High-dimensional changepoint estimation with heterogeneous missingness

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Collaborators

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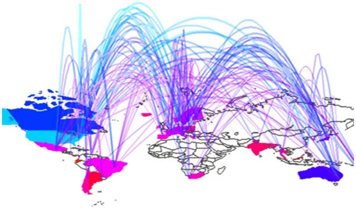
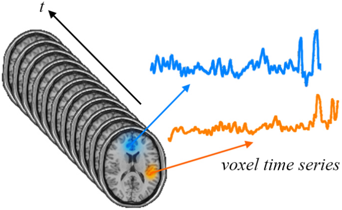
High-dimensional changepoint models

- The evolution of technology enables the collection of vast amounts of time-ordered data:
  - Healthcare devices
  - Covid case numbers
  - Network traffic data
  - Trading data of financial instruments





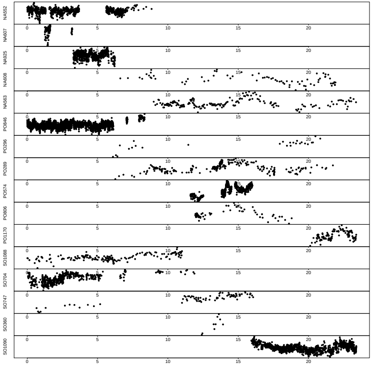
- Changes in the dynamics of the data streams are frequently of interest, leading to a renaissance of research on changepoint analysis.

Missingness in Big Data

- One of the ironies of Big Data is that missingness plays an even more prominent role.
- Consider running complete-case analysis with an $n \times d$ matrix, where each entry is missing independently with 1% probability.
  - When $d = 5$, around 95% of observations are retained.
  - When $d = 300$, only around 5% of observations are retained.
- In high-dimensional time series models, missingness can also arise due to asynchronous measurements.

High-dimensional change with missing data

- Our goal is to estimate the time of a high-dimensional, sparse change in mean, but where our data are corrupted by missingness.



$^{13}C/^{12}C$ in ocean cores 0–23 Ma

- Develop a robust methodology
- Quantify problem difficulty through interaction of signal and missingness

Problem setup

- Observed data $(X \circ \Omega, \Omega)$
  - Full data matrix $X = (X_{j,t}) \in \mathbb{R}^{p\times n}$
  - Revelation matrix $\Omega = (\omega_{j,t}) \in \{0,1\}^{p\times n}$: $\omega_{j,t} = 1$ if $X_{j,t}$ is observed and 0 otherwise.
- Data distribution:
  - Assume $X_t = (X_{1,t}, \ldots, X_{p,t})^\top \sim N_p(\mu_t, \sigma^2 I_p)$ independently with

$$\mu_1 = \cdots = \mu_z = \mu^{(1)} \quad \text{and} \quad \mu_{z+1} = \cdots = \mu_n = \mu^{(2)}.$$

  - Vector of change $\theta := \mu^{(2)} - \mu^{(1)}$ is sparse in the sense that $\|\theta\|_0 \le k \ll p$.
- Missingness mechanism:
  - $\omega_{j,t} \sim \mathrm{Bern}(q_j)$ independently, and independent of X.

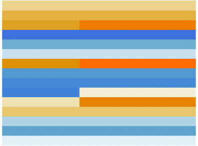
- **Goal**: estimate the changepoint location z.

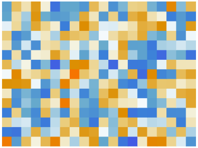
The `MissInspect` methodology

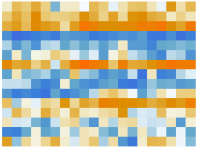
Motivation of methodology

- The `inspect` algorithm (W. and Samworth, 2018) works in the fully observed case:
  - Aggregate component series by finding a projection direction well-aligned with the vector of change.
  - Project data along this direction into a univariate series.
  - Estimate changepoint by the location of the maximum of the CUSUM transform of the projected series.

