

# Analytic Permutation Testing via Kahane–Khintchine Inequalities

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# What is Khintchine's inequality?

## Theorem (Khintchine's Inequality, 1923)

Let  $\varepsilon_1, \dots, \varepsilon_{2n} \stackrel{iid}{\sim} \text{Rademacher}$ .<sup>1</sup> Then, for any  $p \in [1, \infty)$ , there exist finite universal constants  $A_p$  and  $B_p$  such that for any fixed  $x_1, \dots, x_{2n} \in \mathbb{R}$  (or  $\in \mathbb{C}$ ),

$$A_p \left( \sum_{i=1}^{2n} x_i^2 \right)^{1/2} \leq \left\{ \mathbb{E} \left| \sum_{i=1}^{2n} \varepsilon_i x_i \right|^p \right\}^{1/p} \leq B_p \left( \sum_{i=1}^{2n} x_i^2 \right)^{1/2} .$$

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This has a lot of applications in the theory of  $L^p$  spaces such as the existence of Hilbert subspaces of  $L^p[0, 1]$ . Optimal constants are known (Haagerup, 1982).

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# What is the restricted Khintchine inequality?

## Theorem (Restricted Khintchine's Inequality (Spektor, 2018))

Let  $\varepsilon_1, \dots, \varepsilon_{2n}$  be dependent Rademacher random variables such that  $\sum \varepsilon_i = 0$ . Then, for any  $p \in [2, \infty)$ , there exists a finite universal constant  $B_p$  such that for any fixed  $x_1, \dots, x_{2n} \in \mathbb{R}$ ,

$$\left\{ \mathbb{E}_\varepsilon \left| \sum_{i=1}^{2n} x_i \varepsilon_i \right|^p \right\}^{1/p} \leq B_p (\|x\|_2^2 - 2n\bar{x}^2)^{1/2}.$$

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<sup>2</sup>Note: this coincides with the  $2p$ -th moments of a centred Gaussian.

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... but isn't that a permuted t statistic?

For  $s^2$  the sample variance, divide by  $n$  to get

$$\left\{ \mathbb{E}_\pi |\bar{x}_1^{(\pi)} - \bar{x}_2^{(\pi)}|^p \right\}^{1/p} \leq B_p s$$

where  $B_{2p} = [(2p)!/p!]^{1/p}$ .<sup>2</sup>

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# Statistical Hypothesis Testing

## Two sample test

A prototypical problem in statistical hypothesis testing is to determine whether or not two populations have the same mean value.

### Example (Heights of boys and girls at age 10)

Given a data set of 39 boys and 54 girls, the mean heights are

$$\hat{\mu}_{\text{boy}} = 142.2 \text{ cm, and } \hat{\mu}_{\text{girl}} = 140.7 \text{ cm}$$

with a difference of 1.5 cm and a two sample t-test gives a non-significant p-value of 0.26 where

$$\text{p-value} = P(\text{an observed difference} \geq 1.5 \mid \mu_{\text{boy}} = \mu_{\text{girl}})$$

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**Goal:** To use Kahane-Khintchine to construct bounds on such tail probabilities.

Two statistical paradigms:

## 1. **Parametric Statistics**

- ▶ Assume data has a specific distribution (e.g. normal)
- ▶ Working with a finite number of parameters (e.g. mean and variance).
- ▶ Easy to compute but strong assumptions.



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## 2. **Non-parametric Statistics**

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- ▶ Hard to compute but weak assumptions.

A *permutation test* is a type of non-parametric statistical test.

# What is a permutation test?

## Two Sample: setup

Given  $X_1, \dots, X_n, X_{n+1}, \dots, X_{2n}$  with  $EX_i = \mu_1$  for  $i \leq n$  and  $EX_i = \mu_2$  for  $i > n + 1$ ,

$$H_0 : \mu_1 = \mu_2 \quad \text{vs} \quad H_1 : \mu_1 \neq \mu_2.$$

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## Parametric Two Sample Test: t distribution

Compute  $T_0 = \sqrt{n}(\bar{X}_1 - \bar{X}_2)/s$  for sample variance  $s^2$ . Then, for  $T \sim t(2n - 2)$ ,

$$\text{p-value} = P(|T| > |T_0|).$$

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## Nonparametric Two Sample Test: permutation

For a uniformly random permutation  $\pi$  on  $2n$  elements, consider

$$T(\pi) = n^{-1} \left( \sum_{i=1}^n X_{\pi(i)} - \sum_{i=n+1}^{2n} X_{\pi(i)} \right)$$

and p-value =  $P(|T(\pi)| > |T_0| \mid X_1, \dots, X_{2n})$  for  $T_0 = \bar{X}_1 - \bar{X}_2$ .

