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MCGLM - A Python Library

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Outline

Outline

Preamble

Statistics

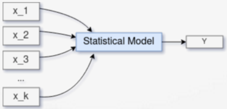
- Statistics has built tools to extract information about data and, consequently, the system that generated it.
- Randomness is an assumption and one of the biggest challenges.
- Statistical models are one of the foremost tools to overcome the inherent randomness in data, countenancing the statistical analysis.

Introduction to Statistical Models

Statistical Models

Statistical models aim to associate a dependent variable y, a.k.a response variable, with a group of independent variables x_i, $i >= 1$.

Statistical Inference leverages statistical model inversely, assessing model's paramaters that are consistent with the dependent data.



Nature might produce distinguish kinds of data.

- Components of response can be independent events.
- Components of response can be dependent events, such as time-series or spatial.
- Components of response can assume real values, positive real values, integer values, or bounded values.

- The first statistical models cover independent data exclusively.
- Over the years, many statistical publications aimed to expand the boundaries of models.
- Nowadays, some models can cover almost all kinds of data.

Outline

Linear Regression is dated to the early nineteenth century. Legendre and Gauss published it.

Statistical Models, History

Linear Regression

Linear Regression is dated to the early nineteenth century. Legendre and Gauss published it.

A vector of observation $\boldsymbol{y}$ with n components is considered independent realizations of a random variable $\boldsymbol{Y}$; the vector $\boldsymbol{\mu}$ defines the mean parameters.
The systematic part of the model specifies the vector $\boldsymbol{\mu}$ by employing a linear operation between regression parameters $\beta_1, ..., \beta_p$ and the covariates. The mathematical notation for the systematic part:

$$\mathrm{E}(Y_i) = \mu_{\mathrm{i}} = \beta_0 + \sum_{j=1}^{p} x_{ij}\beta_j; \qquad i = 1, ..., n.$$

where x_{ij} is the value of the jth covariate for observation i.

Statistical Models, History

Linear Regression

Moreover, as the random part, we assume independence and constant variance of errors. These errors follow a Gaussian distribution with mean 0 and constant variance σ^2.

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The three-part specification

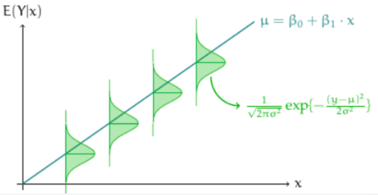
The random component: the components Y have independent Gaussian distribution with $E(\boldsymbol{Y}) = \boldsymbol{\mu}$ and constant variance σ^2;

The systematic component: a linear operation between covariates $x_1, x_2, .., x_p$ and regression parameters produces $\boldsymbol{\eta}$;

The link between the random and the systematic components: $\boldsymbol{\eta} = \boldsymbol{\mu}$;

Statistical Models, History

Linear Regression - A graphical explanation



A graphical explanation for a simple linear regression.

Statistical Models, History

Generalized Linear Models

In 1972, Nelder and Wedderburn went a step further in unifying the theory of statistical modeling and, in particular, regression models, publishing their article on generalized linear models (GLM).

Statistical Models, History

Generalized Linear Models

In 1972, Nelder and Wedderburn went a step further in unifying the theory of statistical modeling and, in particular, regression models, publishing their article on generalized linear models (GLM).
Each component of the random variable Y has a distribution in the exponential family, with density function taking the form

$$\mathrm{f}_y(y;\theta,\phi) = \exp\{(\mathrm{y}\theta - \mathrm{b}(\theta))/\mathrm{a}(\phi) + \mathrm{c}(\mathrm{y},\phi)\}$$

for some specific functions $a(\phi)$, $b(\theta)$ and $c(y,\phi)$. Mean and Variance can be specified as:

$$\mathrm{E}(Y) = b'(\theta). \qquad \mathrm{Var}(Y) = b''(\theta)a(\phi).$$

Statistical Models, History

Generalized Linear Models - Exponential Family

Distribution	Support	Cases
Gaussian	Real Numbers	General Symmetric Distributions.
Binomial(Bernoulli)	Bounded Data	Probability/Odds of an event.
Poisson	Integer Positive	Positive Count Distributions.
Gamma	Real Positive Numbers	Positive Asymmetric Distributions.
Inverse Gaussian	Real Positive Numbers	Positive Asymmetric Distributions.

