Discrepancy Theory and Randomized Controlled Trials

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Harvord Oct 23

BALANCING COVARIATES IN RANDOMIZED EXPERIMENTS USING THE GRAM-SCHMIDT WALK

BY CHRISTOPHER HARSHAW, FREDRIK SÄVJE,
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Chris Harshaw MIT



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Randomized Controlled Trials (RCT) Test medications, procedures or policies Randomly assign subjects to drug or placebo Want the two groups to be similar.

Discrepancy Theory
Divide a group of things (vectors)
into two similar groups.

More similar than Tandom

Outline

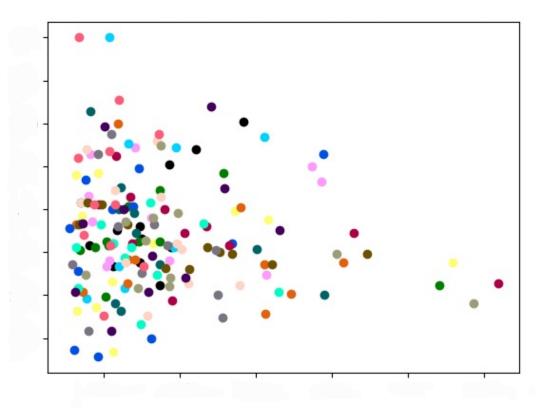
Introduction to Discrepancy Theory

How to analyze RCTs

probability & statistics

Discrepancy theory for RCTs

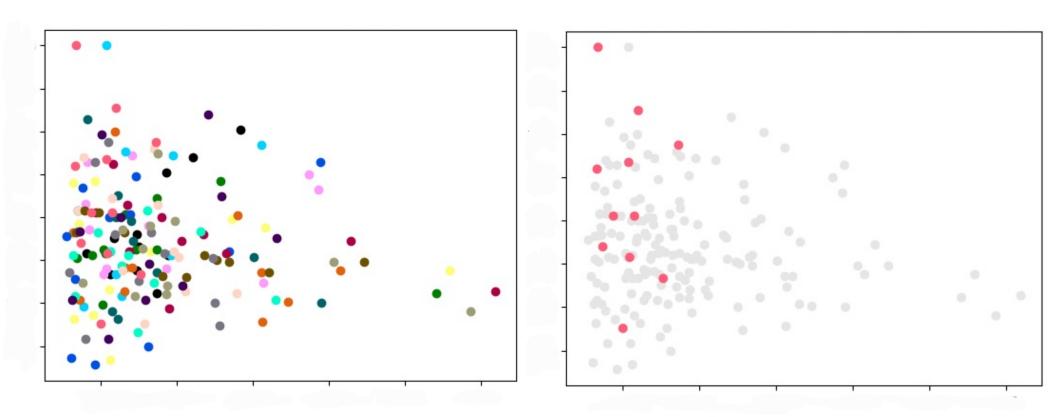
Village-wide maternal health intervention 176 villages, 16 treatments, 11 villages per group





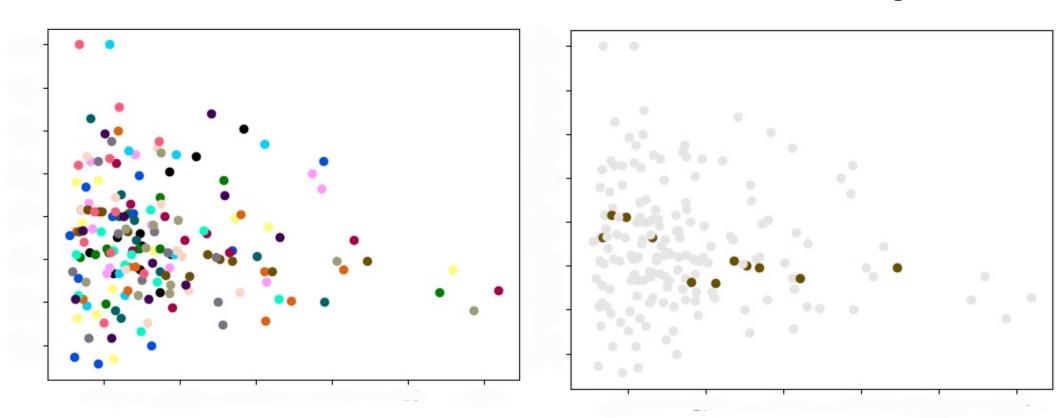
Village-wide maternal health intervention

176 villages, 16 treatments, 11 villages per group



Village-wide maternal health intervention

176 villages, 16 treatments, 11 villages per group



Want to balance many covariates

Distance to hospital

Time to reach hospital when raining

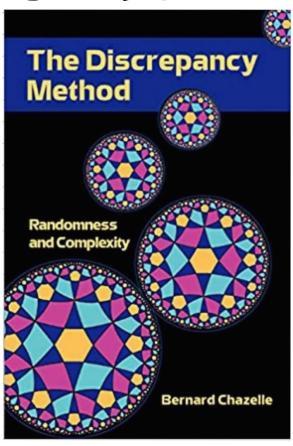
Median income

Average age

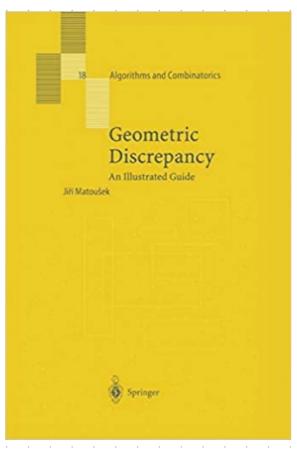
Altitude

Discrepancy Theory

Chazelle



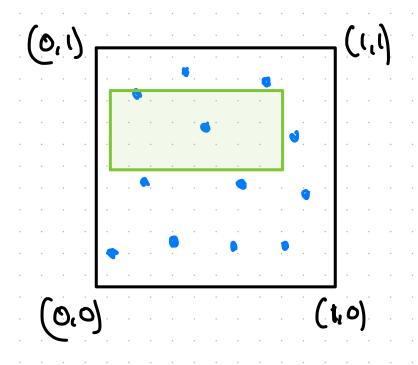
Matoušek



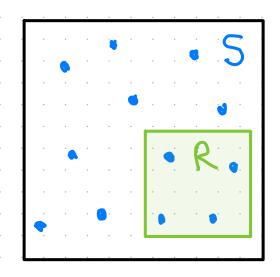
Courses by Aleksandar Nikolov Peng Zhang

