Functional Data Analysis: Part I
Overview and Mean/Covariance Estimation

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Outline

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What is Functional Data?

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- Characteristics of functional data:

  (i) The atom of functional data is a “function”.
  (ii) They are ∞−dimensional data.

Example: Curve Data

- **Curve data**

  - real-valued functions defined on an interval $I \in \mathbb{R}$.

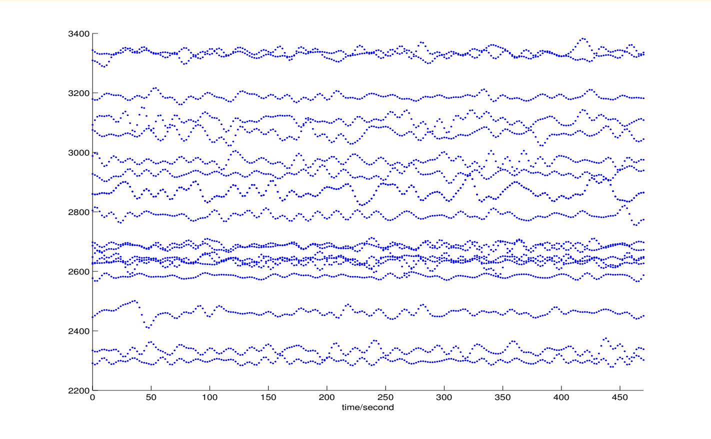
  - one curve per subject

  These curves are usually considered realizations of a stochastic process $X(t)$ in a **Hilbert space**, e.g.

  $L^2(I)$ or RKHS (reproducing kernel Hilbert space).

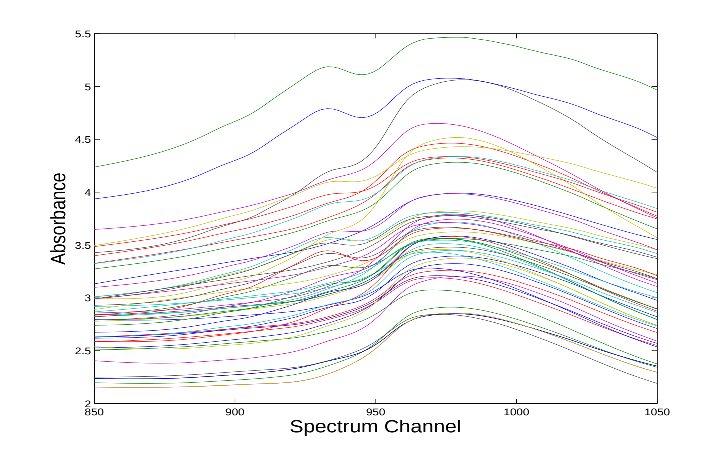
Examples of Functional Data

- fMRI data at a particular voxel for 20 subjects $\Longrightarrow n = 20.$



Examples of Functional Data

- Spectrum data for meat content - here the function is over the spectrum channels of n pieces of meat.



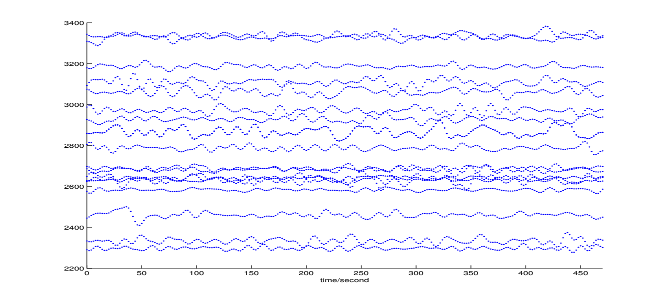
Additional Examples of Functional Data

- 10 minutes EKG recordings of 100 patients.
  $n = 100$
- Daily temperature recording in January at 240 locations.
  $n = 240$
- Daily reproduction (# of eggs) of 1000 female medflies (Mediterranean fruit flies) till death.
  $n = 1000$

Real/Observed Functional Data

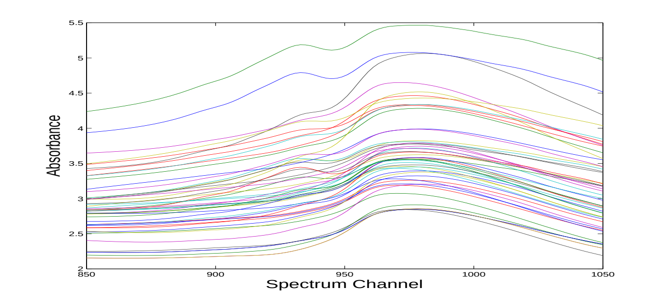
- In reality, functional data are recorded intensely on a time grid $\Longrightarrow$ high-dimensional data.

  * The fMRI data were recorded every two seconds for about 10 minutes (300 time points) $\Longrightarrow$ 300 dimensional data.



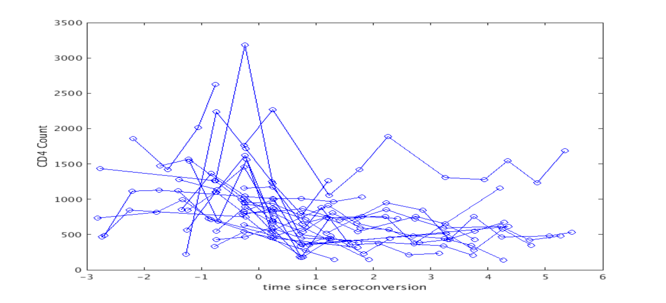
Real/Observed Functional Data

- The spectrum data were recorded at 100 frequency channels (hence 100-dim) and smoothed individually, i.e. pre-smoothed.



Longitudinal Data as Functional Data

- Longitudinal Data - Irregularly sampled functional data.
- They are often only a few measurements per subject, as in medical follow-up or social studies.



Longitudinal AIDS Data

- CD4 counts of 369 patients.

  $n_i = \#$ of repeated measurements for subject i,

  varies with subject.

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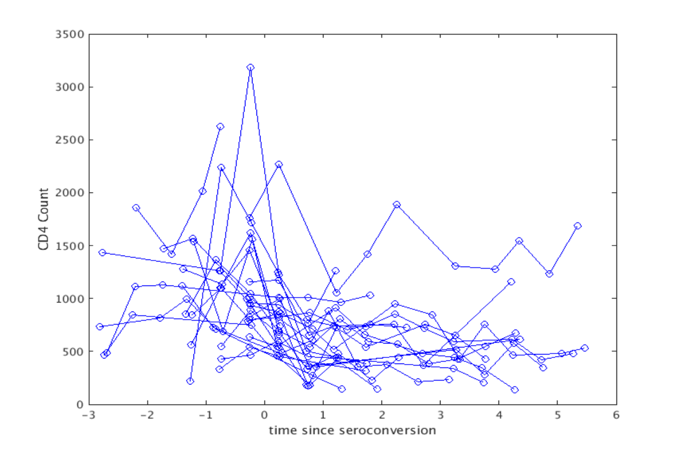
- This results in longitudinal data with uneven $\#$ of measurements at irregular time-points.

