Shape testing for coefficient functions in varying coefficient models

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Outline

- Introduction: varying coefficient models
- Unconstrained estimation in varying coefficient models
- Constrained estimation in varying coefficient models
- Shape testing in varying coefficient models
- Quantile regression in varying coefficient models

... particular shape testing ...

varying coefficient regression model

Y response variable $X^{(1)}, \ldots, X^{(p)}$ covariates

multiple linear regression model: $Y = \beta_0 + \beta_1 X^{(1)} + \ldots + \beta_p X^{(p)} + \varepsilon$

complex data

flexible modelling $\longrightarrow$ **varying coefficient regression model**:

$$Y(\mathbf{T}) = \beta_0(\mathbf{T}) + \beta_1(\mathbf{T}) X^{(1)}(\mathbf{T}) + \ldots + \beta_p(\mathbf{T}) X^{(p)}(\mathbf{T}) + \varepsilon(T)$$

$(Y(T), X^{(1)}(T), \ldots, X^{(p)}(T), T)$ random vector

T takes values in $[0, 1]$ (without loss of generality)

Hastie & Tibshirani (1993), Hoover *et al.* (1998), ... , Honda (2004), Kim (2006), ..., Wang *et al.* (2008), ..., Antoniadis, G. & Verhasselt (2012a), Andriyana (2015), Xie *et al.* (2015), ...

$$
\begin{aligned}
Y(t) &= \beta_0(t) + \beta_1(t)X^{(1)}(t) + \ldots + \beta_p(t)X^{(p)}(t) + \varepsilon(t) \\
&= \mathbf{X}(t)^{\mathsf{T}}\boldsymbol{\beta}(t) + \varepsilon(t)
\end{aligned}
$$

where $\mathbf{X}(t) = \left(\underbrace{X^{(0)}(t)}_{\equiv 1}, X^{(1)}(t), \ldots, X^{(p)}(t) \right)^{\mathsf{T}}$

$\boldsymbol{\beta}(t) = (\beta_0(t), \beta_1(t), \ldots, \beta_p(t))^{\mathsf{T}}$

vector of $(p+1)$ unknown **univariate** regression coefficients at time t

$\beta_0(t)$ is the baseline effect

assume that $\varepsilon(t)$ is a **mean zero** stochastic process at time t

first aim: estimate the **mean regression function**

$$
E(Y(t)|\mathbf{X}(t), t) = \beta_{\mathbf{0}}(\mathbf{t}) + \beta_{\mathbf{1}}(\mathbf{t})X^{(1)}(t) + \ldots + \beta_{\mathbf{p}}(\mathbf{t})X^{(p)}(t)
$$

observational setting: longitudinal data setup

n independent subjects/individuals

for each individual i: measurements repeated over a time period

measurements at time points $t_{i1}, \ldots, t_{iN_i}$

N_i different measurements for response and all explanatory variables:

$Y(t_{ij}) = Y_{ij}$

$X^{(k)}(t_{ij}) = X_{ij}^{(k)} \quad k = 1, \ldots, p \Longrightarrow \mathbf{X}(t_{ij}) \stackrel{\text{not.}}{=} \mathbf{X}_{ij} = (X_{ij}^{(0)}, \ldots, X_{ij}^{(p)})^\mathsf{T}$

total number of observations over all individuals:

$$N = \sum_{i=1}^{n} N_i$$

$$E(Y(t)|\mathbf{X}(t),t) = \boldsymbol{\beta_0(t)} + \boldsymbol{\beta_1(t)}X^{(1)}(t) + \ldots + \boldsymbol{\beta_p(t)}X^{(p)}(t)$$

suppose: each unknown function $\beta_k(t)$, $k = 0, \ldots, p$, can be represented by a B-spline basis expansion

$$\beta_k(t) = \alpha_{k1}B_{k1}(t;\nu_k) + \ldots + \alpha_{km_k}B_{km_k}(t;\nu_k) = \sum_{\ell=1}^{m_k} \alpha_{k\ell}B_{k\ell}(t;\nu_k)$$

$$= \boldsymbol{\alpha}_k^T \mathbf{B}_k(t;\nu_k)$$

$\boldsymbol{\alpha_k} = (\alpha_{\mathbf{k1}}, \ldots, \alpha_{\mathbf{km_k}})^\mathsf{T}$ $\quad$ $\mathbf{B}_k(t;\nu_k) = (B_{k1}(t;\nu_k), \ldots, B_{km_k}(t;\nu_k))^\mathsf{T}$

