BIOST 572: Final Talk

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The Paper

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Semiparametric estimation of regression quantiles with application to standardizing weight for height and age in US children

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Motivational Example

- Data: Observational longitudinal study of obesity from birth to adulthood.
- Overall Goal: Build age-, gender-, height-specific growth charts (under 3 years) to diagnose growth abnormalities.
- Specific Aim: Estimate the reference range for age-, gender-, height-specific weight.
- A simple version: Estimate the reference range for age-, gender-specific BMI.
- Statistical Problem: Estimate covariate specific quantiles in a reference group.
- Other Applications: Regression using placement value/receiver operating characteristic (ROC) regression.

Data Display

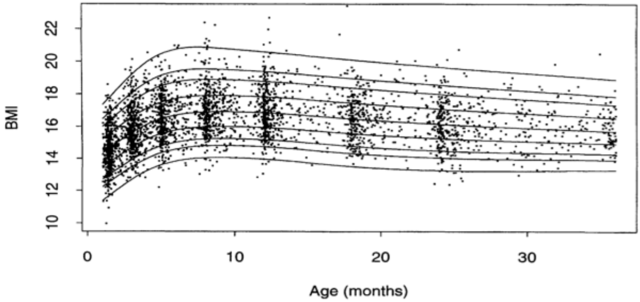


Figure: Estimated 1st, 5th, 10th, 25th,50th, 75th, 90th, 95th and 99th percentiles of BMI as a function of age

Previous Solutions: Bin and Smooth Estimation

- Bin and Smooth Quantiles (BSQ): Empirical quantiles for each narrow interval $X \pm \lambda$, then smoothed it (with splines). (Hamill et al., 1977)
- Bin and Smooth Parameters: Model $f(Y|X)$ by $\theta(X)$, estimate $\theta(X)$ for each narrow interval of $X \pm \lambda$, then smoothed it.
  Cole (1990) let $\theta(X) = \{\mu(X), \sigma(X)\}$ and assume $Y|X$ follows normal distribution with mean $\mu(X)$ and standard deviation $\sigma(X)$.

  $$Y^\alpha = \mu(X) + \sigma(X)z^\alpha,$$

  z^α is the αth quantile for standard normal distribution.
- Limitations: (1) Require large sample size; (2) Curse of dimensionality.

Previous Solutions: Parametric Models

- Idea: Specify a fully parametric model for $Y|X$ indexed by parameter $\boldsymbol{\theta}$, then estimate $\boldsymbol{\theta}$ via likelihood.
- LMS (Cole and Green 1992): Assume Y can be transformed to the standard normal random variable Z as follow:

$$Z = \frac{\{Y/M(X;\boldsymbol{\theta})\}^{L(X;\boldsymbol{\theta})} - 1}{L(X;\boldsymbol{\theta})S(X;\boldsymbol{\theta})},$$

  $M(X;\boldsymbol{\theta})$ is median response, $L(X;\boldsymbol{\theta})$ is Box-Cox power transformation term and $S(X;\boldsymbol{\theta})$ approximate variance.

$$Y^{\alpha}(X;\boldsymbol{\theta}) = M(X;\boldsymbol{\theta})\{1 + z^{\alpha}L(X;\boldsymbol{\theta})S(X;\boldsymbol{\theta})\}^{1/L(X;\boldsymbol{\theta})}$$

- Limitation: (1) The distribution assumption (transformed normal distribution); (2) Sensitivity of the transformation part $L(X)$ to outliers.

Previous Solutions: Nonparametric Models

- Idea: Directly estimate $Y^\alpha(X)$ without assuming certain distribution for Y.
- Quantile Regression (QR): Koenker and Bassett (1978) proposed an M-estimation to obtain $\hat{Y}^\alpha(X)$ that minimize

$$\sum_i \alpha\{Y_i - Y^\alpha(X)\}_+ + (1-\alpha)\{Y_i - Y^\alpha(X)\}_-,$$

  $x_+ = max(0, x)$ and $x_- = max(0, -x)$.
- Limitation: $\hat{Y}^\alpha(X)$ may not be monotone in α.