CD4 Counts of First 25 Patients



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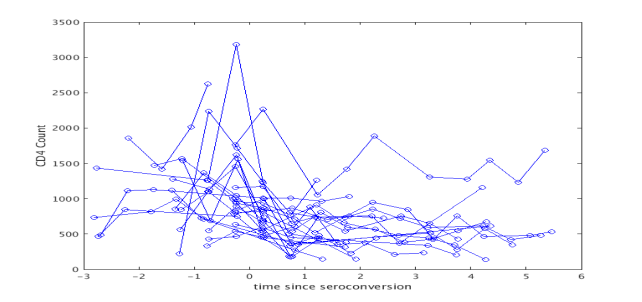
- Longitudinal data have traditionally been modeled by a parametric approach, such as a linear mixed-effects model.

  - However, it may not be easy to spot the pattern due to sparsity of and noise in the longitudinal data.

Longitudinal vs Functional data



- This motivates a data oriented nonparametric approach, which luckily is feasible under mild design conditions.

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  $$Y_{ij} = X_i(t_{ij}) + e_{ij}, \quad j = 1, \ldots, n_i,$$

  where $X_i(t)$ is a smooth random function,
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- A strength of the FDA approach is its ability to handle noise.

Summary

- There are the three types of functional data:

  (i) stochastic processes $\Longrightarrow$ ∞-dimensional data
  (ii) intense/dense functional data $\Longrightarrow$ high dimensional data
  (iii) sparse functional/longitudinal data $\Longrightarrow$ irregular dim. data.

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  (But the observed data may contain noise, a.k.a. measurement error.)

- Nonparametric approaches are typically employed to all three types of functional data.

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- What are the pros and cons for each type of functional data?

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  Answer: We borrow information by smoothing!

  - We can do so because we have a natural ordering of the data.

  - Chen, Chen, M. and W. (2011) proposed a way to reorder multivariate data and convert high-dim data to functional data. (Stay tuned!)

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- The analysis of stochastic processes went even further back to Grenander (1950), Karhunen (1946), Loève (1946), and later include Kleffe (1973) and Dauxois and Poussé (1976).

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- Brain and neuroimaging data are examples of next generation functional data.

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  - What does **"dense"** or **"sparse"** mean?

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- Review of FDA W., Chiou and Müller (2016)

End of Introduction

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Mean and Covariance Function

Data $\{X_1, \ldots, X_n\}$ are i.i.d. copies of a random function $X(t)$:

- Mean function: $\mu(t) = E(X(t))$
- Covariance function: $\Sigma(s,t) = \text{cov}(X(s), X(t))$,
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  where s & $t \in$ interval I.

- Regular functional data - All subjects are measured at the same time grid, $t_1, \ldots, t_m$, often equally spaced $\Longrightarrow$ multivariate data.

  Irregular functional data - The measurement schedule for subject i is $t_{i1}, \ldots, t_{in_i} \Longrightarrow$ longitudinal data.

Estimation of Mean and Covariance Functions: Dense and Regular Functional Data

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- The cross-section mean can further be smoothed slightly to obtain a smooth mean estimate (This requires a dense/intense measurement schedule).

  - **Think how you should smooth to retain the $\sqrt{n}$-consistent of the smooth estimate** .

Estimation of Mean and Covariance Functions: Dense and Regular Functional Data

- Likewise, the sample covariance matrix is also $\sqrt{n}$-consistent and can be slightly smoothed to retain the $\sqrt{n}$-rate of consistency.

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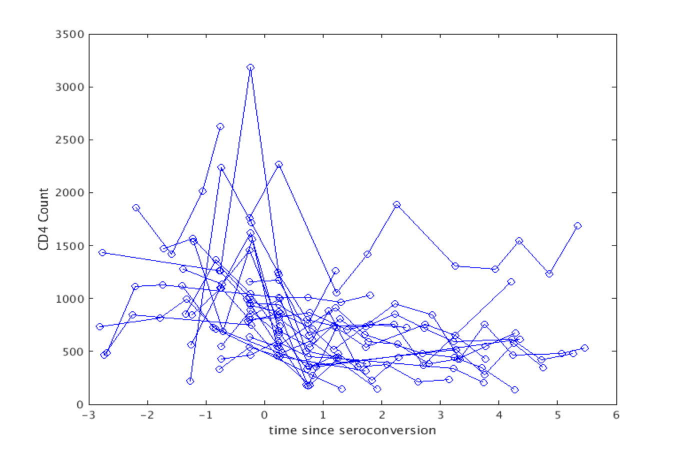
  ("Dense" functional data $\Longleftrightarrow$ $\sqrt{n}$-rate of convergence is feasible.)

- Likewise, 2D smoothing is needed to estimate the covariance function. and $\sqrt{n}$-consistency can be achieved for **dense** functional data.

