Bayesian Mass Balancing of Hydrometallurgical Processes

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Overiew

1. Mass balance overview
2. Bayesian mass balance
   a. Advantages
   b. Results on synthetic data
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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 $\beta_1, \beta_2, \beta_3$
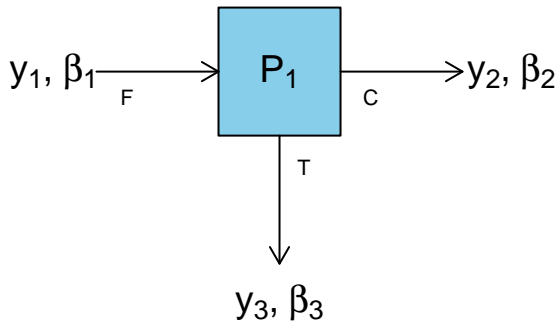
$$y_1 = \beta_1 + \epsilon_1$$
$$y_2 = \beta_2 + \epsilon_2$$
$$y_3 = \beta_3 + \epsilon_3$$

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 $\beta \geq 0$
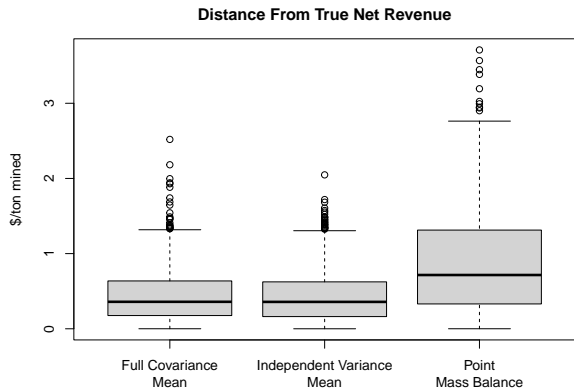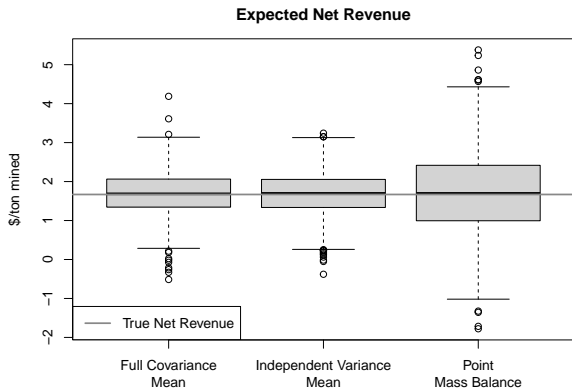- For two models M_1, M_2 if we can find $p(M_1|y)$ and $p(M_2|y)$ we can select the more likely model

Circuit Copper Recovery

Cu Recovery (%)