Recap of the `inspect` methodology







$$\boldsymbol{\mu} \quad + \quad W \quad = \quad X$$

For $a \in \mathbb{S}^{p-1}$,

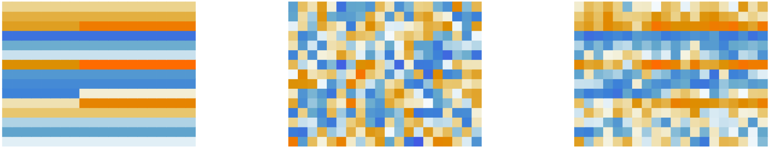
$$a^\top X_t \sim N(a^\top \boldsymbol{\mu}, \sigma^2).$$

Optimal projection direction is $\theta / \|\theta\|_2$.

Recap of the `inspect` methodology

Use CUSUM transformation $\mathcal{T} : \mathbb{R}^{p\times n} \to \mathbb{R}^{p\times(n-1)}$:

$$[\mathcal{T}(M)]_{j,t} := \sqrt{\frac{t(n-t)}{n}}\left(\frac{1}{n-t}\sum_{r=t+1}^{n} M_{j,r} - \frac{1}{t}\sum_{r=1}^{t} M_{j,r}\right).$$



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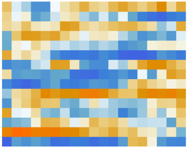

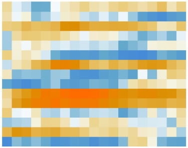

$$A \quad + \quad E \quad = \quad T$$

Define $A := \mathcal{T}(\boldsymbol{\mu})$, $E := \mathcal{T}(W)$ and $T := \mathcal{T}(X)$.

Recap of the `inspect` methodology

- For a single changepoint, $A = \theta\gamma^\top$ for some $\gamma \in \mathbb{R}^{n-1}$.
- Oracle projection direction $\theta/\|\theta\|_2$ is the leading left singular vector of A.
- We could therefore estimate v by

$$\hat{v}_{\max,k} \in \underset{u \in \mathbb{S}^{p-1}(k)}{\operatorname{argmax}} \|u^\top T\|_2.$$

However, computing $\hat{v}_{\max,k}$ is **NP-hard**.

Recap of the `inspect` methodology

- We obtain a computationally efficient projection direction via convex relaxation.

$$\max_{u \in \mathbb{S}^{p-1}(k)} \|u^\top T\|_2 = \max_{u \in \mathbb{S}^{p-1}(k), w \in \mathbb{S}^{n-2}} u^\top T w$$
$$= \max_{u \in \mathbb{S}^{p-1}, w \in \mathbb{S}^{n-2}, \|u\|_0 \le k} \langle uw^\top, T \rangle = \max_{M \in \mathcal{M}} \langle M, T \rangle,$$

where $\mathcal{M} := \{M : \|M\|_* = 1, \mathrm{rk}(M) = 1, \mathrm{nnzr}(M) \le k\}$.

- Therefore, a convex relaxation of the above optimisation problem is to compute

$$\hat{M} \in \operatorname*{argmax}_{M \in \mathcal{S}_1} \big\{ \langle M, T \rangle - \lambda \|M\|_1 \big\},$$

where $\mathcal{S}_1 := \{M \in \mathbb{R}^{p \times (n-1)} : \|M\|_* \le 1\}$.

- Estimate $\theta / \|\theta\|_2$ by the leading left singular vector of $\hat{M}$.

Motivation of methodology

- The `inspect` method (W. and Samworth, 2018) works in the fully observed case:
  - Aggregate component series by finding a projection direction well-aligned with the vector of change.
  - Project data along this direction into a univariate series.
  - Estimate changepoint by the location of the maximum of the CUSUM transform of the projected series.
- In the presence of missingness:
  - Projection of data with missingness does not make sense.
  - But the notion of CUSUM transformation can be extended to the missing data setting.
  - Project the CUSUM transformation instead.

