Bayesian Analysis of Split-Plot Experiments with Non-Normal Responses for Evaluating Non-Standard Performance Criteria

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I. Introduce data set and model

II. Background on GLMM and HGLM

III. Non-Standard Questions

IV. Bayesian Framework

V Conclusions

Film Manufacturing Example

- Mixture-process experiment [Robinson, Myers, and Montgomery (2004)]
- Three components, (X_1,X_2, X_3), melted and mixed in a screw extruder to produce a roll of film
- Pieces are cut from the roll and processed at a particular setting of the process variables, (P_1,P_2,P_3)
- Response is a quality measure reflecting the amount of polarized light that passes through the film.
- Reponse is distinctly non-normal and coefficient of variation is constant…assumed to be gamma distributed

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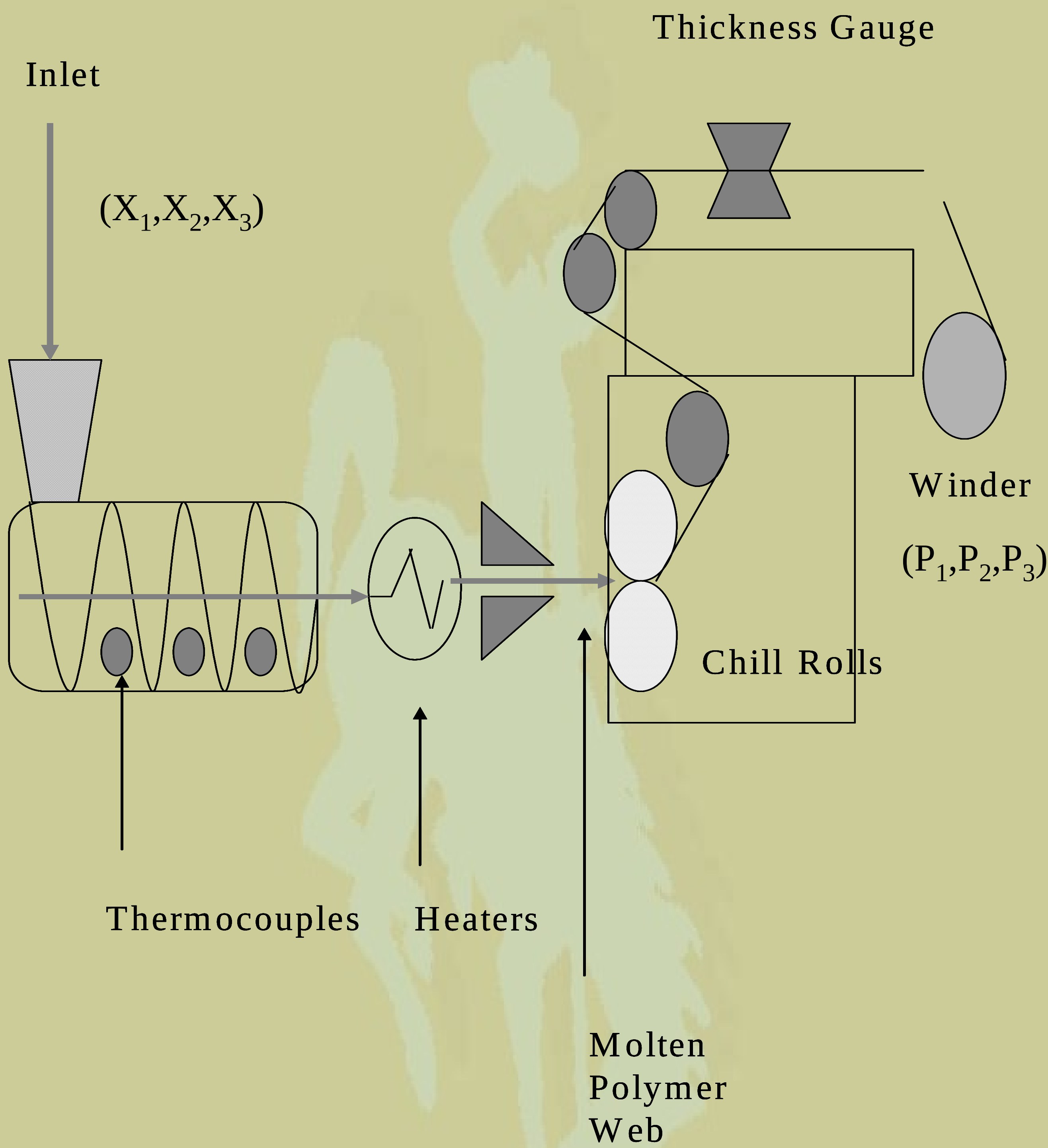
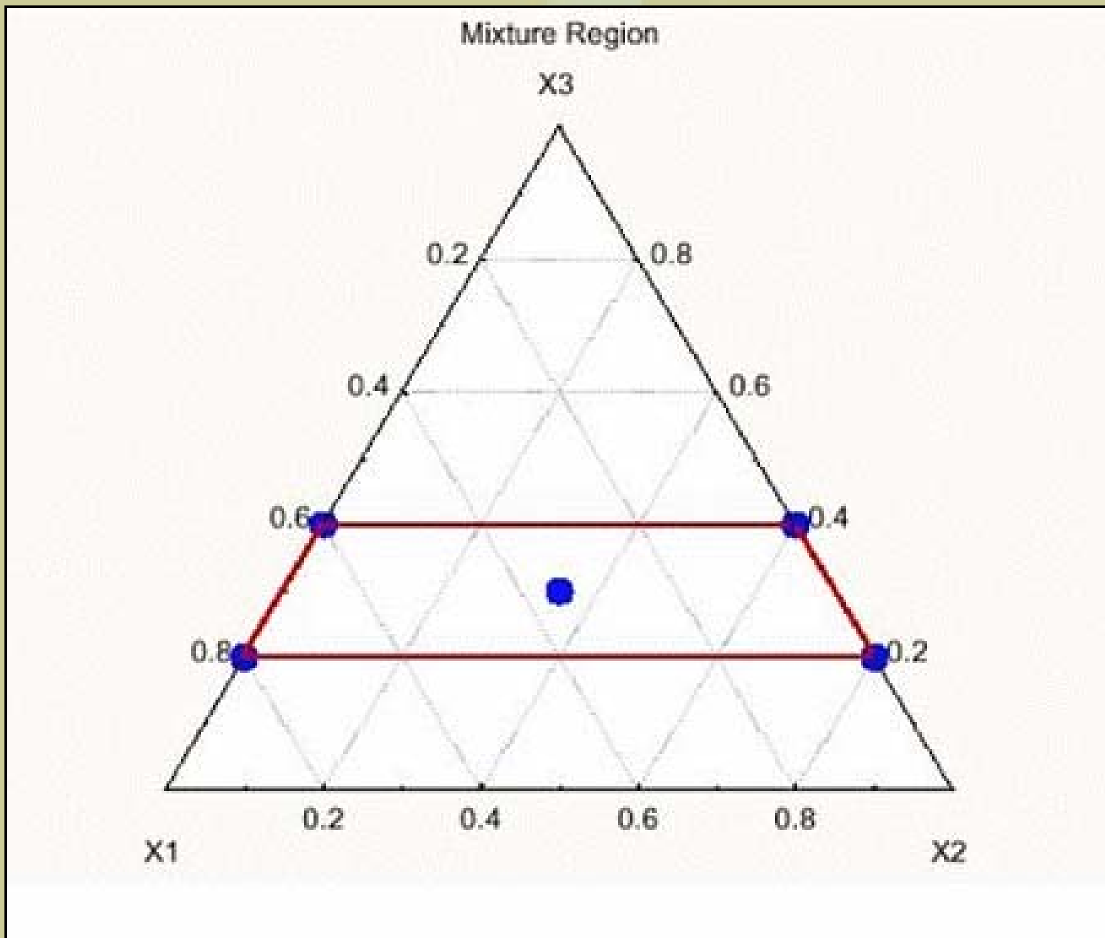

Thickness Gauge
Inlet
(X1,X2,X3)
Winder
(P1,P2,P3)
Chill Rolls
Thermocouples
Heaters
Molten
Polymer
Web



At each mixture, a 2^{3-1} design is run in the process variables.

