VB-LKMR – Simulations

Overview:

We present a variational Bayes inference procedure for lagged kernel machine regression (LKMR) for identifying time windows of susceptibility to exposures of complex metal mixtures. VB-LKMR identifies critical exposure windows of chemical mixtures, and accounts for complex nonlinear and non-additive effects of the mixture at any given exposure window.

This page presents an overview of using VB-LKMR code for simulations, and comparison to a MCMC implementation of LKMR.

We present the code for a simulation of N = 100, where each individual has 3 metal exposures measured at 4 time windows. The simulation code presented here is for a single simulated dataset. For the manuscript, the simulations for multiple datasets were run in parallel on a high performance computing cluster. Alternatively, the simulations could be made into a for loop. Please note that for the manuscript, the simulations were based on N = 300, not N = 100 as we present here.

VB-LKMR simulation:

Run "AnalysisCode_VB_LKMR.R", which simulates a single dataset (N=100) with AR-1 = 0.8 and runs VB-LKMR and MCMC-LKMR. To output tables analogous to Table 1 of the manuscript, run "SummaryAnalysis_VB_LKMR.R" and use the commands below. Note that the columns correspond to "Intercept, Slope, R^2, and RMSE" of the regression $\hat{\boldsymbol{h}}_t$ vs. $\boldsymbol{h}_t$ for t = 1,…,4 time windows. Each row corresponds to a time window, ranging from time window 1 to time window 4. Note that because there is no true effect at time window 1, the slope and R^2 are not applicable to the regression of $\hat{\boldsymbol{h}}$ vs. $\boldsymbol{h}$ so are set to be 0.

```
> print("VB: Intercept, Slope, R^2, RMSE")
[1] "VB: Intercept, Slope, R^2, RMSE"
> print( round(Summary.MFVB, 2) )
      [,1] [,2] [,3] [,4]
[1,]  0.03 0.00 0.00 0.40
[2,]  0.01 0.89 0.93 0.31
[3,] -0.01 0.91 0.96 0.41
[4,] -0.03 0.91 0.99 0.34

> print("MCMC: Intercept, Slope, R^2, RMSE")
[1] "MCMC: Intercept, Slope, R^2, RMSE"
> print(round(Summary.MCMC, 2))
      [,1] [,2] [,3] [,4]
[1,]  0.02 0.00 0.00 0.44
[2,]  0.02 0.92 0.93 0.31
[3,] -0.01 0.90 0.95 0.45
[4,] -0.04 0.91 0.99 0.35
```