



Semiparametric Vector Generalized Linear Models.

Estimation and Computation

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June 7, 2023

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Outline of talk



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Motivating Example

Proposed Model

Fitting the Model

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Introduction

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A Generalized Linear Model (GLM) for modelling data

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- A random component: a reference distributions for Y which originates from an exponential family.
- A systematic component: a linear predictor $\eta_i = \mathbf{X}_i^T \boldsymbol{\beta}$
- A link function: A function which maps $\mathbb{E}[Y_i | \mathbf{X}_i] = \mu_i$ to η_i . In most cases it is more convenient to use the inverse link function $g^{-1}(\mu_i) = \eta_i$.

Common GLMS



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- Poisson Regression: Which assumes $Y_i \sim \text{Po}(\mu_i)$ and $g(\mu_i) = \log(\mathbf{X}_i^T \boldsymbol{\beta})$.
- Logistic Regression: Which assumes $Y_i \sim \text{Ber}(\mu_i)$ and $g(\mu_i) = \frac{\log(\mathbf{X}_i^T \boldsymbol{\beta})}{1 - \log(\mathbf{X}_i^T \boldsymbol{\beta})}$.

A VGLM (Vector Generalized Linear Model) aims to generalize GLMs to multivariate responses, however, multivariate generalizations of common families of probability distributions (e.g., poisson, gamma, ...) are difficult to construct.

Problems Modelling with parametric GLMs and VGLMs



Common problems that occur with parametric modelling

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- requires correct specification of the mean-variance relationship

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- requires correct specification of the mean-variance relationship
- observed data often exhibit over-or under-dispersion relative to the postulated model

For multivariate data, problems arise when specifying a parametric distribution and the response covariance structure. For most cases there is no standard parametric model which could produce a given dataset.

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Motivating Example (Butterfly Dataset)



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Table 1: Snippet of Butterfly Counts for the 3 most common species (Hui et al. 2013; Oliver, Prudic and Collinge 2006)

site	Pieris.rapae	Colias.philodice	Colias.eurytheme	building	vegetation	habitat
1	0	0	0	2.1	10.8	mixed
2	1	1	2	2.1	10.8	mixed
3	1	1	2	19.8	1.7	mixed
4	0	2	1	5.3	0	mixed
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Motivating Example (Butterfly Dataset)



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We would like to fit a joint model, as species could complement or compete with each other within a site.

However, no multivariate generalisation of the poisson distribution allows for both positive and negatively correlated response components.

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This model is a vector generalisation of a Semiparametric Generalized Linear Model ¹, which is based on an exponential tilt reformulation of the joint distribution from which the data originates for which the response distribution F remains unspecified.

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This model is a vector generalisation of a Semiparametric Generalized Linear Model ¹, which is based on an exponential tilt reformulation of the joint distribution from which the data originates for which the response distribution F remains unspecified.

This allows arbitrary nonparametric response distribution parameter F and the mean model parameters β to be simultaneously estimated without loss of information.

¹(P. J. Rathouz and Gao 2009; Huang and P. Rathouz 2012; Huang 2014)

Proposed Model



Given data

$$(\mathbf{Y}_i, \mathbf{X}_i) \in \mathcal{Y} \times \mathcal{X} \subset \mathbb{R}^K \times \mathbb{R}^q, i = 1, \dots, n$$

Proposed Model



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$$(\mathbf{Y}_i, \mathbf{X}_i) \in \mathcal{Y} \times \mathcal{X} \subset \mathbb{R}^K \times \mathbb{R}^q, i = 1, \dots, n$$

Assume these are independent samples originating from some multivariate exponential family. The joint density can be written in the form

$$dF_i(\mathbf{y}) = \exp\{b_i + \boldsymbol{\theta}_i^T \mathbf{y}\} dF(\mathbf{y}), \quad i = 1, \dots, n$$

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Here

- b_i are each observations normalising constant,

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Given data

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Here

- b_i are each observations normalising constant,
- $dF_i(\mathbf{y})$ is an exponential tilt of the response distribution $dF(\mathbf{y})$,
- where the amount of tilting $\boldsymbol{\theta}$ determined by the mean $\boldsymbol{\mu}(\mathbf{X}_i^T \boldsymbol{\beta})$ of the observation \mathbf{Y}_i .