GLMs relies on three components:

- Linear Predictor by a design matrix;
- Link Function which transforms the $\boldsymbol{\eta}$ into $\boldsymbol{\mu}$;
- Exponential distribution model or a Variance function.

Distribution	Canonical link function	Variance function
Poisson	Log	μ
Binomial	Logit	$\mu(\mu - 1)$
Normal	Identity	1
Gamma	Reciprocal	μ^2
Inverse Gaussian	Reciprocal^2	μ^3

The Maximum-likelihood estimator leverages the underlying distribution to find regression and dispersion parameters that maximizes the product of general likelihood.

The Maximum-likelihood estimator leverages the underlying distribution to find regression and dispersion parameters that maximizes the product of general likelihood. Let Y be a N x 1 response vector, X an N x k design matrix and β a k x 1 regression parameter vector. A mathematical notation for GLM might be specified as:

$$
\begin{aligned}
\mathrm{E}(\mathbf{Y}) &= \boldsymbol{\mu} = g^{-1}(\boldsymbol{X}\boldsymbol{\beta}). \\
\mathrm{Var}(\mathbf{Y}) &= \boldsymbol{\Sigma} = \mathrm{V}(\boldsymbol{\mu}; p)^{\frac{1}{2}}(\boldsymbol{\tau}_0\boldsymbol{I})\mathrm{V}(\boldsymbol{\mu}; p)^{\frac{1}{2}}.
\end{aligned}
$$

where g is the link function, $V(\mu; p) = diag(\vartheta(\mu; p))$, is a diagonal matrix whose main entries are given by the variance function $\vartheta(; p)$ applied elementwise to the vector μ. The I denotes the N x N identity, whereas τ_0 and p are the dispersion and power parameters.

Assumptions

Linearity upon the link function;
The random variable Y is independently distributed as some exponential family distribution;

Statistical Models, History

Generalized Linear Models

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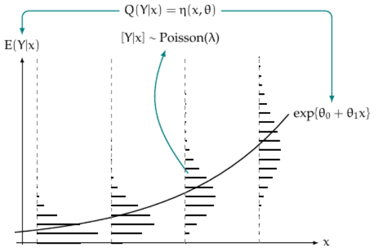

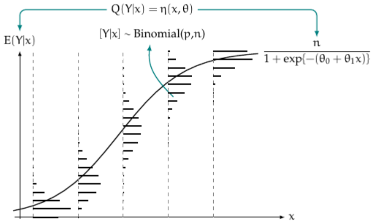

Poisson and Binomial regression.

Statistical Models, History

Quasi-likelihood

In 1974, one of the authors for GLM, Wedderburn, wrote an iconic paper "Quasi-Likelihood Functions, Generalized Linear Models, and the Gauss-Newton Method".

Wedderburn proposed a near likelihood estimator, the quasi-likelihood, which doesn't rely on a distribution model. Yet asymptotically, the convergence is guaranteed.

Quasi-score is an Estimating Equation for Quasi-likelihood functions.

Most of the time, it is unresonable to assume statisticians know the probability model upfront.

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Statistical Models, History

Generalized Estimating Equations

In 1986, Liang and Zeger published the paper "Longitudinal data analysis using generalized linear models", which establishes an extension of generalized linear models to the analysis of longitudinal data.

Statistical Models, History

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For example, the severity of respiratory disease along with the nutritional status, age and family income of children might be observed once every three months for an 18 month period. The dependence of the outcome variable, severity of disease, on the covariates is of interest.

Statistical Models, History

Generalized Estimating Equations

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For example, the severity of respiratory disease along with the nutritional status, age and family income of children might be observed once every three months for an 18 month period. The dependence of the outcome variable, severity of disease, on the covariates is of interest.

This paper introduces estimating equations that give consistent estimates of the regression parameters and of their variances under weak assumptions about the joint distribution. The dispersion parameters remain nuisance.

Statistical Models, History

Generalized Estimating Equations

A correlation matrix establishes the dependence between components of the response variable analyzed.

A list of usual dependence structures for GEEs: independent, autoregressive, exchangeable, unstructured, stationary-M, M-dependent or non-stationary.

Therefore, A GEE has four components:

- Linear Predictor;
- Link function;
- Variance function;
- Correlation Matrix(Dependence Structure).

Copulas

- Copulas can calculate any joint distribution with its marginals, alongside the vital statistical properties of these family distributions.
- Copulas can model the dependence of several random variables. Sklar (1959).
- Estimation by either the classical Maximum Likelihood or a Bayesian-based inference.

