The Polyhedral Structure of Graphical Designs





Catherine Babecki University of Washington, Seattle Featuring Rekha Thomas, Stefan Steinerberger, and David Shiroma





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Spherical Designs

and weights $a_i \in \mathbb{R}$ chosen so that

whenever f is smooth in some suitable way.

Definition: A spherical quadrature rule is a set of points $\{x_1, \ldots, x_n\} \subset \mathbb{S}^d$

 $\frac{1}{|\mathbb{S}^d|} \int_{\mathbb{S}^d} f(x) \, dx \approx \sum_{i=1}^n a_i f(x_i)$





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A spherical *t*-design is a quadrature rule which integrates all polynomials up to degree *t* exactly.





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This is a spherical 5-design!





Extension to Graphs

Definition: G = ([n], E, w) a finite, connected, weighted graph. A subset $S \subset [n]$ with weights a_s averages a function $\varphi : [n] \to \mathbb{R}$ if $\sum_{s \in S} a_s \varphi(s) = \frac{1}{n} \sum_{v \in [n]} \varphi(v).$



 $w: E \to \mathbb{R}_{>0}$





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$$arphi = egin{bmatrix} 1 \ 0 \ -1 \ 1 \ 1 \ -1 \ 0 \ 2 \ -2 \ -1 \ 1 \ 1 \end{bmatrix}$$

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a = (0, 0, 0, 0, 0, 1, 1, 1, 1, 1)





What Functions Should We Average?

Definition: G = ([n], E, w). Eigenvectors of the operator D - A.



• $A \in \mathbb{R}^{n \times n}$ is the weighted adjacency matrix $A_{ij} = w(ij)$ if $ij \in E$ • $D \in \mathbb{R}^{n \times n}$ is the diagonal matrix with $D_{ii} = \deg i = \sum_{ij \in E} w(ij)$





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D - A

 $\begin{bmatrix} 23/15 & 0 & 0 & -1/2 & 0 & -1/2 & -8/15 & 0 & 0 \\ 0 & 23/15 & 0 & -1/2 & -1/2 & 0 & 0 & -8/15 & 0 \\ 0 & 0 & 23/15 & 0 & -1/2 & -1/2 & 0 & 0 & -8/15 \end{bmatrix}$ -11/30-1/3-1/30 -11/3012/5-11/30-11/30-1/30 -11/30-11/3012/5-1/30 31/15-11/30-2/5-2/50 -11/3031/15-2/5-2/50 -11/3031/15-11/30-2/5-2/5







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Definition: G = ([n], E, w). Eigenvectors of the operator D - A.

Eigenvectors by eigenspace

 $\lambda_1 = 0$	1	1	1	1	1	1	1	1	1
$\lambda_2 = 1.069$	6262	.5616	.0646	0264	.256	2291	3059	.2744	.031
	2870	3988	.6858	2798	.1171	.1627	1402	1948	.335
$\lambda_3 = 1.861$.3193	.3193	.3193	.1406	.1406	.1406	4600	4600	46
$\lambda_4 = 2.661$.3248	4014	.0766	.0507	.2150	2658	4852	.5996	11
	.2760	.1433	4193	2776	.1827	.0949	4123	2141	.620
$\lambda_5 = 2.672$.3468	.3458	.3468	4499	4499	4499	.1032	.1032	.103
$\lambda_6 = 3.003$.0724	0995	.0271	.1880	.5015	6894	.2707	3721	.101
	.0731	.0261	0992	6876	.5066	.1810	.2734	.0977	37

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What Eigenspaces?



The first eigenvector by frequency



The second eigenvector by frequency



What Eigenspaces?



The first eigenvector by frequency



The 18th eigenvector by frequency



The second eigenvector by frequency



What Eigenspaces?