The normalising constants $b_i = b(\mathbf{X}_i, \beta, F)$ are defined to be

$$b(\mathbf{X}_i, \beta, F) = -\log \left\{ \int_{\mathcal{Y}} \exp\{\boldsymbol{\theta}_i^T \mathbf{y}\} dF(\mathbf{y}) \right\},$$

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and the vector of tilt parameters $\boldsymbol{\theta}_i = \boldsymbol{\theta}(\mathbf{X}_i, \beta, F) \in \mathbb{R}^K$ is the implicit solution to

$$\mu_{(k)}(\mathbf{X}_{(k)}^T \beta_{(k)}) = \int_{\mathcal{Y}} y_{(k)} \exp\{b_i + \boldsymbol{\theta}_i^T \mathbf{y}\} dF(\mathbf{y}), \quad k = 1, \dots, K$$

Semiparametric Extension



This joint density has the log-likelihood

$$\ell(\beta, F|\mathbf{X}, \mathbf{Y}) = \sum_{i=1}^n \left\{ \log dF(\mathbf{Y}_i) + b_i + \boldsymbol{\theta}_i^T \mathbf{Y}_i \right\}$$

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One way to estimate the densities $dF(\mathbf{Y}_i)$ is by replacing them with the histogram estimators p_i , which are assigned to values in the observed support $\{\mathbf{Y}_i \in \mathbb{R}^k | i = 1, 2, \dots, n\}$

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This produces empirical log-likelihood.

$$\ell(\beta, \mathbf{p}) = \sum_{i=1}^n \log p_i + b_i + \boldsymbol{\theta}_i^T \mathbf{Y}_i$$

Estimation of β and \boldsymbol{p}



$(\hat{\beta}, \hat{\boldsymbol{p}})$ are then the joint maximisers of the empirical log likelihood.

$$(\hat{\beta}, \hat{\boldsymbol{p}}) = \arg \max \ell(\boldsymbol{\beta}, \boldsymbol{p})$$

Estimation of β and p



Subject to empirical analogous of the normalising constraints

$$1 = \sum_{i=1}^n p_i \exp\{b_j + \boldsymbol{\theta}_j^T \mathbf{Y}_i\}, \quad j = 1, 2, 3, \dots, n$$

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$$1 = \sum_{i=1}^n p_i \exp\{b_j + \theta_j^T \mathbf{Y}_i\}, \quad j = 1, 2, 3, \dots, n$$

and the mean constraints

$$\mu_{(k)}(\mathbf{X}_{(k)j}^T \beta_{(k)}) = \sum_{i=1}^n p_i Y_{(k)i} \exp\{b_j + \theta_j^T \mathbf{Y}_i\} \quad j = 1, \dots, n, k = 1, \dots, K$$

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Currently the model is fit computationally in MATLAB using non-linear constrained optimization to maximise the empirical log-likelihood. ²

²The code is available at [github](#).

Constraints



For n observations of a K dimensional response $\mathbf{Y}_i \in \mathbb{R}^K$ the optimization simultaneously solves for $Q + n(2 + K)$ parameters.

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For n observations of a K dimensional response $\mathbf{Y}_i \in \mathbb{R}^K$ the optimization simultaneously solves for $Q + n(2 + K)$ parameters.

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which are subject to $n(K + 1)$ mean and normalising constraints.

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Butterfly Dataset



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$$\mu_{(k)i} = \mathbb{E}[Y_{(k)i} | \mathbf{X}_i] = \exp\{\mathbf{X}_i^T \boldsymbol{\beta}_{(k)}\},$$
$$i = 1, 2, \dots, 66, \quad k = 1, 2, \dots, 14$$

```
butterfly = fit_vspglm(...  
  ["colias.philodice ~ (building,urban,habitat)",...  
  "pieris.rapae ~ (building, urban, habitat)", ...  
  "colias.eurytheme ~ (building, urban, habitat)"], ...  
  tbl, {'log', 'log', 'log'})
```

Figure 1: Formula Syntax to fit 3 separate unconstrained models using the same covariates and log link functions

Butterfly Dataset

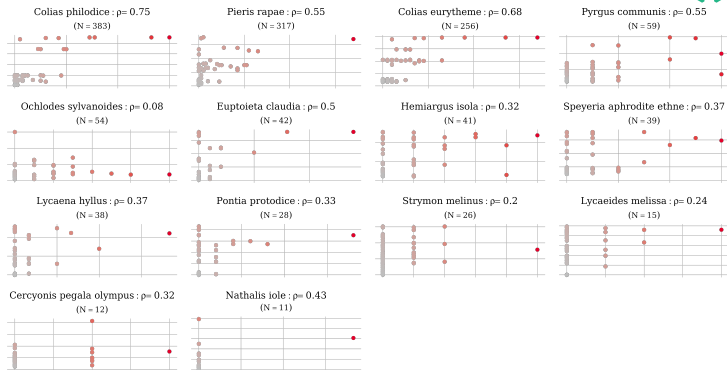


Figure 2: Predictions (y-axis) vs Observed counts (x-axis)

