WQS EXTENSIONS AND RECENT WORK

Data type extensions

- New gWQS package includes capability for evaluating new data types/distributions:
  - Multinomial (generalized logits)
  - Poisson (count data)
  - Negative binomial (over-dispersed count data)

- Later extensions will include
  - Time-to-response data with censoring (e.g., Weibull distribution)
  - Stratification implementation for categorical variables
  - Allowance for interaction of WQS with continuous variable during estimation

Random subset WQS regression

- Two types of ensemble steps
  - *Bootstrap sampling* of observations with replacement
  - *Random subset* selection of variables (e.g., random set of 20 repeated 1000 times)

Allows for WQS regression to be extended to large number of variables – e.g., metabolomics

Extensions: Metabolomics

The methods of metabolomics are not only to understand traditional measures of **biological response** but also to analyze the **exposures** associated with those responses.

May be useful for

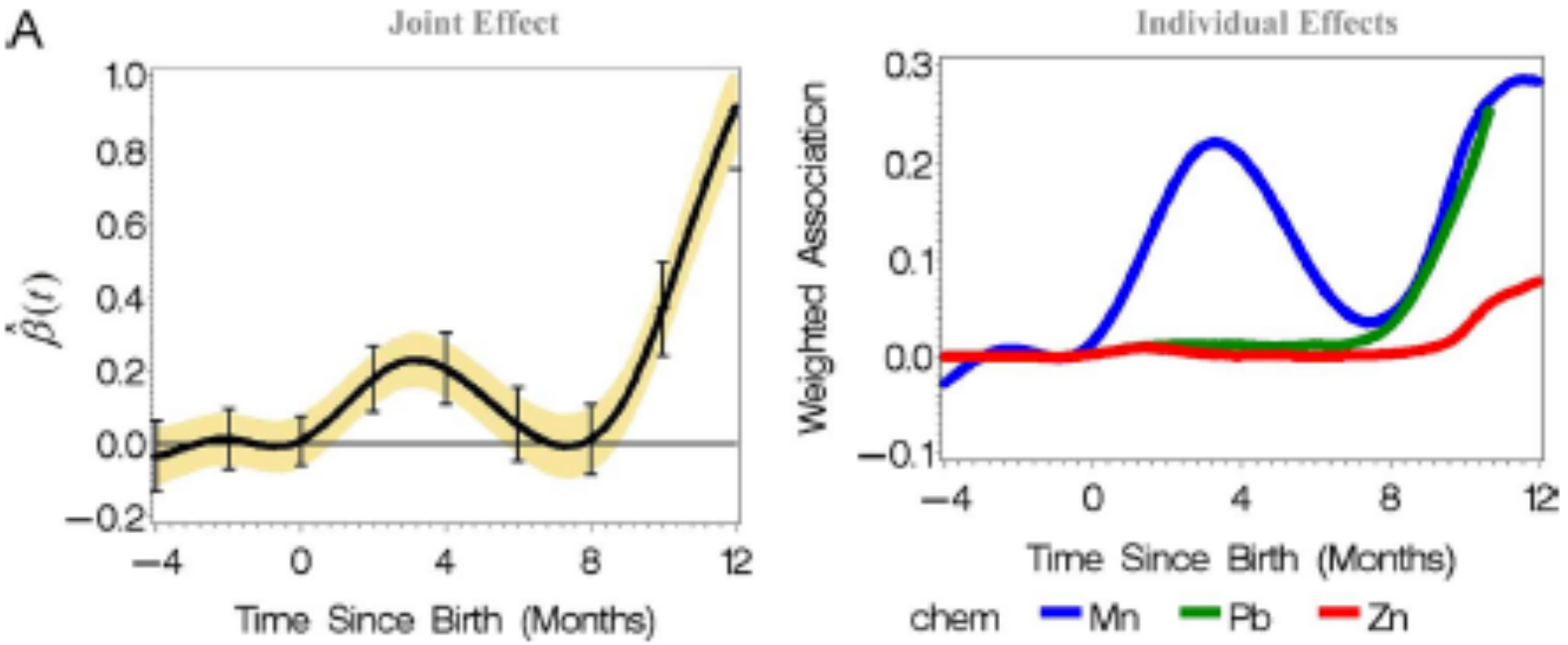
- Biomarker discovery
- Measuring a “mixture effect”

