EXPECTED VALUE OF THE ONE DIMENSIONAL EARTH MOVER'S DISTANCE

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ABSTRACT. From a combinatorial point of view, we consider the Earth Mover's Distance (EMD) associated with a metric measure space. The specific case considered is deceptively simple: Let the finite set $S = \{1, \cdots, n\}$ be regarded as a metric space by restricting the usual Euclidean distance on the real numbers. The EMD is defined on ordered pairs of probability distributions on S. We provide an easy method to compute a generating function encoding the values of EMD in its coefficients, which is related to the Segré embedding from projective algebraic geometry. As an application we use the generating function to compute the expected value of EMD in this one-dimensional case. The EMD is then used in clustering analysis for a specific data set.

1. INTRODUCTION

On the surface, the literature in algebraic combinatorics appears to be quite distant from recent trends in data science. However, after considering a specific data set in detail, we were led to a fascinating overlap.

Fix a positive integer n. We will denote the finite set of integers $\{1, \cdots, n\}$ by $[n]$. By a probability measure on $[n]$ we mean, as usual, a non-negative real number valued function f on the set $[n]$ such that $f(1) + \cdots + f(n) = 1$. Let the set of all probability measures on $[n]$ be denoted $\mathcal{P}_n$, which we view as embedded in $\mathbb{R}^n$ as a compact subset (in fact, a simplex). Given $\mu, \nu \in \mathcal{P}_n$ define

$$\mathcal{J}_{\mu\nu} = \left\{ J : \begin{array}{l} J \text{ is a non-negative real number } n \text{ by } n \text{ matrix such that} \\ \sum_{i=1}^n J_{ij} = \mu_j \text{ for all } j \text{ and } \sum_{j=1}^n J_{ij} = \nu_i \text{ for all } i \end{array} \right\}.$$

We think of $\mathcal{J}_{\mu\nu}$ as the set of joint probability measures on $[n] \times [n]$ with marginals equal to μ and ν.

The *Earth Mover's Distance* is defined as

$$\mathrm{EMD}(\mu, \nu) = \inf_{J \in \mathcal{J}_{\mu\nu}} \sum_{i,j=1}^{n} |i - j| J_{ij}.$$

We remark that the set $\mathcal{P}_n \times \mathcal{P}_n$ is a compact subset of $\mathbb{R}^{2n}$ and so by continuity the infinum is actually a minimum value. Also, the "EMD" is sometimes referred to by other names, for example, in a two dimensional setting, it is called the *image distance*. More generally, it is the Wasserstein metric (see [Mém11]).

The set of all finite distributions, $\mathcal{P}_n$, embeds as a compact polyhedra on a hyperplane in $\mathbb{R}^n$ and inherits Lebesgue measure and has finite volume. We normalize this measure so that the total mass of $\mathcal{P}_n$ is one. We then obtain a probability measure on $\mathcal{P}_n$, which is *uniform*.

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Similarly, $\mathcal{P}_n \times \mathcal{P}_n$ may be embedded in $\mathbb{R}^n \times \mathbb{R}^n$ and can be given the (uniform) product probability measure.

From its definition, the function EMD is a metric on $\mathcal{P}_n$. The subject of this paper concerns the expected value of EMD with respect to the uniform probability measure. In this light, we define a function $\mathcal{M}$ on ordered pairs of non-negative integers, (p, q), as

$$\mathcal{M}_{p,q} = \frac{(p-1)\mathcal{M}_{p-1,q} + (q-1)\mathcal{M}_{p,q-1} + |p-q|}{p+q-1} \tag{1.1}$$

with $\mathcal{M}_{p,q} = 0$ if either p or q is not positive. Let $\mathcal{M}_n = \mathcal{M}_{n,n}$ for any non-negative integer n.

We will prove the following theorem in Section 5.

Theorem 1. *Fix a positive integer n. Let $\mathcal{P}_n \times \mathcal{P}_n$ be given the uniform probability measure defined by Lebesgue measure from the embedding into $\mathbb{R}^{2n}$. The expected value of EMD on $\mathcal{P}_n \times \mathcal{P}_n$ is $\mathcal{M}_n$.*

From a theoretical point of view, this paper concerns the expected value of EMD. The above theorem is obtained as a limit of a discrete version of the EMD, which is described using a generating function. The generating function is a deformation of the Hilbert series of the Segré embedding. Some standard tools from algebraic combinatorics show up in a new way.

However, we will also consider a "real world" data set. Our use of the EMD should be viewed as an attempt at exploratory data analysis rather than rigorous hypothesis testing. Specifically, we consider a network of grade distributions from the University of Wisconsin - Milwaukee campus, where two nodes are joined when the EMD between them falls below a pre-specified distance threshold. The "communities" in this network will be investigated. For example, the spectrum of the corresponding Laplacian matrix (see [Chu97]) will be used to determine the large scale clustering.

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2. Non-technical preliminaries

In this section we describe a *fictional* situation where one encounters discrete distributions. The one dimensional EMD sheds light, and provides motivation.

Dr. X is a new mathematics faculty member at Cool College. During her first semester, she taught Calculus to a group of 30 first year students. The students had all done fairly well in high school, but nobody earned a grade of A in Dr. X's section. The students are complaining.

Dr. Y is surprised with the poor grades. He has been teaching for 30 years now and has never seen a class so upset. He thinks that the poor evaluations in Dr. X's class are due entirely to her students' low grades. The matter is causing some grief in this small department. Campus wide, some believe that standards are being set too high. Others are concerned that students are not learning calculus well enough. Dr. X has noted that some of her students are studying to be structural engineers and states that she won't be caught driving on bridges designed by these students or anybody else from Cool College for that matter. The Dean has been made aware of the situation.

Dr. Z is the Chair of the department and also taught Calculus this term. Noting that Dr. X and Dr. Y had the same section grade point average of 2.5, Dr. Z suggests that everyone calm down and get back to work. Unfortunately, the matter escalates to the Dean, who calls for a meeting and asks to see the grade distributions for the classes.

Dr. X's grades are:

A	B	C	D	F
0	19	8	2	1

Dr. Y's grades are:

A	B	C	D	F
12	2	5	11	0

Dr. Z's grades are:

A	B	C	D	F
2	20	2	3	3

The Dean immediately notices that the grade point average for each section is only 2.5, which seems low when compared to the rest of the courses at Cool College. Dr. Z reminds the dean that grades in math classes are always lower because math is harder than most subjects. Reluctantly, the dean agrees.

However, the data driven Dean wants to further investigate the grade distributions of Dr. X, Dr. Y, and Dr. Z. After consulting with faculty governance it is decided that the one dimensional EMD is the best metric for this comparison. The math department is suspicious of this decision.

