We are free to choose almost any function we like for g, so long as it is invertible, and so long as g^{-1} has the appropriate range.

- For example, in logistic regression, we set $\mu_i = g^{-1}(\eta_i) = \sigma(\eta_i)$.

GLM with canonical link function

- One particularly simple form of link function is to use $g = \psi$.
- This is called the **canonical link function**.
- In this case $\theta_i = \eta_i = \mathbf{w}^\top \mathbf{x}_i$, so the model becomes

$$p(y_i|\mathbf{x}_i, \mathbf{w}, \sigma^2) = \exp\left[\frac{y_i \mathbf{w}^\top \mathbf{x}_i - A(\mathbf{w}^\top \mathbf{x}_i)}{\sigma^2} + c(y_i, \sigma^2)\right].$$

Canonical link functions $g = \psi$ for some GLMs

Distribution	Link $g(\mu)$	$\theta = \psi(\mu)$	$\mu = \psi^{-1}(\theta)$
$\mathcal{N}(\mu, \sigma^2)$	identity	$\theta = \mu$	$\mu = \theta$
$\mathrm{Ber}(\mu)$	logit	$\theta = \log\left(\frac{\mu}{1-\mu}\right)$	$\mu = \sigma(\theta)$
$\mathrm{Poi}(\mu)$	log	$\theta = \log(\mu)$	$\mu = e^{\theta}$
$\mathrm{Ga}(a, b)$	inverse	$\theta = \mu^{-1}$	$\mu = \theta^{-1}$.

Mean and variance of the response variable

- It can be shown that

$$\mathbb{E}[y|\mathbf{x}_i, \mathbf{w}, \sigma^2] = \mu_i = A'(\theta_i)$$
$$\text{var}[y|\mathbf{x}_i, \mathbf{w}, \sigma^2] = \sigma_i^2 = A''(\theta_i)\sigma^2.$$

Example: linear regression

- In linear regression, the response variable follows a normal distribution,

$$
\begin{aligned}
p(y_i|\mu_i, \sigma^2) &= \mathcal{N}(y_i|\mu_i, \sigma^2) \\
&= \frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}} \exp\left[-\frac{1}{2\sigma^2}(y_i - \mu_i)^2\right] \\
&= \exp\left[\frac{y_i\mu_i - \frac{\mu_i^2}{2}}{\sigma^2} - \frac{y_i^2}{2\sigma^2} + \log\left(\frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}}\right)\right] \\
&= \exp\left[\frac{y_i\mu_i - \frac{\mu_i^2}{2}}{\sigma^2} - \frac{1}{2}\left(\frac{y_i^2}{\sigma^2} + \log(2\pi\sigma^2)\right)\right].
\end{aligned}
$$

- For linear regression, $y_i \in \mathbb{R}$.

- The link function is the identity $\theta_i = \mu_i = \mathbf{w}^\top \mathbf{x}_i$.

- With $A(\mu_i) = \mu_i^2/2$, $\mathbb{E}[y_i] = \mu_i$, and $\text{var}[y_i] = \sigma^2$.

Example: logistic regression

- In logistic regression, the response variable follows a Bernoulli distribution

$$
\begin{aligned}
p(y_i|\mu_i, \sigma^2) &= \mu_i^{y_i}(1-\mu_i)^{y_i} \\
&= \exp\left[\log\left(\frac{\mu_i}{1-\mu_i}\right) y_i - (-\log(1-\mu_i))\right].
\end{aligned}
$$

- The link function is the logit, $\log\left(\frac{\mu_i}{1-\mu_i}\right) = \mathbf{w}^\top \mathbf{x}_i$.

- With $A(\theta_i) = -\log(1-\sigma(\theta_i))$, $\mathbb{E}[y_i] = \sigma(\theta_i)$, and $\mathrm{var}[y_i] = \sigma(\theta_i)(1-\sigma(\theta_i))$.

Example: Poisson regression

- In Poisson regression, the response variable follows a Poisson distribution

$$p(y_i|\mathbf{x}_i, \mathbf{w}, \sigma^2) = \exp[y_i \log(\mu_i) - \mu_i - \log(y_i!)].$$

- The link function is $\log$, $\log \mu_i = \mathbf{w}^\top \mathbf{x}_i$.

- With $A(\theta_i) = \exp(\theta_i)$, $\mathbb{E}[y_i] = \exp(\theta_i) = \lambda_i$.

Outline

Log-likelihood for a GLM

- One of the appealing properties of GLMs is that they can be fit using exactly the same methods that we used to fit logistic regression.

- In particular, the log-likelihood has the following form

$$\ell(\mathbf{w}) = \frac{1}{\sigma^2} \sum_{n=1}^{N} \ell_i = \frac{1}{\sigma^2} \sum_{n=1}^{N} [\theta_i y_i - A(\theta_i)],$$

where $\ell_i = \theta_i y_i - A(\theta_i)$.

Gradient for the log-likelihood

- We can compute the gradient vector using the chain rule as follows

$$\begin{aligned}\frac{d\ell_i}{dw_j} &= \frac{d\ell_i}{d\theta_i}\frac{d\theta_i}{d\mu_i}\frac{d\mu_i}{d\eta_i}\frac{d\eta_i}{dw_j} \\ &= (y_i - A'(\theta_i))\frac{d\theta_i}{d\mu_i}\frac{d\mu_i}{d\eta_i}x_{i,j} \\ &= (y_i - \mu_i)\frac{d\theta_i}{d\mu_i}\frac{d\mu_i}{d\eta_i}x_{i,j}.\end{aligned}$$

- If we use a canonical link, $\theta_i = \eta_i$, this simplifies to

$$\mathbf{g}(\mathbf{w}) = \frac{1}{\sigma^2}\left[\sum_{i=1}^{N}(y_i - \mu_i)\mathbf{x}_i\right] = \frac{1}{\sigma^2}\mathbf{X}^\top(\mathbf{y} - \boldsymbol{\mu}),$$

where $\boldsymbol{\mu} = [\mu_1, \cdots, \mu_N]^\top$.