# What is a permutation test?

## The Permutation Test:

- ▶ The distribution of  $T(\pi)$  is discrete supported on the symmetric group  $\mathbb{S}_{2n}$ .
- ▶ Generally, the p-value is estimated via Monte Carlo simulation as  $(2n)!$  is large.
- ▶ It is an *exact test*—i.e. achieves correct significance level for any  $n$ .
- ▶ Main assumption is *exchangeability*—i.e. distribution of  $T$  is invariant under permutations under  $H_0$ .
- ▶ Often applied when the asymptotic behaviour of the test statistic is not known.

## Research Question

1. What is the distribution of  $T : \mathbb{S}_{2n} \rightarrow \mathbb{R}$  for  $\pi$  uniformly distributed on  $\mathbb{S}_{2n}$ ?
2. What is a good upper bound for  $P(T(\pi) > T_0)$ ?

# An analytic approach to permutation testing

## Research Question

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2. What is a good upper bound for  $P(T(\pi) > T_0)$ ?

## The Permutationless Permutation Test

I want to run a permutation test without ever generating a single permutation!



## Theorem 2.1, Univariate Data

### Theorem (K, Spektor, Myroshnychenko)

For  $X_1, \dots, X_n$  with  $X_i$ ,  $i \leq m_1$ , from sample 1 and  $X_i$ ,  $i > m_1$ , from sample 2 with  $s$  the sample standard deviation of  $X_1, \dots, X_n$  and test statistic

$$T(\pi) = \frac{1}{s} \left[ \frac{1}{m_1} \sum_{i=1}^{m_1} X_{\pi(i)} - \frac{1}{m_2} \sum_{i=m_1+1}^n X_{\pi(i)} \right]$$

with  $m_1 = \kappa m_2$  for some  $\kappa \geq 1$ , then

$$P(T(\pi) \geq t) \leq \exp(-nt^2/2[\kappa + 1]^3).$$

# Theorem 2.1, Univariate Data

## Proof Sketch:

1. First prove a weighted restricted variant of Khintchine's inequality.

## Theorem (K, Spektor, Myroshnychenko)

For  $m_1 > m_2 > 0$ , let  $n = m_1 + m_2$  and  $M = m_1 - m_2$  and let  $\kappa m_2 = m_1$  for some rational  $\kappa > 1$ . Let  $\delta_1, \dots, \delta_n$  be weighted dependent Rademacher random variables such that marginally  $P(\delta_i = 1/m_1) = P(\delta_i = -1/m_2) = 1/2$  and such that  $\sum \delta_i = 0$ —i.e. precisely  $m_1$  of the  $\delta_i$  equal  $1/m_1$  and  $m_2$  equal  $-1/m_2$ . For any  $p \in [2, \infty)$ , there exists a positive finite constant  $B_p$  such that for any sequence  $x_1, \dots, x_n \in \mathbb{R}$ ,<sup>3</sup>

$$E|\sum_{i=1}^n \delta_i x_i|^p \leq B_p (\lceil \kappa + 1 \rceil^2 s_n^2 / 2m_2)^{p/2}$$

$s_n^2 = (n-1)^{-1} \sum_{i=1}^n (x_i - \bar{x})^2$  is the sample variance of  $x$ .

<sup>3</sup>This theorem is also valid for  $x_i \in \mathbb{C}$  after standard alterations are made in the proof.

