3: Case Studies

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A key issue in the consolidation process of the nuclear fuel cycle is the **safe disposal of radioactive waste**.

At present, deep geological disposal based on a multibarrier concept is considered the most promising option (visualize a **deep underground chamber** within which radioactive materials such as spent fuel rods are entombed in layers of concrete and other barriers; e.g., PSAC User Group, 1989).

The **safety** of this concept ultimately relies on the safety of the mechanical, chemical and physical barriers offered by the geological formation itself.

In spite of recent worldwide efforts, the physico-chemical behavior of such a disposal system over geological time scales (hundreds or thousands of years) is **far from known with certainty** (e.g., Sinclair, 1996).

**Goal**: Predicting outcomes, including **radioactive dose** for people on the earth’s surface, as a function of factors like time, how far the disposal chamber is underground, ...
Uncertainty

Radioactive dose is estimated by computer simulation models such as AEA’s MASCOT, which numerically solve complex systems of partial differential equations.

The output of such models is deterministic given fixed scenario and parametric inputs, but these are uncertain. Structural and predictive uncertainty are also part of a full uncertainty audit (Fig. 1; Draper, 1997).

![Diagram of MASCOT model](image)

**Figure 1. Illustrating the four potential sources of uncertainty in stochastic modeling of radioactive dose with programs like MASCOT.**

Parametric uncertainty is typically quantified with probability distributions across all the model inputs: the program is run $N$ times, with different stochastically generated inputs each time, obtaining $N$ dose estimates at each of $T$ time points.
Focus on the Mean

Regulatory bodies insist on summarizing the dose distribution \( f \) at a given time point by its mean:
\[
\theta = \int y f(y) \, dy
\]
(even though this may be a very unstably estimated quantity; Sinclair and Robinson, 1994).

**Technical challenge:** \( f \) is typically extremely (positively) skewed, with many zeros and a few comparatively huge values, and the number of Monte Carlo repetitions \( N \) is constrained by time and money (often \( \leq 10,000 \), sometimes \( \leq 500–1000 \)).

With relatively small \( N \), the concern is that **you haven’t seen all of the right tail yet.**

Problem statement in contract proposal:

**To develop an improved understanding of the issue of convergence of probabilistic safety assessment (PSA) calculations, together with specific algorithms that could underlie improved analysis of statistical errors associated with estimating mean values or other statistical performance measures, in the context of risk assessments for long-term safety studies in radioactive waste disposal.**
Recent elaboration by Jim Sinclair:

Given a set of observations, what can I say about the true mean?

Is the internal evidence of my sample distribution sufficient for me to quote a best estimate and some interval limits?

Is the evidence such that I can say I shouldn’t even be estimating a mean unless I get many more samples?

What kind of external information about the distribution, such as knowledge of its general shape, or something like an upper bound, could improve my ability to predict the mean?

Time permitting, can similar questions be answered about other statistics, such as various percentiles of the distribution?

Can the extent to which, say, the 99th percentile is more robustly predictable than the mean be quantified?
An Example of the Data

Consider \( N = 10,000 \) dose values from MASCOT at \( t = 100 \) years, based on a scenario permitting relatively large doses of **Strontium 90 (Sr–90)** with relatively low probability. The outcome examined is **total dose** from three nuclides including Sr–90.

9864 (98.6%) of the 10,000 values are 0; 134 of the other 136 (1.36%) range smoothly from 1.059e–14 to 8.552e–01; the two largest values are 3.866 and 189.3 (!). The sample mean is 0.01964. (The true mean at 100 years, obtained from another program, AEA’s ESCORT, is 9.382e–4 (21 times smaller); the sample mean omitting the largest observation is 7.138e–4.)

Figure 2. A normal quantile-quantile plot of the positive log dose values (the line shows ideal behavior if Gaussian).
Method 1: Naive
Frequentist Nonparametrics

This distribution fairly closely follows a two-part or mixture model, in which each observation is 0 with probability $p$ and lognormal with probability $(1-p)$ (Fig. 2).

Method 1: Central Limit Theorem (CLT). We are trying to estimate $\theta$, the population mean. Why not use $\hat{\theta}_1 =$ the sample mean?

Dose values $D_i, i = 1, \ldots, N$;

Point estimate $\hat{\theta}_1 = \bar{D} = \frac{1}{N} \sum_{i=1}^{N} D_i$. (1)

The standard (frequentist) interval estimate is based on the hope—with such a large $N$—that the distribution of $\hat{\theta}_1$ in repeated sampling from the population density $f$ is close to normal (by the Central Limit Theorem):

95% Interval estimate $\hat{\theta}_1 \pm 1.96 \frac{s_D}{\sqrt{N}}$, (2)

where $s_D$ is the sample standard deviation

$$\sqrt{\frac{1}{N-1} \sum_{i=1}^{N} (D_i - \bar{D})^2}.$$ 

This is a nonparametric method, because no assumptions about $f$ are used (except that its variance is finite).
Method 1: CLT (continued)

Here $\hat{\theta}_1 = \bar{D} = 0.01964$, $s_D = 1.893$, and the 95% interval estimate is

$$0.01964 \pm 1.96 \frac{1.893}{\sqrt{10000}} = (-0.01746, 0.05675),$$

which does include the true value $9.382 \times 10^{-4}$ but has made itself look silly in doing so by going negative. (“Guttman” multiplier 2.68 [Woo, 1989] just makes this problem worse.)

Moreover the largest observation occurred at iteration number 6132, and many of the CLT intervals based on observations $1-k$ for $k < 6132$ fail to cover: only 63% of the 100 “95%” intervals based on observations $1-100$, $1-200$, ... include the true value.