CD4 Counts of First 25 Patients



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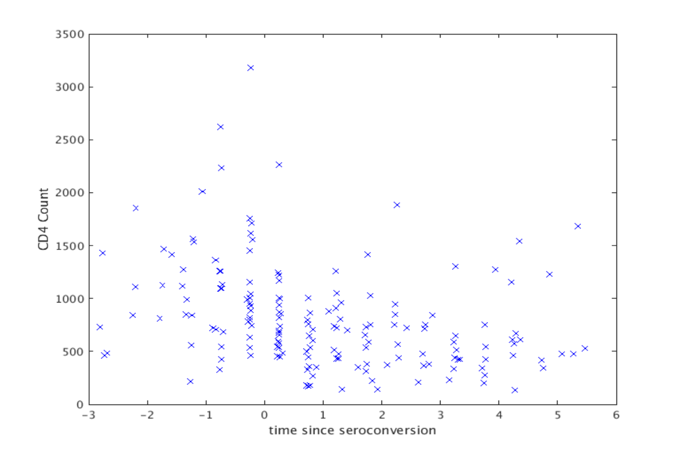
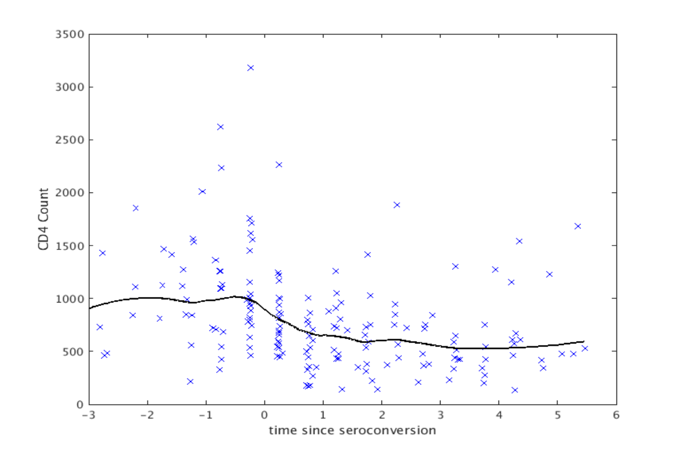
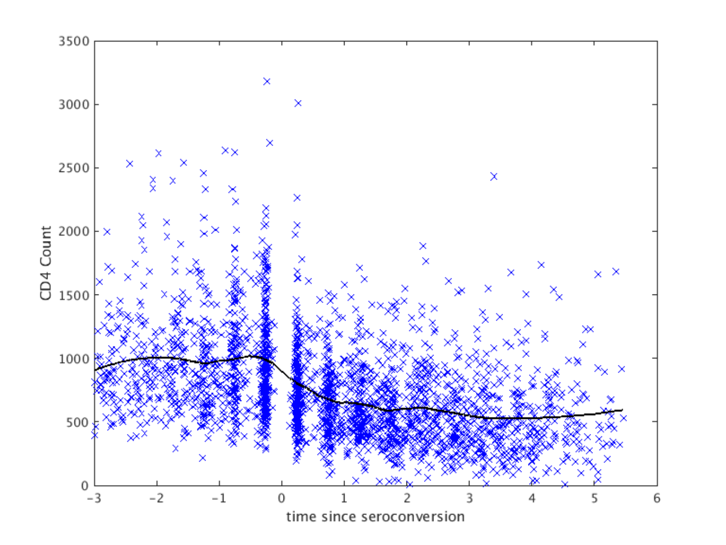


Mean Curve: CD4 Counts of first 25 Patients



Mean Curve: CD4 counts of all patients



Estimation of Mean Function

If we employ the local linear smoother, the estimate for the mean function is:

$$\hat{\mu}(t) = \hat{\beta}_0, \quad \text{where}$$
$$(\hat{\beta}_0, \hat{\beta}_1) = \underset{\beta_0,\beta_1}{\operatorname{argmin}} \quad \sum_{i=1}^{n} \sum_{j=1}^{n_i} \Big[Y_{ij} - \beta_0 - \beta_1 (T_{ij} - t) \Big]^2 K_{h_\mu}(T_{ij} - t).$$

Remarks

- In addition to the local linear (or polynomial) smoother, any smoothing method, such as penalized splines, B-splines, Wavelets, and Fourier filtering, can be employed.

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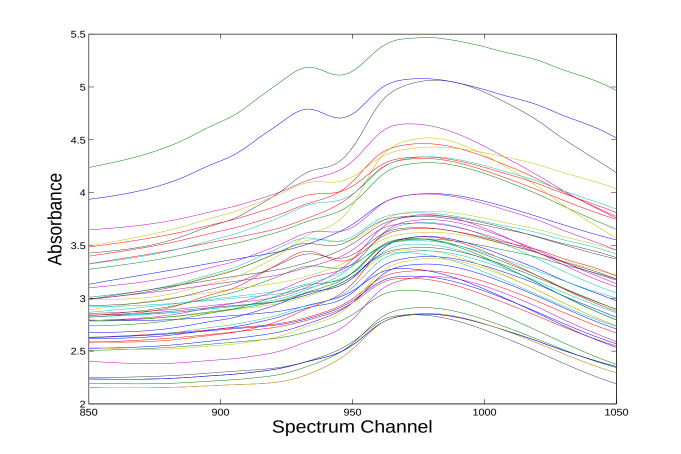
- These smoothing methods (scatter plot smoothers) can also be applied to dense data, whether regular or not, so a unified approach is feasible.
- Another common approach for dense data is to pre-smooth the data from each subject separately, then take the cross-section mean at each time point t.

Remarks

This is the case for the spectrum data.



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- Such a pre-smoothing typically aims at:

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  Hall, M. W. (2006) and Zhang and Chen (2007).

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- However, both depend on the amount of smoothing and design of the dense data, so whether the mission has been accomplished is unclear.

- Because of this uncertainty and because pre-smoothing alters the data, we prefer not to adopt a pre-smoothing approach.

End of Estimation of Mean Function

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  $\Longrightarrow \text{cov}(Y(s), Y(t)) = \text{cov}(X(s), X(t))$, when $s \neq t$,

  $$\text{var}(Y(t)) = \text{cov}(Y(t), Y(t)) = \text{cov}(X(t), X(t)) + \sigma^2(t).$$

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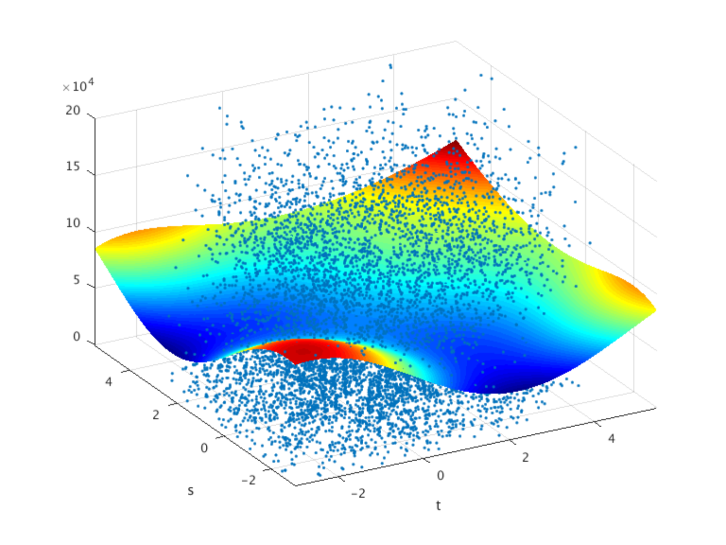
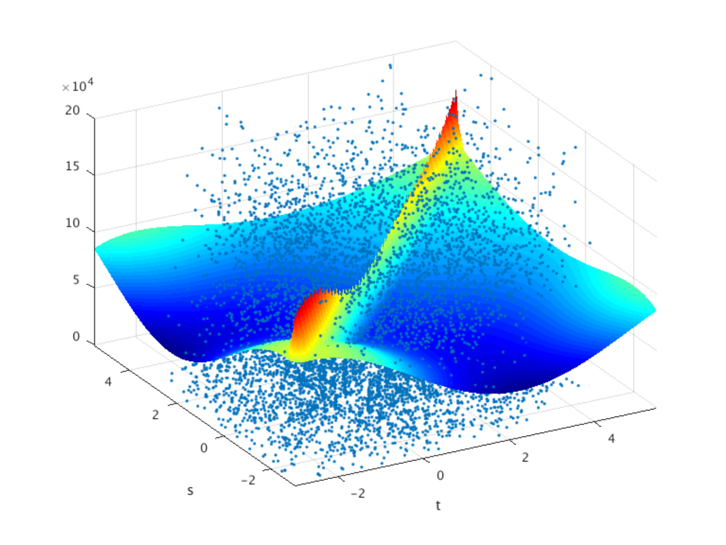
- This means we need to handle the diagonal part of $\text{cov}(Y)$, which corresponds to the variance of Y, differently from the rest of $\text{cov}(Y)$.