Statistical Models, History

Copulas and Mixed Models

Copulas

- Copulas can calculate any joint distribution with its marginals, alongside the vital statistical properties of these family distributions.
- Copulas can model the dependence of several random variables. Sklar (1959).
- Estimation by either the classical Maximum Likelihood or a Bayesian-based inference.

Random Effect Models

- It was introduced by Ronald Fisher back in 1950s to study dependent data. Two level of random components: Fixed Effect and Random Effects.
- Breslow and Clayton (1993) penalized quasi-likelihood.
- Fahrmeir, L. and Lang, S. (2001). Bayesian inference for generalized additive mixed models based on Markov random field priors.

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- MCGLM, 2015. Bonat, Jørgensen; A brand new family of Statistical Models: Multivariate Covariance Generalized Linear Models.
- The model can fit many kinds of dependence, such as longitudinal and spatial dependence. This dependence is specified by the means of dependence matrices and covariance link functions.
- MCGLM can also fit multi-responses at once.

Outline

Project Goals

- This project aims to implement mcglm in Python. Thus far, only R users could access the algorithm.
- The main Python library for statistical models, the statsmodels, implements GEE, Mixed Models and Copulas.
- This brand new-Python library inherits the statsmodels basic methods and interface, delivering a new API that the library itself can wrap.
- The mcglm library leverages numpy, scipy, statsmodels and csr_matrix;
- The numpy uses BLAS and LAPACK, such as R packages.
- The mcglm library implements some dependencies matrices as moving averages, mixed models, and the independent case through methods: mc_ma(), mc_mixed() and mc_id().

Outline

Preamble

Statistical Models, History

Project Goals

Multivariate Covariance Generalized Linear Models

The brand-new library, a Python Implementation

To demonstrate the library usage on two actual examples

The next steps

Multivariate Covariance Generalized Linear Models

Mathematical Notation

Let X_r denote an N x k_r a design matrix and β_r a k_r x 1 regression parameter vector for the response r. The mean and variance for MCGLM are:

$$\begin{aligned} \mathrm{E}(\mathbf{Y}) &= \mathbf{M} = \{g_1^{-1}(\boldsymbol{X}_1\boldsymbol{\beta}_1), \ldots, g_R^{-1}(\boldsymbol{X}_R\boldsymbol{\beta}_R)\}. \\ \mathrm{Var}(\mathbf{Y}) &= \boldsymbol{C} = \boldsymbol{\Sigma}_R \overset{G}{\otimes} \boldsymbol{\Sigma}_b. \end{aligned}$$

The component C is calculated by means of generalized product Kronecker

$$\boldsymbol{\Sigma}_R \overset{G}{\otimes} \boldsymbol{\Sigma}_b = \mathrm{Bdiag}(\tilde{\boldsymbol{\Sigma}}_1, \ldots, \tilde{\boldsymbol{\Sigma}}_R)(\boldsymbol{\Sigma}_b \otimes \boldsymbol{I})\mathrm{Bdiag}(\tilde{\boldsymbol{\Sigma}}_1^T, \ldots, \tilde{\boldsymbol{\Sigma}}_R^T)$$

The matrix $\tilde{\boldsymbol{\Sigma}}_r$ denotes a lower triangular matrix, resulting of a Cholesky decomposition from $\boldsymbol{\Sigma}_r$. The operator Bdiag itemize a block diagonal matriz e $\boldsymbol{I}$ denotes $N \times N$ an identity matrix.

The matrix $\boldsymbol{\Sigma}_r$, a.k.a covariance matrix of the outcome r, is defined by:

$$\boldsymbol{\Sigma}_r = \mathrm{V}(\boldsymbol{\mu}_r; p_r)^{\frac{1}{2}}(\boldsymbol{\Omega}(\boldsymbol{\tau}_r))\mathrm{V}(\boldsymbol{\mu}_r; p_r)^{\frac{1}{2}}.$$

Where $\mathrm{V}(\boldsymbol{\mu}_r; p_r) = \mathrm{diag}(\vartheta(\boldsymbol{\mu}_r; p_r))$ is a diagonal matrix, whose entries are defined by means of variance functions. Each function distinguishes marginal distribution. Finally, the operation omega $\boldsymbol{\Omega}(\boldsymbol{\tau}_r)$, the matrix linear matricial, describes the covariance inhrently to the mean structure.

$$\boldsymbol{\Omega}(\boldsymbol{\tau}_r) = h_r^{-1}(\tau_{r0}Z_{r0} + \cdots + \tau_{rD}Z_{rD}).$$

Where h is a covariance link function specified. The matrices Z specifies the data dependencies.