![Figure 3](image)

Figure 3. Upper and lower 95% Central Limit Theorem intervals, with the true mean superimposed, based on observations $1-100$; $1-200$; ..., $1-10,000$. 73 of these 100 intervals go negative.
Method 1: Simulation Results

I regarded the 10,000 dose values at 100 years as a population to be sampled with replacement. I repeatedly ($S = 5,000$ times) took samples of size $N$ from this population, with $N$ varying from 100 to 1,000,000, and computed the actual coverage of nominal “95%” intervals from the CLT method, with results as shown in Table 1.

Table 1. Actual coverage of nominal 95% intervals based on the Central Limit Theorem, as a function of sample size $N$ (simulation standard errors in parenthesis; results for the 2.68 multiplier were only slightly better).

<table>
<thead>
<tr>
<th>Sample Size ($N$)</th>
<th>Coverage (1.96 Multiplier)</th>
<th>% Left Endpoint</th>
<th>Negative Average Length</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>0.0296 (2.41e–3)</td>
<td>74.7</td>
<td>0.0914 (1.14e–2)</td>
</tr>
<tr>
<td>1,000</td>
<td>0.0976 (4.20e–3)</td>
<td>99.3</td>
<td>0.0757 (3.17e–3)</td>
</tr>
<tr>
<td>5,000</td>
<td>0.391 (6.90e–3)</td>
<td>81.4</td>
<td>0.0656 (1.16e–3)</td>
</tr>
<tr>
<td>10,000</td>
<td>0.622 (6.86e–3)</td>
<td>76.5</td>
<td>0.0565 (6.53e–4)</td>
</tr>
<tr>
<td>25,000</td>
<td>0.878 (4.63e–3)</td>
<td>67.9</td>
<td>0.0434 (2.55e–4)</td>
</tr>
<tr>
<td>50,000</td>
<td>0.909 (4.07e–3)</td>
<td>25.9</td>
<td>0.0324 (1.13e–4)</td>
</tr>
<tr>
<td>100,000</td>
<td>0.930 (3.61e–3)</td>
<td>0.8</td>
<td>0.0231 (5.32e–5)</td>
</tr>
<tr>
<td>500,000</td>
<td>0.950 (3.08e–3)</td>
<td>0.0</td>
<td>0.0105 (2.12e–5)</td>
</tr>
<tr>
<td>1,000,000</td>
<td>0.945 (3.22e–3)</td>
<td>0.0</td>
<td>0.00742 (5.28e–6)</td>
</tr>
</tbody>
</table>

For $N \leq 10,000$ mistakes were always from the interval lying entirely to the left of the true mean. 24.1% of the data sets with $N = 100$ consisted of all zeros, but this dropped to 0% for $N \geq 500$. 
Failure of the CLT

Figure 4. Log mean interval length and coverage rate against log($N$) for the CLT intervals.

log(interval length) vs. log($N$) should be \textbf{linear} if the sample SD is doing its job properly:

\[
\text{length} = 3.92 \cdot \frac{s_N}{\sqrt{N}}, \text{ so for } N \text{ large enough that } s_N \approx \sigma = 1.893,
\]

\[
\log(\text{length}) = 2.004 - 0.5 \log(N); \text{ but the actual curve (Fig. 4) does not approximate this line}
\]

\[
\text{until } N > \exp(10) \approx 22,000.
\]

Not coincidentally, that is just about exactly where the CLT starts producing \textbf{decent performance}: coverage rate against log($N$) shows an ogive shape that does not exceed (say) 0.9 until $N$ is also roughly 22,000 or more.
Failure of the CLT

The reason this method performs so poorly is that even with (say) 7,500 observations going into each average, the distribution of the sample mean is far from Gaussian (Fig. 4.1), because of the extreme skewness of the population.

![Quantile-quantile plot](image)

Figure 4.1. Normal quantile-quantile plot of the 5,000 simulated means in Table 1, each based on $N = 7,500$ observations.
CLT Nightmare
In fact with this population you don’t even begin to get a really decent normal approximation to the mean until $N \geq 100,000$:

![Quantile-Quantile Plot]

Figure 5. Normal quantile-quantile plot of 5,000 simulated means, each based on $N = 100,000$ observations.

![Histogram]

Figure 6. Histogram of the 5,000 simulated means in Fig. 5.
Method 2: Less Naive
Frequentist Nonparametrics

The best frequentist nonparametric confidence interval technology to date is the $\text{BC}_a$ method, based on the bootstrap (Efron and Tibshirani, 1993).

The bootstrap idea in this context is to repeatedly ($B = 1,000$ times, say) choose a sample of size $N$ with replacement from $D_1, \ldots, D_N$, calculate the means of each of these samples, and use the distribution $\mathcal{D}$ of these $B$ means as the basis for confidence intervals.

The percentile method is literal: to produce a 95% interval, choose the $\alpha_1 = 2.5\%$ and $\alpha_2 = 97.5\%$ points of $\mathcal{D}$.

This method works OK with large samples from reasonably “standard” data sets (not too far from Gaussian), but can produce poor coverage for small $N$ and with (e.g.) highly skewed data.

The $\text{BC}_a$ method improves on the percentile method by choosing different $\alpha_1$ and $\alpha_2$ values which yield better (closer to nominal) coverage.
The Bootstrap

This method also makes no use of information about \( f \) apart from assuming its variance is finite.

With the \( N = 10,000 \) dose values at 100 years the BC\(_a\) method yields the nominal 95% interval \((3.64\times10^{-4}, 0.134)\), which also includes the true mean; moreover, BC\(_a\) intervals are incapable of going negative.

However, in the analogue of Fig. 3 for the bootstrap (Fig. 4), it is still true that only 85% of the nominal 95% intervals include the truth.

