1 Simulation Study

We compare the performance of our quantile trend filtering method with the three previously published methods using designs proposed by Racine and Li (2017). The methods compared are

- `npqw`: Racine and Li (2017) constrain the response to follow a smooth location scale model of the form $Y_i = a(X_i) + b(X_i)\epsilon_i$. They estimate the τ_{th} conditional quantile given $X_i = x$ using a kernel estimator

$$q_\tau(x) = \frac{\sum_{i=1}^n \Phi^{-1}_{(Y_i, b(X_i))}(\delta_0) K_h(X_i, x)}{\sum_{i=1}^n K_h(X_i, x)} \tag{1}$$

  defining $\Phi^{-1}_{(Y_i, b(X_i))}(\delta_0)$ as the quantile function of the Normal distribution with mean Y_i and standard deviation $b(X_i)$ evaluated at τ. δ_0 is a function of τ and chosen empirically, h is a tuning parameter and K is a kernel function. Code was obtained from the author for the `quantile-ll` method.

- `qsreg`: Oh et al. (2011) proposed a pseudo-data algorithm for a quantile spline estimator of the form

$$\sum_i \rho_\tau(y_i - g(x_i)) + \lambda \int (g''(x))^2 dx. \tag{2}$$

  If $\rho_\tau(\cdot)$ were differentiable, the solution to this equation would take a form similar to that of the squared loss smoothing spline with weights equal to $\frac{\rho'_\tau(y_i - g(x_i))}{2(y_i - g(x_i))}$. Relying on this idea, Nychka proposed to solve the problem by iteratively solving the weighted smoothing spline. To address the non-differentiability they propose an approximation

$$\rho_{\tau,\delta}(u) = [\tau I(u > 0) + (1 - \alpha) I(u < 0)] u^2/\delta \tag{3}$$

  The function `qsreg` in the `fields` R package was used. The smoothing parameter is chosen automatically using generalized cross validation on the pseudo data.

- `rqss`: Koenker et al. (1994) Koenker proposed smoothing splines using trend filtering with the second order differencing matrix which results in linear splines. The function `rqss` in the `quantreg` package implements this method. The smoothing parameter λ is chosen using a grid search and minimizing

$$SIC(p_\lambda) = log[n^{-1} \sum \rho_\tau(y_i - \widehat{g}(x_i))] + \frac{1}{2n} p_\lambda logn \tag{4}$$

  where $p_\lambda = \sum I(y_i = \widehat{g}_i(x_i))$, which can be thought of as active knots.

- `detrendr_SIC`: Our method where we minimize $\sum_i \rho_\tau(y_i - \theta_i) + \lambda ||D\theta||_1$ and λ is chosen using SIC from above. A single value of λ was chosen by scaling and summing SIC values across all quantiles.

- `detrendr_valid`: Our method where lambda is chosen by leaving out every 5th observation as a validation data set and evaluating the check loss function on the validation data.

- `detrendr_eBIC`: The traditional BIC is given by

$$\mathrm{BIC}(s) = -2\log(L\{\hat{\theta}(s)\}) + \nu(s)\log n \tag{5}$$

where $\theta(s)$ is the parameter θ with those components outside s being set to 0, and $\nu(s)$ is the number of components in s. If we assume an asymmetric Laplace likelihood $L(y|\theta) = \left(\frac{\tau^n(1-\tau)}{\sigma}\right)^n \exp\left\{-\sum_i \rho_\tau(\frac{y_i-\theta_i}{\sigma})\right\}$ and the number of non-zero elements of $D\theta$ as df

$$\mathrm{BIC}(df) = 2\sum_i \frac{1}{\sigma}\rho_\tau(y_i - \theta_i) + df \log n \tag{6}$$

We can choose and $\sigma > 0$ and have found empirically that $\sigma = \frac{1-|1-2\tau|}{2}$ produces stable estimates. Chen and Chen (2008) proposed the extended BIC for large parameter spaces

$$BIC_\gamma(s) = -2\log(L\{\hat{\theta}(s)\}) + \nu(s)\log n + 2\gamma \log \binom{P}{j} \tag{7}$$

where P is the total number of possible parameters and j is the number of parameters included in given model.

