Nonparametric covariance estimation for longitudinal data via tensor product smoothing

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The data:

$$Y_i = (Y_{i1}, Y_{i2}, \ldots, Y_{im})', \qquad i = 1, \ldots, N$$

associated with measurement times

$$t_1 < t_2 < \cdots < t_m.$$

The flaming hoops:

- Covariance matrices (and their estimates) should be positive definite.
  - Constrained optimization is a headache.
- The $\{t_{ij}\}$ may be suboptimal.
  - Observation times may not fall on a regular grid, may vary across subjects.
- More dimensions, more problems (maybe.)
  - Sample covariance matrix falls apart when m is large.

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- Covariance matrices (and their estimates) should be positive definite. A cute little reparameterization $\implies$ unconstrained estimation, meaningful interpretation
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Covariance dress-up: the modified Cholesky decomposition

$$Y = (Y_1, \dots, Y_M)' \sim \mathcal{N}(0, \Sigma).$$

For any positive definite Σ, we can find T which diagonalizes Σ:

$$D = T\Sigma T', \quad T = \begin{bmatrix} 1 & 0 & \dots & & \\ -\phi_{21} & 1 & & & \\ -\phi_{31} & -\phi_{32} & 1 & & \\ \vdots & & & \ddots & \\ -\phi_{M1} & -\phi_{M2} & \dots & -\phi_{M,M-1} & 1 \end{bmatrix} \tag{1}$$

The matrix T is the *Cholesy factor* of the precision matrix.

Now, for the cutest part:

Okay, really:

Imagine regressing Y_j on its predecessors:

$$y_j = \begin{cases} e_1 & j = 1, \\ \sum_{k=1}^{j-1} \phi_{jk} y_k + \sigma_j e_j & j = 2, \ldots, M \end{cases} \tag{2}$$

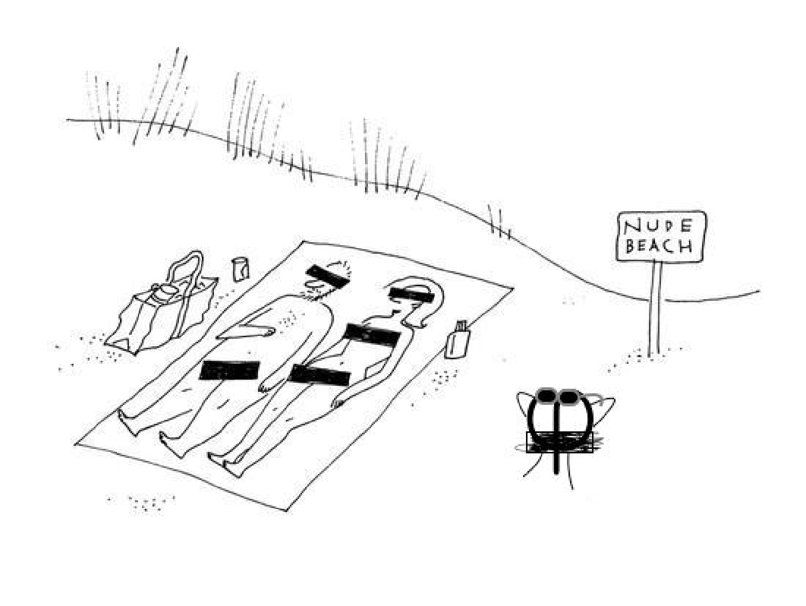
In matrix form:

$$e = TY, \tag{3}$$

and taking covariances on both sides:

$$D = diag\left(\sigma_1^2, \ldots, \sigma_M^2\right) = T\Sigma T'. \tag{4}$$

No constraints on the ϕ_{jk}s!



The regression model tool box: a deep treasure chest of luxury.