![Figure 7](image-url)

Figure 7. Upper and lower 95% bootstrap intervals, with the true mean superimposed, based on observations 1–100; 1–200; ..., 1–10,000. None of these intervals go negative.
Bootstrap Results

Performance in the analogue of Table 1 is a bit better, but still pretty bad:

Table 2. Actual coverage of nominal 95% intervals based on the bootstrap, as a function of sample size $N$ (simulation standard errors in parenthesis; number of simulation repetitions $S = 1000$ except where otherwise indicated).

<table>
<thead>
<tr>
<th>Sample Size ($N$)</th>
<th>Actual Coverage</th>
<th>Mean</th>
<th>Length</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>.0373 (2.68e−3)</td>
<td>.0695 (9.89e−3)</td>
<td></td>
</tr>
<tr>
<td>500</td>
<td>.100 (4.24e−3)</td>
<td>.0727 (4.42e−3)</td>
<td></td>
</tr>
<tr>
<td>1,000</td>
<td>.0938 (4.12e−3)</td>
<td>.0689 (2.99e−3)</td>
<td></td>
</tr>
<tr>
<td>5,000</td>
<td>.394 (6.91e−3)</td>
<td>.0655 (1.16e−3)</td>
<td></td>
</tr>
<tr>
<td>10,000</td>
<td>.632 (6.82e−3)</td>
<td>.0582 (6.65e−4)</td>
<td></td>
</tr>
</tbody>
</table>

(No point in continuing the simulations: very similar to Table 1.)

Mistakes for small $N$ were again always from the interval lying entirely to the left of the true mean. These intervals cover slightly more often than the CLT intervals, and are slightly narrower.

However the coverage is still abysmal, and the $BC_a$ method is slow: it took 25 minutes of CPU time to do the calculations leading to Fig. 5, and 51 hours of CPU time to produce Table 2, on an otherwise unburdened 333Mhz DECalpha workstation.
Method 3: Parametric Bayesian

The data analysis on p. 6 above suggests the following mixture model.

At a particular time $t$, let $D_i$ be the observed dose on simulation run $i = 1, \ldots, N$. Then

$$D_i = \begin{cases} 
0 & \text{with probability } p \\ 
\text{LN}(\mu, \sigma^2) & \text{with probability } (1-p)
\end{cases}, \quad (3)$$

where $\text{LN}(\mu, \sigma^2)$ denotes the lognormal distribution with mean $\mu$ and standard deviation $\sigma$ on the log scale.

In this model the true population mean $\theta$ is given theoretically (Johnson and Kotz, 1970) by

$$\theta = (1-p)e^\mu + \frac{1}{2}\sigma^2. \quad (4)$$

In a Bayesian formulation prior distributions are needed for the parameters $p, \mu, \text{ and } \sigma$ (or $\sigma^2$, or the precision $\tau = \frac{1}{\sigma^2}$).

I have so far used diffuse priors that are relatively flat in the regions of high likelihood for the parameters.

With $N = 10,000$ observations this is reasonable; with $N \leq 1,000$ (say) the priors would probably need to be more informative.
MCMC

One simple initial idea for fitting the mixture model (3): **Gibbs sampling** via **BUGS** (Spiegelhalter et al., 1997).

Unfortunately **BUGS** cannot fit model (3) above, but it can fit a **functionally equivalent** model:

\[
D_i = \begin{cases} 
LN(\mu_1, \sigma_1^2) & \text{with probability } p_1 \\
LN(\mu_2, \sigma_2^2) & \text{with probability } p_2 = (1 - p_1)
\end{cases},
\]

(5)

where the **zeros** in the data set are replaced by values of the form \((\epsilon \pm \text{tiny lognormal noise})\) to correspond to the first component of the mixture.

In this model the **underlying mean** of the distribution of the \(D_i\) is **theoretically**

\[
\theta = p_1 \exp \left( \mu_1 + \frac{1}{2} \sigma_1^2 \right) + p_2 \exp \left( \mu_2 + \frac{1}{2} \sigma_2^2 \right). 
\]

(6)

With the \(N = 10,000\) observations of dose at \(t = 100\) years examined on p. 6, I used initial values that permitted a **short burn-in** (100 iterations):

```r
list( mu = c(-45.03454, NA ), eta = 29.31891, 
p = c( 0.0136, NA ),tau = c( 0.2522539, 0.01351527 ) )
```
model d100.2;

const

N = 10000, mu.mu1.p = 0.0, tau.mu1.p = 1.0E-6,
    mu.eta.p = 0.0, tau.eta.p = 1.0E-6,
    epsilon = 0.001, kappa = 0.437;

var

d[N], mu[2], eta, alpha[2], p[2], tau[2], T[N],
    theta;

data d in "d100.gibbs.dat";
inits in "d100-2.in";

{

    mu[1] ~ dnorm( mu.mu1.p, tau.mu1.p );
    eta ~ dnorm( mu.eta.p, tau.eta.p ) I( 0, );
    alpha[1] <- 1;
    alpha[2] <- 1;
    p[] ~ ddirch( alpha[] );
    tau[1] ~ dgamma( epsilon, epsilon );
    tau[2] ~ dgamma( epsilon, epsilon );

    for ( i in 1:N ) {

        T[i] ~ dcat( p[] );
        d[i] ~ dlnorm( mu[ T[i] ], tau[ T[i] ] );

    }


}
Extreme Behavior of Lognormal Model

With values for the parameters similar to those in the dose data at 100 years (with 0's changed to lognormal draws centered at a very small positive value) \((\mu_1 = -45.0, \sigma_1 = 1.99, \mu_2 = -15.7, \sigma_2 = 8.60, p = 0.986)\), formula (6) gives a shock: \(\theta\) comes out \(2.46e+7!\)

To look at this from another angle, I repeatedly (10,000 times) sampled 10,000 draws from model (5) and calculated the mean of these draws.

