TOPICS IN TWO-SAMPLE TESTING

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Contents

Chapter 1

Stein's method

In this chapter we present an introduction to Stein's method of exchangeable pairs which we use to prove the core theoretical result of this thesis: a rate of convergence bound for the randomization distribution.

1.1 Introduction

Stein's method provides a means of bounding the distance between two probability distributions in a given probability metric. When applied with the normal distribution as the target, this results in central limit type theorems. Several flavors of Stein's method (e.g. the method of exchangeable pairs) proceed via auxiliary randomization. We reproduce Stein's proof of the Hoeffding combinatorial central limit theorem (HCCLT) with explicit calculation of various constants. It will be instructive to follow the proof of the HCCLT because our proof proceeds in a similar fashion but with the following generalizations: an approximate contraction property, less cancellation of terms due to separate estimation of various denominators, and non-unit variance of an r.v. in the exchangeable pair.

1.2 Hoeffding combinatorial CLT

Theorem 1.1. *Let* $\{a_{ij}\}_{i,j}$ *be an* $n \times n$ *matrix of real-valued entries that is row- and column-centered and scaled such that the sums of the squares of its elements equals* $n-1$*:*

$$\sum_{j=1}^{n} a_{ij} = 0 \tag{1.1}$$

$$\sum_{i=1}^{n} a_{ij} = 0 \tag{1.2}$$

$$\sum_{i=1,j=1}^{n} a_{ij}^2 = n - 1 \tag{1.3}$$

Let Π *be a random permutation of* $\{1, \ldots, n\}$ *drawn uniformly at random from the set of all permutations:*

$$P(\Pi = \pi) = \frac{1}{n!}. \tag{1.4}$$

Define

$$W = \sum_{i=1}^{n} a_{i\Pi(i)} \tag{1.5}$$

to be the sum of a random diagonal. Then

$$|P(W \le w) - \Phi(w)| \le \frac{C}{\sqrt{n}} \left[\sqrt{\sum_{i,j=1}^{n} a_{ij}^4} + \sqrt{\sum_{i,j=1}^{n} |a_{ij}|^3} \right]. \tag{1.6}$$

Proof. In order to construct our exchangeable pair, we introduce the ordered pair of random variables (I, J) independent of Π that represents a uniformly at random draw from the set of all non-null transpositions:

$$P(I = i, J = j) = \frac{1}{n(n-1)} \quad i, j \in \{1, \ldots, n\}, i \neq j. \tag{1.7}$$

Define the random permutation Π' by

$$\Pi'(i) = \Pi \circ (I, J) = \begin{cases} \Pi(J) & i = I \\ \Pi(I) & i = J \\ \Pi(i) & \text{else.} \end{cases} \tag{1.8}$$

We construct our exchangeable pair by defining

$$W' = \sum_{i=1}^{n} a_{i\Pi'(i)} = W - a_{I\Pi(I)} + a_{I\Pi(J)} - a_{J\Pi(J)} + a_{J\Pi(I)}. \tag{1.9}$$

We now verify the contraction property:

$$\begin{aligned}
\mathbb{E}[W - W'|\Pi] &= \mathbb{E}[a_{I\Pi(I)} - a_{I\Pi(J)} + a_{J\Pi(J)} - a_{J\Pi(I)}|\Pi] \\
&= \frac{2}{n}\sum_{i=1}^{n} a_{i\Pi(i)} - \frac{2}{n}\frac{1}{n-1}\sum_{i,j=1, i\neq j}^{n} a_{i\Pi(j)} \\
&= \frac{2}{n}W - \frac{2}{n}\frac{1}{n-1}\left[\sum_{i,j=1}^{n} a_{i\Pi(j)} - \sum_{i}^{n} a_{i\Pi(i)}\right] \\
&= \frac{2}{n}W + \frac{2}{n}\frac{1}{n-1}W - \frac{2}{n}\frac{1}{n-1}\left[\sum_{i=1}^{n}\sum_{j=1}^{n} a_{i\Pi(j)}\right] \\
&= \frac{2}{n}W\left(1 + \frac{1}{n-1}\right) - 0 \\
&= \frac{2}{n-1}W
\end{aligned}$$

This satisfies our contraction property with

$$\lambda = \frac{2}{n-1}. \tag{1.10}$$

To bound the variance component, compute

$$
\begin{aligned}
\mathbb{E}[(W-W')^2|\Pi] &= \mathbb{E}[(a_{I\Pi(I)} - a_{I\Pi(J)} + a_{J\Pi(J)} - a_{J\Pi(I)})^2|\Pi] \\
&= \mathbb{E}[a_{I\Pi(I)}^2 + a_{J\Pi(J)}^2 + a_{I\Pi(J)}^2 + a_{J\Pi(I)}^2 \\
&\quad - 2a_{I\Pi(I)}a_{I\Pi(J)} - 2a_{J\Pi(J)}a_{J\Pi(I)} - 2a_{I\Pi(I)}a_{J\Pi(I)} - 2a_{J\Pi(J)}a_{I\Pi(J)} \\
&\quad + 2a_{I\Pi(I)}a_{J\Pi(J)} + 2a_{I\Pi(J)}a_{J\Pi(I)}|\Pi] \\
&= \frac{2}{n}\sum_{i=1}^n a_{i\Pi(i)}^2 + \frac{2}{n}\frac{1}{n-1}\sum_{i,j=1,i\neq j}^n a_{i\Pi(j)}^2 \\
&\quad - \frac{4}{n}\frac{1}{n-1}\sum_{i,j=1,i\neq j}^n a_{i\Pi(i)}a_{i\Pi(j)} - \frac{4}{n}\frac{1}{n-1}\sum_{i,j=1,i\neq j}^n a_{i\Pi(i)}a_{j\Pi(i)} \\
&\quad + \frac{2}{n}\frac{1}{n-1}\sum_{i,j=1,i\neq j}^n a_{i\Pi(i)}a_{j\Pi(j)} + \frac{2}{n}\frac{1}{n-1}\sum_{i,j=1,i\neq j}^n a_{i\Pi(j)}a_{j\Pi(i)} \\
&= \frac{2}{n}\sum_{i=1}^n a_{i\Pi(i)}^2 + \frac{2}{n}\frac{1}{n-1}\left(\sum_{i,j=1}^n a_{i\Pi(j)}^2 - \sum_{i=1}^n a_{i\Pi(i)}^2\right) \\
&\quad - \frac{4}{n}\frac{1}{n-1}\sum_{i=1}^n\left(a_{i\Pi(i)}\sum_{j=1}^n\left(a_{i\Pi(j)} + a_{j\Pi(i)}\right) - 2a_{i\Pi(i)}^2\right) \\
&\quad + \frac{2}{n}\frac{1}{n-1}\left(\sum_{i,j=1,i\neq j}^n a_{i\Pi(i)}a_{j\Pi(j)} + a_{i\Pi(j)}a_{j\Pi(i)}\right) \\
&= \frac{2}{n}\left(1 - \frac{1}{n-1}\right)\sum_{i=1}^n a_{i\Pi(i)}^2 + \frac{2}{n} \\
&\quad + \frac{8}{n}\frac{1}{n-1}\sum_{i=1}^n a_{i\Pi(i)}^2 \\
&\quad + \frac{2}{n}\frac{1}{n-1}\sum_{i=1}^n\sum_{j=1}^n\left(a_{i\Pi(i)}a_{j\Pi(j)} + a_{i\Pi(j)}a_{j\Pi(i)}\right) - \frac{4}{n}\frac{1}{n-1}\sum_{i=1}^n a_{i\Pi(i)}^2 \\
&= \frac{2}{n} + \frac{2(n+2)}{n(n-1)}\sum_{i=1}^n a_{i\Pi(i)}^2 + \frac{2}{n(n-1)}\sum_{i,j=1,i\neq j}^n (a_{i\Pi(i)}a_{j\Pi(j)} + a_{i\Pi(j)}a_{j\Pi(i)})
\end{aligned}
\tag{1.11}
$$

Theorem 1.2 (The c_r-inequality)**.** *Let $r > 0$. Suppose that $\mathbb{E}|X|^r < \infty$ and $\mathbb{E}|Y|^r <$*

∞. *Then*

$$\mathbb{E}|X+Y|^r < c_r(\mathbb{E}|X|^r + \mathbb{E}|Y|^r), \tag{1.12}$$

where $c_r = 1$ *when* $r \leq 1$ *and* $c_r = 2^{r-1}$ *when* $r \geq 1$.

Corollary 1.3. *Suppose that* $\mathrm{Var}(X) < \infty$ *and* $\mathrm{Var}(Y) < \infty$. *Then*

$$\mathrm{Var}(X+Y) < 2(\mathrm{Var}(X) + \mathrm{Var}(Y)). \tag{1.13}$$

Proof. This follows immediately by applying Theorem 1.2 to the centered random variables $X' = X - \mathbb{E}[X]$ and $Y' = Y - \mathbb{E}[Y]$. $\square$

From (1.11) and corollary 1.3,

$$\begin{aligned}
\mathbb{E}[(W-W')^2|\Pi] = \mathrm{Var}\Bigg(&\frac{2(n+2)}{n(n-1)}\sum_{i=1}^{n} a_{i\Pi(i)}^2 \\
&+\frac{2}{n(n-1)}\sum_{i,j=1,i\neq j}^{n}(a_{i\Pi(i)}a_{j\Pi(j)} + a_{i\Pi(j)}a_{j\Pi(i)})\Bigg) \\
\leq 2\Bigg(&\frac{4(n+2)^2}{n^2(n-1)^2}\mathrm{Var}\left(\sum_{i=1}^{n} a_{i\Pi(i)}^2\right) + \\
&\frac{4}{n^2(n-1)^2}\mathrm{Var}\left(\sum_{i,j=1,i\neq j}^{n}(a_{i\Pi(i)}a_{j\Pi(j)} + a_{i\Pi(j)}a_{j\Pi(i)})\right)\Bigg) \\
\leq \frac{32}{n^2}&\mathrm{Var}\left(\sum_{i=1}^{n} a_{i\Pi(i)}^2\right) + \frac{32}{n^4}\mathrm{Var}\left(\sum_{i,j=1,i\neq j}^{n}(a_{i\Pi(i)}a_{j\Pi(j)} + a_{i\Pi(j)}a_{j\Pi(i)})\right)
\end{aligned} \tag{1.14}$$

for $n \geq 2$ since $n-1 \geq n/2 \implies \frac{1}{(n-1)^2} \leq \frac{4}{n^2}$ for $n \geq 2$.

First, we address the first term in (1.14):

$$\mathrm{Var}\left(\sum_{i=1}^{n} a_{i\Pi(i)}^2\right) = \sum_{i=1}^{n}\mathrm{Var}(a_{i\Pi(i)}^2) + \sum_{i,j=1,i\neq j}^{n}\mathrm{Cov}(a_{i\Pi(i)}^2, a_{j\Pi(j)}^2),$$

with

$$\begin{aligned}
\sum_{i,j=1,i\neq j}^{n} \mathrm{Cov}(a_{i\Pi(i)}^2, a_{j\Pi(j)}^2) &= \sum_{i,j=1,i\neq j}^{n} \left(\frac{1}{n(n-1)} \sum_{k,l=1,k\neq l}^{n} a_{ik}^2 a_{jl}^2 - \left(\frac{1}{n}\sum_k a_{ik}^2\right)\left(\frac{1}{n}\sum_l a_{jl}^2\right)\right) \\
&= \sum_{i,j=1,i\neq j}^{n} \left(\frac{1}{n(n-1)} \sum_{k,l=1}^{n} a_{ik}^2 a_{jl}^2 - \frac{1}{n^2}\sum_k \sum_l a_{ik}^2 a_{jl}^2 - \frac{1}{n(n-1)}\sum_k a_{ik}^2 a_{jk}^2 \right) \\
&= \frac{1}{n^2(n-1)} \sum_{i,j=1,i\neq j}^{n} \sum_{k,l=1}^{n} a_{ik}^2 a_{jl}^2 - \frac{1}{n(n-1)} \sum_{i,j=1,i\neq j}^{n} \sum_k a_{ik}^2 a_{jk}^2 \\
&\leq \frac{(n-1)^2}{n^2(n-1)} \\
&\leq \frac{1}{n}
\end{aligned}$$

It will be convenient to express our bound as a multiple of $\sum_{i,j=1}^n a_{i,j}^4$, so we establish a lower bound on that quantity. Our scaling is such that $\sum_{i,j=1}^n a_{i,j}^2 = n-1$, so if we write $\mathbf{a} := [a_{11}^2\ a_{12}^2 \ldots a_{nn}^2]^T$ out as a vector, $\mathbf{a}^T\mathbf{1} = n-1$. By Cauchy-Schwarz,

$$\begin{aligned}
(n-1)^2 &= (\mathbf{a}^T\mathbf{1})^2 \\
&\leq ||\mathbf{a}||_2^2 ||\mathbf{1}||_2^2 \\
&= n^2 \sum_{i,j=1}^{n} a_{i,j}^4.
\end{aligned}$$

Therefore, $\sum_{i,j=1}^n a_{i,j}^4 \geq 1$, so

$$\sum_{i,j=1,i\neq j}^{n} \mathrm{Cov}(a_{i\Pi(i)}^2, a_{j\Pi(j)}^2) \leq \frac{1}{n} \sum_{i,j=1}^{n} a_{i,j}^4. \tag{1.15}$$

For the second term in (1.14) we again apply corollary 1.3:

$$\mathrm{Var}\left(\sum_{i,j=1,i\neq j}^{n} (a_{i\Pi(i)}a_{j\Pi(j)} + a_{i\Pi(j)}a_{j\Pi(i)}) \right) < 2\,\mathrm{Var}\,(X) + 2\,\mathrm{Var}\,(Y)\,,$$

where $X = \sum_{i,j=1,i\neq j}^{n} a_{i\Pi(i)}a_{j\Pi(j)}$ and $Y = \sum_{i,j=1,i\neq j}^{n} a_{i\Pi(j)}a_{j\Pi(i)}$. We note that

$$X = \sum_{i=1}^{n} a_{i\Pi(i)} \sum_{j=1,j\neq i}^{n} a_{j\Pi(j)} = W^2 - \sum_{i=1}^{n} a_{i\Pi(i)}^2. \tag{1.16}$$

TODO: ... Maybe finish this up later? □

1.3 Exchangeable Pairs

TODO: Add a lot of development for exchangeable pairs. For now, focusing on generalizing the theorems in "Normal Approximation by Stein's Method."

Theorem 5.5 in "Normal Approximation by Stein's Method" concerns variance 1 exchangeable random variables. Our setting has the variance tending to 1, so we first prove a slight generalization of the theorem. Large parts of the proof are copied verbatim from the book.

1.4 Preliminaries

Definition 1.4 (Approximate Stein Pair)**.** *Let (W, W') be an exchangeable pair. If the pair satisfies the "approximate linear regression condition"*

$$\mathbb{E}[W - W'|W] = \lambda(W - R) \tag{1.17}$$

where R is a variable of small order and $\lambda \in (0, 1)$, then we call (W, W') an approximate Stein pair.