| —— Distribution | —— Mean | ···· Interval Bounds |
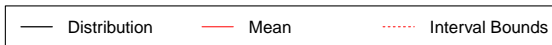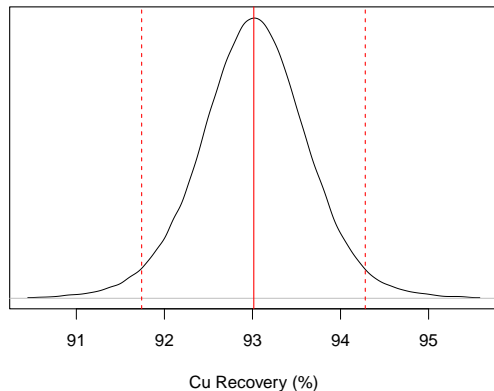
Bayesian Data Reconsciliation
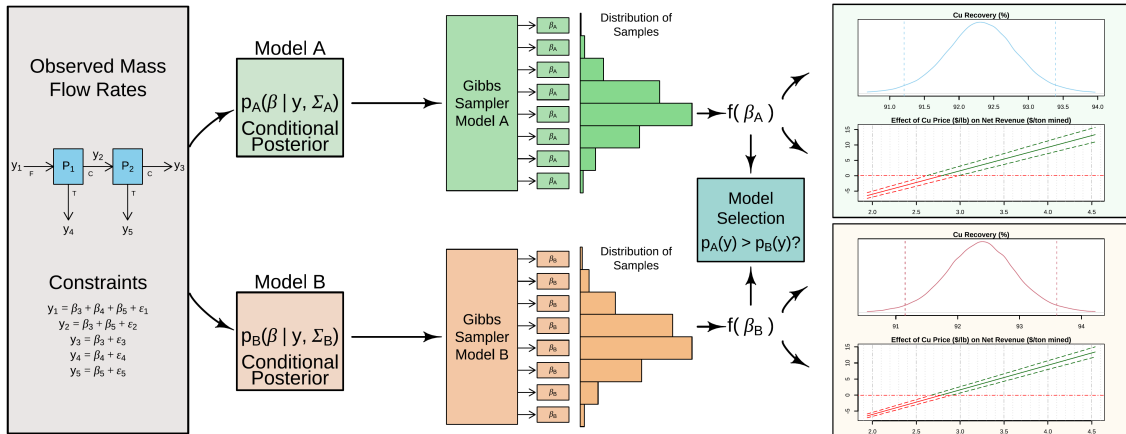
# Results - Accuracy On Simulated Data

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
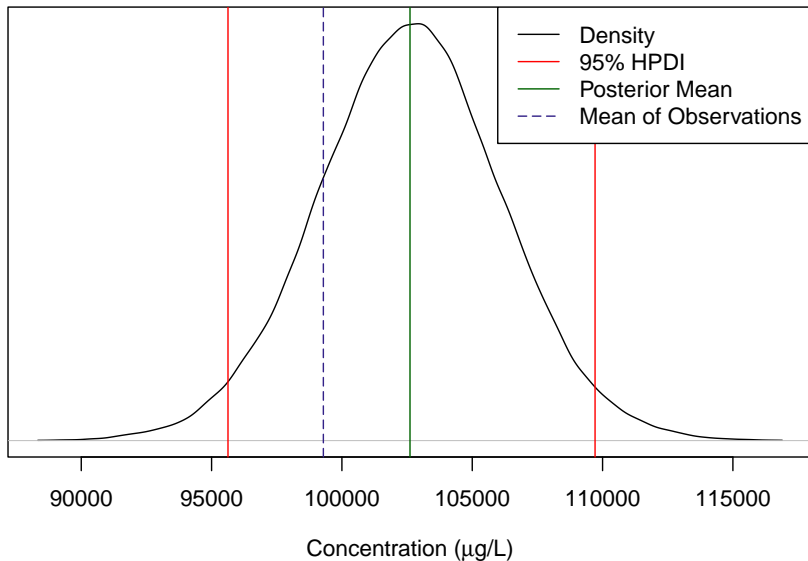
Running Your own Data with `BayesMassBal` in R

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

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

```r
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")
```
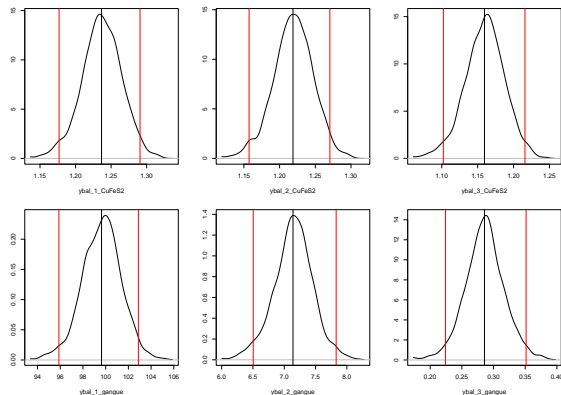
Error correlation

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

Model comparison via

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

See `vignette("Two_Node_Process")` for details

Thank You!!

Contact Info

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Info on `BayesMassBal`

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

Website: `skoermer.github.io/BayesMassBal`

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