The smallest of the 10,000 means was 5.33e–6, and their median was 0.0787; but their mean was \(1.36e+4\), and the biggest was \(9.88e+7!\)

The problem is that the lognormal distribution is extremely sensitive to assumptions about the rate at which the tails fall off toward 0 in the normal distribution.

With a mean of –15.7 and an SD of 8.60 on the log scale, the median observation on the dose scale would be 1.52e–7, but one time in 10,000 you would get a value like \(\exp(-15.7 + 3.72 \cdot 8.60) = 1.21e+7\) (which contributes .0001 \(1.21e+7 = 1.21e+4\) to the mean), one time in 100,000 you would get something like \(\exp(-15.7 + 4.26 \cdot 8.60) = 1.32e+9\) (which adds another 1.32e+4), and so on.
Parametric Bayesian Results

One possible fix is to use a truncated lognormal model: in the second component,
\[ \log(D_i) = \mu_2 + \sigma_2 e_i, \] with \( e_i \sim N(0,1) \) truncated at \(-A\) and \( A \) (or just at \( A \)). Then for this component of the mixture \( V[\log(D_i)] = \kappa \sigma_2^2 \) with

\[
\kappa = 1 - \frac{2 \Phi^{-1}(1 - \gamma) \phi[\Phi^{-1}(1 - \gamma)]}{1 - 2 \gamma}, \tag{7}
\]

where \( \gamma = \Phi(-A) \).

Table 2.5. Rough estimates in the truncated lognormal mixture model as a function of the number of points \( k \) set aside in each tail.

<table>
<thead>
<tr>
<th>( k )</th>
<th>( \hat{\mu}_2 )</th>
<th>( \hat{\sigma}_2 )</th>
<th>( \hat{\theta} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-15.68</td>
<td>8.601</td>
<td>24,086,800.</td>
</tr>
<tr>
<td>1</td>
<td>-15.71</td>
<td>8.352</td>
<td>585,834.</td>
</tr>
<tr>
<td>3</td>
<td>-15.71</td>
<td>7.988</td>
<td>6,739.</td>
</tr>
<tr>
<td>4</td>
<td>-15.72</td>
<td>7.843</td>
<td>1,176.</td>
</tr>
<tr>
<td>5</td>
<td>-15.73</td>
<td>7.692</td>
<td>248.8</td>
</tr>
<tr>
<td>6</td>
<td>-15.74</td>
<td>7.539</td>
<td>60.89</td>
</tr>
<tr>
<td>8</td>
<td>-15.77</td>
<td>7.250</td>
<td>5.086</td>
</tr>
<tr>
<td>10</td>
<td>-15.79</td>
<td>6.952</td>
<td>0.5939</td>
</tr>
<tr>
<td>12</td>
<td>-15.82</td>
<td>6.695</td>
<td>0.08936</td>
</tr>
<tr>
<td>14</td>
<td>-15.83</td>
<td>6.434</td>
<td>0.01645</td>
</tr>
</tbody>
</table>

To bring \( \theta \) in line with the true mean, \( k = 14 \) (about \( \gamma = 10\% \) in each tail) corresponds to \( \kappa \doteq 0.43 \).
Parametric Bayesian Results

Figs. 8–11 and Table 3 present exploratory results with this model on the modified 100-year dose data, using a burn-in of 500 and a monitoring run of 5000 draws (this took 4.5 hours of CPU time at 333Mhz).

![Sigma squared for mixture component 2](image)

Figure 8. Time series trace for $\sigma_2^2$, showing a bit of positive serial correlation (0.26) but not enough to be worrisome (the traces for the other parameters are similar).

![QQ plot](image)

Figure 8.1. qqplot of log(predictive dose) against log(actual dose) at 100 years.
Bayesian Results (continued)

Figure 9. Density traces of the marginal posterior distributions of $\mu_1$ and $\mu_2$, both of which are not far from normal.

Figure 10. Density traces of the marginal posterior distributions of $\sigma_1^2$ and $\sigma_2^2$, both of which exhibit the sort of skewness you would expect for variances.
Bayesian Results (continued)

Figure 11. Density traces of the marginal posterior distributions of $p_1$ and $\log(\theta)$. NB $\theta$'s distribution is even heavier-tailed than lognormal.

Table 3. Numerical summaries of the posterior distributions for the parameters of model (5) with the 100-year dose data ($\kappa = 0.43$).

<table>
<thead>
<tr>
<th>Variable</th>
<th>Posterior Mean</th>
<th>SD*</th>
<th>Maximum Likelihood Estimate</th>
<th>SE**</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p_1$</td>
<td>0.986</td>
<td>1.16e-3</td>
<td>0.986</td>
<td>1.16e-3</td>
</tr>
<tr>
<td>$\mu_1$</td>
<td>-45.0</td>
<td>0.0203</td>
<td>-45.0</td>
<td>0.0199</td>
</tr>
<tr>
<td>$\sigma_1^2$</td>
<td>3.96</td>
<td>0.0563</td>
<td>3.96</td>
<td>0.0563</td>
</tr>
<tr>
<td>$p_2$</td>
<td>0.0139</td>
<td>1.16e-3</td>
<td>0.0139</td>
<td>1.16e-3</td>
</tr>
<tr>
<td>$\mu_2$</td>
<td>-16.0</td>
<td>0.812</td>
<td>-15.7</td>
<td>0.738</td>
</tr>
<tr>
<td>$\sigma_2^2$</td>
<td>82.5</td>
<td>11.9</td>
<td>74.0</td>
<td>10.0</td>
</tr>
<tr>
<td>$\theta$</td>
<td>28.0</td>
<td>959 (!)</td>
<td>0.076</td>
<td>0.205</td>
</tr>
</tbody>
</table>

SD = standard deviation

NB median($\theta$) = 0.058, $q_{85} = 1.0$, max = 47728 (!), 95% central interval = (9.35e-4, 19.2); 95% maximum likelihood CI = (3.92e-4, 14.7)
Method 4: Bayesian Nonparametrics

**Method 3 coverage properties.** I repeatedly (100 times) drew samples of size 10,000 with replacement from the modified 100-year dose data and used **BUGS** to construct 95% interval estimates of the true mean 0.0196 (based on the 2.5% and 97.5% points of the simulated posterior distributions).

