

Bayesian Mass Balancing of Hydrometallurgical Processes

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Overview

- ① Mass balance overview
- ② Bayesian mass balance
 - a. Advantages
 - b. Results on synthetic data
 - c. Results on real data
- ③ Conducting a Bayesian mass balance with your data in R

Definitions - Data Reconciliation aka *Mass Balance*

Goal: For process P_1 filter noisy mass flow rate observations y_1, y_2, y_3 to find $\beta_1, \beta_2, \beta_3$

$$y_1 = \beta_1 + \epsilon_1$$

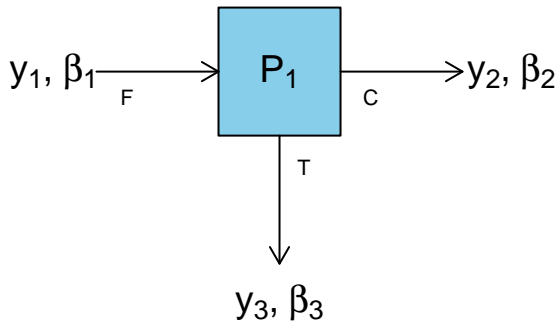
$$y_2 = \beta_2 + \epsilon_2$$

$$y_3 = \beta_3 + \epsilon_3$$

Under assumption of steady state:

$$\beta_1 = \beta_2 + \beta_3$$

Do $\epsilon_1, \epsilon_2, \epsilon_3$ covary?



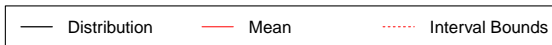
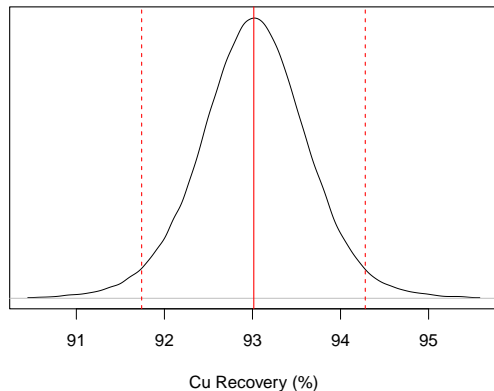
Definitions - Bayesian Inference

- Utilizes Bayes' Rule:

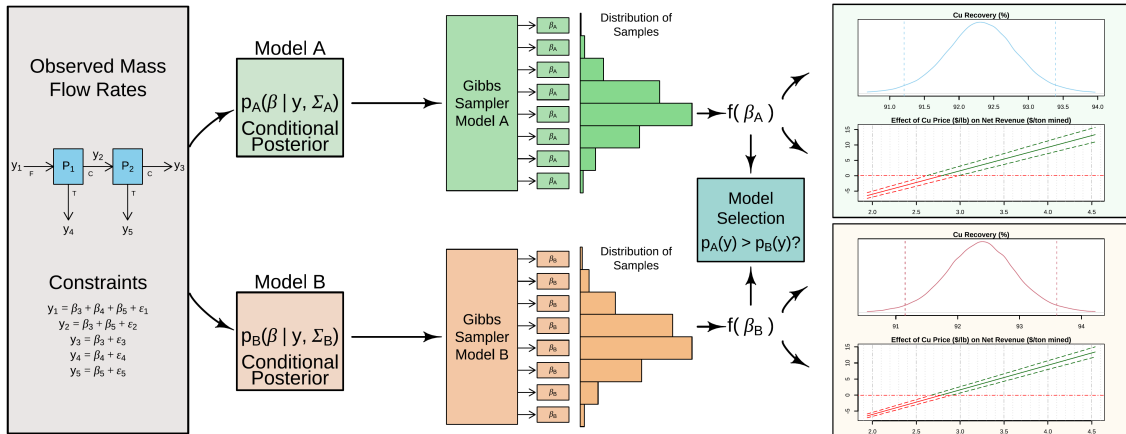
$$p(\beta|y) = \frac{p(y|\beta)p(\beta)}{p(y)}$$

- Provides a distribution of β instead of a point estimate
- Typically utilize algorithms to draw random samples from $p(\beta|y)$, which we can then plug into other formulae
- Can include *a-priori* data on of β : $p(\beta)$, we know all $\beta \geq 0$
- For two models M_1, M_2 if we can find $p(M_1|y)$ and $p(M_2|y)$ we can select the more likely model

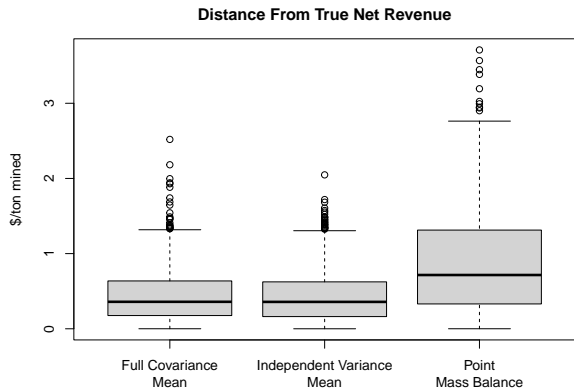
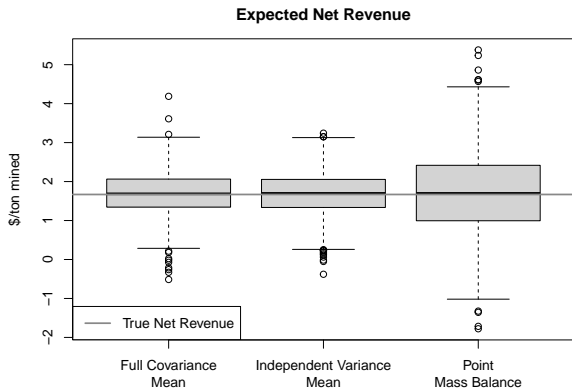
Circuit Copper Recovery