New method: Semiparametric Models (SM)

- Allow the shape depend on X and do not specify specific distribution for Y. Model $\mu(X)$ and $\sigma(X)$ parametrically to gain efficiency.
- General model

$$Y_i = \mu(X_i; \boldsymbol{\theta}) + \sigma(X_i; \boldsymbol{\theta})\varepsilon(X_i),$$

$\mu(X_i; \boldsymbol{\theta})$ is the location parameter, $\sigma(X_i; \boldsymbol{\theta})$ is the scale parametre, i.e. $\sqrt{Var(Y_i|X_i)}$, and $\varepsilon(X_i)$ is from baseline distribution with mean zero, unit varaince. Denote baseline distribution function by $F_0(z, X) = P(\varepsilon(X) \leq z|X)$, we have

$$Y^\alpha(X; \boldsymbol{\theta}, F_0) = \mu(X_i; \boldsymbol{\theta}) + \sigma(X_i; \boldsymbol{\theta})Z^\alpha(X),$$

$Z^\alpha(X)$ is the αth quantile of $\varepsilon(X)$, i.e.

$$F_0(Z^\alpha(X), X) = \alpha.$$

Quasi-likelihood

Using independent working correlation and use normal distribution as working model for $Y|X$, we obtain quasi-likelihood score equation as below:

$$
\begin{aligned}
0 &= \frac{\partial \mu(X;\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} \frac{Y-\mu(X;\boldsymbol{\beta})}{Var(Y|X)} \\
0 &= \frac{\partial \sigma^2(X;\gamma)}{\partial \gamma} \frac{(Y-\mu(X;\boldsymbol{\beta}))^2-\sigma^2(X;\gamma)}{Var[(Y-\mu(X;\boldsymbol{\beta}))^2|X]} \\
&= \frac{\partial \sigma^2(X;\gamma)}{\partial \gamma} \frac{(Y-\mu(X;\boldsymbol{\beta}))^2-\sigma^2(X;\gamma)}{2Var(Y|X)^2}
\end{aligned}
$$

Model details

- We can use splines to model $\mu(X)$ and $\sigma(X)$. Let $\boldsymbol{\theta} = \{\beta_1, \cdots, \beta_p, \gamma_1, \cdots, \gamma_q\}$, $R(X) = \{R_1(X), \cdots, R_p(X)\}$ and $S(X) = \{S_1(X), \cdots, S_q(X)\}$ are pre-specified regression spline basis functions.

$$\mu(X) = \sum_{k=1}^{p} \beta_k R_k(X), \log\{\sigma(X)\} = \sum_{k=1}^{q} \gamma_k S_k(X)$$

The scores becomes

$$\begin{aligned} 0 &= \sum_i R(X_i)^T \frac{Y_i - \mu(X_i; \boldsymbol{\beta})}{\sigma^2(X_i; \gamma)} \\ 0 &= \sum_i S(X_i)^T \frac{(Y_i - \mu(X_i; \boldsymbol{\beta}))^2 - \sigma^2(X_i; \gamma)}{\sigma^2(X_i; \gamma)} \end{aligned}$$

Estimate Baseline Function

- Obtain the estimated residuals

$$\hat{e}_i(X_i) = \frac{Y_i - \mu(X_i; \hat{\beta})}{\sigma(X_i; \hat{\gamma})},$$

- Special case: F_0 does not depend on X.

$$\hat{F}_0(z, X) = n^{-1} \sum_{i=1}^{n} I(\hat{e}_i \leq z).$$

- Step function $\Rightarrow$ continuous function.

$$\hat{F}_0(z, X) = n^{-1} \sum_{i=1}^{n} K_{\lambda_2}(z, \hat{e}_i),$$

where $K_{\lambda_2}(z, \hat{e}_i) = \Phi\{(z - \hat{e}_i)/\lambda_2\}$. $\hat{F}_0(z, X)$ is monotonically increasing in z.

Estimate Baseline Function

- General case: F_0 does depend on X.

$$\hat{F}_0(z, X) = \frac{\sum_{i=1}^{n} w_{\lambda_1}(X, X_i) I(\hat{e}_i \leq z)}{\sum_{i=1}^{n} w_{\lambda_1}(X, X_i)},$$

  where $w_{\lambda_1}(X, X_i) = \phi((X - X_i)/\lambda_1)$.
- Continuous version:

$$\hat{F}_0(z, X; \lambda_1, \lambda_2) = \frac{\sum_{i=1}^{n} w_{\lambda_1}(X, X_i) K_{\lambda_2}(z, \hat{e}_i)}{\sum_{i=1}^{n} w_{\lambda_1}(X, X_i)},$$

- For λ_1 and λ_2, we can use either fixed value or allow them to be functions of X.
- Estimate αth quantile by $\mu(x, \hat{\beta}) + \sigma(x, \hat{\gamma}) \hat{F}_0^{-1}(\alpha, X)$.