Discrepancy Theory:

Illustration by points and axis-parallel rectangles in [0,1]2



Problem: find $S = \{x', ..., x''\} \subseteq [0, 1]^2$ so that for all rectangles R, $\frac{|S \cap R|}{|S|} \approx \text{volume}(R)$

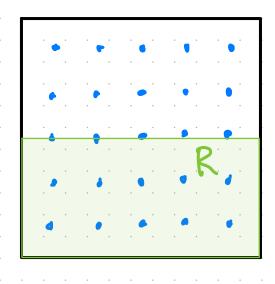


How good can this approximation be?

$$\frac{|S \cap R|}{|S|} = \frac{4}{12} = \frac{1}{3}$$

Given
$$S = \{x', ..., x''\} \subseteq [0,1]^2$$
 and rectangle R
discrepancy is $\left| \frac{|S \cap R|}{|S|} - volume(R) \right|$

Want small discrepancy for all R



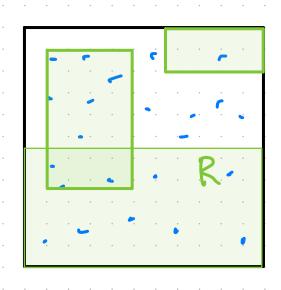
Given
$$S = \{x', ..., x''\} \subseteq [0,1]^2$$
 and rectangle R
discrepancy is $\left| \frac{|S \cap R|}{|S|} - volume(R) \right|$.

Want small discrepancy for all R

$$R = [0,1] \times [0,12]$$

Given n, find
$$S = \{x', ..., x''\} \subseteq [0,1]^2$$
 so that $\forall R$ discrepancy $\left| \frac{|S \cap R|}{|S|} - \text{volume}(R) \right|$ is small

Theorem (Van der Corput 35)



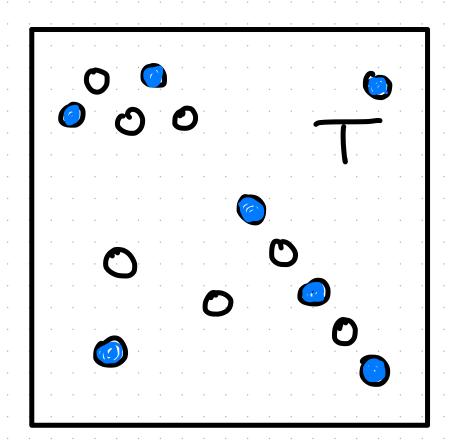
There exists S such that
for all R,
discrepancy & closn

for some constant C.

A Partitioning Problem

Given
$$T \in [0,1]^2$$
 and n , find $S \in T$, $|S| = n + s + s$.

 $|S| = n + s + s$
 $|S| = n + s$



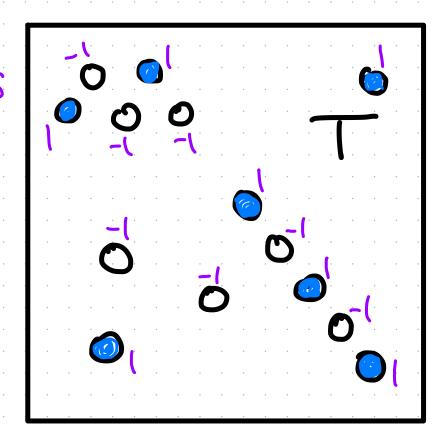
S approximates T and so does T-S

A Partitioning Problem

Given
$$T \in [0,1]^2$$
 and n , find $S \in T$, $|S|=n$ $S+$.

 $HR \left| \frac{|S \cap R|}{|S|} - \frac{|T \cap R|}{|T|} \right| \text{ is small}$

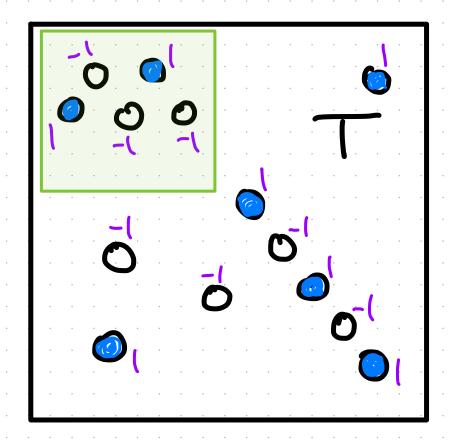
Let
$$= 1 \text{ if } j \in S$$
 $0 \text{ or } j \in S$ -1 o.w.



S approximates T

and so does T-S

A Partitioning Problem



Each rectangle gives a subset of T

Discrepancy for Set Systems

Define [n] = {1,..., n}

Given S, c[n], Szc[n],..., Szc[n]

Find Z:[n] -> {±1} s.t.

Vi [] ES; is small

Define disc(z) = max [[] = z(j) |

Discrepancy for Set Systems

For uniform random Z,

$$Pr[disc(Z) \leq \int 2n ln(2n)] > 0$$

Discrepancy for Set Systems

Define disc(z) =
$$\max_{i} \left(\sum_{j \in S_i} z(j) \right)$$

$$Pr\left[disc(z) \leq \int 2n \ln(2d)\right] > 0$$

Spencer 85

$$\exists z \text{ s.t. } disc(z) \leq 6Jd \text{ when } d \in \Omega$$

Discrepancy for Set Systems -> Vectors

Given S, c[n], Szc[n],..., Szc[n] let X be the incidence matrix of the sets

$$\chi(i,j) = \begin{cases} 1 & \text{if } i \in Si \\ 0 & \text{o.} \omega. \end{cases} \qquad (\chi_z)(i) = \sum_{j \in Si} z(j)$$

$$disc(z) = \max_{i} \left(\sum_{j \in S_i} z(j) \right) = \|Xz\|_{\infty}$$

where
$$\|v\|_{\infty} \stackrel{\text{def}}{=} \max_{j} |v(j)|$$

Let
$$X = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$
 so $X_2 = \sum_{i=1}^{n} Z(i) X_i$

Discrepancy for Vectors

Spencer 85

Given $X_1 \in [-1,1]^d$, ..., $X_n \in [-1,1]^d$, $X = \begin{pmatrix} x_1 & x_2 & ... & x_n \\ 1 & 1 & 1 \end{pmatrix}$

Was unknown if could find z in polynomial time.