The Model

1. Conditional Mean

Response follows a GLM family and to account for correlation among subplot units (pieces of film) a random effect defined for whole plot units (rolls)

$$E(\mathbf{y}|\boldsymbol{\delta}) = \boldsymbol{\mu},\ Var(\mathbf{y}|\boldsymbol{\delta}) = \phi\ V(\boldsymbol{\mu})$$

$\boldsymbol{\delta}$ is the vector of random effects

Linear predictor written as

$$\boldsymbol{\eta} = \boldsymbol{g}(\boldsymbol{\mu}) = \mathbf{X}^{*}\boldsymbol{\beta}^{*} + \mathbf{Z}\boldsymbol{\delta}$$

ex. $g^{-1}(\mu \mid \delta_i) = exp(\mathbf{x}_i^{*}\boldsymbol{\beta}^{*} + \delta_i)$

2. Random effects

The random effects in $\boldsymbol{\delta}$ assumed to have some user-specified probability distribution

GLMMs and HGLMs

- GLMMs and HGLMs can be fit using R as well as SAS GLIMMIX

- Inference primarily focuses upon the response mean and variance…model parameter estimates have asymptotically normal distributions and using Taylor series linearizations, inferential properties on the conditional and marginal means are derived [see Robinson et al (2004, 2006) and Lee and Nelder (1996)].

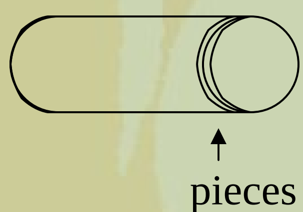
- Although the mean and variance are interesting, the engineer may have questions related to quantiles of the response distribution

  Ex. Given a mixture-process setting, what percent of film pieces will yield responses greater than 150?

  Ex. For a given mixture-process setting, 80% of the product will exceed what amount?

Scenarios for interest in quantiles

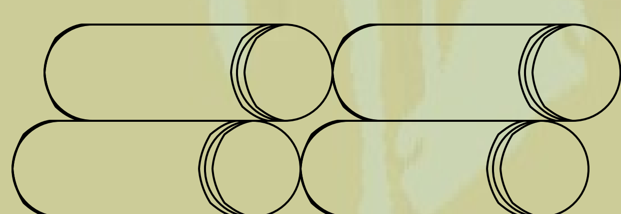
- Scenario 1: Assume an arbitrary mixture-process combination and that a single roll of film is produced with this combination. For a single roll of film, what percent of film pieces will exceed 150? (# film pieces arbitrarily large or small)



$x1$=0.35, $x2$=0.35, $x3$=0.30

$p1$=1, $p2$=-1, $p3$=-1

- Scenario 2: Same as above but assume the process yields an arbitrarily large number of rolls of film for the given mixture-process setting. What percent of film pieces across the population of rolls will have film quality exceeding 150?



y is a quality measure of reflective light

$$y \sim Gamma(\alpha, \theta)$$

Questions of interest need integration of estimated response distribution

Q1: $\int_{150}^{\infty} \hat{f}(y)\, dy$

Q2: $\int_{0}^{q} \hat{f}(y)\, dy = 0.2$

Need estimates of α and θ

Recall for a Gamma,

$$E(y) = \alpha/\theta \Rightarrow \hat{\theta} = \hat{\alpha}/\hat{E}(y)$$

Bayesian framework provides a forum for straight-forward inference on integrals above

Bayesian Inference Framework

Bayesian approach combines prior information on the model parameters[$\boldsymbol{\Theta}' = \left(\alpha, \boldsymbol{\delta}', \boldsymbol{\beta}^{*'}, \sigma_\delta\right)$] with the information that the data provides about the model parameters

The prior information on the model parameters described by the *prior* probability density $\pi\left(\boldsymbol{\Theta}\right)$ which is the product of pdfs for each of the parameters in $\boldsymbol{\Theta}$

Information on the parameters from the data is captured by the likelihood $f\left(\mathbf{y} \mid \boldsymbol{\Theta}\right)$, which is the product of gamma pdf's

$$\theta_i = \alpha \big/ E\left(y_i \mid \boldsymbol{\Theta}\right) = \alpha \big/ \exp\left(\mathbf{x}_i' \boldsymbol{\beta}^{*'} + \delta_{roll_i}\right)$$

