Envelope Quantile Regression

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Joint work with Shanshan Ding, Guangyu Zhu and Lan Wang
Outline

- Envelope model (Cook, Li and Chiaromonte, 2010)
- Envelope quantile regression
Multivariate linear regression

\[ Y = \alpha + \beta X + \varepsilon \]

- \( Y \in \mathbb{R}^r \): multivariate response / multiple output
- \( X \in \mathbb{R}^p \): non-stochastic predictors centered at 0
- \( \varepsilon \in \mathbb{R}^r \): mean 0 and covariance \( \Sigma > 0 \)
- \( \alpha \in \mathbb{R}^r \): unknown intercept
- \( \beta \in \mathbb{R}^{r \times p} \): unknown coefficients
- \( n \): sample size
Envelope model

Goal:
- Achieve efficient estimation in $\beta$.

Mechanism:
- Remove immaterial information in the data.
SE for 2 elements in $\widehat{\beta}$:

- Standard model: 1.60, 1.61
- Envelope model: 0.188, 0.187
Schematic representation of standard analysis

\[ Z. \text{Su, G. Zhu and X. Chen} \]

The direction marked as \( E \Sigma (B) \perp \) is invariant to the changes in \( X \). This indicates that the linear combination \( \Gamma^T_0 Y \) is the immaterial part, where \( \text{span}(\Gamma^T_0) = E \Sigma (B) \perp \). Then \( \Gamma^T Y \) is the material part, where \( \text{span}(\Gamma^T) = E \Sigma (B) \). Having identified the material and immaterial parts, a data point 'X' is first projected onto the envelope subspace \( E \Sigma (B) \) to remove the immaterial information and then projected onto the \( Y_1 \) axis. The projection path is marked as \( B_1 \) and \( B_2 \) in the right panel of Figure 1. Note that the two distribution curves are well separated which indicates we have obtained efficiency gains. The standard error is 1.60 for the standard estimator of \( \beta_1 \) and 0.188 for the envelope estimator. In other words, the sample size should be more than 70 times the original sample size for the standard model to achieve a comparable standard error.

Fig. 1. Left panel: Illustration of inference under the standard model. Right panel: Illustration of inference under the envelope model. The red "o" mark girls and the blue "+" mark boys.

Now we formally introduce the envelope subspace and envelope model. As the response vector \( Y \) can be decomposed into the material part \( \Gamma^T Y \) and the immaterial part \( \Gamma^T_0 Y \), we assume that they satisfy the following two conditions: (i) \( \Gamma^T_0 Y | X \sim \Gamma^T_0 Y \) and (ii) \( \text{cov}(\Gamma^T Y, \Gamma^T_0 Y | X) = 0 \). Together these conditions imply that \( \Gamma^T_0 Y \) depends on neither \( X \) nor \( \Gamma^T Y \) and therefore \( \Gamma^T_0 Y \) is immaterial to the regression. Cook et al. showed that (i) and (ii) are equivalent to the following conditions (a) \( B \subseteq \text{span}(\Gamma) \), where \( B = \text{span}(\beta) \) and (b) \( \Sigma = \Sigma_1 + \Sigma_2 = P \Gamma \Sigma P \Gamma + Q \Gamma \Sigma Q \Gamma \).

When (b) holds, \( \text{span}(\Gamma) \) is a reducing subspace of \( \Sigma \) (Conway, 1990). The envelope subspace \( E \Sigma (B) \) is then defined as the smallest reducing subspace of \( \Sigma \) that contains \( B \) (Cook et al., 2010). Consequently, \( E \Sigma (B) \) can be used to decompose \( \Sigma \) into variation from the material and immaterial parts of \( Y \): \( \Sigma_1 = \text{var}(P \Gamma Y) \) and \( \Sigma_2 = \text{var}(Q \Gamma Y) \). We call (1) an envelope model when (a) and (b) hold.
Working mechanism of envelope model

\[ E(\Sigma(B)) \perp \]