Discrepancy for Vectors

Spencer 85

Given
$$X_i \in [-1,1]^d$$
, ..., $X_n \in [-1,1]^d$, $X = \begin{pmatrix} x_1 & x_2 & ... & x_n \\ 1 & 1 & 1 \end{pmatrix}$

Bansal 10 Can find z in polynomial time.

Followed by many other algorithms for many discrepancy problems

We still do not know the right constant. Is it 2?

Euclidean Discrepancy for Vectors

Bárány-Grinberg '81+ Beck-Fiala '81

Given X1, ..., $X_n \in \mathbb{R}^d$, $\|X_i\|_2 \le 1$ for all i $\exists z \in \{\pm 1\}^n$ s.t. $\|\sum_i z(i) x_i\|_2 = \|X_i\|_2 \le Jd$

Counnot improve
$$Jd: X_1 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} X_2 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} X_3 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} X_4 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} X_5 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} X_5 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} X_5 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} X_5 = \begin{pmatrix}$$

Euclidean Discrepancy for Vectors

Bárány-Grinberg '81+ Beck-Fiala '81 (algorithmic)

Thm 1 Given X,, ..., Xn ERd, IIXille = 1 for all i

∃ Z € [=1]" s.t. ||Xz||2 = Jd

Charikar, Newman and Nikolou 11:

Is NP-hard to distinguish

from

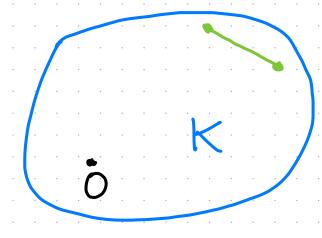
Banaszczykś 198 Theorem

Generalizes Euclidean discrepancy

Given $X_1, ..., X_n \in \mathbb{R}^d$, $\|X_i\|_2 \le 1$ for all iThen 1 says $\exists z \in \{\pm 1\}^n$ s.t. $\sum_i z(i) \times i \in B_{id}(0)$

Banaszczyk:

For all convex k with Goussian measure $\geq \frac{1}{2}$ $\exists z \in \{\pm 1\}^n \text{ s.t. } Zz(i) \times i \in 5k$



Banaszczykś 198 Theorem

Generalizes Euclidean discrepancy

Given
$$X_1, ..., X_n \in \mathbb{R}^d$$
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Banaszczyk:

For all convex k with Goussian measure $\geq \frac{1}{2}$ $\exists z \in \{\pm 1\}^n \text{ s.t. } \sum_{i} z(i) \times i \in 5k$

Gaussian measure =
$$Pr[xeK] = \frac{1}{(2\pi)^{d/2}} \int e^{-\frac{1}{2}||x||_{2}^{2}} dx$$

 $x \in \mathcal{N}(0, Id)$ $x \in K$

Banaszczykś 198 Theorem

Given $X_1, ..., X_n \in \mathbb{R}^d$, $\|X_i\|_2 \le 1$ for all iThan 1 says $\exists z \in \{\pm 1\}^n$ s.t. $\sum_i z(i) \times i \in B_{\overline{id}}(0)$

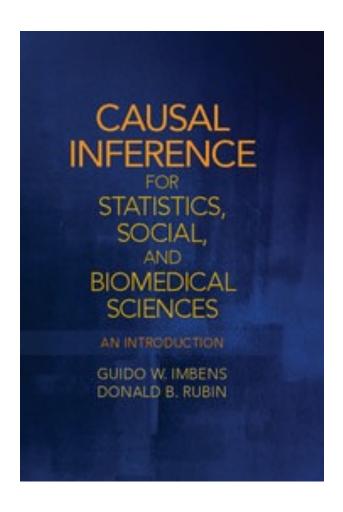
Banaszczyk:

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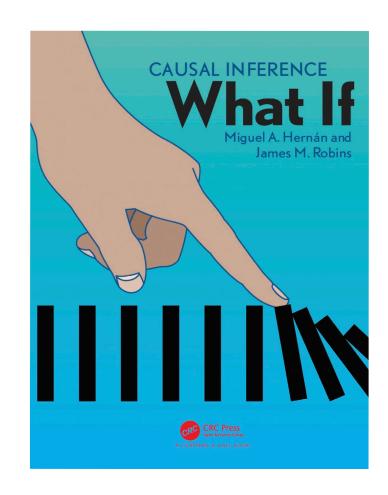
Efficient algorithm, Gram-Schmidt Walk

Bansal, Dodush, Garg, Lovett 19

Randomized Controlled Trials

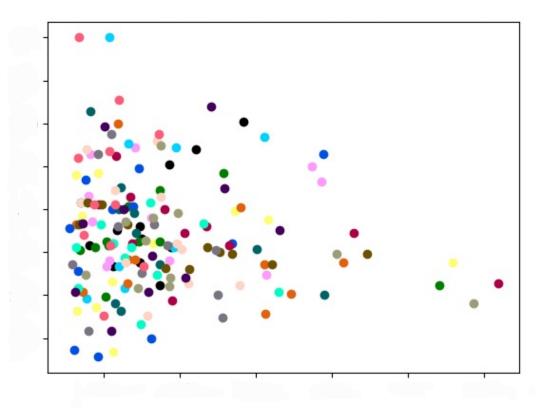


Imbens & Rabin



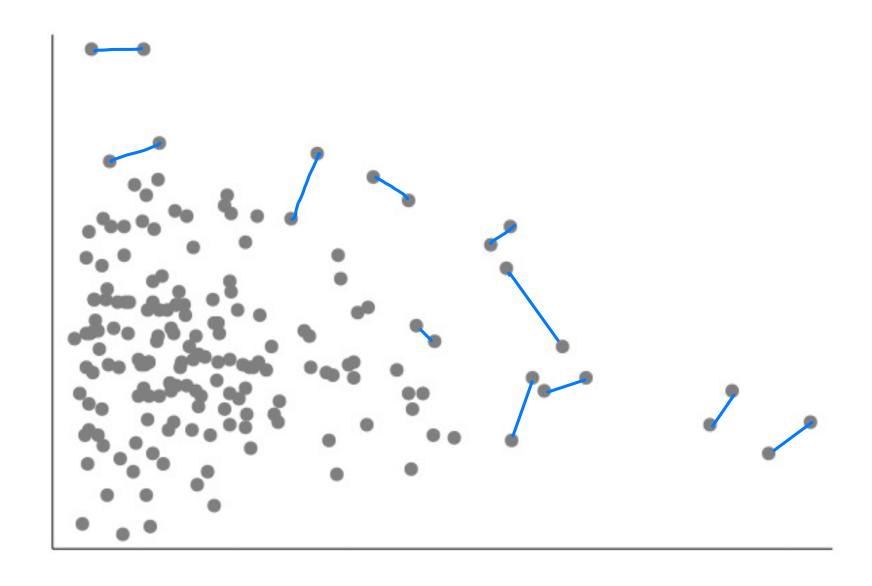
Hernán & Robins

Village-wide maternal health intervention 176 villages, 16 treatments, 11 villages per group

