

Nonparametric covariance estimation for longitudinal data via tensor product smoothing

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The data:

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

associated with measurement times

$$t_1 < t_2 < \dots < t_m.$$

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
- ▶ The $\{t_{ij}\}$ may be messy.
Frame covariance estimation as function estimation.
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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 :

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

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:

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

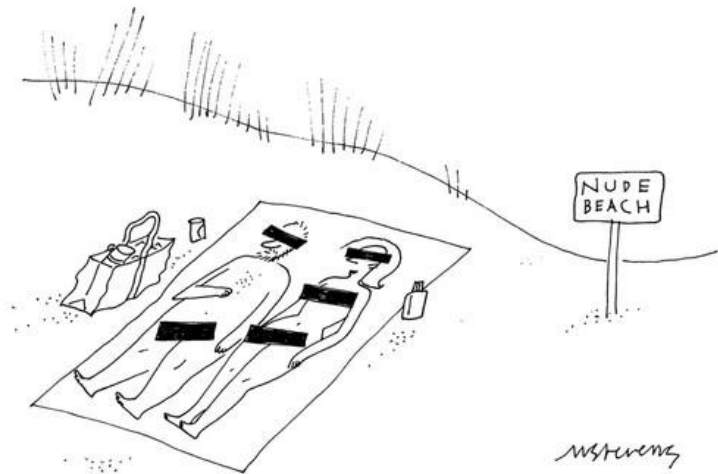
In matrix form:

$$e = TY, \quad (3)$$

and taking covariances on both sides:

$$D = \text{diag}(\sigma_1^2, \dots, \sigma_M^2) = T\Sigma T'. \quad (4)$$

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 2 for a varying coefficient model:

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

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

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

(Iterated) penalized maximum likelihood estimation

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

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

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

Rotate the input axes:

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

Then ϕ becomes

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

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

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

Smooth ANOVA models

Decompose

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

so Model 5 becomes

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

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 8 becomes

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

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

$$B = [1_p \mid B_l \mid B_m \mid B_{lm}] \quad (11)$$

where

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

The null and penalized subspaces of P

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 Basis

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:

$$B = \left[1_p \mid B_1 \mid B_2 \mid B_3 \mid B_4 \mid B_5 \right], \quad (12)$$

where

$$B_3 = m \square B_1$$

$$B_4 = B_2 \square l$$

$$B_5 = B_2 \square B_1$$