This indicates that the linear combination \( \Gamma^T_0 Y \) is the immaterial part, where \( \text{span}(\Gamma^T_0) = E(\Sigma(B)) \perp \). Then \( \Gamma^T Y \) is the material part, where \( \text{span}(\Gamma) = E(\Sigma(B)) \). Having identified the material and immaterial parts, a data point 'X' is first projected onto the envelope subspace \( E(\Sigma(B)) \) to remove the immaterial information and then projected onto the \( Y_1 \) axis. The projection path is marked as \( B_1 \) and \( B_2 \) in the right panel of Figure 1. Note that the two distribution curves are well separated which indicates we have obtained efficiency gains. The standard error is 1.60 for the standard estimator of \( \beta_1 \) and 0.188 for the envelope estimator. In other words, the sample size should be more than 70 times the original sample size for the standard model to achieve a comparable standard error.

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The Envelope Model

\((\Gamma, \Gamma_0)\): \(r \times r\) orthogonal matrix.

- \(\Gamma^T Y\): Material part
- \(\Gamma_0^T Y\): Immaterial part

\[ \Gamma_0^T Y|X \sim \Gamma_0^T Y, \quad \Gamma_0^T Y \perp \Gamma^T Y|X. \]
Working mechanism of envelope model

\[ \Gamma = (1, -1)^T, \quad \Gamma_0 = (1, 1)^T. \]

\[ \Gamma^T Y = Y_1 - Y_2, \quad \Gamma_0^T Y = Y_1 + Y_2. \]
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\[ \Gamma_0^T Y | X \sim \Gamma_0^T Y, \quad \Gamma_0^T Y \perp \Gamma^T Y | X. \]
Formal definition of envelope

\[ \Gamma_0^T Y \mid X \sim \Gamma_0^T Y \iff \mathcal{B} \subseteq \text{span}(\Gamma), \mathcal{B} = \text{span}(\beta). \]

\[ \Gamma_0^T Y \perp \Gamma^T Y \mid X \iff \Sigma = P_{\Gamma} \Sigma P_{\Gamma} + Q_{\Gamma} \Sigma Q_{\Gamma}. \]
(\text{span}(\Gamma) \text{ is a reducing subspace of } \Sigma)

**Definition:** The \(\Sigma\)-envelope of \(\mathcal{B}\), represented by \(\mathcal{E}_\Sigma(\mathcal{B})\), is the smallest reducing subspace of \(\Sigma\) containing \(\mathcal{B}\).
Coordinate form of the envelope model

\[ Y = \alpha + \Gamma \eta X + \varepsilon \]
\[ \Sigma = \Sigma_1 + \Sigma_2 = \Gamma \Omega \Gamma^T + \Gamma_0 \Omega_0 \Gamma_0^T \]

\[ \beta = \Gamma \eta. \]
\[ \text{span}(\Gamma) = \mathcal{E}_\Sigma (\mathcal{B}). \]
\[ u: \text{dimension of } \mathcal{E}_\Sigma (\mathcal{B}), \; u \leq r. \]
\[ \Omega > 0, \; \Omega_0 > 0. \]
Maximum likelihood estimators

To be estimated: \( u, \alpha, \mathcal{E}_\Sigma(B), \eta, \Omega \) and \( \Omega_0 \).

Estimate \( u \):

- Likelihood based methods: LRT, AIC, BIC, ...
- Nonparametric methods: Cross validation, permutation tests ...

Given \((X_i, Y_i)_{i=1,\ldots,n}\), log-likelihood function:

\[
-n \log(|\Sigma_1+\Sigma_2|) - \frac{1}{2} \sum_{i=1}^{n} [(Y_i-\alpha-\Gamma\eta X_i)^T (\Sigma_1+\Sigma_2)^{-1} (Y_i-\alpha-\Gamma\eta X_i)]
\]
Maximum likelihood estimators

\[ \hat{E}_\Sigma(B) = \arg\min_{\text{span}(\Gamma) \in \mathbb{G}^{r\times u}} (\log |\Gamma^T \hat{\Sigma}_{\text{res}} \Gamma| + \log |\Gamma^T \hat{\Sigma}_{Y}^{-1} \Gamma|). \]

Grassmann manifold \( \mathbb{G}^{r\times u} \): the set of all \( u \) dimensional subspaces in an \( r \) dimensional space.

