

Bayesian Optimal Change Point Detection in High Dimension

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Problem Setting

- ▶ Suppose we observe a sequence of random vectors X_1, \dots, X_n independently from p -dimensional Gaussian distributions:

$$X_i \stackrel{\text{ind.}}{\sim} N_p(\mu_i, \Sigma_i), \quad i = 1, \dots, n.$$

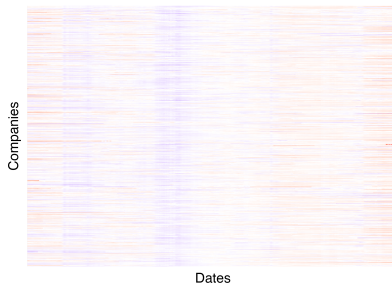
- ▶ We consider the high-dimensional setting:
 - ▶ The number of variables p grows to infinity with the sample size n .
 - ▶ p can be significantly larger than n .
- ▶ Assume changes occur in the mean vector or covariance matrix, with unknown number and locations.

Background

Comparative Genomic Hybridization Microarray



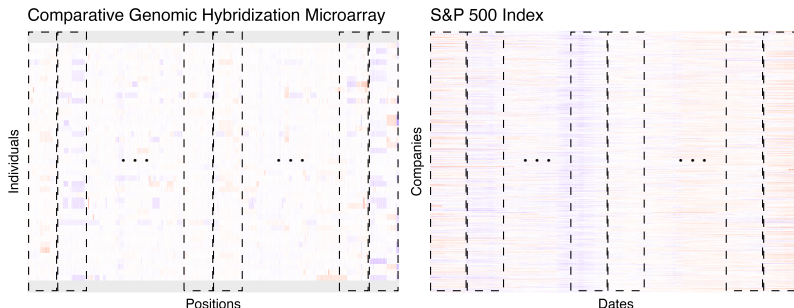
S&P 500 Index



Approach:

- Define a sliding window of size n_w and perform two-sample tests within it to detect changes.

Background



Challenges:

- ▶ How can we efficiently compute the Bayes factor for high-dimensional data?
- ▶ How can we determine the optimal window size?

mxPBF for Two-Sample Mean Test

- ▶ For two-sample tests, we will use mxPBF, introduced by Lee et al. (2023), which is designed for high-dimensional data.
- ▶ Let the hypothesis of interest be:

$$H_0^\mu : \mu_i = \mu_{i+1} \quad \text{for all } 1 \leq i \leq n-1 \quad \text{vs} \quad H_1^\mu : \text{not } H_0^\mu.$$

- ▶ For $n_w + 1 \leq l \leq n - n_w + 1$, consider the model:

$$X_{l-n_w}, \dots, X_{l-1} \mid \mu_{l-1}, \Sigma \stackrel{\text{i.i.d.}}{\sim} N_p(\mu_{l-1}, \Sigma),$$

$$X_l, \dots, X_{l+n_w-1} \mid \mu_l, \Sigma \stackrel{\text{i.i.d.}}{\sim} N_p(\mu_l, \Sigma),$$

- ▶ We can sequentially perform the following hypothesis:

$$H_0^{\mu,l} : \mu_{l-1} = \mu_l \quad \text{vs} \quad H_1^{\mu,l} : \mu_{l-1} \neq \mu_l.$$

mxPBF for Two-Sample Mean Test

- ▶ For a given integer $1 \leq j \leq p$, we can marginalize the model as:

$$\begin{aligned} X_{l-n_w,j}, \dots, X_{l-1,j} &| \mu_{l-1,j}, \sigma_{jj} \stackrel{\text{i.i.d.}}{\sim} N(\mu_{l-1,j}, \sigma_{jj}), \\ X_{l,j}, \dots, X_{l+n_w-1,j} &| \mu_{l,j}, \sigma_{jj} \stackrel{\text{i.i.d.}}{\sim} N(\mu_{l,j}, \sigma_{jj}). \end{aligned}$$

- ▶ Then, the marginalized hypothesis becomes:

$$H_{0,j}^{\mu,l} : \mu_{l-1,j} = \mu_{l,j} \quad \text{vs} \quad H_{1,j}^{\mu,l} : \mu_{l-1,j} \neq \mu_{l,j}.$$

- ▶ This approach avoids inverse calculation and allows obtaining the Bayes factor for $p \geq n - 2$, though ignores the data's dependence structure.