# Theorem 2.1, Univariate Data

## Proof Sketch:

2. Use Markov's / Chernoff's inequality to translate moment bounds into tail probability bounds.

## Lemma

For a centred symmetric univariate random variable  $Z \in \mathbb{R}$  such that  $E|Z|^{2p} \leq (2p)!C^p/p!$  for some constant  $C > 0$ . Then,

$$P(Z > t) \leq e^{-t^2/4C}.$$

## Proof.

The moment generating function is bounded as follows:

$$Ee^{\lambda Z} = \sum_{p=0}^{\infty} \frac{\lambda^p E Z^p}{p!} = \sum_{p=0}^{\infty} \frac{\lambda^{2p} E Z^{2p}}{(2p)!} \leq \sum_{p=0}^{\infty} \frac{\lambda^{2p} C^p}{p!} \leq e^{\lambda^2 C}.$$

The result follows as  $P(Z > t) \leq e^{-\lambda t} Ee^{\lambda Z}$ . □

## A More General Setting

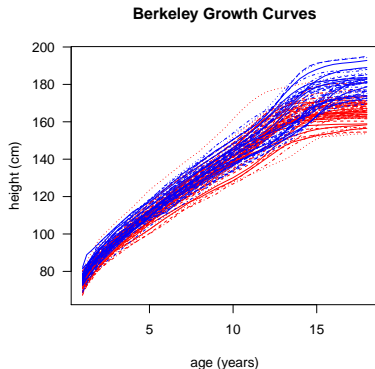
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**Problem:** Univariate data (i.e.  $X \in \mathbb{R}$ ) is boring! Statisticians care about more complex data (e.g.  $X \in L^p$ ).

# A More General Setting

**Problem:** Univariate data (i.e.  $X \in \mathbb{R}$ ) is boring! Statisticians care about more complex data (e.g.  $X \in L^P$ ).

Instead of comparing the heights of girls and boys at age 10, compare the entire growth curves or compare the covariance operators.



# What is the Kahane-Khintchine Inequality?

## Theorem (Kahane-Khintchine Inequality, 1964)

Let  $(\mathcal{X}, \|\cdot\|)$  be a Banach space. For any  $p, p' \in [1, \infty)$ , there exists a universal finite constant  $C_{p,p'} > 0$  such that for any sequence of  $X_1, \dots, X_n \in \mathcal{X}$

$$\left\{ \mathbb{E} \left\| \sum_{i=1}^n \varepsilon_i X_i \right\|^p \right\}^{1/p} \leq C_{p,p'} \left\{ \mathbb{E} \left\| \sum_{i=1}^n \varepsilon_i X_i \right\|^{p'} \right\}^{1/p'}$$

where  $\varepsilon_i$  are iid Rademacher random variables.

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where  $\varepsilon_i$  are iid Rademacher random variables.

Optimal constants are not currently known for this inequality in our setting of interest. Though, optimal constants are known in other cases (Latała & Oleszkiewicz, 1994).

## Theorem 2.2, Commutative $L^q$ Spaces

### Theorem (K, Spektor, Myroshnychenko)

Let  $m = n/2$ ,  $\|\cdot\|_{S^q}$  be the  $q$ -Schatten norm for matrices or operators, and  $\varepsilon_1, \dots, \varepsilon_n$  be Rademacher random variables such that  $\sum_{i=1}^n \varepsilon_i = 0$ . Let  $X_1(t), \dots, X_n(t)$  be continuous functions on a compact interval with empirical covariance operator  $\hat{\Sigma}(s, t) = (n-1)^{-1} \sum_{i=1}^n X_i(s)X_i(t)$ . Let  $q \in [1, \infty)$  with norm  $\|\cdot\|_{L^q}$ . For  $T(\pi) = \|\sum_{i=1}^n \varepsilon_i X_i\|_{L^q}$ , there exists a universal constant  $c > 0$  such that

$$P(T(\pi) \geq t) \leq \exp\left(-t^2/c \|\hat{\Sigma}^{1/2}\|_{S^q}^2\right).$$