Lemma 1.5. *If (W, W') is an exchangeable pair, then $\mathbb{E}[g(W, W')] = 0$ for all anti-symmetric measurable functions such that the expected value exists.*

Here is a slight generalization of Lemma 2.7:

Lemma 1.6. *Let (W, W') be an approximate Stein pair and $\Delta = W - W'$. Then*

$$\mathbb{E}[W] = \mathbb{E}[R] \quad \textit{and} \quad \mathbb{E}[\Delta^2] = 2\lambda\mathbb{E}[W^2] - 2\lambda\mathbb{E}[WR] \quad \textit{if } \mathbb{E}[W^2] < \infty. \tag{1.18}$$

Furthermore, when $\mathbb{E}[W^2] < \infty$*, for every absolutely continuous function* f *satisfying* $|f(w)| \leq C(1 + |w|)$*, we have*

$$\mathbb{E}[Wf(W)] = \frac{1}{2\lambda} = \mathbb{E}[(W - W')(f(W) - f(W'))] + \mathbb{E}[f(W)R]. \tag{1.19}$$

Proof. From (1.17) we have

$$\mathbb{E}[\mathbb{E}[W - W'|W]] = \mathbb{E}[\lambda(W - R)] = \lambda\mathbb{E}[W] - \lambda\mathbb{E}[R].$$

We also have

$$\mathbb{E}[\mathbb{E}[W - W'|W]] = \mathbb{E}[W] - \mathbb{E}[\mathbb{E}[W'|W]] = \mathbb{E}[W] - \mathbb{E}[W'] = 0$$

using exchangeability. Equating the two expressions yields

$$\mathbb{E}[W] = \mathbb{E}[R]$$

As an intermediate computation,

$$\begin{aligned}
\mathbb{E}[W'W] &= \mathbb{E}[\mathbb{E}[W'W|W]] \\
&= \mathbb{E}[W\mathbb{E}[W'|W]] \\
&= \mathbb{E}[W((1 - \lambda)W + \lambda R)] \quad \text{from (1.17)} \\
&= (1 - \lambda)\mathbb{E}[W^2] + \lambda\mathbb{E}[WR].
\end{aligned} \tag{1.20}$$

Then

$$\begin{aligned}
\mathbb{E}[\Delta^2] &= \mathbb{E}[(W - W')^2] \\
&= \mathbb{E}[W^2] + \mathbb{E}[W'^2] - 2\mathbb{E}[W'W] \\
&= 2\mathbb{E}[W^2] - 2((1 - \lambda)\mathbb{E}[W^2] + \lambda\mathbb{E}[WR]) \quad \text{from (1.20)} \\
&= 2\lambda\mathbb{E}[W^2] - 2\lambda\mathbb{E}[WR].
\end{aligned} \tag{1.21}$$

By the linear growth assumption on f, $\mathbb{E}[g(W, W')]$ exists for the antisymmetric function $g(x,y) = (x-y)(f(y)+f(x))$. By Lemma 1.5,

$$\begin{aligned} 0 &= \mathbb{E}[(W-W')(f(W')+f(W))] \\ &= \mathbb{E}[(W-W')(f(W')-f(W))] + 2\mathbb{E}[f(W)(W-W')] \\ &= \mathbb{E}[(W-W')(f(W')-f(W))] + 2\mathbb{E}[f(W)\mathbb{E}[(W-W')|W]] \\ &= \mathbb{E}[(W-W')(f(W')-f(W))] + 2\mathbb{E}[f(W)(\lambda(W-R))]. \end{aligned}$$

Rearranging the expression yields

$$\mathbb{E}[Wf(W)] = \frac{1}{2\lambda}\mathbb{E}[(W-W')(f(W)-f(W'))] + \mathbb{E}[f(W)R]. \tag{1.22}$$

□

This is just a small part of Lemma 2.4:

Lemma 1.7. *For a given function $h : \mathbb{R} \to \mathbb{R}$, let f_h be the solution to the Stein equation. If h is absolutely continuous, then*

$$||f_h|| \leq 2||h'||. \tag{1.23}$$

1.5 Main Theorem

Generalization of Theorem 5.5:

Theorem 1.8. *If T, T' are mean 0 exchangeable random variables with variance $\mathbb{E}[T^2]$ satisfying*

$$\mathbb{E}[T'-T|T] = -\lambda(T-R)$$

for some $\lambda \in (0,1)$ and some random variable R, then

$$\begin{aligned} \sup_{t\in\mathbb{R}} |P(T \leq t) - \Phi(t)| \leq (2\pi)^{-1/4}\sqrt{\frac{\mathbb{E}[|T'-T|^3]}{\lambda}} + \frac{1}{2\lambda}\sqrt{\mathrm{Var}(\mathbb{E}[(T'-T)^2|T])} \\ + |\mathbb{E}[T^2]-1| + \mathbb{E}|TR| + \mathbb{E}[|R|] \end{aligned}$$

Proof. For $z \in \mathbb{R}$ and $\alpha > 0$ let f be the solution to the Stein equation

$$f'(w) - wf(w) = h_{z,\alpha}(w) - \Phi(z) \tag{1.24}$$

for the smoothed indicator

$$h_{z,\alpha}(w) = \begin{cases} 1 & w \leq z \\ 1 + \frac{z-w}{\alpha} & z < w \leq z + \alpha \\ 0 & w > z + \alpha. \end{cases} \tag{1.25}$$

Therefore,

$$\begin{aligned} |P(W \leq z) - \Phi(z)| &= |\mathbb{E}[(f'(W) - Wf(W))]| \\ &= \left|\mathbb{E}\left[f'(W) - \frac{(W'-W)(f(W') - f(W))}{2\lambda} + f(W)R\right]\right| \\ &= \left|\mathbb{E}\left[f'(W)\left(1 - \frac{(W'-W)^2}{2\lambda}\right)\right.\right. \\ &\quad \left.\left. + \frac{f'(W)(W'-W)^2 - (f(W') - f(W))(W'-W)}{2\lambda} + f(W)R\right]\right| \\ &:= |\mathbb{E}[J_1 + J_2 + J_3]| \\ &\leq |\mathbb{E}[J_1]| + |\mathbb{E}[J_2]| + |\mathbb{E}[J_3]|. \end{aligned} \tag{1.26}$$

It is known from Chen and Shao (2004) that for all $w \in \mathbb{R}, 0 \leq f(w) \leq 1$ and $|f'(w)| \leq 1$. Then

$$|\mathbb{E}[J_3]| \leq \mathbb{E}[|J_3|] = \mathbb{E}[|f(W)R|] \leq \mathbb{E}[|R|] \tag{1.27}$$

and

$$
\begin{aligned}
|\mathbb{E}[J_1]| &= \left|\mathbb{E}\left[f'(W)\left(1-\frac{(W'-W)^2}{2\lambda}\right)\right]\right| \\
&\leq \mathbb{E}\left[\left|f'(W)\left(1-\frac{(W'-W)^2}{2\lambda}\right)\right|\right] \\
&\leq \mathbb{E}\left[\left|\left(1-\frac{(W'-W)^2}{2\lambda}\right)\right|\right] \\
&= \frac{1}{2\lambda}\mathbb{E}[|2\lambda-\mathbb{E}[(W'-W)^2|W]|] \\
&= \frac{1}{2\lambda}\mathbb{E}[|2\lambda(\mathbb{E}[W^2]-\mathbb{E}[WR])-\mathbb{E}[(W'-W)^2|W]+2\lambda(1-\mathbb{E}[W^2]+\mathbb{E}[WR])|] \\
&\leq \frac{1}{2\lambda}\mathbb{E}[|2\lambda(\mathbb{E}[W^2]-\mathbb{E}[WR])-\mathbb{E}[(W'-W)^2|W]|]+\mathbb{E}[|(1-\mathbb{E}[W^2]+\mathbb{E}[WR])|]
\end{aligned} \tag{1.28}
$$

Note that

$$\mathbb{E}[\mathbb{E}[(W'-W)^2|W]]=\mathbb{E}[\Delta^2]=2\lambda(\mathbb{E}[W^2]-\mathbb{E}[WR]), \tag{1.29}$$

so

$$\frac{1}{2\lambda}\mathbb{E}[|2\lambda(\mathbb{E}[W^2]-\mathbb{E}[WR])-\mathbb{E}[(W'-W)^2|W]|]\leq\frac{1}{2\lambda}\sqrt{\mathrm{Var}(\mathbb{E}[(W'-W)^2|W])}. \tag{1.30}$$

Combining with (1.28),

$$
\begin{aligned}
|\mathbb{E}[J_1]| &\leq \frac{1}{2\lambda}\sqrt{\mathrm{Var}(\mathbb{E}[(W'-W)^2|W])}+\mathbb{E}[|1-\mathbb{E}[W^2]+\mathbb{E}[WR]|] \\
&\leq \frac{1}{2\lambda}\sqrt{\mathrm{Var}(\mathbb{E}[(W'-W)^2|W])}+\mathbb{E}[|1-\mathbb{E}W^2|]+\mathbb{E}|WR|
\end{aligned} \tag{1.31}
$$

Lastly, we bound the second term,

$$
\begin{aligned}
J_2 &= \frac{1}{2\lambda}(W'-W)\int_W^{W'}(f'(W)-f'(t))dt \\
&= \frac{1}{2\lambda}(W'-W)\int_W^{W'}\int_t^W f''(u)dudt \\
&= \frac{1}{2\lambda}(W'-W)\int_W^{W'}(W'-u)f''(u)du.
\end{aligned} \tag{1.32}
$$

To show the final equality, consider separately the cases $W \leq W'$ and $W' \leq W$. For the former,

$$
\begin{aligned}
-\frac{1}{2\lambda}(W'-W)\int_W^{W'}\int_W^t f''(u)dudt &= -\frac{1}{2\lambda}(W'-W)\int_W^{W'}\int_u^{W'} f''(u)dtdu \\
&= -\frac{1}{2\lambda}(W'-W)\int_W^{W'}(W'-u)f''(u)du.
\end{aligned}
$$

For the latter,

$$
\begin{aligned}
\frac{1}{2\lambda}(W'-W)\int_W^{W'}\int_t^{W} f''(u)dudt &= -\frac{1}{2\lambda}(W'-W)\int_{W'}^{W}\int_t^{W} f''(u)dudt \\
&= -\frac{1}{2\lambda}(W'-W)\int_{W'}^{W}\int_{W'}^{u} f''(u)dtdu \\
&= -\frac{1}{2\lambda}(W'-W)\int_{W'}^{W}(u-W')f''(u)du.
\end{aligned}
$$

Since W and W' are exchangeable,

$$
\begin{aligned}
|\mathbb{E}[J_2]| &= \left|\mathbb{E}\left[\frac{1}{2\lambda}(W'-W)\int_W^{W'}(W'-u)f''(u)du\right]\right| \\
&= \left|\mathbb{E}\left[\frac{1}{2\lambda}(W'-W)\int_W^{W'}\left(\frac{W+W'}{2}-u\right)f''(u)du\right]\right| \\
&\leq \left|\mathbb{E}\left[||f''||\frac{1}{2\lambda}|W'-W|\int_{\min(W,W')}^{\max(W,W')}\left|\frac{W+W'}{2}-u\right|du\right]\right| \qquad (1.33)\\
&= \left|\mathbb{E}\left[||f''||\frac{1}{2\lambda}\frac{|W'-W|^3}{4}\right]\right| \\
&\leq \frac{\mathbb{E}[|W'-W|^3]}{4\alpha\lambda},
\end{aligned}
$$

where the final inequality follows from the fact that $|h'_{z,\alpha}(x)| \leq 1/\alpha$ for all $x \in \mathbb{R}$ and Lemma 1.7.

Collecting the bounds, we obtain

$$\begin{aligned}
P(W \leq z) &\leq \mathbb{E}[h_{z,\alpha}(W)] \\
&\leq Nh_{z,\alpha} + \frac{\mathbb{E}[|W' - W|^3]}{4\alpha\lambda} + \frac{1}{2\lambda}\sqrt{\mathrm{Var}(\mathbb{E}[(W' - W)^2|W])} \\
&\quad + |1 - \mathbb{E}[W^2]| + \mathbb{E}|WR| + \mathbb{E}|R| \qquad (1.34) \\
&\leq \Phi(z) + \frac{\alpha}{\sqrt{2\pi}} + \frac{\mathbb{E}[|W' - W|^3]}{4\alpha\lambda} + \frac{1}{2\lambda}\sqrt{\mathrm{Var}(\mathbb{E}[(W' - W)^2|W])} \\
&\quad + |\mathbb{E}[W^2] - 1| + \mathbb{E}|WR| + \mathbb{E}|R|
\end{aligned}$$

The minimizer of the expression is

$$\alpha = \frac{(2\pi)^{1/4}}{2}\sqrt{\frac{\mathbb{E}[|W' - W|^3]}{\lambda}}. \tag{1.35}$$

Plugging this in, we get the upper bound

$$\begin{aligned}
P(W \leq z) - \Phi(z) \leq (2\pi)^{-1/4}\sqrt{\frac{\mathbb{E}[|W' - W|^3]}{\lambda}} + \frac{1}{2\lambda}\sqrt{\mathrm{Var}(\mathbb{E}[(W' - W)^2|W])} \\
+ |\mathbb{E}[W^2] - 1| + \mathbb{E}|WR| + \mathbb{E}|R|
\end{aligned} \tag{1.36}$$

Proving the corresponding lower bound in a similar manner completes the proof of the theorem. □

Chapter 2

Main Proof

In this chapter, we prove the core theoretical result of this thesis: a rate of convergence bound for the randomization distribution of the t-statistic, using theorem 1.8 of chapter 1.

2.1 Motivation

Motivated by concerns regarding normality assumptions in the hypothesis being tested, Fisher [5] proposed a nonparametric randomization test. Also known as a permutation test, Fisher applied this novel test to Charles Darwin's *Zea mays* data and noted that the achieved significance level was very similar to that observed in the parametric test. Indeed, Diaconis and Holmes [3] used efficient Gray code based calculations to show that the randomization distribution looked remarkably normal. For more history on the development of randomization procedures, see Zabell [12] or David [2]. Diaconis and Lehmann [4] in their comment on Zabell's paper further expanded on some properties of these randomization tests.

Ludbrook and Dudley [7] have written about the advantages of permutation tests, especially in biomedical research, and outlined two models of statistical inference: the so-called population model, formally introduced by Newman and Pearson [8], and Fisher's randomization model [5]. Add some more on these two models...

Under the randomization model and using the language of triangular arrays, Lehmann [6] proved a weak convergence result of the randomization distribution of the t-statistic to the standard normal distribution, however, there is no known Berry-Esseen type bound for this rate of convergence.

Introduced by Stein [11], the eponymous technique provides a powerful means with which to handle dependencies among collections of random variables, a common criticism of classical Fourier analytic methods. In addition, one can easily obtain bounds on rates of convergence. Bentkus and Götze [1] first obtained a Berry-Esseen bound for Student's statistic in the independent but non-identically distributed setting with additional work by Shao [10].

We use Stein's method of exchangeable pairs to prove a conservative bound of $O(N^{-1/4})$ on the rate of convergence of the randomization t-distribution to the standard normal distribution.

2.2 Set-up

We observe two samples with equal sample size: $S_1 = \{u_i\}_{i=1}^N$ and $S_2 = \{u_i\}_{i=N+1}^{2N}$. Since we consider the t-statistic under different permutations, it will be convenient to re-write the sample values relative to the null permutation π_0: $S_1 = \{u_{\pi_0(i)}\}_{i=1}^N$ and $S_2 = \{u_{\pi_0(i)}\}_{i=N+1}^{2N}$. Student's two-sample t-statistic is given by

$$\begin{aligned}
T_\Pi(\{u_{\Pi(i)}\}_{i=1}^N, \{u_{\Pi(i)}\}_{i=N+1}^{2N}) &= \frac{\bar{u}_{1,\Pi} - \bar{u}_{2,\Pi}}{\sqrt{\frac{\frac{1}{N-1}\sum_{i=1}^N (u_{\Pi(i)} - \bar{u}_{1,\Pi})^2}{N} + \frac{\frac{1}{N-1}\sum_{i=N+1}^{2N} (u_{\Pi(i)} - \bar{u}_{2,\Pi})^2}{N}}} \\
&= \frac{1}{\sqrt{\frac{N}{N-1}}} \frac{\sum_{i=1}^N u_{\Pi(i)} - \sum_{i=N+1}^{2N} u_{\Pi(i)}}{\sqrt{\sum_{i=1}^N (u_{\Pi(i)} - \bar{u}_{1,\Pi})^2 + \sum_{i=N+1}^{2N} (u_{\Pi(i)} - \bar{u}_{2,\Pi})^2}} \\
&= \sqrt{\frac{N-1}{N}} \frac{q_\Pi}{d_\Pi},
\end{aligned}$$

where

$$q_\Pi = \left(\sum_{i=1, i\neq I}^{N} u_{\Pi(i)} + u_{\Pi(I)} - \sum_{i=N+1, i\neq J}^{2N} u_{\Pi(i)} - u_{\Pi(J)} \right)$$

$$d_\Pi = \sqrt{\sum_{i=1}^{N} (u_{\Pi(i)} - \bar{u}_{1,\Pi})^2 + \sum_{i=N+1}^{2N} (u_{\Pi(i)} - \bar{u}_{2,\Pi})^2}$$

$$\bar{u}_{1,\Pi} = \frac{1}{N} \sum_{i=1}^{N} u_{\Pi(i)} \text{ and } \bar{u}_{2,\Pi} = \frac{1}{N} \sum_{i=N+1}^{2N} u_{\Pi(i)}$$

In order to perform hypothesis testing, we compute the observed value of $T_{\Pi=\pi_0}$ and compare that with the randomization distribution of T_Π. We shall create an exchangeable pair (T_Π, T'_Π) by considering a uniformly random transposition (I, J). WLOG, take $I \leq J$. We apply this transposition to the group labels. Note that if $I, J \in \{1, \ldots, N\}$ or $I, J \in \{N+1, \ldots, 2N\}$ then $T'_\Pi = T_\Pi$, where T'_Π is the t-statistic under this random transposition. That is, the t-statistic is invariant to within-group transpositions: the only changes occur when $1 \leq I \leq N$ and $N+1 \leq J \leq 2N$. With this in mind, let's redefine our transposition to be uniformly at random over the N^2 cases where $1 \leq I \leq N$ and $N+1 \leq J \leq 2N$. Thus,

$$\begin{aligned}
T'_\Pi(\{u_{\Pi(i)}\}_{i=1}^{N}, \{u_{\Pi(i)}\}_{i=N+1}^{2N}) &= T_{\Pi\circ(I,J)}(\{u_{\Pi\circ(I,J)(i)}\}_{i=1}^{N}, \{u_{\Pi\circ(I,J)(i)}\}_{i=N+1}^{2N}) \\
&= \sqrt{\frac{N-1}{N}} \frac{q'_\Pi}{d'_\Pi} \\
q'_\Pi &= \left(\sum_{i=1, i\neq I}^{N} u_{\Pi(i)} + u_{\Pi(J)} - \sum_{i=N+1, i\neq J}^{2N} u_{\Pi(i)} - u_{\Pi(I)} \right) \\
&= q_\Pi - 2u_{\Pi(I)} + 2u_{\Pi(J)} \\
d'_\Pi &= \sqrt{\sum_{i=1}^{N} (u_{\Pi(i)} - \bar{u}'_{1,\Pi})^2 + \sum_{i=N+1}^{2N} (u_{\Pi(i)} - \bar{u}'_{2,\Pi})^2}.
\end{aligned}$$

2.3 Assumptions

Recall that the t-statistic is invariant up to sign under linear transformations, so we can mean-center and scale so that $\sum_{i=1}^{2N} u_i = 0$ and $\sum_{i=1}^{2N} u_i^2 = 2N$. The transformation that achieves this centering and scaling is given by

$$z_i = \sqrt{\frac{2N}{\sum(u_i - \bar{u})^2}}(u_i - \bar{u}), \tag{2.1}$$

so we just assume that the u_i's have already been transformed. This can be seen as a very mild assumption: only $u_i = c$ for all i cannot be scaled in this way.