Model Y_j, e_j as

$$Y_j = Y(t_j), \quad e_j = e(t_j),$$
$$e(s) \sim \mathcal{WN}(0,1),$$

Swap the standard regression model **??** for a varying coefficient model:

$$\phi_{jk} = \phi(t_j, t_k),$$

$$y(t_j) = \sum_{k=1}^{j-1} \phi(t_j, t_k)\, y(t_k) + \sigma(t_j)\, e(t_j) \tag{5}$$

The $\{\phi_{jk}\}$ are called *generalized autoregressive parameters.*
The $\{\sigma_j^2\}$ are called the *innovation variances.*

(Iterated) penalized maximum likelihood estimation

1. Fix $\sigma_{ij}^2 = \sigma_{ij0}^2$, $i = 1, \ldots, N$,$j = 1, \ldots, M$.
2. Find $\phi_0 = arg \min_{\phi} - 2L_{\phi}\left(\phi, y_1, \ldots, y_N\right) + \lambda J\left(\phi\right)$
3. Fix $\phi = \phi_0$.
4. Find $\sigma_0^2 = arg \min_{\sigma^2} - 2L_{\sigma}^2\left(\sigma^2, y_1, \ldots, y_N\right) + \lambda J\left(\sigma^2\right)$

$$-2L_{\phi}\left(\phi, y_1, \ldots, y_N\right) = \sum_{i=1}^{N} \sum_{j=2}^{m_i} \sigma_{ij0}^{-2} \left(y_{ij} - \sum_{k=1}^{j-1} \phi\left(t_{ij}, t_{ik}\right) y_{ik} \right)^2$$

Regularization of $\phi(s,t)$ is more intuitive if we transform the s-t axis.

Rotate the input axes:

$$l = s - t$$
$$m = \frac{1}{2}(s+t).$$

Then ϕ becomes

$$\phi^*(l,m) = \phi^*\left(s-t, \frac{1}{2}(s+t)\right)$$
$$= \phi(s,t).$$

Take $\hat{\phi}^*$ to be the minimizer of

$$-2L + \lambda J(\phi^*)$$

Smooth ANOVA models

Decompose

$$\phi^*(l, m) = \mu + \phi_1(l) + \phi_2(m) + \phi_{12}(l, m), \tag{7}$$

so Model **??** becomes

$$y(t_j) = \sum_{k=1}^{j-1} \Big[\mu + \phi_1(l_{jk}) + \phi_2(m_{jk}) + \phi_{12}(l_{jk}, m_{jk}) \Big] y(t_k) + \sigma(t_j)\, e(t_j) \tag{8}$$

We can use B-splines to construct the model basis.

Represent the main effects as

$$\begin{aligned} \phi_1(l) &= \sum_{c=1}^{c_l} B_c(l; q_l)\,\theta_{lc}, \\ \phi_2(m) &= \sum_{c'=1}^{c_m} B_{c'}(m; q_m)\,\theta_{mc'}, \end{aligned} \tag{9}$$

and the interaction term by the tensor product of the marginal bases **??** and **??**:

$$\phi_{12}(l, m) = \sum_{c=1}^{c_l}\sum_{c'=1}^{c_m} B_c(l; q_l)\,B_{c'}(m; q_m)\,\theta_{cc'} \tag{10}$$

PS-ANOVA model basis

In matrix notation, Model **??** becomes

$$E\left[Y|W\right] = WB\theta,$$

where W is the matrix of covariates holding the past values of Y, and B is the B-spline regression basis:

$$B = \left[\ 1_p \mid B_l \mid B_m \mid B_{lm}\ \right] \tag{11}$$

where

$$\begin{aligned} B_{lm} &= B_m \,\square\, B_l \\ &\equiv \left(B_m \otimes 1'_{c_l}\right) \odot \left(1'_{c_m} \otimes B_l\right). \end{aligned}$$

Difference penalty had to regulate.

For $f(x) = \sum_{i=1}^{p} B_i(x)\,\theta_i$, approximate

$$\int_0^1 \left(f''(x)\right)^2 \, dx = \int_0^1 \left\{ \sum_{i=1}^{p} B_i''(x)\,\theta_i \right\}^2 dx \\ = k_1 \sum_i \left(\Delta^2 \theta_i\right)^2 + k_2, \tag{12}$$

by

$$||D_2\theta||^2, \qquad D_2\theta = \left(\Delta^2\theta_1, \ldots, \Delta^2\theta_{p-2}\right)'$$

In general, $\boxed{\text{approximate } \int_0^1 \left(f^{(d)}\right)^2 dx \text{ with } ||D_d\theta||^2}$

PS-ANOVA Penalty

Estimate B-spline coefficients by minimizing

$$(Y - WB\theta)'(Y - WB\theta) + \theta' P\theta$$

where

$$P = \text{blockdiag}(0,\ P_1,\ P_2,\ P_{12}), \tag{13}$$

$$P_i = \lambda_i D'_{d_i} D_{d_i}$$

$$P_{12} = \lambda_3 D'_{d_1} D_{d_1} \otimes I_{cm} + \lambda_4 I_{c_l} \otimes D'_{d_2} D_{d_2}$$

