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Regression-based approaches for simulation meta-modelling in the presence of heterogeneity and correlation

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Presentation Outline

Motivation: Simulation Meta-Modelling

- Simulation studies are used to inform recommendations and support decision-making on competing outputs simulated under comparable conditions.
- Simulations typically involve running m replications for each of n unique input combinations/design points.
- However, as $m, n \nearrow \infty$ simulation analysis can become enormously time-consuming.
- The use of *meta-models* to obtain a functional approximation of the (black-box) relationship between the inputs and outputs addresses this issue.

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Use of Common Random Numbers (CRNs)

- CRNs are used as a variance-reduction technique for simulation experiments.
- This approach uses the same pseudo-random number stream for each of the design points to subject all scenarios to the same statistical environment.
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Simulation Output Types

- In combat simulation experiments, output metrics of interest may also be categorical and/or discrete variables, not just continuous.
- Meta-modelling approaches for continuous variables have been extensively covered (see e.g. Chen et al. [2009] for a review of these methods), although meta-modelling with binary, discrete, or count outputs has received very little attention.
  - Meckesheimer et al. [2001] tackle the problem of meta-modelling with piecewise-continuous responses, but their approach does not accommodate the meta-modelling of strictly binary, discrete, or count outputs.
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Main Contributions

- We discuss a framework for a regression-based meta-modelling of simulation experiments with continuous, binary, and count outputs.
- Specifically, we illustrate the use of **estimated generalized least squares (EGLS)** [Kleijnen, 1992], **finite mixture GLMs** [Wedel and DeSarbo, 1995], and **heteroskedastic binary regression** [Alvarez and Brehm, 1995].
- Our framework also accounts for possible *heterogeneity* and *correlation* induced by the use of CRNs.
- We focus on regression-based approaches as these structures are more interpretable compared to other methods. A regression-based approach also lends itself more easily to sensitivity analyses, design point comparison, and ranking of alternatives.

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Notation

- $\mathbf{x}_i = (1, x_{i,1}, \ldots, x_{i,L})^\top$ denotes the regressors (incl. higher-order or interaction terms) for each design point $i = 1, \ldots, n$.
- $\mathbf{X}$ is the $n \times (L+1)$ matrix whose ith row is $\mathbf{x}_i^\top$.
- Let $\{w_{i;r}\}_{r=1}^m$ be the m realizations of the (continuous) output variable w_i.
- Let $\bar{\mathbf{w}} = (\bar{w}_1, \ldots, \bar{w}_n)^\top$, where $\bar{w}_i = \frac{1}{m}\sum_{r=1}^m w_{i;r}$, be the vector of simulation output averages.
- $\beta = (\beta_0, \beta_1, \ldots, \beta_L)^\top$ is the vector of unknown regression coefficients.
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Generalized Least Squares (GLS)

- We assume the linear input-output relationship

$$w_i = \mathbf{x}_i^\top \beta + \epsilon_i, \qquad \text{where } \mathrm{Var}[\epsilon|X] = \Sigma$$

where $\Sigma = [\sigma_{i,j}]$ is an unknown positive semi-definite $n \times n$ matrix with possibly unequal diagonal entries and nonzero off-diagonal entries.

- The GLS estimator of β is

$$\hat{\beta}^{GLS} = (\mathbf{X}^\top \Sigma^{-1} \mathbf{X})^{-1} \mathbf{X}^\top \Sigma^{-1} \bar{\mathbf{w}},$$

which can be calculated if Σ is known.

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Estimated Generalized Least Squares (EGLS)

- Given repeated measurements of the output for each i, we can estimate Σ by the sample covariance matrix $\hat{\Sigma} = [\hat{\sigma}_{i,j}]$, where

$$\hat{\sigma}_{i,j} = \frac{1}{m-1}\sum_{r=1}^{m}(w_{i;r} - \bar{w}_i)(w_{j;r} - \bar{w}_j), \qquad i,j = 1,\ldots,n.$$

- Using $\hat{\Sigma}$ in the GLS estimator results to the *estimated* GLS (EGLS) estimator

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Tests of Significance via Jackknifing

- For each $r = 1, \ldots, m$, we calculate the EGLS estimate $\hat{\beta}^{J:(-r)}$ after removing the rth replication.