The dean's goal is to quantify the difference between pairs of grade distributions, to help identify outlying grading schemes. The dean begins by comparing Dr. Y's grades to Dr. X's, and notices that if the 12 A grades in Dr. Y's section were moved down to B, 5 C grades moved up to B, 8 D grades moved up to C, and one D grade moved down to F, then the distributions would be identical. Obviously, the dean would not literally change the grades – that would be upsetting to some of the students. But, as a thought experiment, it (minimally) involves moving 26 grades. The following matrix

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 12 & 2 & 5 & 0 & 0 \\ 0 & 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

encodes the "conversion". That is, if the rows and columns correspond to the grades (A,B,C,D,F) then the entry in row i and column j records how many grades to move from position i in Dr.Y's grade book to position j in Dr. X's grade book. The entries on the diagonal reflect *no* "Earth" movement, while the entries in the first sub and super diagonals reflect *one* unit of movement. The row sums are Dr. X's grade distribution, while the column sums are Dr. Y's grade distribution. In total, the value of the EMD is 26. Is that a lot? Let's see.

Dr. Z and Dr. Y's distributions compare as follows: move 10 B's up one unit to a grade of A, to reflect the fact that Dr. Y had 12 grades of A. "He sure did have a lot of A grades" says Dr. Z. Dr. Y assures us that it is because of his superb teaching techniques developed over the years. Dr. Z does not want to comment, but seems suspicious of this claim. "Moving along" says the dean. We move 5 grades down from B to C, and 3 grades from B to D. This latter change is noted as a jump across *two* positions which will "cost" 2 units in the EMD Since there are 3 grades to move, this makes an overall contribution of 6. Finally, 2 C grades are moved down to D, and the 3 F grades in Dr. Z's section would be moved to D in Dr. Y's. The dean notes that Dr. Y didn't have any failing students. Dr. Y again assures everyone that his teaching ensures that nobody ever fails on his watch. Dr. X thinks that he just passes them through, but Dr. Y assures her that he, of course, doesn't do that. The Chair declines to enter the debate. Dr. Y exclaims, "You can't be neutral", and "you better stand up for something."

The Dr. Z and Dr. Y matrix is

$$\begin{bmatrix} 2 & 10 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 & 0 \\ 0 & 3 & 2 & 3 & 3 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Again, the off diagonal terms contribute to the EMD. Note that the 3 in row four, column two counts as $2 \times 3 = 6$ units of movement. Interestingly, the total EMD is again 26.

Finally, Dr. Z and Dr. X are compared. The joint matrix is

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 2 & 17 & 0 & 0 & 0 \\ 0 & 3 & 2 & 3 & 0 \\ 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

The total EMD is 10, which the dean notes is significantly less than 26. The dean concludes that Dr. Y is an outlier compared to the rest of the department. Dr. Y is upset and decides to retire. Dr. Z says that in that case we are going to need to hire next year. Dr. X agrees to serve on the hiring committee, if she receives a course release. Dr. Z is not sure how they would cover her classes in that case. The dean suggests increasing class size.

Finally, Dr. Z expresses concerns about using EMD to make these decisions – perhaps someone should look at the expected value of EMD.

3. Technical Preliminaries

In this section we recall some basic notation from combinatorics and linear algebra that are used throughout the paper.

3.1. **Notation from linear algebra.** Given positive integers n and m let $\mathbb{M}_{n,m}$ be the vector spaces of real matrices with n rows and m columns. Throughout, we assume that the field of scalars is the real numbers, $\mathbb{R}$. For i and j with $1 \leq i \leq n$, $1 \leq j \leq m$ we let $e_{i,j}$ denote the n by m matrix with 1 in the i-th row, j-th column, and 0 elsewhere. A matrix, $M \in \mathbb{M}_{n,m}$ is written as $M = (M_{i,j})$ where $M_{i,j}$ is the entry in the i-th row and j-th column.

So, $M = \sum M_{i,j} e_{i,j}$. We assume standard notation for the algebra of matrices. For example, the "dot product" of $X, Y \in \mathbb{M}_{n,m}$ is

$$\langle X, Y\rangle = \mathrm{Trace}(X^T Y).$$

In the case that $m = 1$ we write $e_i = e_{i,1}$ for $1 \le i \le n$. Let $\mathrm{V} = \mathbb{M}_{n,1}$ denote the n-dimension real vector space consisting of column vectors of length n. The set $\{e_1, \cdots, e_n\}$ is a basis for V. For our purposes a very useful alternative basis is given by

$$\omega_j = \sum_{i=1}^{j} e_i$$

where $1 \le j \le n$. We call the set of ω_j the *fundamental* basis for V.

Let the orthogonal complement, $\omega_n^{\perp}$, to ω_n be denoted by

$$\mathrm{V}_0 = \{v \in \mathrm{V} \mid \langle v, \omega_n\rangle = 0\}.$$

Column vectors in V_0 have coordinates that sum to zero. We let π_0 denote the orthogonal projection from V onto V_0,

$$\begin{array}{rccc} \pi_0 : & \mathrm{V} & \to & \mathrm{V}_0 \\ & v & \mapsto & \pi_0(v) \end{array}$$

defined by the formula

$$\pi_0(v) = v - \frac{\langle v, \omega_n\rangle}{n}\omega_n.$$

Note that the image of π_0 is V_0, and contains ω_n. For $1 \le j \le n-1$, let $\tilde{\omega}_j = \pi_0(\omega_j)$. Observe that $\tilde{\omega}_1, \cdots, \tilde{\omega}_{n-1}$ span V_0, and by considering dimension, are a basis for V_0. We will call this set the *fundamental* basis for V_0.

The subspace V_0 has another basis that is of importance for us:

$$\Pi = \{\alpha_1, \cdots, \alpha_{n-1}\}$$

where $\alpha_j = e_j - e_{j+1}$. We refer to Π as the *simple* basis for V_0. An essential point is that Π is dual to the fundamental basis. That is $\langle \alpha_i, \tilde{\omega}_j\rangle = \delta_{i,j}$ where

$$\delta_{i,j} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

Definition 1. Let $\mathcal{E} : V \to \mathbb{R}$ be defined as

$$\mathcal{E}(v) = |v_1| + |v_1 + v_2| + |v_1 + v_2 + v_3| + \cdots + |v_1 + \cdots + v_n|$$

for $v = \sum v_j e_j \in \mathrm{V}$.

Observe that since $V_0 \subset V$, $\mathcal{E}$ is defined on V_0 by restriction.