The *posterior* distribution combines the information in $\pi\left(\boldsymbol{\Theta}\right)$ and $f\left(\mathbf{y} \mid \boldsymbol{\Theta}\right)$ using Bayes' Theorem

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WinBUGS Code

```
Model   {

        For(i in 1:52) {
                y[i] ~dgamma(alpha,theta[i])
                theta[i]<-alpha/mu[i]
                mu[i]<-exp(
                beta[1]*x1[i]+beta[2]*x2[i]+beta[3]*x3[i]+
                ...+ delta[roll[i]])

        }

        for (j in 1:13) {
                delta[j]~dnorm(0,taudelta)  #taudelta is a whole plot precision
        }
        #priors
        taudelta ~ dgamma(0.001,0.001)
        sigmadelta<- 1 /sqrt( taudelta)

        for(k in 1:13){
                beta[k]~ dnorm(0.0,1.0E-6)
        }

        alpha<-1/ralpha
        ralpha~dgamma(0.001,0.001) I(0.01,100)
}
```

$f(\mathbf{y}\,|\,\boldsymbol{\Theta})$ → (likelihood: the For(i in 1:52) loop)

$\pi(\boldsymbol{\Theta})$ → (priors: the for (j in 1:13) loop)

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WinBUGs Output

After allowing for a burn-in period of 4000 MCMC draws, 100,000 draws requested and then a thinning in which every 10^{th} draw selected

The remaining 10,000 draws for the parameters in Θ estimates the posterior distribution of the parameters in Θ

To summarize the posteriors of each of the parameters, the sample means and standard deviations of each of the respective posteriors was used

For this data set, the Bayesian analysis is comparable to the GLMM analysis using PQL from SAS Proc GLIMMIX

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Comparing GLMM and WinBUGs Output

Regression coefficients and uncertainty:

	Bayesian Analysis		GLMM PQL Analysis	
Effect	Estimate	Standard Dev.	Estimate	Standard Error
x1	**6.146**	**0.408**	**6.113**	**0.371**
x2	**4.022**	**0.407**	**3.984**	**0.386**
x3	**1.332**	**0.878**	**1.234**	**0.805**
*x1*x2*	**10.51**	**2.472**	**10.727**	**2.323**
p1	**-0.697**	**0.584**	**-0.688**	**0.499**
p2	**0.272**	**0.533**	**0.366**	**0.499**
p3	**0.224**	**0.597**	**0.305**	**0.499**
*x1*p1*	**1.19**	**0.827**	**1.189**	**0.697**
*x2*p1*	**1.981**	**0.820**	**1.962**	**0.713**
*x1*p2*	**-0.098**	**0.753**	**-0.224**	**0.697**
*x2*p2*	**-0.897**	**0.758**	**-1.031**	**0.713**
*x1*p3*	**-0.380**	**0.840**	**-0.490**	**0.697**
*x2*p3*	**-0.036**	**0.843**	**-0.145**	**0.713**

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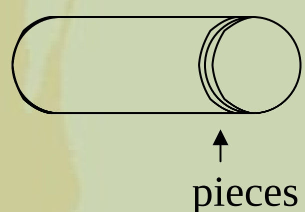
Gamma shape parameter, random effects, and variance of random effects

Effect	Bayesian Analysis Estimate	Bayesian Analysis Standard Dev.	GLMM PQL Analysis Estimate	GLMM PQL Analysis Standard Error
α	**4.2580**	**1.1300**	**4.7214**	**1.2190**
δ_1	**0.0174**	**0.2442**	**0.0408**	**0.2410**
δ_2	**0.0710**	**0.2209**	**0.1298**	**0.2165**
δ_3	**0.1350**	**0.2352**	**0.2299**	**0.2179**
δ_4	**0.0663**	**0.2124**	**0.1273**	**0.2165**
δ_5	**-0.2095**	**0.2648**	**-0.3346**	**0.2117**
δ_6	**-0.0108**	**0.2087**	**-0.0268**	**0.2165**
δ_7	**0.0806**	**0.2169**	**0.1540**	**0.2165**
δ_8	**0.1526**	**0.2370**	**0.2606**	**0.2117**
δ_9	**-0.0205**	**0.2443**	**-0.0408**	**0.2410**
δ_{10}	**-0.1953**	**0.2564**	**-0.3290**	**0.2165**
δ_{11}	**0.0347**	**0.2165**	**0.0715**	**0.2179**
δ_{12}	**-0.0286**	**0.2082**	**-0.0553**	**0.2165**
δ_{13}	**-0.1298**	**0.2303**	**-0.2274**	**0.2117**
σ_δ^2	**0.0572**	**0.1098**	**0.0837**	**0.0659**

