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► **To cite this version:**

Christophe Dutang. Some explanations about the IWLS algorithm to fit generalized linear models. 2017. hal-01577698

**HAL Id: hal-01577698**

**<https://hal.science/hal-01577698>**

Preprint submitted on 27 Aug 2017

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# Some explanations about the IWLS algorithm to fit generalized linear models

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*August 2017*

This short note focuses on the estimation procedure generally used for generalized linear models (GLMs), see e.g. McCullagh, P. (1984). Generalized linear models. European Journal of Operational Research, 16(3), 285-292.

## 1 Fitting GLMs

### 1.1 Definition of the log-likelihood and the score function

The parametrization of the exponential family generally used for GLMs is given by the following density or mass probability function:

$$f_Y(y; \theta, \phi) = e^{\frac{y\theta - b(\theta)}{a(\phi)} + c(y, \phi)}, y \in S,$$

where  $S$  is the support of the distribution, typically  $\mathbb{N}$  or  $\mathbb{R}$ , and  $a, b, c$  are known smooth functions.

Note that  $E(Y) = b'(\theta) = \mu$  and  $Var(Y) = \phi b''(\theta) = \phi V(\mu)$ . Let us start with the iid case, where  $Y_i$  are independent and identically distributed. In that case, the score is defined as

$$S(\theta) = \frac{\partial \log f_Y(Y; \theta, \phi)}{\partial \theta} = \frac{Y - b'(\theta)}{a(\phi)}.$$

It is well known that  $E(S) = 0$  and  $Var(S) = -E(S'(\theta)) = b''(\theta)/\phi$ .

Now, we focus on the GLM context. That is  $Y_i \sim \mathcal{F}_{exp}(\theta_i, \phi_i)$  for all  $i = 1, \dots, n$  where the explanatory variables are linked to the expectation by

$$g(b'(\theta_i)) = g(\mu_i) = \beta_1 x_{i1} + \dots + \beta_p x_{ip},$$

with  $p < n$  for identifiability reasons. Note that an intercept is generally included so that  $x_{i1} = 1$  for all  $i$ . The log-density of  $Y_i$  is

$$l_i(\beta_i) = \log f_{Y_i}(y_i; \theta_i(\beta_i), \phi_i) = \frac{y_i \theta_i(\beta_i) - b(\theta_i(\beta_i))}{a(\phi_i)} + c(y_i, \phi_i).$$

The log-likelihood of the GLM for observations  $y_1, \dots, y_n$  is simply obtained by adding  $l_i$  contributions

$$L(\beta) = \sum_{i=1}^n l_i(\beta_i) = \sum_{i=1}^n \left( \frac{y_i \theta_i(\beta_i) - b(\theta_i(\beta_i))}{a(\phi_i)} + c(y_i, \phi_i) \right).$$

A common choice for the dispersion parameter is  $\phi_i = \phi/w_i$  with  $w_i$  a known weight.

The score function is defined as the expectation of the gradient of the log-likelihood. Using  $\theta_i = (b')^{-1}(g^{-1}(\beta_1 x_{i1} + \dots + \beta_p x_{ip}))$ ,  $\eta_i = \beta_1 x_{i1} + \dots + \beta_p x_{ip}$ ,  $(f^{-1})' = 1/f' \circ f^{-1}$ ,  $((f')^{-1})' = 1/f'' \circ (f')^{-1}$ , we derive the partial derivative

$$\frac{\partial \theta_i}{\partial \beta_j} = ((b')^{-1})'(g^{-1}(\eta_i)) \times (g^{-1})'(\eta_i) \times x_{ij} = \frac{1}{b''((b')^{-1}(g^{-1}(\eta_i)))} \times \frac{x_{ij}}{g'(g^{-1}(\eta_i))} = \frac{1}{b''(\theta_i)} \times \frac{x_{ij}}{g'(\mu_i)}.$$