Priors

- ▶ Let $\bar{\mathbf{X}}_{a:b,j} = (b - a + 1)^{-1} \sum_{i=a}^b \mathbf{X}_{ij}$ and $\gamma_{n_w} = (n_w \vee p)^{-\alpha}$.
- ▶ Priors under $H_{0,j}^{\mu,l}$:
 - ▶ $\mu_j \mid \sigma_{jj} \sim N\left(\bar{\mathbf{X}}_{(l-n_w):(l+n_w-1),j}, \frac{\sigma_{jj}}{2n_w\gamma_{n_w}}\right)$
 - ▶ $\pi(\sigma_{jj}) \propto \sigma_{jj}^{-1}$
- ▶ Priors under $H_{1,j}^{\mu,l}$:
 - ▶ $\mu_{l-1,j} \mid \sigma_{jj} \sim N\left(\bar{\mathbf{X}}_{(l-n_w):(l-1),j}, \frac{\sigma_{jj}}{n_w\gamma_{n_w}}\right)$
 - ▶ $\mu_{l,j} \mid \sigma_{jj} \sim N\left(\bar{\mathbf{X}}_{l:(l+n_w-1),j}, \frac{\sigma_{jj}}{n_w\gamma_{n_w}}\right)$
 - ▶ $\pi(\sigma_{jj}) \propto \sigma_{jj}^{-1}$

The Maximum Pairwise Bayes Factor

- ▶ We can get the resulting log pairwise Bayes factor as a closed form:

$$\log B_{10}^{\mu}(\mathbf{X}_{(l-n_w):(l+n_w-1),j}) := \log \frac{p(\mathbf{X}_{(l-n_w):(l+n_w-1),j} \mid H_{1,j}^{\mu,l})}{p(\mathbf{X}_{(l-n_w):(l+n_w-1),j} \mid H_{0,j}^{\mu,l})}$$

- ▶ Then, the mxPBF is:

$$B_{max,10}^{\mu,n_w}(X_n) := \max_{n_w+1 \leq l \leq n-n_w+1} \max_{1 \leq j \leq p} B_{10}^{\mu}(X_{(l-n_w):(l+n_w-1),j})$$

- ▶ We can reject $H_0^{\mu} : \mu_i = \mu_{i+1}$ for all i , i.e., detect a change, if the mxPBF exceeds a prespecified threshold.

Choice of Hyperparameters

- ▶ The choice of the hyperparameter α is critical for performance.
- ▶ We adopt the hyperparameter selection method from Lee et al. (2023), which controls the empirical False Positive Rate (FPR).
 1. Given an observed data matrix X , calculate the sample mean $\hat{\mu}$ and sample covariance matrix $\hat{\Sigma}$.
 2. Generate N simulated datasets $\{X_{\text{sim}}^{(s)} \in \mathbb{R}^{n \times p}\}_{s=1}^N$ using $\hat{\mu}$ and $\hat{\Sigma}$.
 3. For each s , calculate the mxPBF $B_{\text{max},10,\alpha}(X_{\text{sim}}^{(s)})$.
 4. Calculate the empirical FPR as

$$\widehat{\text{FPR}}_{\alpha} = N^{-1} \sum_{s=1}^N I(B_{\text{max},10,\alpha}(X_{\text{sim}}^{(s)}) > C_{\text{th}}).$$