Uncertainty

- Scenario 1: Assume an arbitrary mixture-process combination and that a single roll of film is produced with this combination. Also assume an arbitrarily large number of pieces of film come from a single roll. For a single roll of film, what percent of film pieces will exceed 150?



$x1$=0.35, $x2$=0.35, $x3$=0.30

$p1$=1, $p2$=-1, $p3$=-1

For this scenario, we are concerned with the distributional properties of film pieces within a given roll

Overall uncertainty is a function of parameter uncertainty from the estimation of model parameters as well as the random effect associated with the specific roll

Recall that our response is assumed gamma with parameters α and θ

The linear predictor is given by

$$\eta = \mathbf{x}'\boldsymbol{\beta}^* + \delta$$

$$\mathbf{x}'\boldsymbol{\beta}^* = \sum_{j=1}^{3} \beta_j x_j + \beta_{12} x_1 x_2 + \sum_{k=1}^{3} \gamma_k p_k + \sum_{j=1}^{2} \sum_{k=1}^{3} \psi_{jk} x_j p_k$$

We have posteriors for each of model parameters and thus for the linear predictor η

For a log link, conditional mean response is then

$$E\left(y \mid \delta\right) = g^{-1}\left(\eta\right) = exp\left(\eta\right)$$

A separate gamma density then exists for each MCMC draw since each draw provides a value of α as well as a value of $\theta = \alpha / exp\left(\eta\right)$

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Recall that our goal is to provide inference on the proportion of film pieces, for a given roll, that will yield responses greater than 150

$$\int_{150}^{\infty} \hat{f}(y)\, dy$$

The integral is easily obtained using a cdf command in a software package since the quanities needed for the cdf command are the response value of interest (150) and the values of α and θ

Recall that each MCMC draw provides a realization of α and θ and by doing the integration for each draw, one has the posterior distribution of the quantity of interest

Note that point estimates of α and θ can also be easily found using a PQL analysis of the GLMM from Proc GLIMMIX…however the uncertainty associated with this estimate would be *challenging* to derive

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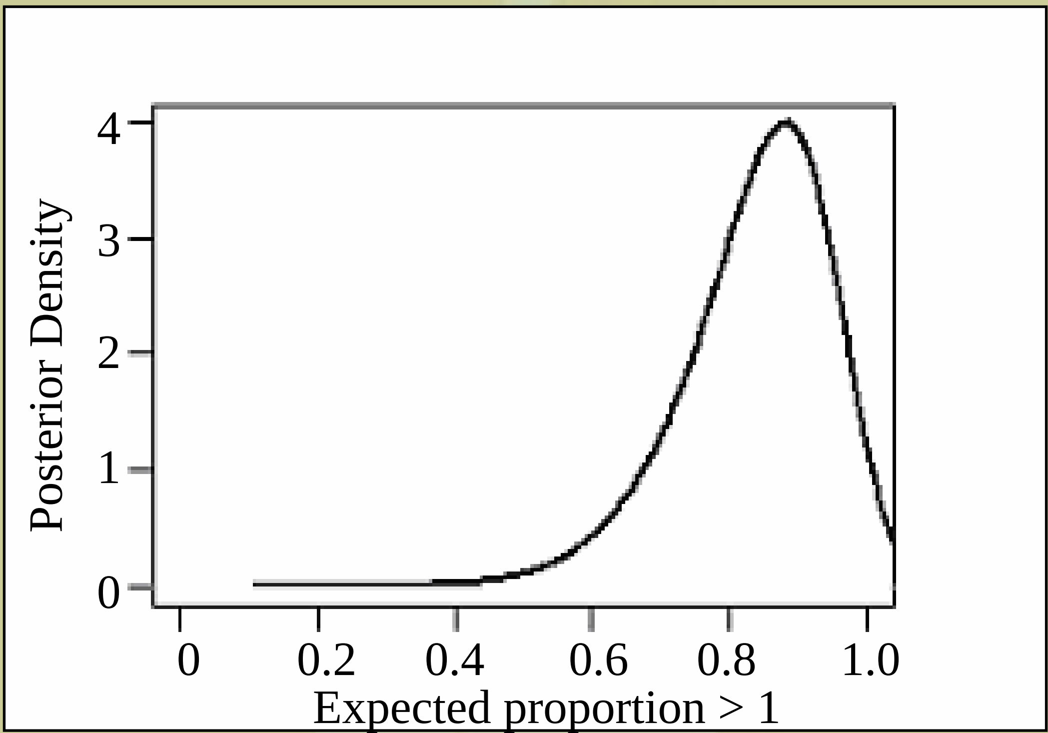
Posterior distribution of $P(y > 150 \mid \delta)$