Therefore, using this partial derivative w.r.t.  $\beta_j$  leads to the following score

$$S_j(\beta) = \frac{\partial L(\beta)}{\partial \beta_j} = \sum_{i=1}^n U_i(\theta_i) \frac{\partial \theta_i}{\partial \beta_j} = \sum_{i=1}^n \frac{y_i - b'(\theta_i)}{a(\phi_i)} \frac{1}{b''(\theta_i)} \frac{x_{ij}}{g'(\mu_i)} = \sum_{i=1}^n \frac{y_i - \mu_i}{a(\phi_i)V(\mu_i)} \frac{x_{ij}}{g'(\mu_i)}$$

where  $\mu_i = b'(\theta_i)$  and  $V(\mu_i) = b''(\theta_i)$  for  $j = 1, \dots, p$ . The parameter  $\beta$  is found by solving the score equations

$$S_j(\beta) = 0, \quad j = 1, \dots, p.$$

## 1.2 Objective of the optimization procedure

The question we may ask is whether it is equivalent to solve the score function or to minimize the opposite of the log-likelihood by the (exact) Newton method?

Consider  $f : \mathbb{R}^n \mapsto \mathbb{R}$  a twice differentiable function with a gradient vector  $g(x) = \nabla f(x)$ , and a Hessian matrix  $H(x) = \nabla^2 f(x)$ . Let  $F : \mathbb{R}^n \mapsto \mathbb{R}^n$  be a differentiable function. The Jacobian matrix is denoted by  $\text{Jac } F(x) \in \mathbb{R}^{n \times n}$ .

From classical optimization books, e.g. Nocedal, J. & Wright, S. J. (2006), Numerical Optimization, Springer Science+Business Media, a (local) optimization method consists in computing the following sequence  $x_{k+1} = x_k + d_k$  where  $d_k$  is computed according to a scheme. In addition, a globalization technique may be used in conjunction such as a line search. But, the globalization scheme is seldom done for fitting GLMs.

The exact Newton method (also called the Newton-Raphson method) to find the minimum of a function  $f$  uses the direction  $d_k = -H(x_k)^{-1}g(x_k)$ . In comparison, the steepest descent method to find the minimum of  $f$  considers  $d_k = -g(x_k)$ . Furthermore, the exact Newton method to find the root of  $F$  uses the direction  $d_k = -\text{Jac}(x_k)^{-1}F(x_k)$ . Hence, the direction is exactly the same between the minimization problem and the root problem, when the root function  $F$  is the gradient  $\nabla f$  of the objective. Hence, finding the roots of the score equations is equivalent to maximizing the log-likelihood.

## 1.3 Derivation of the Newton method for the score equations

The Newton method to find the root of the score equations is

$$\beta^{(k+1)} = \beta^{(k)} - \text{Jac } S \left( \beta^{(k)} \right)^{-1} S(\beta^{(k)}).$$

The exponent  $(k)$  is used to denote the  $k$ th iteration since subscript are used for indexing observation and/or component. Let us compute the Jacobian of the score or the Hessian of the log-likelihood.

$$\begin{aligned} \frac{\partial^2 L(\beta)}{\partial \beta_j \partial \beta_l} &= \sum_{i=1}^n \frac{\partial}{\partial \beta_l} \left( \frac{y_i - b'(\theta_i)}{a(\phi_i)} \right) \frac{1}{b''(\theta_i)} \frac{x_{ij}}{g'(\mu_i)} + \sum_{i=1}^n \frac{\partial}{\partial \beta_l} \left( \frac{1}{b''(\theta_i)} \right) \frac{y_i - b'(\theta_i)}{a(\phi_i)} \frac{x_{ij}}{g'(\mu_i)} \\ &\quad + \sum_{i=1}^n \frac{\partial}{\partial \beta_l} \left( \frac{x_{ij}}{g'(\mu_i)} \right) \frac{y_i - b'(\theta_i)}{a(\phi_i)} \frac{1}{b''(\theta_i)}. \end{aligned}$$

The first term is

$$\frac{\partial}{\partial \beta_l} \left( \frac{y_i - b'(\theta_i)}{a(\phi_i)} \right) = \frac{-b''(\theta_i)}{a(\phi_i)} \times \frac{\partial \theta_i}{\partial \beta_l} = \frac{-b''(\theta_i)}{a(\phi_i)} \times \frac{1}{b''(\theta_i)} \times \frac{x_{il}}{g'(\mu_i)} = \frac{-x_{il}}{a(\phi_i)g'(\mu_i)}.$$