We also assume that the pooled sample standard deviation is non-zero for all permutations:

$$d_\Pi = \sqrt{\sum_{i=1}^{N}(u_{\Pi(i)} - \bar{u}_{1,\Pi})^2 + \sum_{i=N+1}^{2N}(u_{\Pi(i)} - \bar{u}_{2,\Pi})^2} > 0 \tag{2.2}$$

This estimate is zero if and only if there exists a grouping that is constant in each group. The condition also implies that the sample mean for any group is strictly less than 1 in absolute value. In fact, this assumption subsumes the former.

The mean-centering assumption implies that $\sum_{i=1}^{N} u_{\Pi(i)} = -\sum_{i=N+1}^{2N} u_{\Pi(i)}$ and hence that $\bar{u}_{1,\Pi} = -\bar{u}_{2,\Pi}$ for all Π.

Here we establish an equality with d_Π that will prove easier to work with:

$$\begin{aligned}
d_\Pi^2 &= \sum_{i=1}^{N}(u_{\Pi(i)} - \bar{u}_{1,\Pi})^2 + \sum_{i=N+1}^{2N}(u_{\Pi(i)} - \bar{u}_{2,\Pi})^2 \\
&= \sum_{i=1}^{2N} u_{\Pi(i)}^2 - N\bar{u}_{1,\Pi}^2 - N\bar{u}_{2,\Pi} \\
&= 2N - N\bar{u}_{2,\Pi}^2 - N\bar{u}_{2,\Pi}^2 \\
&= 2N(1 - \bar{u}_{2,\Pi}^2)
\end{aligned}$$

Since $d_\Pi > 0$, it follows that $|\bar{u}_{2,\Pi}| < 1$. Define

$$B = \max_{\Pi} |\bar{u}_{2,\Pi}| < 1. \tag{2.3}$$

2.4 Preliminaries

Here we collect useful bounds and other results.

In order to bound various moments of $\bar{u}_{2,\Pi}$ under the permutation distribution, we use a result of Serfling's [9]:

Proposition 2.1. *Consider sampling without replacement from a finite list of values $u_1, \ldots, u_{2N}$. Let $u_\Delta = \max_i u_i - \min_i u_i$. Then for $p > 0$,*

$$\begin{aligned}
\mathbb{E}[\bar{u}_{2,\Pi}^p] &\leq \frac{\Gamma(p/2+1)}{2^{p/2+1}} \left[\frac{N+1}{2N} u_\Delta^2\right]^{p/2} (2N)^{-p/2} \\
&\leq \frac{\Gamma(p/2+1)}{2^{p/2+1}} \left[\frac{N+1}{4N} u_\Delta^2\right]^{p/2} N^{-p/2} \\
&:= f_{c_1}(p) N^{-p/2}.
\end{aligned} \tag{2.4}$$

By assumption (2.3),

$$(d_\Pi)^{-p} = \frac{1}{(2N(1-\bar{u}_{2,\Pi}^2))^{p/2}} \leq \frac{1}{(2N(1-B^2))^{p/2}} := f_{c_2}(p) N^{-p/2}. \tag{2.5}$$

The transposition (I, J) also affects the denominator of T'_Π, and we need to quantify the difference between the denominators of T_Π and T'_Π. Letting $\bar{u}'^2_{2,\Pi}$ denote the sample mean of the second group after the transposition,

$$\begin{aligned}
\bar{u}'^2_{2,\Pi} &= \left(\bar{u}_{2,\Pi} - \frac{1}{N} u_{\Pi(J)} + \frac{1}{N} u_{\Pi(I)}\right)^2 \\
&= \bar{u}_{2,\Pi}^2 + 2\bar{u}_{2,\Pi} \left(-\frac{1}{N} u_{\Pi(J)} + \frac{1}{N} u_{\Pi(I)}\right) + \frac{1}{N^2} (u_{\Pi(I)} - u_{\Pi(J)})^2
\end{aligned}$$

We consider the difference

$$\begin{aligned}
h_\Pi &= d_\Pi^2 - d_\Pi'^2 \\
&= 2N - 2N\bar{u}_{2,\Pi}^2 - 2N + 2N\bar{u}_{2,\Pi}'^2 \\
&= 4\bar{u}_{2,\Pi}(u_{\Pi(I)} - u_{\Pi(J)}) + \frac{2}{N}(u_{\Pi(I)} - u_{\Pi(J)})^2
\end{aligned}$$

Therefore, by the c_r-inequality,

$$\begin{aligned}
\mathbb{E}[h_\Pi^p] &= \mathbb{E}\left|4\bar{u}_{2,\Pi}(u_{\Pi(I)} - u_{\Pi(J)}) + \frac{2}{N}(u_{\Pi(I)} - u_{\Pi(J)})^2\right|^p \\
&\le 2^{p-1}\left(\mathbb{E}|4\bar{u}_{2,\Pi}(u_{\Pi(I)} - u_{\Pi(J)})|^p + \mathbb{E}\left|\frac{2}{N}(u_{\Pi(I)} - u_{\Pi(J)})^2\right|^p\right) \\
&\le 2^{p-1}\left[(4u_\Delta)^p\mathbb{E}\left|\bar{u}_{2,\Pi}\right|^p + \left(\frac{2}{N}u_\Delta^2\right)^p\right] \\
&\le 2^{p-1}(4u_\Delta)^p f_{c_1}(p)N^{-p/2} + 2^{p-1}(2u_\Delta^2)^p N^{-p} \\
&:= f_{c_3}(p)N^{-p/2}. \qquad (2.6)
\end{aligned}$$

Now we establish a bound on the difference $d_\Pi - d_\Pi'$ via a bound on the remainder of a zeroth order Taylor approximation. Write

$$d_\Pi' = \sqrt{d_\Pi^2 - h_\Pi} = f(h_\Pi) = f(0) + R_0(h_\Pi) = d_\Pi + R_0(h_\Pi)$$

By Taylor's theorem, the remainder of the zeroth-order expansion takes the form

$$R_0(h_\Pi) = \frac{f'(\xi_L)}{1}h_\Pi = \frac{-h_\Pi}{2\sqrt{d_\Pi^2 - \xi_L}}, \quad \text{where } \xi_L \in [0, h_\Pi].$$

We are approximating d_Π' by a constant and bounding the error via a function of the first derivative. This is a sufficient approximation because the squared difference h_Π is not so big relative to the flattening out of the square root function. Now

$$|d_\Pi - d_\Pi'| \le |R_0(h_\Pi)| \le \frac{|h_\Pi|}{2\sqrt{d_\Pi^2 - \xi_L}} \le \frac{|h_\Pi|}{2\sqrt{d_\Pi^2 - \max(0, h_\Pi)}}$$

Recall that $h_\Pi = d_\Pi^2 - d_\Pi'^2$, so

$$d_\Pi^2 - \max(0, d_\Pi^2 - d_\Pi'^2) = \begin{cases} d_\Pi^2 & \text{if } d_\Pi^2 - d_\Pi'^2 \le 0 \\ d_\Pi'^2 & \text{if } d_\Pi^2 - d_\Pi'^2 > 0 \end{cases}$$

Therefore,

$$|d_\Pi - d'_\Pi| \le \frac{|h_\Pi|}{2\min(d_\Pi, d'_\Pi)} \le \max\left(\frac{|h_\Pi|}{2d_\Pi}, \frac{|h_\Pi|}{2d'_\Pi}\right) \le \frac{|h_\Pi|}{2d_\Pi} + \frac{|h_\Pi|}{2d'_\Pi}.$$

The important thing to do is to isolate $|h_\Pi|$, which is small in expectation, but not absolutely. By the c_r-inequality,

$$\begin{aligned}
\mathbb{E}|d_\Pi - d'_\Pi|^p &\le 2^{p-1}\left(\mathbb{E}\left|\frac{h_\Pi}{2d_\Pi}\right|^p + \mathbb{E}\left|\frac{h_\Pi}{2d'_\Pi}\right|^p\right) \\
&\le 2^{-1}\left(\sqrt{\mathbb{E}[h_\Pi^{2p}]\mathbb{E}[d_\Pi^{-2p}]} + \sqrt{\mathbb{E}[h_\Pi^{2p}]\mathbb{E}[d_\Pi'^{-2p}]}\right) \\
&\le \sqrt{f_{c_3}(2p)N^{-2p/2} f_{c_2}(2p)N^{-2p/2}} \qquad \text{by (2.6) and (2.5)} \\
&:= f_{c_4}(p)N^{-p}.
\end{aligned} \tag{2.7}$$

With

$$q_\Pi = N\bar{u}_{1,\Pi} - N\bar{u}_{2,\Pi} = -2N\bar{u}_{2,\Pi}, \tag{2.8}$$

(2.4), and noting that q_Π and q'_Π are exchangeable,

$$\mathbb{E}[q_\Pi'^p] = \mathbb{E}[q_\Pi^p] = \mathbb{E}[(-2N\bar{u}_{2,\Pi})^p] \le 2^p N^p f_{c_1}(p) N^{-p/2} := f_{c_5}(p). \tag{2.9}$$

$$\begin{aligned}
\mathbb{E}\left[\left(\frac{q'_\Pi}{d_\Pi d'_\Pi}\right)^p\right] &\leq \sqrt{\mathbb{E}|q'_\Pi|^{2p}\mathbb{E}|d_\Pi d'_\Pi|^{-2p}} \\
&\leq \sqrt{\mathbb{E}|q_\Pi|^{2p}\sqrt{\mathbb{E}|d_\Pi|^{-4p}\mathbb{E}|d'_\Pi|^{-4p}}} \\
&= \sqrt{\mathbb{E}|q_\Pi|^{2p}\mathbb{E}|d_\Pi|^{-4p}} \\
&\leq \sqrt{f_{c_5}(2p)N^{2p/2}f_{c_2}(4p)N^{-4p/2}} \quad \text{from (2.9) and (2.5)} \\
&:= f_{c_6}(p)N^{-p/2}. \qquad (2.10)
\end{aligned}$$

2.5 Proof

T_Π and T'_Π are exchangeable by construction:

$$\begin{aligned}
P(\Pi = \pi, \Pi' = \pi') &= P(\Pi' = \pi' | \Pi = \pi) P(\Pi = \pi) \\
&= \frac{1}{N^2}\mathbb{1}_{\{\pi' = \pi\circ(i,j), 1\leq i\leq N, N+1\leq j\leq 2N\}} P(\Pi = \pi') \\
&= \frac{1}{N^2}\mathbb{1}_{\{\pi = \pi'\circ(i,j), 1\leq i\leq N, N+1\leq j\leq 2N\}} P(\Pi = \pi') \\
&= P(\Pi' = \pi | \Pi = \pi') P(\Pi = \pi') \\
&= P(\Pi = \pi', \Pi' = \pi)
\end{aligned}$$

Since (Π, Π') are exchangeable, $(T_\Pi, T'_\Pi) = (T(\Pi), T(\Pi'))$ are exchangeable as well. T_Π, and thus T'_Π by exchangeability, have mean zero by symmetry. Let π^* identify the permutation that reverses the order of the indices after applying the original permutation π. That is, $\pi^* = (2N, \dots, 1) \circ \pi$. Since indices 1 to N correspond to the first group and $N+1$ to $2N$ to the second, π^* flips the groups after π, so $T_{\pi^*} = -T_\pi$.

$$\begin{aligned}
P(T_\Pi = t) &= \sum_{\pi : T_\pi = t} P(\Pi = \pi) \\
&= \sum_{\pi : T_\pi = t} P(\Pi = \pi^*) \quad \text{by exchangeability} \\
&= \sum_{\pi^* : T_{\pi^*} = -t} P(\Pi = \pi^*) \quad \text{since } T_{\pi^*} = -T_\pi \text{ and } \pi \mapsto \pi^* \text{ is bijective} \\
&= P(T_\Pi = -t)
\end{aligned}$$

For convenience, we restate theorem 1.8 of chapter 1:

Theorem 1.8. *If T_Π, T'_Π are mean 0 exchangeable random variables with variance $\mathbb{E}T_\Pi^2$ satisfying*

$$\mathbb{E}[T'_\Pi - T_\Pi | T_\Pi] = -\lambda(T_\Pi - R_\Pi)$$

for some $\lambda \in (0,1)$ and some random variable R_Π, then

$$\begin{aligned}
\sup_{t\in\mathbb{R}} |P(T_\Pi \le t) - \Phi(t)| \le (2\pi)^{-1/4} \sqrt{\frac{\mathbb{E}|T'_\Pi - T_\Pi|^3}{\lambda}} + \frac{1}{2\lambda}\sqrt{\mathrm{Var}(\mathbb{E}[(T'_\Pi - T_\Pi)^2|T_\Pi])} \\
+ |\mathbb{E}T_\Pi^2 - 1| + \mathbb{E}|T_\Pi R_\Pi| + \mathbb{E}|R_\Pi|
\end{aligned}$$

The difference of our exchangeable pair is given by

$$\begin{aligned}
T'_\Pi - T_\Pi &= \sqrt{\frac{N-1}{N}} \left(\frac{q'_\Pi}{d'_\Pi} - \frac{q_\Pi}{d_\Pi} \right) \\
&= \sqrt{\frac{N-1}{N}} \frac{1}{d_\Pi} \left(q'_\Pi - q_\Pi + q'_\Pi \frac{(d_\Pi - d'_\Pi)}{d'_\Pi} \right) \\
&= \sqrt{\frac{N-1}{N}} \frac{1}{d_\Pi} \left(2u_{\Pi(J)} - 2u_{\Pi(I)} + q'_\Pi \frac{(d_\Pi - d'_\Pi)}{d'_\Pi} \right). \qquad (2.11)
\end{aligned}$$

Note that

$$\sqrt{\frac{N-1}{N}}\mathbb{E}\left[\frac{1}{d_\Pi}(2u_{\Pi(J)}-2u_{\Pi(I)})\middle|\Pi=\pi\right] = \sqrt{\frac{N-1}{N}}\frac{2}{d_\Pi}\frac{1}{N^2}\sum_{I=1}^{N}\sum_{I=N+1}^{2N}(u_{\Pi(J)}-u_{\Pi(I)})$$
$$= -\frac{2}{N}T_\Pi$$

Therefore,

$$\sqrt{\frac{N-1}{N}}\mathbb{E}\left[\frac{1}{d_\Pi}(2u_{\Pi(J)}-2u_{\Pi(I)})\middle|\Pi=\pi\right] = \sqrt{\frac{N-1}{N}}\mathbb{E}\left[\frac{1}{d_\Pi}(2u_{\Pi(J)}-2u_{\Pi(I)})\middle|T_\Pi\right]$$

and

$$\lambda = \frac{2}{N}.$$

$$\begin{aligned}\mathbb{E}[T'_\Pi - T_\Pi|T_\Pi] &= -\lambda T_\Pi + \sqrt{\frac{N-1}{N}}\mathbb{E}\left[\frac{q'_\Pi}{d_\Pi}\frac{(d_\Pi-d'_\Pi)}{d'_\Pi}\middle|T_\Pi\right]\\ &= -\lambda\left(T_\Pi - \left(\frac{N}{2}\right)\sqrt{\frac{N-1}{N}}\mathbb{E}\left[\frac{q'_\Pi}{d_\Pi}\frac{(d_\Pi-d'_\Pi)}{d'_\Pi}\middle|T_\Pi\right]\right)\end{aligned}$$

so

$$R_\Pi = \left(\frac{N}{2}\right)\sqrt{\frac{N-1}{N}}\frac{1}{d_\Pi}\mathbb{E}\left[q'_\Pi\frac{(d_\Pi-d'_\Pi)}{d'_\Pi}\middle|T_\Pi\right]. \tag{2.12}$$

Proposition 2.2. $|\mathbb{E}T_\Pi^2 - 1| \le c_2 N^{-1}$

Proof.

$$\begin{aligned}\mathbb{E}T_\Pi^2 &= \frac{N-1}{N}\mathbb{E}\left[\left(\frac{q_\Pi}{d_\Pi}\right)^2\right] &(2.13)\\ &= \frac{N-1}{N}\mathbb{E}\left[\frac{4N^2\bar{u}_{2,\Pi}^2}{2N-2N\bar{u}_{2,\Pi}^2}\right] \qquad \text{from (2.8)}\\ &= 2(N-1)\mathbb{E}\left[\frac{\bar{u}_{2,\Pi}^2}{1-\bar{u}_{2,\Pi}^2}\right]\\ &= 2(N-1)\mathbb{E}[g(\bar{u}_{2,\Pi})], &(2.14)\end{aligned}$$

where $g(x) = \frac{x^2}{1-x^2}$. Now we proceed to calculate moments of $\bar{u}_{2,\Pi}$.