Let[1] $v = \sum_{i=1}^{n-1} c_i \alpha_i \in \mathrm{V}_0$. Then, $\mathcal{E}(v) = \sum_{i=1}^{n-1} |c_i|$. This fact is easily seen since the fundamental basis is dual to the simple basis, and

$$\langle v, \omega_j\rangle = v_1 + \cdots + v_j$$

for $1 \le j \le n$.

In Section 5, we will prove that

$$\mathrm{EMD}(\mu, \nu) = \mathcal{E}(\mu - \nu) \tag{3.1}$$

[1]We use the lowercase letter "c" because it is the first letter in "coefficient."

for all $\mu, \nu \in \mathcal{P}_n$. This allows for a much more explicit combinatorial analysis of EMD. For situations in which the metric space is not a subset of the real line, the analysis is more difficult. Indeed, EMD is often computed as an optimization problem that minimizes the "Cost" under the constraints imposed by the marginal distribution. Consequently, the computational complexity is the same as for linear programming.

3.2. **Compositions and related combinatorics.** Let $\mathbb{N}$ be the set of non-negative integers. Given $s \in \mathbb{N}$, and a positive integer n, define:

$$\mathcal{C}(s,n) = \{(a_1, a_2, \cdots, a_n) \in \mathbb{N}^n : a_1 + \cdots + a_n = s\}.$$

An element of the set $\mathcal{C}(s,n)$ will be referred to as a *composition* of s into n parts[2]. It is an elementary fact that there are $\binom{s+n-1}{n-1}$ compositions, and therefore for fixed n, the number of compositions of s grows as a polynomial function of s with degree $n-1$. An essential fact for this paper is the asymptotic approximation

$$\binom{s+n-1}{n-1} \sim \frac{s^{n-1}}{(n-1)!}.$$

As in the introduction, given compositions μ and ν of s we let $\mathcal{J}_{\mu\nu}$ denote the set of n by n matrices with row sums μ and column sums ν. There is a slight difference here in that we are not requiring μ and ν to be normalized to sum to one. In the same light, EMD can be extended as a metric on $\mathcal{C}(s,n)$.

We fix [3] an n by n matrix C with i-th row and j-th column entry to be $|i-j|$. That is,

$$C = \begin{bmatrix} 0 & 1 & 2 & \cdots & n-1 \\ 1 & 0 & 1 & \cdots & n-2 \\ 2 & 1 & 0 & \cdots & n-3 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ n-1 & n-2 & n-3 & \cdots & 0 \end{bmatrix}.$$

So, for $\mu, \nu \in \mathcal{C}(s,n)$ and regarding the set $\mathcal{J}_{\mu\nu}$ as non-negative integer matrices with prescribed row and column sums, we arrive at

$$\mathrm{EMD}(\mu,\nu) = \min_{J \in \mathcal{J}_{\mu\nu}} \langle J, C \rangle,$$

which is a discrete version of EMD. When we take $s \to \infty$ we recover the value referred to in the introduction.

The function, EMD, may be further generalized to the case where C has p rows and q columns, with i,j entry $|i-j|$. In this case μ has p components and ν has q components (each compositions of s). This generalization will be needed in an induction argument in Section 5. However, applications need only consider the $p = q$ case.

A further generalization beyond the scope of this paper is to consider more general "cost" matrices than C. Indeed, this is equivalent to a variation of the metric.

[2]We use the caligraphic letter "$\mathcal{C}$" to denote the set of "compositions."

[3]Note that here we are using the upper case roman letter "C" because it is the first letter of the word "Cost."

4. Generating Functions

In algebraic combinatorics, it is often useful to record discrete data in a (multi-variate) formal power series. This is our point of view, and so we define

$$H_n(z,t) := \sum_{s=0}^{\infty} \left(\sum_{(\mu,\nu)\in \mathcal{C}(s,n)\times\mathcal{C}(s,n)} z^{\mathrm{EMD}(\mu,\nu)} \right) t^s.$$

where t and z are (formal) indeterminates. Now we see that the coefficient of t^s in $H_n(z,t)$ is a polynomial in z whose coefficients record the distribution of the values of EMD.

It is useful to see the first few values of H:

$$\begin{aligned} H_1(z,t) &= \frac{1}{1-t} \\ H_2(z,t) &= \frac{tz+1}{(1-t)^2(1-tz)} \\ H_3(z,t) &= \frac{-t^3z^4 - t^2(2z+1)z^2 + t(z+2)z + 1}{(1-t)^3(1-tz)^2\,(1-tz^2)} \end{aligned}$$

As before, when considering p by q matrices we can analogously define $H_{p,q}(z,t)$. We also extend the definition so that $H_{p,q} = 0$ if either of p or q is not positive. We obtain a similar series, namely

$$H_{p,q}(z,t) := \sum_{s=0}^{\infty} \left(\sum_{(\mu,\nu)\in \mathcal{C}(s,p)\times\mathcal{C}(s,q)} z^{\mathrm{EMD}(\mu,\nu)} \right) t^s.$$

Note that if $p < q$ we can regard p-tuples as q-tuples, so the function EMD is defined.

Theorem 2. *For positive integers p and q,*

$$H_{p,q}(z,t) = \frac{H_{p-1,q}(z,t) + H_{p,q-1}(z,t) - H_{p-1,q-1}(z,t)}{1 - z^{|p-q|}t}$$

if $(p,q) \neq (1,1)$ and $H_{1,1} = \frac{1}{1-t}$.

This proof will also be given in Section 5, after we have developed some of the consequences in the remainder of this section.

4.1. **The partially ordered set $[p]\times[q]$.** Recall that a *partially ordered set* is a set S together with a relation, $\preceq$, which is required to be reflexive, antisymmetric and transitive. Given positive integers p and q we define $S = [p]\times[q]$, and

$$(i,j) \preceq (i',j') \iff i'-i \in \mathbb{N} \text{ and } j'-j \in \mathbb{N}$$

for $1 \le i, i' \le p$ and $1 \le j, j' \le q$.

It is important to note that not all elements are comparable with respect to this order. For example, if $p = q = 2$, clearly $(1,2) \not\preceq (2,1)$ and $(2,1) \not\preceq (1,2)$. We say that $(1,2)$ and $(2,1)$ are incomparable. A subset of S in which all pairs are comparable is called a *chain*.