Mixed model representation

In matrix notation, Model **??** is given by

$$E\left[Y|W\right] = WB\theta,$$

where W is the matrix of covariates holding the past values of Y, and B is the B-spline regression basis:

$$B = [\ 1_p \mid B_l \mid B_m \mid B_{lm}\ ] \tag{14}$$

$$B_{lm}\left(B_m \otimes 1'_{c_l}\right) \odot \left(1'_{c_m} \otimes B_l\right),$$

and

$$\theta = (\mu,\ \theta_l,\ \theta_l,\ \theta_{lm})'$$

Mixed model representation

Find transformation M to map

$$B \to [\ X \mid Z\ ], \qquad \theta \to (\beta, \alpha)'$$

such that

$$BM = [\ X \mid Z\ ], \qquad B\theta = X\beta + Z\alpha$$

Applying M to basis **??** and penalty **??**, Model **??** becomes

$$\begin{gathered} Y = W\left(X\beta + Z\alpha\right) + e, \\ \alpha \sim \mathcal{N}\left(0, G\right), \quad e \sim \mathcal{N}\left(0, D\right) \end{gathered} \tag{15}$$

The $\{\lambda_j\}$ become

$$\lambda_j = \frac{\sigma^2}{\tau_j^2}$$

where $\operatorname{diag}(G) = \left\{\tau_j^2\right\}$.

Decomposition of ϕ^* *for* $d_l = d_m = 2$

	$\{1\}$	$\{m\}$	$\{B_{j'}(m)\}$
$\{1\}$	$\{1\}$	$\{m\}$	$\{B_{j'}(m)\}$
$\{l\}$	$\{l\}$	$l \times m$	$l \times \{B_{j'}(m)\}$
$\{B_j(l)\}$	$\{B_j(l)\}$	$m \times \{B_j(l)\}$	$\{B_j(l)\, B_{j'}(m)\}$

Nested PS-ANOVA

Re-express ϕ_{12}:

$$\phi_{12}(l,m) = g_1(l)\left[\sum_{r=1}^{d_m-1} m^r\right] + \left[\sum_{r=1}^{d_l-1} l^r\right] g_2(m) + h(l,m),$$

For $d_l = d_m = 2$,

$$\phi_{12}(l,m) = g_1(l)\ m + l\ g_2(m) + h(l,m)$$

with basis:

$$B = \left[\, 1_p \mid B_1 \mid B_2 \mid B_3 \mid B_4 \mid B_5 \,\right], \tag{16}$$

where

$$B_3 = m \,\square\, B_1 \qquad B_5 = B_2 \,\square\, B_1$$

$$B_4 = B_2 \,\square\, l$$

Nested PS-ANOVA

$$P = \text{blockdiag}\left(0,\ P_1,\ P_2,\ P_3,\ P_4,\ P_5\right), \qquad (17)$$

$$P_i = \lambda_i D'_{d_i} D_{d_i}$$

$$P_{12} = \lambda_3 D'_{d_1} D_{d_1} \otimes I_{c_m} + \lambda_4 I_{c_l} \otimes D'_{d_2} D_{d_2}$$

Nested PS-ANOVA

Re-express ϕ_{12}:

$$\phi_{12}(l,m) = g_{lr}(l)\left[\sum_{r=1}^{d_m-1} m^r\right] + \left[\sum_{r=1}^{d_l-1} l^{r'}\right] g_{mr'}(m) + h(l,m),$$

For $d_l = d_m = 2$,

$$\phi_{12}(l,m) = g_{l1}(l)\; m + l\; g_{m1}(m) + h(l,m)$$

with basis:

$$B = \left[\, 1_p \mid B_1 \mid B_2 \mid B_3 \mid B_4 \mid B_5 \,\right], \tag{18}$$

where

$$B_3 = m \,\square\, B_1 \qquad B_5 = B_2 \,\square\, B_1$$

$$B_4 = B_2 \,\square\, l$$

Nested PS-ANOVA

$$P = \text{blockdiag}\left(0,\ P_1,\ P_2,\ P_3,\ P_4,\ P_5\right)$$

Remove the redundant columns, and give each penalized component its own random effect:

$$B$$