Finally, Σ_b the R x R correlation matrix between outcomes, calculated by the Pearson estimator.

Getting back to the mean.

$$\mathrm{E}(\mathbf{Y}) \quad = \quad \mathbf{M} = \{g_1^{-1}(\boldsymbol{X}_1\boldsymbol{\beta}_1), \ldots, g_r^{-1}(\boldsymbol{X}_r\boldsymbol{\beta}_r)\}.$$

Where M is a vector of $(\mu_1, .., \mu_r)$. The vector β_r is the regressor vector for the outcome r, and g_r^{-1} is the inverse of the link function for the outcome r.

MCGLM five components:

- Linear Predictor;
- Link function;
- Variance function;
- Z matrices for the dependence specification;
- Covariance link function.

Multivariate Covariance Generalized Linear Models

Estimation and Inference

- MCGLM implements the second-moment assumptions, grounded on two moments for the estimation: the mean and the variance.
- There are two optimization algorithms and two estimating equations.
- The estimation produces two groups of parameters: regression and dispersion.

Multivariate Covariance Generalized Linear Models

The second-moment assumptions

Mean - Quasi-score function

$$\psi_{\boldsymbol{\beta}}(\boldsymbol{\beta}, \boldsymbol{\lambda}) = \boldsymbol{D}^\top \boldsymbol{C}^{-1}(\mathcal{Y} - \mathcal{M}).$$

Where $\boldsymbol{D} = \nabla_{\boldsymbol{\beta}} \mathcal{M}$ and $\nabla_{\boldsymbol{\beta}}$ denotes the gradient operator.
Fisher scoring algorithm.
Finally, matrices *sensitivity* and *variability* of $\psi_{\boldsymbol{\beta}}$ are given by:

$$\mathrm{S}_{\boldsymbol{\beta}} = -\boldsymbol{D}^\top \boldsymbol{C}^{-1} \boldsymbol{D} \quad \text{and} \quad \mathrm{V}_{\boldsymbol{\beta}} = \boldsymbol{D}^\top \boldsymbol{C}^{-1} \boldsymbol{D}.$$

Variance - Pearson Estimating Equation Function

$$\psi_{\boldsymbol{\lambda}}(\boldsymbol{\beta}, \boldsymbol{\lambda}) = \mathrm{tr}(W_{\boldsymbol{\lambda}}(\boldsymbol{r}^\top \boldsymbol{r} - \boldsymbol{C})).$$

Where $W_{\boldsymbol{\lambda}_i} = -\partial \boldsymbol{C}^{-1}/\partial \boldsymbol{\lambda}_i$ and $\boldsymbol{r} = \mathcal{Y} - \mathcal{M}$ for the dispersion parameters.

Modified Chaser algorithm.

The entry (i, j) of the $Q \times Q$ *sensitivity* matrix of $\psi_{\boldsymbol{\lambda}}$ is given by,

$$\mathrm{S}_{\boldsymbol{\lambda}_{ij}} = \mathrm{E}\left(\frac{\partial}{\partial \boldsymbol{\lambda}_i}\psi_{\boldsymbol{\lambda}_j}\right) = -\mathrm{tr}\left(W_{\boldsymbol{\lambda}_i}\boldsymbol{C}W_{\boldsymbol{\lambda}_j}\boldsymbol{C}\right).$$

The entry (i, j) of the $Q \times Q$ *variability* matrix of $\psi_{\boldsymbol{\lambda}}$ is given by

$$\mathrm{V}_{\boldsymbol{\lambda}_{ij}} = \mathrm{Cov}(\psi_{\boldsymbol{\lambda}_i}, \psi_{\boldsymbol{\lambda}_j}) = 2\mathrm{tr}(W_{\boldsymbol{\lambda}_i}\boldsymbol{C}W_{\boldsymbol{\lambda}_j}\boldsymbol{C}) + \sum_{l=1}^{NR} k_l^{(4)}(W_{\boldsymbol{\lambda}_i})_{ll}(W_{\boldsymbol{\lambda}_j})_{ll},$$