Covariance Surface of $X(t)$

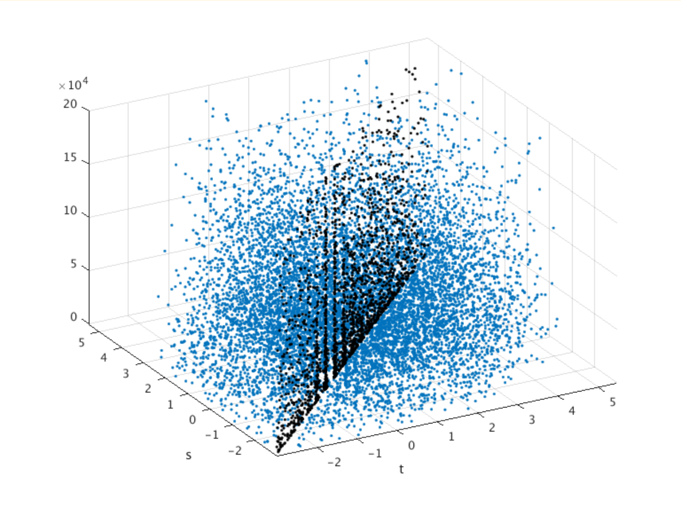


Covariance of $Y(t)$



Raw Covariance Plot: Diagonal Data in Black

$$[Y(t_{ij}) - \hat{\mu}(t_{ij})][Y(t_{ik}) - \hat{\mu}(t_{ik})],\ \forall\ i, j, k$$



Raw Covariance with Diagonal Data Removed

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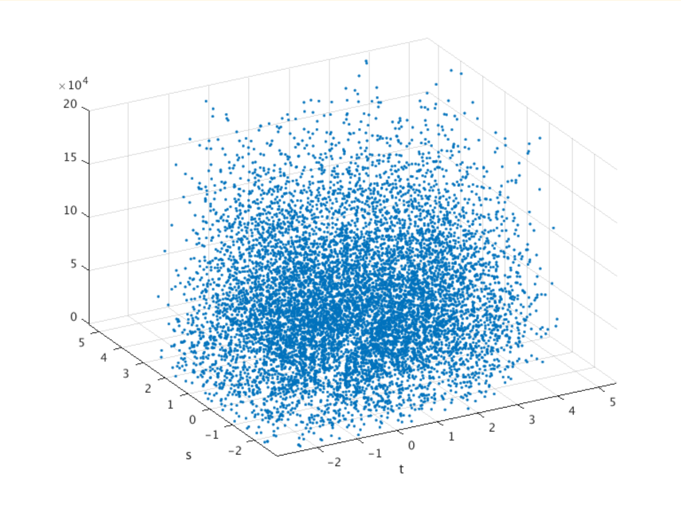
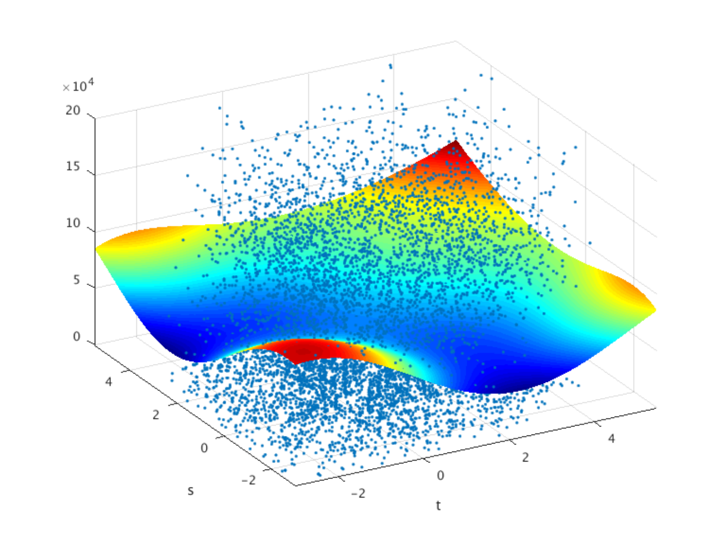


2D Smoother to Estimate the Covariance of $X(t)$



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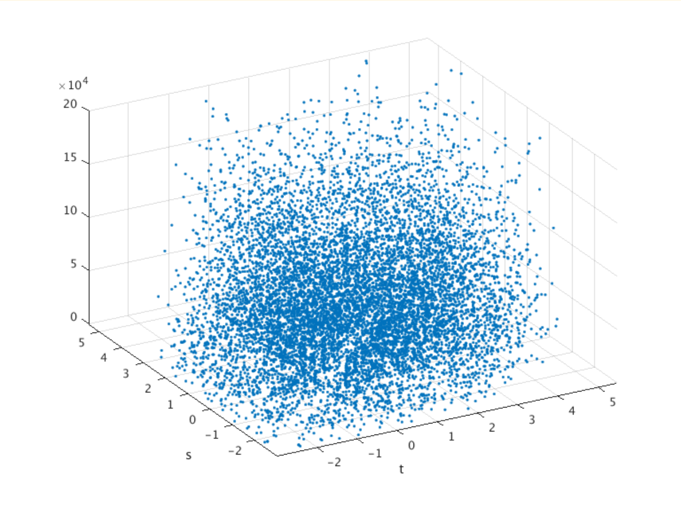
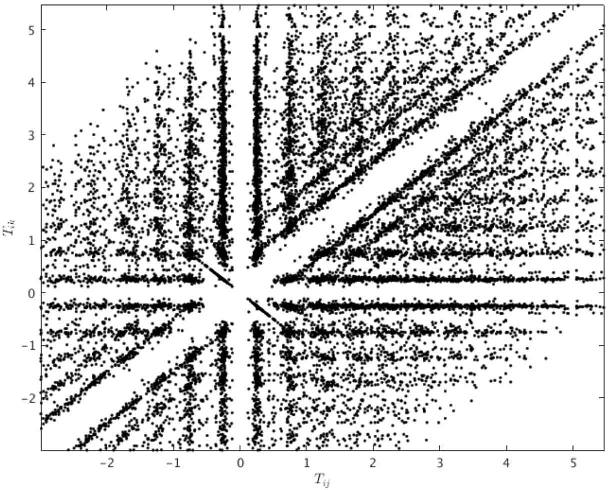
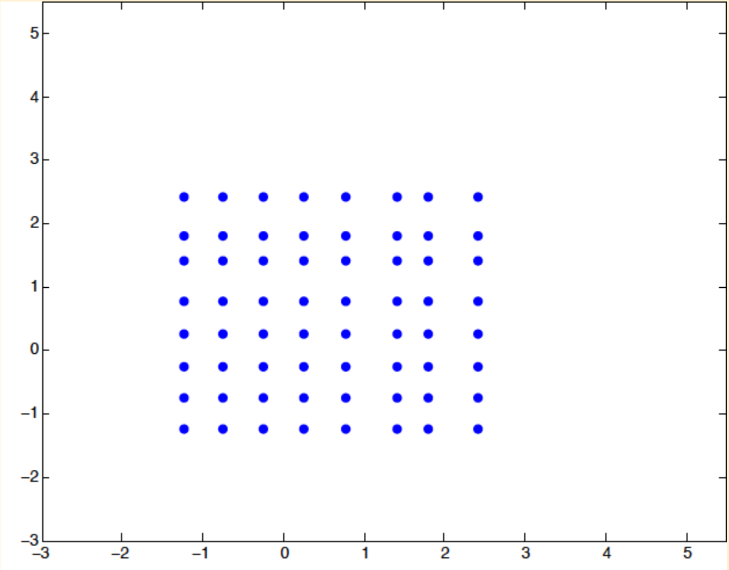