Nonparametric kernel estimator (NKE) based on Y_i

- A nonparametric way will be use

$$\hat{F}(z, X) = \frac{\sum_{i=1}^{n} w_{\lambda_1}(X, X_i) I(Y_i \leq z)}{\sum_{i=1}^{n} w_{\lambda_1}(X, X_i)},$$

  then estimate αth quantile by $\hat{F}^{-1}(\alpha, X)$
- To estimate $\hat{F}(z, X)$, assuming a uniform distribution for X,

$$\begin{aligned} Bias &= \frac{1}{4}\ddot{F}(z, X)\lambda_1^2\sigma_W^2 \\ Var &= (n\lambda_1)^{-1} F(z, X) \int W(u)^2 du \end{aligned}$$

- Optimal weight is $\lambda_1^* = \left(\frac{n^{-1}F(z,X)\int W(u)^2 du}{\ddot{F}(z,X)^2\sigma_W^4}\right)^{1/5}$.
- Minimum mean square error (MSE) is in order of $n^{-2/5}$.

Multiple covariates

- Estimating equation part: Use two set of spline basis $R(X_1)$, $R(X_2)$ and $S(X_1)$, $S(X_2)$. Use their tensor product to generate the new basis $R(X) = R(X_1) \otimes R(X_2)$, $S(X) = [S(X_1), S(X_2)]$.
- Baseline estimator: Not approximate indicator function by continuous one. For kernel $W(X)$, can use any multivariate kernel, for example the tensor product of two univariate kernel $W_1(X_1) \times W_2(X_2)$. In application, they use $W(X) = W_1(X_1)$.

Simulation: Methods Comparing

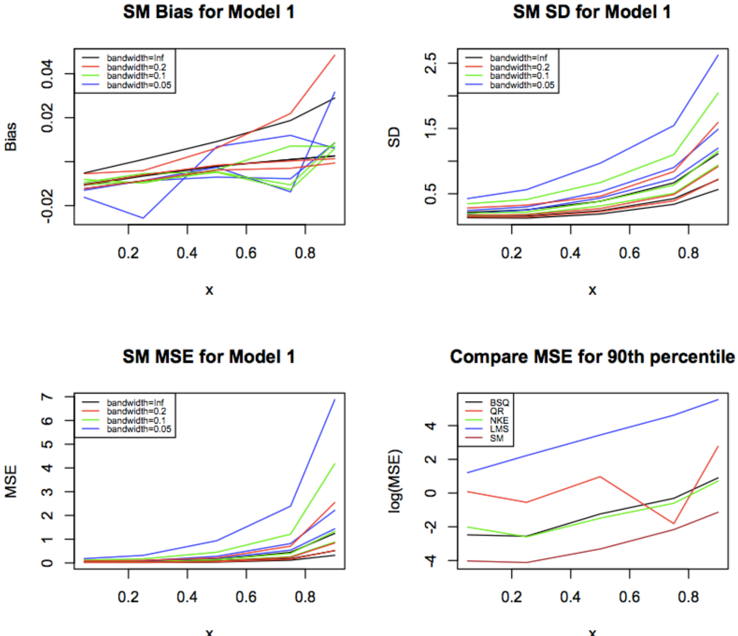
Assume univariate covariate X follows the standard uniform distribution.

- Methods: BSQ=Bin smoothed quantile, QR=Quantile regression, NKE=Nonparametric kernel smooth estimator, LMS=LMS parametric method, SM=Semiparametric method
- Model 1:

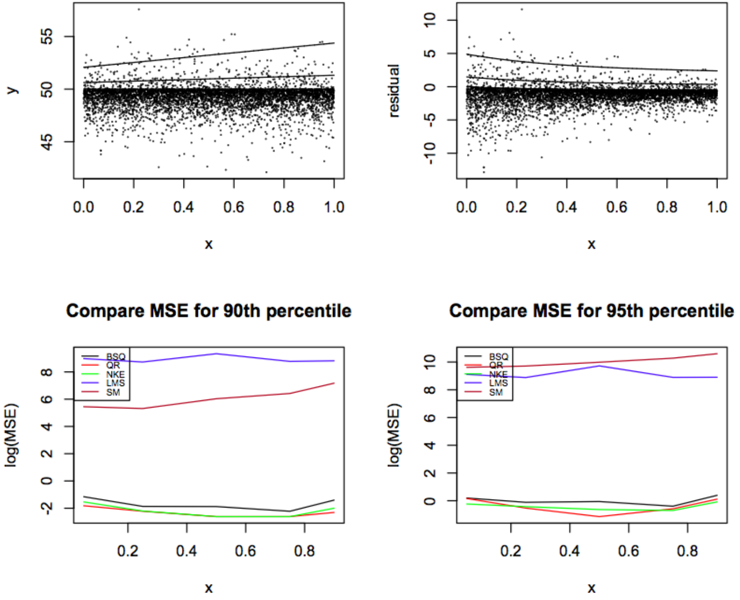
$$\mu(X) = 50 + 10X, \log(\sigma(X)) = 1 + 2X,$$

  and $\varepsilon(X)$ follows the standard normal distributions.
- Model 2: $(Y - 50)|X$ follows the mixture distribution $0.1 Exp(0.9 + X) + 0.9(-Exp(0.1 + X))$.
- All sample size is $n = 5000$ and bias, variance and MSE calculated from 1000 simulations.