Multivariate Covariance Generalized Linear Models

The second-moment assumptions

The python mcglm library implements modified chaser algorithm to solve the system of equations $\psi_{\boldsymbol{\beta}} = \mathbf{0}$ and $\psi_{\boldsymbol{\lambda}} = \mathbf{0}$, defined by:

$$
\begin{aligned}
\boldsymbol{\beta}^{(i+1)} &= \boldsymbol{\beta}^{(i)} - \mathrm{S}_{\boldsymbol{\beta}}^{-1}\psi_{\boldsymbol{\beta}}(\boldsymbol{\beta}^{(i)}, \boldsymbol{\lambda}^{(i)}) \\
\boldsymbol{\lambda}^{(i+1)} &= \boldsymbol{\lambda}^{(i)} - \alpha\mathrm{S}_{\boldsymbol{\lambda}}^{-1}\psi_{\boldsymbol{\lambda}}(\boldsymbol{\beta}^{(i+1)}, \boldsymbol{\lambda}^{(i)}).
\end{aligned} \tag{1}
$$

The second-moment assumptions derive two group of parameters: $\boldsymbol{\theta} = (\boldsymbol{\beta}^\top, \boldsymbol{\lambda}^\top)^\top$, where $\boldsymbol{\beta} = (\boldsymbol{\beta}_1^\top, \ldots, \boldsymbol{\beta}_R^\top)^\top$ and $\boldsymbol{\lambda} = (\rho_1, \ldots, \rho_{R(R-1)/2}, p_1, \ldots, p_R, \boldsymbol{\tau}_1^\top, \ldots, \boldsymbol{\tau}_R^\top)^\top$. The dispersion vector ρ, p and τ refer to correlation coefficients, power and dispersion parameters, respectively.

Let $\hat{\boldsymbol{\theta}} = (\hat{\boldsymbol{\beta}}^\top, \hat{\boldsymbol{\lambda}}^\top)^\top$ the estimator of estimating equation of $\boldsymbol{\theta}$. The asymptotic distribution of $\hat{\boldsymbol{\theta}}$ is:

$$\hat{\boldsymbol{\theta}} \sim \mathrm{N}(\boldsymbol{\theta}, \mathrm{J}_{\boldsymbol{\theta}}^{-1})$$

where $\mathrm{J}_{\boldsymbol{\theta}}^{-1}$ is the inverse of Godambe matrix,

$$\mathrm{J}_{\boldsymbol{\theta}}^{-1} = \mathrm{S}_{\boldsymbol{\theta}}^{-1} \mathrm{V}_{\boldsymbol{\theta}} \mathrm{S}_{\boldsymbol{\theta}}^{-T},$$

where $\mathrm{S}_{\boldsymbol{\theta}}^{-T} = (\mathrm{S}_{\boldsymbol{\theta}}^{-1})^T$.

Multivariate Covariance Generalized Linear Models

Specification - Candidates, from R package.

- Link Function: identity, logit, log, probit, cauchy, cloglog, loglog, negative binomial, reciprocal.
- Variance Function: constant, binomialP, binomialPQ, tweedie, geometric tweedie, poisson tweedie.
- Covariance Function: identity, expm, inverse.

Multivariate Covariance Generalized Linear Models

Matrix Linear Predictor - Feasible Models

- linear regression.
- quasi likelihood models.
- double generalized linear models.
- linear mixed model.
- moving average models.
- exchangeable or compound symmetry.
- unstructured models(popular in longitudinal data analysis).
- conditional autoregressive models(time series, spatial and space-time data).
- models in quantitative genetic and phylogenetic.
- models for Twin and family data.

Multivariate Covariance Generalized Linear Models

Matrix Linear Predictor - Examples

The compound symmetry or exchangeable structure.

$$\boldsymbol{\Omega}(\boldsymbol{\tau}) = \tau_0 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \tau_1 \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}.$$

Unstructured.

$$\boldsymbol{\Omega}(\boldsymbol{\tau}) = \tau_0 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \tau_1 \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \tau_2 \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} + \tau_3 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

Moving Average, 2-window.

$$\boldsymbol{\Omega}(\boldsymbol{\tau}) = \tau_0 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \tau_1 \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} + \tau_2 \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}.$$

Gaussian Pseudo Log Likelihood (plogLik):

$$\text{plogLik}(\boldsymbol{\theta}) = -\frac{NR}{2}\log(2\pi) - \frac{1}{2}\log|\hat{\boldsymbol{C}}| - (\mathcal{Y} - \hat{\mathcal{M}})^\top \hat{\boldsymbol{C}}^{-1}(\mathcal{Y} - \hat{\mathcal{M}}).$$

