Markov Bases for Noncommutative Fourier Analysis of Ranked Data

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Abstract

To calibrate Fourier analysis of S_5 ranking data by Markov chain Monte Carlo techniques, a set of moves (Markov basis) is needed. We calculate this basis, and use it to provide a new statistical analysis of two data sets. The calculation involves a large Gröbner basis computation (45825 generators), but reduction to a minimal basis and reduction by natural symmetries leads to a remarkably small basis (14 elements). Although the Gröbner basis calculation is infeasible for S_6, we exploit the symmetry of the problem to calculate a Markov basis for S_6 with 7,113,390 elements in 58 symmetry classes. We improve a bound on the degree of the generators for a Markov basis for S_n and conjecture that this ideal is generated in degree 3.

1 Election data with five candidates

Table 1 shows the results of an election. A population of 5738 voters was asked to rank five candidates for president of a national professional organization. The table shows the number of voters choosing each ranking. For example, 29 voters ranked candidate 5 first, candidate 4 second, . . . , and candidate 1 last, resulting in the entry 54321 = 29. Table 2 shows a simple summary of the data: the proportion of voters ranking candidate i in position j. For example, 28.0% of the voters ranked candidate 3 first and 23.1% of the voters ranked candidate 3 last.

Table 2 is a natural summary of the 120 numbers in Table 1, but is it an adequate summary? Does it capture all the "juice" in the data? In this paper,

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Table 1
American Psychological Association voting data: the number of voters that ranked the 5 candidates in a given order.

Ranking	# votes	Ranking	# votes	Ranking	# votes	Ranking	# votes
54321	29	43521	91	32541	41	21543	36
54312	67	43512	84	32514	64	21534	42
54231	37	43251	30	32451	34	21453	24
54213	24	43215	35	32415	75	21435	26
54132	43	43152	38	32154	82	21354	30
54123	28	43125	35	32145	74	21345	40
53421	57	42531	58	31542	30	15432	40
53412	49	42513	66	31524	34	15423	35
53241	22	42351	24	31452	40	15342	36
53214	22	42315	51	31425	42	15324	17
53142	34	42153	52	31254	30	15243	70
53124	26	42135	40	31245	34	15234	50
52431	54	41532	50	25431	35	14532	52
52413	44	41523	45	25413	34	14523	48
52341	26	41352	31	25341	40	14352	51
52314	24	41325	23	25314	21	14325	24
52143	35	41253	22	25143	106	14253	70
52134	50	41235	16	25134	79	14235	45
51432	50	35421	71	24531	63	13542	35
51423	46	35412	61	24513	53	13524	28
51342	25	35241	41	24351	44	13452	37
51324	19	35214	27	24315	28	13425	35
51243	11	35142	45	24153	162	13254	95
51234	29	35124	36	24135	96	13245	102
45321	31	34521	107	23541	45	12543	34
45312	54	34512	133	23514	52	12534	35
45231	34	34251	62	23451	53	12453	29
45213	24	34215	28	23415	52	12435	27
45132	38	34152	87	23154	186	12354	28
45123	30	34125	35	23145	172	12345	30

Table 2
First order statistics: The proportion of voters who ranked candidate i in position j. This is a scaled version of the Fourier transform of Table 1 at the permutation representation.

	Rank				
Candidate	1	2	3	4	5
1	18.3	26.4	22.8	17.4	14.8
2	13.5	18.7	24.6	24.6	18.3
3	28.0	16.7	13.8	18.2	23.1
4	20.4	16.9	18.9	20.2	23.3
5	19.6	21.0	19.6	19.2	20.3

we develop tools to answer such questions using Fourier analysis and algebraic techniques.

In Section 2, we give a general exposition of how noncommutative Fourier analysis can be used to analyze group valued data with summary given by a representation ρ. In order to use Markov chain Monte Carlo techniques to calibrate the Fourier analysis, we define an exponential family and toric ideal associated to a finite group G and integer representation ρ. A generating set of the toric ideal can be used to run a Markov chain to sample from data on the group. For example, the 14 moves in Table 3 allow us to randomly sample from the space of data on S_5 with fixed first order summary (Table 2).

In Section 3 we show how this basis (Table 3) was computed - either using Gröbner bases or by utilizing symmetry. We describe extensive computations of the basis for ranked data on at most 6 objects. From these computations, we conjecture that the toric ideal for S_n is generated in degree 3. In Section 4, we show this ideal for S_n is generated in degree $n-1$, improving a result of Diaconis and Sturmfels (1998), and we describe the degree 2 moves. Finally, in Section 5, we apply these methods to analyze the data in Table 1 and an example from Diaconis and Sturmfels (1998).