Simulation Result: Model 1



Simulation Result: Model 2



Data Analysis

Can follow the procedures below

- Step 1: Fit the nonparametric quantile regression to see whether certain quantile $Y^\alpha(X)$ and/or distribution $F(z, X)$ change over X.
- Step 2: If step 1 no, use the nonparametric kernel smooth estimator.
- Step 3: If step 1 yes, fit a semiparametric quantile regression model and then check whether the residual distribution $F_0(z, X)$ change over X.
- Step 4: If step 3 no, fit a semiparametric quantile regression model assuming same baseline.
- Step 5: If step 3 yes, choose between the semiparametric quantile regression with kernel smooth and the nonparametric kernel smooth estimator.

Example

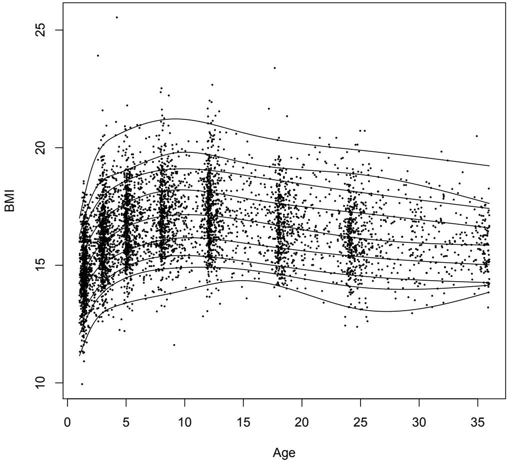


Figure: Fitted 1st, 5th, 10th, 25th, 50th, 75th, 90th, 95th and 99th percentiles from nonparametric quantile regression

Example

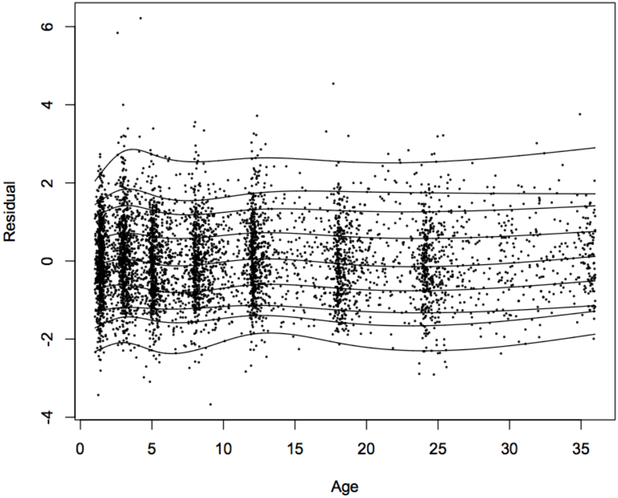


Figure: Fitted 1st, 5th, 10th, 25th, 50th, 75th, 90th, 95th and 99th percentiles from nonparametric quantile regression for residuals

Example

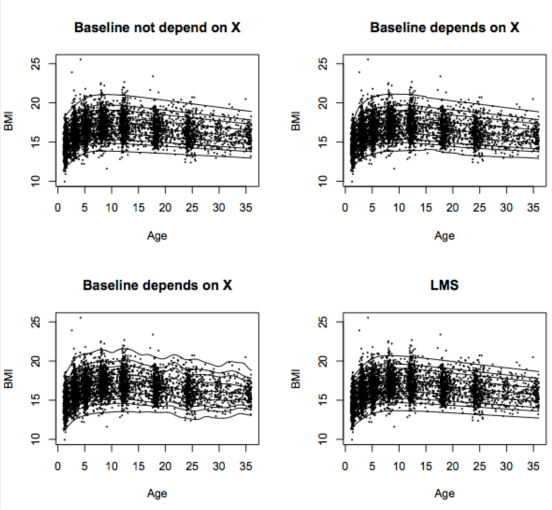


Figure: Fitted 1st, 5th, 10th, 25th, 50th, 75th, 90th, 95th and 99th percentiles from four methods