- Writing

$$L_{j,t} := \sum_{r=1}^{t} \omega_{j,t}, \quad R_{j,n-t} := \sum_{j=n-t+1}^{n} \omega_{j,t}, \quad N_j := L_{j,n} + R_{j,n}.$$

- The MissCUSUM transformation $\mathcal{T}^{\text{Miss}} : \mathbb{R}^{p\times n} \times \{0,1\}^{p\times n} \to \mathbb{R}^{p\times(n-1)}$ is defined such that $T_\Omega := \mathcal{T}^{\text{Miss}}(X \circ \Omega, \Omega)$ satisfies

$$(T_\Omega)_{j,t} := \sqrt{\frac{L_{j,t}R_{j,n-t}}{N_j}}\left(\frac{1}{R_{j,n-t}} \sum_{r=t+1}^{n} (X\circ\Omega)_{j,r} - \frac{1}{L_{j,t}} \sum_{r=1}^{t} (X\circ\Omega)_{j,r}\right),$$

  when $\min\{L_{j,t}, R_{j,t}\} > 0$ and 0 otherwise.
- When the data are fully-observed, i.e. Ω is an all-one matrix, $\mathcal{T}^{\text{Miss}}$ reduces to the standard CUSUM transformation.

How to aggregate signal

- Given the MissCUSUM transformed matrix $T_\Omega = \mathcal{T}^{\mathrm{Miss}}(X \circ \Omega, \Omega)$, we want to find a good projection direction to aggregate signal across coordinates.
- T_Ω can be viewed as a perturbation of A_Ω, the MissCUSUM transformation of $\big(\mathbb{E}(X) \circ \Omega, \Omega\big)$.
- A_Ω can in turn be viewed as a perturbation of a rank one matrix with a leading left singular vector $\theta \circ \sqrt{\boldsymbol{q}}$, where $\sqrt{\boldsymbol{q}} := (\sqrt{q_1}, \ldots, \sqrt{q_p})^\top$.
- This suggests an 'oracle projection direction' of $\theta \circ \sqrt{\boldsymbol{q}} / \|\theta \circ \sqrt{\boldsymbol{q}}\|$.

Estimating the oracle projection direction

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- We can estimate $\theta \circ \sqrt{\boldsymbol{q}}/\|\theta \circ \sqrt{\boldsymbol{q}}\|$ by looking at 'sparse leading left singular vector' of T_Ω

$$\max_{(v,w)\in\mathbb{B}^p\times\mathbb{B}^{n-1}} \quad v^\top T_\Omega w \qquad \text{subject to} \quad \|v\|_0 \le k.$$

- Problem non-convex and requires knowledge of k.
- W. and Samworth (2018) adopts a semidefinite relaxation approach to convexify the problem. But this the fact that A_Ω is not rank one means the semi-definite relaxation is too coarse in this case.
- We instead relax it into a bi-convex problem

$$(\hat{v}, \hat{w}) \in \operatorname*{argmax}_{(v,w)\in\mathbb{B}^p\times\mathbb{B}^{n-1}} \left\{ v^\top T_\Omega w - \lambda \|v\|_1 \right\}$$

- Additional benefit: directly exploits the row sparsity pattern.

The `MissInspect` algorithm

Algorithm 1: Pseudocode of the `MissInspect` algorithm

Input: $X_\Omega = X \circ \Omega \in \mathbb{R}^{p\times n}$, $\Omega \in \{0,1\}^{p\times n}$, $\lambda > 0$

$T_\Omega \leftarrow \mathcal{T}^{\mathrm{Miss}}(X_\Omega, \Omega)$;

Find $(\hat{v}, \hat{w}) \in \mathrm{argmax}_{\tilde{v}\in\mathbb{B}^{p-1}, \tilde{w}\in\mathbb{B}^{n-2}} \big\{ \langle T_\Omega, \tilde{v}\tilde{w}^\top \rangle - \lambda \|\tilde{v}\|_1 \big\}$;