2 Fourier analysis of group valued data

Let G be a finite group (in our example, $G = S_5$). Let $f\colon G \to \mathbb{Z}$ be any function on G. For example, if $g_1, g_2, \ldots, g_N$ is a sample of points chosen from a distribution on G, take $f(g)$ to be the number of sample points g_i that are equal to g. We view f interchangeably as either a function on the group or an element of the group ring $\mathbb{Z}[G]$. Recall that a map $\rho\colon G \to GL(V_\rho)$ is a matrix representation of G if $\rho(st) = \rho(s)\rho(t)$ for all $s, t \in G$. The dimension d_ρ of

Table 3
S_5 moves: there are 29890 moves in 14 symmetry classes of sizes 200-7200

Move	Number	Move	Number
$\begin{bmatrix} 53412 \\ 54321 \end{bmatrix} - \begin{bmatrix} 53421 \\ 54312 \end{bmatrix}$	450	$\begin{bmatrix} 45231 \\ 54312 \end{bmatrix} - \begin{bmatrix} 45312 \\ 54231 \end{bmatrix}$	600
$\begin{bmatrix} 54123 \\ 54231 \\ 54312 \end{bmatrix} - \begin{bmatrix} 54132 \\ 54213 \\ 54321 \end{bmatrix}$	200	$\begin{bmatrix} 53412 \\ 54123 \\ 54231 \end{bmatrix} - \begin{bmatrix} 53421 \\ 54132 \\ 54213 \end{bmatrix}$	3600
$\begin{bmatrix} 45123 \\ 54231 \\ 54312 \end{bmatrix} - \begin{bmatrix} 45132 \\ 54213 \\ 54321 \end{bmatrix}$	200	$\begin{bmatrix} 45123 \\ 53412 \\ 54231 \end{bmatrix} - \begin{bmatrix} 45132 \\ 53421 \\ 54213 \end{bmatrix}$	7200
$\begin{bmatrix} 43512 \\ 54123 \\ 54231 \end{bmatrix} - \begin{bmatrix} 43521 \\ 54132 \\ 54213 \end{bmatrix}$	3600	$\begin{bmatrix} 43512 \\ 53241 \\ 54123 \end{bmatrix} - \begin{bmatrix} 43521 \\ 53142 \\ 54213 \end{bmatrix}$	3600
$\begin{bmatrix} 45231 \\ 52341 \\ 53412 \end{bmatrix} - \begin{bmatrix} 45312 \\ 52431 \\ 53241 \end{bmatrix}$	7200	$\begin{bmatrix} 45132 \\ 52341 \\ 53412 \end{bmatrix} - \begin{bmatrix} 45312 \\ 52431 \\ 53142 \end{bmatrix}$	3600
$\begin{bmatrix} 34512 \\ 45123 \\ 53241 \end{bmatrix} - \begin{bmatrix} 34521 \\ 45213 \\ 53142 \end{bmatrix}$	600	$\begin{bmatrix} 34521 \\ 45213 \\ 53142 \end{bmatrix} - \begin{bmatrix} 35142 \\ 43521 \\ 54213 \end{bmatrix}$	600
$\begin{bmatrix} 35142 \\ 43521 \\ 54213 \end{bmatrix} - \begin{bmatrix} 35241 \\ 43512 \\ 54123 \end{bmatrix}$	600	$\begin{bmatrix} 34521 \\ 45312 \\ 52143 \end{bmatrix} - \begin{bmatrix} 35142 \\ 42513 \\ 54321 \end{bmatrix}$	1440

the representation ρ is the dimension of V_ρ as a $\mathbb{C}$-vector space. We say that a ρ is integer-valued if $\rho_{ij}(g) \in \mathbb{Z}$ for all $g \in G$ and for all $1 \leq i, j \leq d_\rho$. We denote the set of irreducible representations of G by $\hat{G}$.

An analysis of $f(g)$ may be based on the Fourier transform. The Fourier transform of f at ρ is

$$\hat{f}(\rho) = \sum_{g \in G} f(g)\rho(g). \tag{1}$$

The Fourier transform at all the irreducible representations $\rho \in \hat{G}$ determines f through the Fourier inversion formula

$$f(g) = \frac{1}{|G|} \sum_{\rho \in \hat{G}} d_\rho \operatorname{Tr}(\hat{f}(\rho)\rho(g^{-1})), \tag{2}$$

which can be rewritten as $f(g) = \sum_{\rho \in \hat{G}} f|_{V_\rho}(g)$, where

$$f|_{V_\rho}(g) = \frac{d_\rho}{|G|} \sum_{h \in G} \chi_\rho(h) f(gh). \tag{3}$$

This decomposition shows the contributions to f from each of the irreducible representations of G. For example, if a few of the $f|_{V_\rho}$ are large, we can analyze these components in order to understand the structure of f. See Diaconis (1988, 1989) for background, proofs, and previous literature.