Butterfly Dataset

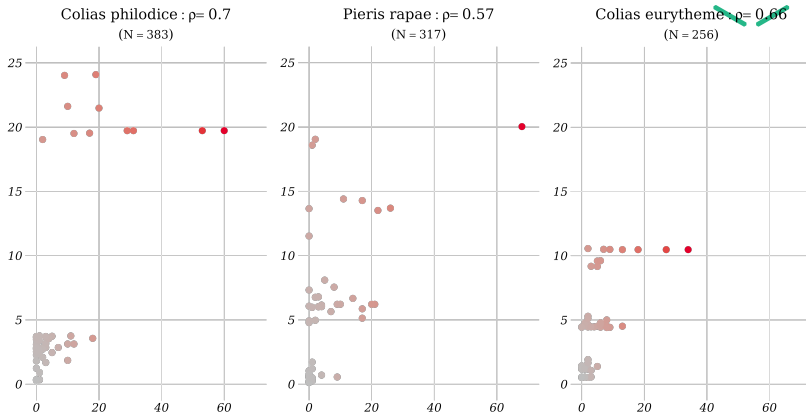


Figure 3: Predictions (y-axis) vs Observed counts (x-axis) for the 3 butterfly species with the greatest number of observed counts

Sorbinil Dataset



Contains $n = 41$ observations of itching scores (Y_L, Y_R) for the left and right eye after the application of sorbinil or a placebo, measured on a 9 point Likert scale between 0 and 4 with increments of 0.5.

Table 3: Snippet of Sorbinil dataset (Rosner, Glynn and Lee 2006)

$n = 6$		$n = 14$		$n = 14$		$n = 7$	
Sorbinil Left	Sorbinil Right	Sorbinil Left	Placebo Right	Placebo Left	Sorbinil Right	Placebo Left	Placebo Right
2	2	1	1.5	2.5	2	3	3
1	1	2	2.5	2.5	2.5	2	3
0.5	2	3	1	3	3	2.5	2.5
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots

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The following symmetric model was found to be adequate

$$\mu_L = \beta_0 + \beta_1 \mathcal{I}_L, \quad \mu_R = \beta_0 + \beta_1 \mathcal{I}_R$$

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$$\mu_L = \beta_0 + \beta_1 \mathcal{I}_L, \quad \mu_R = \beta_0 + \beta_1 \mathcal{I}_R$$

This model finds a significant effect that sorbinil reduces itching scores by 0.43.

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$$\mu_L = \beta_0 + \beta_1 \mathcal{I}_L, \quad \mu_R = \beta_0 + \beta_1 \mathcal{I}_R$$

This model finds a significant effect that sorbinil reduces itching scores by 0.43.

The code to fit this symmetric model is

```
sorbinil = fit_vspglm(["(Y_L, Y_R) ~ (I_L & I_R)"], tbl, {'id'})
```

Sorbinil Dataset

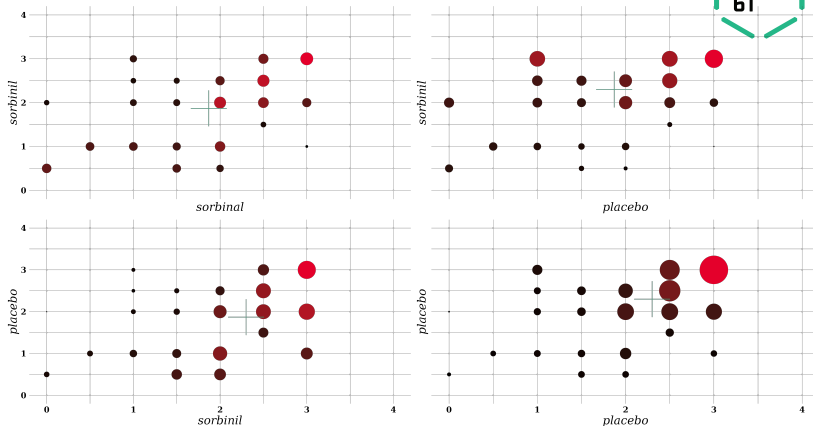








Figure 4: Reweighted Sorbinil pmf at group medians (left eye = y axis, right eye = x axis). Medians are indicated by the green cross. Areas with greater probability mass colored in vermilion.