Given a p by q matrix, J, we define the support as

$$\mathrm{support}(J) := \{(i,j) : J_{ij} > 0\}.$$

Proposition 3. *Let p and q be positive integers, and $s \in \mathbb{N}$. For $\mu \in \mathcal{C}(s,p)$, $\nu \in \mathcal{C}(s,q)$ and $J \in \mathcal{J}_{\mu\nu}$, there exists a $J' \in \mathcal{J}_{\mu\nu}$ such that the support of J' is a chain in $[p] \times [q]$, and $\langle J', C\rangle \leq \langle J, C\rangle$.*

Proof. Suppose there exists incomparable $(i,j),(i',j')$ such that $J_{ij}, J_{i'j'} > 0$. Without loss of generality assume $i' < i$, $j < j'$, and $0 < J_{ij} \leq J_{i'j'}$. We construct J' as follows:

$$\begin{bmatrix} & & \\ & & J_{i'j'} \\ & & \\ & J_{ij} & \\ & & \end{bmatrix}$$

For $(k,l) \notin \{(i,j),(i',j'),(i',j),(i,j')\}$ let $J'_{kl} = J_{kl}$. Next, let $J'_{ij} = 0$ and

$$J'_{i'j'} = J_{i'j'} - J_{ij}$$

which is non-negative. And,

$$J'_{i'j} = J_{i'j} + J_{ij}$$
$$J'_{ij'} = J_{ij'} + J_{ij}.$$

□

The point here is that we will only need to consider matrices J with support on a chain.

4.2. **A special case of the Robinson-Schensted-Knuth correspondence.** In this subsection we recall, in detail, a special case of the Robinson-Schensted-Knuth correspondence (RSK), see [Ful97]. For those familiar with RSK, we consider the case where the Young diagrams have only one row. For non-experts, the exposition here does not require any knowledge of RSK.

Given $\mu \in \mathcal{C}(s,n)$ with $\mu = (\mu_1, \cdots, \mu_n)$ we define the *word* of μ to be a finite weakly increasing sequence of positive integers, $w = w(\mu) = w_1 w_2 w_3 \cdots$ where the number of times k occurs in w is equal to μ_k.

As an example, if $\mu = (3,0,2,1,0)$ then

$$w = 111334.$$

Note that the length of the word is equal to $s = \sum \mu_i$, and all elements of w are at most n.

Next, for $s \in \mathbb{N}$ and positive integers p and q, we define

$$R(p,q;s) := \left\{ J \in \mathbb{M}_{p,q} : (\forall i,j), J_{ij} \in \mathbb{N}, \sum_{i,j} J_{ij} = s \text{ and support}(J) \text{ is a chain} \right\}$$

Proposition 4. *For a given $s \in \mathbb{N}$ and positive integers p and q, we have a bijection, Φ, between $\mathcal{C}(s,p) \times \mathcal{C}(s,q)$ and $R(p,q;s)$.*

Proof. Given $(\mu,\nu) \in \mathcal{C}(s,p) \times \mathcal{C}(s,q)$, let u, v be the words of μ and ν respectively,

$$u = u_1 u_2 u_3 \cdots u_s$$

with $1 \leq u_i \leq p$, and

$$v = v_1 v_2 v_3 \cdots v_s$$

with $1 \le v_i \le q$. Define a p by q matrix by

$$J_{ij} = |\{k : (u_k, v_k) = (i, j)\}|$$

for $1 \le i \le p$ and $1 \le j \le q$. We define $\Phi(\mu, \nu) = J$. Given J, we can recover μ and ν as the row and column sums of J. □

4.3. **Rank one matrices and the Segré embedding.** The rank of a p by q matrix is k if the dimension of the row (equivalently, column) space is k. In elementary linear algebra one proves that a matrix has rank at most k iff the determinants of all $k+1$ by $k+1$ minors vanish. We let $\mathbb{D}^{\le k}(p, q)$ denote the set of p by q matrices with rank at most k, which is a closed affine algebraic set, called a *determinantal variety.* For a relatively recent expository article about the role these varieties play in algebraic geometry and representation theory see [EHP14].

In this section we consider the $k = 1$ case, in our context. Define $P : \mathbb{R}^p \times \mathbb{R}^q \to \mathbb{M}_{p,q}$ by

$$P(v, w) = vw^T$$

for $v \in \mathbb{R}^p$ and $w \in \mathbb{R}^q$. Note that if $P(v, w) \ne 0$ then the rank is 1. In fact, the image of P consists of those matrices with rank at most 1. So if $p, q > 1$ then P is not surjective.

Injectivity of P fails as well since for non-zero $c \in \mathbb{R}$, v, w we have $P(v, w) = P(cv, \frac{1}{c}w)$. However, if we pass to projective space we recover an injective map.

In this light, let $\mathbb{RP}^n$ be an n-dimensional real projective space, that is:

$$\mathbb{RP}^n = \{\mathbb{R}v : 0 \ne v \in \mathbb{R}^{n+1}\}$$

where $\mathbb{R}v$ denotes the 1-dimensional subspace spanned by non-zero v. We will also write $\mathbb{RP}^n := \mathbb{P}(\mathbb{R}^{n+1})$.

The *Segré* embedding,

$$\mathbb{P}(\mathbb{R}^p) \times \mathbb{P}(\mathbb{R}^q) \to \mathbb{P}(\mathbb{R}^{pq})$$

is defined as follows: First, we note that we can identify $\mathbb{R}^{pq}$ with the p by q matrices by choosing bases. Given an ordered pair of projective points (i.e. one dimensional subspaces) we can choose non-zero vectors v and w respectively. The value of the Segré is the one dimensional subspace in $\mathbb{M}_{p,q}$ spanned by the matrix $P(v, w)$. It is easily checked that this map is well defined and injective.

The image of the Segré gives rise to a projective variety structure on the set-cartesian product of the two projective varieties. The projective coordinate algebra of the Segré is intimately related to $H_{p,q}(z, t)$, which we will see next.

Let m_{ij} be a choice of (algebraically independent) indeterminates. We consider the polynomial algebra

$$\mathcal{A}_{p,q} = \mathbb{R}[m_{ij} : 1 \le i \le p, 1 \le j \le q].$$

Next for $1 \le i < i' \le p$, and $1 \le j < j' \le q$ define

$$\Delta(i, i'; j, j') = \begin{vmatrix} m_{ij} & m_{ij'} \\ m_{i'j} & m_{i'j'} \end{vmatrix}.$$

The ideal, $\mathcal{I}$, generated by the $\Delta(i, i'; j, j')$ vanishes exactly on the matrices of rank 1. Conversely, any polynomial function that vanishes on the rank at most 1 matrices is in $\mathcal{I}$. The algebra of coordinate functions on the rank at most 1 matrices is then isomorphic to the quotient of $\mathcal{A}_{p,q}$ by $\mathcal{I}$. Define $\mathcal{R}(p, q) := \mathcal{A}_{p,q}/\mathcal{I}$.

The point here is that monomials involving variable which have indices that are not comparable with respect to $\preceq$ may be replaced (modulo $\mathcal{I}$) with comparable indices. This process may be thought of as "straightening" and is related to the non-negative integer matrices J with support in a chain. The matrix J should be thought of as the exponents in a monomial.