Mean-centering the u_i has the effect of mean-centering $\bar{u}_{2,\Pi}$:

$$\mathbb{E}[\bar{u}_{2,\Pi}] = \frac{1}{N}\mathbb{E}\left[\sum_{i=N+1}^{2N} u_{\Pi(i)}\right] = \frac{1}{N}\sum_{i=N+1}^{2N} \mathbb{E}[u_{\Pi(i)}] = \frac{1}{N}\sum_{i=N+1}^{2N}\frac{1}{2N}\sum_{j=1}^{2N} u_j = 0$$

Under independence, $\mathrm{Var}(\bar{u}_{2,\Pi})$ would be $\frac{1}{N}$ given the scaling. However, the negative dependence induced by the permutation structure approximately halves this value. The scaling is such that $\mathrm{Var}(u_{\Pi(i)}) = 1$. Under independence and with $i \neq j$, $\mathrm{Var}(u_{\Pi(i)} + u_{\Pi(j)}) = 2$. Summing only 2 (out of $2N$) values under permutation dependence, $\mathrm{Var}(u_{\Pi(i)} + u_{\Pi(j)}) = 2 - \frac{2}{2N-1}$.

We can't use Serfling's result here because we need more than just an upper bound.

$$\begin{aligned}
\mathrm{Var}(\bar{u}_{2,\Pi}) &= \frac{1}{N^2}\mathbb{E}\left[\left(\sum_{i=N+1}^{2N} u_{\Pi(i)}\right)^2\right] \\
&= \frac{1}{N^2}\mathbb{E}\left[\sum_{i=N+1}^{2N} u_{\Pi(i)}^2 + \sum_{i=N+1}^{2N}\sum_{j=N+1,j\neq i}^{2N} u_{\Pi(i)}u_{\Pi(j)}\right] \\
&= \frac{1}{N^2}\sum_{i=N+1}^{2N}\frac{1}{2N}\sum_{j=1}^{2N} u_j^2 + \frac{1}{N^2}\sum_{i=N+1}^{2N}\sum_{j=N+1,j\neq i}^{2N} \mathbb{E}[u_{\Pi(i)}u_{\Pi(j)}] \\
&= \frac{1}{N} + \frac{1}{N^2}\sum_{i=N+1}^{2N}\sum_{j=N+1,j\neq i}^{2N}\frac{1}{2N}\frac{1}{2N-1}\sum_{k=1}^{2N}\sum_{l=1,l\neq k}^{2N} u_k u_l \\
&= \frac{1}{N} + \frac{1}{N^2}\sum_{i=N+1}^{2N}\sum_{j=N+1,j\neq i}^{2N}\frac{1}{2N}\frac{1}{2N-1}\left(\left(\sum_{k=1}^{2N} u_k\right)^2 - \sum_{k=1}^{2N} u_k^2\right) \\
&= \frac{1}{N} + \frac{1}{N^2}\sum_{i=N+1}^{2N}\sum_{j=N+1,j\neq i}^{2N}\frac{1}{2N}\frac{1}{2N-1}\left(0^2 - 2N\right) \\
&= \frac{1}{N} + \frac{1}{N}(N^2 - N)\left(-\frac{1}{2N-1}\right) \\
&= \frac{2N-1}{N(2N-1)} + \frac{1-N}{N(2N-1)} \\
&= \frac{1}{2N-1}
\end{aligned}$$

Having established the first two moments, we compute the third degree Taylor expansion and bound the error in the approximation. By Taylor's theorem, we expand the function $g(\bar{u}_{2,\Pi}) = \frac{\bar{u}_{2,\Pi}^2}{1-\bar{u}_{2,\Pi}^2}$ around $\mathbb{E}[\bar{u}_{2,\Pi}] = 0$:

$$g(\bar{u}_{2,\Pi}) = \frac{\bar{u}_{2,\Pi}^2}{1-\bar{u}_{2,\Pi}^2} = g(0) + g'(0)\bar{u}_{2,\Pi} + \frac{g''(0)}{2!}\bar{u}_{2,\Pi}^2 + \frac{g^{(3)}(0)}{3!}\bar{u}_{2,\Pi}^3 + R_3(\bar{u}_{2,\Pi}),$$

where $R_3(\bar{u}_{2,\Pi}) = \frac{g^{(4)}(\xi_L)}{4!}\bar{u}_{2,\Pi}^4$, with $\xi_L \in [0, \bar{u}_{2,\Pi}]$.

From (2.14) and evaluating the Taylor series, we have

$$\mathbb{E}[g(\bar{u}_{2,\Pi})] = \frac{\mathbb{E}T_\Pi^2}{2(N-1)} = \mathbb{E}[\bar{u}_{2,\Pi}^2 + R_3(\bar{u}_{2,\Pi})].$$

Therefore,

$$\begin{aligned}
\left|\frac{\mathbb{E}T_\Pi^2}{2(N-1)} - \mathbb{E}[\bar{u}_{2,\Pi}^2]\right| &= \left|\frac{\mathbb{E}T_\Pi^2}{2(N-1)} - \frac{1}{2N-1}\right| \\
&\leq \mathbb{E}|R_3(\bar{u}_{2,\Pi})| \\
&= \mathbb{E}\left|\frac{24(5\xi_L^4 + 10\xi_L^2 + 1)}{4!(\xi_L - 1)^5}\bar{u}_{2,\Pi}^4\right| \\
&\leq \mathbb{E}\left|\frac{24(5\bar{u}_{2,\Pi}^4 + 10\bar{u}_{2,\Pi}^2 + 1)}{4!(\bar{u}_{2,\Pi} - 1)^5}\bar{u}_{2,\Pi}^4\right| \\
&\leq \frac{5B^4 + 10B^2 + 1}{|B-1|^5}\mathbb{E}[\bar{u}_{2,\Pi}^4] \\
&\leq \frac{5B^4 + 10B^2 + 1}{|B-1|^5} f_{c_1}(4)N^{-2} \qquad \text{by (2.4)} \\
&:= c_1 N^{-2}
\end{aligned}$$

$$
\begin{aligned}
|\mathbb{E}T_\Pi^2 - 1| - \frac{1}{2N-1} &\le \left|\mathbb{E}T_\Pi^2 - 1 + \frac{1}{2N-1}\right| \\
&= \left|\mathbb{E}T_\Pi^2 - \frac{2(N-1)}{2N-1}\right| \\
&= 2(N-1)\left|\frac{\mathbb{E}T_\Pi^2}{2(N-1)} - \frac{1}{2N-1}\right| \\
&\le c_1 2(N-1)N^{-2}
\end{aligned}
$$

This implies that

$$
|\mathbb{E}T_\Pi^2 - 1| \le \frac{1}{2N-1} + c_1\frac{2N-2}{N^2} \le \frac{1+2c_1}{N} := c_2 N^{-1}
$$

□

Proposition 2.3. $\frac{1}{2\lambda}\sqrt{\mathrm{Var}(\mathbb{E}[(T'_\Pi - T_\Pi)^2 | T_\Pi])} \le N^{-1}c_3\sqrt{20 + 16\frac{\sum_{i=1}^{2N} u_i^4}{N^2}}$

Proof. With two applications of the c_r inequality, we can bound the variance of the sum by a constant times the sum of the variances. Suppose X, Y, and Z have finite variances. Then, with the centered random variables represented by $\tilde{X}, \tilde{Y}$, and $\tilde{Z}$, we have that

$$
\begin{aligned}
\mathrm{Var}(X+Y+Z) &= \mathrm{Var}(\tilde{X}+\tilde{Y}+\tilde{Z}) \\
&= \mathbb{E}|(\tilde{X}+\tilde{Y})+\tilde{Z}|^2 \\
&\le 2\mathbb{E}|\tilde{X}+\tilde{Y}|^2 + 2\mathbb{E}|\tilde{Z}|^2 \\
&\le 2(2\mathbb{E}[\tilde{X}^2] + 2\mathbb{E}[\tilde{Y}^2]) + 2\mathbb{E}[\tilde{Z}^2] \\
&\le 4(\mathrm{Var}(X) + \mathrm{Var}(Y) + \mathrm{Var}(Z))
\end{aligned}
$$

From (2.11),

$$\begin{aligned}
\mathrm{Var}(\mathbb{E}[(T'_\Pi - T_\Pi)^2|\Pi = \pi]) &= \mathrm{Var}\left(\frac{N-1}{N}\mathbb{E}\left[\left(\frac{2u_{\Pi(J)} - 2u_{\Pi(I)}}{d_\Pi} + T'_\Pi\frac{d_\Pi - d'_\Pi}{d_\Pi}\right)^2\middle|\Pi = \pi\right]\right) \\
&\leq \mathrm{Var}\left(\mathbb{E}\left[\left(\frac{2u_{\Pi(J)} - 2u_{\Pi(I)}}{d_\Pi} + T'_\Pi\frac{d_\Pi - d'_\Pi}{d_\Pi}\right)^2\middle|\Pi = \pi\right]\right) \\
&\leq 4(\mathrm{Var}(X) + \mathrm{Var}(Y) + \mathrm{Var}(Z))
\end{aligned}$$

where

$$\begin{aligned}
X &= \mathbb{E}\left[\left(\frac{2u_{\Pi(J)} - 2u_{\Pi(I)}}{d_\Pi}\right)^2\middle|\Pi = \pi\right] \\
Y &= \mathbb{E}\left[\left(T'_\Pi\frac{d_\Pi - d'_\Pi}{d_\Pi}\right)^2\middle|\Pi = \pi\right] \\
Z &= 2\mathbb{E}\left[\left(\frac{2u_{\Pi(J)} - 2u_{\Pi(I)}}{d_\Pi}T'_\Pi\frac{d_\Pi - d'_\Pi}{d_\Pi}\right)\middle|\Pi = \pi\right]
\end{aligned}$$

The X term will dominate, so we can afford to use coarser methods on Y and Z.

The $\mathbb{E}[u_{\Pi(J)} - u_{\Pi(I)}|\Pi = \pi]$ term is common to applications of Stein's method of exchangeable pairs. However, there is a complication in the d_Π random variable in the denominator. Our strategy will be to calculate the two variances separately with some necessary additional terms.

First, we prove an intermediate result regarding the variance of a product of random variables

$$W = (d_\Pi)^{-2} \text{ and } V = \mathbb{E}[(u_{\Pi(J)} - u_{\Pi(I)})^2|\Pi = \pi].$$

Then $\mathrm{Var}(X) = 4\,\mathrm{Var}(WV)$ since d_Π is $\sigma(\Pi)$-measurable and

$$\begin{aligned}
\mathrm{Var}(WV) &= \mathrm{Var}(W(V - \mathbb{E}V) + W\mathbb{E}V) \\
&\leq 2\,\mathrm{Var}(W(V - \mathbb{E}V)) + 2\,\mathrm{Var}(W\mathbb{E}V) \\
&\leq 2\mathbb{E}[W^2(V - \mathbb{E}V)^2] + 2(\mathbb{E}V)^2\,\mathrm{Var}(W) \\
&\leq 2(f_{c_2}(2))^2 N^{-2}\,\mathrm{Var}(V) + 2u_\Delta^4\,\mathrm{Var}(W). \qquad (2.15)
\end{aligned}$$

$$\begin{aligned}
\mathrm{Var}(W) &= \mathrm{Var}((d_\Pi)^{-2}) \\
&= \mathrm{Var}\left(\frac{1}{2N(1-\bar{u}_{2,\Pi}^2)}\right) \\
&= \frac{1}{4N^2}\left[\mathbb{E}\left[\left(\frac{1}{1-\bar{u}_{2,\Pi}^2}\right)^2\right] - \left(\mathbb{E}\left[\frac{1}{1-\bar{u}_{2,\Pi}^2}\right]\right)^2\right] \\
&= \frac{1}{4N^2}[\mathbb{E}h(\bar{u}_{2,\Pi}) - (\mathbb{E}\tilde{h}(\bar{u}_{2,\Pi}))^2],
\end{aligned}$$

where

$$h(x) = \left(\frac{1}{1-x^2}\right)^2 = 1 + 2x^2 + 3x^4 + \ldots \text{ and } \tilde{h}(x) = \frac{1}{1-x^2} = 1 + x^2 + x^4 + \ldots$$

By Taylor's theorem,

$$\mathbb{E}\left[\left(\frac{1}{1-\bar{u}_{2,\Pi}^2}\right)^2\right] = 1 + 2\left(\frac{1}{2N-1}\right) + \mathbb{E}[R_3(\bar{u}_{2,\Pi})],$$

with

$$\mathbb{E}|R_3(\bar{u}_{2,\Pi})| \leq \frac{24(35B^4 + 42B^2 + 3)}{4!(B-1)^6} f_{c_1}(4)N^{-2} := c_4 N^{-2}$$

Re-arranging, we get

$$\left| \mathbb{E}\left[\left(\frac{1}{1-\bar{u}_{2,\Pi}^2} \right)^2 \right] - 1 - \frac{2}{2N-1} \right| \leq c_4 N^{-2}.$$

Applying Taylor's theorem to $\tilde{h}$:

$$\mathbb{E}\left[\frac{1}{1-\bar{u}_{2,\Pi}^2} \right] = 1 + \frac{1}{2N-1} + \mathbb{E}[\tilde{R}_3(\bar{u}_{2,\Pi})],$$

with

$$\mathbb{E}|\tilde{R}_3(\bar{u}_{2,\Pi})| \leq \frac{24(5B^4+10B^2+1)}{4!(B-1)^5} f_{c_1}(4) N^{-2} := c_5 N^{-2}$$

Squaring, applying the bound, and re-arranging yields

$$\left| \left(\mathbb{E}\left[\frac{1}{1-\bar{u}_{2,\Pi}^2} \right] \right)^2 - \left(1 + \frac{1}{2N-1} \right)^2 \right| \leq 2\left(1 + \frac{1}{2N-1} \right) c_5 N^{-2} + c_5^2 N^{-4}$$