RS WQS regression seems to work well in high dimensions (Curtin et al 2018, *under review*)

Lagged WQS Regression

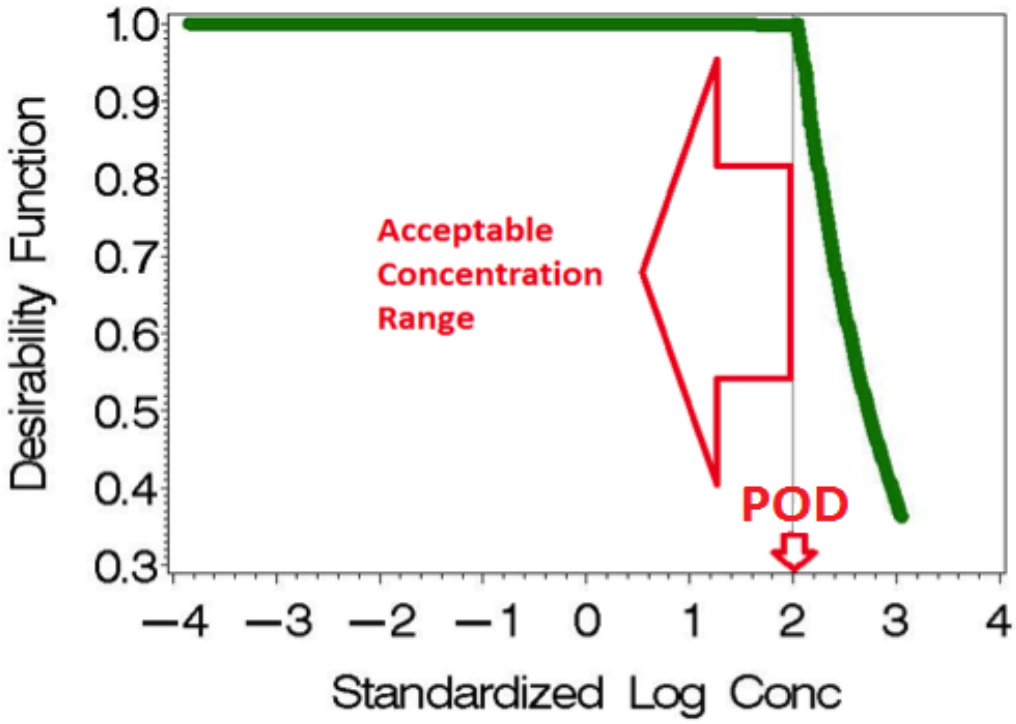
(Bello et al, Env Res, 2017)

Lagged WQS regression is a reverse DLM on an iteratively weighted WQS index.



Acceptable Concentration Region (ACR) models (Gennings et al 2018 ENV INT)

Incorporates the concept of **regulatory guideline values** into a nonlinear regression model



ACR model example

For single chemicals

$$d_m^{low} = \begin{cases} 1, & X_m < \delta_m^{low} \\ \exp\left[-\gamma_m^{low}\left(X_m - \delta_m^{low}\right)\right], & X_m \geq \delta_m^{low} \end{cases}$$

$$g(\mu_i) = \begin{cases} \beta_0 + \beta_1(1) + Z_i^T\theta, & X_i < \delta^{low} \\ \beta_0 + \beta_1(\exp\left[-\gamma^{low}\left(X_i - \delta^{low}\right)\right]) + Z_i^T\theta, & X_i \geq \delta^{low} \end{cases}$$

For mixtures

$$g(\mu_i) = \beta_0 + \beta_1(d_1 \times d_2 \times \ldots \times d_M)^{\frac{1}{M}} + Z_i^T\gamma$$

$$= \beta_0 + \beta_1 MDF + Z_i^T\gamma$$

THANK YOU!