The first eigenvector by frequency



Averages the first 6 eigenvectors



The second eigenvector by frequency



Average annual precipitation, 1981-2010









Definitions

G = ([n], E, w). Order the eigenspaces $\Lambda_1 < \Lambda_2 < \ldots < \Lambda_m$

S averages a basis for the first k eigenspaces with these weights.

 $w: E \to \mathbb{R}_{>0}$

Definition: A k-graphical design is $S \subset [n]$ and weights $a_s \in \mathbb{R}$ such that

Stefan Steinerberger



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)	1	1	1	1	1	1	1	1	1
69	6262	.5616	.0646	0264	.256	2291	3059	.2744	.031
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61	.3193	.3193	.3193	.1406	.1406	.1406	4600	4600	46
61	.3248	4014	.0766	.0507	.2150	2658	4852	.5996	11
	.2760	.1433	4193	2776	.1827	.0949	4123	2141	.626
72	.3468	.3458	.3468	4499	4499	4499	.1032	.1032	.103
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Definition: A k-graphical design is $S \subset [n]$ and weights $a_s \in \mathbb{R}$ such that

 $a_1 = a_3 = .0342, a_2 = .1111, a_6 = .5328, a_8 = .2876$ $S = \{1, 2, 3, 6, 8\}$







What Kind Of Quadrature Weights?







An arbitrarily weighted 3-design

 $a_w \in \mathbb{R}$

A positively weighted 3-design

The unweighted icosahedral graph with

 $\Lambda_1 < \Lambda_4 < \Lambda_3 < \Lambda_2.$

 $a_w \geq 0$



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A combinatorial 2-design $a_w \in \{0, 1\}$

 $a_w \geq 0$





Notation:

- matrix U, rows are the eigenvectors
- $\mathbf{k} = \{\lambda_2, \ldots, \lambda_k\}$
- $\overline{\mathbf{k}} = \{\lambda_1, \lambda_{k+1}, \dots, \lambda_m\}.$
- U_k , $U_{\overline{k}}$ = submatrices of corresponding eigenvectors
- \mathcal{U}_k , $\mathcal{U}_{\overline{k}}$ = columns of corresponding submatrices
- $P_{\overline{k}} = \operatorname{conv}(\mathcal{U}_{\overline{k}})$ is an *eigenpolytope* (Chris Godsil)







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U =



Λ_1	
Λ_2	
Λ_3	
Λ_4	

m = 4





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m = 4, k = 3







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Theorem (B., Thomas, Shiroma):

{ Minimal positively }
weighted k-designs }

 $S \subset [n]$ is a k-design \checkmark





$$\left\{ \begin{array}{l} \text{Facets of} \\ P_{\overline{k}} = \operatorname{conv}(\mathcal{U}_{\overline{k}}) \end{array} \right\}$$
$$V \setminus S \text{ is a facet}$$



The Truncated Tetrahedral Graph

find a minimal 4-graphical design?

	1	1	1	1	1	1	1	1	1	1	1	1]
	-1	-1.5	-0.5	1.5	2	1.5	-0.5	-1.5	-1	1	0	0
	2	1.5	1.5	-0.5	-1	-1.5	-1.5	-0.5	-1	0	1	0
	-1	-0.5	-1.5	-1.5	-1	-0.5	1.5	1.5	2	0	0	1
	0	-1	1	-1	0	1	-1	1	0	0	0	0
T —	-1	0	1	-1	1	0	0	0	0	-1	1	0
/	0	0	0	0	1	-1	1	0	-1	-1	0	1
	-1	0	1	0	-1	0	1	0	-1	1	0	0
	-1	0	0	1	-1	0	0	1	-1	0	1	0
	-1	1	0	0	-1	1	0	0	-1	0	0	1
	1	-1	0	0	-1	1	1	-1	0	-1	1	0
	0	-1	1	1	-1	0	0	-1	1	-1	0	1



eigenvalue 0

1

5

4

3



The Truncated Tetrahedral Graph











The Truncated Tetrahedral Graph



That Weighted Graph From Before

$\lambda_1 = 0$	1	1	1	1	1	1	1	1	1
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The Petersen Graph