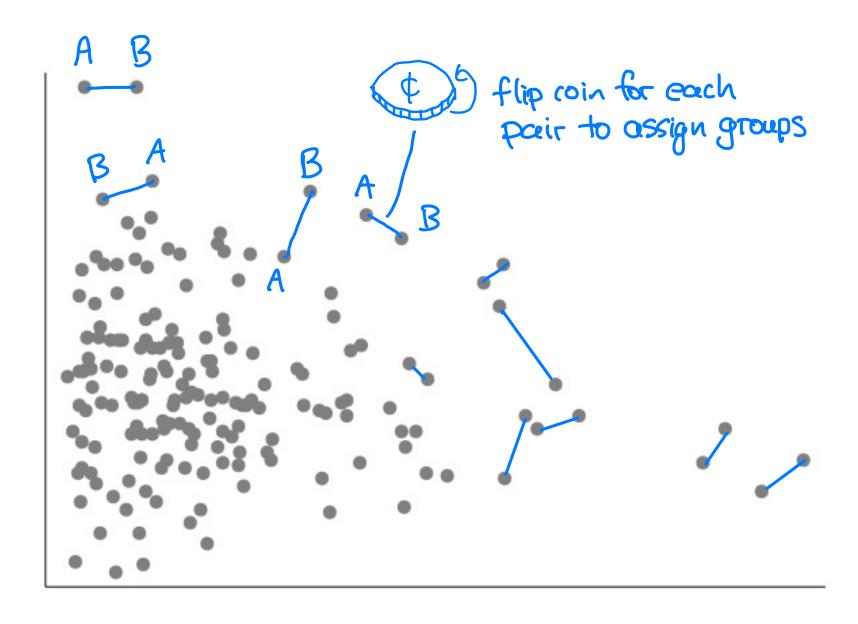




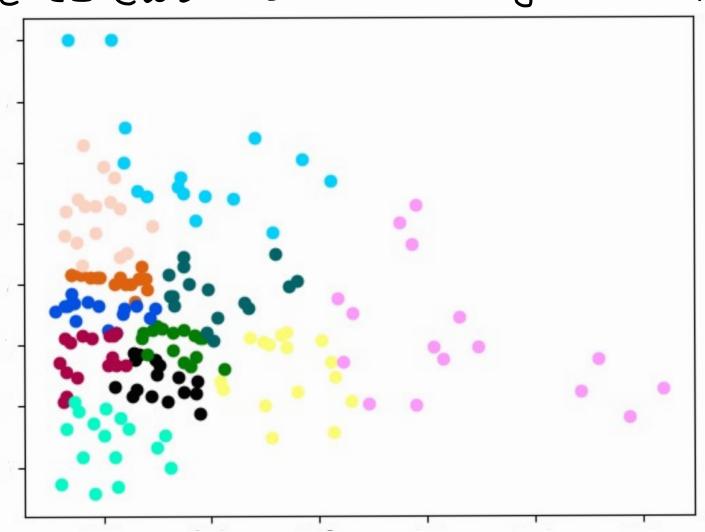
Matching for two groups



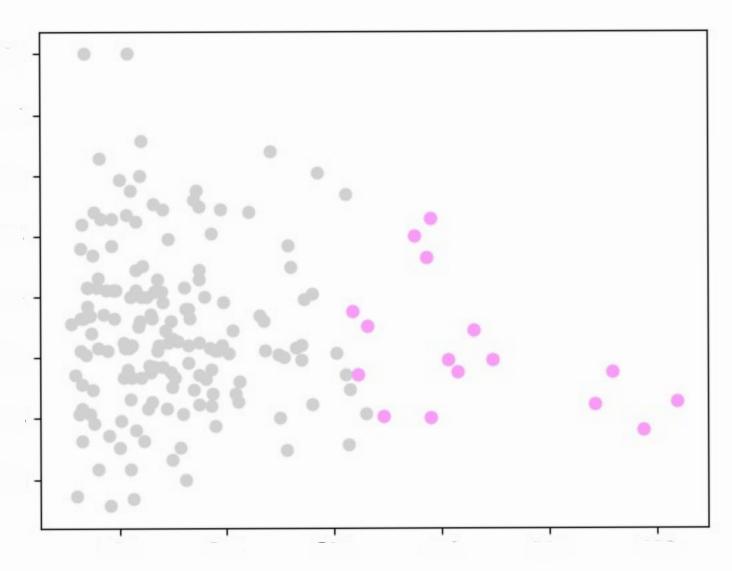
Matching for two groups



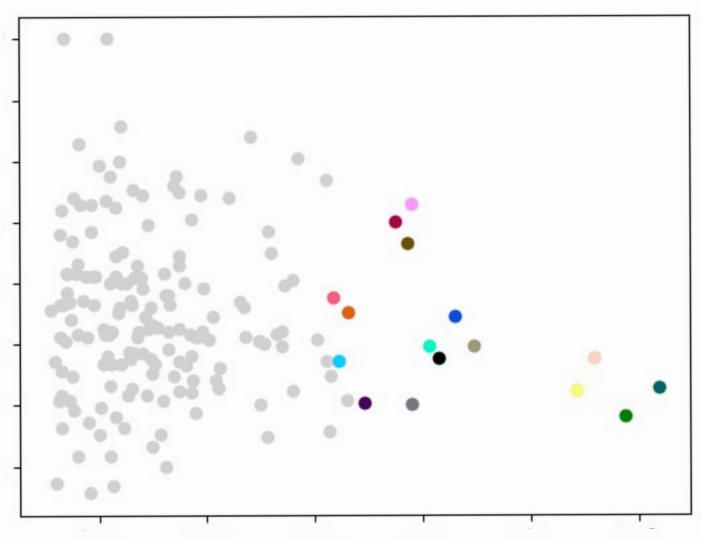
Create 11 clusters of 16 villages each



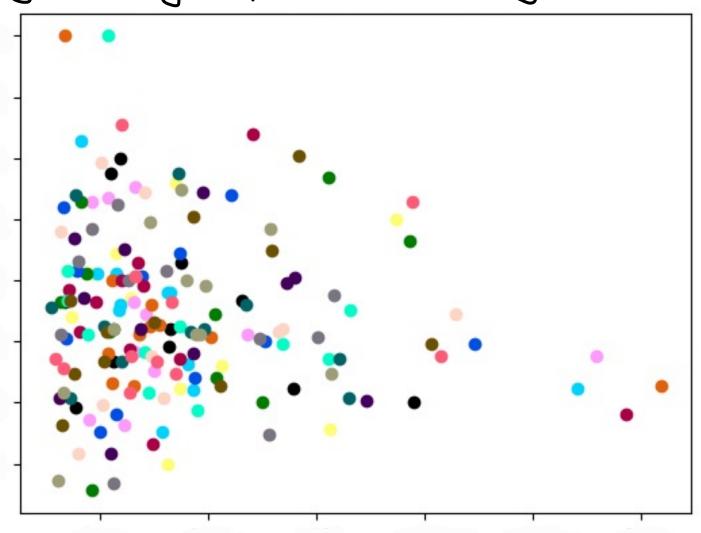




Choose a random bijection from villages to treatments

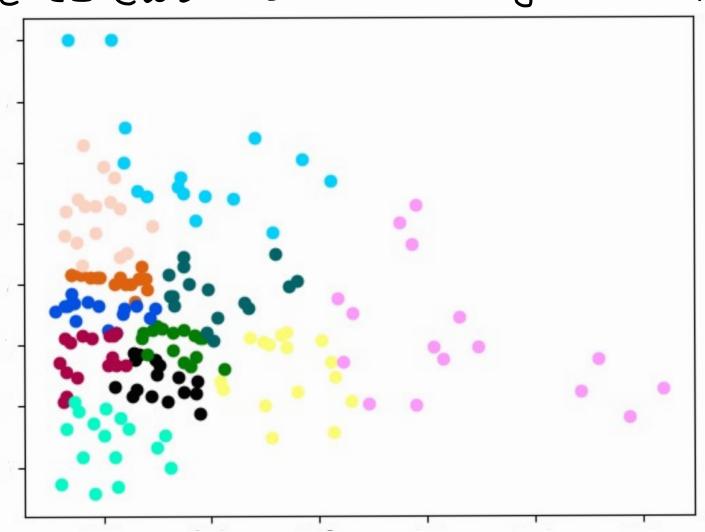


Assign each cluster independently to get 16 groups of 11 villages each



Blocking for many treatment groups

Create 11 clusters of 16 villages each

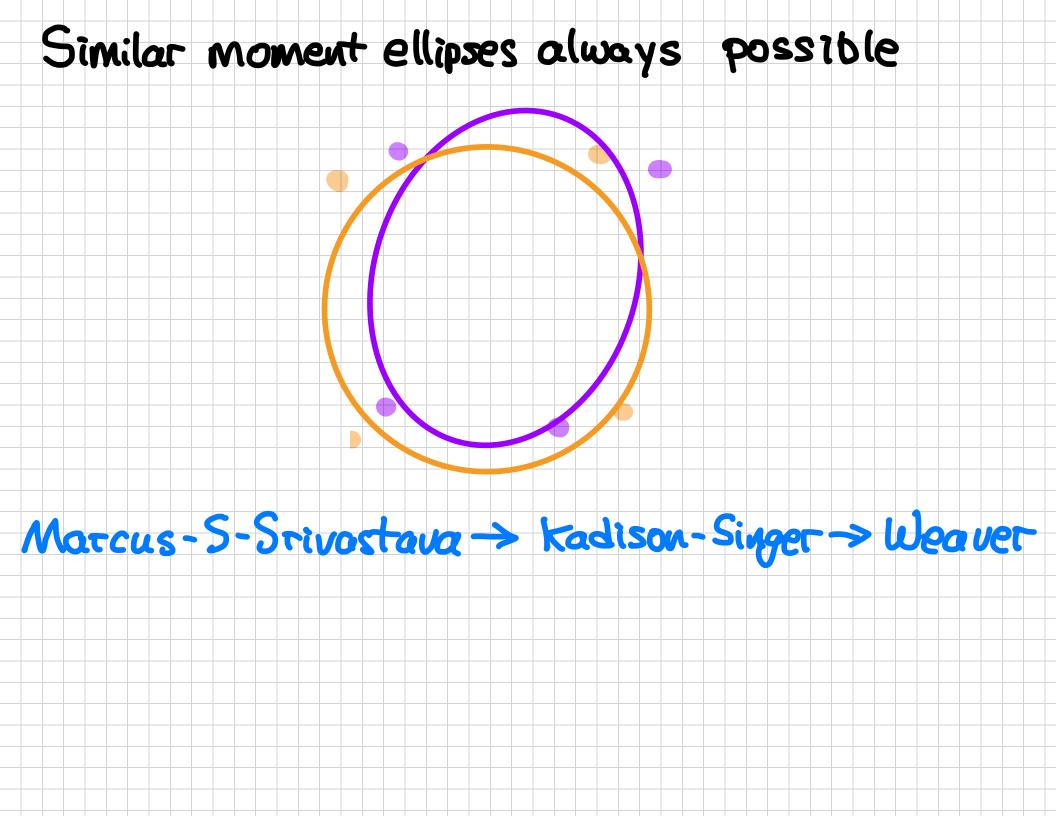


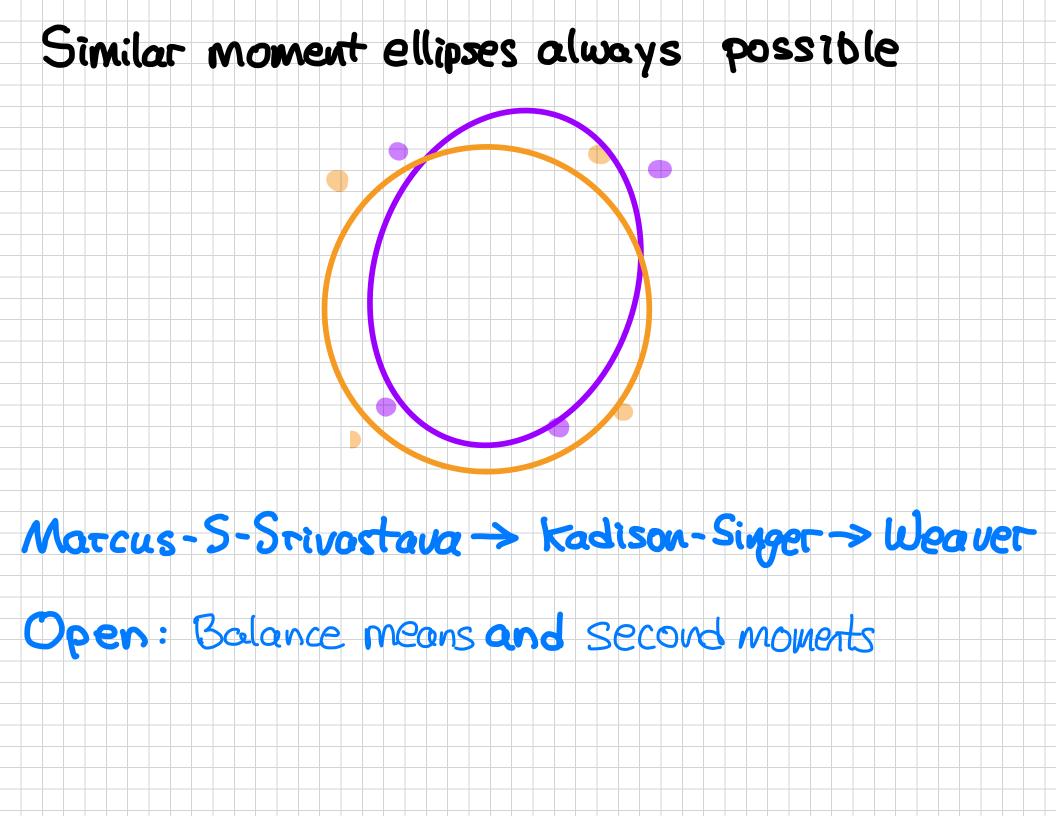
Discrepancy Theory

Can make means similar

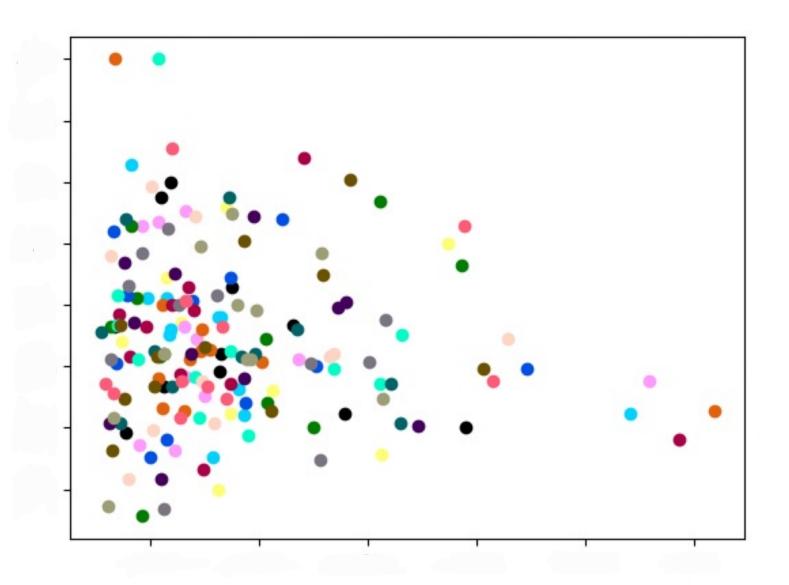
Discrepancy Theory

Can make means similar





Balanced Everything



Randomization

Allows one to argue results unlikely to be due to a poor assignment.

Need randomization for confidence intervals

Can balance better on average