With $\kappa = 0.43$, actual coverage was **89%** (with simulation SE 3.1%), but the intervals were extremely long (median length 238 (!), mean length 409 (!)).

**Tentative conclusion:** Intervals probably still wider than necessary for decent coverage. How well will this method work with small $N$ (500, say)? Still have to actually implement truncated lognormal idea instead of $\kappa$ approximation. (Work in progress.)

**Method 4: Bayesian Nonparametrics.** A sample of size $N = 1000$ from the 100-year dose data would only be expected to have about **14** values from the non-zero part of the distribution.

Clearly with such samples it would be necessary to **teach** the interval-generating process about the right tail, above and beyond what it can learn directly from the data (the lack of such a way to learn is why the bootstrap fails).
Bayesian Nonparametrics (continued)

One approach: the parametric Bayesian Method 3. But the lognormal is only approximately “correct” at \( t = 100 \) years, and the approximation may well be even more vague at other times and for other scenarios.

It would be good to be able to build a model that is centered at the lognormal, but which can adapt to other distributions when the data suggest this is necessary.

Continuing Part 3, a fairly recently developed modeling approach based on Pólya trees (Lavine, 1992, 1994; Walker et al., 1998), first studied by Ferguson (1974), is promising.

Consider just the \( n = 136 \) non-zero dose values \( Y_i \) in the 100-year data. One way to write the parametric Bayesian lognormal model is

\[
\begin{align*}
\log(Y_i) & = \mu + \sigma e_i \\
(\mu, \sigma^2) & \sim p(\mu, \sigma^2) \\
e_i & \overset{\text{IID}}{\sim} N(0, 1),
\end{align*}
\]

for some prior distribution \( p(\mu, \sigma^2) \) on \( \mu \) and \( \sigma^2 \).

The Pólya trees idea is to replace the last line of (7), which expresses certainty about the distribution of the \( e_i \), with a distribution on the set of possible distributions \( F \) for the \( e_i \).
The new model is

\[
\log(Y_i) = \mu + \sigma e_i \\
(\mu, \sigma^2) \sim \rho(\mu, \sigma^2) \\
(e_i | F) \overset{\text{iid}}{\sim} F \quad \text{(mean 0, SD 1)} \\
F \sim \text{PT} (\Pi, A_c).
\] (9)

Here (a) \( \Pi = \{B_\epsilon\} \) is a binary tree partition of the real line, where \( \epsilon \) is a binary sequence which locates the set \( B_\epsilon \) in the tree.

You get to choose these sets \( B_\epsilon \) in a way that centers the Pólya tree on any distribution you want, in this case the standard normal.

This is done by choosing the cutpoints on the line, which define the partitions, based on the quantiles of \( N(0, 1) \):

<table>
<thead>
<tr>
<th>Level</th>
<th>Sets</th>
<th>Cutpoint(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>((B_0, B_1))</td>
<td>(\Phi^{-1}(\frac{1}{2}) = 0)</td>
</tr>
<tr>
<td>2</td>
<td>((B_{00}, B_{01}, B_{10}, B_{11}))</td>
<td>(\Phi^{-1}(\frac{1}{4}) = -0.674, \Phi^{-1}(\frac{1}{2}) = 0, \Phi^{-1}(\frac{3}{4}) = +0.674)</td>
</tr>
<tr>
<td>:</td>
<td>:</td>
<td>:</td>
</tr>
</tbody>
</table>

(\( \Phi \) is the \( N(0, 1) \) CDF.) In practice this process has to stop somewhere; I use a tree defined down to level \( M = 8 \), which is like working with random histograms, each with \( 2^8 = 256 \) bins.
Pólya Trees (continued)

And (b) Walker et al. (1998):

A helpful image is that of a particle cascading through the partitions $B_\epsilon$. It starts [on the real line] and moves into $B_0$ with probability $C_0$ or into $B_1$ with probability $C_1 = 1 - C_0$. In general, on entering $B_\epsilon$ the particle could either move into $B_{\epsilon 0}$ or into $B_{\epsilon 1}$. Let it move into the former with probability $C_{\epsilon 0}$ or into the latter with probability $C_{\epsilon 1} = 1 - C_{\epsilon 0}$. For Pólya trees, these probabilities are random, beta variables, $(C_{\epsilon 0}, C_{\epsilon 1}) \sim \text{beta}(\alpha_{\epsilon 0}, \alpha_{\epsilon 1})$ with non-negative $\alpha_{\epsilon 0}$ and $\alpha_{\epsilon 1}$. If we denote the collection of $\alpha$'s by $\mathcal{A}$, a particular Pólya tree distribution is completely defined by $\Pi$ and $\mathcal{A}$.

To make a Pólya tree distribution choose a continuous distribution with probability 1, the $\alpha$'s have to grow quickly as the level $m$ of the tree increases. Following Walker et al. (1998) I take

$$\alpha_\epsilon = c m^2$$

whenever $\epsilon$ defines a set at level $m$,

and this defines $\mathcal{A}_c$.