- For each $\ell = 1, \ldots, L$, calculate m pseudo-values

$$J_{\ell;r} = m\hat{\beta}_\ell^{EGLS} - (m-1)\hat{\beta}_\ell^{J:(-r)}, \qquad r = 1, \ldots, m$$

  and the average $\bar{J}_\ell = \frac{1}{m} J_{\ell;r}$.

- Assuming $J_{\ell,m}$ are i.i.d. normal, a $100(1-\alpha)\%$ CI for β_ℓ is

$$\bar{J}_\ell \pm t_{1-\frac{\alpha}{2},m-1} \times S_\ell^J, \qquad \text{where } S_\ell^J = \sqrt{\frac{\sum_{r=1}^m (J_{\ell;r} - \bar{J}_\ell)^2}{m-1}}.$$

- Jackknifing requires $m - 1 > n$ to ensure that $\hat{\beta}^{J:(-r)}$ is well-defined for each r.

Heterogeneity for Non-Continuous Outputs

- We define *heterogeneity* as the case where there may exist smaller *latent classes* of unique design points where the base and main effects (i.e. regression coefficients) may differ across latent classes.
- This heterogeneity can be modelled using a finite mixture of GLMs [Wedel and DeSarbo, 1995], which can accommodate continuous, binary, and count output types among others.

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Finite Mixture GLMs

- Let S be the (unknown) number of latent classes.
- For each i, define $\mathbf{u}_i = (u_{i,1}, \ldots, u_{i,S})$, where $u_{i,s} = 1$ if design point i belongs to class s.
  - $\mathbf{u}_i$ has a *categorical distribution* with probabilities $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_S)$.
  - Note that $\mathbf{u}_i$ is unobserved.
- Conditional on design point i belonging to class s, w_i has pdf/pmf $f_i^{(s)}(w; \beta_s)$ belonging to the exponential family.
  - $\beta_s = (\beta_{s,0}, \beta_{s,1}, \ldots, \beta_{s,L})^\top$ denotes the regression parameters for latent class s.
  - $\beta = (\beta_1^\top, \ldots, \beta_S^\top)$ is the collection of all regression parameters
- The conditional mean $\mu_i^{(s)} = \mathbb{E}[w_i | \mathbf{x}_i, u_{i,s}]$ is related to $\boldsymbol{\beta}_s$ via an appropriate link function $g(\mu_i^{(s)}) = \mathbf{x}_i^\top \boldsymbol{\beta}_s$.

Finite Mixture GLMs

- Estimates for $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are obtained by maximizing the *complete log-likelihood*

$$L_c(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \sum_{i=1}^{n} \sum_{s=1}^{S} u_{i,s} \ln f_i^{(s)}(w_i; \boldsymbol{\beta}_s) + \sum_{i=1}^{n} \sum_{s=1}^{S} u_{i,s} \ln \alpha_s .$$

- Since the complete likelihood function involves unobserved data, maximum likelihood estimation is achieved using the EM algorithm [Dempster et al., 1977; Wedel and DeSarbo, 1995].

- S must also be estimated; we do so by calculating the log-likelihood, the AIC, and the BIC for a pre-specified set of values for S and select the value which maximizes the likelihood or minimizes the AIC/BIC.

- We use the **flexmix** package in R [Leisch, 2004] to estimate finite mixture GLMs.

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Illustration: Heteroskedastic Probit Regression

- Suppose we observe $w_i = \mathbf{1}(y_i^* > 0)$, where $\mathbf{1}(\cdot)$ is the indicator function and y_i^* is a latent variable of the form $y_i^* = \mathbf{x}_i^\top \boldsymbol{\beta} + \epsilon_i$.

- Assuming $\epsilon_i \sim N(0, \sigma_i^2)$, reflecting heteroskedasticity in the latent error, the *heteroskedastic* probit model is specified as

$$\Phi^{-1}(p_i) = \frac{\mathbf{x}_i^\top \beta}{\sigma_i}, \qquad h(\sigma_i) = h(1) + \mathbf{z}_i^\top \gamma,$$

  where $p_i = \mathbb{P}(w_i = 1 | \mathbf{x}_i) = \mathbb{E}[w_i | \mathbf{x}_i]$.