This is not an optimization problem.

100 balanced but very different assignments



1. Franework & Mathematical Formalization

2. Algorithm

The Gram-Schmidt Walk Design is Robust: never much worse than iid random

Balanced: much better when covariates correlate with outcomes

Neyman-Rubin Model of Experiments

Consider two treatment groups: A = Test and B = Control

Two potential outcomes for subject i observe a(i) if $i \in A$ b(i) if $i \in B$

Can not observe both

Assignment is only source of randomness Response to treatment is NOT random

Designs

The design is the distribution of A, B

uniform: Pr[ie A] = 1/2, independently

balanced: A uniform subset of half

Matching: divide subjects into disjoint pairs (i.i) assign $i \rightarrow A$, $j \rightarrow B$ or

 $i \rightarrow B, \quad j \rightarrow A$

with prob 1/2

Neyman-Rubin Model for Experiments

Two potential outcomes for subject i observe a(i) if i \(A \) prob 1/2 b(i) if i \(B \) prob 1/2

Can not observe both

Want to measure average treatment effect
$$T = \frac{1}{n} \sum_{i} a(i) - b(i)$$
 (ATE)

Horvitz-Thompson Estimator

Estimate
$$T = \frac{1}{n} \sum_{i} a(i) - b(i)$$

by
$$\hat{\tau} = \frac{2}{n} \left(\sum_{i \in A} a(i) - \sum_{i \in B} b(i) \right)$$

Are not using difference of means $\frac{1}{|A|} \sum_{i \in A} a(i) - \frac{1}{|B|} \sum_{i \in B} b(i)$

Differs from Horvitz-Thompson when lAlt IBI

Precision

Confidence Interval

Formula for error of estimator

Set
$$Z(i) = \begin{cases} 1 & i \in A \\ -1 & i \in B \end{cases}$$

$$n(\hat{\tau} - \tau) = z^{T}(\alpha + b) = z^{T}\mu \text{ where } \mu^{\text{eff}}\alpha + b$$

$$nT = \sum_{i} a(i) - b(i)$$

$$\bigcap_{i \in A} \widehat{z} = 2\sum_{i \in B} \alpha(i) - 2\sum_{i \in B} b(i)$$

$$\Pi(\hat{\tau} - \tau) = \sum_{i \in A} (a(i) + b(i)) - \sum_{i \in B} (a(i) + b(i))$$

How show Pr[|î-t|>t] is small?