Now we combine bounds to get

$$\begin{aligned}
&\left|\mathbb{E}\left[\left(\frac{1}{1-\bar{u}_{2,\Pi}^2}\right)^2\right]-\left(\mathbb{E}\left[\frac{1}{1-\bar{u}_{2,\Pi}^2}\right]\right)^2\right| \\
&=\left|\mathbb{E}\left[\left(\frac{1}{1-\bar{u}_{2,\Pi}^2}\right)^2\right]-\left(\mathbb{E}\left[\frac{1}{1-\bar{u}_{2,\Pi}^2}\right]\right)^2+\frac{1}{(2N-1)^2}-\frac{1}{(2N-1)^2}\right| \\
&\leq\left|\mathbb{E}\left[\left(\frac{1}{1-\bar{u}_{2,\Pi}^2}\right)^2\right]-\left(\mathbb{E}\left[\frac{1}{1-\bar{u}_{2,\Pi}^2}\right]\right)^2+\frac{1}{(2N-1)^2}\right|+\left|\frac{1}{(2N-1)^2}\right| \\
&\leq\left|\mathbb{E}\left[\left(\frac{1}{1-\bar{u}_{2,\Pi}^2}\right)^2\right]-1-\frac{2}{2N-1}-\left(\left(\mathbb{E}\left[\frac{1}{1-\bar{u}_{2,\Pi}^2}\right]\right)^2-\left(1+\frac{1}{2N-1}\right)^2\right)\right|+\left|\frac{1}{(2N-1)^2}\right| \\
&\leq c_4N^{-2}+2\left(1+\frac{1}{2N-1}\right)c_5N^{-2}+c_5^2N^{-4}+\left|\frac{1}{(2N-1)^2}\right| \\
&\leq (c_4+3c_5+c_5^2+\frac{1}{4})N^{-2} \\
&:= c_6N^{-2}
\end{aligned}$$

Therefore, $\operatorname{Var}(W)\leq\frac{c_6}{4}N^{-4}$ and

$$\operatorname{Var}(X)\leq 8(f_{c_2}(2))^2N^{-2}\operatorname{Var}(V)+8u_\Delta^4\frac{c_6}{4}N^{-4}$$

with

$$\begin{aligned}
\operatorname{Var}(V)&=\operatorname{Var}(\mathbb{E}[(u_{\Pi(J)}-u_{\Pi(I)})^2|\Pi=\pi]) \\
&=\operatorname{Var}(\mathbb{E}[u_{\Pi(J)}^2+u_{\Pi(I)}^2-2u_{\Pi(J)}u_{\Pi(I)}|\Pi=\pi]) \\
&=\operatorname{Var}\left(\frac{1}{N^2}\sum_{I=1}^{N}\sum_{J=N+1}^{2N}(u_{\pi(J)}^2+u_{\pi(I)}^2-2u_{\pi(J)}u_{\pi(I)})\right) \\
&=\operatorname{Var}\left(\frac{1}{N^2}\left(N\sum_{K=1}^{2N}u_K^2-\sum_{I=1}^{N}\sum_{J=N+1}^{2N}2u_{\pi(J)}u_{\pi(I)}\right)\right) \\
&=\frac{4}{N^4}\sum_{I=1}^{N}\sum_{J=N+1}^{2N}\sum_{K=1}^{N}\sum_{L=N+1}^{2N}\operatorname{Cov}(u_{\pi(I)}u_{\pi(J)},u_{\pi(K)}u_{\pi(L)})
\end{aligned}$$

since $\sum_{K=1}^{2N} u_K^2 = 2N$ is a constant. We proceed by calculating

$$\mathrm{Cov}(u_{\pi(I)}u_{\pi(J)}, u_{\pi(K)}u_{\pi(L)}) = \mathbb{E}[u_{\pi(I)}u_{\pi(J)}u_{\pi(K)}u_{\pi(L)}] - \mathbb{E}[u_{\pi(I)}u_{\pi(J)}]\mathbb{E}[u_{\pi(K)}u_{\pi(L)}].$$

The index sets for variables I and J (and K and L) are disjoint, so

$$\mathbb{E}[u_{\pi(I)}u_{\pi(J)}] = \mathbb{E}[u_{\pi(K)}u_{\pi(L)}] = \frac{1}{2N}\frac{1}{2N-1}\sum_{I=1}^{2N} u_I \sum_{J=1, J\neq I}^{2N} u_J = -\frac{1}{2N-1}$$

for all values of I, J, K, L in the sum. Therefore,

$$\mathbb{E}[u_{\pi(I)}u_{\pi(J)}] = \mathbb{E}[u_{\pi(K)}u_{\pi(L)}] = \frac{1}{(2N-1)^2}.$$

However, K could equal I and L could equal J, which changes the mass assigned by the permutation distribution, necessitating a separate treatment for each case.

Case $I \neq J \neq K \neq L$:

$$
\begin{aligned}
&\mathbb{E}[u_{\pi(I)}u_{\pi(J)}u_{\pi(K)}u_{\pi(L)}] \\
&= \frac{1}{2N}\frac{1}{2N-1}\frac{1}{2N-2}\frac{1}{2N-3}\sum_{I=1}^{2N}\sum_{J=1,J\neq I}^{2N}\sum_{K=1,K\neq I,J}^{2N}\sum_{L=1,L\neq I,J,K}^{2N} u_I u_J u_K u_L \\
&= \frac{1}{2N}\frac{1}{2N-1}\frac{1}{2N-2}\frac{1}{2N-3}\sum_{I=1}^{2N} u_I \sum_{J=1,J\neq I}^{2N} u_J \sum_{K=1,K\neq I,J}^{2N} u_K(-u_I - u_J - u_K) \\
&= \frac{1}{2N}\frac{1}{2N-1}\frac{1}{2N-2}\frac{1}{2N-3}\sum_{I=1}^{2N} u_I \sum_{J=1,J\neq I}^{2N} u_J((-u_I - u_J)(-u_I - u_J) + (u_I^2 + u_J^2 - 2N)) \\
&= \frac{1}{2N}\frac{1}{2N-1}\frac{1}{2N-2}\frac{1}{2N-3}\sum_{I=1}^{2N} u_I \sum_{J=1,J\neq I}^{2N} u_J(2u_I^2 - 2N + 2u_J^2 + 2u_I u_J) \\
&= \frac{1}{2N}\frac{1}{2N-1}\frac{1}{2N-2}\frac{1}{2N-3}\sum_{I=1}^{2N} u_I \left((2u_I^2 - 2N)(-u_I) + 2\sum_{J=1,J\neq I}^{2N} u_J^3 + 2u_I(2N - u_I^2)\right) \\
&= \frac{1}{2N}\frac{1}{2N-1}\frac{1}{2N-2}\frac{1}{2N-3}\sum_{I=1}^{2N} u_I \left(-4u_I^3 + 6Nu_I + 2\left(\sum_{J=1}^{2N} u_J^3 - u_I^3\right)\right) \\
&= \frac{1}{2N}\frac{1}{2N-1}\frac{1}{2N-2}\frac{1}{2N-3}\left(-6\sum_{I=1}^{2N} u_I^4 + 12N^2\right)
\end{aligned}
$$

for $N^2(N-1)^2$ terms in the sum.

Case $I = K$ and $J = L$:

$$
\begin{aligned}
\mathbb{E}[u_{\pi(I)}^2 u_{\pi(J)}^2] &= \frac{1}{2N}\frac{1}{2N-1}\sum_{I=1}^{2N}\sum_{J=1,J\neq I}^{2N} u_I^2 u_J^2 \\
&= \frac{1}{2N}\frac{1}{2N-1}\sum_{I=1}^{2N} u_I^2(2N - u_I^2) \\
&= \frac{2N}{2N-1} - \frac{1}{2N}\frac{1}{2N-1}\sum_{I=1}^{2N} u_I^4
\end{aligned}
$$

for N^2 terms in the sum.

Case $I = K, J \neq L$ or $I \neq K, J = L$:

$$
\begin{aligned}
\mathbb{E}[u^2_{\pi(I)}u_{\pi(J)}u_{\pi(K)}] &= \frac{1}{2N}\frac{1}{2N-1}\frac{1}{2N-2}\sum_{I=1}^{2N}\sum_{J=1,J\neq I}^{2N}\sum_{K=1,K\neq I,J}^{2N} u_I^2 u_J u_K \\
&= \frac{1}{2N}\frac{1}{2N-1}\frac{1}{2N-2}\sum_{I=1}^{2N}\sum_{J=1,J\neq I}^{2N} u_I^2 u_J(0-u_I-u_J) \\
&= -\frac{1}{2N}\frac{1}{2N-1}\frac{1}{2N-2}\left(\sum_{I=1}^{2N} u_I^3 \sum_{J=1,J\neq I}^{2N} u_J + \sum_{I=1}^{2N} u_I^2 \sum_{J=1,J\neq I}^{2N} u_J^2\right) \\
&= -\frac{1}{2N}\frac{1}{2N-1}\frac{1}{2N-2}\left(\sum_{I=1}^{2N} -u_I^4 + \sum_{I=1}^{2N} u_I^2(2N-u_I^2)\right) \\
&= \frac{1}{2N}\frac{1}{2N-1}\frac{1}{2N-2}\left(2\sum_{I=1}^{2N} u_I^4 - 4N^2\right)
\end{aligned}
$$

for $2N^2(N-1)$ terms in the sum.

Putting it all together, we have

$$
\begin{aligned}
&\mathrm{Var}(\mathbb{E}[(u_{\Pi(J)}-u_{\Pi(i)})^2]|\Pi=\pi) \\
&= \frac{4}{N^4}(N^2(N-1)^2)\left(\frac{1}{(2N)(2N-1)(2N-2)(2N-3)}\left(-6\sum_{i=1}^{2N} u_i^4 + 12N^2\right) - \frac{1}{(2N-1)^2}\right) \\
&+ \frac{4}{N^4}N^2\left(\frac{2N}{2N-1} - \frac{1}{2N}\frac{1}{2N-1}\sum_{i=1}^{2N} u_i^4 - \frac{1}{(2N-1)^2}\right) \\
&+ \frac{4}{N^4}(2N^2(N-1))\left(\frac{1}{2N}\frac{1}{2N-1}\frac{1}{2N-2}\left(2\sum_{i=1}^{2N} u_i^4 - 4N^2\right) - \frac{1}{(2N-1)^2}\right) \\
&\leq \frac{48}{4N^2} + \frac{8}{N^2} + \frac{16\sum_{i=1}^{2N} u_i^4}{N^4} \\
&= \left(20 + 16\left(\sum_{i=1}^{2N} u_i^4\right)N^{-2}\right)N^{-2}
\end{aligned}
$$

Therefore,

$$\mathrm{Var}(X) \leq 8(f_{c_2}(2))^2 \left(20 + 16\left(\sum_{i=1}^{2N} u_i^4\right) N^{-2}\right) N^{-4} + 8u_\Delta^4 \frac{c_6}{4} N^{-4}$$

Because the latter two terms are much smaller in order, we can apply coarser techniques. In particular, we use the following bound:

$$\mathrm{Var}(\mathbb{E}[U|V]) = \mathrm{Var}(U) - \mathbb{E}(\mathrm{Var}(U|V)) \leq E[U^2]$$

Applying to the second term,

$$\begin{aligned}
\mathrm{Var}(Y) &= \mathrm{Var}\left(\mathbb{E}\left[\left(T'_\Pi \frac{d_\Pi - d'_\Pi}{d_\Pi}\right)^2 \middle| \Pi = \pi\right]\right) \\
&\leq \mathbb{E}\left[\left(\frac{q'_\Pi}{d_\Pi d'_\Pi}(d_\Pi - d'_\Pi)\right)^4\right] \\
&\leq \sqrt{\mathbb{E}\left[\left(\frac{q'_\Pi}{d_\Pi d'_\Pi}\right)^8\right] \mathbb{E}[(d_\Pi - d'_\Pi)^8]} \\
&\leq \sqrt{f_{c_6}(8) N^{-8/2} f_{c_4}(8) N^{-8}} \text{ from (2.10), (2.7)} \\
&= \sqrt{f_{c_6}(8) f_{c_4}(8)} N^{-6} \\
&:= c_7 N^{-6}
\end{aligned}$$

And to the third,

$$\begin{aligned}
\operatorname{Var}(Z) &= 4\operatorname{Var}\left(\mathbb{E}\left[\left(\frac{2u_{\Pi(J)} - 2u_{\Pi(I)}}{d_\Pi} T'_\Pi \frac{d_\Pi - d'_\Pi}{d_\Pi}\right)\middle| \Pi = \pi\right]\right) \\
&\leq 16u_\Delta^2 \mathbb{E}\left[\left(\frac{1}{d_\Pi}\frac{q'_\Pi}{d_\Pi d'_\Pi}(d_\Pi - d'_\Pi)\right)^2\right] \\
&\leq 16u_\Delta^2 f_{c_2}(2)N^{-2/2}\sqrt{\mathbb{E}\left[\left(\frac{q'_\Pi}{d_\Pi d'_\Pi}\right)^4\right]\mathbb{E}[(d_\Pi - d'_\Pi)^4]} \text{ from (2.5)} \\
&\leq 16u_\Delta^2 f_{c_2}(2)N^{-1}\sqrt{f_{c_6}(4)N^{-4/2}f_{c_4}(4)N^{-4}} \text{ from (2.10), (2.7)} \\
&\leq 16u_\Delta^2 f_{c_2}(2)(f_{c_6}(4))^{-1/2}(f_{c_4}(4))^{-1/2}N^{-4} \\
&:= c_8 N^{-4}
\end{aligned}$$

$$\begin{aligned}
&\frac{1}{2\lambda}\sqrt{\operatorname{Var}(\mathbb{E}[(T'_\Pi - T_\Pi)^2 | T_\Pi])} \\
&= N\sqrt{(\operatorname{Var}(X) + \operatorname{Var}(Y) + \operatorname{Var}(Z))} \\
&\leq N\sqrt{8(f_{c_2}(2))^2\left(20 + 16\left(\sum_{i=1}^{2N} u_i^4\right)N^{-2}\right)N^{-4} + 8u_\Delta^4\frac{c_6}{4}N^{-4} + c_7N^{-6} + c_8N^{-4}} \\
&:= N^{-1}c_3\sqrt{20 + 16\frac{\sum_{i=1}^{2N} u_i^4}{N^2}}
\end{aligned}$$

□

Proposition 2.4. $(2\pi)^{-1/4}\sqrt{\frac{\mathbb{E}|T'_\Pi - T_\Pi|^3}{\lambda}} < (2\pi)^{-1/4}c_9N^{-1/4}$.

Proof. The strategy is to break apart the remainder term from the main piece. From

(2.11),

$$\begin{aligned}
\mathbb{E}|T'_\Pi - T_\Pi|^3 &= \left(\frac{N-1}{N}\right)^{3/2} \mathbb{E}\left[d_\Pi^{-3}\left|2u_{\Pi(J)} - 2u_{\Pi(I)} + q'_\Pi \frac{d_\Pi - d'_\Pi}{d'_\Pi}\right|^3\right] \\
&\le 8\left(8u_\Delta^3 \mathbb{E}[d_\Pi^{-3}] + \sqrt{\mathbb{E}\left[\left(\frac{q'_\Pi}{d_\Pi d'_\Pi}\right)^6\right]\mathbb{E}[(d_\Pi - d'_\Pi)^6]}\right) \\
&\le 64u_\Delta^3 f_{c_2}(3)N^{-3/2} + 8\sqrt{f_{c_6}(6)N^{-6/2}f_{c_4}(6)N^{-6}} \text{ from (2.5), (2.10), (2.7)} \\
&\le \frac{c_9^2}{2}N^{-3/2}
\end{aligned}$$

Therefore,

$$(2\pi)^{-1/4}\sqrt{\frac{\mathbb{E}|T'_\Pi - T_\Pi|^3}{\lambda}} \le (2\pi)^{-1/4}c_9 N^{-1/4}.$$

$\square$

Proposition 2.5. $\mathbb{E}|R| \le \frac{1}{2}\sqrt{f_{c_6}(2)f_{c_4}(2)}N^{-1/2}$.

Proof.

$$\begin{aligned}
\mathbb{E}|R| &= \mathbb{E}\left|\left(\frac{N}{2}\right)\sqrt{\frac{N-1}{N}}\frac{1}{d_\Pi}\mathbb{E}\left[q'_\Pi \frac{(d_\Pi - d'_\Pi)}{d'_\Pi}\middle| T_\Pi\right]\right| \\
&\le \frac{N}{2}\mathbb{E}\left|\frac{q'_\Pi}{d_\Pi d'_\Pi}(d_\Pi - d'_\Pi)\right| \\
&\le \frac{N}{2}\sqrt{\mathbb{E}\left|\frac{q'_\Pi}{d_\Pi d'_\Pi}\right|^2 \mathbb{E}[d_\Pi - d'_\Pi]^2} \\
&\le \frac{N}{2}\sqrt{f_{c_6}(2)N^{-2/2}f_{c_4}(2)N^{-2}} \text{ from (2.10), (2.7)} \\
&= \frac{1}{2}\sqrt{f_{c_6}(2)f_{c_4}(2)}N^{-1/2}
\end{aligned}$$

$\square$

Proposition 2.6. $\mathbb{E}|T_\Pi R| \le \frac{1}{2}(f_{c_6}(4)f_{c_4}(4))^{1/4}\sqrt{2+2c_1}N^{-1/2}$.