Example 1 *This analysis is most familiar for the cyclic group C_n where it becomes the discrete Fourier transform*

$$\hat{f}(j) = \sum_{k=0}^{n-1} f(k) e^{-2\pi i jk/n}, \qquad f(k) = \frac{1}{n} \sum_{j=0}^{n-1} \hat{f}(j) e^{2\pi i kj/n} \tag{4}$$

In (4), if a few of the $\hat{f}(j)$ are much larger than the rest, then f is well understood as approximately a sum of a few periodic components.

Table 4
Squared length (divided by 120) of the projection of the APA data into the 7 isotypic subspaces of S_5.

	S^5	$S^{4,1}$	$S^{3,2}$	$S^{3,1,1}$	$S^{2,2,1}$	$S^{2,1,1,1}$	$S^{1,1,1,1,1}$
d_ρ^2	1	16	25	36	25	16	1
Data	2286	298	459	78	27	7	0

Table 5
Second order summary for the APA data

	Rank									
Candidate	1,2	1,3	1,4	1,5	2,3	2,4	2,5	3,4	3,5	4,5
1,2	-137	-20	18	140	111	22	4	6	-97	-46
1,3	476	-88	-179	-209	-147	-169	-160	107	128	241
1,4	-189	51	113	24	-9	98	99	-65	23	-146
1,5	-150	57	47	45	43	49	56	-48	-53	-48
2,3	-42	84	19	-61	30	-16	82	-76	-39	72
2,4	157	-20	-43	-25	-93	-76	-56	8	38	112
2,5	22	-44	7	15	-117	69	25	62	99	-138
3,4	-265	-7	72	199	39	140	85	19	-52	-233
3,5	-169	10	88	70	78	44	47	-51	-36	-80
4,5	296	-24	-142	-130	-5	-163	-128	38	-9	267

For the symmetric group S_n, the permutation representation assigns permutation matrices $\rho(\pi)$ to permutations π. Thus, if $f(\pi)$ is the number of rankers choosing π, $\hat{f}(\rho)$ is a $n \times n$ matrix with (i,j) entry the number of rankers ranking item i in position j (as in Table 2). The irreducible representations of S_5 are indexed by the seven partitions of five and are written as S^λ where λ is a partition of 5. For our data, (2) gives a decomposition of f into 7 parts. Table 4 shows the lengths of the projection of Table 1 onto the seven isotypic subspaces of S_5.

The largest contribution to the data occurs from the trivial representation S^5. We call the projection onto $S^5 \oplus S^{4,1}$ the first order summary; it was shown in Table 2 above. We see that the projection onto $S^{3,2}$ is also sizable while the rest of the projections are relatively negligible. This suggests a data-analytic look at the projection into $S^{3,2}$. Table 5 shows this projection in a natural coordinate system. This projection is based on the permutation representation of S_5 on unordered pairs $\{i,j\}$. Table 5 is an embedding of a 25 dimensional space into a 100 dimensional space so that its coordinates are easy to interpret. See Diaconis (1989) for further explanation.

The largest number in Table 5 is 476 in the $\{1, 3\}, \{1, 2\}$ position corresponding to a large positive contribution to ranking candidates one and three in the top two positions. There is also a large positive contribution for ranking candidates four and five in the top two positions. Since Table 5 gives the projection of f onto a subspace orthogonal to $S^5 \oplus S^{4,1}$, the popularity of individual candidates has been subtracted out. We can see the "hate vote" against the pair of candidates one and three (and the pair four and five) from the last column. Finally, the negative entries for e.g., pairs one and four, one and five, three and four, three and five show that voters don't rank these pairs in the same way.

The preceding analysis is from Diaconis (1989) which used it to show that noncommutative spectral analysis could be a useful adjunct to other statistical techniques for data analysis.

The data is from the American Psychological Association – a polarized group of academicians and clinicians who are on very uneasy terms (the organization almost split in two just after this election). Candidates one and three are in one camp, candidates four and five from the other. Candidate two seems disliked by both camps. The winner of the election depends on the method of allocating votes. For example, the Hare system or plurality voting would elect candidate three. However, other widely used voting methods (Borda's sum of ranks or Coomb's elimination system) elect candidate one. For details and further analysis of the data, see Stern (1993).

To explain the perturbation analysis in Section 5, it is useful to consider a simple exponential model for group-valued data.

Definition 2 *Let ρ be an integer valued representation of a finite group G. Then the exponential family of G and ρ is given by the family of probability distributions on G*

$$P_\Theta(g) = Z^{-1}\, \mathrm{e}^{\mathrm{Tr}(\Theta\rho(g))} \tag{5}$$

where the normalizing constant is $Z = \sum_{g\in G} \mathrm{e}^{\mathrm{Tr}(\Theta\rho(g))}$ and Θ is a $n \times n$ matrix of parameters to be chosen to fit the data.