## Theorem 2.3, Non-commutative $L^q$ Spaces

### Theorem (K, Spektor, Myroshnychenko)

Let  $\|\cdot\|_{S^q}$  be the  $q$ -Schatten norm for a matrix or operator and  $\varepsilon_1, \dots, \varepsilon_n$  be Rademacher random variables such that  $\sum_{i=1}^n \varepsilon_i = 0$ . For  $d, d' > 1$ , let  $X_1, \dots, X_n \in \mathbb{R}^{d \times d'}$  be a collection of  $n$  fixed matrices (or let  $X_1, \dots, X_n$  be a collection of bounded linear operators). For  $T(\pi) = \|\sum_{i=1}^n \varepsilon_i X_i\|_{S^q}$ , there exists a universal constant  $c > 0$  such that

$$P(T(\pi) > t) \leq \exp(-t^2/cS^2)$$

where  $S = \max\{\|(\sum_{i=1}^n X_i X_i^*)^{1/2}\|_{S^q}, \|(\sum_{i=1}^n X_i^* X_i)^{1/2}\|_{S^q}\}$  with  $X_i^*$  the adjoint operator.

### **Proof Sketch:**

1. Use similar tricks for inserting the dependency condition into Kahane's inequality in the commutative and non-commutative settings.
2. Use Markov / Chernoff and the bound on the moment generating function to bound the tail probability.

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The stats journals were unhappy that these bounds are based on unknown constants.

# The Beta Transformation in $\mathbb{R}$

In statistics, we want a p-value to be a Uniform  $[0, 1]$  random variable under the null hypothesis, but our bound on the p-value follows a more general beta distribution.

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## Proposition (K, Spektor, Myroshnychenko)

*Under the setting of Theorem 2.1 (univariate data) with  $n$  sufficiently large,*

$$P(\exp\{-nT(\pi)^2/2\lceil\kappa+1\rceil^3\} < u) \leq C_0 I\left(u; \frac{\lceil\kappa+1\rceil^3}{2+\kappa+\kappa^{-1}}, \frac{1}{2}\right)$$

*where  $I(u; \alpha, \beta)$  is the regularized incomplete beta function and*

$$C_0 = \frac{\left(\frac{\lceil\kappa+1\rceil^3}{2+\kappa+\kappa^{-1}}\right)^{1/2} \Gamma\left(\frac{\lceil\kappa+1\rceil^3}{2+\kappa+\kappa^{-1}}\right)}{\Gamma\left(\frac{1}{2} + \frac{\lceil\kappa+1\rceil^3}{2+\kappa+\kappa^{-1}}\right)}.$$

# Beta Transformation, Proof Sketch

1. Note that  $nT_0^2/(2 + \kappa + \kappa^{-1})$  is approximately  $\chi^2(1)$  via the CLT.
2. For  $Z \sim \chi^2(1)$ , bound

$$\begin{aligned} \mathbb{P}\left(e^{-Z/c} \leq u\right) &= \mathbb{P}(Z \geq -c \log u) \\ &= (2\pi)^{-1/2} \int_{-c \log u}^{\infty} x^{-1/2} e^{-x/2} dx \\ &= \left(\frac{c}{2\pi}\right)^{1/2} \int_0^u (-\log y)^{-1/2} y^{c/2-1} dy \\ &\leq \left(\frac{c}{2\pi}\right)^{1/2} \int_0^u (1-y)^{1/2-1} y^{c/2-1} dy \\ &= \frac{(c/2)^{1/2} \Gamma(c/2)}{\Gamma((c+1)/2)} I(u; c/2, 1/2) \end{aligned}$$

# The Beta Transform in Banach Space

## Theorem (K, Spektor, Myroshnychenko)

Let  $(\mathcal{X}, \|\cdot\|)$  be a Banach space with separable dual space  $\mathcal{X}^*$ , and let  $h : \mathbb{R} \rightarrow \mathbb{R}$  be monotonically increasing. For any random variable  $X$  taking values in  $\mathcal{X}$  such that  $\mathbb{E}h(\|X\|)^2 < \infty$  and  $\sup_{X \in \mathcal{X}} h(\|X\|) < U < \infty$  and for  $u \in (0, 1)$  and some constants  $C, c, \alpha, \beta > 0$ ,

$$\mathbb{P} \left( e^{-h(\|X\|)/c} < u \right) \leq CI(u; \alpha, \beta)$$

where  $I(u; \alpha, \beta)$  is the incomplete beta function for  $c$  sufficiently large.