Bayesian Data Reconciliation



Results - Accuracy On Simulated Data

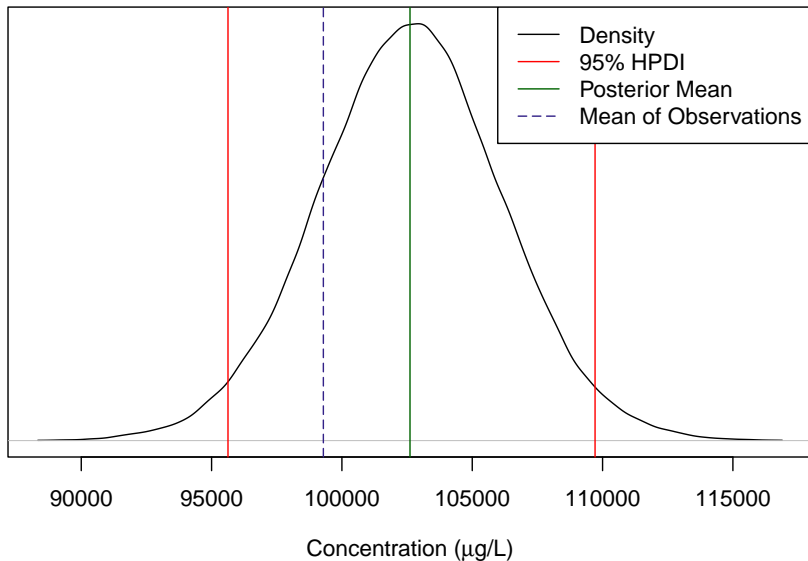


Rare Earth Element (REE) Solvent Extraction (SX) Pilot Plant

- Process for concentrating REEs from acid mine drainage
- Five banks of mixer settlers, each bank in a counter-current configuration
 - ▶ Extraction
 - ▶ Scrubbing
 - ▶ Stripping
 - ▶ Saponification
 - ▶ Acid Wash
- Samples at 10 locations taken hourly for 44 hours
- Time of steady state determined, then mass balance conducted



SX Plant Results - Total REE Concentration in Stripping Solution



Running Your own Data with BayesMassBal in R

First

```
install.packages("BayesMassBal")  
library(BayesMassBal)
```

Review how to organize data and specify constraints using:

```
vignette("Two_Node_Process")
```

Additionally the following code will provide the folder on your computer of example files you can use to model spreadsheets for importing your data via .csv.

```
system.file("extdata", "twonode_constraints.csv",  
            package = "BayesMassBal")  
system.file("extdata", "twonode_example.csv",  
            package = "BayesMassBal")
```

BayesMassBal in R: Importing Your Data

Next, open a new R script (Ctrl + Shift + N), and save your script in the same folder as your data and constraints.

Then in RStudio go to Session -> Set Working Directory -> To Source File Location so R knows where to find your data.

Import your data and constraints:

```
y <- importObservations(file = "Plant_Flow_Rates.csv")  
X <- constrainProcess(file= "Plant_Constraints.csv")
```

BayesMassBal in R: Running the Mass Balance

```
bmb.indep.out <- BMB(X = X, y = y, BTE =c(2000, 80000,1),  
                    cov.structure ="indep")
```

```
summary(bmb.indep.out, export = "results.csv")
```

```
## Mass Flow Rates:
```

```
##
```

```
## CuFeS2:
```

```
## -----
```

```
## Sampling Location Expected Value      95% LB      95% UB  
##           1           1.23654171 1.17682739 1.29068863  
##           2           1.21876650 1.15726110 1.27041060  
##           3           1.15947522 1.10223404 1.21587636  
##           4           0.01777521 0.01087145 0.02415583  
##           5           0.05929128 0.04984514 0.06996186
```

BayesMassBal Additional Features

```
plot(bmb.indep.out, ...,  
     layout = "dens")
```

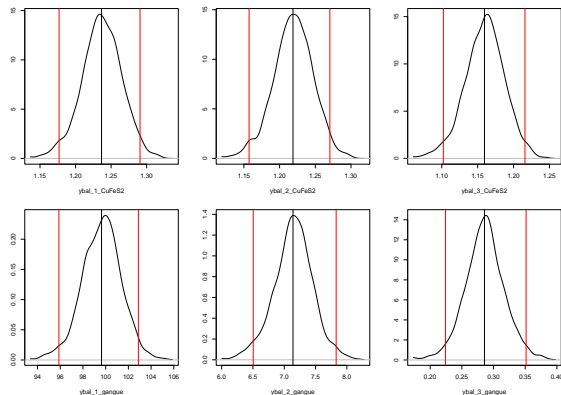
Error correlation

```
BMB(X = X, y = y,  
     cov.structure = "component")
```

Model comparison via

```
BMB(..., lml = TRUE)
```

See vignette("Two_Node_Process") for details



Thank You!!

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Info on BayesMassBal

CRAN: CRAN.R-project.org/package=BayesMassBal

Website: skoermer.github.io/BayesMassBal

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