Three simulation designs from Racine and Li (2017) were considered. For all designs X_i was generated as a uniformly spaced sequence in $[0, 1]$ and the response Y was generated as

$$Y_i = sin(2\pi x_i) + \epsilon_i(x_i)$$

The three error distributions considered were

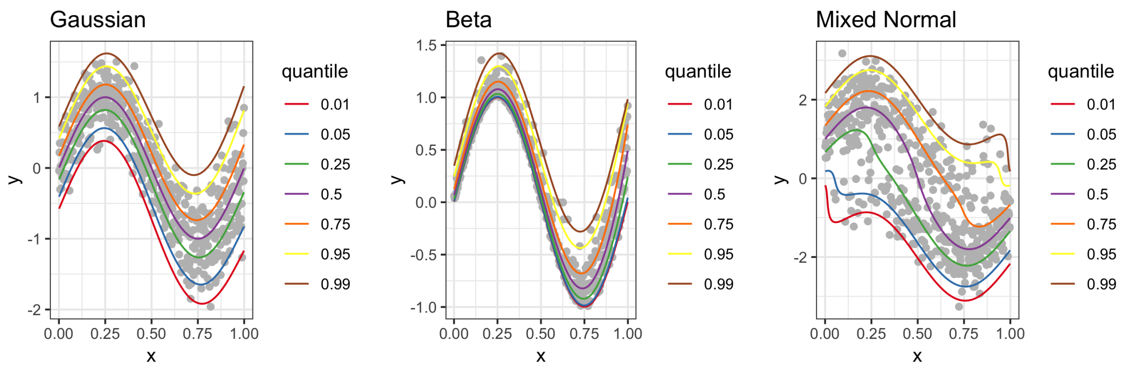
- Gaussian: $\epsilon_i(x_i) \sim N\left(0, \left(\frac{1+x_i^2}{4}\right)^2\right)$

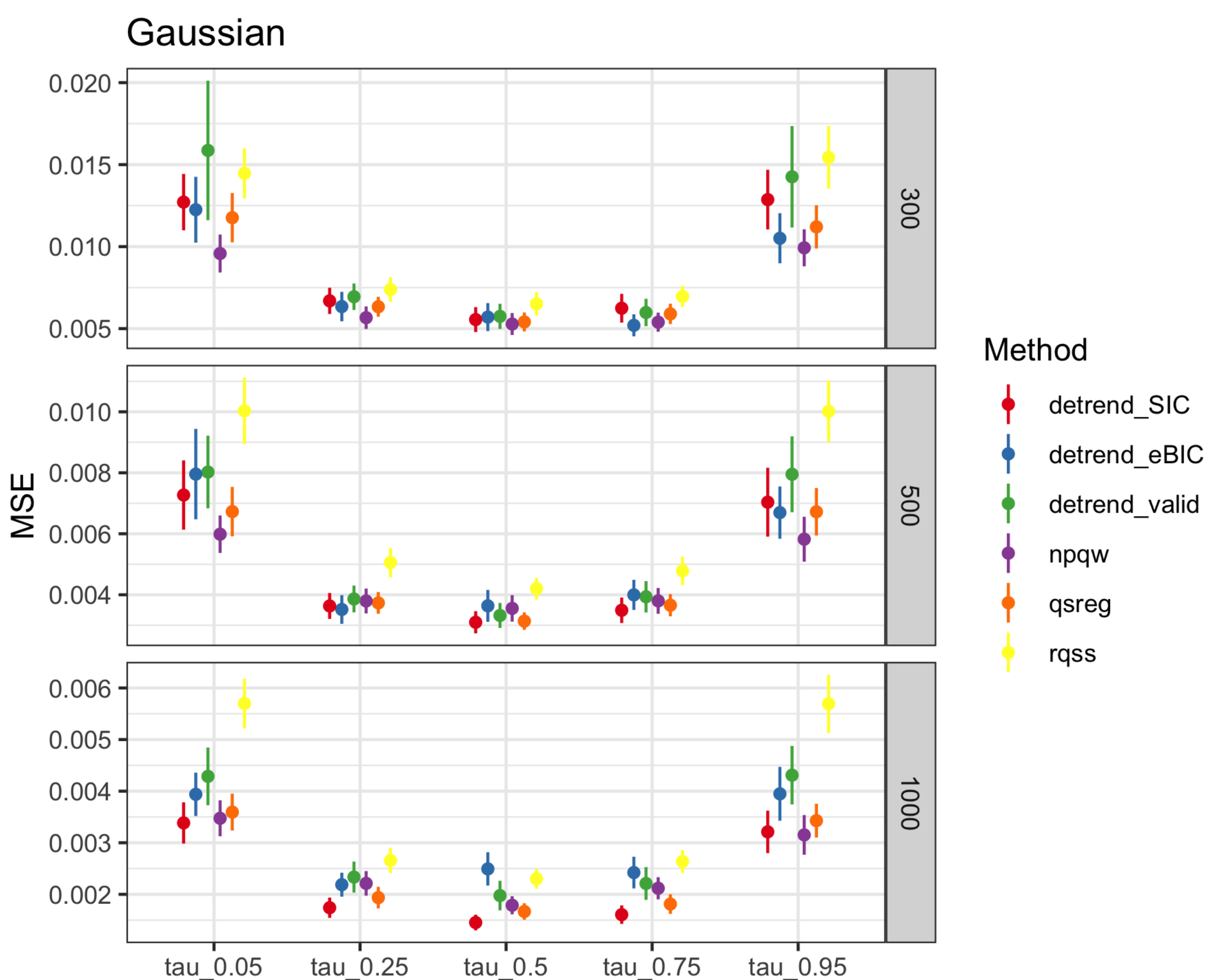
- Beta: $\epsilon_i \sim Beta(1, 11 - 10x_i)$