$c > 0$ is a kind of tuning constant: with small $c$ the posterior distribution for the CDF of the $e_i$ will be based almost completely on $\hat{F}_n$, the empirical CDF (the “data distribution”) for the $e_i$, whereas with large $c$ the posterior will be based almost completely on the prior centering distribution, in this case $N(0,1)$. 
Prior to Posterior Updating

Prior to posterior updating is easy with Pólya trees: if

\[
F \sim PT(\Pi, \mathcal{A})
\]

\[
(Y_i|F) \overset{\text{IID}}{\sim} F
\]

and (say) \(Y_1\) is observed, then the posterior \(p(F|Y_1)\) for \(F\) given \(Y_1\) is also a Pólya tree with

\[
(\alpha_\epsilon|Y_1) = \begin{cases} 
\alpha_\epsilon + 1 & \text{if } Y_1 \in B_\epsilon \\
\alpha_\epsilon & \text{otherwise}
\end{cases}.
\]

In other words the updating follows a Pólya urn scheme (e.g., Feller, 1968): at each level of the tree, if \(Y_1\) falls into a particular partition set \(B_\epsilon\), then 1 is added to the \(\alpha\) for that set.
Inference for $\mu$ and $\sigma^2$

With $Y = (Y_1, \ldots, Y_n)$ as the vector of non-zero dose values, as usual Bayes’ Theorem gives

$$p(\mu, \sigma^2 | Y) \propto p(\mu, \sigma^2) l(\mu, \sigma^2 | Y). \quad (13)$$

Here I use the conjugate prior for $\mu$ and $\sigma^2$,

$$\sigma^2 \sim \chi^{-2}(\nu_p, \sigma_p^2)$$

$$(\mu | \sigma^2) \sim N \left( \mu_p, \frac{\sigma^2}{\kappa_p} \right) \quad (14)$$

($\chi^{-2}$ denotes the distribution of the reciprocal of a $\chi^2$ variate), and $l(\mu, \sigma^2 | Y)$ is the likelihood function (the sampling distribution for $Y$ given $\mu$ and $\sigma^2$, re-interpreted as a function of $\mu$ and $\sigma^2$ for fixed $Y$).

(13) is hard to use to draw inferences about $\mu$ and $\sigma^2$ for two reasons: (a) there is the usual difficulty in extracting marginal information about $\mu$ or $\sigma^2$ singly, and (b) $l(\mu, \sigma^2 | Y)$ is not directly evaluable, and depends in a complicated way on something that is directly computable, the conditional likelihood $l(\mu, \sigma^2 | Y, F)$.

Figs. 12–14 plot the conditional likelihood, which has a remarkable, almost fractal, character in this nonparametric setting.
Figure 12. *The conditional log likelihood function for μ given a particular estimate of F based on the 100 year data and with σ² = 73.99. The log likelihood in the parametric version of this model is much smoother.*

Figure 13. *The (joint) conditional log likelihood function for μ and σ² with the 100 year data. The global maximum is barely visible near (μ, σ²) = (–15, 80).*
Figure 14. A contour plot of the same (joint) conditional log likelihood function for $\mu$ and $\sigma^2$ as in Fig. 13. Now the global max is easier to spot, as the only place with a conditional log likelihood of 0.6.

To overcome the computational problems I again use MCMC. Walker et al. (1998) sketch a Metropolis within Gibbs algorithm for a model like (8), except they pretend that $\sigma^2$ is known. I have extended this algorithm to the more realistic case of unknown $\sigma^2$.

(Sample $F$ from its full conditional given $(\mu, \sigma^2)$ (easy: just Pólya updating), and use a random-walk Metropolis to sample $[\mu, \log(\sigma^2)]$, given $F$, with a bivariate normal proposal distribution. On each MCMC sweep renormalize $F$ to have mean 0 and SD 1.)
Inference for $\theta$

It still remains to relate all this to $\theta_Y = E(Y)$ (and to incorporate the mixture aspect of model (5)).

With $W = \log(Y)$, each iteration of the MCMC obtains an estimate of the CDF $F_W$ (in the form of a histogram estimate of the density $f_W$ with $2^M = 256$ bins). But

$$\theta_Y = E(Y) = E(e^W) = \int_{-\infty}^{\infty} e^w f_W(w) \, dw,$$  \hspace{2cm} (15)

so $\theta_Y$ can be estimated from each MCMC iteration by

$$\hat{\theta}_Y = \sum_{j=1}^{2^M} e^{w_j^*} \hat{p}_j(w_j^*),$$  \hspace{2cm} (16)

where the $\hat{p}$’s are the current bin proportions and the $w_j^*$ are the bin centers.

As an example of the results, Figs. 15–18 present posterior summaries based on 5,000 monitoring iterations, arising from the following modeling inputs: (Pólya tree prior) $M = 8, c = 1$ (NB and the centering distribution was the standard normal Winsorized to $\pm 2.42$ (roughly the 0.008 point of the distribution), to damp down the tail); (prior on $\mu_2$ and $\sigma_2^2$) $\nu_p = \kappa_p = 50, \mu_p = -15.7$ and $\sigma_p^2 = 74.0$ (the sample mean and variance of the log($y_i$)); and Metropolis proposal distribution bivariate normal with covariance matrix

$$\Sigma = K \begin{pmatrix} 0.54 & 0.000 \\ 0.00 & 0.015 \end{pmatrix},$$  \hspace{2cm} (17)

(the matrix values are based on Fisher information), with $K = 0.5$ (Metropolis acceptance rate 76%).
Results

Figure 15. *Time series trace, kernel density trace, autocorrelation and partial autocorrelation functions for $\mu_2$.***
Results (continued)

Figure 16. Time series trace, kernel density trace, autocorrelation and partial autocorrelation functions for $\sigma_2^2$. 
Figure 17. Time series trace, kernel density trace, autocorrelation and partial autocorrelation functions for log(θ).
Figure 18. Prior (standard normal) for CDF $F$ of standardized $\log(y)$ and density trace of sample of $y$ values (bold lines), with 25 density traces of MCMC draws from the posterior of $F$ (dotted lines). Note the compromise effected between the prior and the sample with $c = 1$. 
Results (continued)

Preliminary results are given in Table 4 for the 100 year data, using \( c = 1 \) as a kind of compromise tuning constant. The sample mean of the \( e^y \) values in the data was 1.44.