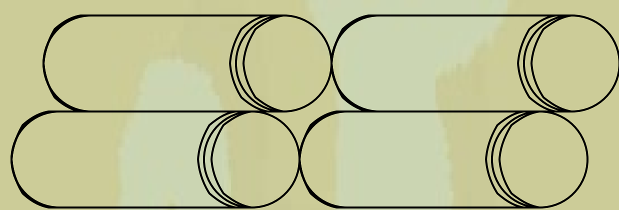


Credible interval obtained using the 2.5% and 97.5% quantiles of the posterior

point estimate: **0.858**

95% C.I.: **(0.598,0.973)**

- Scenario 2: Same as before but assume the process yields an arbitrarily large number of rolls of film for the given mixture-process setting.



x1=0.35, *x2*=0.35, *x3*=0.30

p1=1, *p2*=-1, *p3*=-1

Assume these settings are optimal and many rolls produced at these settings

In previous setting, linear predictor given by

$$\eta = \mathbf{x}'\boldsymbol{\beta}^* + \delta$$

Now, linear predictor given by

$$\eta_{pop} = \mathbf{x}'\boldsymbol{\beta}^* + \xi \qquad \xi \sim N\left(0, \sigma_\delta^2\right)$$

δ represents the uncertainty associated with a given roll whereas the uncertainty across a population of rolls is what is taken into account by a randomly generated value of $\xi \sim N\left(0, \sigma_\delta^2\right)$

The Bayesian analysis provides the posterior distribution of σ_δ and thus, for each MCMC draw, a value of the linear predictor $\eta_{pop} = \mathbf{x}'\boldsymbol{\beta}^* + \xi$ is tabulated

The mean of the gamma density is now the mean across a population of rolls or

$$\mu_{pop} = E_\xi\left[exp\left(\eta_{pop}\right)\right]$$

To estimate μ_{pop}, a large number of values of ξ are generated and subsequently, $exp\left(\eta_{pop}\right)$ is calculated and an arithmetic mean is taken

For each MCMC draw, one then has $\hat{\theta}_{pop} = \hat{\alpha} / \hat{\mu}_{pop}$ and $\hat{\alpha}$

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Recall that our goal is to provide inference on the proportion of film pieces, across a population of rolls, that will yield responses greater than 150

$$\int_{150}^{\infty} \hat{f}(y)\, dy$$

Note that this is the same as what was done in scenario 1 except that we now use the gamma density with the marginal mean instead of the conditional mean

Credible interval obtained using the 2.5% and 97.5% quantiles of the posterior

point estimate: **0.842**

95% C.I.: **(0.258,0.994)**

μ_{pop}

point estimate: 0.858

95% C.I.: (0.598,0.973)

$\mu \mid \delta$

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Conclusions

- For non-normal response split-plots, GLMMs and HGLMs are standard fare for analyses…these analyses focus primarily upon the mean
- When interest is on other characteristics of the response (specific quantiles, proportion within specifications, etc.), inferences using GLMM or HGLM theory may require many levels of approximations or boot-strapping
- Bayesian modeling framework easily allows for inferences on response quantiles by working with the posterior distributions
- Application of the Bayesian modeling framework to robust design is also natural and demonstrated in Robinson, Anderson-Cook and Hamada (2007)