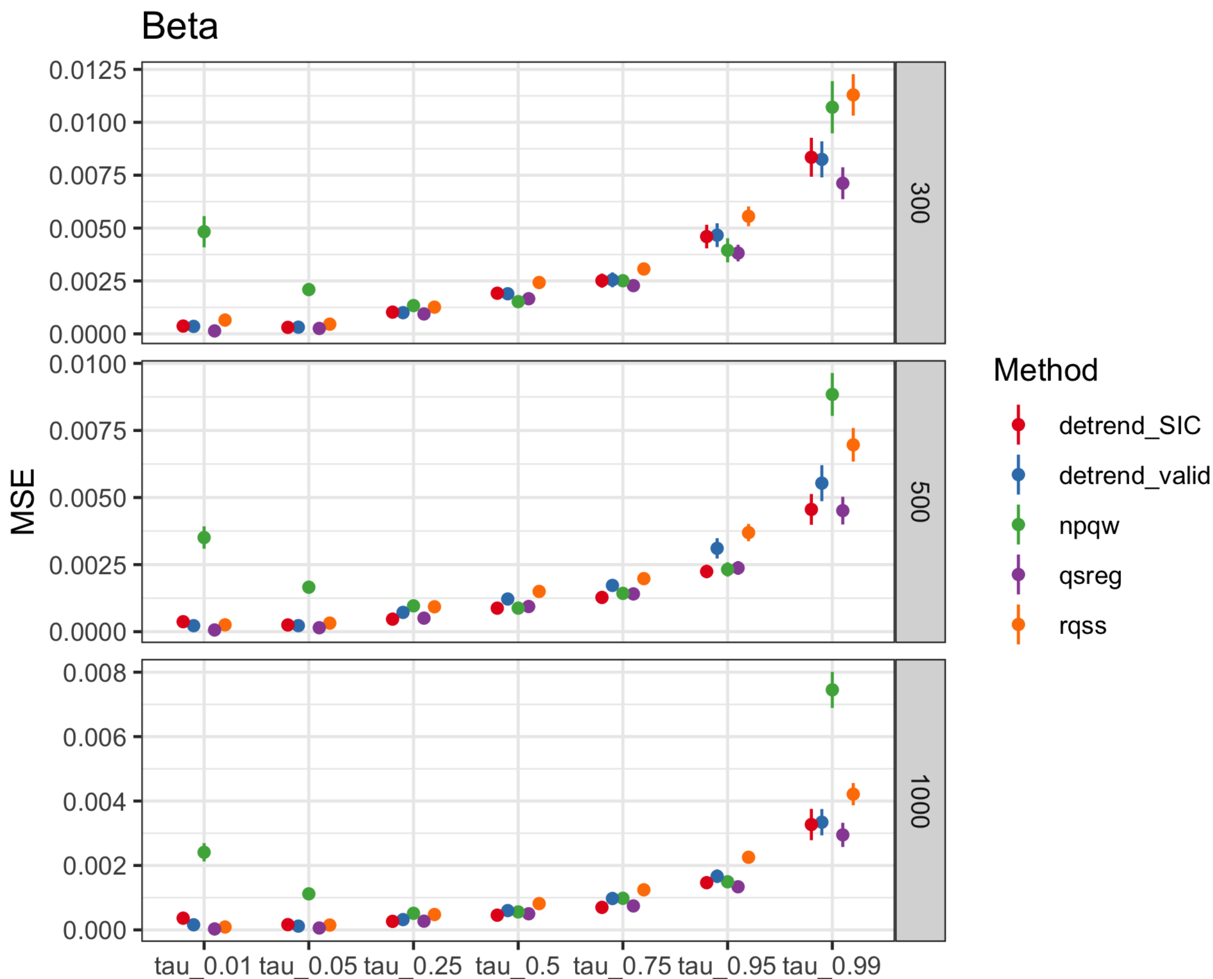
- Mixed normal: ϵ_i is simulated from a mixture of $N(-1, 1)$ and $N(1, 1)$ with mixing probability x_i.