For example let $G = S_n$ and ρ be the usual permutation representation. Then if Θ is the zero matrix, P_Θ is the uniform distribution. If $\Theta_{1,1}$ is nonzero and $\Theta_{i,j}$ is zero otherwise, the model P_Θ corresponds to item one being ranked first with special probability, the rest ranked randomly. Such models have been studied by Silverberg (1984); Verducci (1982); Diaconis (1989). See Marden (1995) for a book-length treatment of models for permutation data.

From the Darmois-Koopman-Pitman Theorem (e.g., Diaconis and Freedman, 1984, Theorem 3.1), we deduce

Proposition 3 *The model (5) has the property that a sufficient statistic for*

Θ based on data $f(\pi)$ is the Fourier transform $\hat{f}(\rho)$. Furthermore, (5) is the unique model characterized by this property.

Definition 4 *Given a finite group G and an integer valued representation ρ of dimension d_ρ define the toric ideal of G at ρ as $I_{G,\rho} = \ker(\phi_{G,\rho})$, where*

$$\phi_{G,\rho}\colon \mathbb{C}[x_g \mid g \in G] \longrightarrow \mathbb{C}[t_{ij}^{\pm 1} \mid 1 \le i,j \le d_\rho]$$
$$x_g \longmapsto \prod_{1\le i,j\le d_\rho} t_{ij}^{\rho_{ij}(g)}.$$

This ideal is the vanishing ideal of the exponential family from Definition 2. It will be our main object of study in Sections 3 and 4.

As suggested by Fisher (1973), tests of goodness of fit of the model (5) should be based on the conditional distribution of the data f given the sufficient statistic $\hat{f}(\rho)$. By an elementary calculation,

$$P_\Theta(f|\hat{f}(\rho)) = w^{-1} \prod_{\sigma\in G} \frac{1}{f(\sigma)!}, \quad \text{where} \quad w = \sum_{\substack{g\in\mathbb{Z}[G] \\ \hat{g}(\rho)=\hat{f}(\rho)}} \prod_{\sigma\in G} \frac{1}{g(\sigma)!}. \tag{6}$$

Observe that the conditional distribution in (6) is free of the unknown parameter Θ.

The original justification for the Fourier decomposition is model free (nonparametric). The first order summary in Table 2 is a natural object to look at and the second order summary was analyzed because of a sizable projection to $S^{3,2}$ in Table 4. It is natural to wonder if the second order summary is real or just a consequence of finding patterns in any set of numbers. To be honest, the APA data is not a sample (those 5,972 who choose to vote are likely to be quite different from the bulk of the 100,000 or so APA members). If the first order summary is accepted "as is", the largest probability model for which $\hat{f}(\rho)$ captures all the structure in the data is the exponential family (5). It seems natural to use the conditional distribution of the data given $\hat{f}(\rho)$ as a way of perturbing things. The uniform distribution on data with fixed $\hat{f}(\rho)$ is a much more aggressive perturbation procedure. Both are computed and compared in Section 5.

3 Computing Markov bases for permutation data

To carry out a test based on Fisher's principles, we use Markov chain Monte Carlo to draw samples from the distribution (6).

Table 6
Markov bases for S_3 and S_4 and the size of their symmetry classes.

S_3 Move	Number	S_4 Move	Number
$\begin{bmatrix}123\\231\\312\end{bmatrix}-\begin{bmatrix}132\\213\\321\end{bmatrix}$	1	$\begin{bmatrix}1234\\2143\end{bmatrix}-\begin{bmatrix}1243\\2134\end{bmatrix}$	18
		$\begin{bmatrix}2314\\2431\\4123\end{bmatrix}-\begin{bmatrix}2134\\2413\\4321\end{bmatrix}$	144
		$\begin{bmatrix}1324\\2134\\3214\end{bmatrix}-\begin{bmatrix}1234\\2314\\3124\end{bmatrix}$	16

Definition 5 *A* Markov basis *for a finite group G and a representation ρ is a finite subset of "moves" $g_1, \ldots, g_B \in \mathbb{Z}[G]$ with $\hat{g}_i(\rho) = 0$ such that any two elements in $\mathbb{N}[G]$ with the same Fourier transform at the representation ρ can be connected by a sequence of moves in that subset.*

In Diaconis and Sturmfels (1998) it was explained how Gröbner basis techniques could be applied to find such Markov bases.

Proposition 6 *A generating set of $I_{G,\rho}$ (see Definition 4) is a Markov basis for the group G and the representation ρ.*

We will write I_{S_n} for our main example, the ideal of S_n with the permutation representation ρ. The representation $\rho\colon \mathbb{N}[S_n] \to \mathbb{N}^{n^2}$ sends an element of S_n to its permutation matrix. The elements $\mathbf{b} \in \mathbb{N}^{n^2}$ with $\rho^{-1}(\mathbf{b})$ non-empty are the *magic squares*, that is, matrices with non-negative integer entries such that all row and column sum are equal. We write an element $\pi_1 + \cdots + \pi_m \in \mathbb{N}[S_n]$ as a tableau $\begin{bmatrix}\pi_1(1) & \ldots & \pi_1(n)\\ \vdots & & \vdots \\ \pi_m(1) & \ldots & \pi_m(n)\end{bmatrix}$. In this notation, a Markov basis element is written as a difference of two tableaux. For example, the degree 2 element of the Markov basis for S_5, $\begin{bmatrix}13452\\14325\end{bmatrix} - \begin{bmatrix}13425\\14352\end{bmatrix}$, corresponds to adding one to the entries 13452 and 14325 in Table 1 and subtracting one from the entries 13425 and 14352.

