LKMR – Simulations

Overview:

We present lagged kernel machine regression (LKMR) for identifying time windows of susceptibility to exposures of complex metal mixtures. 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 LKMR code for simulations, and comparison to Bayesian kernel machine regression (BKMR) and JKBKMR (joint kernel BKMR).

We present the code for the base case simulation of N = 100, where each individual has 5 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.

LKMR simulation:

Run "Sim_Code.R", which simulates a dataset with AR-1 = 0.8 and runs LKMR, BKMR and JKBKMR. To output tables analogous to Table 1 of the manuscript, use the commands below. Note that the columns correspond to "Intercept, Slope, R^2, RMSE and Coverage" 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.

```
> round(mat.res.gfl,2) #LKMR
     Intercept Slope Rsquared RMSE Coverage
[1,]     -0.02  0.00     0.00 0.53     0.99
[2,]     -0.03  0.85     0.77 0.50     0.98
[3,]     -0.05  1.00     0.84 0.67     0.97
[4,]      0.13  0.94     0.96 0.48     1.00

> round(mat.res.bkr,2) #BKMR
     Intercept Slope Rsquared RMSE Coverage
[1,]     -0.04  0.00     0.00 1.59     0.87
[2,]     -0.09  1.71     0.58 1.64     0.91
[3,]     -0.14  2.28     0.90 2.31     0.64
[4,]      0.15  1.48     0.97 1.29     0.81

> round(mat.res.1kernel.all,2) #JKBKMR
     Intercept Slope Rsquared RMSE Coverage
[1,]     -0.81  0.00     0.00 1.05     1.00
[2,]     -0.28  0.75     0.63 0.69     1.00
[3,]     -0.49  0.66     0.48 1.29     0.96
[4,]     -0.33  0.65     0.70 1.33     0.94
```