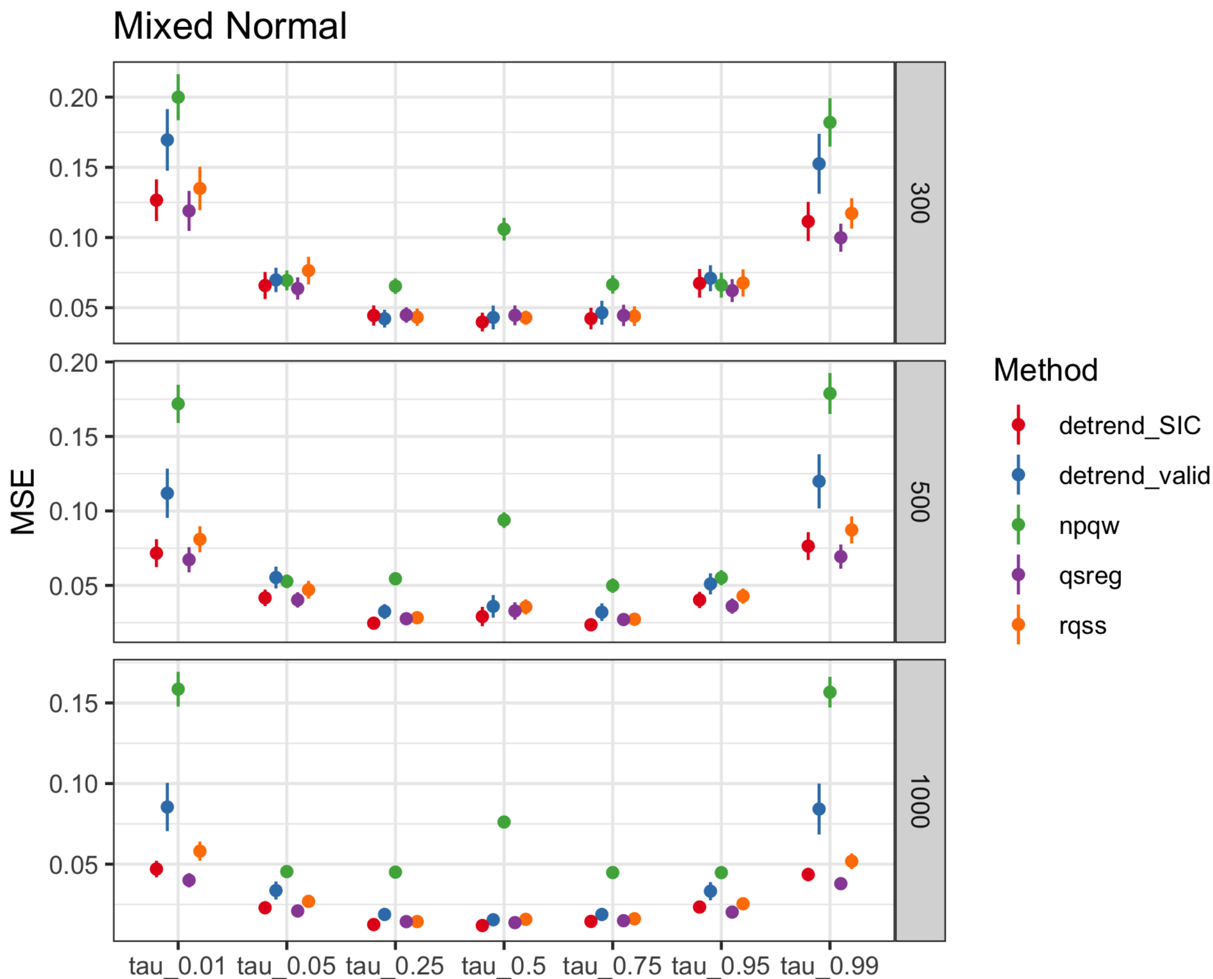
100 datasets were generated of sizes 300, 500 and 1000. The MSE was calculated as $\frac{1}{n}\sum_i(\hat{q}_\tau(x_i) - q_\tau(x_i))^2$. The plots below show the mean MSE $\pm$ twice the standard error by method, quantile level and sample size.

