Analyzing the provided simulated dataset

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1 Introduction

In this vignette we go through the analysis of a simulated dataset included in the dpeaqms package.

2 The Data

The dataset consists of 12 samples divided into $G = 4$ groups i.e. CTL ($g = 1$), TRT1($g = 2$), TRT2 ($g = 3$) and TRT3 ($g = 4$) with 3 samples in each group. The simulation scenario assumed the availibility of 6 isobaric tags. This necessitates the use of two experiments ($E = 2$) with six tagged samples per experiment. Two samples from each the groups CTL, TRT1 and TRT2 were used in the first experiments while one sample from each of the groups CTL, TRT1 and TRT2 were used in the second in addition to the three samples from the TRT3 group.

3 Analyzing the Simulated Dataset

Load the library and the simulated dataset using the commands

```
library(dpeaqms)
data(dpeaqms.simulatedDataset1)
```

A simple analysis with the prior parameters set to their defaults can be performed using the command

```
simdataSamples <- dpeaqms.mcmc(msmsdata=dpeaqms.simulatedDataset1,
                               controlGroup='CTL', transform=FALSE,
                               samples=1000, thin=100, burnin=100000)
```

This will draw 1000 model parameters parameter samples from the probability distribution of the model parameters given the data. The "transform" parameter specifies that the intensity data is not to be log transformed. The "samples" parameter specifies the number of samples to be taken. The "thin" sample specifies the number of iterations of the MCMC algorithm to skip between successive samples. Finally the "burnin" parameter specifies the number of initial iterations of the MCMC algorithm to discard before starting to draw samples.

4   Outputing the Results

The MCMC sample obtained by running the commands in the previous section can be analyzed using standard tools from the coda package. The MCMC sample can also be summarized using a function from the package

```
dpeaqms.extract.sample(msmsdata=dpeaqms.simulatedDataset1,
                       mcmc_sample=simdataSample, numberOfMCMCSamples=1000,
                       controlGroup='CTL', summaryOnly=T)
```