$\hat{z} \leftarrow \mathrm{median}\Big(\mathrm{argmax}_{t\in[n-1]} \big|(\hat{v}^\top T_\Omega)_t\big|\Big)$;

Output: $\hat{z}$

Algorithm 2: Pseudocode for an iterative procedure optimising (2)

Input: $T_\Omega \in \mathbb{R}^{p\times(n-1)}$, $\lambda \in \big(0, \|T_\Omega\|_{2\to\infty}\big)$

$\tilde{v} \leftarrow$ leading left singular vector of T_Ω;

repeat

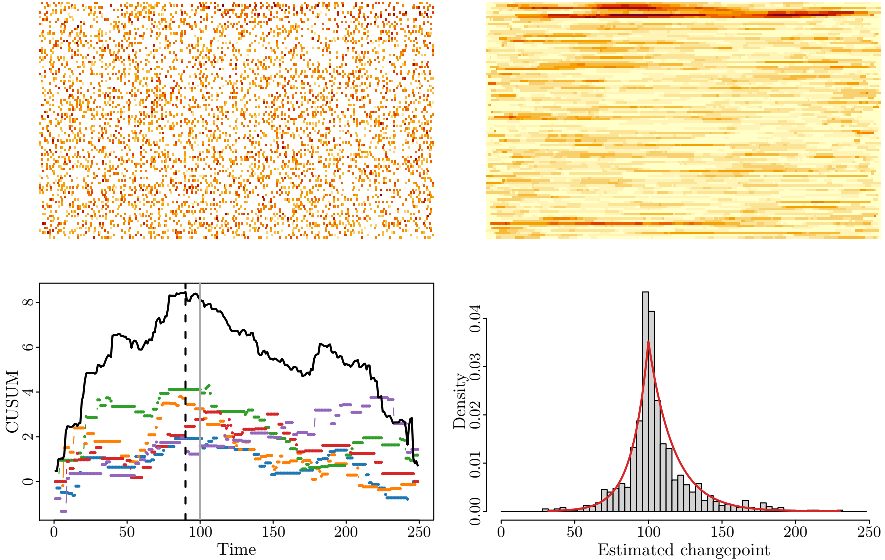
$\quad \tilde{w} \leftarrow \frac{T_\Omega^\top \tilde{v}}{\|T_\Omega^\top \tilde{v}\|_2}$;

$\quad \tilde{v} \leftarrow \frac{\mathrm{soft}(T_\Omega \tilde{w}, \lambda)}{\|\mathrm{soft}(T_\Omega \tilde{w}, \lambda)\|_2}$;

until *convergence*;

Output: $(\hat{v}, \hat{w}) = (\tilde{v}, \tilde{w})$

Illustration of the algorithm in action



Parameters: $p = 100$, $n = 250$, $z = 100$, $k = 10$, $\|\theta\|_2 = 2$, $q_j = 0.2\ \forall\, j$

Theoretical guarantees

Projection direction estimation

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- Let $\tau := n^{-1}\min\{z, n-z\}$. Define the 'observation rate-weighted signal ℓ_2 norm':

$$\|\theta\|_{2,\boldsymbol{q}} := \left(\sum_{j=1}^{p} \theta_j^2 q_j\right)^{1/2}$$

Proposition. Let $(\hat{v}, \hat{w})$ be the optimiser in Step 2 of Algorithm 1, applied with $\lambda = 2\sigma\sqrt{n\log(pn)}$. Then with probability at least $1 - 6/(kn)$, we have

$$\sin\angle(\hat{v}, \theta \circ \sqrt{\boldsymbol{q}}) \leq \frac{64\sigma}{\tau\|\theta\|_{2,\boldsymbol{q}}}\sqrt{\frac{k\log(pn)}{n}} + \frac{112\|\theta\|_2}{\tau\|\theta\|_{2,\boldsymbol{q}}}\sqrt{\frac{6\log(kn)}{n}}.$$

- First term represents estimation error caused by noise in data: $\|\theta\|_{2,\boldsymbol{q}}/\sigma$ is the signal-to-noise ratio
- Second term reflects error due to incomplete observation: $\|\theta\|_{2,\boldsymbol{q}}^2/\|\theta\|_2^2$ may be regarded as 'signal-weighted observation probability'.