More generally, the situation here may be put into the context of Gröbner basis. The cost matrix C used here gives a weight to each matrix coefficient. This weight can then be extended (say, lexicographically) to a well ordering of the monomials that is compatible with multiplication. That is, a *term order* (see [CLO98]). The minors generating the ideal $\mathcal{I}$ are indeed a Gröbner basis. The complement of the ideal of leading terms is then a vector space basis for the quotient by $\mathcal{I}$.

For $s \in \mathbb{N}$, let $\mathcal{A}^s_{p,q}$ denote the subspace of homogeneous degree s polynomials, and set $\mathcal{R}^s_{p,q} = \mathcal{A}^s_{p,q}/(\mathcal{A}^s_{p,q} \cap \mathcal{I})$. Since $\mathcal{I}$ is generated by homogeneous polynomials, we have

$$\mathcal{R}_{p,q} = \bigoplus_{s=0}^{\infty} \mathcal{R}^s_{p,q}.$$

That is, we have an algebra gradation by polynomial degree.

The polynomial functions on $\mathbb{R}^p$ (resp. $\mathbb{R}^q$) will be denoted $\mathcal{A}_p$ (resp. $\mathcal{A}_q$). Given vectors $v \in \mathbb{R}^p$ and $w \in \mathbb{R}^q$ an element of the tensor product $\mathcal{A}_p \otimes \mathcal{A}_q$ defines a function on $\mathbb{R}^p \times \mathbb{R}^q$ with value $f(v)g(w)$. Given an element $(v, w) \in \mathbb{R}^p \times \mathbb{R}^q$, and $f \otimes g \in \mathcal{A}_p \otimes \mathcal{A}_q$, the value of $f \otimes g$ on (v, w) is given by $f(v)g(w)$. Extending by linearity we obtain an algebra isomorphism from the polynomials on $\mathbb{R}^p \times \mathbb{R}^q$ to the tensor product algebra $\mathcal{A}_p \otimes \mathcal{A}_q$.

The quadratic map P, defined above, gives rise to an algebra homomorphism,

$$P^* : \mathcal{R}_{p,q} \to \mathcal{A}_p \otimes \mathcal{A}_q,$$

defined such that $P^*(F)$ is a function on $\mathbb{R}^p \times \mathbb{R}^q$ from a function F on $\mathbb{D}^{\leq 1}_{p,q}$. This is done via the usual adjoint map given by $[P^*(F)](v, w) = F(P(v, w))$.

The image of P^* is given as the "diagonal" subalgebra:

$$\bigoplus_{s=0}^{\infty} \mathcal{A}^s_p \otimes \mathcal{A}^s_q.$$

From our point of view, the significance of this structure is as follows:

- The dimension
$$\dim \left(\mathcal{A}^s_p \otimes \mathcal{A}^s_q\right) = \binom{s+p-1}{p-1}\binom{s+q-1}{q-1},$$
which is equal to the cardinality of $\mathcal{C}(p, s) \times \mathcal{C}(q, s)$. That is, a basis may be parameterized by a pair of compositions.
- The (finite dimensional) vector space $\mathcal{R}^s_{p,q}$ will have a dimension also equal to the above since P^* is an isomorphism.
- The bijection Φ from Proposition 4 establishes that the above dimension is given by the cardinality of $R(p, q; s)$.
- A basis for $\mathcal{R}^s_{p,q}$ may be given by the monomials of the form $\prod m_{ij}^{P_{ij}}$ where $P \in R(p, q; s)$.
- These monomials correspond to the monomials in $\mathcal{A}^s_p \times \mathcal{A}^s_q$ with exponents $(\mu, \nu) \in \mathcal{C}(s, p) \times \mathcal{C}(q, s)$.

4.4. **The specialization and a derivative.** It is relatively easy to see, from the definition, that

$$H_{p,q}(0,t) = \frac{1}{(1-t)^{\min(p,q)}}.$$

We next turn to the specialization $H_{p,q}(1,t)$, which turns out to be the Hilbert series of the rank at most 1 matrices. That is to say

$$H_{p,q}(1,t) = \sum_{s=0}^{\infty} (\dim \mathcal{R}^s_{p,q}) t^s.$$

In [EW03] this series was computed in Equation (6.4) as

$$H_{p,q}(1,t) = \frac{\sum_{i=0}^{\min(p-1,q-1)} \binom{p-1}{i}\binom{q-1}{i} t^i}{(1-t)^{p+q-1}}.$$

In this sense, $H(z,t)$ interpolates between the generating function for compositions and the Hilbert series of the determinantal varieties (at least in the rank one case). Moreover, for generic z we have a relationship to the EMD.

Our motivation comes from the expected value of the EMD. Therefore, it is natural to compute the partial derivative of $H_{p,q}(z,t)$ with respect to z, and then set $z = 1$. From the definition of $H_{p,q}$,

$$\left.\frac{\partial H_{p,q}(z,t)}{\partial z}\right|_{z=1} = \sum_{s=0}^{\infty} \left(\sum_{(\mu,\nu) \in \mathcal{C}(s,p) \times \mathcal{C}(s,q)} EMD(\mu,\nu) \right) t^s$$

To expand this we start with

$$H_{p,q}(z,t) = \frac{H_{p-1,q} + H_{p,q-1} - H_{p-1,q-1}}{1 - z^{|p-q|} t},$$

the recursion relationship from Theorem 2. Then let the partial derivative of $H_{p,q}$ with respect to z be denoted $H'_{p,q}$. We find the derivative using the "quotient rule"

$$H'_{p,q}(z,t) = \frac{\partial}{\partial z} H_{p,q}(z,t) = \tag{4.1}$$

$$\frac{(H'_{p-1,q} + H'_{p,q-1} - H'_{p-1,q-1})(1 - z^{|p-q|}t) + |p-q| z^{|p-q|-1} t (H_{p-1,q} + H_{p,q-1} - H_{p-1,q-1})}{(1 - z^{|p-q|}t)^2}.$$

When $z = 1$ this becomes

$$\begin{aligned} H'_{p,q}(1,t) = \frac{1}{(1-t)^2} \Big(\Big(H'_{p-1,q}(1,t) + H'_{p,q-1}(1,t) - H'_{p-1,q-1}(1,t) \Big) \Big(1 - t \Big) + \\ |p-q| t \Big(H_{p-1,q}(1,t) + H_{p,q-1}(1,t) - H_{p-1,q-1}(1,t) \Big) \Big). \end{aligned} \tag{4.2}$$

