Semiparametric Vector Generalized Linear Models.

Estimation and Computation

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Outline of talk

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GLMs

A Generalized Linear Model (GLM) for modelling data

$$(Y_i, \boldsymbol{X}_i) \in \mathcal{Y} \times \mathcal{X} \subset \mathbb{R} \times \mathbb{R}^q, i = 1, \ldots, n$$

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

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- Poisson Regression: Which assumes $Y_i \sim \mathrm{Po}(\mu_{\mathrm{i}})$ and $g(\mu_i) = \log(\mu_i) = \eta_i$ $(g^{-1}(\eta_i) = \exp\{\boldsymbol{X}_i^T \boldsymbol{\beta}\} = \mu_i)$.

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

VGLMs

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.

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Common problems that occur with parametric modelling

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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)

This dataset contains 66 counts of 14 species of butterflies in Boulder Colorado, USA.

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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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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Vector Generalisation

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

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Vector Generalisation

This model is a vector generalisation of a Semiparametric Generalized Linear Model [1], which is based on a 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 $\boldsymbol{\beta}$ 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

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

Proposed Model

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

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

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

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Here

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

Model Tilt Parameters

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

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

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

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

Semiparametric Extension

This joint density has the log-likelihood

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

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

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This produces empirical log-likelihood.

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

Estimation of β and p

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

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

Estimation of β and p

Subject to empirical analogous of the normalising constraints

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

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and the mean constraints

$$\mu_{(k)}(\boldsymbol{X}_{(k)j}^T \boldsymbol{\beta}_{(k)}) = \sum_{i=1}^{n} p_i Y_{(k)i} \exp\{b_j + \boldsymbol{\theta}_j^T \boldsymbol{Y}_i\} \quad j = 1, \ldots, n, k = 1, \ldots, K$$

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Code

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

[2] The code is available at github.