At the time of writing Diaconis and Sturmfels (1998), finding a Gröbner basis for I_{S_5} was computationally infeasible. Due to an increase in computing power and the development of the software `4ti2` (Hemmecke and Hemmecke, 2003), we were able to compute a Gröbner and a minimal basis of I_{S_5}.

This computation involved finding a Gröbner basis of a toric ideal involving 120 indeterminates. It took `4ti2` approximately 90 hours of CPU time on a 2GHz machine and produced a basis with 45,825 elements. The Markov basis had 29890 elements, 1050 of degree 2 and 28840 of degree 3, see Tables 3 and 7. Using `4ti2`, we have also computed Markov bases of the ideals I_{S_n} for $n = 3$ and $n = 4$, they are shown in Table 6.

Although the calculation for S_6 is currently not possible using Gröbner basis methods, there is a natural group action that reduces the complexity of this problem. The group $S_n \times S_n$ acts on $\mathbb{N}^{n^2}$ by permuting rows and columns. If we permute the rows and columns of a magic square, we still have a magic square, therefore, this action lifts to a group action on the Markov basis of I_{S_n}. In terms of tableaux, one copy of S_n acts by permuting columns of the tableau, the other acts by permuting the labels in the tableau. We have calculated orbits under this action, notice that the symmetrized bases are remarkably small (Table 7).

To calculate a Markov basis for I_{S_6}, we had to construct the fiber over every magic square with sum at most 5 (by Theorem 8) and then pick moves such that every fiber is connected by these moves (see Sturmfels, 1996, Theorem 5.3). For degrees 2 and 3 this was relatively straightforward (e.g., there are 20,933,840 six by six magic squares with sum 3). For these degrees, we constructed all squares and then calculated orbits of the group action and calculated the fiber for each orbit (there were 11 orbits in degree 2 and 103 in degree 3).

However, there are 1,047,649,905 six by six magic squares of degree 4 and 30,767,936,616 of degree 5 (from Beck and Pixton, 2003), so complete enumeration was not possible. Instead, we first randomly generated millions of magic squares with sums 4 or 5 using another Markov chain. We broke these down into orbits, keeping track of the number of squares we had found. For example, we needed to generate 30 million squares of degree 5 to find a representative for each orbit. We were left with 2804 orbits for degree 4 and 65481 orbits for degree 5. For degree 5, the proof of Theorem 8 shows that we only need to consider magic squares with norm squared less that 50, leaving 13196 orbits to check. The fibers were calculated by a depth first search with pruning. Remarkably, the computation showed that I_{S_6} is generated in degree 3, see Table 7.

The entire calculation for S_6 took about 2 weeks, with the vast majority of the time spent calculating orbits of degree 5 squares. Our data and code (in perl) are available for download at `http://math.berkeley.edu/~eriksson`. The code could be easily adapted to calculate other Markov bases with a good degree bound and a large symmetry group. Our calculations and Table 7 suggest the following conjecture:

Conjecture 7 *The ideal I_{S_n} is generated in degree 3.*

4 Structure of the toric ideal I_{S_n}

Theorem 6.1 of Diaconis and Sturmfels (1998) shows that every reverse lexicographic Gröbner basis of I_{S_n} has degree at most n. By considering only minimal generators and not a full Gröbner basis, we are able to strengthen

Table 7
Number of generators and symmetry classes of generators by degree in a Markov basis for I_{S_n}.

	Degree 2		Degree 3		Degree 4		Degree 5		Degree 6	
n	all	sym	all	sym	all	sym	all	sym	all	sym
3	0	0	1	1						
4	18	1	160	2	0	0				
5	1050	2	28840	12	0	0	0	0		
6	57150	7	7056240	51	0	0	0	0	0	0

this degree bound.

Theorem 8 *The ideal I_{S_n} is generated in degree $n-1$ for $n > 3$.*

PROOF. Since we know that I_{S_n} is generated in degree n, we need to show that the fibers over all magic squares with sum n are each connected by moves of degree $n-1$ or less. Let S and T be tableaux in $\rho^{-1}(\mathbf{b})$, where $\mathbf{b}$ is a magic square with sum n. Suppose that the first row of S and the first row of T differ in exactly k places. Then we claim that there is a degree $k+1$ move that can be applied to S to get a tableaux $S' \in \rho^{-1}(\mathbf{b})$ with the same first row as T.