Before proceeding it is useful to see some initial values:

$$H'_{1,1} = 0 \qquad H'_{1,2} = \frac{t}{(1-t)^3} \qquad H'_{1,3} = \frac{3t}{(1-t)^4}$$

$$H'_{2,1} = \frac{t}{(1-t)^3} \qquad H'_{2,2} = \frac{2t}{(1-t)^4} \qquad H'_{2,3} = \frac{t(3t+5)}{(1-t)^5}$$

$$H'_{3,1} = \frac{3t}{(1-t)^4} \qquad H'_{3,2} = \frac{t(3t+5)}{(1-t)^5} \qquad H'_{3,3} = \frac{8t(t+1)}{(1-t)^6}$$

Both $H_{p,q}(1,t)$ and $H'_{p,q}(1,t)$ are rational functions. We anticipate that their numerators are

$$W_{p,q}(t) := (1-t)^{p+q-1} H_{p,q}(1,t)$$

and

$$N_{p,q}(t) := (1-t)^{p+q} H'_{p,q}(1,t).$$

Thus, multiplying by $(1-t)^{p+q}$ on both sides of Equation 4.2 gives:

$$N_{p,q} = \frac{1}{(1-t)^2}\Big(\big((1-t)(N_{p-1,q}+N_{p,q-1}) - (1-t)^2 N_{p-1,q-1}\big)(1-t) + |p-q|t\big((1-t)^2(W_{p-1,q}+W_{p,q-1}) - (1-t)^3 W_{p-1,q-1}\big)\Big)$$

or

$$N_{p,q} = N_{p-1,q} + N_{p,q-1} - (1-t)N_{p-1,q-1} + |p-q|t(W_{p-1,q} + W_{p,q-1} - (1-t)W_{p-1,q-1}) \tag{4.3}$$

If we also note that

$$W_{p,q} = W_{p-1,q} + W_{p,q-1} - (1-t)W_{p-1,q-1}.$$

we ultimately obtain

$$N_{p,q} = N_{p-1,q} + N_{p,q-1} - (1-t)N_{p-1,q-1} + |p-q|tW_{p,q}.$$

An easy induction shows that both $W_{p,q}(t)$ and $N_{p,q}(t)$ are polynomials in t.

Before proceeding it is instructive to recall our goal of finding the expected value of the EMD. In this light, define

$$\mathcal{N}(p,q;s) := \sum_{(\mu,\nu)\in\mathcal{C}(s,p)\times\mathcal{C}(s,q)} \mathrm{EMD}(\mu,\nu)$$

for $s \in \mathbb{N}$ and positive integers p and q. The expected value of EMD will be then obtained from

$$\lim_{s\to\infty} \frac{1}{s} \frac{\mathcal{N}(p,q;s)}{\binom{s+p-1}{p-1}\binom{s+q-1}{q-1}}$$

which we will show in the proof of the main theorem to be $\mathcal{M}_{p,q}$. Note that we use the letter "$\mathcal{M}$" for *mean*, and the letter "$\mathcal{N}$" for *numerator*.

Proposition 5. *Given positive integers p and q,*

$$\frac{N_{p,q}(t)}{(1-t)^{p+q}} = \sum_{s=0}^{\infty} \mathcal{N}(p,q;s)t^s$$

Proof. We have seen that

$$\left.\frac{\partial H}{\partial z}\right|_{z=1} = \frac{N_{p,q}(t)}{(1-t)^{p+q}}.$$

Differentiating the definition $H_{p,q}(z,t)$ term by term and then setting $z=1$ gives the result. □

Using Equation 4.3 and the formula for $W_{p,q}(t)$ one can efficiently compute $N_{p,q}(t)$ for specific values of p and q. Expanding $\frac{1}{(1-t)^{p+q}}$ in a series involves only binomial coefficients. We are then led to an efficient method for finding the expected value of EMD on $\mathcal{C}(s,p) \times \mathcal{C}(s,q)$ for any given values of p, q and s.

Some initial data for $N_{n,n}(t)$ for $n = 1, \cdots, 12$ are:

0
$2t$
$8t(t+1)$
$4t\left(5t^2+14t+5\right)$
$8t\left(5t^3+27t^2+27t+5\right)$
$2t\left(35t^4+308t^3+594t^2+308t+35\right)$
$16t\left(7t^5+91t^4+286t^3+286t^2+91t+7\right)$
$8t\left(21t^6+378t^5+1755t^4+2860t^3+1755t^2+378t+21\right)$
$16t\left(15t^7+357t^6+2295t^5+5525t^4+5525t^3+2295t^2+357t+15\right)$
$2t\left(165t^8+5016t^7+42636t^6+142120t^5+209950t^4+142120t^3+42636t^2+5016t+165\right)$
$8t\left(55t^9+2079t^8+22572t^7+99484t^6+203490t^5+\right.$
$\left.203490t^4+99484t^3+22572t^2+2079t+55\right)$
$4t\left(143t^{10}+6578t^9+88803t^8+499928t^7+1352078t^6+1872108t^5+\right.$
$\left.1352078t^4+499928t^3+88803t^2+6578t+143\right)$

After looking at the above data, we conjecture:

Conjecture 1. *The $N_{n,n}(t)$ are polynomials in t with non-negative integer coefficients. Furthermore, the coefficients are unimodal and "palindromic" – that is the coefficient of t^i matches the coefficient of t^{d-i} where d is the polynomial degree.*

In the next section we will use Proposition 5 to find the asymptotic value as $s \to \infty$ for fixed values of p and q.

5. Proofs of the theorems

For $v \in \mathbb{R}^n$, we defined

$$\mathcal{E}(v) = |v_1| + |v_1+v_2| + |v_1+v_2+v_3| + \cdots + |v_1+\cdots+v_n|$$

in Section 3.

In this section we shall prove that for all n and for $\mu, \nu \in \mathcal{P}_n$, $\mathcal{E}(\mu - \nu) = EMD(\mu, \nu)$. By continuity it will suffice to show that this is true on a dense subset of $\mathcal{P}_n$. Specifically, we will consider the special case that if μ (resp. ν) is of the form

$$\mu = \left(\frac{a_1}{s}, \cdots, \frac{a_n}{s}\right)$$

for some positive integer s and $(a_1, \cdots, a_n) \in \mathcal{C}(s, n)$. As $s \to \infty$, such points are dense in $\mathcal{P}_n$

For $p \leq n$ (resp. $q \leq n$) we can regard $\mathcal{C}(s, p)$ (resp. $\mathcal{C}(s, q)$) as being embedded in $\mathcal{C}(s, n)$ by appending zeros onto the right.

By induction on $p + q$ we will show that for any non-negative integer s,

$$\mathrm{EMD}(\mu, \nu) = \mathcal{E}(\mu - \nu)$$

for $\mu \in \mathcal{C}(s, p)$ and $\nu \in \mathcal{C}(s, q)$.