# Beta Transform, Proof Sketch

1. For  $Z = h(\|X\|) \in \mathbb{R}^+$ , rewrite as a countable supremum  $Z = \sup_{\phi \in B^*} h(\phi(X))$  and apply Talagrand's concentration inequality:  $P(Z \geq EZ + t) \leq \exp\left(\frac{-t^2}{a+bt}\right)$  for positive constants  $a$  and  $b$  depending on  $Eh(\|X\|)^2$  and  $\sup_{X \in \mathcal{X}} h(\|X\|)$ .
2. Use a bunch of inequalities and calculus to get that

$$\begin{aligned} \exp\left(\frac{-t^2}{a+bt}\right) &\leq e^{-t/b} \left[ \left(1 + \frac{bt}{a}\right)^a \right]^{1/b^2} \\ &\leq e^{-t/b} \sum_{k=0}^a \frac{1}{k!} \left(\frac{t}{b}\right)^k = \int_t^\infty \frac{x^{a-1} e^{-x/b}}{b^a \Gamma(a)} dx \end{aligned}$$

3. Then proceed similarly to the univariate case to get

$$\begin{aligned} P\left(e^{-(Z-EZ)/c} \leq u\right) &\leq \frac{c^a}{b^a \Gamma(a)} \int_0^u (1-y)^{a-1} y^{c/b-a-1} dy \\ &= CI(u; a, c/b - a) \end{aligned}$$

# The Empirical Beta Transform

In practice, we do not know the universal constants emerging from Kahane's inequality and Talagrand's inequality, so instead we perform a small simulation to estimate the parameters of the beta distribution  $\alpha$  and  $\beta$ .

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## Empirical Beta Transform

Compute p-value  $p_0$  from test statistic  $T_0$ .

Choose  $r > 1$ , the number of permutations to simulate—e.g.  $r = 10$ .

Draw  $\pi_1, \dots, \pi_r$  from  $\mathbb{S}_n$  uniformly at random.

Compute p-values  $p_1, \dots, p_r$  from test statistics  $T_{\pi_1}, \dots, T_{\pi_r}$ .

Find the method of moments estimator for  $\alpha$  and  $\beta$ .

Estimate first and second central moments of the  $p_i$  by  $\bar{p}$  and  $s^2$ .

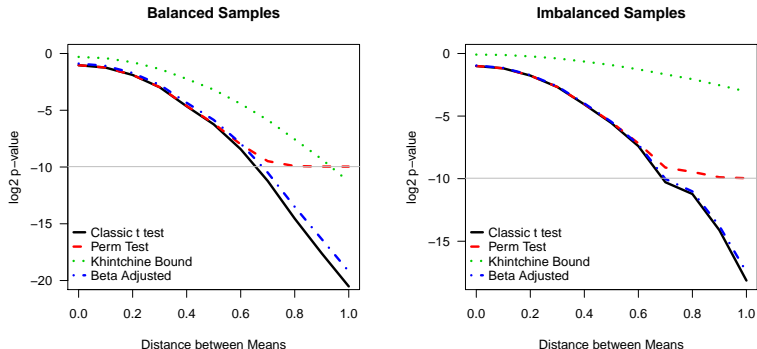
Estimate  $\hat{\alpha} = \bar{p}^2(1 - \bar{p})/s^2 - \bar{p}$ .

Estimate  $\hat{\beta} = [\bar{p}(1 - \bar{p})/s^2 - 1][1 - \bar{p}]$ .

Return the adjusted p-value  $I(p_0; \hat{\alpha}, \hat{\beta})$ .

# But does it work on simulated data?

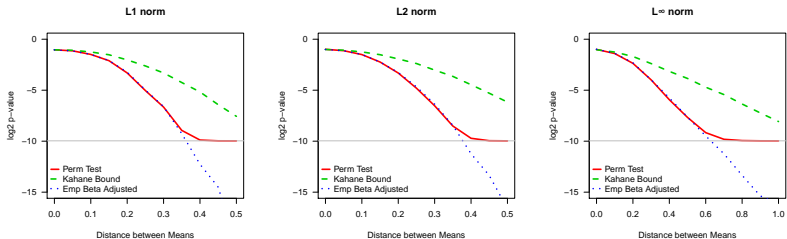
## Simulated Univariate Gaussian Data



On the left,  $m_1 = m_2 = 100$ . On the right,  $m_1 = 140, m_2 = 60$ .