\( \hat{\Gamma} \): an orthogonal basis of \( \hat{E}_\Sigma(B) \).

Estimate other parameters

- \( \hat{\beta} = P_{\hat{\Gamma}} \hat{\beta}_{\text{ols}} \).
- \( \hat{\eta} = \hat{\Gamma}^T \hat{\beta}_{\text{ols}} \).
- \( \hat{\Omega} = \hat{\Gamma}^T \hat{\Sigma}_{\text{res}} \hat{\Gamma} \).
- \( \hat{\Omega}_0 = \hat{\Gamma}_0^T \hat{\Sigma}_Y \hat{\Gamma}_0 \).
- \( \hat{\alpha} = \bar{Y} \).
Asymptotic variance

\[ \sqrt{n}\{\text{vec}(\hat{\beta}) - \text{vec}(\beta)\} \xrightarrow{d} N(0, V) \]

- Under the standard model

\[ V = \Sigma_X^{-1} \otimes \Sigma. \]

- Under the envelope model

\[ V = \Sigma_X^{-1} \otimes \Gamma \Omega \Gamma^T + (\eta^T \otimes \Gamma_0) M^{-1} (\eta^T \otimes \Gamma_0)^T, \]

where

\[ M = \eta \Sigma_X \eta^T \otimes \Omega_0^{-1} + \Omega \otimes \Omega_0^{-1} + \Omega^{-1} \otimes \Omega_0 - 2I_u \otimes I_{r-u}. \]
Efficiency gains

**Theorem (Cook, Li and Chiaromonte, 2010)**

The envelope estimator is always more efficient than or as efficient as the standard estimator asymptotically.

**Remark**

The efficiency gains are substantial especially when $\|\Sigma_1\| \ll \|\Sigma_2\|$. 
Berkeley guidance study, $\|\Sigma_1\| \ll \|\Sigma_2\|$

Standard model: 1.60, 1.61

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Berkeley guidance study, $\|\Sigma_1\| \gg \|\Sigma_2\|$
Recent developments

New models and methods

- Heteroscedastic envelope model
- Inner envelope model
- Scaled envelope model
- Partial envelope model
- Weighted envelope model

Connection with other areas

- Envelopes and partial least squares
- Envelopes and reduced rank regression
- Sparse envelopes and variable selection
- Bayesian envelope model
- Tensor envelope model
- Envelopes in generalized linear model

Software

- MATLAB toolbox *envlp*
- R package *envlp*
Quantile regression

- \( Y \): univariate response
- \( X \in \mathbb{R}^p \): predictor vector, mean \( \mu_X \) and variance \( \Sigma_X \)

The \( \tau \)-th conditional quantile of \( Y \) is

\[
Q_Y(\tau \mid X = x) = \inf\{y : F_Y(y \mid X = x) \geq \tau\}, \quad 0 < \tau < 1.
\]

Linear quantile regression model

\[
Q_Y(\tau \mid X) = \mu_\tau + \beta^T_\tau X.
\]
Estimation

The standard method to estimate $\mu_\tau$ and $\beta_\tau$ is to solve

$$(\tilde{\mu}_\tau, \tilde{\beta}_\tau) = \arg \min_{\mu_\tau \in \mathbb{R}, \beta_\tau \in \mathbb{R}^p} \sum_{i=1}^{n} \rho_\tau(Y_i - \mu_\tau - \beta_\tau^T X_i).$$

$(\tilde{\mu}_\tau, \tilde{\beta}_\tau)$ is also a root of the estimating equation

$$\frac{1}{n} \sum_{i=1}^{n} (1, X_i^T) \begin{bmatrix} I(Y_i < \mu_\tau + \beta_\tau^T X_i) - \tau \end{bmatrix} = O_p(n^{-1/2}).$$
Envelope Quantile Regression

Let \( (\Gamma_\tau, \Gamma_{0\tau}) \) be a \( p \times p \) orthogonal matrix.