 $U_{\overline{2}} =$

The Petersen Graph

The eigenpolytope is 5-dimensional and has face vector

(10, 4)

 $U_{\overline{2}} =$

22 facets come in two types: 12 are simplices and 10 have 6 vertices

$$\lambda_1 = 0^{(1)}, \lambda_2 = 5^{(4)}, \text{ and } \lambda_3 = 2^{(5)}$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & -1 & 0 & 1 & 1 & 0 & -1 & 0 & 0 \\ 1 & -1 & -1 & 0 & 1 & 1 & -1 & 0 & 0 \\ 1 & -1 & -1 & 0 & 1 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 & 1 & -1 & 0 \\ 0 & -1 & -1 & 0 & 1 & 0 & 0 & 0 & 1 \end{bmatrix}$$

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$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & -1 & 0 & 1 & 1 & 0 & -1 & 0 & 0 \\ 1 & -1 & -1 & 0 & 1 & 1 & -1 & 0 & 0 \\ 1 & -1 & -1 & 0 & 1 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 & 1 & -1 & 0 \\ 0 & -1 & -1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & -1 & -1 & 0 & 1 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Oriented matroid duality for vector configurations:

 $(U^*)^\top$

 $\mathcal{U}^* = 0$

Gale duality for polytopes:

$$U = \begin{bmatrix} 1 & 1 & -1 & -1 & 0 & 0 \\ 0 & 0 & -1 & -1 & 1 & 1 \\ 1 & 2 & 3 & 4 & 5 & 6 \end{bmatrix}$$

Gale duality for polytopes:

Gale duality for polytopes:

only if 0 is in the relative interior of $conv\{u_i : i \in I\}$.

Theorem: For $I \subseteq [n]$, $\operatorname{conv}\{u_i^* : i \in [n] \setminus I\}$ is a face of $\operatorname{conv}(\mathcal{U}^*)$ if and

Two Consequences

Existence and Bounds

Theorem (B., Thomas, Shiroma): For $k = 1, \ldots, m-1$ there is a positively weighted k-designof size at most $\sum_{i=1}^{k} \dim \Lambda_i$

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Organization

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Organization

Two Consequences

Cross-Polytopes

The d-dimensional cross polytope is $\Diamond_d = \operatorname{conv}\{\pm e_i : i \in [d]\}$

		vertex						
	e_1	$-e_{1}$	• • •	• • •	• • •	e_d	$-e_d$	
$\lambda_1 = 0$				$\mathbb{1}^{\top}$				
$\lambda_2 = 2d$	e_1	e_1	•••	e_{d-1}	e_{d-1}	-1	-1	
$\lambda_3 = 2d - 2$	e_1	$-e_{1}$	• • •	• • •	• • •	e_d	$-e_d$	

Families

Cross-Polytopes

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vertex

•••	•••	• • •	e_d	$-e_d$
	$\mathbb{1}^{\top}$			
• • •	e_{d-1}	e_{d-1}	-1	-1
• • •	• • •	• • •	e_d	$-e_d$

 $\Lambda_1 < \Lambda_3 < \Lambda_2$ $P_{\bar{\mathbf{2}}}$ is the *d*-simplex 2-designs are antipodal points

Families

Cubes

Linear error correcting codes make 'good' graphical designs on the graphs of cubes

Cubes

The eigenpolytopes of the cube can be thought of as generalized cut polytopes

Bonisoli's Theorem for linear equidistant codes provides surprisingly small graphical designs on the cube, equivalently, very large faces of these polytopes

Cubes

More generally, if a graph comes from an association scheme, graphical designs are a generalization of classical t-designs

A random neighbor is chosen with equal probability

A random neighbor is chosen with equal probability

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Initial measure: μ_0 $\mu_{k+1} = AD^{-1}\mu_k$ Stationary distribution: $D^{-1} \mathbb{1}$ normalized

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Random Walks + Graphical Designs

then

Convergence to the stationary distribution controlled by $|\lambda_{l+1}|$!