Table 4. Parametric versus nonparametric results with the nonzero part of the 100 year data.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Parametric Posterior</th>
<th>Nonparametric Posterior</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mu_2 )</td>
<td>-16.0 0.812</td>
<td>-15.9 1.17</td>
</tr>
<tr>
<td>( \sigma^2_2 )</td>
<td>82.5 11.9</td>
<td>76.1 15.1</td>
</tr>
<tr>
<td>( \theta_Y )</td>
<td>28.0 959</td>
<td>14.7 78.7</td>
</tr>
</tbody>
</table>

(median of \( \theta_Y = 1.80 \), 95% central interval = (0.0660, 102.8))

Note that the nonparametric approach results in larger posterior SDs for \( \mu_2 \) and \( \sigma^2_2 \) (correctly acknowledging greater uncertainty) but a smaller posterior SD for \( \theta \) (correctly damping down the extreme lognormal tail).

It appears from a small preliminary simulation that by varying \( c \) from 0.1 to 10 it is possible to obtain actual coverage close to 95% for nominal 95% intervals with this approach without unnecessarily wide intervals (work in progress).
We describe parametric and BNP approaches to modeling count data and demonstrate advantages of BNP modeling using empirical, predictive, graphical and formal model comparisons ($LS$ and $LS_{FS}$).

We examine models suitable for analyzing data in control (C) and treatment (T) setting as in the IHGA case study (Hendriksen et al. 1984; Part 1) in which a number of elderly people were randomized in C group, receiving standard care, and T group, which also received in-home geriatric assessment (IHGA).

The outcome of interest was number of hospitalizations during two years.

**Parametric random-effects Poisson** (PREP) model is natural choice for $C$ and $T$ data sets (in parallel):

\[
(y_i|\theta_i) \overset{\text{ind}}{\sim} \text{Poisson}(\exp(\theta_i)) \\
(\theta_i|G) \overset{\text{iid}}{\sim} G \\
G \equiv N(\mu, \sigma^2)
\]  

(18)

assuming a parametric CDF $G$ for latent variables $\theta_i$ (random effects).

What if this assumption is wrong?

Want to remove the parametric assumption on distribution of random effects by building a prior model on CDF $G$ that may be centered on $N(\mu, \sigma^2)$, but permits adaptation (learning from data).
Dirichlet Process Mixture Model

• Specifying prior for an unknown distribution requires a stochastic process with realizations (sample paths) that are CDFs.

• We use Dirichlet process (DP), in notation \( G \sim DP(\alpha, G_0) \), where \( G_0 \) is the center or base distribution of the process and \( \alpha \) a precision parameter (Ferguson 1973, Antoniak 1974).

• Poisson DP mixture model:

\[
(y_i \mid \theta_i)^{ind} \sim \text{Poisson}(\exp(\theta_i)) \\
(\theta_i \mid G)^{iid} \sim G \\
G \sim \text{DP}(\alpha G_0), \quad G_0 \equiv G_0(\cdot; \psi),
\]

where \( i = 1, \ldots, n \) (we refer to (19) as BNP model 1).

• Equivalent formulation of the Poisson DP mixture model:

\[
(y_i \mid G)^{iid} \sim f(\cdot; G) = \int \text{Poisson}(y_i; \exp(\theta)) dG(\theta), \quad G \sim \text{DP}(\alpha G_0),
\]

where \( i = 1, \ldots, n \) and \( G_0 = N(\mu, \sigma^2) \).

• MCMC implemented for a marginalized version of DP mixture. Key idea: \( G \) is integrated out over its prior distribution, (Antoniak 1974, Escobar and West 1995), resulting in \([\theta_1, \ldots, \theta_n \mid \alpha, \psi]\) that follows Pólya urn structure (Blackwell and MacQueen, 1973).

• Specifically, \([\theta_1, \ldots, \theta_n \mid \alpha, \psi]\) is

\[
g_{r0}(\theta_{r1} \mid \mu_r, \sigma_r^2) \prod_{i=2}^{n_r} \left\{ \frac{\alpha_r}{\alpha_r + i - 1} g_{r0}(\theta_{ri} \mid \mu_r, \sigma_r^2) + \frac{1}{\alpha_r + i - 1} \sum_{\ell=1}^{i-1} \delta_{\theta_{r\ell}}(\theta_{ri}) \right\}.
\]
DP Mixture Model with Stochastic Order

- There are cases when treatment always has an effect, only the extent of which is unknown. This can be expressed by introducing stochastic order for the random effects distributions: $G_1(\theta) \geq G_2(\theta), \theta \in R$, denoted by $G_1 \leq_{st} G_2$.

- Posterior predictive inference can be improved under this assumption if we incorporate stochastic order in the model. To that end we introduce a prior over the space $\mathcal{P} = \{(G_1, G_2) : G_1 \leq_{st} G_2\}$.

- A convenient way to specify such a prior is to work with subspace $\mathcal{P}'$ of $\mathcal{P}$, where $\mathcal{P}' = \{(G_1, G_2) : G_1 = H_1, G_2 = H_1H_2\}$, with $H_1$ and $H_2$ d.f.-s on $R$, and then place independent DP priors on $H_1$ and $H_2$.

- Note: to obtain a sample $\theta$ from $G_2 = H_1H_2$, independently draw $\theta_1$ from $H_1$ and $\theta_2$ from $H_2$, and then set $\theta = \max(\theta_1, \theta_2)$.