5. Choose $\hat{\alpha}$ that achieves a pre-specified FPR.

Theoretical Foundation

- ▶ Given a class of distributions for X_n , with K_0 denoting the number of change points and i_1, \dots, i_{K_0} representing their locations.
- ▶ We define the localization rate for change point detection as ϵ , if:

$$\mathbb{P}_0 \left(\hat{K} = K_0, \max_{1 \leq k \leq K_0} \frac{|i_k - \hat{i}_k|}{n} \leq \epsilon \right) \rightarrow 1.$$

- ▶ Consistency of the Bayes factor implies that:
 1. $B_{10}(X_n) \xrightarrow{P} 0$ under H_0
 2. $\{B_{10}(X_n)\}^{-1} \xrightarrow{P} 0$ under H_1
- ▶ It has been demonstrated that mxPBF is consistent and achieves nearly minimax-optimal localization rate.

Multiscale Approach

- ▶ Choosing the optimal window size is case-specific and difficult when data knowledge is limited.
- ▶ To address this issue and enhance stability across scenarios, we propose a multiscale approach inspired by Avanesov and Buzun (2018).
- ▶ The approach simultaneously considers a set of window sizes $\mathcal{N} = \{n_w^{(r)} : r = 1, \dots, |\mathcal{N}|\}$ and makes a decision based on a majority rule.
- ▶ Under mild conditions, the approach inherits the theoretical properties of a single window.
- ▶ It has been shown that the proposed multiscale method outperforms existing state-of-the-art methods across various scenarios.

Combined method

- ▶ In practice, it is often uncertain whether changes occur in the mean, covariance, or both.
- ▶ In such cases, we sequentially apply both of the proposed change point detection methods.
 1. Given a data matrix X and a window size n_w , apply a sliding window approach to center the observations.
 2. Apply the change point detection method to covariance matrices.
 - 2-1. If one or more change points are detected, partition the data based on the estimated change points.
 3. Apply the proposed change point detection method for mean vectors to the uncentered data or each segment.
 4. Combine the change points detected in both mean and covariance structures.

Comparative Genomic Hybridization Microarray Data

- ▶ Log intensity ratio of fluorescence levels in DNA fragments.
- ▶ 2215×43 matrix.

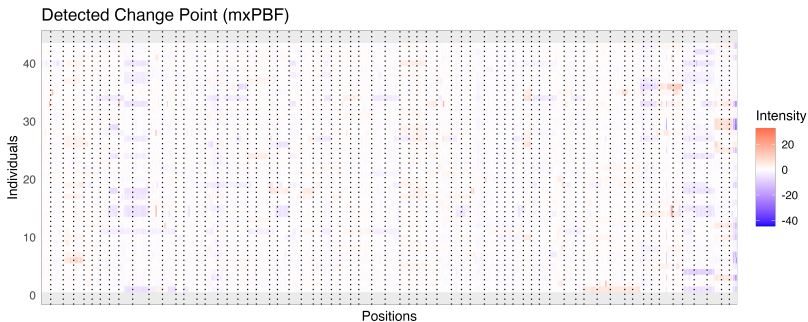


Figure: Log-intensity ratio measurements from microarray data of 43 individuals, with vertical dotted lines marking the identified change points.

S&P 500 Index Data

- ▶ Daily log returns of the closing stock prices from January 2015 to December 2016.
- ▶ 380×479 matrix.

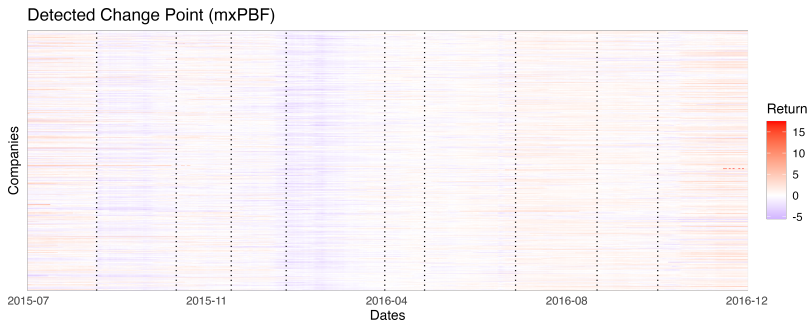


Figure: Log returns of 479 companies within the S&P 500 are displayed, with vertical dotted lines indicating the identified change points.