Figure 1: Simulated data with true quantiles $\tau \in \{0.01, 0.05, 0.25, 0.5, .75, 0.95, 0.99\}$






Beta
MSE
0.0125
0.0100
0.0075
0.0050
0.0025
0.0000
0.0100
0.0075
0.0050
0.0025
0.0000
0.008
0.006
0.004
0.002
0.000
300
500
1000
tau_0.01
tau_0.05
tau_0.25
tau_0.5
tau_0.75
tau_0.95
tau_0.99
Method
detrend_SIC
detrend_valid
npqw
qsreg
rqss



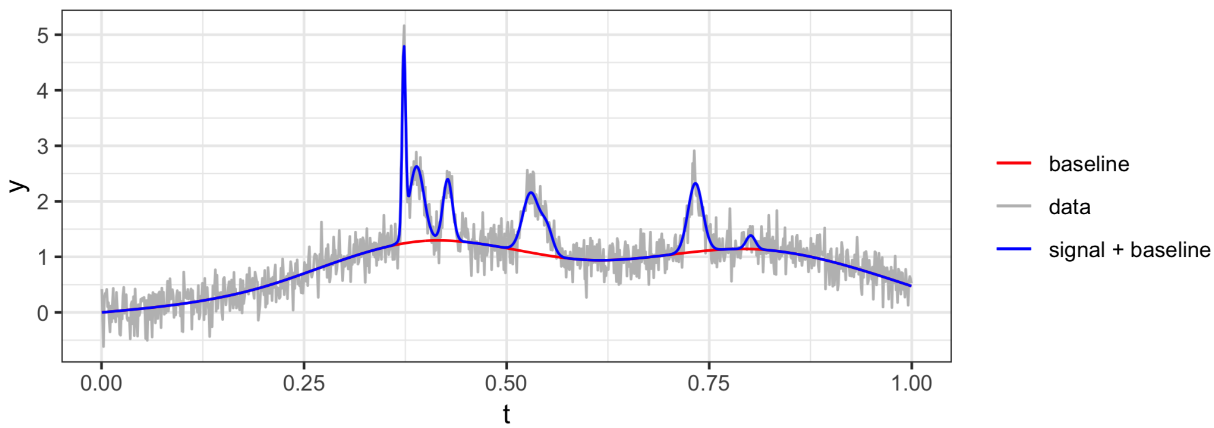
2 Peaks Simulation

We use another simulation design based on the applied problem we aim to solve. We assume that the measured data can be represented by

$$Y(t) = s(t) + b(t) + \epsilon \tag{8}$$

where $s(t)$ is the true signal at time t, $b(t)$ is the drift component that varies smoothly over time and $\epsilon \sim N(0, \sigma^2)$ is an error component. We assume t is a uniformly spaced sequence between 0 and 1. We generate $b(t)$ using a cubic natural spline basis function with degrees of freedom sampled from 2 to 10 with equal probability, and coefficients drawn from a normal distribution with mean and variance equal to 1. The true signal function is assumed to be zero with Gaussian peaks. The number of peaks is sampled from 5 to 15 with equal probability with centers uniformly distributed between 0.1 and 0.9 and bandwidths uniformly

Figure 2: Example of simulated peaks, baseline, and observed measurements.



distributed between $2/n$ and $2/n + .01$. One hundred datasets were generated for $n = 500$ and $n = 1000$. We compare the methods ability to estimate the baseline using a low quantile, $\tau \in \{0.05, 0.1\}$ and calculate the MSE using the simulated baseline value as the standard. The npqw method performs significantly worse than the other methods and is not included in the figures.

Figure 3: MSEs compared to the simulated baseline function.