Constraints

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

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

Butterfly Dataset

```
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

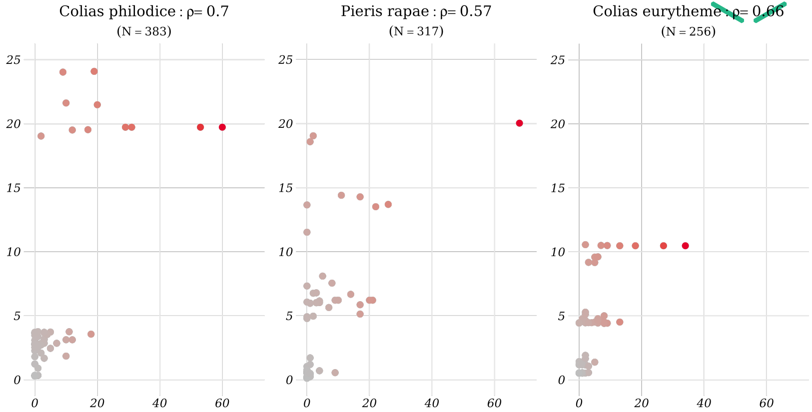

Figure 2: Predictions (y-axis) vs Observed counts (x-axis) for the 3 butterfly species with the greatest number of observed counts

Butterfly Dataset (14d)

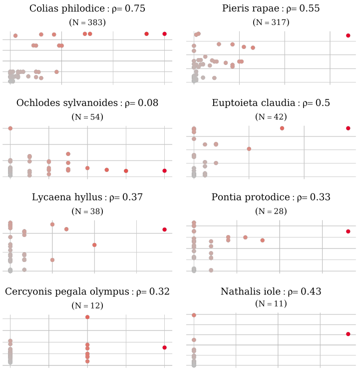

Figure 3: Predictions (y-axis) vs Observed counts (x-axis)

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
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

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

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The code to fit this symmetric model is

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

Sorbinil Dataset

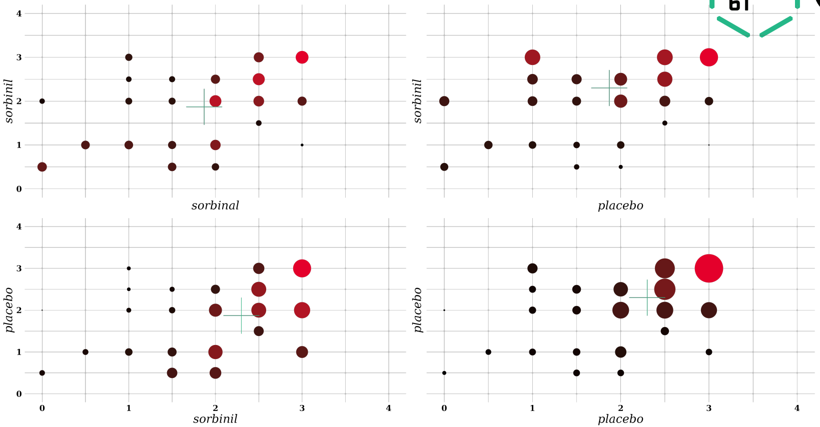

Figure 4: Reweighted Sorbinal pmf at group medians (left eye = y axis, right eye = x axis). Medians are indicated by the green cross. Areas with greater probability mass colored in vermillion.

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Trivariate Poisson Model

$$
\begin{aligned}
\alpha &\sim \mathcal{N}(0, \sigma_0^2), \quad \sigma \in \mathbb{R}_+ \\
\boldsymbol{X} &\sim \ \mathrm{U}[-1, 1]^3 \\
Y_1 | \alpha, \boldsymbol{X}_{(1)} &\sim \mathrm{Pois}(\exp(\boldsymbol{X}_{(1)}^T \boldsymbol{\beta}_{(1)} + \alpha)) \\
Y_2 | \alpha, \boldsymbol{X}_{(2)} &\sim \mathrm{Pois}(\exp(\boldsymbol{X}_{(2)}^T \boldsymbol{\beta}_{(2)} + 0.5\alpha)) \\
Y_3 | \alpha, \boldsymbol{X}_{(3)} &\sim \mathrm{Pois}(\exp(\boldsymbol{X}_{(3)}^T \boldsymbol{\beta}_{(3)} - 0.3\alpha))
\end{aligned}
$$

Trivariate Poisson Simulation Results

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

β	$\hat{\beta}$	$\lvert\beta - \hat{\beta}\rvert$	Errors		$p \leqslant 0.05$	CI		
			$\hat{\sigma}$	$\bar{se}(\hat{\beta})$		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

$$
\begin{aligned}
\alpha &\sim \mathcal{N}(0,\ \sigma_0^2) \\
\boldsymbol{X} &\sim \mathrm{U}[-1,1]^3 \\
\boldsymbol{Y}_1 | \boldsymbol{X}_{(1)}, \alpha &\sim \mathcal{N}(\boldsymbol{X}_{(1)}^T \boldsymbol{\beta}_{(1)} + \alpha,\ \sigma_1^2) \\
\boldsymbol{Y}_2 | \boldsymbol{X}_{(2)}, \alpha &\sim \mathrm{Pois}(\exp(\boldsymbol{X}_{(2)}^T \boldsymbol{\beta}_{(2)} + 0.5\alpha)) \\
\boldsymbol{Y}_3 | \boldsymbol{X}_{(3)}, \alpha &\sim \mathrm{Gamma}(\lambda,\ \exp(\boldsymbol{X}_{(3)}^T \boldsymbol{\beta}_{(3)} - 0.3\alpha))
\end{aligned}
$$

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	$\hat{\beta}$	$\lvert\beta - \hat{\beta}\rvert$	Errors		$p \leqslant 0.05$	CI		
				$\hat{\sigma}$	$\bar{\text{se}}(\hat{\beta})$		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	$\hat{\beta}$	$\lvert\beta - \hat{\beta}\rvert$	Errors		$p \leqslant 0.05$	CI		
			$\hat{\sigma}$	$\bar{\text{se}}(\hat{\beta})$		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