Simulation Study

- ▶ We compare our methods with those from:
 - ▶ Dette (Dette et al., 2022)
 - ▶ Geomcp (Grundy et al., 2020)
 - ▶ Inspect (Wang and Samworth, 2018)
 - ▶ Edivisive (Matteson and James, 2014)
- ▶ Settings for mxPBF:
 - ▶ Set of window sizes $\mathcal{N} = \{25, 60, 100\}$
 - ▶ Number of generated samples $N = 300$
 - ▶ Prespecified FPR = 0.05
 - ▶ Threshold $C_{\text{th}} = 10$
- ▶ 50 replications for each scenario.
- ▶ Evaluation metrics: F1 score and Hausdorff distance.

Performance When Data Including CPs in Mean

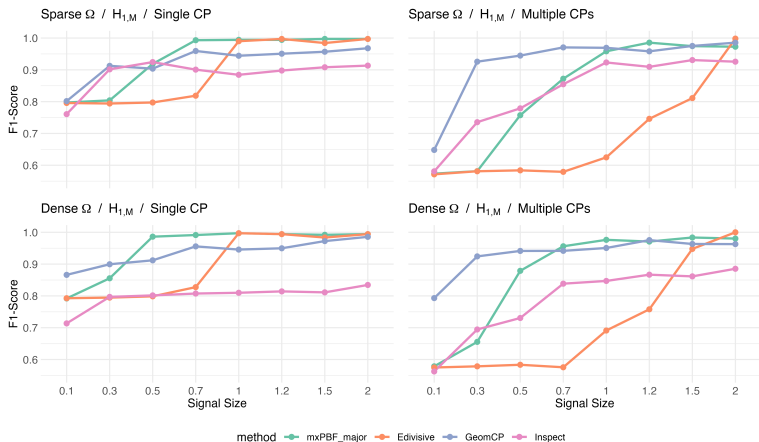


Figure: F1 scores based on 50 simulated datasets under $H_{1,M}$ with $p = 200$.

Performance When Data Including CPs in Covariance

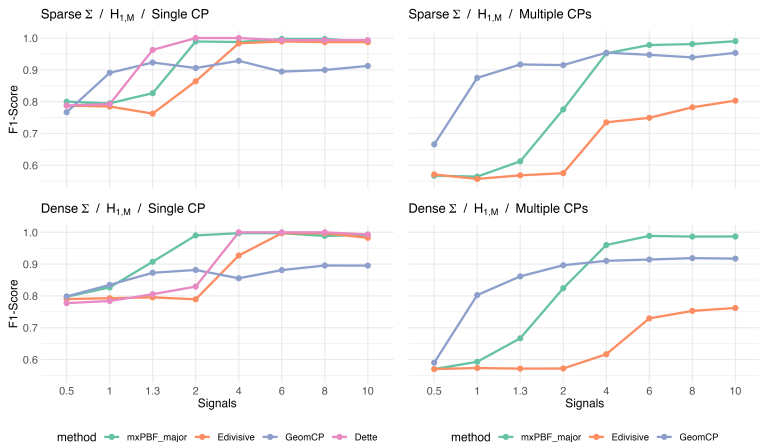


Figure: F1 scores based on 50 simulated datasets under $H_{1,M}$ with $p = 200$.