- Specifying independent DP priors on mixing distributions $H_1$ and $H_2$ we obtain the following model:

\[
\begin{align*}
Y_{1i} & \mid \theta_i \ iid \overset{\text{ind}}{\sim} \text{Poisson}(\exp(\theta_i)), i = 1, n_1 \\
Y_{2k} & \mid \theta_{1n_1+k}, \theta_{2k} \ iid \overset{\text{ind}}{\sim} \text{Poisson}(\exp(\max(\theta_{1n_1+k}, \theta_{2k}))), k = 1, n_2 \\
\theta_{1i} & \mid H_1 \ iid \overset{\text{id}}{\sim} \ H_1, i = 1, n_1 + n_2 \\
\theta_{2k} & \mid H_2 \ iid \overset{\text{id}}{\sim} \ H_2, k = 1, n_2 \\
H_r & \mid \alpha_r, \mu_r, \sigma_r^2 \sim \text{DP}(\alpha_r H_{r0})
\end{align*}
\]

(21)

where the base distributions of Dirichlet processes, $H_{10}$ and $H_{20}$, are again Normal with parametric priors on hyperparameters. We refer to (21) as BNP model 2.

- We implement a standard MCMC with an extension for stochastic order (Gelfand and Kottas, 2002).
Posterior Predictive Distributions

- To create a level playing field to compare quality of PREP and BNP models we compute predictive distributions for future data, based on predictive distribution for latent variables and posterior parameter samples.

- For BNP model 1 the posterior predictive for a future $Y^\text{new}$ is

$$[Y^\text{new} | \text{data}] = \int \int \text{Poisson}(Y^\text{new}; \exp(\theta^\text{new}))(\theta^\text{new} | \eta)[\eta | \text{data}],$$

where $\theta^\text{new}$ is associated with $Y^\text{new}$ and $\eta$ collects all model parameters except $\theta$s (we use bracket notation of Gelfand and Smith (1990) to denote distribution function).

- The posterior predictive for latent variables, induced by Pólya urn structure of DP, is

$$[\theta^\text{new} | \eta] = \frac{\alpha}{\alpha + n} G_{r0}(\theta^\text{new} | \mu_r, \sigma^2) + \frac{1}{\alpha + n} \sum_{\ell=1}^{n} n_\ell \delta_{\theta_\ell}(\theta^\text{new}).$$

(23)
Simulation data sets for control (C) and treatment (T) variables (D1: C and T both Gaussian; D2: C skewed, T bimodal; D3: C Gaussian, T bimodal, \( \bar{n} \geq 10 \)).
Prior (lower [blue] circles) and posterior (upper [red] circles) predictive distributions for PREP model (top) and BNP model 1 (bottom) for data set $D_3$ with bimodal random effects.
Posterior Inference for \( G \)

- Perhaps more interestingly, using generic approach for inference about random mixing distribution, we can obtain \([G \mid \text{data}]\), based on which we can compute posterior of any linear functional of \( G \), e.g. \([E(y \mid G)]\).

- With \( G \sim DP(\alpha G_0) \), following Ferguson (1973) and Antoniak (1974),

\[
[G \mid \text{data}] = \int [G \mid \theta, \alpha, \psi]d[\theta, \alpha, \psi \mid \text{data}]. \tag{24}
\]

where \([G' \mid \theta, \alpha, \psi] \) is also a DP with parameters

\[
\alpha' = \alpha + n \quad \text{and}
\]

\[
G'_0(\cdot | \psi) = \frac{\alpha}{\alpha + n} G_0(\cdot | \psi) + \frac{1}{\alpha + n} \sum_{i=1}^{n} 1_{(-\infty, \theta_i]}(\cdot), \tag{25}
\]

where \( \theta = (\theta_1, ..., \theta_n) \) and \( \psi \) collects parameters of \( G_0 \).

- Using (24), (25) and the definition of DP we develop computationally efficient approach to obtaining posterior sample paths from \([G \mid \text{data}]\).
Normal random effects (data set $D_1$): Posterior MCMC estimates of the random effects distributions for PREP model (first row) and BNP model 1 (second row).

When PREP is correct it (naturally) yields narrower uncertainty bands.
Skewed and bimodal random effects (data set $D_2$): Posterior MCMC estimates of random effects distributions for PREP model (first row) and BNP model 1 (second row).

When PREP is incorrect it continues to yield narrower uncertainty bands that unfortunately fail to include the truth, whereas BNP model 1 adapts successfully to the data-generating mechanism.
Bimodal random effects in $T$ (data set $D_3$): Posterior MCMC estimates of random effects distributions for BNP model 1 (first row) and BNP model with stochastic order (second row).

Extra assumption of stochastic order, when true, yields narrower uncertainty bands (as it should).
$LS$ and $LS_{FS}$
For PREP and BNP Models

$LS$ (left panel) versus full-sample log-score $LS_{FS}$ (right panel) for PREP and BNP models for all 3 data sets $(C$ and $T), D_{1,C}, \ldots, D_{3,T}$.

When PREP is correct $(1C, 1T, 3C)$, $LS$ and $LS_{FS}$ for PREP and BNP nearly coincide (as they should), but when PREP is incorrect $(2C, 2T, 3T)$ both kinds of $LS$ give a clear preference for BNP model 1 (also as they should).
Conclusions

• The BNP methods we illustrate here allow the fitting of random-effects models without making restrictive (and potentially incorrect) parametric distributional assumptions about the random effects; these methods provide posterior inference for the unknown random effects distribution $G$ and associated functionals of interest, as well as predictive distributions for future data (useful for model comparison).

• In Milovan’s dissertation work, besides the BNP models shown here, we have also considered one more BNP model, with bivariate base distribution for DP to induce dependence between random effects $C$ and $T$ distributions.

• All BNP models exhibit superior performance compared to their parametric counterparts on all data sets not generated from the parametric model (e.g., with random effects drawn from skewed and bimodal distributions).
References