Rate of location estimation

- With a good projection direction estimator, `MissInspect` algorithm produces good changepoint location estimator.
- We analyse a sample-splitting variant of Algorithm 1
  - Odd time points for projection direction estimation
  - Even time points for changepoint estimation after projection
- Two different rates of convergence of the location estimator depending on how much we are willing to assume on $\boldsymbol{q}$:
  - slow rate: algorithm works well even if some coordinates are almost completely missing.
  - fast rate: when at least a logarithmic number of observations are seen in each coordinate.

Slow and fast rates

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Theorem. Set tuning parameter $\lambda = 2\sigma\sqrt{n\log(pn)}$. There exists universal constants c, C such that if

$$\frac{1}{\tau}\sqrt{\frac{\log(pn)}{n}}\left(\frac{\sigma\sqrt{k}}{\|\theta\|_{2,\boldsymbol{q}}} + \frac{\|\theta\|_2}{\|\theta\|_{2,\boldsymbol{q}}}\right) \le c,$$

then with probability at least $1 - 22/n$, we have

$$\frac{|\hat{z} - z|}{n\tau} \le C\sqrt{\frac{\log(kn)}{n\tau}}\left(\frac{\sigma}{\|\theta\|_{2,\boldsymbol{q}}} + \frac{\|\theta\|_2}{\|\theta\|_{2,\boldsymbol{q}}}\right).$$

Slow and fast rates

Theorem. Set tuning parameter $\lambda = 2\sigma\sqrt{n\log(pn)}$. There exists universal constants c, C such that if

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Theorem. Under the same assumption as the above theorem, assume in addition that $n\tau^2 \min_j q_j \ge C_1 k \log(pn)$ for $C_1 > 0$, then with probability at least $1 - 23/n$, we have for some $C_2 > 0$ that

$$\frac{|\hat{z} - z|}{n\tau} \le \frac{C_2 \log(pn)}{n\tau}\left(\frac{\sigma^2}{\|\theta\|_{2,\boldsymbol{q}}^2} + \frac{\|\theta\|_\infty^2}{\|\theta\|_{2,\boldsymbol{q}}^2}\right).$$

Lower bound

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- Let $P_{n,p,z,\theta,\sigma,\boldsymbol{q}}$ denote our row-homogeneous missingness model, with changepoint at z.
- Let $\hat{\mathcal{Z}}$ be the set of all estimators of z.

Theorem. Let $M \geq 1$ satisfy $\|\theta\|_\infty \leq M \min_{j\in[p]:\theta_j\neq 0} |\theta_j|$. If $\max\{\sigma^2, \|\theta\|_\infty^2/(2M^2)\} \geq \|\theta\|_{2,\boldsymbol{q}}^2$, then there exists $c > 0$, depending only on M, such that for $n \geq 3$,

$$\inf_{\tilde{z}\in\hat{\mathcal{Z}}} \max_{z\in[n-1]} \mathbb{E}_{P_{n,p,z,\theta,\sigma,\boldsymbol{q}}} \frac{|\tilde{z}(X\circ\Omega,\Omega) - z|}{n} \geq \frac{c}{n} \min\left\{\frac{\sigma^2}{\|\theta\|_{2,\boldsymbol{q}}^2} + \frac{\|\theta\|_\infty^2}{\|\theta\|_{2,\boldsymbol{q}}^2}, n\right\}.$$