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CPD in Covariance Structure

- ▶ The method in the covariance structure is quite similar.
- ▶ Assume that the data has a zero mean:

$$X_i \stackrel{\text{ind.}}{\sim} N_p(0, \Sigma_i), \quad i = 1, \dots, n.$$

- ▶ We consider the following hypothesis test:

$$H_0^\Sigma : \Sigma_i = \Sigma_{i+1} \quad \text{for all } 1 \leq i \leq n-1 \quad \text{vs} \quad H_1^\Sigma : \text{not } H_0^\Sigma.$$

- ▶ Given n_w and l , this hypothesis becomes:

$$H_0^{\Sigma, l} : \Sigma_{l-1} = \Sigma_l \quad \text{vs} \quad H_1^{\Sigma, l} : \Sigma_{l-1} \neq \Sigma_l,$$

meaning that H_0^Σ holds if and only if $H_0^{\Sigma, l}$ is true for all l .

Testing the Existence of CP

- We apply the mxPBF idea (Lee et al., 2021) once again to construct the Bayes factor for hypothesis testing.
- For a given pair (i, j) with $1 \leq i \neq j \leq p$, the marginalized models are defined as follows:

$$X_{(l-n_w):(l-1),i} \mid X_{(l-n_w):(l-1),j} \stackrel{\text{i.i.d.}}{\sim} N_{n_w} (a_{l-1,ij} X_{(l-n_w):(l-1),j}, \tau_{l-1,ij} I_{n_w}),$$

$$X_{l:(l+n_w-1),i} \mid X_{l:(l+n_w-1),j} \stackrel{\text{i.i.d.}}{\sim} N_{n_w} (a_{l,ij} X_{l:(l+n_w-1),j}, \tau_{l,ij} I_{n_w}),$$

where $\Sigma_l = (\sigma_{l,ij})$, $a_{l,ij} = \sigma_{l,ij}/\sigma_{l,jj}$, and $\tau_{l,ij} = \sigma_{l,ii}(1 - \rho_{l,ij}^2)$.

- The resulting hypotheses are:

$$H_{0,ij}^{\Sigma,l} : a_{1,ij} = a_{2,ij} \text{ and } \tau_{1,ij} = \tau_{2,ij} \quad \text{vs} \quad H_{1,ij}^{\Sigma,l} : \text{not } H_{0,ij}^{\Sigma,l}.$$

Testing the Existence of CP

- The resulting log PBF is:

$$\begin{aligned} & \log B_{10}^{\Sigma} (X_{(l-n_w):(l+n_w-1),i}, X_{(l-n_w):(l+n_w-1),j}) \\ &= \frac{1}{2} \log \left(\frac{\gamma_{n_w}}{1 + \gamma_{n_w}} \right) + 2 \log \Gamma \left(\frac{n_w}{2} + a_0 \right) - \log \{ \Gamma(n_w + a_0) \Gamma(a_0) \} \\ &+ a_0 \log \left(\frac{b_{01,ij} b_{02,ij}}{b_{0,ij}} \right) - \left(\frac{n_w}{2} + a_0 \right) \log \left(b_{01,ij} + \frac{n_w}{2} \hat{\tau}_{1l-1,ij} \right) \\ &- \left(\frac{n_w}{2} + a_0 \right) \log \left(b_{02,ij} + \frac{n_w}{2} \hat{\tau}_{2l,ij} \right) + (n_w + a_0) \log (b_{0,ij} + n_w \hat{\tau}_{l,ij}), \end{aligned}$$

where Γ is the Gamma function and

$$\hat{\tau}_{ij} = \frac{X_{(l-n_w):(l+n_w-1),i}^T (I_{2n_w} - H_{X_{(l-n_w):(l+n_w-1),j}}) X_{(l-n_w):(l+n_w-1),i}}{2n_w}.$$

Testing the Existence of CP

- ▶ For each l , we define the mxPBF as:

$$B_{\max,10}^{\Sigma,l,n_w}(X_n) := \max_{1 \leq i \neq j \leq p} B_{10}^{\Sigma}(X_{(l-n_w):(l+n_w-1),i}, X_{(l-n_w):(l+n_w-1),j})$$

- ▶ The final mxPBF, used for testing the existence of change points, is:

$$B_{\max,10}^{\Sigma,n_w}(X_n) := \max_{n_w+1 \leq l \leq n-n_w+1} B_{10}^{\Sigma,l,n_w}(X_n)$$

- ▶ Given a threshold $C_{cp} > 0$, we reject H_0^{Σ} if

$$B_{\max,10}^{\Sigma,n_w}(X_n) > C_{cp}$$

- ▶ Once the existence of change points is confirmed, we can proceed to estimate their locations.