$m_k = u_k + \nu_k$ $\quad$ $u_k + 1 =$ number of knot points

where $\{B_{k\ell}(\cdot;\nu_k) : \ell = 1, \ldots, u_k + \nu_k = m_k\}$ is the ν_k-th degree B-spline basis with $u_k + 1$ equidistant knots for the k-th component

normalized B-splines: $\displaystyle\sum_{\ell=1}^{m_k} B_{k\ell}(t;\nu_k) = 1$

$$\boxed{\beta_k(t_{ij}) = \sum_{\ell=1}^{m_k} \alpha_{k\ell} B_{k\ell}(t_{ij};\nu_k)}$$

$\alpha_{k\ell}$ unknown coefficients

the **B-spline estimates** of the coefficients: minimize

$$S(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \frac{1}{N_i} \sum_{j=1}^{N_i} \left(Y_{ij} - \sum_{k=0}^{p} \underbrace{\sum_{\ell=1}^{m_k} \alpha_{k\ell} B_{k\ell}(t_{ij};\nu_k)}_{=\beta_k(t_{ij})} X_{ij}^{(k)} \right)^2$$

with respect to $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_0^\mathsf{T}, \ldots, \boldsymbol{\alpha}_p^\mathsf{T})^\mathsf{T}$, where $\boldsymbol{\alpha}_k = (\alpha_{k1}, \ldots, \alpha_{km_k})^\mathsf{T}$

what is the solution to this minimization problem ?

it is better to write all this in matrix notation

$$S(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \frac{1}{N_i} \sum_{j=1}^{N_i} \left(Y_{ij} - \sum_{k=0}^{p} \sum_{\ell=1}^{m_k} \alpha_{k\ell} B_{k\ell}(t_{ij};\nu_k) X_{ij}^{(k)} \right)^2$$
$$= \sum_{i=1}^{n} (\mathbf{Y}_i - \mathbf{U}_i \boldsymbol{\alpha})^T \mathbf{W}_i (\mathbf{Y}_i - \mathbf{U}_i \boldsymbol{\alpha})$$

$$\mathbf{Y}_i = (Y_{i1}, \ldots, Y_{iN_i})^{\mathsf{T}}$$

$$\mathbf{B}(t) = \begin{pmatrix} B_{01}(t;\nu_0) & \ldots & B_{0m_0}(t;\nu_0) & 0 \ldots 0 & 0 & \ldots & 0 \\ 0 & \ldots & 0 & \ddots & 0 & \ldots & 0 \\ 0 & \ldots & 0 & 0 \ldots 0 & B_{p1}(t;\nu_p) & \ldots & B_{pm_p}(t,\nu_p) \end{pmatrix}$$

$$\mathbf{U}_{ij}^{\mathsf{T}} = \mathbf{X}_{ij}^{\mathsf{T}} \mathbf{B}(t_{ij}) \in I\!R^{1 \times m_{\text{tot}}} \qquad \mathbf{X}_{ij} = \left(1, X^{(1)}(t_{ij}), \ldots, X^{(p)}(t_{ij})\right)^{\mathsf{T}}$$

$$\mathbf{U}_i = (\mathbf{U}_{i1}^{\mathsf{T}}, \ldots, \mathbf{U}_{iN_i}^{\mathsf{T}})^{\mathsf{T}} \in I\!R^{N_i \times m_{\text{tot}}} \quad \text{and} \quad m_{\text{tot}} = \sum_{k=0}^{p} m_k$$

$$\mathbf{W}_i = \text{diag}\left(N_i^{-1}, \ldots, N_i^{-1}\right) \in I\!R^{N_i \times N_i}$$

(a diagonal matrix with N_i times N_i^{-1} on the diagonal)

$$S(\boldsymbol{\alpha}) = \sum_{i=1}^{n} (\mathbf{Y}_i - \mathbf{U}_i\boldsymbol{\alpha})^T \mathbf{W}_i (\mathbf{Y}_i - \mathbf{U}_i\boldsymbol{\alpha})$$

if $\sum_{i=1}^{n} \mathbf{U}_i^T \mathbf{W}_i \mathbf{U}_i$ is invertible then $S(\boldsymbol{\alpha})$ has a unique minimizer

$$\boxed{\widehat{\boldsymbol{\alpha}} = \Big(\sum_{i=1}^{n} \mathbf{U}_i^T \mathbf{W}_i \mathbf{U}_i\Big)^{-1} \sum_{i=1}^{n} \mathbf{U}_i^T \mathbf{W}_i \mathbf{Y}_i}$$

where $\widehat{\boldsymbol{\alpha}} = (\widehat{\boldsymbol{\alpha}}_0^\mathsf{T}, \ldots, \widehat{\boldsymbol{\alpha}}_p^\mathsf{T})^\mathsf{T}$ and $\widehat{\boldsymbol{\alpha}}_k = (\widehat{\alpha}_{k1}, \ldots, \widehat{\alpha}_{km_k})^\mathsf{T}$ for $k = 0, \ldots, p$