-  Huang, Alan (2014). "Joint estimation of the mean and error distribution in generalized linear models". In: *Journal of the American Statistical Association* 109.505, pp. 186–196.
-  Huang, Alan and Paul Rathouz (2012). "Proportional likelihood ratio models for mean regression". In: *Biometrika* 99.1, pp. 223–229.
-  Hui, Francis K. et al. (2013). "To mix or not to mix: comparing the predictive performance of mixture models vs. separate species distribution models". In: *Ecology* 94.9, pp. 1913–1919.
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-  Rathouz, Paul J. and Liping Gao (2009). "Generalized linear models with unspecified reference distribution". In: *Biostatistics* 10.2, pp. 205–218.
-  Rosner, Bernard, Robert J Glynn and Mei-Ling T Lee (2006). "Extension of the rank sum test for clustered data: Two-group comparisons with group membership defined at the subunit level". In: *Biometrics* 62.4, pp. 1251–1259.

Trivariate Poisson Model



$$\alpha \sim \mathcal{N}(0, \sigma_0^2), \quad \sigma \in \mathbb{R}_+$$

$$\mathbf{X} \sim \text{U}[-1, 1]^3$$

$$Y_1 | \alpha, \mathbf{X}_{(1)} \sim \text{Pois}(\exp(\mathbf{X}_{(1)}^T \boldsymbol{\beta}_{(1)} + \alpha))$$

$$Y_2 | \alpha, \mathbf{X}_{(2)} \sim \text{Pois}(\exp(\mathbf{X}_{(2)}^T \boldsymbol{\beta}_{(2)} + 0.5\alpha))$$

$$Y_3 | \alpha, \mathbf{X}_{(3)} \sim \text{Pois}(\exp(\mathbf{X}_{(3)}^T \boldsymbol{\beta}_{(3)} - 0.3\alpha))$$

Trivariate Poisson Simulation Results



Table 4: Simulation results for trivariate Poisson model using a sample size of $n = 200$ and $N = 1000$ simulations

β	$\hat{\beta}$	$ \beta - \hat{\beta} $	Errors		$p \leq 0.05$	CI		
			$\hat{\sigma}$	$\text{se}(\hat{\beta})$		90%	95%	99%
0.4	0.40	0.004	0.13	0.12	0.88	0.89	0.94	0.99
-0.8	-0.79	0.002	0.13	0.14	0.99	0.93	0.96	0.99
0	0.001	0.001	0.13	0.12	0.05	0.89	0.95	0.99

Trivariate Mixed Effects Simulation



$$\alpha \sim \mathcal{N}(0, \sigma_0^2)$$

$$\mathbf{X} \sim \text{U}[-1, 1]^3$$

$$\mathbf{Y}_1 | \mathbf{X}_{(1)}, \alpha \sim \mathcal{N}(\mathbf{X}_{(1)}^T \boldsymbol{\beta}_{(1)} + \alpha, \sigma_1^2)$$

$$\mathbf{Y}_2 | \mathbf{X}_{(2)}, \alpha \sim \text{Pois}(\exp(\mathbf{X}_{(2)}^T \boldsymbol{\beta}_{(2)} + 0.5\alpha))$$

$$\mathbf{Y}_3 | \mathbf{X}_{(3)}, \alpha \sim \text{Gamma}(\lambda, \exp(\mathbf{X}_{(3)}^T \boldsymbol{\beta}_{(3)} - 0.3\alpha))$$

Trivariate Mixed Effects Simulation Results



Table 5: Simulation results for trivariate mixed effects model using a sample size of $n = 200$ and $N = 1000$ simulations

Margin	β	$\hat{\beta}$	$ \beta - \hat{\beta} $	Errors		$p \leq 0.05$	CI			
				$\hat{\sigma}$	$\text{se}(\hat{\beta})$			90%	95%	99%
Normal	1	1.005	0.0058	0.17	0.18	1	0.90	0.95	0.99	
Poisson	-0.5	-0.49	0.0005	0.13	0.13	0.96	0.83	0.88	0.93	
Gamma	0.4	0.39	0.004	0.12	0.13	0.85	0.89	0.93	0.97	

Multivariate Normal Simulation Results



Table 6: Simulation results for bivariate normal model using sample size of $n = 200$ and $N = 1000$ simulations

β	$\hat{\beta}$	$ \beta - \hat{\beta} $	Errors		$p \leq 0.05$	CI		
			$\hat{\sigma}$	$\text{se}(\hat{\beta})$		90%	95%	99%
-1	-0.99	0.0004	0.11	0.11	1	0.91	0.95	0.99
0	-0.0004	0.0004	0.11	0.11	0.05	0.90	0.95	0.99
0.5	0.49	0.009	0.14	0.13	0.95	0.88	0.94	0.98
2.2	2.19	0.003	0.14	0.14	1	0.90	0.94	0.98