To change the first row of S to make it agree with the first row of T, we have to permute k elements of the first row of S. But to remain in the fiber, this means we must also permute (at most) k other rows of S. For example, if the first row of S is $123\ldots n$ and the first row of T is $213\ldots n$, we would also have to pick the row of S with a 2 in the first column and the row with a 1 in the second column. Once we have picked the (at most) k rows of S that must be changed, it follows from Birkhoff's theorem (e.g., van Lint and Wilson, 2001, Theorem 5.5) that we can change these k rows and the first row to make a new tableau $S' \in \rho^{-1}(\mathbf{b})$ that agrees with T in one row.

We applied a degree $k+1$ move and are left with S' and T being connected by a degree $n-1$ move, so as long as we have $k+1 \leq n-1$, we are done. That is, for every pair (S,T) of tableaux in a degree n fiber, we must show that there is a row of S and a row of T that differ in at most $n-2$ places.

Given such a pair (S,T), introduce an $n \times n$ matrix M where the entries M_{ij} are the number of entries that row i of S and row j of T agree. Notice that if $M_{ij} \geq 2$, we have rows i in S and j in T that differ in at most $n-2$ places and are done.

Suppose that row i of S is $(\pi_i(1), \ldots, \pi_i(n))$. The row sum $\sum_{j=1}^n M_{ij}$ counts the total number of times that $\pi_i(j)$ appears in column j for each j. This is exactly $\sum_{k=1}^{n} \mathbf{b}(k, \pi(k))$. Summing over all rows, we see that every entry of $\mathbf{b}$ gets counted its cardinality number of times. That is,

$$\sum_{1 \le i,j \le n} M_{ij} = \sum_{1 \le i,j \le n} \mathbf{b}(i,j)^2 = ||\mathbf{b}||^2$$

Now since each row of $\mathbf{b}$ sums to n, we have that $||\mathbf{b}||^2 \ge n^2$, with equality only if $\mathbf{b}(i,j) = 1$ for all i, j. If this $||\mathbf{b}||^2 > n^2$, then one of the M_{ij} must be larger than 1, and we are done.

Therefore, we only have to consider the fiber over $\mathbf{b}_1 = \begin{pmatrix} 1 & 1 & \dots & 1 \\ \vdots & & & \vdots \\ 1 & 1 & \dots & 1 \end{pmatrix}$. Elements of this fiber are tableaux such that every row and every column is a permutation of $\{1, \dots, n\}$ ("Latin squares"). Two tableaux are connected by a degree $n-1$ move if they have a row in common. We claim that if $n > 3$, this graph is connected. (Note that for $n = 3$, there are two components and a degree 3 move for S_3, see Table 7.)

For fixed $\nu \in S_n$, the set T_ν of all tableaux in $\rho^{-1}(\mathbf{b}_1)$ that have ν as a row is connected by definition. Form the graph G_n where the vertices are elements $\nu \in S_n$ and there is an edge between λ and ν if λ and ν occur in a tableau together. Then if this graph is connected, the whole fiber over $\mathbf{b}_1$ is connected by degree $n-1$ moves.

First, we claim that λ and ν occur together in a tableau if and only if λ is a derangement with respect to ν (i.e., if λ and ν are disjoint from each other). The derangement condition is clearly necessary. Sufficiency follows from Birkhoff's theorem: if λ is a derangement with respect to ν, then the square $\mathbf{b}_1 - \rho(\lambda) - \rho(\nu)$ has non-negative entries and row and column sums $n-2$, therefore, it it the sum of $n-2$ permutation matrices. Thus, G_n is the graph where two permutations are connected by an edge when they are disjoint.

Now note that $[1, 2, \dots, n-2, n-1, n]$ and $[3, 4, \dots, n, 1, 2]$ are connected in G_n since the second is a cyclic shift of the first. Then, if $n > 3$, $[3, 4, \dots, n, 1, 2]$ and $[1, 2, \dots, n-2, n, n-1]$ are also connected. Thus $[1, 2, \dots, n]$ and $[1, 2, \dots, n-2, n, n-1]$ are connected, so applying transpositions keeps us in the same connected component of G_n. But S_n is generated by transpositions, so G_n is connected and therefore $\rho^{-1}(\mathbf{b}_1)$ is connected by moves of degree $n-1$. $\square$

Remark 9 *From partial computations with* `CaTS` *(Jensen, 2003) for $n = 4$, it appears that every Gröbner basis for S_4 contains degree 4 elements, while the Markov basis for S_4 needs only degree 3. Furthermore, our Gröbner basis for S_5 contained degree 5 elements. Therefore, it is possible that the degree n Gröbner basis of Diaconis and Sturmfels (1998) is the Gröbner basis of smallest degree.*