- \( \Gamma_T \tau X \): material part
- \( \Gamma_{0\tau}^T X \): immaterial part

Assume that

- \( Q_Y(\tau \mid X) = Q_Y(\tau \mid \Gamma_T^T X) \)
- \( \text{cov}(\Gamma_T^T X, \Gamma_{0\tau}^T X) = 0. \)
Envelope Quantile Regression

Assume that

- \( Q_Y(\tau \mid X) = Q_Y(\tau \mid \Gamma_T^T X) \iff \beta_\tau \in \text{span}(\Gamma_\tau) \)
- \( \text{cov}(\Gamma_T^T X, \Gamma_0^T X) = 0 \iff \text{span}(\Gamma_\tau) \) is a reducing subspace of \( \Sigma_X \).

The \( \Sigma_X \)-envelope of \( \beta_\tau \), denoted by \( \mathcal{E}_{\Sigma_X}(\beta_\tau) \), is the smallest reducing subspace of \( \Sigma_X \) containing \( \beta_\tau \).

Example: If \( \Sigma_X = AA^T + cI_p \), where \( A \in \mathbb{R}^{p \times k}, k < p \), and \( c > 0 \), then the dimension of \( \mathcal{E}_{\Sigma_X}(\beta_\tau) \) is at most \( k + 1 \).
Assume that

- \( Q_Y(\tau \mid X) = Q_Y(\tau \mid \Gamma_T^T X) \iff \beta_\tau \in \text{span}(\Gamma_\tau) \)
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Envelope Quantile Regression

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Coordinate form of the envelope quantile regression

\[ Q_Y(\tau \mid X) = \mu_\tau + \eta_\tau^T \Gamma_\tau X \]
\[ \Sigma_X = \Gamma_\tau \Omega_\tau \Gamma_\tau^T + \Gamma_0 \Omega_0 \Gamma_0^T \]

- \( \beta_\tau = \Gamma_\tau \eta_\tau \).
- \( \Gamma_\tau \in \mathbb{R}^{p \times u_\tau} \) is an orthonormal basis of \( \mathcal{E}_{\Sigma_X}(\beta_\tau) \).
- \( u_\tau \): dimension of \( \mathcal{E}_{\Sigma_X}(\beta_\tau) \), \( u_\tau \leq p \).
- \( \Omega_\tau > 0, \Omega_0 > 0 \).
Estimation

To be estimated: \( u_\tau, \mu_\tau, \mathcal{E}_{\Sigma_X}(\beta_\tau), \eta_\tau, \mu_X, \Omega_\tau \) and \( \Omega_{0\tau} \).

Estimate \( u_\tau \):
- Cross validation

Estimate \( \theta = (\mu_\tau, \text{vec}^T(\Gamma_\tau), \text{vec}^T(\eta_\tau), \mu_X^T, \text{vech}^T(\Omega_\tau), \text{vech}^T(\Omega_{0\tau}))^T \)
- Generalized method of moments (GMM)

Estimating equation

\[
h_n(\theta) = \left( \frac{1}{n} \sum_{i=1}^{n} (1, X_i^T) \begin{bmatrix} 1 & \eta_\tau^T \Gamma_\tau^T X_i \end{bmatrix} - \tau \right)
\]

\[
= \begin{bmatrix} \mu_X - \bar{X} \\
\text{vech}(\Gamma_\tau \Omega_\tau \Gamma_\tau^T + \Gamma_{0\tau} \Omega_{0\tau} \Gamma_{0\tau}^T) - \text{vech}(S_X) \end{bmatrix}
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} g(X_i, Y_i; \theta).
\]

\( \hat{\theta} = \arg \min_{\theta} h_n(\theta)^T \hat{\Delta} h_n(\theta) \)

\( \hat{\Delta} \) is a \( \sqrt{n} \)-consistent estimator of \( \mathbb{E}(g(X_i, Y_i; \theta)g^T(X_i, Y_i; \theta))^{-1} \).
Efficiency gains