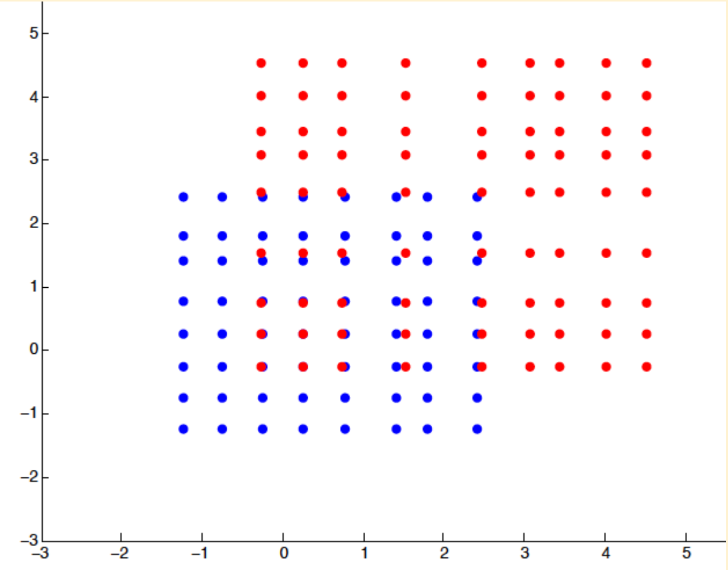
Design Plot for Covariance: $(t_{ij}, t_{ik}),\ \forall\ i, j \neq k$



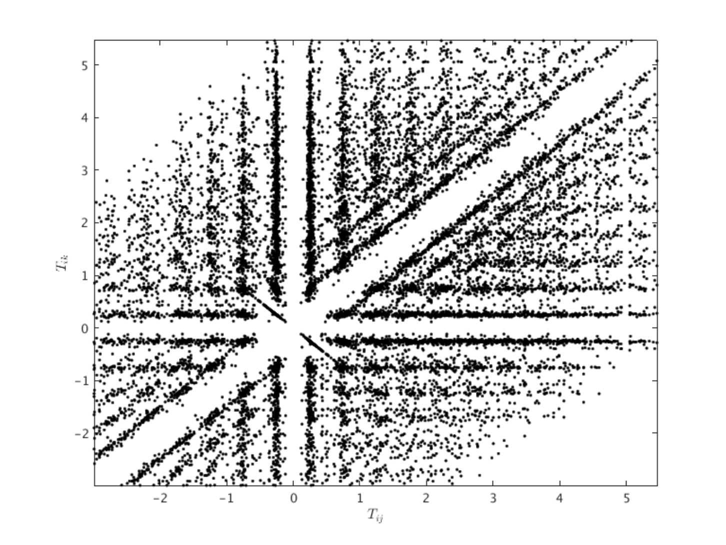
Design Plot for One Subject: $(t_{ij}, t_{ik}), \forall j, k$



Design Plot for Two Subjects: $(t_{ij}, t_{ik}), \forall j, k$



Design Plot for All Subjects: $(t_{ij}, t_{ik}),\ \forall\ i, j, k$



Estimated Covariance Surface of $X(t)$

Let $D_{ijl} = (Y_{ij} - \hat{\mu}(t_{ij}))(Y_{il} - \hat{\mu}(t_{il}))$, be the raw covariances.

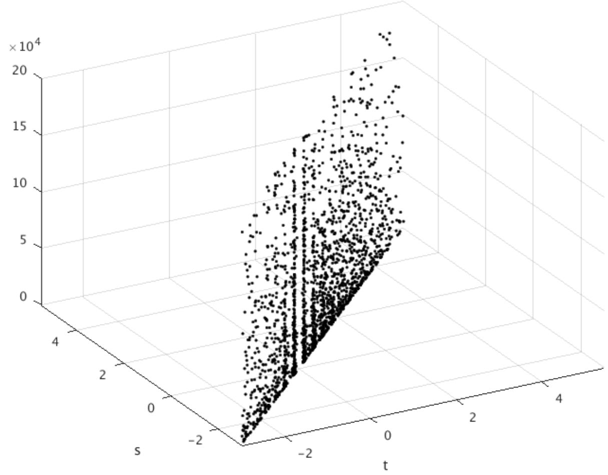
Employing a local linear smoother, the estimate for $\Sigma(s, t)$ is:

$\hat{\Sigma}(s, t) = \hat{\beta}_0$, where

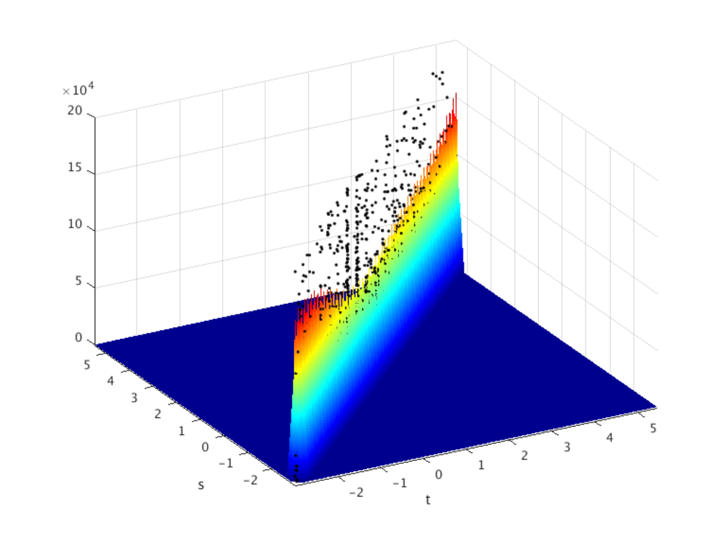
$$(\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2) = \underset{\beta_0, \beta_1, \beta_2}{\operatorname{argmin}} \sum_{i=1}^{n} \sum_{1 \le j \ne l \le n_i} \Big[D_{ijl} - \beta_0$$

$$- \beta_1(t_{ij} - s) - \beta_2(t_{il} - t) \Big]^2 K_{h_\Sigma}(t_{ij} - s) K_{h_\Sigma}(t_{il} - t).$$

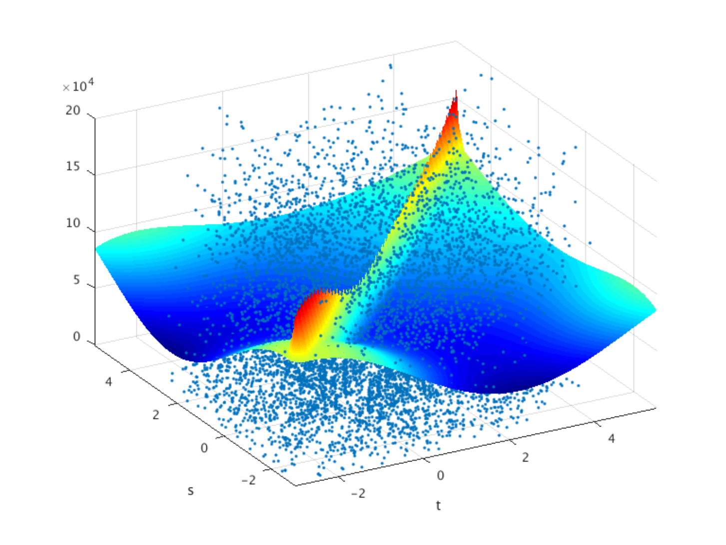
Raw Variance Plot: $[Y(t_{ij}) - \mu(t_{ij})]^2, \ \forall\ i, j$



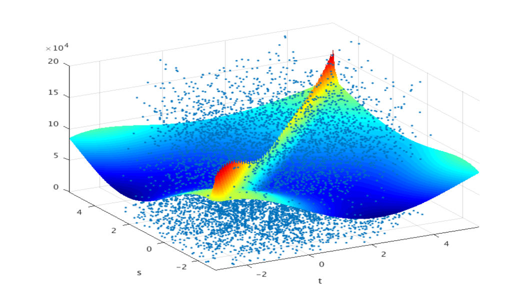
Estimated Variance function of $Y(t)$



Estimated Covariance & Variance of $Y(t)$



Estimates of $\sigma^2(t)$: Variance of Measurement Errors



$\sigma^2(t) = \mathsf{var}(Y(t)) - \mathsf{var}(X(t)).$

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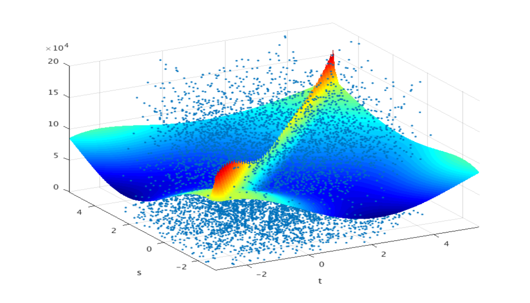

$\sigma^2(t) = \mathsf{var}(Y(t)) - \mathsf{var}(X(t))$.

When $\sigma^2(t) = \sigma^2$ for all t, one can estimate σ^2 by $\int_I \hat{\sigma}^2(t)dt$.

Due to boundary effects, PACE replaces I by a sub-interval.

PACE (Matlab) Package for FDA: http://www.stat.ucdavis.edu/PACE/

fdapace: R-package of PACE

- An R-package, **fdapace**, is now available in CRAN.

  - But it only contains a few core functions in PACE.

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- fdapace is still under construction - Feedback welcome!

End of Covariance Estimation

Outline

Theory: Mean and Covariance Estimation (Zhang and W., 2016)

- So far, we have used "**scatter plot smoothers**" to estimate the mean and covariance functions.

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- Another way to assign weights is to give equal weights, $\frac{1}{n}$, to all subjects as proposed in Li and Hsing (2010).

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- A referee requested that we develop a general theory using a general weight function, which covers both weighing schemes.
- As a result, an optimal weighing scheme based on convex combinations of the two weights was developed.

Estimation of Mean Function

- Equal weight per observation (Yao, Müller and W., 2005)

$$\hat{\mu}_{obs}(t) = \hat{\beta}_0 \text{ where}$$

$$(\hat{\beta}_0, \hat{\beta}_1) = \underset{\beta_0, \beta_1}{\operatorname{argmin}} \quad \sum_{i=1}^{n} \sum_{j=1}^{n_i} \left[Y_{ij} - \beta_0 - \beta_1 (T_{ij} - t) \right]^2 K_{h_\mu}(T_{ij} - t).$$

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- Equal weight per subject (Li and Hsing, 2010)

$$\hat{\mu}_{sub}(t) = \hat{\beta}_0 \text{ where}$$

$$(\hat{\beta}_0, \hat{\beta}_1) = \underset{\beta_0, \beta_1}{\operatorname{argmin}} \quad \sum_{i=1}^{n} \mathbf{\frac{1}{n_i}} \sum_{j=1}^{n_i} \left[Y_{ij} - \beta_0 - \beta_1 (T_{ij} - t) \right]^2 K_{h_\mu}(T_{ij} - t).$$

Estimation of Mean Function

- A general weighing scheme (Zhang and W,, 2016),

  \- weight $\mathbf{w_i}$ for subject i, where $\sum_{i=1}^{n} n_i w_i = 1$.

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- The OBS scheme uses $w_i = \frac{1}{\sum_{i=1}^{n} n_i} \Rightarrow$ the same for all subjects.

  The SUBJ scheme uses $w_i = \frac{1}{n n_i}$.