# But does it work on simulated data?

## Simulated Multivariate Gaussian Data



For data in  $\mathbb{R}^{12}$  with sample sizes  $m_1 = m_2 = 50$  for  $\ell^1$ ,  $\ell^2$ , and  $\ell^\infty$  norms.

## Extending to k sample testing

Under the one-way ANOVA model,  $X_{i,j} = \mu + \tau_i + \varepsilon_{i,j}$  we can test

$$\text{Pairwise} \quad H_0^{(ij)} : \tau_i = \tau_j \quad H_1^{(ij)} : \tau_i \neq \tau_j$$

$$\text{Global} \quad H_0 : \tau_1 = \dots = \tau_k = 0 \quad H_1 : \exists \tau_i \neq 0.$$

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## Extension to Banach Spaces

Note that the global test statistic can be considered as an  $\ell^2$  direct sum of  $\kappa = \binom{k}{2}$  Banach spaces. For a sequence  $(\mathcal{X}_i, \|\cdot\|_i)$  and elements  $X_i \in \mathcal{X}_i$ ,

$$(X_i)_{i=1}^n \in \left( \bigoplus_{i=1}^{\kappa} \mathcal{X}_i \right)_{\ell^2}$$

with norm  $\|(X_i)_{i=1}^n\| = (\sum_{i=1}^n \|X_i\|_i^2)^{1/2}$ .

# Synchronized Test: Analytic Variant

Let  $X^{(i)}$  be the vector of observations from population  $i$  and let

$$X = \begin{pmatrix} X^{(1)} & X^{(1)} & \dots & X^{(k-1)} \\ X^{(2)} & X^{(3)} & \dots & X^{(k)} \end{pmatrix}.$$

be the  $(2m) \times \binom{k}{2}$  matrix of pairwise comparisons. Then, for  $\varepsilon$  multivariate Rademacher such that  $\sum \varepsilon_j = 0$ , we have the test statistic  $T = \|X^T \varepsilon\|_{\ell^2}$



# Synchronized Test: Analytic Variant

Let  $X^{(i)}$  be the vector of observations from population  $i$  and let

$$X = \begin{pmatrix} X^{(1)} & X^{(1)} & \dots & X^{(k-1)} \\ X^{(2)} & X^{(3)} & \dots & X^{(k)} \end{pmatrix}.$$

be the  $(2m) \times \binom{k}{2}$  matrix of pairwise comparisons. Then, for  $\varepsilon$  multivariate Rademacher such that  $\sum \varepsilon_j = 0$ , we have the test statistic  $T = \|X^T \varepsilon\|_{\ell^2}$

The squared test statistic  $T^2 = \sum_{i,j=1}^{2m} a_{i,j} \varepsilon_i \varepsilon_j$  is a degree 2 homogeneous Rademacher chaos with  $a_{i,j}$  the  $ij$ th entry in  $XX^T$ .

## Theorem 3.1, k-sample testing

### Theorem (K, Spektor, Myroshnychenko)

Let  $T = \|X^T \varepsilon\|_{\ell^2}$  for  $X$  the above  $2m \times \binom{k}{2}$  matrix and  $\varepsilon_i$  such that  $\sum_{i=1}^{2m} \varepsilon_i = 0$ . Then, for some universal constant  $c$ ,

$$P(T > t) \leq \exp[-t^2/cS]$$

where  $S = \|XX^T\|_{S^2}$ .

# Theorem 3.1, k-sample testing

## Proof Sketch

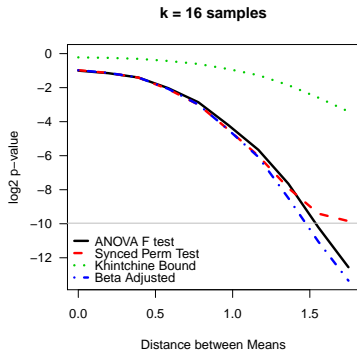
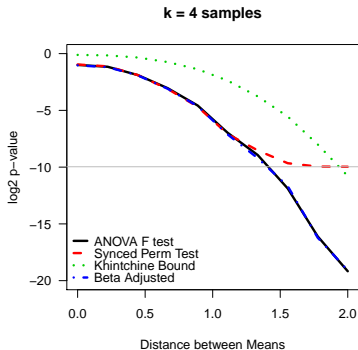
1. Extend the ideas in Spektor (2018) from Rademacher sums to homogeneous Rademacher chaoses of degree 2.
2. Apply a decoupling inequality from Kwapien (1987)