Numerical studies

Choice of the tuning parameter

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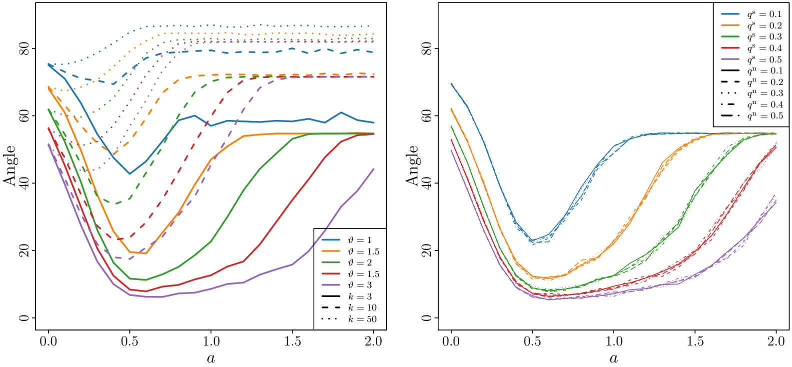
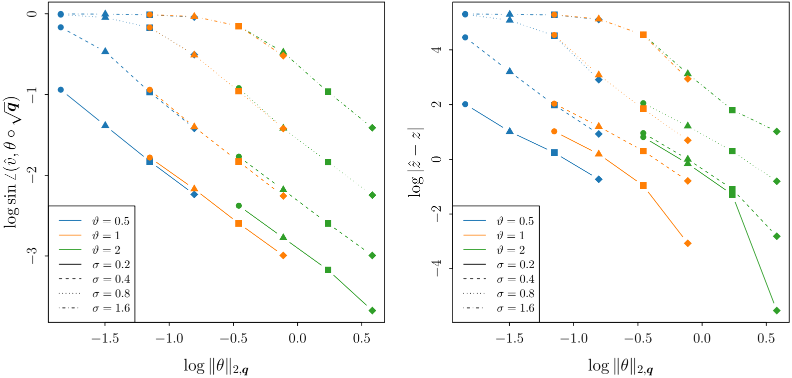
- The tuning parameter $\lambda = 2\sigma\sqrt{n\log(pn)}$ is convenient for theoretical analysis but often a bit conservative in practice.
- Examine the performance of the projection direction estimator for $\lambda = a\sigma\sqrt{n\log(pn)}$ by varying a.
- Best choice around $a = 1/2$.



Validation of theory

- We show via simulation that the quantity $\|\theta\|_{2,\boldsymbol{q}}$ indeed captures the appropriate interaction between signal and missingness in this problem.



Parameters: $n = 1200$, $p = 1000$, $z = 400$, $k = 3$, $\theta = \vartheta k^{-1/2}(\mathbf{1}_k^\top, \mathbf{0}_{p-k}^\top)^\top$, $\boldsymbol{q} = q\mathbf{1}_p$ with $q \in \{0.1, 0.2, 0.4, 0.8\}$ denoted by circles, triangles, squares and diamonds.

Comparison with competitors

- `ImputeInspect` algorithm
  - First impute missing data using the `softImpute` matrix completion algorithm (since the mean matrix of $X \circ \Omega$ is low-rank), then run the `inspect` procedure on the imputed data.
- `IteratedMeanImputation` algorithm
  - Iterate between imputing missing value using segment means and estimate of the changepoint using `inspect` on the imputed data.
- `GeneralisedLikelihoodRatio` algorithm
  - At each timepoint, compute the generalised likelihood ratio statistic for testing equality in mean for data on the left and right of that point. Estimate change by maximising the test statistics.