Theorem (Steinerberger & Thomas): If μ_0 defines an ℓ -graphical design, $\sum_{v \in V} \left| \mu_k(v) - \frac{1}{n} \right|^2 \le \lambda_{\ell+1}^{2k}.$

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Converges in one step :)

Complexity Results: A Road Map

A polytope P described by its n vertices

G = ([n], E, w) with P as an eigenpolytope

An orthonormal basis for \mathbb{R}^n

Complexity Results

Creating Graphs from Orthonormal Bases

Lemma (B. and Shiroma): The algorithm **Input:** an orthonormal basis \mathcal{B} of $\mathbb{1}_n^{\perp}$ and a set partition of [n-1]**Output:** G = ([n], E, w), with nontrivial eigenvectors \mathcal{B} , eigenspaces specified by the partition can be done in $\mathcal{O}(n^3)$ time.

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Step 1: derive constraints on the eigenvalues from expressing

 $M = \text{Diag}(0, \lambda_2, \ldots, \lambda_n)$

 $D - A = B^{\top} M B$

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full-dimensional polyhedral cone of eigenvalues which provide valid graphs

Step 2: wiggle!

Embedding Polytopes in Graphs

Theorem (B. and Shiroma): The algorithm **Input:** A polytope P described by its n vertices equivalent to P. can be done in $\mathcal{O}(n^3)$ time.

- **Output:** G = ([n], E, w) which has an eigenpolytope combinatorially

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Universality of Eigenpolytopes

Corollary (B. and Shiroma): Every combinatorial polytope appears as the eigenpolytope of a positively weighted graph.

The following decision problem is strongly NP-complete. *Instance*: A polytope P described by its vertices *Question*: Is P simplicial?

.

Theorem (Chandrasekaran-Kabadi-Murty, Dyer, Fukuda-Liebling-Margot):

simplicial polytope = every facet is a simplex

Complexity Results

The following decision problem is strongly NP-complete. *Instance*: A polytope P described by its vertices *Question*: Is P simplicial?

Theorem (B. and Shiroma): The following decision problem is strongly NP-complete. Instance: G = ([n], E, w) with an eigenspace ordering and $k \in \{2, \ldots, m-1\}$ Question: Does G have a k-graphical design with cardinality smaller than the "facet bound"?

of size at most $\sum_{i=1}^{k} \dim \Lambda_i$.

Theorem (Chandrasekaran-Kabadi-Murty, Dyer, Fukuda-Liebling-Margot):

simplicial polytope = every facet is a simplex

Theorem: For each $k = 1, \ldots, m-1$ there is a positively weighted k-design

Theorem (Dyer, Linial): The following counting problem is #P-complete. *Instance*: A polytope P described by its vertices *Question*: How many facets does P have?

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Theorem (B. and Shiroma): The following counting problem is #P-complete. *Instance*: G = ([n], E, w) with an eigenspace ordering and $k \in \{2, ..., m-1\}$ Question: How many positively weighted k-graphical designs does G have?

A (very silly) LP Relaxation

The following LP finds a (not necessarily minimal or minimum) positively weighted k-graphical design.

$\min \|x\|_1 \qquad \text{s.t. } U_k x = 0, \ \mathbb{1}^\top x = 1, x \ge 0$

Complexity Results

A (very silly) LP Relaxation

weighted k-graphical design.

The following LP finds a (not necessarily minimal or minimum) positively

$\min \|x\|_1 \qquad \text{s.t. } U_k x = 0, \ \mathbb{1}^\top x = 1, x \ge 0$

the support of a positively weighted 100-design on the similarity graph of the 1000 most common English words.

https://code.google.com/archive/p/word2vec/

Complexity Results