While I_{S_n} is difficult to compute, it is easy to classify the degree 2 part of the Markov basis. To do so, first assume that all entries of the magic square $\mathbf{b}$ are either 1 or 0. Then the squares with non-trivial $\rho^{-1}(\mathbf{b})$ are those that can be put in a block diagonal form with $k \geq 2$ blocks and each block of size at least 2. Such a magic square has a fiber of size 2^{k-1}, corresponding to choosing, for each block, an orientation of the two permutations that sum to that block (since the order of the rows in a tableau don't matter, there are only $k-1$ such choices). Therefore, we need $2^{k-1}-1$ moves to make such a fiber connected. It is a standard fact (e.g., Stanley, 1997, Chapter 1) that the number of partitions of n into k blocks each of size at least 2 (denoted $p_2(n;k)$) satisfies

$$\sum_{n\geq 0} p_2(n;k)q^n = q^{2k}\prod_{i=1}^{k}\frac{1}{1-q^i}$$

Then let $D_2(n)$ be the number of degree 2 moves, up to symmetry, in a Markov basis for S_n. If a magic square contains a 2, it can be thought of as coming from $D_2(n-1)$, so putting everything together, we have

$$D_2(n) = D_2(n-1) + \sum_{k=2}^{\lfloor \frac{n}{2} \rfloor}(2^{k-1}-1)[q^{n-2k}]\prod_{i=1}^{k}\frac{1}{1-q^i},$$

where $[q^j](\sum a_i q^i) := a_j$. For example, $D_2(9) = 47$.

5 Statistical analysis of the election data

In order to run a Markov chain fixing $\hat{f}(\rho)$ on data f, we use the Markov basis $\{g_1, \ldots, g_B\}$ as calculated above. Then, starting from f, choose i uniformly in $\{1, 2, \ldots, B\}$ and choose $\epsilon = \pm 1$ with probability 1/2. If $f + \epsilon g_i \geq 0$ (coordinate-wise), the Markov chain moves to $f + \epsilon g_i$. Otherwise, the Markov chain stays at f. This gives a symmetric connected Markov chain on the data sets with a fixed value of $\hat{f}(\rho)$. As such, it has a uniform stationary distribution. To get a sample from the hypergeometric distribution (6), the Metropolis algorithm or the Gibbs sampler can be used (see Liu, 2001).

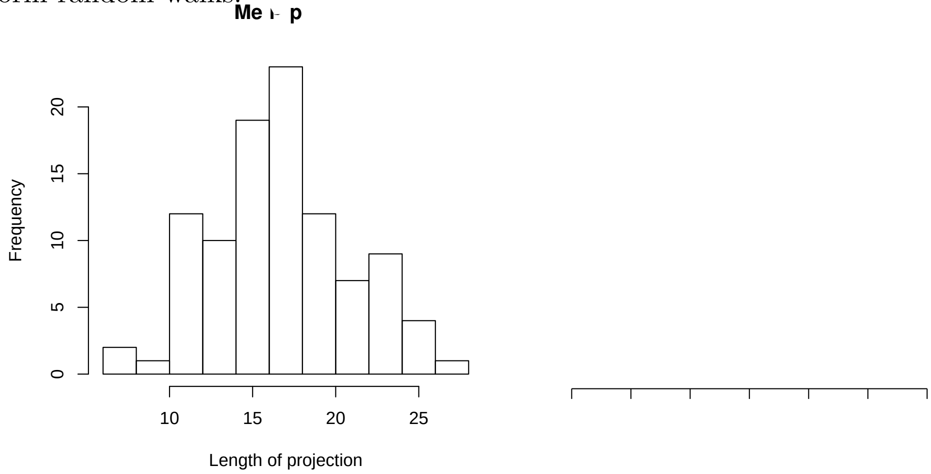
Given a symmetrized basis, we can still perform a random walk. Pick, at random, an element g of $S_n \times S_n$. Pick a move from the symmetrized basis at random, apply g to it (permuting columns and renaming entries), then use the resulting move in the Markov chain. This again gives a symmetric Markov chain that converges to the uniform distribution.

In this section, we apply the Markov basis for S_5 to analyze Table 1. The second and third rows of Table 8 show the average sum of squares for 100 samples from the hypergeometric distribution (6) (row 2) and from the uniform distribution

Table 8
Squared length (divided by 120) of the projection of the APA data into the 7 isotypic subspaces of S_5. Also, the averages of this projection for 100 random draws for 3 perturbations.

	S^5	$S^{4,1}$	$S^{3,2}$	$S^{3,1,1}$	$S^{2,2,1}$	$S^{2,1,1,1}$	$S^{1,1,1,1,1}$
Data	2286	298	459	78	27	7	0
Hypergeometric	2286	298	16	19	10	6	0
Uniform	2286	298	511	672	436	295	25
Bootstrap	2286	303	469	93	37	13	1

Fig. 1. Distribution of the length of the projection to $S^{3,2}$ with the Metropolis and uniform random walks.