the **B-spline estimate** of $\boldsymbol{\beta}(t)$ is then

$$\widehat{\boldsymbol{\beta}}(t) = \mathbf{B}(t)\widehat{\boldsymbol{\alpha}} = (\widehat{\beta}_0(t), \ldots, \widehat{\beta}_p(t))^\mathsf{T} \quad \text{with} \quad \widehat{\beta}_k(t) = \sum_{\ell=1}^{m_k} \widehat{\alpha}_{k\ell} B_{k\ell}(t; \nu_k)$$

what about the asymptotic behaviour of this estimator?

notations:

$u^{\max} = \max_{0 \le k \le p} u_k$ maximal number of knot points

we allow $u^{\max}$ to grow with the sample size n, and denote it $u_n^{\max}$

$\rho_n = \inf_{\mathbf{g}^* \in \mathcal{G}} \|\boldsymbol{\beta} - \mathbf{g}^*\|_\infty$ assume: $\rho_n \to 0$ as $n \to \infty$

$$\|\boldsymbol{\beta} - \mathbf{g}^*\|_\infty = \max_{0 \le k \le p} \|\beta_k - g_k^*\|_\infty = \max_{0 \le k \le p} \left(\sup_t |\beta_k(t) - g^*(t)|\right)$$

where $\mathbf{g}^* = (g_0^*, \ldots, g_p^*)^\mathsf{T} \in \mathcal{G}$

$\mathcal{G} = \mathcal{G}_{\nu_0}(\mathcal{K}_0) \times \ldots \times \mathcal{G}_{\nu_p}(\mathcal{K}_p)$ $\mathcal{K}_k$ are sets of knots in $[0,1]$ for $k = 0, \ldots, p$

$\mathcal{G}_\nu(\mathcal{K})$ = space of spline functions of degree ν with set of knots $\mathcal{K}$

$B^r([0,1])$ = set of real-valued functions on $[0,1]$, who have a bounded r-th derivative

e.g. $r = 2$, $\nu = 3$, $\rho_n = O\left((u_n^{\max})^{-2}\right)$

theoretical results

- uniform consistency of $\widehat{\beta}_k(\cdot)$, estimator of $\beta_k(\cdot)$; + rate
- uniform consistency of $\widehat{\beta}_k^{(v)}(\cdot)$, estimator of $\beta_k^{(v)}(\cdot)$; + rate

$v = 0, \ldots, \nu_k$

Corollary.

Suppose $\beta_k(\cdot) \in B^{\nu_k+1}([0,1])$ for $k = 0, \ldots, p$. Then, under Assumptions 1—5,

$$\|\widehat{\boldsymbol{\beta}}^{(v)} - \boldsymbol{\beta}^{(v)}\|_\infty = O_P\left((u_n^{\mathsf{max}})^v \rho_n + (u_n^{\mathsf{max}})^{v-\nu_n^{\mathsf{min}}-1} + (u_n^{\mathsf{max}})^v r_n\right)$$

for $v = 0, \ldots, \nu_n^{\mathsf{min}}$, where $\nu_n^{\mathsf{min}} = \min_{0 \le k \le p} \nu_k$

$$r_n^2 = \frac{(u_n^{\mathsf{max}})^2}{n^2} \sum_{i=1}^{n} \left(\frac{1}{N_i} \left(1 - \frac{1}{u_n^{\mathsf{max}}}\right) + \frac{1}{u_n^{\mathsf{max}}} \right)$$

Assumption 1:

1. The observation times $t_{ij},\ j = 1, \ldots, N_i,\ i = 1, \ldots, n$, are chosen independently according to a distribution function $F_T(t)$ on $[0, 1]$. Moreover, they are independent of the response and the covariate process $\{(Y_i(t), X_i^{(1)}(t), \ldots, X_i^{(p)}(t))\},\ i = 1, \ldots, n$.
   The distribution function $F_T(t)$ has a Lebesgue density $f_T(t)$ that is bounded away from zero and infinity, uniformly over all $t \in [0, 1]$, that is, $\exists$ positive constants M_1 and M_2 such that $M_1 \leqslant f_T(t) \leqslant M_2$ for all $t \in [0, 1]$.
2. The eigenvalues $\eta_0(t), \ldots, \eta_p(t)$ of $\mathbf{\Sigma}(t) = E(\mathbf{X}(t)\mathbf{X}(t)^\mathsf{T})$ are bounded away from zero and infinity, uniformly over all $t \in [0, 1]$, that is, $\exists$ positive constants M_3 and M_4 such that $M_3 \leqslant \eta_0(t) \leqslant \ldots \leqslant \eta_p(t) \leqslant M_4$ for all $t \in [0, 1]$.
3. $\exists$ a positive constant M_5 such that $|X^{(k)}(t)| \leqslant M_5$ for all $t \in [0, 1]$ and $k = 0, \ldots, p$.
4. $\exists$ a positive constant M_6 such that $E(\varepsilon^2(t)) \leqslant M_6 < \infty$ for all $t \in [0, 1]$.
5. $\limsup_{n\to\infty}\left(\frac{\max_k m_k}{\min_k m_k}\right) < \infty$.