Important notation

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- SUB: harmonic mean of n_i,

$$\bar{N}_H = \frac{n}{\sum_{i=1}^{n} \frac{1}{n_i}}, \quad \frac{\bar{N}_{S2}}{(\bar{N})^2} \to 1.$$

Asymptotic Normality

- OBS:

$$[\Gamma_{obs}(t)]^{-1/2}\{\hat{\mu}_{obs}(t) - \mu(t) - \underbrace{\frac{1}{2}h_\mu^2\sigma_K^2\mu^{(2)}(t)}_{\text{asymptotic bias}}\} \xrightarrow{d} \mathcal{N}(0,1), \quad \text{where}$$

$$\underbrace{\Gamma_{obs}(t)}_{\text{asymptotic variance}} = \|K\|^2\frac{\Sigma(t,t)+\sigma^2}{n\bar{N}h_\mu f(t)} + \frac{(\bar{N}_{S2}-\bar{N})}{n(\bar{N})^2}\Sigma(t,t).$$

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$$[\Gamma_{sub}(t)]^{-1/2}\{\hat{\mu}_{sub}(t) - \mu(t) - \underbrace{\frac{1}{2}h_\mu^2\sigma_K^2\mu^{(2)}(t)}_{\text{asymptotic bias}}\} \xrightarrow{d} \mathcal{N}(0,1), \quad \text{where}$$

$$\underbrace{\Gamma_{sub}(t)}_{\text{asymptotic variance}} = \|K\|^2\frac{\Sigma(t,t)+\sigma^2}{n\bar{N}_H h_\mu f(t)} + \frac{1}{n}\left(1-\frac{1}{\bar{N}_H}\right)\Sigma(t,t)$$

Rates of Convergence

1. Non-dense: Slower than $\sqrt{n}$-rate.

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   Sparse data $=$ finite n_i, is a special case.

2. Dense:$\sqrt{n}$-rate, with asymptotic bias
   (between non- and parametric paradigm)

3. Ultra-dense: $\sqrt{n}$-rate, no asymptotic bias
   (Parametric paradigm)

Partition of Functional Data: OBS

Assume $\limsup_n (\bar{N}_{S2})/(\bar{N})^2 < \infty$.

1. **Non-Dense data**: When $\bar{N}/n^{1/4} \to 0$ and $h_\mu \asymp (n\bar{N})^{-1/5}$,

$$\sqrt{n\bar{N}h_\mu}\,\left[\hat{\mu}_{obs}(t) - \mu(t) - \frac{1}{2}h_\mu^2\sigma_K^2\mu^{(2)}(t)\right] \xrightarrow{d} \mathcal{N}\left(0, \|K\|^2\frac{\Sigma(t,t)+\sigma^2}{f(t)}\right).$$

2. **Dense data**: When $\bar{N}/n^{1/4} \to C$ and $h_\mu/n^{-1/4} \to C_1$ where $0 < C, C_1 < \infty$,

$$\sqrt{n\frac{(\bar{N})^2}{\bar{N}_{S2}}}\,\left[\hat{\mu}_{obs}(t) - \mu(t) - \frac{1}{2}h_\mu^2\sigma_K^2\mu^{(2)}(t)\right] \xrightarrow{d} \mathcal{N}\left(0, \|K\|^2\frac{\Sigma(t,t)+\sigma^2}{f(t)\cdot C_1} + \Sigma(t,t)\right).$$

3. **Ultra-Dense data**: When $\bar{N}/n^{1/4} \to \infty$, $h_\mu = o(n^{-1/4})$, and $h_\mu\bar{N} \to \infty$,

$$\sqrt{n\frac{(\bar{N})^2}{\bar{N}_{S2}}}\,\left[\hat{\mu}_{obs}(t) - \mu(t)\right] \xrightarrow{d} \mathcal{N}\left(0, \Sigma(t,t)\right).$$

Partition of Functional Data: SUB

1. **Non-Dense data**: When $\bar{N}_H/n^{1/4} \to 0$ and $h_\mu \asymp (n\bar{N}_H)^{-1/5}$,

$$\sqrt{n\bar{N}_H h_\mu}\,\left[\hat{\mu}_{sub}(t) - \mu(t) - \frac{1}{2}h_\mu^2\sigma_K^2\mu^{(2)}(t)\right] \xrightarrow{d} \mathcal{N}\left(0, \|K\|^2\frac{\Sigma(t,t)+\sigma^2}{f(t)}\right).$$

2. **Dense data**: When $\bar{N}_H/n^{1/4} \to C$ and $h_\mu/n^{-1/4} \to C_1$ where $0 < C, C_1 < \infty$,

$$\sqrt{n}\,\left[\hat{\mu}_{sub}(t) - \mu(t) - \frac{1}{2}h_\mu^2\sigma_K^2\mu^{(2)}(t)\right] \xrightarrow{d} N\left(0, \|K\|^2\frac{\Sigma(t,t)+\sigma^2}{f(t)C\cdot C_1} + \Sigma(t,t)\right).$$

3. **Ultra-Dense data**: When $\bar{N}_H/n^{1/4} \to \infty$, $h_\mu = o(n^{-1/4})$, and $h_\mu\bar{N}_H \to \infty$,

$$\sqrt{n}\,\left[\hat{\mu}_{sub}(t) - \mu(t)\right] \xrightarrow{d} \mathcal{N}\left(0, \Sigma(t,t)\right).$$

- This shows $\hat{\mu}_{sub}(t)$ is asymptotically equivalent to the sample mean when the true curves $X_i(t)$ can be observed without any measurement errors.

Comparison of Two Schemes

1. **Asymptotic bias**: both $= \frac{1}{2}h_\mu^2\sigma_K^2\mu^{(2)}(t)$.

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1. **Asymptotic bias**: both $= \frac{1}{2}h_\mu^2\sigma_K^2\mu^{(2)}(t)$.
2. **Asymptotic variance**:
   - **Non-dense data**: var$(\hat{\mu}_{obs}) \leq$ var$(\hat{\mu}_{sub})$, so OBS is more efficient.
   - **Ultra-dense data**: var$(\hat{\mu}_{obs}) \geq$ var$(\hat{\mu}_{sub})$, so SUB is more efficient.

L^2 Convergence

- Equal weight per observation:

$$\|\hat{\mu}_{obs} - \mu\|_2 = O_p\left(h_\mu^2 + \sqrt{\left(\frac{\bar{N}_{S2}}{(\bar{N})^2} + \frac{1}{\bar{N}h_\mu}\right)\frac{1}{n}}\right).$$

- Equal weight per subject:

$$\|\hat{\mu}_{sub} - \mu\|_2 = O_p\left(h_\mu^2 + \sqrt{\left(1 + \frac{1}{\bar{N}_H h_\mu}\right)\frac{1}{n}}\right)$$

Uniform Convergence

- Equal weight per observation:

$$\sup_{t\in[0,1]} \left|\hat{\mu}_{obs}(t) - \mu(t)\right| = O\left(h_\mu^2 + \sqrt{\left(\frac{\bar{N}_{S2}}{(\bar{N})^2} + \frac{1}{\bar{N}h_\mu}\right)\frac{\log(n)}{n}}\right) \quad a.s.$$

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Optimal Weighing Scheme

- Optimal weights for a convex combination of the two estimators exists.