Theorem

The envelope quantile regression estimator is always more efficient than or as efficient as the standard quantile regression estimator asymptotically.
Envelope Quantile Regression

**Example** Boston housing data
506 owner-occupied homes in suburbs of Boston

- **Y**: House value
- **X**: 13 attributes of the house (crime rate, nitric oxides concentrations, pupil-teacher ratio, etc)

**Table 1**: SE of quantile regression (QR) estimator and envelope quantile regression (EQR) estimator ($\tau = 0.5$, $\hat{u}_\tau = 3$)

<table>
<thead>
<tr>
<th></th>
<th>$\beta_1$</th>
<th>$\beta_2$</th>
<th>$\beta_3$</th>
<th>$\beta_4$</th>
<th>$\beta_5$</th>
<th>$\beta_6$</th>
<th>$\beta_7$</th>
<th>$\beta_8$</th>
<th>$\beta_9$</th>
<th>$\beta_{10}$</th>
<th>$\beta_{11}$</th>
<th>$\beta_{12}$</th>
<th>$\beta_{13}$</th>
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<tbody>
<tr>
<td>QR</td>
<td>.41</td>
<td>.33</td>
<td>.25</td>
<td>.75</td>
<td>.40</td>
<td>.60</td>
<td>.38</td>
<td>.36</td>
<td>.59</td>
<td>.53</td>
<td>.25</td>
<td>.22</td>
<td>.57</td>
</tr>
<tr>
<td>EQR</td>
<td>.18</td>
<td>.20</td>
<td>.16</td>
<td>.75</td>
<td>.12</td>
<td>.32</td>
<td>.15</td>
<td>.17</td>
<td>.17</td>
<td>.16</td>
<td>.20</td>
<td>.22</td>
<td>.24</td>
</tr>
<tr>
<td>Ratio</td>
<td>2.2</td>
<td>1.6</td>
<td>1.6</td>
<td>1.0</td>
<td>3.3</td>
<td>1.8</td>
<td>2.6</td>
<td>2.1</td>
<td>3.4</td>
<td>3.4</td>
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</tr>
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Envelope Quantile Regression

Example Boston housing data
506 owner-occupied homes in suburbs of Boston

■ Y: House value
■ X: 13 attributes of the house (crime rate, nitric oxides concentrations, pupil-teacher ratio, etc)

Table 2: SE of quantile regression (QR) estimator and envelope quantile regression (EQR) estimator ($\tau = 0.9$, $\hat{u}_\tau = 2$)

<table>
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<th></th>
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<tbody>
<tr>
<td>QR</td>
<td>1.25</td>
<td>.51</td>
<td>.87</td>
<td>4.88</td>
<td>1.00</td>
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<td>1.28</td>
<td>.85</td>
<td>.73</td>
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<td>4.0</td>
</tr>
</tbody>
</table>
Envelope Quantile Regression

Example
Salary data for 337 non-pitchers for 1992 Major League Baseball season

- $Y$: Salary of baseball player’s
- $X$: 12 measures of the player’s previous year’s performance (batting average, on-base percentage, number of runs, hits, doubles, triples, home runs, batted in, walks, strike-outs, stolen bases and errors)

### Table 3: SE ratios of QR estimator over EQR estimator.

<table>
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<tr>
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<tbody>
<tr>
<td>$\tau = 0.5$</td>
<td>1.8</td>
<td>1.9</td>
<td>6.8</td>
<td>5.5</td>
<td>2.8</td>
<td>1.1</td>
<td>3.3</td>
<td>5.7</td>
<td>2.6</td>
<td>1.3</td>
<td>1.2</td>
<td>1.0</td>
</tr>
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<td>2.8</td>
<td>3.3</td>
<td>29.5</td>
<td>21.8</td>
<td>8.0</td>
<td>2.8</td>
<td>4.6</td>
<td>8.4</td>
<td>8.0</td>
<td>5.0</td>
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Thank you!