example

- data from the National Institute of Mental Health Schizophrenia Collaborative Study
- response variable: 'severity of the illness', measured on a numerical scale from 1 (normal, not ill) to 7 (among most extremely ill)
- most patients were measured at weeks 0, 1, 3 and 6
  a few patients were additionally measured at weeks 2, 4 and 5

  hence, N_i is between 4 and 7
- $n = 437$ patients were randomly assigned to either receive a drug or a placebo
- Drug=binary variable : Drug=1, patient received the drug
  Drug=0, patient received a placebo
- consider a varying coefficient model:

$$Y(\text{week}) = \beta_0(\text{week}) + \beta_1(\text{week})\,\text{Drug} + \varepsilon(\text{week})$$

- number of knots are determined by a 4-fold cross validation (with the number of knots ranging from 1 to 8)

mean fits ($\widehat{E}(Y(t) \mid \mathbf{X}(t), t)$) for the placebo group and the drug group

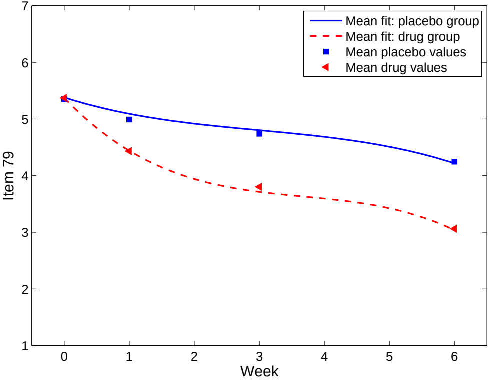
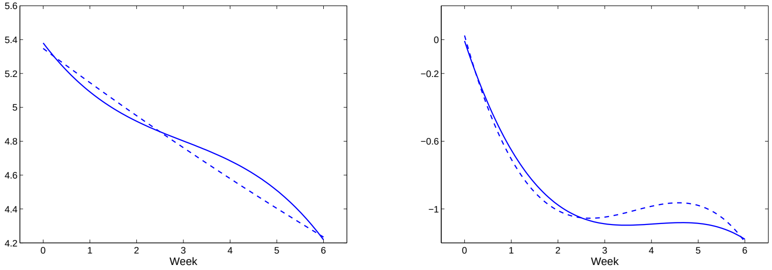


Figure: Schizophrenia data. The mean fits for the placebo and the drug group. The squares and triangles are the mean response measurements at weeks 0, 1, 3 and 6, of the placebo group and drug group, respectively.

- **how does the drug affects the severity of the illness of patients?**
- **how does a possible effect evolve over time?**



(a) (b)

Figure: Schizophrenia data. Estimates of coefficient functions $\beta_0(\cdot)$ and $\beta_1(\cdot)$, using cubic splines (full lines) and splines with degree vector $(3, 2)$ (dashed lines).

- negative $\beta_1(\cdot)$ which is decreasing: drug is effective
- the drug effect drops quickly to reach a steady effect of -1 from week 3 onwards

main goal: testing for various shape constraints on the coefficient functions in a varying coefficient model

- testing

$$\begin{aligned} H_0 : &\quad \beta_k(\cdot) \text{ is monotone increasing} \\ \text{versus } H_1 : &\quad \beta_k(\cdot) \text{ is not monotone increasing} \end{aligned}$$

- testing

$$\begin{aligned} H_0 : &\quad \beta_k(\cdot) \text{ is a convex function} \\ \text{versus } H_1 : &\quad \beta_k(\cdot) \text{ is not a convex function} \end{aligned}$$

- simultaneous testing (e.g.)

$$\begin{aligned} H_0 : &\quad \beta_1(\cdot) \text{ is monotone decreasing} \quad \text{and} \quad \beta_3(\cdot) \text{ is convex} \\ \text{versus } H_1 : &\quad \neg H_0 \end{aligned}$$

- constrained spline estimation: **monotonicity**

which constraints need to be added on the B-spline coefficients to obtain a monotone B-spline estimate ?