The second term is

$$\frac{\partial}{\partial \beta_l} \left( \frac{1}{b''(\theta_i)} \right) = -\frac{\partial(b''(\theta_i))}{\partial \beta_l} \frac{1}{(b''(\theta_i))^2} = -\frac{b'''(\theta_i)}{(b''(\theta_i))^2} \frac{\partial \theta_i}{\partial \beta_l} = -\frac{b'''(\theta_i)}{(b''(\theta_i))^3} \frac{x_{il}}{g'(\mu_i)} = -\frac{b'''(\theta_i)}{(V(\mu_i))^3} \frac{x_{il}}{g'(\mu_i)}.$$

The third term is

$$\frac{\partial}{\partial \beta_l} \left( \frac{x_{ij}}{g'(\mu_i)} \right) = -\frac{x_{ij}}{(g'(\mu_i))^2} \frac{\partial(g'(\mu_i))}{\partial \beta_l} = -\frac{x_{ij}g''(\mu_i)}{(g'(\mu_i))^2} \frac{\partial \mu_i}{\partial \beta_l} = -\frac{x_{ij}x_{il}g''(\mu_i)}{(g'(\mu_i))^3},$$

since

$$\frac{\partial \mu_i}{\partial \beta_l} = \frac{\partial(b'(\theta_i))}{\partial \beta_l} = b''(\theta_i) \frac{\partial \theta_i}{\partial \beta_l} = b''(\theta_i) \times \frac{1}{b''(\theta_i)} \times \frac{x_{il}}{g'(\mu_i)} = \frac{x_{il}}{g'(\mu_i)}.$$

Recalling that the Hessian matrix is defined as

$$H(\beta, y_1, \dots, y_n) = \left( \frac{\partial^2 L(\beta)}{\partial \beta_j \partial \beta_l} \right)_{j,l},$$

and using  $b''(\theta) = V(\mu)$ , we get

$$\begin{aligned} \frac{\partial^2 L(\beta)}{\partial \beta_j \partial \beta_l} &= -\sum_{i=1}^n \frac{x_{il}}{a(\phi_i)g'(\mu_i)} \frac{1}{b''(\theta_i)} \frac{x_{ij}}{g'(\mu_i)} - \sum_{i=1}^n \frac{b'''(\theta_i)}{(V(\mu_i))^3} \frac{x_{il}}{g'(\mu_i)} \frac{y_i - b'(\theta_i)}{a(\phi_i)} \frac{x_{ij}}{g'(\mu_i)} \\ &\quad - \sum_{i=1}^n \frac{x_{ij}x_{il}g''(\mu_i)}{(g'(\mu_i))^3} \frac{y_i - b'(\theta_i)}{a(\phi_i)} \frac{1}{b''(\theta_i)} \\ &= -\sum_{i=1}^n \frac{x_{il}x_{ij}}{a(\phi_i)(g'(\mu_i))^2 V(\mu_i)} - \sum_{i=1}^n \frac{b'''(\theta_i)x_{il}x_{ij}(y_i - \mu_i)}{(V(\mu_i))^3 (g'(\mu_i))^2 a(\phi_i)} - \sum_{i=1}^n \frac{x_{ij}x_{il}g''(\mu_i)(y_i - \mu_i)}{(g'(\mu_i))^3 \mu_i a(\phi_i)}. \end{aligned}$$

In practice, we use the expectation of this matrix w.r.t. the random variable  $Y_i$ . This procedure is known as the Fisher scoring method. Hence, two terms will cancel because  $E(Y_i) = \mu_i$ . So

$$\bar{H}(\beta) = E(H(\beta, Y_1, \dots, Y_n)) = \left( -\sum_{i=1}^n \frac{x_{il}x_{ij}}{a(\phi_i)(g'(\mu_i))^2 V(\mu_i)} \right)_{j,l}.$$

This matrix can be rewritten as the product of three matrices  $\bar{H}(\beta) = -X^T W(\beta) X$  where

$$W(\beta) = \begin{pmatrix} \frac{1}{a(\phi_1)(g'(\mu_1))^2 V(\mu_1)} & & \\ & \ddots & \\ & & \frac{1}{a(\phi_n)(g'(\mu_n))^2 V(\mu_n)} \end{pmatrix}, X = \begin{pmatrix} x_{11} & \dots & x_{1p} \\ \vdots & & \vdots \\ x_{n1} & \dots & x_{np} \end{pmatrix}.$$