Proof.

$$\begin{aligned}
\mathbb{E}|T_\Pi R| &= \mathbb{E}\left|T_\Pi\left(\frac{N}{2}\right)\sqrt{\frac{N-1}{N}}\frac{1}{d_\Pi}\mathbb{E}\left[q'_\Pi\frac{(d_\Pi - d'_\Pi)}{d'_\Pi}\middle|T_\Pi\right]\right| \\
&\le \frac{N}{2}\mathbb{E}\left|T_\Pi\frac{q'_\Pi}{d_\Pi d'_\Pi}(d_\Pi - d'_\Pi)\right| \\
&\le \frac{N}{2}\sqrt{\mathbb{E}T_\Pi^2\mathbb{E}\left[\left(\frac{q'_\Pi}{d_\Pi d'_\Pi}\right)^2(d_\Pi - d'_\Pi)^2\right]} \\
&\le \frac{N}{2}\sqrt{\mathbb{E}T_\Pi^2\sqrt{\mathbb{E}\left[\left(\frac{q'_\Pi}{d_\Pi d'_\Pi}\right)^4\right]\mathbb{E}[(d_\Pi - d'_\Pi)^4]}} \\
&\le \frac{N}{2}\sqrt{\mathbb{E}T_\Pi^2\sqrt{f_{c_6}(4)N^{-4/2}f_{c_4}(4)N^{-4}}} \text{ from (2.10), (2.7)} \\
&= \frac{N^{-1/2}}{2}(f_{c_6}(4)f_{c_4}(4))^{1/4}\sqrt{\mathbb{E}T_\Pi^2} \\
&\le \frac{1}{2}(f_{c_6}(4)f_{c_4}(4))^{1/4}\sqrt{2+2c_1}N^{-1/2}
\end{aligned}$$

because $\mathbb{E}T_\Pi^2 \le 1 + \frac{1+2c_1}{N} \le 2 + 2c_1$. □

Collecting the results of propositions 2.2, 2.3, 2.4, 2.5, 2.6, we have

$$\begin{aligned}
\sup_{t\in\mathbb{R}}|P(T_\Pi \le t) - \Phi(t)| &\le (2\pi)^{-1/4}\sqrt{\frac{\mathbb{E}|T'_\Pi - T_\Pi|^3}{\lambda}} + \frac{1}{2\lambda}\sqrt{\mathrm{Var}(\mathbb{E}[(T'_\Pi - T_\Pi)^2|T_\Pi])} \\
&\quad + |\mathbb{E}T_\Pi^2 - 1| + \mathbb{E}|T_\Pi R_\Pi| + \mathbb{E}|R_\Pi| \\
&\le N^{-1}c_3\sqrt{20 + 16\frac{\sum_{i=1}^{2N}u_i^4}{N^2}} + (2\pi)^{-1/4}c_9N^{-1/4} + c_2N^{-1} \\
&\quad + \frac{1}{2}(f_{c_6}(4)f_{c_4}(4))^{1/4}\sqrt{2+2c_1}N^{-1/2} + \frac{1}{2}\sqrt{f_{c_6}(2)f_{c_4}(2)}N^{-1/2}
\end{aligned}$$

Chapter 3

Simulations

This chapter is a computational companion to chapter 2.

3.1 Preliminaries

First, we provide simulations accompanying section 2.4. We generate i.i.d. samples $\{u_i\}_{i=1}^{N} \sim \mathcal{N}(-1,1)$ and $\{u_i\}_{i=N+1}^{2N} \sim \mathcal{N}(1,1)$ for exponentially spaced values of $N \in \{\text{floor}(10^{.5+.5i})\}_{i=1}^{7}$. The u_i are scaled and centered, and for each N, we perform $10,000$ permutations.

We plot Monte Carlo estimates of the means of each term, scaled by the rate of our bound, along with 95%ile bootstrap confidence intervals for different values of $p \in \{2,4,6,8\}$.

Due to the flatness of the curves, we conclude that the bounds we have proved are of the correct rate. In addition, we can observe the behavior of the constants as functions of p. For instance, our $f_{c_3}(p)$ constant for $\mathbb{E}[h_{\mathrm{II}}^{p}]$ appears to be an exponential function of p.

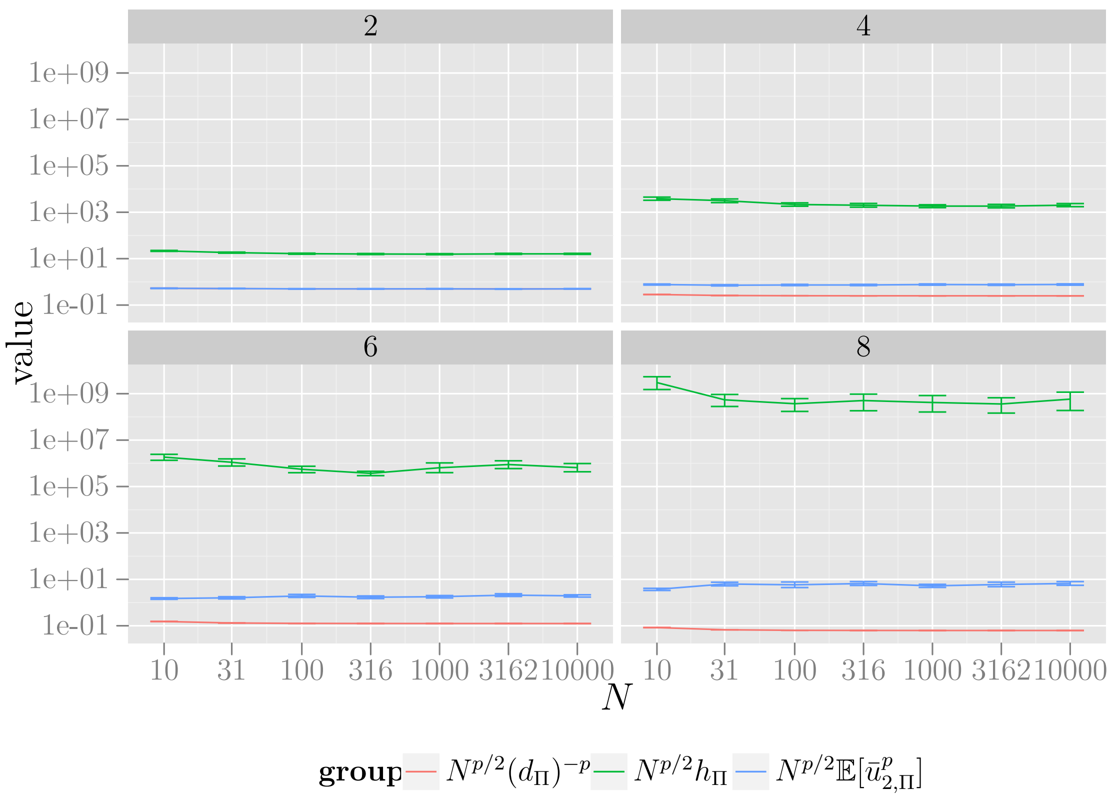


Figure 3.1: Log-log plots of values scaled by proven upper bounds of rates, faceted on p.

Here, to compute the corresponding "prime" random variables, in each permutation we pick a transposition uniformly at random among transpositions that switch groups.

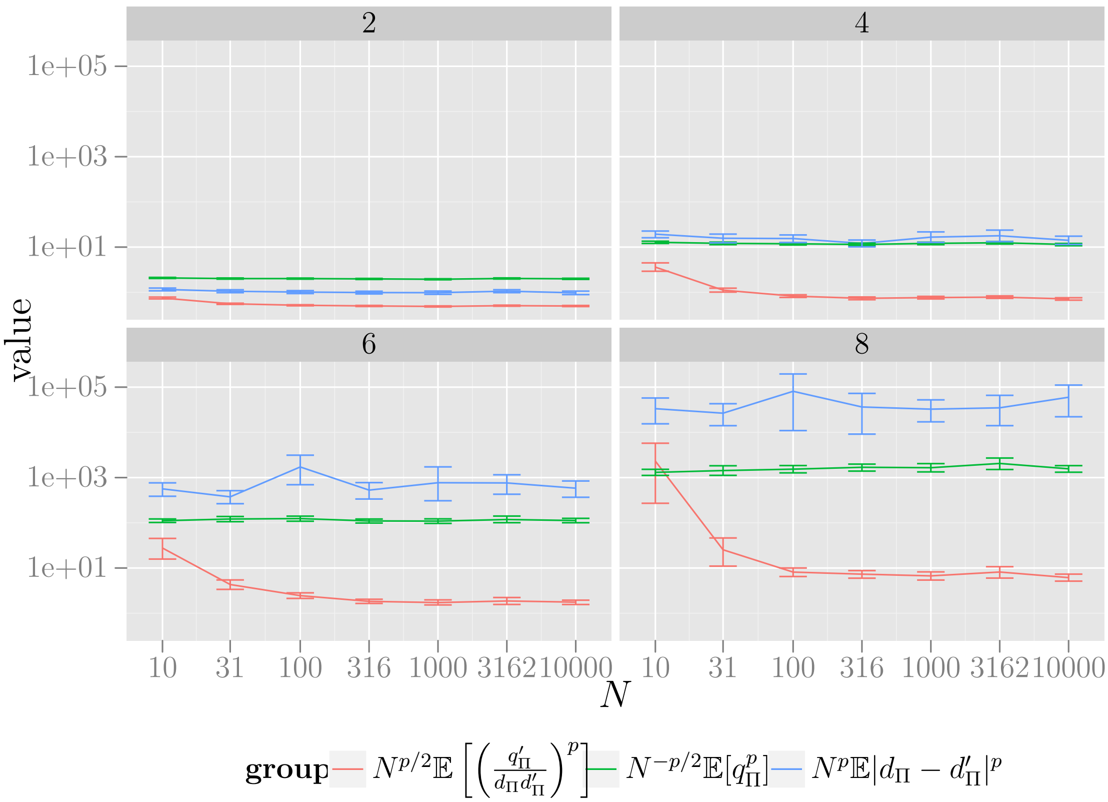


Figure 3.2: Log-log plots of values scaled by proven upper bounds of rates, faceted on p.

It is possible that the bound of rate $N^{-p/2}$ on $\mathbb{E}\left[\left(\frac{q'_\Pi}{d_\Pi d'_\Pi}\right)^p\right]$ is a bit conservative.

3.2 Approximate Regression Condition

From the approximate regression condition

$$\mathbb{E}[T'_{\Pi} - T_{\Pi}|T_{\Pi}] = -\lambda(T_{\Pi} - R_{\Pi})$$

we get

$$\mathbb{E}[T'_{\Pi}|T_{\Pi}] = (1-\lambda)T_{\Pi} - \lambda R_{\Pi}.$$

That is, the conditional expectation of T'_{Π} on T_{Π} is expected to lie near the line $(1-\lambda)T_{\Pi}$ with a small perturbation of order $1/N$ (recall that $\lambda = 2/N$).

For various values of N, we compute 20 permutations that correspond with 20 values of T_{Π}. For each T_{Π}, we draw a transposition (I, J) uniformly at random from the space of our allowable transpositions, repeating this 100 times.

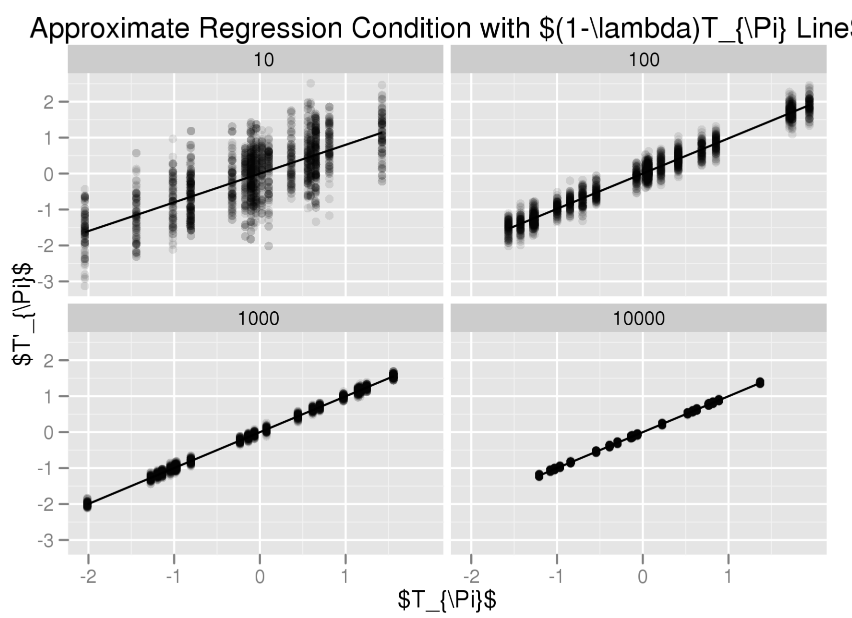


Figure 3.3: Faceted on per-group sample size, N.

The approximate regression condition appears to hold visually.

3.3 Main Bounds

Here we simulate the main bounds under the same setting as the previous section.

3.3.1 Failure of Monte Carlo

Again, we simulate the conditional expectations of the form $\mathbb{E}[f(T'_\Pi, T_\Pi)|T_\Pi]$ with 1,000 draws from the uniform distribution on all group-switching transpositions (I, J).

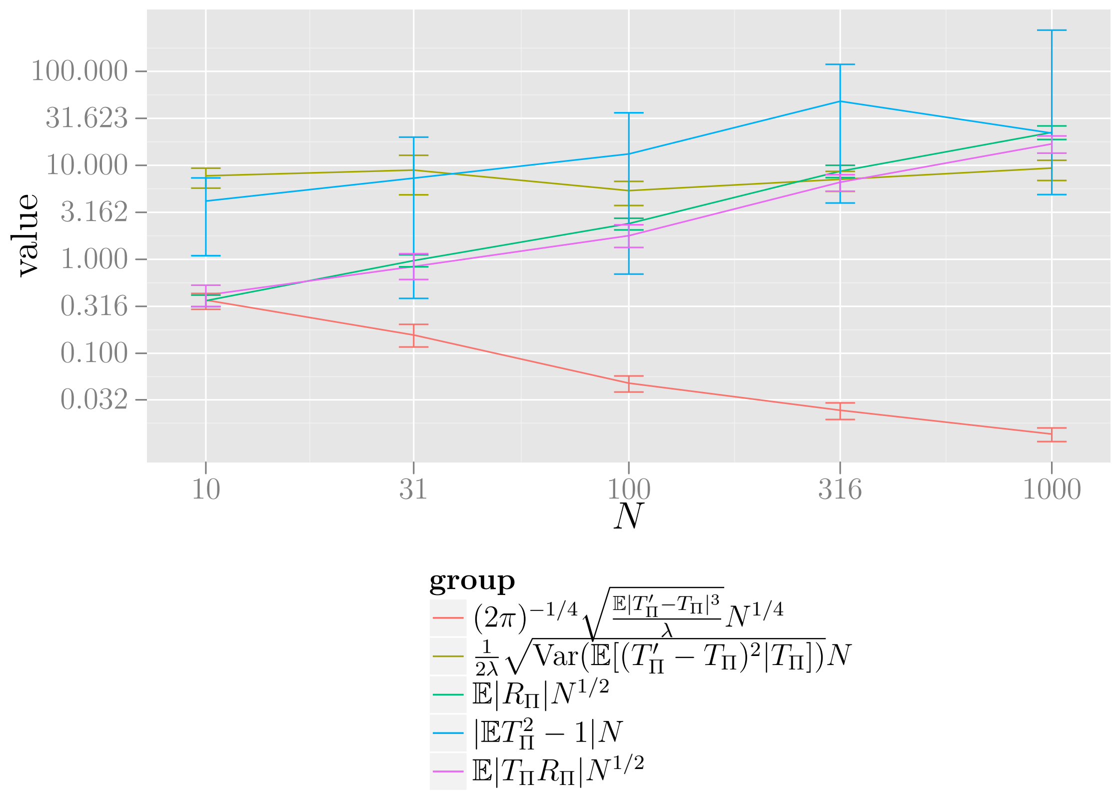


Figure 3.4: Log-log plot of values for each term in the bound, simulating the conditional expectation by Monte Carlo (1,000 MC draws, 100 permutations each).