- spline function $g(t) = \sum_{\ell=1}^{m} \gamma_\ell B_\ell(t;\nu)$ with distance $1/u$ between equidistant knot points

  the derivative of g is:

$$g'(t) = \sum_{\ell=1}^{m} \gamma_\ell B_\ell^{'}(t;\nu) = u \sum_{\ell=1}^{m-1} \Delta\gamma_{\ell+1} B_\ell(t;\nu-1) \quad \Delta\gamma_{\ell+1} = \gamma_{\ell+1} - \gamma_\ell$$

- in general: **if** $\Delta\gamma_{\ell+1} \geq 0 \quad \forall \ell,$ **then** $g(\cdot)$ is monotone increasing
- **Lemma**

  If $\nu = 2$, then $g'(t) \geq 0$ for all $t \in [0,1]$ **if and only if** $g'(\xi_i) \geq 0$ for $i = 0, 1, \ldots, u$

  hence, monotonicity of $g(t)$ in the knots $\xi_0, \cdots, \xi_u$ is equivalent to monotonicity on the whole domain $[\xi_0, \xi_u]$

- for **quadratic splines**:
  - for $g(t) = \sum_{\ell=1}^{m} \gamma_\ell B_\ell(t;2)$
  - denote the matrix $\mathbf{S} \in I\!R^{(u+1)\times(u+2)}$ which consists of B-spline derivatives *at the knots*; $\mathbf{S}_{ij} = B'_j(\xi_{i-1};2)$
    due to the lemma:

    g is increasing *if and only if*

    $$\mathbf{S}\boldsymbol{\gamma} \geq \mathbf{0} \in I\!R^{u+1} \qquad \text{where } \boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_m)^{\mathsf{T}}$$

    Wang & Meyer (2011), Meyer (2012)

- for **cubic splines** ($\nu = 3$): for imposing monotonicity we need to impose quadratic constraints at the knots

  Akhim, G. & Verhasselt (2017)

- or, for cubic or higher order splines: impose general constraint (e.g. via penalty term)

  see e.g. Bollaerts *et al.* (2006), Akhim, G. & Verhasselt (2017)

- testing for **monotonicity**:

H_0 : $\beta_k(\cdot)$ is monotone increasing versus H_1 : $\beta_k(\cdot)$ is not monotone increasing

or equivalently

$$H_0: \quad \beta_k'(t) \geq 0 \quad \forall t \in [0,1] \qquad \text{versus} \qquad H_1: \quad \neg H_0$$

(for testing whether $\beta_k(\cdot)$ is monotone decreasing, replace $X^{(k)}$ by $-X^{(k)}$)

- • using **quadratic spline approximation**
  - translate monotonicity constraint into linear constraint on B-spline coefficients: define $\mathbf{C} = (\mathbf{0}_1, \mathbf{S}, \mathbf{0}_3)$ where

    $\mathbf{0}_1 \in I\!R^{(u_k+1)\times\sum_{j=0}^{k-1} m_j}$ and
    $\mathbf{0}_3 \in I\!R^{(u_k+1)\times\sum_{j=k+1}^{d} m_j}$ are matrices with entries 0

    $\mathbf{S} \in I\!R^{(u_k+1)\times(u_k+2)}$ = matrix of derivatives at the knots of B-splines corresponding to coefficient $\beta_k(\cdot)$: $\mathbf{S}_{ij} = B_{kj}'(\xi_{k,i-1}; 2)$
  - the estimate $\widehat{\beta}_k$ is increasing **if and only if** $\mathbf{C}\widehat{\alpha} \geq 0$

based on this: what would be an appropriate test statistic ?

possible test statistic (Wang & Meyer (2011)) : $\boxed{\min(\mathbf{C}\widehat{\boldsymbol{\alpha}})}$

pseudo algorithm to test the hypothesis H_0 is:

1. determine the unconstrained estimator $\widehat{\boldsymbol{\alpha}}$, and calculate the minimum of the slopes at the knots

$$s_{\min} = \min(\mathbf{C}\widehat{\boldsymbol{\alpha}})$$

2. if $s_{\min}$ is non-negative, do not reject H_0
3. if $s_{\min} < 0$, determine the distribution of $s_{\min}$ under H_0 and calculate the α percentile Q_α
4. if $s_{\min}$ is smaller than the α percentile, then reject H_0

how to access the distribution of $s_{\min}$ under H_0?

two approaches: bootstrap procedure
OR relying on asymptotic normality result

♣ first approach: **bootstrap procedure**

- calculate residuals

$$\widehat{\varepsilon}_{ij} = Y_{ij} - \sum_{k=0}^{p} X_{ij}^{(k)} \widehat{\beta}_k(t_{ij}) \qquad \widehat{\boldsymbol{\beta}}(\cdot) \text{ unconstrained B-spline estimator}$$