Proof. If $p = q = 1$ the result is trivial since there is only one composition of s. Consider $p + q \geq 2$. Without loss of generality assume $p \leq q$.

We proceed by induction on s (inside the induction on $p + q$). If $s = 0$ the statement is vacuous, and so the basis is clear.

For positive integer s let J be a p-by-q non-negative integer matrix such that J has row and column sums μ and ν respectively and $\langle J, C\rangle$ is minimal. We shall show that $\langle J, C\rangle = \mathcal{E}(\mu - \nu)$.

If the first row (resp. column) of J is zero we can delete it and reduce to the induction hypothesis on $p + q$. Therefore, we assume that there is a positive entry in the first row (resp. column) of J. If $J_{11} > 0$ then we can subtract J_{11} from s and reduce to the induction hypothesis on s.

We are therefore left with $J_{11} = 0$ and the existence of $i > 1$, $j > 1$ with $J_{1j} > 0$ and $J_{i1} > 0$. However, $(1, j)$ and $(i, 1)$ are incomparable in the poset $[p] \times [q]$. However, by Proposition 3 we can assume that the support of J is a chain. Equation 3.1 follows. □

Proof of Theorem 2. The vector space of degree s homogeneous polynomial functions on the rank at most one p-by-q matrices is denoted $\mathcal{R}^s_{p,q}$. By Proposition 3, we obtain a basis for this space by considering the monomials

$$\prod_{i=1}^{p} \prod_{j=1}^{q} x_{ij}^{J_ij}$$

where J is a non-negative integer matrix with support on a chain. The row and column sums of J are a pair of compositions of s with p and q parts respectively. We denote these by μ and ν (Proposition 4). If we weight each of the monomials by $z^{\mathrm{EMD}(\mu,\nu)} t^s$ and sum as a formal series to obtain the Hilbert series of of $\mathcal{R}_{p,q}$,

$$\sum_{s=0}^{\infty} \left(\sum_{(u,v) \in \mathcal{C}(s,p) \times \mathcal{C}(s,q)} z^{\mathrm{EMD}(u,v)} \right) t^s$$

which we recognize as the definition of $H_{p,q}(z, t)$.

Each monomial has a non-negative integer matrix J as its exponents, with support on a chain. This chain terminates at or before $x_{p,q}^{J_{p,q}}N$. From Equation 3.1 The variable $x_{p,q}$ is weighted by $z^{|p-q|}t$, and contributes

$$\sum_{J_{p,q}=0}^{\infty} \left(z^{|p-q|}t\right)^{J_{p,q}}$$

to all monomials. The geometric series sums to $\frac{1}{1-z^{|p-q|}t}$.

The preceding variables in the monomial may contain $x_{p,j}$ for some $1 \leq j \leq q$, or $x_{i,q}$ for some $1 \leq i \leq p$, but not both – since the exponent matrix has support in a chain. In the former case these monomials are in the sum $H_{p,q-1}$, while in the latter are counted in $H_{p,q-1}$.

The sum $H_{p-1,q} + H_{p,q-1}$ over counts monomials. That is to say, if a monomial has exponent with support involving variables $x_{i,j}$ with $i < p$ and $j < q$ then it is counted once in $H_{p-1,q}$ and once in $H_{p,q-1}$. It also appears once in $H_{p-1,q-1}$. We therefore observe that such monomials are counted exactly once in the expression

$$H_{p-1,q} + H_{p,q-1} - H_{p-1,q-1}.$$

Finally, we see that **all** such monomials are counted exactly once in the product

$$\frac{H_{p-1,q} + H_{p,q-1} - H_{p-1,q-1}}{1 - z^{|p-q|}t}$$

if $(p,q) \neq (1,1)$ and $H_{1,1} = \frac{1}{1-t}$. □

5.0.1. *Limiting values as $s \to \infty$.*

Proof of Theorem 1. Fix positive integers p and q. The coefficient of t^s in $\frac{1}{(1-t)^{p+q}}$ is

$$\binom{s+p+q-1}{p+q-1} = \frac{s^{p+q-1}}{(p+q-1)!} + \text{ lower order term in } s.$$

And, we have

$$N_{p,q}(t) = c_0 + c_1 t + c_2 t^2 + \cdots + c_k t^k$$

for some non-negative integers $c_0, \cdots, c_k$. Thus the coefficient of t^s in

$$\frac{N_{p,q}(t)}{(1-t)^{p+q}}$$

is therefore asymptotic to

$$N_{p,q}(1)\frac{s^{p+q-1}}{(p+q-1)!}$$

We will next find an in-homogeneous three term recursive formula for $N_{p,q}(1)$ from Equation 4.3.

First we observe that $W_{p,q}(1) = \binom{p+q-2}{p-1}$. Therefore, we have

$$N_{p,q}(1) = N_{p-1,q} + N_{p,q-1} + |p-q|\binom{p+q-2}{p-1}.$$

Then we divide by $(p+q-1)!$ to obtain the asymptotic. However, our goal is to obtain the expected value of EMD. So, in light of Proposition 5, we will need to divide by

$$\binom{s+p-1}{p-1}\binom{s+q-1}{q-1} \sim \frac{s^{p+q-2}}{(p-1)!(q-1)!}.$$

Thus, we find that the expected value is

$$\mathcal{M}_{p,q} = \frac{(p-1)!(q-1)!}{(p+q-1)!} N_{p,q}(1),$$

which we can rewrite as

$$\mathcal{M}_{p,q} = \frac{(p-1)\mathcal{M}_{p-1,q} + (q-1)\mathcal{M}_{p,q-1} + |p-q|}{p+q-1}.$$