The MC error is too large, and we see some scaled bounds actually increase.

3.3.2 Exact Conditional Expectation Calculations

Here we T' for all N^2 group-switching transpositions (I, J):

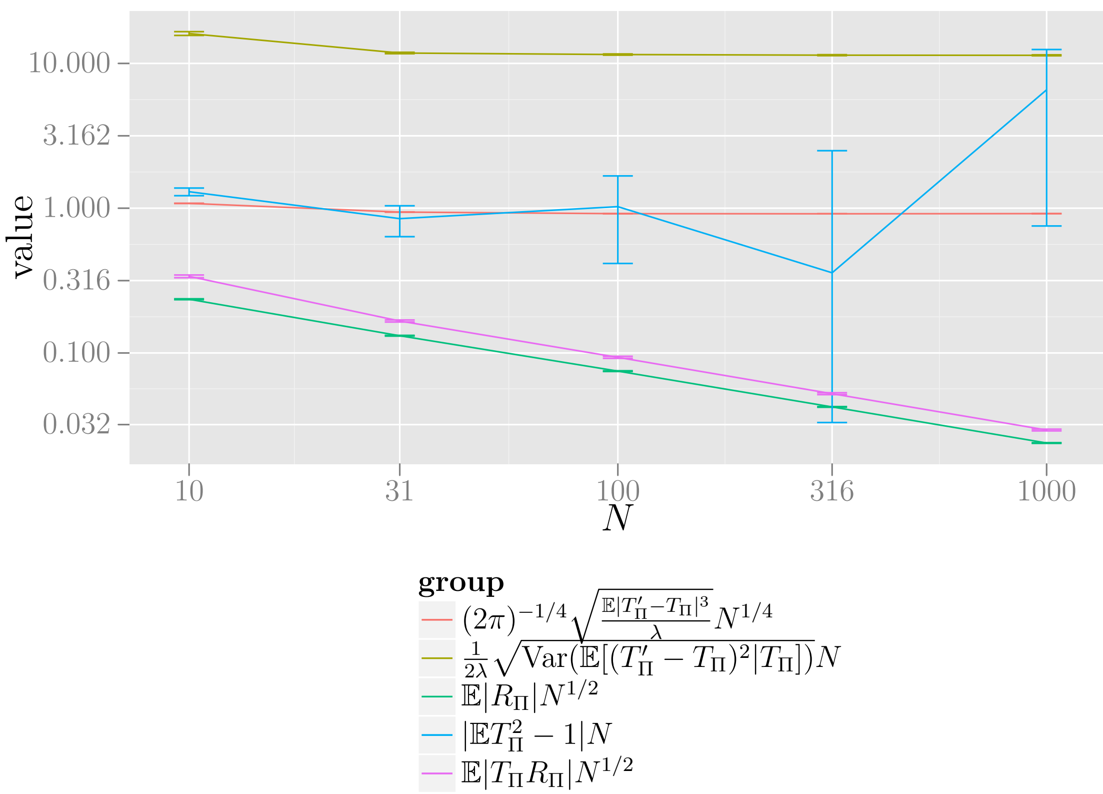
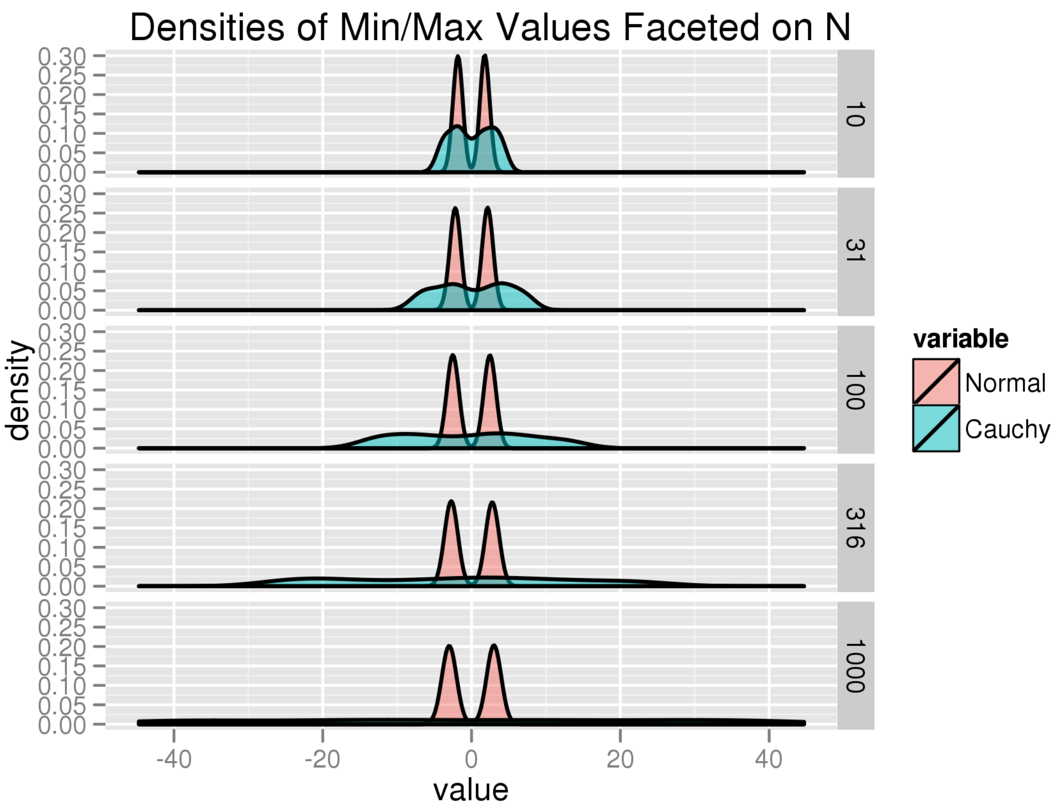


Figure 3.5: Log-log plot of values for each term in the bound, calculating the conditional expectation exactly (200,000 permutations each).

Our bounds appear to be of the correct order or slightly conservative in some cases. The bounds on the remainder terms ($\mathbb{E}|R_\Pi|$ and $\mathbb{E}|T_\Pi R_\Pi|$) are of order $N^{1/2}$, but the true rates are probably lower.

3.4 True Rate

To assess the true rate of convergence, we consider two settings: the earlier Normal setting and group draws from a Cauchy distribution with location parameters -1 and 1 depending on the group. Our bounds include a dependence on $u_\Delta = \max_i u_i - \min_i u_i$. To better understand the differences between these two models, we simulate the minimum and maximum scaled (mean 0 and sum of squares $2N$) values:



For $N = 1000$, the Normal model typically has u_Δ values around 6. In contrast, the Cauchy model has u_Δ values closer to 40.

Here, we plot the empirical Kolmogorov-Smirnov test statistic in the following three settings:

1. a standard Normal draw of size N (repeated N times to get the empirical distribution)

2. the permutation t-statistic under Cauchy sampling (N permutations)

3. the permutation t-statistic under Normal sampling (N permutations)

We also add the sum of the five unscaled, simulated bound terms $(200,000$ permutations) from the previous section.

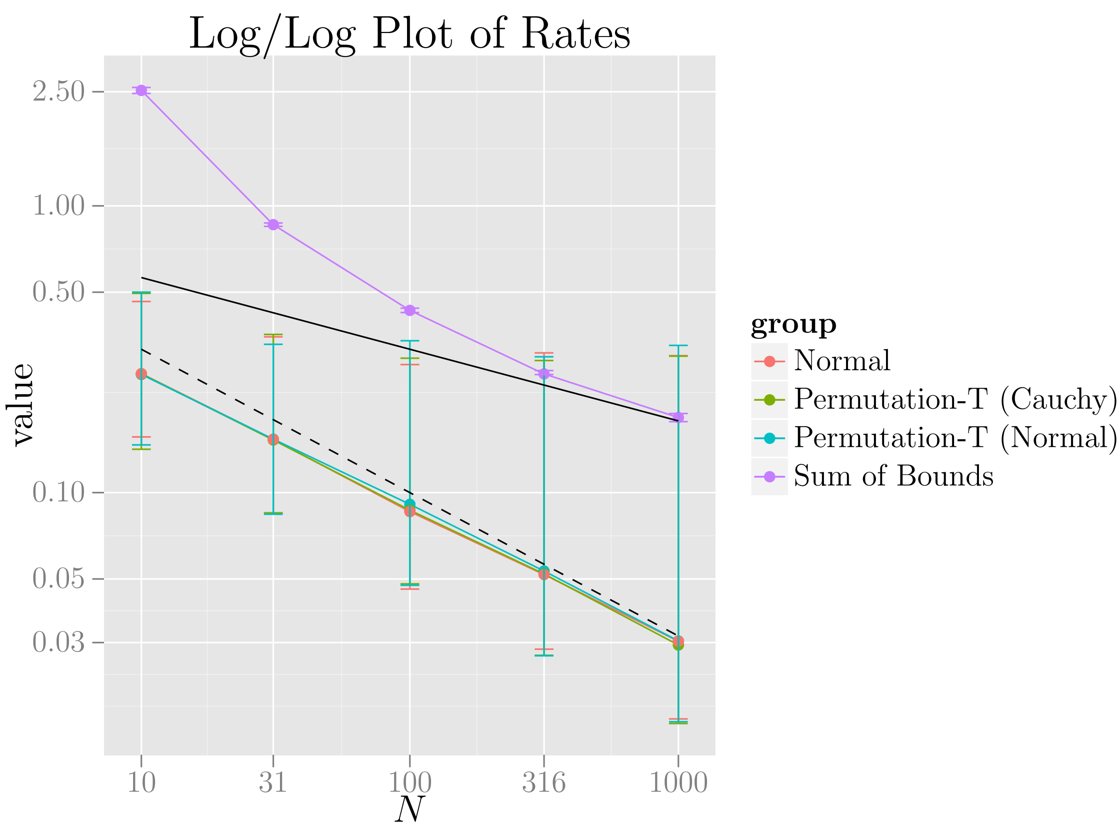


Figure 3.6: Solid black line: $N^{-1/4}$; dashed black line: $N^{-1/2}$

It's not a fair comparison to place the sum of the bounds on the same plot because that was computed over $200,000$ separate permutations instead of the 500 shared by the other three. Still, we can draw some general conclusions. The normal and two permutation-t K-S statistics decay perfectly at a rate of $N^{-1/2}$, and our bound follows a rate of $N^{-1/4}$, suggesting that the true rate of convergence is the former. Also, the error-bars seem to be increasing in size but are actually roughly constant due to the log-log scale.

Chen et al. [**?**] provide a simple example (pp.154-155) in which the sum of i.i.d. random variables yields

$$E|W' - W|^3 = \frac{4}{N^{3/2}}$$

with $\lambda = N^{-1}$. This leads to an $O(N^{-1/4})$ bound, which is suboptimal and apparently not uncommon when applying this kind of theorem.

3.5 Efficient Updates

Instead of conditioning on the value of T_Π, we condition on the observed permutation π. For N observations in each group, there are $N^2 T'_\Pi$ values that come from swapping one value in the first group with one value in the second. T'_Π should not differ much from T_Π, and calculating the t-statistics from scratch is inefficient.

We use an efficient t-statistic update rule to easily calculate millions of t-statistics. The two sample t-statistic is given by

$$T_\Pi = \frac{\bar{x} - \bar{u}}{\sqrt{\frac{2}{n}}\sqrt{\frac{1}{2}(S_X^2 + S_U^2)}},$$

where $S_X^2 = \frac{1}{N-1}(\sum_{i=1}^N x_i^2 - n\bar{x}^2)$.

Let T_{x_i,u_j} be the result of T' by swapping x_i with u_j:

$$\begin{aligned}
\Delta &\equiv u_j - x_i \\
\bar{x}_{x_i,u_j} &= \bar{x} - \frac{1}{N}x_i + \frac{1}{N}u_j = \bar{x} + \frac{\Delta}{N} \\
\bar{u}_{x_i,u_j} &= \bar{u} + \frac{1}{N}x_i - \frac{1}{N}u_j = \bar{u} - \frac{\Delta}{N} \\
S^2_{X_{x_i,u_j}} &= \frac{1}{N-1}(\sum_{k=1}^{N} x_k^2 - x_i^2 + u_j^2) - \frac{N}{N-1}\bar{x}^2_{x_i,u_j} \\
S^2_{U_{x_i,u_j}} &= \frac{1}{N-1}(\sum_{k=1}^{N} u_k^2 + x_i^2 - u_j^2) - \frac{N}{N-1}\bar{u}^2_{x_i,u_j} \\
\bar{x}^2_{x_i,u_j} &= \bar{x}^2 + \frac{2\Delta}{N}\bar{x} + \frac{\Delta^2}{N} \\
\bar{u}^2_{x_i,u_j} &= \bar{u}^2 - \frac{2\Delta}{N}\bar{u} + \frac{\Delta^2}{N}
\end{aligned}$$

Then

$$\begin{aligned}
T_{x_i,u_j} &= \frac{\bar{x}_{x_i,u_j} - \bar{u}_{x_i,u_j}}{\sqrt{\frac{2}{N}}\sqrt{\frac{1}{2}(S^2_{X_{x_i,u_j}} + S^2_{U_{x_i,u_j}})}} \\
&= \frac{\bar{x} - \bar{u} + \frac{2\Delta}{N}}{\sqrt{\frac{2}{N}}\sqrt{\frac{1}{2(N-1)}[\sum_{k=1}^{N}(x_k^2 + u_k^2) - N(\bar{x}^2 + \bar{u}^2 + \Delta(\frac{2\bar{x}}{n} - \frac{2\bar{u}}{n}) + \frac{2}{n^2}\Delta^2)]}}.
\end{aligned}$$

Only the terms involving Δ need to be recomputed for each of the N^2 swaps.

Consider a naïve implementation based on a double for-loop and recomputing each t-statistic anew versus a vectorized approach using the update formula:

```
computeAllCond2 <- function(T, N, u, l, x, y){
    minus <- which(l == -1)
    plus <- which(l == 1)
    Tprime <- 1:(N^2)
    for(j in 1:N){
      for(k in 1:N){
        swap <- c(minus[j], plus[k])
```

```
        l[swap] <- l[rev(swap)]
        Tprime[N*(j-1)+k] <- t.test(u[l==1], u[l==-1], var.equal=TRUE)$statistic
        l[swap] <- l[rev(swap)]
      }
    }
    data.frame("T" = T, "Tprime" = Tprime, "N" = N, "lambda" = 2 / N)
}

computeAllCond <- function(T, N, u, l, x, y){
  del <- rep(y, length(x)) - rep(x, each = length(y))
  xbar <- mean(x)
  ybar <- mean(y)
  Tprime <- -(xbar - ybar + 2/N*del) /
    (sqrt(2/N)*sqrt(sum(u^2)/(2*(N-1)) - 1/2*N/(N-1)*(xbar^2 + ybar^2 + 2*del/N*(x
  data.frame("T" = T, "Tprime" = Tprime, "N" = N, "lambda" = 2 / N)
}
```

We observe roughly a 2,000 times increase in speed on a problem instance of size $N = 100$. With byte-compilation and additional tuning, a four order of magnitude increase is possible.

```
> system.time(computeAllCond2(T, N, u, l, x, y))
   user  system elapsed
  7.333   0.000   7.334
> system.time(computeAllCond(T, N, u, l, x, y))
   user  system elapsed
  0.005   0.000   0.004
> sum((sort(computeAllCond(T, N, u, l, x, y)$Tprime) - sort(computeAllCond2(T, N,
[1] 3.137579e-27
dat <- ldply(rep(floor(10^(seq(1, 3.5, by=.5))), each = 8),
simulateBounds, .parallel = TRUE, .progress = "text")
> print(object.size(dat), units = "Gb")
```

```
2.6 Gb
```

3.6 A Different Exchangeable Pair

Rather than only consider transpositions that swap one element of the first group with one from the second group, we have a few different choices. Let's take the other extreme, where we consider all $(2N)^2$ transpositions, including null transpositions. There are N^2 transpositions within each group, for a total of $2N^2$. Each of these does not change the t-statistic. We previously only considered the N^2 transpositions where $I < J$. There are another N^2 with $I > J$. These transpositions have exactly the same effect as the previous group $(I, J) = (J, I)$, and all within-group transpositions have no effect.