- obtain **pseudo responses under H_0**

$$Y_{ij}^{\mathsf{ps}} = \sum_{k=0}^{p} X_{ij}^{(k)} \widehat{\beta}_k^{\mathsf{cs}}(t_{ij}) + \widehat{\varepsilon}_{ij} \quad \text{for } i = 1, \ldots, n \quad \text{and } j = 1, \ldots, N_i$$

where

$$\widehat{\boldsymbol{\beta}}^{\mathsf{cs}} = (\widehat{\beta}_0^{\mathsf{cs}}, \ldots, \widehat{\beta}_p^{\mathsf{cs}})^{\mathsf{T}}$$

is the *constrained estimate* putting the constraint on β_k

bootstrap procedure to determine the distribution of $s_{\min}$ under H_0 is

- Step 1: resample n subjects (with all its repeated measurements) with replacement from

$$\{(Y_{ij}^{\textsf{ps}}, X_{ij}, t_{ij}) : i = 1, \ldots, n, j = 1, \ldots, N_i\}$$

  to obtain the bootstrap sample
  $\{(Y_{ij}^{\textsf{ps}*}, X_{ij}^*, t_{ij}^*) : i = 1, \ldots, n, j = 1, \ldots, N_i^*\}$
- Step 2: repeat the above sampling procedure B times
- Step 3: obtain the test statistic $s_{\min}^*$ from each bootstrap sample and derive the empirical distribution based on all $s_{\min}^*$
- Step 4:
  consider the α percentile $\widehat{Q}_\alpha$ of the empirical distribution in Step 3;

  reject H_0 if $s_{\min} < \widehat{Q}_\alpha$;

  else do not reject H_0

♣ second approach: via **asymptotic normality result**
(see Wang & Meyer (2011))

what about the variance-covariance matrix of the B-spline estimators ?

- the B-splines estimator

$$\widehat{\boldsymbol{\alpha}} = \Big(\sum_{i=1}^{n} \mathbf{U}_i^T \mathbf{W}_i \mathbf{U}_i\Big)^{-1} \sum_{i=1}^{n} \mathbf{U}_i^T \mathbf{W}_i \mathbf{Y}_i = (\mathbf{U}^\intercal \mathbf{W} \mathbf{U})^{-1} \mathbf{U}^\intercal \mathbf{W} \mathbf{Y}$$

  with additional notations

$$\mathbf{U} = (\mathbf{U}_1, \ldots, \mathbf{U}_n)^\intercal \in I\!R^{N \times m_{\text{tot}}} \quad \mathbf{W} = \text{diag}\Big(\mathbf{W}_1, \ldots, \mathbf{W}_n\Big) \in I\!R^{N \times N}$$

- observations under the model: $\mathbf{Y} \approx \mathbf{U}\boldsymbol{\alpha} + \boldsymbol{\varepsilon}$
- denote by $\mathbf{V}$ the variance-covariance matrix of $\boldsymbol{\varepsilon} = (\boldsymbol{\varepsilon}_1, \ldots, \boldsymbol{\varepsilon}_n)^\intercal$ a matrix of dimension $N \times N$
- denote $\mathcal{X} = \{(t_{ij}, \mathbf{X}_{ij}) : i = 1, \ldots, n, j = 1, \ldots, N_i\}$
- conditioning on $\mathcal{X}$, one obtains: $E(\widehat{\boldsymbol{\alpha}} \mid \mathcal{X}) \approx \boldsymbol{\alpha}$ and $\text{Cov}(\widehat{\boldsymbol{\alpha}} \mid \mathcal{X}) \approx (\mathbf{U}^\intercal \mathbf{W} \mathbf{U})^{-1} \mathbf{U}^\intercal \mathbf{W} \mathbf{V} \mathbf{W} \mathbf{U} (\mathbf{U}^\intercal \mathbf{W} \mathbf{U})^{-1}$

what now further in case of normal errors?

$$\boldsymbol{\varepsilon} = (\varepsilon_1, \ldots, \varepsilon_n)^\top \sim N(\mathbf{0}, \mathbf{V})$$

- recall that we need to evaluate
  $P\left(\min(\mathbf{C}\widehat{\boldsymbol{\alpha}}) \leq r\right) = P\left(s_{\min} \leq r\right), \; r \in \mathbb{R}$
- since $E(\mathbf{Y}|\mathcal{X}) \approx \mathbf{U}\boldsymbol{\alpha}$, we have that $\mathbf{C}\widehat{\boldsymbol{\alpha}}$ is, conditioned on $\mathcal{X}$, approximately normal with mean $\mathbf{C}\boldsymbol{\alpha}$ and variance-covariance matrix

$$\boldsymbol{\Sigma} = \mathbf{C}(\mathbf{U}^\top \mathbf{W}\mathbf{U})^{-1}\mathbf{U}^\top \mathbf{W}\mathbf{V}\mathbf{W}\mathbf{U}(\mathbf{U}^\top \mathbf{W}\mathbf{U})^{-1}\mathbf{C}^\top$$