- The scale model $h(\sigma_i) = h(1) + \mathbf{z}_i^\top \gamma$ consists of:
  1. A scale link function $h(\cdot)$ (usually the log, square root, or identity function)
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  2. A vector of regressors $\mathbf{z}_i$ (not necessary equal to $\mathbf{x}_i$)
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Illustration: Heteroskedastic Probit Regression

- Suppose we observe $w_i = \mathbf{1}(y_i^* > 0)$, where $\mathbf{1}(\cdot)$ is the indicator function and y_i^* is a latent variable of the form $y_i^* = \mathbf{x}_i^\top \boldsymbol{\beta} + \epsilon_i$.

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- Aside from the probit link $g(p) = \Phi^{-1}(p)$, we can also use the logit link $g(p) = \ln(p/(1-p))$. See Koenker and Yoon [2009] for other appropriate link functions.
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Presentation Outline

Introductory Notes and Assumptions

- We consider the main effects (intercept term plus first-order terms)
- We assume a 5% level of significance for all hypothesis tests/confidence intervals. We focus on individual tests of significance.
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Data Description

- Outputs: *mission success* (binary), *number of red infantry defeated* (count), *number of red vehicles destroyed* (count)
- Inputs: *Option* ("A", "B", "C", or "D"), *F1* ("Direct" or "Indirect"), *F2* ("25" or "75"), and *F3* ("Low", "Medium", or "High")
- There are $n = 48$ distinct input combinations, each of which is repeated $m = 200$ times.
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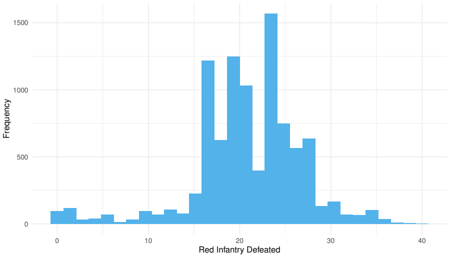
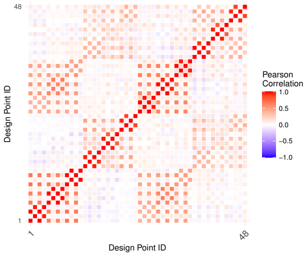
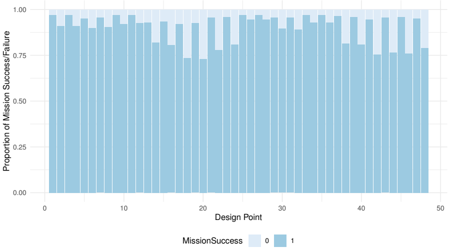


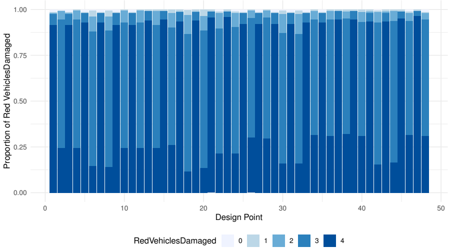
(a) Histogram of RID



(b) Correlation heat map for RID across design points



(a) MS by design point



(b) RVD by design point

Table: OLS, EGLS, and finite mixture Gaussian regression estimates for number of red infantry defeated.

	OLS (HC se)		EGLS Est.		EGLS 95% Jackknifed CI		FM Gaussian Regression Class 1		Class 2		Class 3	
Intercept	23.340	*	23.454	*	23.039	24.489	22.981	*	22.405	*	23.234	*
Option B	-1.029	*	-1.255	*	-2.338	-0.789	-2.607	*	0.385	*	-0.952	*
Option C	-0.105		-0.035		-0.795	0.278	0.177	*	-0.069		1.140	*
Option D	-1.119	*	-1.193	*	-2.263	-0.744	-1.833	*	-0.194	*	-1.066	*
F1 Indirect	-2.839	*	-2.933	*	-3.808	-2.426	-1.779	*	-1.891	*	-2.789	*
F2 75	0.009		0.007		-0.001	0.070	-0.064	*	0.007		-0.228	*
F3 Low	-0.816	*	-0.647	*	-1.044	-0.166	-1.408	*	-0.191	*	-1.158	*
F3 Medium	-0.280	*	-0.309	*	-0.820	-0.071	-0.349	*	0.075	*	-0.738	*
Log-Lik	-30433.70						54.68					
AIC	60885.41						-51.37					
BIC	60949.94						2.89					