1. Estimate MSE $\stackrel{\text{def}}{=} [E(\hat{\tau} - \tau)^2]$ Chebysheu: $Pr[|\hat{\tau} - \tau| > c\sqrt{MSE}] \leq \frac{1}{C^2}$

2. Higher moments and Sub-Gaussian Concentration

Mean Squared Error

MSE
$$(\hat{\tau}) = \frac{1}{n^2} \mathbb{E}(z^T \mu)^2$$

$$= \frac{1}{n^2} \mathbb{E}(\mu^T z)(z^T \mu)$$

$$= \frac{1}{n^2} \mu^T (\mathbb{E} z z^T) \mu$$

$$= \frac{1}{n^2} \mu^T Z \mu$$

 $Z(i) = \begin{cases} 1 & i \in A \\ -1 & i \in B \end{cases}$

Mean Squared Error

$$MSE(\hat{\tau}) = \frac{1}{n^2} \left[E(z^T \mu)^2 \right]$$

$$= \frac{1}{n^2} \left[E(\mu^T z)(z^T \mu) \right]$$

 $Z(i) = \begin{cases} 1 & i \in A \\ -1 & i \in B \end{cases}$

We can know Z, but not ju So, want | Zllz small

Measure Robustness by 117112

There is a μ such that $\mu^{T} Z \mu = \|\mu\|^{2} \|Z\|_{2}$ So, worst-case mean squared error
is captured by $\|Z\|_{2}$

Robustness-iid case

For Z uniform in
$$\{\pm 1\}^n$$

 $Z = Cou(z) = I$ and $||Z|| = 1$

Uniform Design Maximizes Robustness

For Z uniform in $\{\pm 1\}^n$ Z = Cou(z) = I and $\|Z\| = 1$

For every other design, 11711>1

To get lower variance, give up a little in worst case need nice μ or helpful covariates

MSE - Random Balanced, IAI=1B1

For uniform
$$Z = 11 = 0$$

 $Z = \frac{1}{n-1} (I - \frac{1}{n} 11) (|Z||_2 = \frac{n}{n-1})$

MSE - Random Balanced, IAI= IBI

For uniform
$$z$$
 s.t. $z^T 1 = 0$

$$Z = \frac{1}{n-2} \left(I - \frac{1}{n} 1 1^T \right) \quad \|Z\|_2 = \frac{n}{n-1}$$

$$MSE = \frac{1}{(n-1)^2} \|\mu - \frac{1}{n} 1^T \mu\|_2^2$$

$$small if$$

$$larger than$$

$$\frac{1}{n^2} \quad \text{far from } 0$$

Can be worse than iid, but often preferred, especially if a, b = 0

Covariates

$$X_{1}, \dots, X_{n} \in \mathbb{R}^{d}$$

$$X = \begin{pmatrix} 1 & 1 \\ x_{1}, \dots & x_{n} \end{pmatrix}$$

Can help if μ close to row span of X

Ideal case:
$$\mu = X^T \beta$$

Gives
$$n^2 MSE(\hat{\tau}) = \mu^T Z \mu = \beta^T X Z X^T \beta$$

$$\leq ||\beta||_2^2 ||XZX^T||_2$$

As don't know B, will try to make $\|XZX^T\|_2$ small

Impact of Balance and Robustness

$$MSE(\hat{\tau}) \leq \frac{1}{n^2} \min_{\beta \in \mathbb{R}^d} \left[\sigma_z \left\| \mu - \chi^T \beta \right\|_2^2 + \sigma_x \left\| \beta \right\|_2^2 + Cross + term \right]$$

$$error of complexity safe to linear fit of \beta ignore$$

$$\sigma_{x} = \|x \neq x^{T}\|_{2}$$
 measures Balance

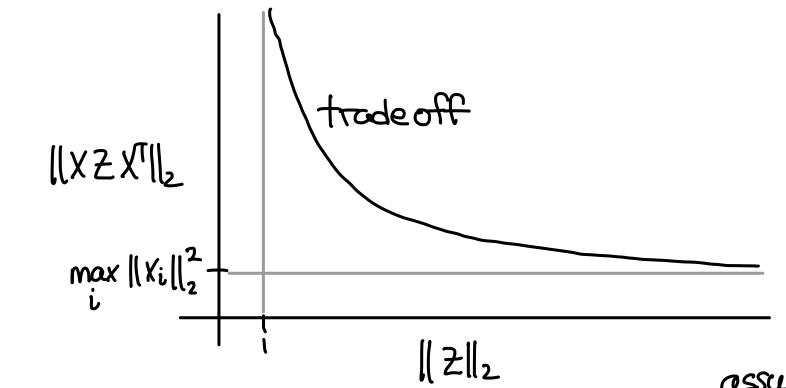
Balance - Robustness Tradeoff

Robustness

Balance

$$\|XZX^T\|_2 \ge 1$$

in general



assuming $\|x_i\|_2 \leq 1$

Matching Design

$$\|Z\|_{2} = 2$$

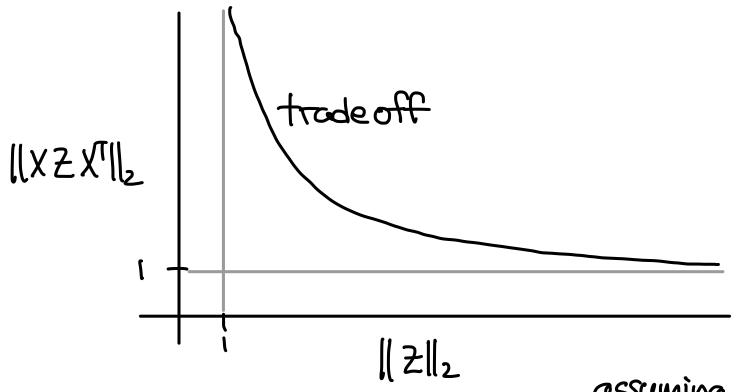
$$Z = \begin{cases} 1 - 100000 \\ -1 & 10000 \\ 000 - 1 & 1000 \\ 00000 \\ 00000 \\ 1 \end{cases}$$