$$\begin{aligned} \mathbb{E}_\varepsilon |T^2|^p &= \left[ \mathbb{E}_\pi \mathbb{E}_\delta \left| \sum_{i,j=1}^m \delta_i \delta_j b_{i,j,\pi} \right|^p \right]^{1/p} \\ &\leq B_p^2 C \left[ \mathbb{E}_\pi \mathbb{E}_\delta \left| \sum_{i,j=1}^m \delta_i \delta_j b_{i,j,\pi} \right|^2 \right]^{1/2} \leq 2B_p^2 C \|XX^T\|_{S^2} \end{aligned}$$

3. Then use Markov/Chernoff again with a little help from the Legendre duplication formula and Watson's formula to get the correct coefficients.

# And it also works on simulated data!

## Simulated $k$ samples of univariate Gaussian data



# Really Cool Data Application 1: Speech Sounds

Testing differences between

- ▶ 12 spoken vowel sounds (phonemes)
- ▶ Taken from recordings of 4 speakers while controlling for gender (male/female) and country of origin (Canada/China).
- ▶ Using experimental designs—i.e. the Latin square design and the randomized block design.

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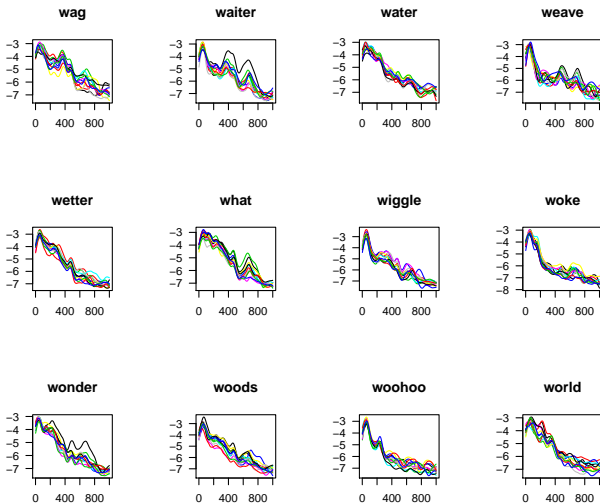
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The only other way to analyze this data would be to run a large scale simulation based permutation test requiring an estimated 35 million SVD calculations with estimated runtime of 74 days on my Intel Core i7-7567U CPU.

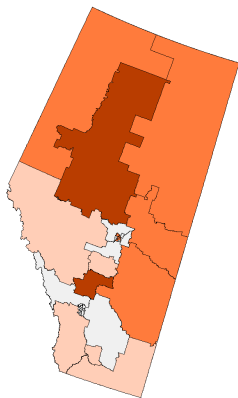
# Really Cool Data Application 1: Speech Sounds

## Log periodograms of one of the speakers



## Alberta 2019 Electoral Results:

- ▶ Testing for local autocorrelation at each riding in Alberta—i.e. testing if election results correlated or uncorrelated with the neighbouring results.
- ▶ Test statistics take the form a measure of matrix association like  $\gamma_{AB} := \sum_{i,j=1}^n a_{i,j}b_{i,j}$ .
- ▶ Considering the map as a graph  $\mathcal{G}$  with a measurement  $y_i$  taken at each vertex, the permutation test permutes the location of the vertices.





# Summary of Results

- ▶ Adapted the restricted Khintchine inequality to bounding permutation p-values for the unpaired t-test.
- ▶ Extended this result for imbalanced samples
- ▶ Extended this via the Kahane-Khintchine inequality to
  - ▶ Commutative Banach Spaces: Multivariate, Functional Data
  - ▶ Non-Commutative Banach Spaces: Matrices and Operators
- ▶ Developed a k-sample test based on the synchronized permutation test.
- ▶ Extended this to more advanced experimental designs.
- ▶ Able to apply such tools to a diverse collection of data sets.

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Thank you for listening