Consistency of mxPBF

- ▶ To support the proposed change point detection method, we establish the consistency of the mxPBF.
- ▶ Consistency of the mxPBF $B_{\max, 10}^{n_w}$ implies that:
 1. $B_{\max, 10}^{n_w}(X_n) \xrightarrow{P} 0$ under H_0
 2. $\{B_{\max, 10}^{n_w}(X_n)\}^{-1} \xrightarrow{P} 0$ under H_1
- ▶ We first assume the following condition for the window size n_w :

Condition (A1)

$n_w \leq n/2$ and $\epsilon_{n_w} := \log(n_w \vee p)/n_w = o(1)$ as $n \rightarrow \infty$.

Consistency in Mean Structure

Theorem 2.1

Suppose we observe $X_i \stackrel{\text{ind.}}{\sim} N_p(\mu_{0i}, \Sigma_0)$, $i = 1, \dots, n$, and consider the hypothesis above. Assume a window size n_w satisfies condition (A1). Let $C_{2,\text{low}} = 2 + \epsilon$ and $C_2 = 2 + 2\epsilon$ for some small constant $\epsilon > 0$.

(i) Suppose H_0^μ is true.

if $p(n - 2n_w + 1)(n_w \vee p)^{-C_{2,\text{low}}} = o(1)$ and

$$\alpha > 2[1 + 2\{C_2 \log(n_w \vee p)\}^{-1/2}]/(1 - 3\sqrt{C_2 \epsilon n_w}) := \alpha_{n_w, p},$$

then $B_{\max, 10}^{\mu, n_w}(X_n) = O_p\{(n_w \vee p)^{-c}\}$, for some $c > 0$.

(ii) Suppose H_1^μ is true. If there exist indices k and j such that

$$\{i_k - i_{k-1}\} \wedge \{i_{k+1} - i_k\} \geq n_w \text{ and}$$

$$\frac{(\mu_{0i_k, j} - \mu_{0i_{k+1}, j})^2}{\sigma_{0, jj}} \geq K \log(n_w \vee p)/n_w := \xi_{n_w, p}^2(\star), \text{ for some } K,$$

then $\{B_{\max, 10}^{\mu, n_w}(X_n)\}^{-1} = O_p\{(n_w \vee p)^{-c'}\}$, for some $c' > 0$.

Consistency in Mean Structure

- ▶ Enikeeva and Harchaoui (2019) proposed a test for change point detection in mean under sparse alternatives.
- ▶ Their test can detect a change point if:
 - (1) $\|\mu_{0i_1} - \mu_{0i_2}\|_2^2 \geq C\sqrt{p \log(p \log n)}/\{i_1(1 - i_1/n)\}$ in the *moderate sparsity regime*.
 - (2) $\|\mu_{0i_1} - \mu_{0i_2}\|_2^2 \geq C's_0 \log p/\{i_1(1 - i_1/n)\}$ in the *high sparsity regime*, for some positive constants C and C' .
- ▶ In contrast, our condition (\star) in Theorem 2.1 can be seen as:

$$\max_{1 \leq k \leq K_0} \|\mu_{0i_k} - \mu_{0i_k}\|_{\max}^2 \geq K^* \log(n_w \vee p)/n_w,$$

which is not directly comparable.

Localization Rate in Mean Structure

- ▶ Wang and Samworth (2018) proposed a change point estimation method for high-dimensional mean vectors based on a sparse projection.

- ▶ To obtain the localization rate for change point detection, they assumed:

$$\min_{1 \leq k \leq K_0} \|\mu_{0i_k} - \mu_{0i_{k+1}}\|_2^2 \geq C\sigma^2 \frac{s_0 \log(np)}{n\tau^2},$$

where $\tau \leq n^{-1} \min_{0 \leq k \leq K_0} (i_{k+1} - i_k)$.