(row 3) with $\hat{f}(\rho)$ fixed. Both sets of numbers are based on a Markov chain simulation using a symmetrized version of the minimal basis. In each case, starting from the original data set, the chain was run 10,000 steps and the current function recorded. From here, the chain was run 10,000 further steps, and so on until 100 functions were recorded. While the running time of 10,000 steps is arbitrary, wide variation in the running time did not appreciably change the results.

A histogram of the 100 values of the length of the projection into $S^{3,2}$ under each distribution is shown in Figure 1. These show some of variability but nothing exceptional. The histograms for the other projections are very similar.

Consider first the hypergeometric distribution leading to row 2 of Table 8 and Figure 1. A natural test of goodness of fit of the model (5) for the APA data may be based on the conditional distribution of the squared length of the projection of the data into $S^{3,2}$. From the random walk under the null model, this should be about 15 ± 5. For the actual data, this projection is 459. This gives a definite reason to reject the null model. Our look at the data projected into $S^{3,2}$ and the analysis that emerged in Section 2 confirms this conclusion.

Table 9
Length of projections onto the 5 isotypic subspaces for the S_4 data and three tests.

	S^4	$S^{3,1}$	$S^{2,2}$	$S^{2,1,1}$	$S^{1,1,1,1}$
Data	462	381	268	49	4
Metropolis	462	381	169	37	8
Uniform	462	381	277	228	80
Bootstrap	462	381	269	56	7

In Diaconis and Efron (1985), the uniform distribution of the data conditional on a sufficient statistic was suggested as an antagonistic alternative to the null hypothesis when the data strongly rejects a null model. The idea is to help quantify if the data is really far from the null, or practically close to the null and just rejected because of a small deviation but a large sample size (see the discussion in the last section of Diaconis and Efron, 1985). From Figure 1, we see that the actual projected length 459 is roughly typical of a pick from the uniform. This affirms the strong rejection of (5) and points to a need to look at the structure of the higher order projection on its own terms.

An appropriate stability analysis was left open in Diaconis (1989). If the data in Table 1 were a sample from a larger population, the sampling variability adds noise to the signal. How stable is the analysis above to natural stochastic perturbations? One standard approach is shown in the last row of Table 8. This is based on a boot-strap perturbation of the data in Table 1. Here, the votes of all 5972 rankers are put in a hat and a sample of size 5972 is drawn from the hat with replacement to give a new data set. The sum of squares decomposition is repeated. This resampling step (from the original population) was repeated 100 times. The entries in the last row of Table 8 show the average squared length of these projections. We see that they do not vary much from the original sum of squares. While not reported here, the boot-strap analogue of the second order analysis in Table 8 was quite stable. We conclude that sampling variability is not an important issue for this example.

In Diaconis and Sturmfels (1998) an S_4 example was analyzed. However, the data was analyzed using only the uniform distribution, which only tells half of the story. The analysis under hypergeometric sampling gives an important supplement. Briefly, a sample of 2262 German citizens were asked to rank order the desirability of four political goals. The data and a first order summary appears in Diaconis and Sturmfels (1998). The sizes of the projections for the data and the random walks appear in Table 9. We have noted a typographical error in the data, the 2431 entry should be 59.

The projection of the data into the second order subspace $S^{2,2}$ has squared length 268. The boot-strap analysis (Line 4 in Table 9) shows this is stable under sampling perturbations. The hypergeometric analysis (line 2 of Table 9) suggests that for the specific data, relatively large projections onto the second order space are typical, even if the first order model holds. This is quite different than the previous example. Still, the observed 268 is sufficiently much larger than 169 that a look at the second order projection is warranted. The uniform analysis points to the actual projection being typical, this again suggests a serious look at the second order projection.

As a side remark, the software `LattE` (De Loera et al., 2003) can be used to count how many data sets have a given first order summary. For our S_4 example, these correspond to lattice points inside a convex polytope with 6285 vertices in $\mathbb{R}^{24}$. `LattE` computes (in only 523.12 seconds) that there are 11606690287805167142987310121 (approximately 10^{28}) elements of $\mathbb{N}[S_4]$ with the same first order summary as our S_4 example.

6 Conclusions

In this paper, we have given a general methodology for studying group valued data where the summary we are interested in is given by a representation of the group and analyzed in detail the case of ranked data. This suggests a family of interesting toric ideals: to each finite group G and representation ρ we associate a toric ideal (Definition 4).

For practical purposes, it would be nice to have a general algorithm to analyze ranked data with n candidates. We ran Markov chains using just the degree 2 moves, but they seemed to mix very poorly. However, our computations and Conjecture 7 suggest that finding all (or even some) degree 3 moves in addition to the degree 2 moves would allow for a good random walk.

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