- we obtain the expression

$$P\left(s_{\min} \leq r\right) = 1 - P\left(s_{\min} > r\right) = 1 - \int \cdots \int_{\{\mathbf{z}|\mathbf{z}-r\mathbf{1}\geq 0\}} \phi(\mathbf{z}; \mathbf{C}\boldsymbol{\alpha}, \boldsymbol{\Sigma}) d\mathbf{z}$$

  where $\mathbf{z}, \mathbf{1} = (1, 1, \ldots, 1)^\top \in \mathbb{R}^{(u_k+1)\times 1}$

  $\phi(\cdot\,; \mathbf{C}\boldsymbol{\alpha}, \boldsymbol{\Sigma})$=multivariate normal density with mean $\mathbf{C}\boldsymbol{\alpha}$ and covariance $\boldsymbol{\Sigma}$
- this probability can only be calculated if $\boldsymbol{\alpha}$ and $\mathbf{V}$ are known ...

consistency of the test, based on asymptotic normality result

probability of committing an error of Type II tends to 0, when $n \to \infty$

Theorem 2

Assume that $u_n^{\text{max}} \rho_n + (u_n^{\text{max}})^{\nu_k} + u_n^{\text{max}} r_n = o(1)$. Under Assumptions 1—5, if $\inf_{t \in [0,1]} \beta_k'(t) = \delta > 0$, then

$$\lim_{n \to \infty} P(s_{\text{min}} < \min(0, \widehat{Q}_\alpha)) = 0$$

- • using **cubic spline approximation**
  - test statistic: $\min_{t \in \text{Grid}} \widehat{\beta}_k'(t)$
  - first approach: bootstrap procedure similar as before
  - second approach: now rely on the asymptotic behaviour of the derivative estimates

- testing for **convexity** testing

$$H_0: \quad \beta_k(\cdot) \text{ is a convex function}$$
$$\text{versus } H_1: \quad \beta_k(\cdot) \text{ is not a convex function}$$

or equivalently

$$H_0: \beta_k''(t) \geq 0 \text{ for all } t \text{ in } [0,1] \qquad \text{versus} \qquad H_1: \neg H_0$$

- similar to before, but now focusing on the estimates of the second derivative function
- here distinction between
  - use of cubic spline approximation
  - use of quartic (or higher order) spline approximation

- **simultaneous testing** : example

$$H_0: \quad \beta_1(\cdot) \text{ is monotone decreasing} \quad \text{and} \quad \beta_3(\cdot) \text{ is convex}$$

$$\text{versus } H_1: \quad \neg H_0$$

- test statistic:

$$\mathbf{s} = \left(\min_{t \in \text{Grid}} \widehat{\beta}_1'(t), \min_{t \in \text{Grid}} \widehat{\beta}_3''(t) \right)$$

- use bootstrap type of procedure
- use Bonferroni type of correction

we looked at: conditional mean

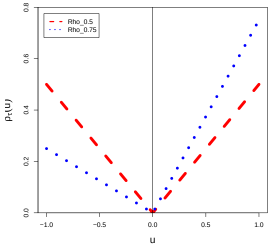
other quantities of interest: **conditional quantiles** (quantile regression)

what about the objective function $S(\alpha)$?

conditional mean	$\sum_{i=1}^{n} \frac{1}{N_i} \sum_{j=1}^{N_i} \left(Y_{ij} - \sum_{k=0}^{p} \sum_{\ell=1}^{m_k} \alpha_{k\ell} B_{k\ell}(t_{ij}; \nu_k) X_{ij}^{(k)} \right)^2$
conditional quantile (order τ)	$\sum_{i=1}^{n} \frac{1}{N_i} \sum_{j=1}^{N_i} \rho_\tau \left(Y_{ij} - \sum_{k=0}^{p} \sum_{\ell=1}^{m_k} \alpha_{k\ell} B_{k\ell}(t_{ij}; \nu_k) X_{ij}^{(k)} \right)$

$$\rho_\tau(z) = \begin{cases} \tau\, z & \text{if } z > 0 \\ -(1-\tau)\, z & \text{otherwise} \end{cases}$$

check function



in both contexts: **homoscedasticity** $\Longleftrightarrow$ **heteroscedasticity**