- This can be used inside a (stochastic) gradient descent procedure.

Hessian for the log-likelihood

- For improved efficiency, we could use a second-order method.
- If we use a canonical link, the Hessian is given by

$$\mathbf{H}(\mathbf{w}) = -\frac{1}{\sigma^2}\sum_{i=1}^{N}\frac{d\mu_i}{d\theta_i}\mathbf{x}_i\mathbf{x}_i^\top = -\frac{1}{\sigma^2}\mathbf{X}^\top\mathbf{\Sigma}\mathbf{X},$$

  where $\mathbf{\Sigma} = \mathrm{diag}\left(\frac{d\mu_1}{d\theta_1}, \cdots, \frac{d\mu_N}{d\theta_N}\right)$.

- This can be used inside the Iterative Reweighted Least Squares (IRLS) algorithm.

Iterative reweighted least squares (IRLS) algorithm

- The Iterative Reweighted Least Squares algorithm is a particular case of the Newton's method.

- The updated parameters are obtained by iteratively solving a weigthed least squares problem.

A least squares problem

- Remember that a least squares (LS) problem refers to

$$LS(\mathbf{w}) = \min_{\mathbf{w}} \sum_{i=1}^{N} (y_i - \mathbf{w}^\top \mathbf{x}_i)^2,$$

  for a dataset $\mathcal{D} = \{\mathbf{x}_i, y_i\}_{i=1}^{N} = \{\mathbf{X}, \mathbf{y}\}$.

- It can be shown that the vector **w** that minimises $LS(\mathbf{w})$ is given as

$$\mathbf{w} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

A weigthed least squares problem

- A weighted least squares (*WLS*) problem refers to

$$WLS(\mathbf{w}) = \min_{\mathbf{w}} \sum_{i=1}^{N} r_i (y_i - \mathbf{w}^\top \mathbf{x}_i)^2,$$

  for a dataset $\mathcal{D} = \{\mathbf{x}_i, y_i, r_i\}_{i=1}^N = \{\mathbf{X}, \mathbf{R}, \mathbf{y}\}$, with $\mathbf{R} = \mathrm{diag}(r_1, \ldots, r_N)$.

- It can be shown that the vector $\mathbf{w}$ that minimises $WLS(\mathbf{w})$ is given as

$$\mathbf{w} = (\mathbf{X}^\top \mathbf{R} \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{R} \mathbf{y}.$$

Iterative reweighted least squares problem

- Newton's method for the log-likelihood of the GLM follows as

$$
\begin{aligned}
\mathbf{w}_{k+1} &= \mathbf{w}_k - \mathbf{H}_k^{-1}\mathbf{g}_k \\
&= \mathbf{w}_k + (\mathbf{X}^\top \Sigma_k \mathbf{X})^{-1}\mathbf{X}^\top(\mathbf{y} - \boldsymbol{\mu}_k) \\
&= (\mathbf{X}^\top \Sigma_k \mathbf{X})^{-1}[\mathbf{X}^\top \Sigma_k \mathbf{X}\mathbf{w}_k + \mathbf{X}^\top(\mathbf{y} - \boldsymbol{\mu}_k)] \\
&= (\mathbf{X}^\top \Sigma_k \mathbf{X})^{-1}\mathbf{X}^\top \Sigma_k \mathbf{z}_k,
\end{aligned}
$$

  where $\mathbf{z}_k = \mathbf{X}\mathbf{w}_k + \Sigma_k^{-1}(\mathbf{y} - \boldsymbol{\mu}_k)$ is known as the **working response**.

- At iteration k, the solution for $\mathbf{w}_{k+1}$ has a similar form to the solution for a weigthed least squared problem replacing $\mathbf{R}$ for Σ_k, and $\mathbf{y}$ for $\mathbf{z}_k$.

- The name IRLS is due to at each iteration, we solve a weighted least squares problem, where the weight matrix Σ_k changes at each iteration.

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`GeneralizedLinearRegression()`

- It uses IRLS (Iterative Reweigthed Least Squares) for optimisation.

- It only allows ℓ_2 regularisation.

- `LinearRegression()` uses L-BFGS, and allows for ℓ_1, ℓ_2 and elastic net regularization.

- `LogisticRegression()` also uses L-BFGS, and allows for ℓ_1, ℓ_2 and elastic net regularization.

`GeneralizedLinearRegression()`

- Spark currently only supports up to 4096 features through its `GeneralizedLinearRegression` interface.

- It will throw an exception if this constraint is exceeded.

GLM available in Spark

- It includes the following families

Family	**Response type**	**Supported links**
Gaussian	Continuous	Indentity*, Log, Inverse
Binomial	Binary	Logit*, Probit, CLogLog
Poisson	Count	Log*, Identity, Sqrt
Gamma	Continuous	Inverse*, Identity, Log
Tweedie	Zero-inflated continuous	Power link function

where * stands for canonical link.

- The parameters are set using `setFamily` and `setLink`.