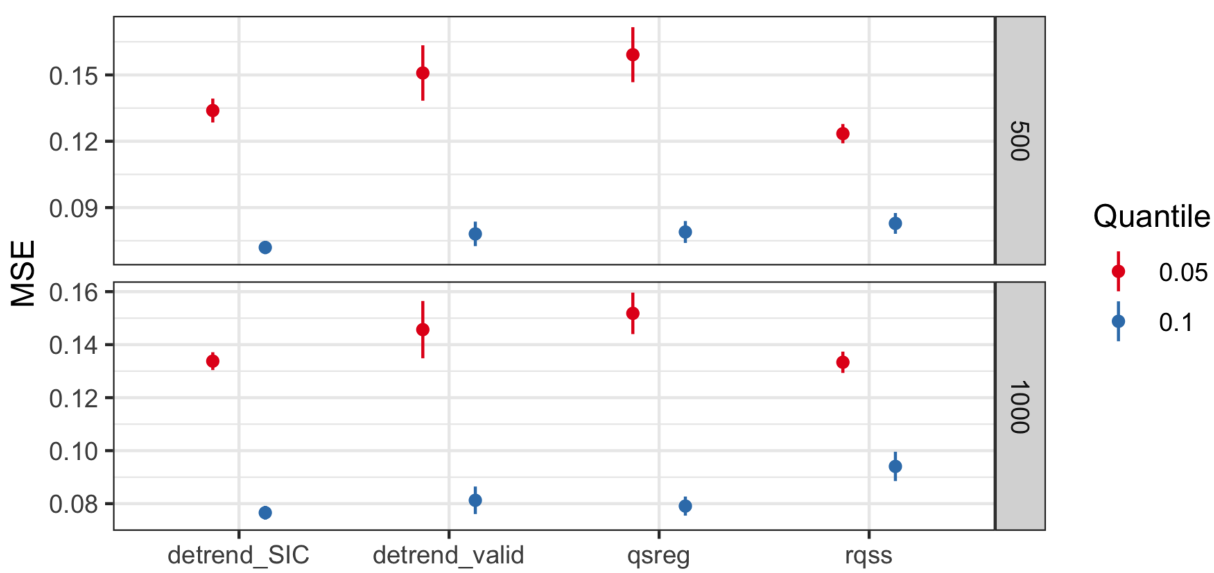
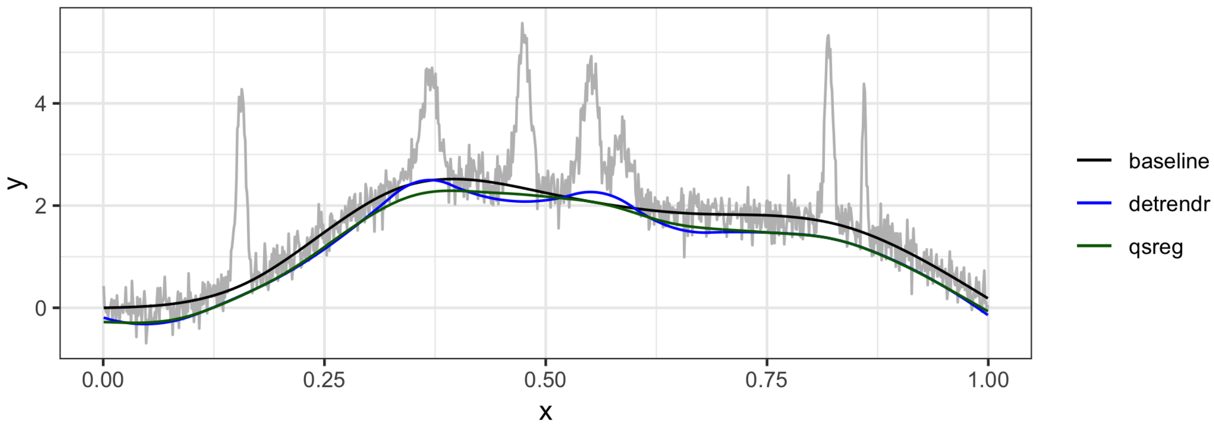


Figure 4: Example baseline fit.



References

Chen, J. and Chen, Z. (2008), "Extended Bayesian information criteria for model selection with large model spaces," *Biometrika*, 95, 759–771.

Koenker, R., Ng, P., and Portnoy, S. (1994), "Quantile smoothing splines," *Biometrika*, 81, 673–680.

Oh, H.-S., Lee, T. C. M., and Nychka, D. W. (2011), "Fast Nonparametric Quantile Regression With Arbitrary Smoothing Methods," *Journal of Computational and Graphical Statistics*, 20, 510–526.

Racine, J. S. and Li, K. (2017), "Nonparametric conditional quantile estimation: A locally weighted quantile kernel approach," *Journal of Econometrics*, 201, 72–94.