The (expected) Newton method is

$$\beta^{(k+1)} = \beta^{(k)} + \left( X^T W(\beta^{(k)}) X \right)^{-1} S(\beta^{(k)}).$$

Let us write matricially the score vector

$$S_j(\beta) = \sum_{i=1}^n \frac{y_i - \mu_i}{\phi_i V(\mu_i)} \frac{x_{ij}}{g'(\mu_i)} = \sum_{i=1}^n (y_i - \mu_i) x_{ij} g'(\mu_i) \times \frac{1}{\phi_i (g'(\mu_i))^2 V(\mu_i)} = X^T W(\beta) \tilde{Y}(\beta)$$

where we define a new vector  $\tilde{Y}(\beta) = ((y_i - \mu_i)g'(\mu_i))_i \in \mathbb{R}^n$ . The (expected) Newton method can be reformulated as

$$\beta^{(k+1)} = \beta^{(k)} + \left( X^T W(\beta^{(k)}) X \right)^{-1} X^T W(\beta^{(k)}) \tilde{Y}(\beta^{(k)}).$$

## 1.4 Reformulation as an iterative weighted least square (IWLS) problem

Let us rewrite  $\beta$  as a matrix product

$$\beta = \left( X^T W(\beta^{(k)}) X \right)^{-1} X^T W(\beta^{(k)}) X \beta = \left( X^T W(\beta^{(k)}) X \right)^{-1} X^T W(\beta^{(k)}) \tilde{X},$$

where  $\tilde{X}(\beta) = X\beta$  is the vector of linear predictor  $\eta_i$ . In other words, the (expected) Newton method can be factorized as

$$\beta^{(k+1)} = \left( X^T W(\beta^{(k)}) X \right)^{-1} X^T W(\beta^{(k)}) \left( \tilde{X}(\beta^{(k)}) + \tilde{Y}(\beta^{(k)}) \right) = \left( X^T W(\beta^{(k)}) X \right)^{-1} X^T W(\beta^{(k)}) Z(\beta^{(k)})$$

with a new vector  $Z(\beta) = (\eta_i(\beta) + (y_i - \mu_i(\beta)) g'(\mu_i(\beta)))_i$ .

That is  $\beta^{(k+1)}$  is the solution of a weighted least square problem with weights  $W^{(k)}$ , response vector  $Z^{(k)}$  and explanatory variable  $X^{(k)}$ .

## 1.5 The IWLS Algorithm

The iterative weighted least square algorithm used to fit GLM is as follows

1. Initialization:

- (a) Use original data with a small shift  $\mu_i^{(0)} = y_i + 0.1$  to compute  $\eta_i^{(0)} = g(\mu_i^{(0)})$ .
- (b) Compute working responses  $Z^{(0)} = (\eta_i^{(0)} + (y_i - \mu_i^{(0)}) g'(\mu_i^{(0)}))_i$ .
- (c) Compute working weights  $W^{(0)} = \text{diag}(w_1, \dots, w_n)$  and  $w_i = \frac{1}{a(\phi_i)(g'(\mu_i^{(0)}))^2 V(\mu_i^{(0)})}$ .
- (d) Solve the system to get  $\beta^{(0)}$

$$X^T W^{(0)} X \beta^{(0)} = X^T W^{(0)} Z^{(0)}.$$

2. Iteration: for  $k = 1, \dots, m$  do

- (a) Compute working responses  $Z^{(k)} = (z_i)_i$  and  $z_i = \eta_i(\beta^{(k)}) + (y_i - \mu_i(\beta^{(k)})) g'(\mu_i(\beta^{(k)}))$ .
- (b) Compute working weights  $W^{(k)} = \text{diag}(w_1, \dots, w_n)$  and  $w_i = \frac{1}{a(\phi_i)(g'(\mu_i(\beta^{(k)})))^2 V(\mu_i(\beta^{(k)}))}$ .
- (c) Solve the system to get  $\beta^{(k+1)}$

$$X^T W^{(k)} X \beta^{(k+1)} = X^T W^{(k)} Z^{(k)}.$$

- (d) Verify convergence on the deviance:  $\|Dev(\beta^{(k+1)}) - Dev(\beta^{(k)})\| \leq \epsilon$ .

In practice the linear system  $X^T W^{(k)} X \beta^{(k+1)} = X^T W^{(k)} Z^{(k)}$  is solved via a QR decomposition, see e.g. Green (1984).