Note: Breusch-Pagan test on OLS: p-value $< 2.2e^{-16}$; OLS $R^2 = 6.645\%$; Rao's lack-of-fit F test for ELGS: test statistic $= 1.69$, p-value $= 0.0041$.

Table: Homoskedastic and heteroskedastic binary regression (with probit and logit link functions) and finite mixture logistic regression results for mission success.

	Homoskedastic				Heteroskedastic				FM Logistic Regression			
	Probit		Logit		Probit		Logit		Class 1		Class 2	
Intercept	1.2041	*	2.0124	*	0.8818	*	1.4441	*	0.8785	*	1.0220	*
Option B	-0.8926	*	-1.4877	*	-0.4215		-0.7117		-0.2800	*	-0.4215	*
Option C	-0.1523		-0.2569		-0.0361		-0.0623		0.0320		-0.3944	*
Option D	-0.7843	*	-1.3804	*	-0.2456		-0.4194		-0.2879	*	-0.2895	
F1 Indirect	-0.8402	*	-1.3954	*	-0.7586	*	-1.2322	*	-0.2872	*	-0.3758	*
F2 75	-0.0772		-0.1370		-0.0441		-0.0787		-0.0199		-0.0321	
F3 Low	-0.2634	*	-0.4357	*	-0.0961		-0.1632		-0.0934	*	0.0280	
F3 Medium	0.0352		0.0616		0.0038		0.0054		0.0010		0.0877	
Log-Lik	-713.01		-712.38		-703.60		-703.60		-744.37			
AIC	1442.00		1440.80		1437.30		1437.27		1526.75			
BIC	1482.73		1481.47		1513.65		1513.62		1623.46			
LR Test p-val.					0.0091		0.0145					
AR	0.7114		0.7114		0.9024		0.9024					
Bal. AR	0.6716		0.6716		0.5000		0.5000					

Table: Results of the Poisson (P), quasi-Poisson (QP), Conway-Maxwell Poisson (CMP), negative binomial (NB), and Poisson-lognormal mixture (PLN) regression for number of red vehicles damaged.

	P		QP		CMP		NB		PLN	
Intercept	1.3621	*	1.3621	*	15.8125	*	1.3621	*	1.3723	*
Option B	0.0023		0.0023		0.0219		0.0023		-0.0053	
Option C	0.0084		0.0084		0.0813		0.0084		0.0081	
Option D	0.0184		0.0184	*	0.1765	*	0.0184		0.0111	
F1 Indirect	-0.2186	*	-0.2186	*	-2.0633	*	-0.2186	*	-0.2228	*
F2 75	0.0007		0.0007		0.0064		0.0007		0.0003	
F3 Low	-0.0288	*	-0.0288	*	-0.2760	*	-0.0288	*	-0.0274	*
F3 Medium	-0.0018		-0.0018		-0.0165		-0.0018		0.0005	
Log-lik	-15488.30				-8752.54		-15488.33		-15299.16	
AIC	30993.00				17523.08		30995.00			
BIC	31049.97				17587.60		31059.18		-15340.40	
Dispersion	0.0874		0.0875		0.0932					

Note: FM Poisson regression returns $S = 1$ as optimal $\Rightarrow$ usual Poisson regression

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- Our analysis using finite mixture GLMs has shown that there is significant heterogeneity in the base and main effects to the mean of the continuous and binary outputs.
- The results arising from the finite mixture GLMs, however, must be appraised via a qualitative assessment of the design points that are clustered together in latent classes to determine why such a clustering was derived from the data.
- As it is likely that there is some degree of under- or overdispersion in the output metrics, especially for count data, simulation meta-modelling via a joint modelling of the mean and dispersion [see e.g. Smyth, 1989]

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