Comparison with competitors

ν	k	ϑ	$\angle(\hat{v}^{\mathrm{MI}}, \theta \circ \sqrt{\boldsymbol{q}})$	$\angle(\hat{v}^{\mathrm{II}}, \theta)$	$\lvert\hat{z}^{\mathrm{MI}} - z\rvert$	$\lvert\hat{z}^{\mathrm{II}} - z\rvert$	$\lvert\hat{z}^{\mathrm{IMI}} - z\rvert$	$\lvert\hat{z}^{\mathrm{GLR}} - z\rvert$
0.1	3	1	**71.4**	86.8	**141.7**	468.0	184.1	212.4
0.1	3	2	**40.6**	56.7	**36.5**	304.8	147.7	139.8
0.1	3	3	**26.1**	40.1	**14.5**	257.5	101.0	66.6
0.1	44	1	**82.6**	88.9	**185.9**	468.9	187.6	209.4
0.1	44	2	**63.5**	83.2	**66.9**	404.5	133.7	118.3
0.1	44	3	**49.0**	72.8	**18.7**	308.6	90.8	52.0
0.1	2000	1	**86.5**	88.2	**180.0**	485.0	184.1	219.6
0.1	2000	2	**76.9**	87.6	**121.2**	457.3	138.9	137.5
0.1	2000	3	**67.7**	82.9	50.4	376.9	79.2	**41.0**
0.5	3	1	**32.3**	81.0	**11.9**	358.4	150.8	176.0
0.5	3	2	**13.6**	42.1	**1.6**	7.2	44.8	10.5
0.5	3	3	**9.6**	24.8	**0.7**	6.9	7.6	2.1
0.5	44	1	**62.7**	88.4	**50.1**	438.5	159.4	207.1
0.5	44	2	**37.3**	73.6	**2.3**	174.2	41.8	7.3
0.5	44	3	**26.9**	58.1	**0.7**	1.8	3.3	1.6
0.5	2000	1	**77.5**	88.6	**114.3**	448.1	162.5	202.9
0.5	2000	2	**59.2**	85.5	**6.7**	338.6	40.6	6.8
0.5	2000	3	**52.0**	72.4	**1.7**	48.2	3.9	**1.7**

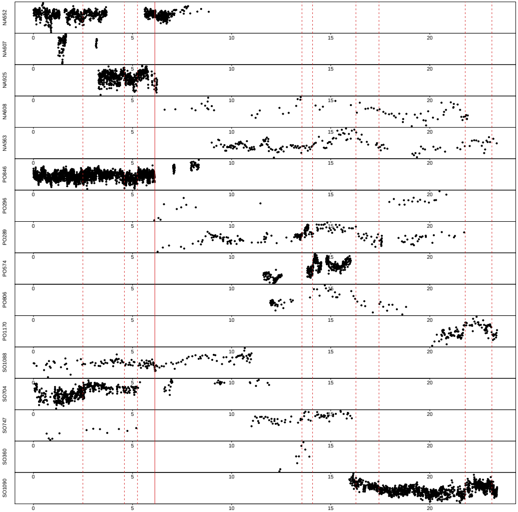
Parameters: $n = 1200$, $p = 2000$, $z = 400$, $q_1, \ldots, q_p \stackrel{\mathrm{iid}}{\sim} \mathrm{Beta}\big(10\nu, 10(1-\nu)\big)$

Real data analysis

- Oceanographic dataset covering the Neogene geological period (Samworth and Poore, 2005; Poore et al., 2006).
- Cores were extracted from North Atlantic, Pacific and Southern Oceans measuring ratio of abundance of $^{13}\mathrm{C}$ to $^{12}\mathrm{C}$ isotope ratio in microfossils at different depths (proxy for geological age).
- 7369 observations at 6295 distinct time points.
- Due to physical constraints and heterogeneity in the analysis carried out in different cores, appropriate to treat the series as data with missingness.

Real data analysis

- The most prominent change at 6.13Ma was previously identified as a time of rapid change in oceanographic current flows (Poore et al., 2006).



Summary

- We propose a new method for high-dimensional changepoint estimation in the presence of missing data.
- A good projection direction for aggregation is estimated after applying a MissCUSUM transformation to the data.
- Theory reveals interesting interaction between signal and missingness in this problem.
- Algorithm implemented in the `InspectChangepoint` R package on CRAN.

Main reference

- Follain, B., Wang, T. and Samworth, R. J. (2022) High-dimensional changepoint estimation with heterogeneous missingness. *J. Roy. Statist. Soc., Ser. B*, to appear.