## 2 Numerical illustration

In this section, we carry out simple examples of GLMs on simulated datasets in the R statistical software, R Core Team (2017), R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria. URL <https://www.R-project.org/>.

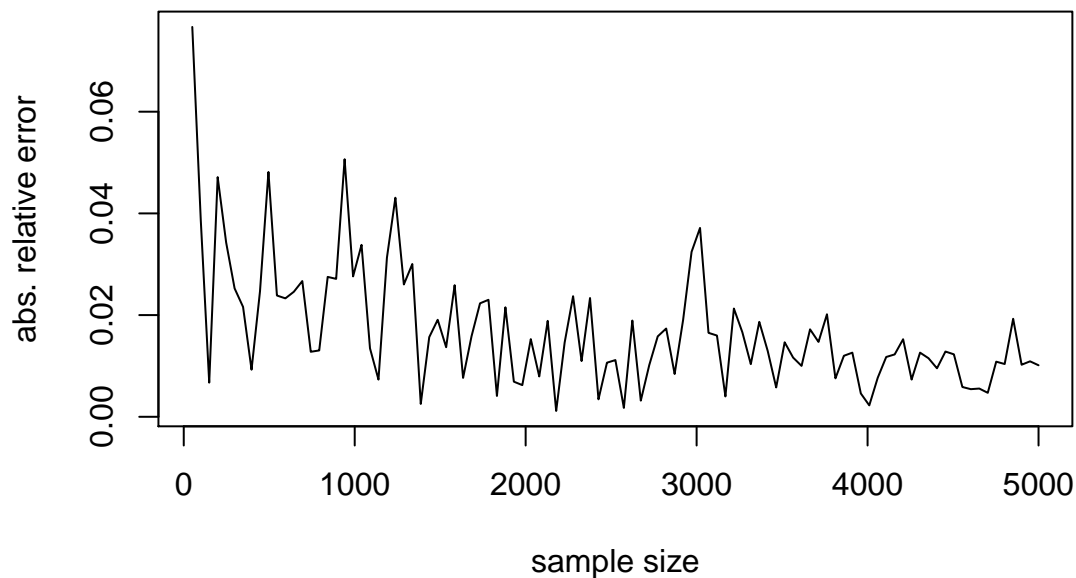
## 2.1 Poisson regression

A Poisson distribution has the following probability mass function  $P(X = x) = \lambda^x e^{-\lambda} / x!$  for  $x \in \mathbb{N}$ . We rewrite as

$$\log(f(x)) = x \log(\lambda) - \log(x!) - \lambda = \frac{x \log(\lambda) - \lambda}{1} - \log(x!).$$

So  $\theta = \log(\lambda) \Leftrightarrow \lambda = e^\theta$ ,  $b(x) = e^x$ ,  $\phi = 1$ ,  $a(x) = x$  and  $c(x, \phi) = -\log(x!)$ . In particular  $(b')^{-1}(x) = \log(x)$ .

Below we make a simple Poisson regression with a single categorical variable where an explicit solution exists. We plot the absolute relative error of the GLM estimator.



## 2.2 Gamma regression

A gamma distribution has the following density function  $f(x) = \frac{\lambda^\alpha x^{\alpha-1} e^{-\lambda x}}{\Gamma(\alpha)}$  for  $x \in \mathbb{X} = \mathbb{R}_+$ ,  $\lambda, \alpha > 0$ . We rewrite as

$$\log(f(x)) = \frac{\frac{-\lambda}{\alpha} x - (-\log(-\frac{-\lambda}{\alpha}))}{1/\alpha} + \alpha \log(\alpha) + (\alpha - 1) \log(x) - \log(\Gamma(\alpha))$$

So  $\theta = \frac{-\lambda}{\alpha}$ ,  $\Theta = \mathbb{R}_-$ ,  $\phi = 1/\alpha$ ,  $a(x) = x$ ,  $b(x) = -\log(-x)$  and

$$c(x, \phi) = \log(1/\phi)/\phi + (1/\phi - 1) \log(x) - \log(\Gamma(1/\phi)).$$

In particular  $(b')^{-1}(x) = 1/x$ . Below we make a simple gamma regression with a single categorical variable where an explicit solution exists. We plot the absolute relative error of the GLM estimator.