For x,,...xn uniform in unit ball in IRd and best possible matching

$$\mathbb{E} \| XZX^{\mathsf{T}} \|_{2} \ge const \cdot \frac{1-2/d}{d}$$

For all $\phi \in (O(1), obtains$

$$\|Z\|_2 \leq \frac{1}{\phi} \|XZX^T\|_2 \leq \frac{1}{1-\phi}$$



assuming $\|x_i\|_2 \in 1$

For all $\phi \in (O(1), obtains$

$$\|Z\|_2 \leq \frac{1}{\phi} \|XZX^T\|_2 \leq \frac{1}{1-\phi}$$

$$Z \leq (\phi I + (\iota - \phi) \chi^{\mathsf{T}} \chi)^{-1}$$

$$MSE(\hat{\tau}) \leq \frac{1}{N^2} \min_{\beta \in \mathbb{R}^d} \left[\frac{1}{\phi} \|\mu - \chi_{\beta}^T\|^2 + \frac{1}{1-\phi} \|\beta\|^2 \right]$$

is a ridge regression regularized least squares

$$|| \text{Small when}$$

$$| \mu \text{ near span}$$

$$| \text{of } \chi$$

$$| \text{of } \chi$$

$$| \text{MSE}(\hat{\tau}) \leq \frac{1}{N^2} \min_{\substack{\beta \in \mathbb{R}^d \\ \text{with } n}} \left[\frac{1}{\beta} || \mu - \chi_{\beta}^T ||^2 + \frac{1}{1-\phi} || \beta ||^2 \right]$$

$$| \text{Grows} \qquad \text{Fixed as }$$

$$| \text{with } n \qquad \text{n grows}$$

In asymptotic regimes

for n >> d, want $\phi \rightarrow 1$ Almost as robust as iid,

but can have much lower MSE

For all $\phi \in (O(1), obtains)$

$$\|Z\|_2 \leq \frac{1}{\phi} \|XZX^T\|_2 \leq \frac{1}{1-\phi}$$

$$MSE(\hat{z}) \leq \frac{1}{N^2} \min_{B \in \mathbb{R}^d} \left[\frac{1}{\phi} \|\mu - \chi_B^T\|^2 + \frac{1}{1-\phi} \|\beta\|^2 \right]$$

With sub-Gaussian tails

Gram-Schmidt Walk of Bansal, Dadush, Garg, Lovett '19

A polynomial-time algorithm that on input $x_1, ..., x_n$ with $\|x_i\|_2 \le 1$ chooses a random $z \in \{\pm 1\}^n$

$$X_z = \sum_i z(i) x_i$$
 is $\int 40 - subgaussian$

-> Polynomial-time algorithm for Banaszczyk's Discrepancy Theorem

Gram-Schmidt Walk of Bansal, Dadush, Garg, Lovett '19

A polynomial-time algorithm that on input $x_1, ..., x_n$ with $\|x_i\|_2 \le 1$ chooses a random $z \in \{\pm 1\}^n$

so that || X Z X T || 2 = 40 1

$$X_z = \sum_i z(i) \times i$$
 is $\sqrt{10} - subgaussian$

Harshow, Sävje, S, Zhang

Choose tradeoff parameter $\phi \in (0,1)$

Run GSW on augmented covariate vectors

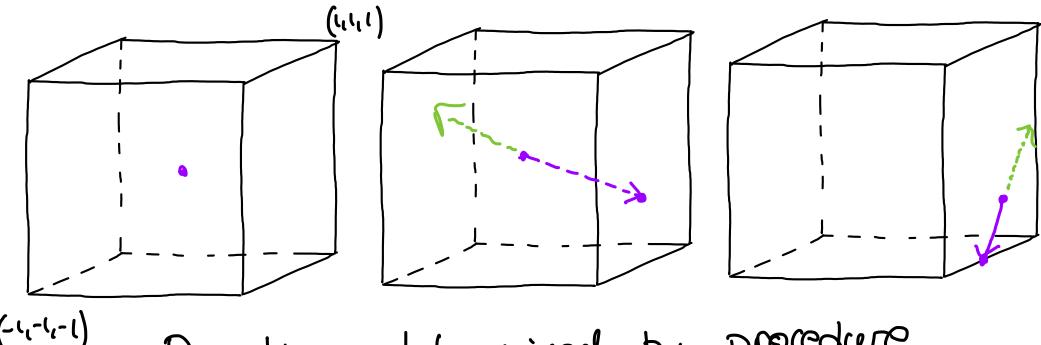
$$b_{i} = \left(\frac{\int \phi e_{i}}{\int l - \phi \times i} \right)$$
 elementary unit vector

Input matrix =
$$\begin{pmatrix} \int \phi & I \\ \int I - \phi & X \end{pmatrix}$$

And, randomly permute their order. *

Gram-Schmidt Walk Algorithm (BDGL)

Start with z=lo,...,o). Move inside [-1,1]



Directions determined by procedure like Gram-Schmidt.

Random steps provide Martingale

See also Beck-Fiala 181, Deville-Tillé 104

Improving GSW would require assumptions

Tradeoff within constant of optimal

Even for d fixed, $n \rightarrow \infty$, x; from nice distribution $\|XZX^T\|_2 \gtrsim 1$

Zhang 22: 3c>O st. NP-hard to distinguish

3 Z ||XZXT||=0

from YZ ||XZXT||≥c

In Practice

Can choose design after examining X and extensive simulation.

Can include functions of covariates.

Can weight covariates

Use ML, or regression, to adjust ??

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Can choose design after examining X and extensive simulation.

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Use ML, or regression, to adjust ??

$$MSE(\hat{\tau}) \leq \frac{1}{N^2} \min_{B \in \mathbb{R}^d} \left[\frac{1}{\phi} \|\mu - \chi_B^T\|^2 + \frac{1}{1-\phi} \|\beta\|^2 \right]$$

Open Problems

Online vetsion (see Kulkarni-Reis-Rothvoss)

Other relations between X and M?

Matrix Spencer Conjecture

Komlos Conjecture: $\exists c s+.$ $\forall x_1,...,x_n \text{ with } ||x_i||_2 \leq 1 \text{ for all } i$ $\exists z \in \exists 1 \end{cases}^n s+. ||z \neq i| x_i||_{\infty} \in C$

To learn more ...







Statistics > Methodology

[Submitted on 8 Nov 2019 (v1), last revised 4 Feb 2022 (this version, v5)]

Balancing covariates in randomized experiments with the Gram-Schmidt Walk design

Christopher Harshaw, Fredrik Sävje, Daniel Spielman, Peng Zhang

VI: CS style exposition

U2: For experimentalists and statisticians more results
different simulations

13, 14, 15, 16: adding stuff referees request 17: CLT, variance estimator, CI, +

Packages for Julia and R on Gittlub