Nonparametric covariance estimation for longitudinal data via tensor product smoothing

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The data:

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

associated with measurement times

$$t_1 < t_2 < \cdots < t_{M_i}.$$

Goal: estimate

$$Cov\,(Y) = \Sigma$$

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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The flaming hoops:

- Covariance matrices (and their estimates) should be positive definite. A cute little reparameterization $\Longrightarrow$ unconstrained estimation, meaningful interpretation
- The $\{t_{ij}\}$ may be messy.
  Frame covariance estimation as function estimation.
- More dimensions, more problems (maybe.)

Figure: Regulate like Nate Dogg.

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:

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

Now, for the cutest part:

Okay, really:

Regress Y_j on $Y_{(1:j-1)} = (Y_1, \ldots, Y_{j-1})'$:

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

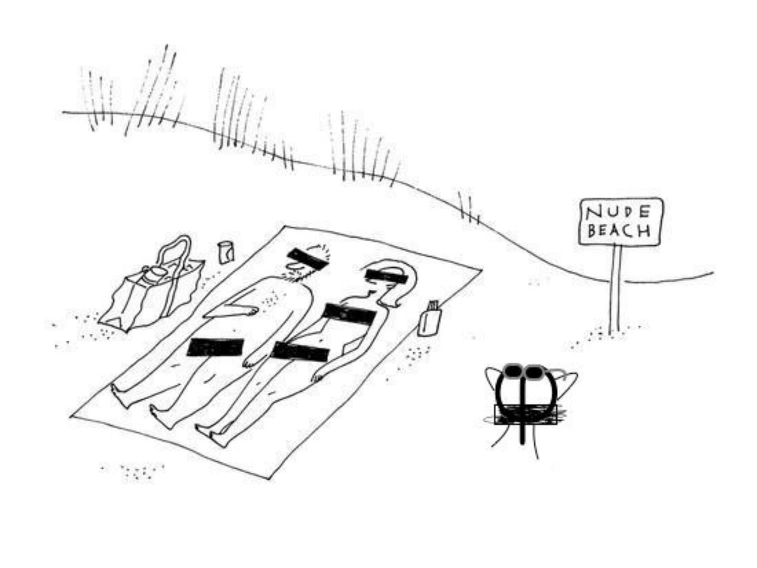
In matrix form:

$$e = TY, \tag{2}$$

and taking covariances on both sides:

$$D = diag\left(\sigma_1^2, \ldots, \sigma_M^2\right) = T \Sigma T'. \tag{3}$$

No constraints on the ϕ_{jk}s!



The regression model tool box is a deep, luxurious toolbox.

$$Y_j \longrightarrow Y(t_j) \qquad e_j \longrightarrow e(t_j)$$
$$\phi_{jk} \longrightarrow \phi(t_j, t_k) \qquad \sigma_j^2 \longrightarrow \sigma^2(t_j)$$

$$y(t_j) = \sum_{k=1}^{j-1} \phi(t_j, t_k)\, y(t_k) + \sigma(t_j)\, e(t_j), \tag{4}$$

where

$$e(s) \sim \mathcal{WN}(0, 1)$$

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

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

Reparameterize ϕ:

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

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

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

Smooth ANOVA models

Decompose

$$\phi^* (l, m) = \mu + \phi_1 (l) + \phi_2 (m) + \phi_{12} (l, m), \tag{6}$$

so Model 4 becomes

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

Approximate ϕ_1, ϕ_2, ϕ_{12} with B-splines.

$$
\begin{aligned}
\phi_1(l) &= \sum_{c=1}^{c_l} B_c(l; q_l)\,\theta_{lc} = B_l\theta_l, \\
\phi_2(m) &= \sum_{c'=1}^{c_m} B_{c'}(m; q_m)\,\theta_{mc'} = B_m\theta_m \\
\phi_{12}(l, m) &= \sum_{c=1}^{c_l}\sum_{c'=1}^{c_m} B_c(l; q_l)\,B_{c'}(m; q_m)\,\theta_{cc'} = B_{lm}\theta_{lm}
\end{aligned}
\tag{7}
$$

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

Difference penalty had to regulate.

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

$$\begin{aligned}\int_0^1 \left(f''(x)\right)^2 \, dx &= \int_0^1 \left\{ \sum_{i=1}^{p} B_i''(x)\,\theta_i \right\}^2 dx \\ &= k_1 \sum_i \left(\Delta^2 \theta_i\right)^2 + k_2,\end{aligned} \tag{8}$$

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

$$B \equiv [\, 1_p \mid B_l \mid B_m \mid B_{lm} \,], \qquad \theta \equiv (\mu, \theta_l, \theta_m, \theta_{lm})'$$

Find θ minimizing

$$(Y - WB\theta)' \, D^{-1} \, (Y - WB\theta) + \theta' P \theta$$

$$P = \begin{bmatrix} 0 & & & \\ & \underbrace{\lambda_l D'_{d_l} D_{d_l}}_{P_l} & & \\ & & \underbrace{\lambda_l D'_{d_l} D_{d_l}}_{P_m} & \\ & & & \underbrace{\tau_l D'_{d_l} D_{d_l} \otimes I_{c_m} + \tau_m I_{c_l} \otimes D'_{d_m} D_{d_m}}_{P_{lm}} \end{bmatrix}$$

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Mixed model representation

Find transformation $\mathrm{Q} = \left[\; \mathrm{Q}_n \; \middle| \; \mathrm{Q}_s \; \right]$ to map

$$
\begin{aligned}
BQ &= \left[\; BQ_0 \; \middle| \; BQ_1 \; \right] \qquad\qquad B\theta = X\beta + Z\alpha \\
&= \left[\; X \; \middle| \; Z \; \right]
\end{aligned}
$$

to reparameterize the ill-posed Model 9 as

$$
Y = W\left(X\beta + Z\alpha\right) + e \tag{10}
$$

$$
\alpha \sim \mathcal{N}\left(0, G\right), \quad e \sim \mathcal{N}\left(0, \sigma^2 D\right)
$$

Smoothing parameter selection = variance component estimation

$G = \sigma^2 F^{-1}$ where

$$F = \begin{bmatrix} F_l & & \\ & F_m & \\ & & F_{lm} \end{bmatrix} = \begin{bmatrix} \lambda_l \tilde{\Delta}_l & & \\ & \lambda_m \tilde{\Delta}_m & \\ & & F_{lm} \end{bmatrix},$$

$$F_{lm} = \begin{bmatrix} \tau_l \tilde{\Delta}_l & & \\ & \tau_m \tilde{\Delta}_m & \\ & & \tau_m \tilde{\Delta}_m \otimes I_{c_l - d_l} + I_{c_m - d_m} \otimes \tau_l \tilde{\Delta}_l \end{bmatrix}$$

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 $d_l = d_m = 2$,

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

$$B = \left[\; 1_p \mid B_1 \mid B_2 \mid B_3 \mid B_4 \mid B_5 \;\right], \tag{11}$$

where

$$B_3 = m \,\square\, B_1, \qquad B_4 = B_2 \square\, l, \qquad B_5 = B_2 \,\square\, B_1$$

Nested PS-ANOVA Penalty

$$P = \mathrm{blockdiag}\left(0,\; P_1,\; P_2,\; P_3,\; P_4,\; P_5\right), \tag{12}$$