The pseudo *Akaike* information criterion pAIC is given by

$$\text{pAIC}(\boldsymbol{\theta}) = 2(P + Q) - 2\text{plogLik}(\boldsymbol{\theta}).$$

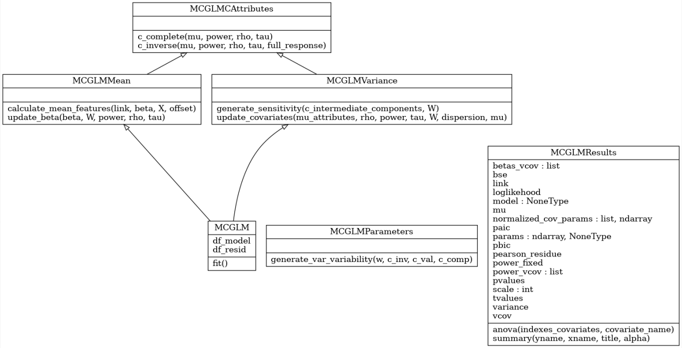
The pseudo *Bayesian* information criterion pBIC is given by

$$\text{pBIC}(\boldsymbol{\theta}) = logNR(P + Q) - 2\text{plogLik}(\boldsymbol{\theta}).$$

Outline

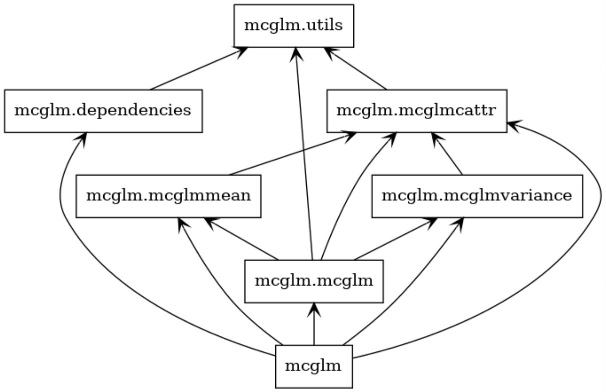
Python Implementation

Classes



Python Implementation

Packages



Python Implementation

Interface

```
from mcglm import MCGLM, mc_id

mcglm = MCGLM(endog=y, exog=X, z=[mc_id(X)], link="log", variance="tweedie",
power=2)

mcglmresults = mcglm.fit()
mcglmresults.summary()
```

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Python Implementation

Unit Testing

92% of test coverage

```
============================================ 26 passed in 2.80s ============================================
jean@pop-os:~/dev/Github/mcglm$ poetry run coverage report
Name                          Stmts   Miss  Cover
-------------------------------------------------
mcglm/__init__.py                 7      0   100%
mcglm/dependencies.py            43      3    93%
mcglm/mcglm.py                  473     75    84%
mcglm/mcglmcattr.py             252     21    92%
mcglm/mcglmmean.py               55      0   100%
mcglm/mcglmvariance.py           36      0   100%
mcglm/utils.py                   20      0   100%
tests/__init__.py                 0      0   100%
tests/test_dependencies.py       32      0   100%
tests/test_mcglm.py             283      0   100%
-------------------------------------------------
TOTAL                          1201     99    92%
```

Python Implementation

Available Functions

- Link Functions: logit, identity, log, probit, cauchy, cloglog, loglog, negative binomial, reciprocal.
- Variance Functions: constant, tweedie, binomialP, binomialPQ, geom_tweedie, poisson_tweedie.
- Covariance Functions: identity.

Python Implementation

Variance Function - options

Variance Function	Formula
constant	1
tweedie	μ^p
binomialP	$\mu(1-\mu)$
binomialPQ	$\mu^p(1-\mu)^q$
poisson_tweedie	$\mu + \mu^p$
geom_tweedie	$\mu^2 + \mu^p$

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To demonstrate the library usage on two actual examples.

https://github.com/jeancmaia/mcglm/blob/main/nbks/qualification_examples.ipynb

Outline

The next steps

Tasks to be accomplished

- I aim to sustain my final defense by the second week of January 2023;
- To craft and publish open and practical documentation for users on `medium.com`;
- To refine the article for submitting to a scientific journal;
- To apply the final suggestions of my board of examiners;