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- Optimal weights:

$$\alpha^* = \frac{c_{n2}}{c_{n1} + c_{n2}},$$

where c_{n1} and c_{n2} are respectively the asymptotic variance of $\hat{\mu}_{obj}$ and $\hat{\mu}_{sub}$.

Optimal Weighing Scheme

- Let $\hat{\mu}_{\alpha^*}$ be the estimate with the optimal weights, $w_i = \alpha^* \frac{1}{n\bar{N}} + (1-\alpha^*)\frac{1}{nN_i}$.

  $$\Rightarrow \|\hat{\mu}_{\alpha^*} - \mu\|_2 = O_p\left(h_\mu^2 + \sqrt{\frac{c_{n1}c_{n2}}{c_{n1}+c_{n2}}}\right).$$

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- Since $\frac{c_{n1}c_{n2}}{c_{n1}+c_{n2}} \le \min\{c_{n1}, c_{n2}\}$, the rate for $\hat{\mu}_{\alpha^*}$ is always at least as good as those for $\hat{\mu}_{obj}$ and $\hat{\mu}_{sub}$.

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- Simulation results in Zhang and W. (2016) show superior performance of $\hat{\mu}_{\alpha^*}$.

End of Theory for Mean Function

Covariance Estimate with General Weights

- Let $D_{ijl} = (Y_{ij} - \hat{\mu}(T_{ij}))(Y_{il} - \hat{\mu}(T_{il}))$ be the raw covariance based on a mean estimate $\hat{\mu}$.

- Let $\mathbf{v_i}$ be the weight attached to each observation for the ith subject with $\sum_{i=1}^{n} n_i(n_i - 1)\mathbf{v_i} = 1$.

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- Let $\mathbf{v_i}$ be the weight attached to each observation for the ith subject with $\sum_{i=1}^{n} n_i(n_i - 1)\mathbf{v_i} = 1$.

- A general covariance estimator based on the weights $\mathbf{v_i}$ is: $\hat{\Sigma}(s,t) = \hat{\beta}_0$, where

$$(\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2) = \underset{\beta_0,\beta_1,\beta_2}{\operatorname{argmin}} \sum_{i=1}^{n} \mathbf{v_i} \sum_{1 \le j \ne l \le n_i} \Big[D_{ijl} - \beta_0 - \beta_1(T_{ij} - s) - \beta_2(T_{il} - t) \Big]^2 K_{h_\Sigma}(T_{ij} - s) K_{h_\Sigma}(T_{il} - t)$$

Covariance Estimators: Two Special Cases

1. $D_{ijl} = (Y_{ij} - \hat{\mu}_{obs}(T_{ij}))(Y_{il} - \hat{\mu}_{obs}(T_{il}))$ and $\mathbf{v_i} = \frac{1}{\sum_{i=1}^{n} n_i(n_i-1)}$ $\Longrightarrow$ OBS scheme.

2. $D_{ijl} = (Y_{ij} - \hat{\mu}_{sub}(T_{ij}))(Y_{il} - \hat{\mu}_{sub}(T_{il}))$ and $v_i = 1/(n_i(n_i-1))$ $\Longrightarrow$ SUB scheme.

Asymptotic Normality

Let

$$
\begin{aligned}
V_1(s,t) &= \mathrm{Var}[(Y_1-\mu(T_1))(Y_2-\mu(T_2)) \mid T_1=s, T_2=t]; \\
V_2(s,t) &= \mathrm{Cov}\left([Y_1-\mu(T_1)][Y_2-\mu(T_2)], [Y_1-\mu(T_1)][Y_3-\mu(T_3)] \mid T_1=s, T_2=t, T_3 \right. \\
V_3(s,t) &= \mathrm{Cov}\left([Y_1-\mu(T_1)][Y_2-\mu(T_2)], [Y_3-\mu(T_3)][Y_4-\mu(T_4)] \mid T_1=s, T_2=t, T_3 \right.
\end{aligned}
$$

$$
\Gamma_\gamma^{-1/2}\left[\hat{\gamma}(s,t)-\gamma(s,t)-\frac{1}{2}h_\gamma^2\sigma_K^2\left(\frac{\partial^2\gamma}{\partial s^2}(s,t)+\frac{\partial^2\gamma}{\partial t^2}(s,t)\right)+o_p(h_\gamma^2)\right] \xrightarrow{d} \mathcal{N}(0,1),
$$

where

$$
\begin{aligned}
\Gamma_\gamma = [1+\mathbf{I}(\mathbf{s}=\mathbf{t})]\Bigg[&\frac{\sum_{i=1}^n n_i(n_i-1)v_i^2}{h_\gamma^2}\|K\|^4\frac{V_1(s,t)}{f(s)f(t)}+\frac{\sum_{i=1}^n n_i(n_i-1)(n_i-2)v_i^2}{h_\gamma} \\
&\times\frac{f(s)V_2(t,s)+f(t)V_2(s,t)}{f(s)f(t)}\Bigg]+\left[\sum_{i=1}^n n_i(n_i-1)(n_i-2)(n_i-3)v_i^2\right]V_3(s,t),
\end{aligned}
$$

and $\mathbf{I}(\cdot)$ is the indicator function.

Summary for Covariance Estimation

Unified asymptotic normality for general weight functions:

1. Three partitions: non-dense, dense, and ultra-dense.

2. Two special weighing schemes:
   $\hat{\Sigma}_{obs}$ more efficient for non-dense data;
   $\hat{\Sigma}_{sub}$ more efficient for ultra-dense data.

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3. Discontinuity of the asymptotic variance of the covariance estimates:

   Asymptotic variance expressions are different between $s = t$ and $s \neq t$.

Discontinuity of the Asymptotic Variance

Technical Explanation:

$E[K_h(T-t)K_h(T-s)] = 0$, for $s \neq t$ when $h \to 0$ for K on an interval;

$E[K_h(T-t)K_h(T-s)] = \|K\|^2 f(t)/h + o(1/h)$, for $s = t$.

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- **Intuitive explanation?**

End of Asymptotic Theory

References for Mean and Covariance Estimation

- Yao Mueller and W. (2005, JASA)
- Li and Hsing (2010, AoS)
- Zhang and W. (2016, Ann. Stat.)
- **Additional References:**

  Stainiswalis and Lee (1998, JASA),
  Yao (2005, J. Mult. Analy.),

End of Part I