- ▶ This assumption implies:

$$\min_{1 \leq k \leq K_0} \|\mu_{0i_k} - \mu_{0i_{k+1}}\|_{\max}^2 \geq C\sigma^2 \frac{\log(np)}{\delta_n \tau}.$$

- ▶ On the other hand, our condition (\star) in Theorem 2.1 implies:

$$\min_{1 \leq k \leq K_0} \|\mu_{0i_k} - \mu_{0i_{k+1}}\|_{\max}^2 \geq C_\star \sigma^2 \frac{\log(n_w \vee p)}{\delta_n},$$

for some constant $C_\star > 0$, which is a much weaker.

Consistency in Covariance Structure

- We now introduce the following conditions to guarantee consistency of the mxPBF in covariance structure.

Condition (A2)

$$\min_{i \neq j} \tau_{0,ij} \gg \{\log(n_w \vee p)\}^{-1}.$$

Condition (A3)

There exist an index k and a pair (i, j) with $i \neq j$ satisfying

$$\{\log(n_w \vee p)\}^{-1} \ll \tau_{0i_k,ij} \wedge \tau_{0i_{k+1},ij} \leq \tau_{0i_k,ij} \vee \tau_{0i_{k+1},ij} \ll (n_w \vee p),$$

$$\frac{\tau_{0i_k,ij}}{\tau_{0i_{k+1},ij}} \vee \frac{\tau_{0i_{k+1},ij}}{\tau_{0i_k,ij}} > \frac{1 + C_{bm}\sqrt{\epsilon_{n_w}}}{1 - 4\sqrt{C_1\epsilon_{n_w}}}$$

for the constant $C_1 > 1$ and some constant $C_{bm}^2 > 8(\alpha + 1)$.

Consistency in Covariance Structure

- ▶ Avanesov and Buzun (2018) proposed a testing procedure based on a bootstrap and multiscale approach for change point detection.
- ▶ They defined:
 - ▶ \mathcal{N} be a set of window sizes.
 - ▶ n_- be the minimum window size in \mathcal{N} .
 - ▶ d be the maximum number of nonzero entries in any column of the true precision matrix.
- ▶ To prove the consistency of the proposed test, they assumed
 - (1) $d|\mathcal{N}|^3\{\log(np)\}^{10} = o\left((s \wedge n_-^2)^{1/4}\right)$
 - (2) $d|\mathcal{N}|\{\log(np)\}^7 = o\left((s \vee n_-)^{1/2}\right)$, where $s \leq n$ is the number of subsamples used to construct bootstrap statistics.
 - (3) Sparsity and irrepresentability conditions of the precision matrix.
 which are stronger than those required for mxPBF.

Localization Rate in Covariance Structure

- ▶ Wang et al. (2021) proposed two procedures to detect change points in covariance structures for sub-Gaussian random vectors.
- ▶ Their second procedure, called WBSIP, assumes
 - ▶ $p \leq \delta_n / \{8(\log n)^{1+\xi}\}$ (roughly)
 - ▶ For any $\xi > 0$, there exists a constant $C > 0$ such that

$$\min_k \|\Sigma_{0i_k} - \Sigma_{0i_{k+1}}\|^2 \geq \frac{Cp(\log n)^{1+\xi}}{n_w}.$$

- ▶ On the other hand, condition (A3) is satisfied if

$$\min_k \|\Sigma_{0i_k} - \Sigma_{0i_{k+1}}\|_{\max}^2 \geq \frac{C' \log(n_w \vee p)}{n_w},$$

for some constant $C' > 0$.

- ▶ Their condition always implies ours in their settings, since

$$\|\Sigma_{0i_k} - \Sigma_{0i_{k+1}}\| \leq p \|\Sigma_{0i_k} - \Sigma_{0i_{k+1}}\|_{\max}.$$