The only changes should be to adjust the weights when taking conditional expectations (the weights should be 1/2) and to divide λ by 2. The new λ is N^{-1}.

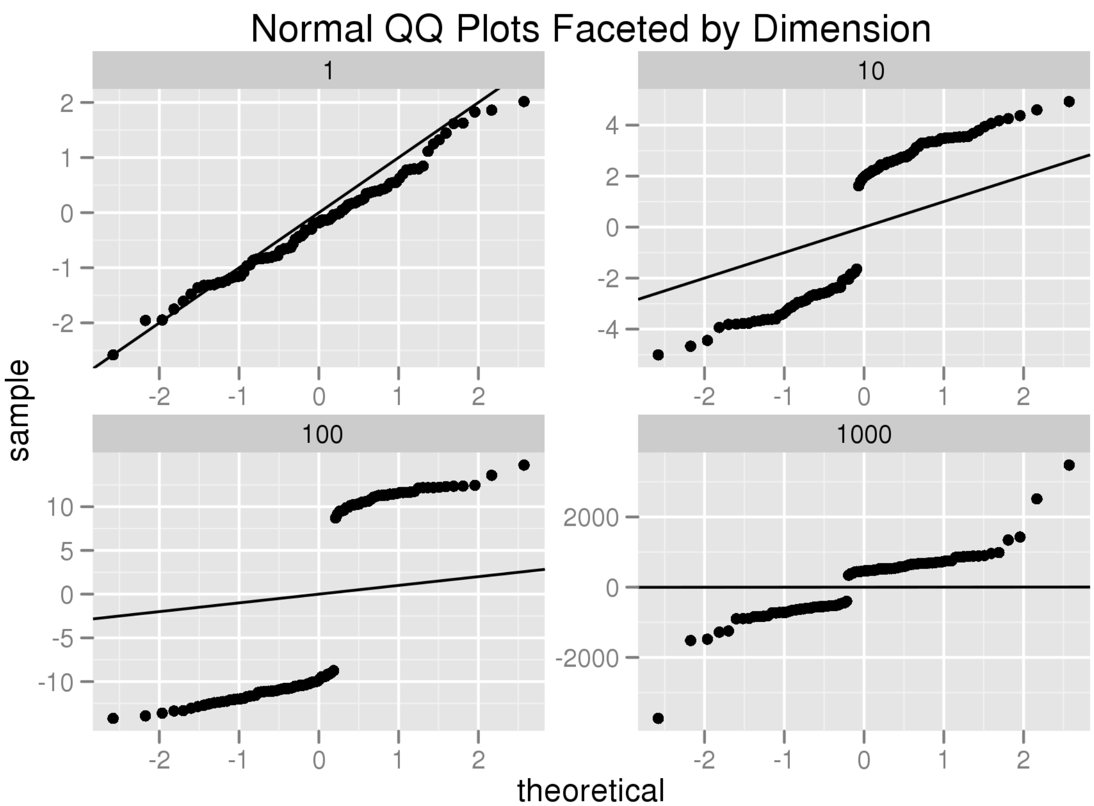
However, every term involving the conditional expectation also has a division by lambda, so any decrease in the c.e. is cancelled out by a corresponding decrease in λ, so there is no change in any of the simulations.

It's nice that the calculations are invariant to change in the exchangeable pair. Whether that holds true for more drastic changes (e.g. swapping more than 2 elements) is not known.

3.7 Generalizations (Null Distribution)

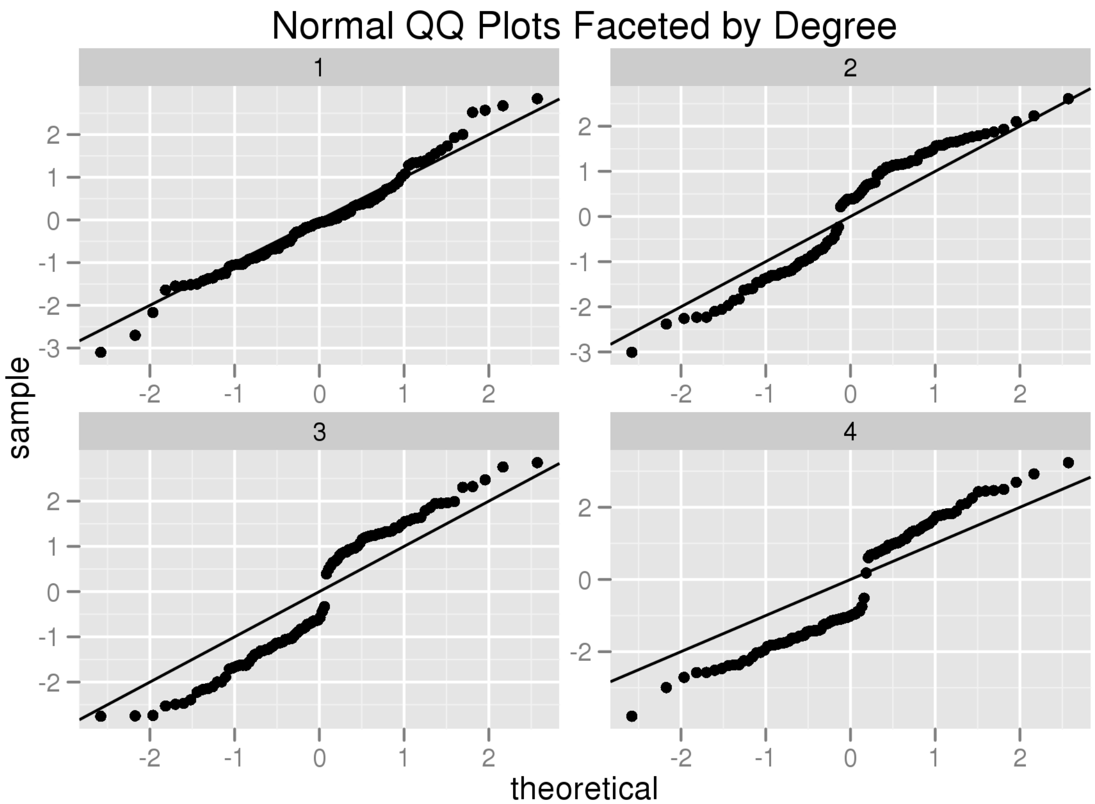
It is natural to consider generalizations from the univariate data, linear kernel setting. We explore whether the randomization distribution is still Normal with multivariate data and/or a non-linear kernel. Should the null distribution be non-Normal, we further attempt to determine whether the approximate regression condition holds.

We generate 100 observations with dimensionality 1, 10, 100, and 1000. For each set of data, we permute 100 times and plot the Friedman statistic (t-statistic on SVM fitted values) with a linear kernel against the standard Normal quantiles. Note that we take the sign of the Friedman statistic to be positive or negative with equal probability for ease of comparing distributions.



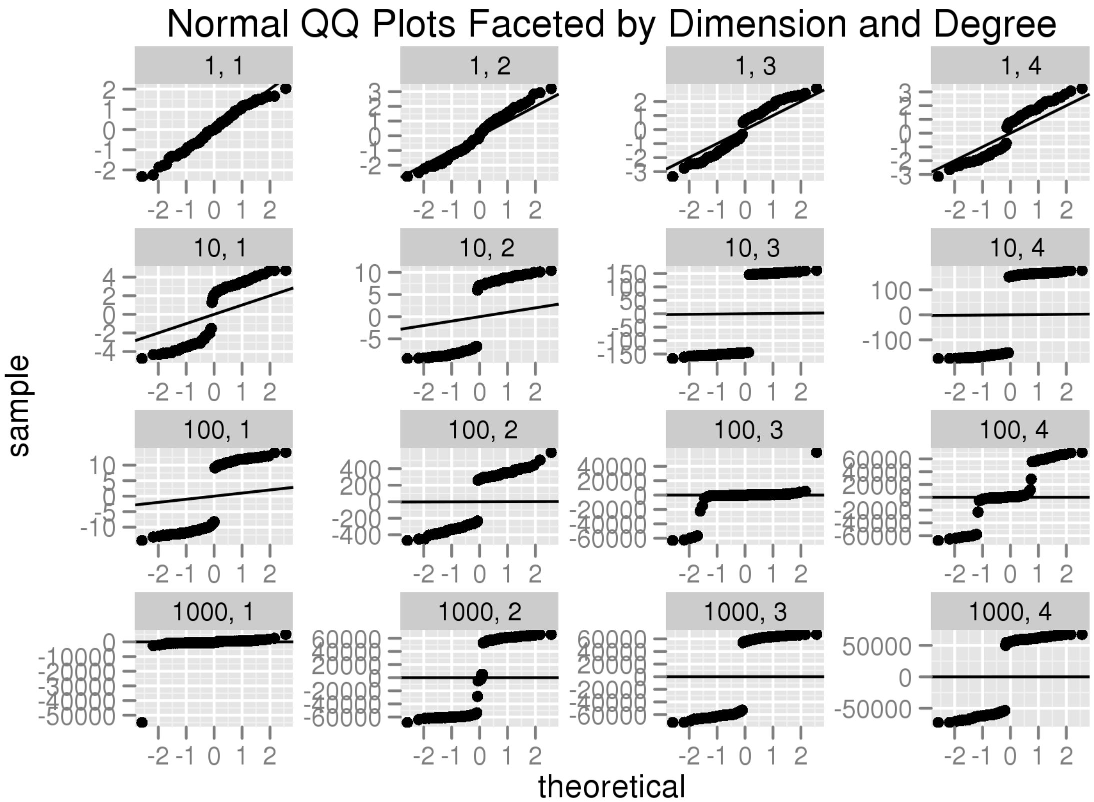
At a sample size of 100 and with univariate data, the standard Normal is a close fit. With increasing dimensionality, the Friedman statistic gets more and more extreme. One possible explanation is that it becomes easier to separate two sets of points as the dimensionality increases.

Here we look at univariate data but with an inhomogeneous kernel $(k(x, x') = (< x, x' > +1)^d)$ of degree d:



The polynomial kernel for degrees greater than 1 yields null distributions with fatter tails than the standard Normal.

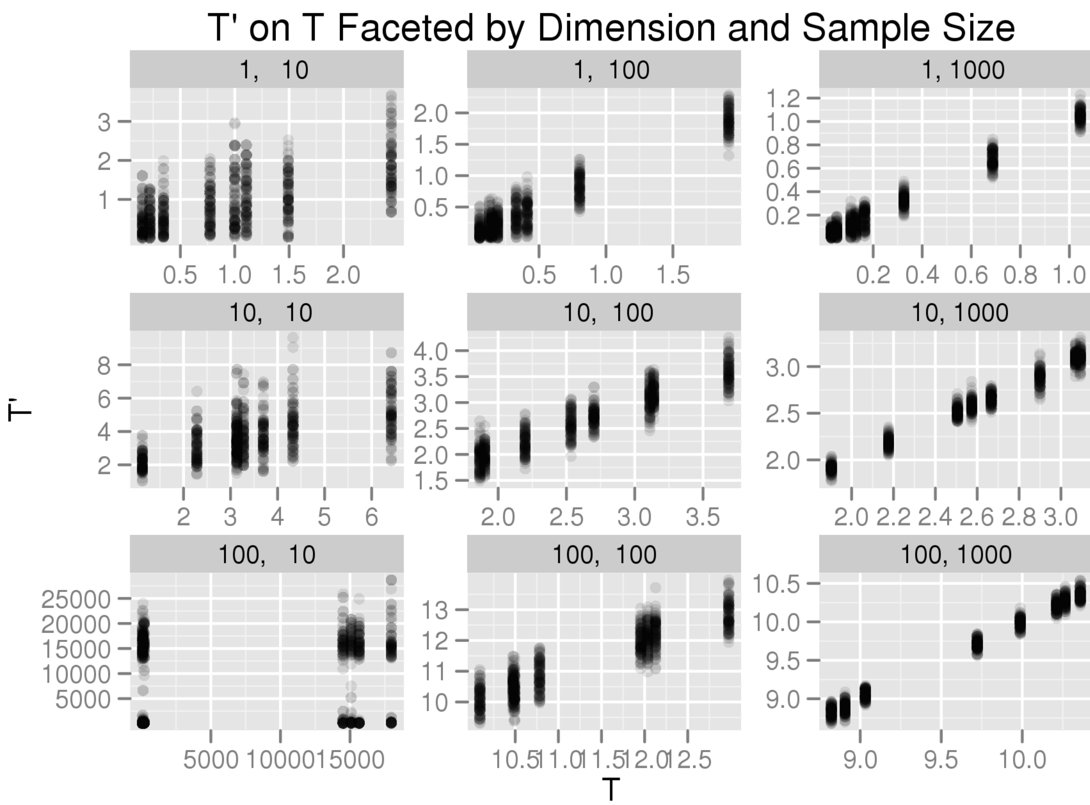
Here we look at the effects of both dimension of the underlying data and degree of the inhomogeneous kernel:



3.8 Generalizations (Approximate Regression Condition)

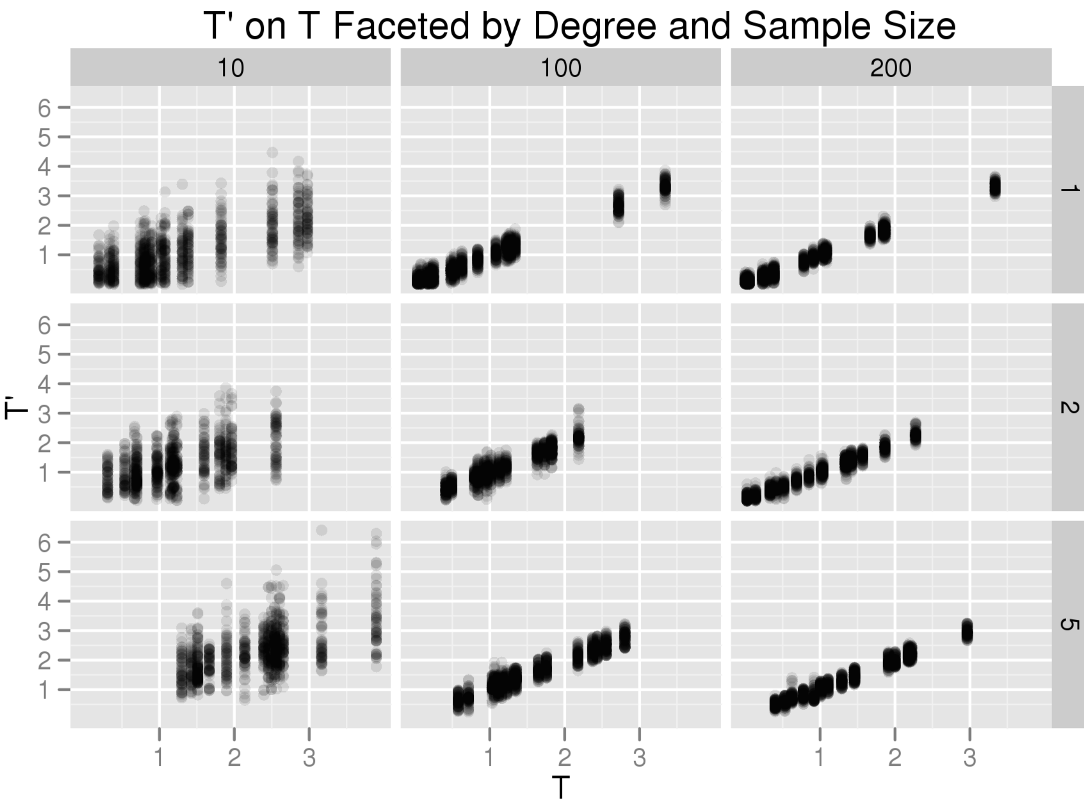
Here we plot T' on T, where T' results from swapping labels and refitting the SVM. Note that here we don't assign the statistics random signs because there is no clear way to maintain the coupling between T and T'.

The dimensions (rows) are 1, 10, and 100, and the sample sizes (columns) are 10, 100, and 1000.



Across a row, it is clear that a larger sample size decreases the variability of T' about T. And down a column, it is clear that increasing dimensionality results in a greater departure from (folded) Normality. It is not clear whether the reduction in variability is of order $1/N$.

Here we look at sample sizes (columns) of 10, 100, and 200 and inhomogeneous polynomial kernel degrees (rows) of 1, 2, and 5.



We again observe an approximately linear plus noise relationship between T' and T with the noise decreasing in sample size.

Chapter 4

Friedman's Test

4.1 a

blah

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