general setting model

$$\begin{aligned} Y(T) &= \beta_0(T) + \beta_1(T)X^{(1)}(T) + \cdots + \beta_p(T)X^{(p)}(T) + \widetilde{\varepsilon} \\ &= \mathbf{X}^{\mathsf{T}}(T)\boldsymbol{\beta}(T) + V(\mathbf{X}(T), T)\,\varepsilon(T) \end{aligned}$$

where $\varepsilon(T)$ is independent of $(\mathbf{X}(T), T)$

special settings: | $V(\mathbf{X}(T), T) = V(T)$ simple heteroscedastic setting | $V(\mathbf{X}(T), T) = V$ a constant homoscedastic setting

assumptions to ensure identifiability needed in all settings

Andriyana (2015), Andriyana & G. (2017), Andriyana *et al.* (2017), ...

general heteroscedastic varying coefficient model

$$Y(T) = \beta_0(T) + \beta_1(T)X^{(1)}(T) + \ldots + \beta_p(T)X^{(p)}(T) + V(\mathbf{X}(T), T)\,\varepsilon(T)$$

$$\mathbf{V}\left(\mathbf{X}(\mathbf{T}), \mathbf{T}\right) = \exp\left\{\gamma_{\mathbf{0}}(\mathbf{T}) + \gamma_{\mathbf{1}}(\mathbf{T})\mathbf{X}^{(\mathbf{1})}(\mathbf{T}) + \ldots + \gamma_{\mathbf{p}}(\mathbf{T})\mathbf{X}^{(\mathbf{p})}(\mathbf{T})\right\}$$

from the model and the error structure:

$$Y(T) = \underbrace{\mathbf{X}^{\mathsf{T}}(T)\boldsymbol{\beta}(T)}_{\text{signal part}} + \underbrace{\exp\left\{\mathbf{X}^{\mathsf{T}}(T)\boldsymbol{\gamma}(T)\right\}}_{\text{variability part}}\,\varepsilon(T)$$

where $\boldsymbol{\beta}(t) = (\beta_0(t), \beta_1(t), \ldots, \beta_p(t))^{\mathsf{T}}$

and $\boldsymbol{\gamma}(t) = (\gamma_0(t), \gamma_1(t), \ldots, \gamma_p(t))^{\mathsf{T}}$

aims: estimate all unknown coefficient functions (in the signal and the variability part!)

estimate all conditional quantiles

shape testing for the coefficient functions, the β_k's and the γ_ℓ's

$$Y(T) = \beta_0(T) + \beta_1(T)X^{(1)}(T) + \ldots + \beta_p(T)X^{(p)}(T) + V(\mathbf{X}(T), T)\,\varepsilon(T)$$

what is the expression for the conditional quantile function?

denote the conditional quantile of order τ $(0 < \tau < 1)$ of $\varepsilon(T)$ given $(\mathbf{X}(T), T)$ by

$$a^{\tau}(T) = \inf\{y : P\{\varepsilon(T) \le y \mid (\mathbf{X}(T), T)\} \ge \tau\} = q_{\tau}(\varepsilon(T) \mid \mathbf{X}(T), T)$$

τ-th conditional quantile of $Y(T)$ given $(\mathbf{X}(T), T)$ is

$$\boxed{q_{\tau}(Y(T)|\mathbf{X}(T), T) = \mathbf{X}^{\mathsf{T}}(T)\boldsymbol{\beta}(T) + V(\mathbf{X}(T), T)\,a^{\tau}(T)}$$

- **estimation methods**
  - for identifiability reasons, and for estimating the variability function: adapt approach of He (1997)
  - basic assumptions:
    - **(H1)**: the conditional median quantile of the error term equals zero: $q_{0.5}\left\{\varepsilon(T) \mid \mathbf{X}(T), T\right\} = 0$
    - **(H2)**: $q_{0.5}\Big\{\ln|\varepsilon(T)| \mid \mathbf{X}(T), T\Big\} = 0$
  - the estimation consists of three steps:
    1. estimate the conditional median function
    2. estimate the variability function $V(\mathbf{X}(T), T)$
    3. estimate the conditional quantile function

various testing problems:

- testing for constancy
- testing for monotonicity
- testing for convexity/concavity
- shape testing for both signal and variability part

tests involving some or all coefficient functions in

the signal part: $\boldsymbol{\beta}(t) = (\beta_0(t), \beta_1(t), \ldots, \beta_p(t))^\mathsf{T}$

the variability part: $\boldsymbol{\gamma}(t) = (\gamma_0(t), \gamma_1(t), \ldots, \gamma_p(t))^\mathsf{T}$

- ◇ likelihood ratio type of tests
- ◇ other tests: based on looking at differences of B-spline coefficients

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