□

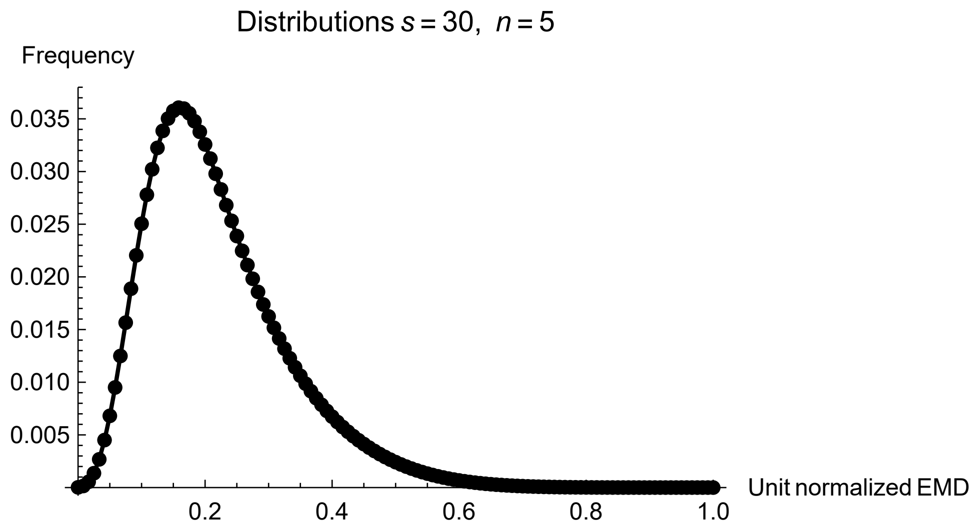
In Theorem 1, the EMD has been normalized so that μ and ν are probability distributions. To translate from the value on pairs of compositions of s this amounts to multiplying by $\frac{1}{s}$. Note that since the order of the pole at $t=1$ in $H_{p,q}(1,t)$ is one less than the order of the pole at $t=1$ in $H'(1,t)$ we see that the (normalized) EMD is approaching a constant as $s \to \infty$. Alternatively, we could not normalize and then obtain linear growth, $s\mathcal{M}_{p,q}$.

The following is a table with approximate values of $\mathcal{M}_{p,q}$ for $1 \leq p, q, \leq 12$,

$$\begin{pmatrix}
0 & 0.5000 & 1.000 & 1.500 & 2.000 & 2.500 & 3.000 & 3.500 & 4.000 & 4.500 & 5.000 & 5.500 \\
0.5000 & 0.3333 & 0.6667 & 1.100 & 1.567 & 2.048 & 2.536 & 3.028 & 3.522 & 4.018 & 4.515 & 5.013 \\
1.000 & 0.6667 & 0.5333 & 0.8000 & 1.190 & 1.631 & 2.095 & 2.572 & 3.057 & 3.545 & 4.037 & 4.531 \\
1.500 & 1.100 & 0.8000 & 0.6857 & 0.9143 & 1.274 & 1.693 & 2.142 & 2.609 & 3.086 & 3.569 & 4.057 \\
2.000 & 1.567 & 1.190 & 0.9143 & 0.8127 & 1.016 & 1.352 & 1.753 & 2.189 & 2.646 & 3.116 & 3.594 \\
2.500 & 2.048 & 1.631 & 1.274 & 1.016 & 0.9235 & 1.108 & 1.425 & 1.810 & 2.235 & 2.683 & 3.146 \\
3.000 & 2.536 & 2.095 & 1.693 & 1.352 & 1.108 & 1.023 & 1.193 & 1.494 & 1.866 & 2.280 & 2.720 \\
3.500 & 3.028 & 2.572 & 2.142 & 1.753 & 1.425 & 1.193 & 1.114 & 1.273 & 1.560 & 1.920 & 2.324 \\
4.000 & 3.522 & 3.057 & 2.609 & 2.189 & 1.810 & 1.494 & 1.273 & 1.198 & 1.348 & 1.623 & 1.972 \\
4.500 & 4.018 & 3.545 & 3.086 & 2.646 & 2.235 & 1.866 & 1.560 & 1.348 & 1.277 & 1.419 & 1.684 \\
5.000 & 4.515 & 4.037 & 3.569 & 3.116 & 2.683 & 2.280 & 1.920 & 1.623 & 1.419 & 1.351 & 1.486 \\
5.500 & 5.013 & 4.531 & 4.057 & 3.594 & 3.146 & 2.720 & 2.324 & 1.972 & 1.684 & 1.486 & 1.422
\end{pmatrix}$$

Definition 2. Averaging $\frac{\mathcal{E}(\mu-\nu)}{s}$ over $(\mu,\nu) \in \mathcal{C}(s,n) \times \mathcal{C}(s,n)$ gives rise to the expected value of the discrete EMD. Taking $s \to \infty$ gives the expected value of the *normalized EMD* on $\mathcal{P}_n$. Observe that the maximum value of normalized EMD on $\mathcal{P}_n$ is $n-1$. The *unit normalized EMD* will be defined as the EMD scaled by $\frac{1}{n-1}$. (This scaling makes $\mathcal{P}_n$ into a metric space with diameter 1.)

In the situation that we look at the discrete case where $\mathcal{P}_n$ is replaced by $\mathcal{C}(s,n)$, we calculated the exact histogram for the unit normalized distance:



The mean of the distribution shown in the above histogram is obtained expanding

$$\frac{8t\left(5t^3+27t^2+27t+5\right)}{(1-t)^{10}}$$

around $t=0$ and taking the coefficient of t^{30}, and then dividing by $\binom{30+5-1}{5-1}^2$ (the number of ordered pairs of distributions). The approximate value is 26.2938.

For the unit normalized distance we divide by $120 = 30(5-1) = s(n-1)$. That is, we divide by s to obtain a probability distribution, and then divide by $n-1$ to scale the diameter to 1. The unit normalized mean is approximately, 0.219115.

In the case that $s \to \infty$, the mean decreases slightly from the $s = 30$ case. Again, the scaling sets the diameter of the metric space $\mathcal{P}_n$ to 1. Thus, the expected value of the unit normalized EMD is

$$\widetilde{\mathcal{M}}_n := \frac{\mathcal{M}_n}{n-1}.$$

Recall the notation that $\mathcal{M}_n = \mathcal{M}_{n,n}$, for positive integer n.

It should be noted that all values of $\widetilde{\mathcal{M}}_n$ are rational numbers, We have the following approximate values of $\widetilde{\mathcal{M}}_n$ for $n = 2, \cdots, 12$,

n	2	3	4	5	6	7	8	9	10	11	12
$\widetilde{\mathcal{M}}_n$	0.3333	0.2667	0.2286	0.2032	0.1847	0.1705	0.1591	0.1498	0.1419	0.1351	0.1293

Note that the above are the limiting values as $s \to \infty$. For finite s and n we can compute the exact mean of the unit normalized EMD by expanding

$$\frac{N_{p,q}(t)}{(1-t)^{p+q}}$$

in the case when $p = q = n$ and then dividing by $s(n-1)\binom{s+n-1}{n-1}^2$. We show the approximate values in the table below.

$s \backslash n$	2	3	4	5	$\cdots$	12
1	0.5000	0.4444	0.4167	0.4000		0.3611
2	0.4444	0.3889	0.3600	0.3422		0.2991
3	0.4167	0.3600	0.3300	0.3113		0.2649
4	0.4000	0.3422	0.3113	0.2918		0.2428
5	0.3889	0.3302	0.2985	0.2784		0.2272
10	0.3636	0.3020	0.2681	0.2462		0.1881
15	0.3542	0.2912	0.2561	0.2333		0.1716
20	0.3492	0.2854	0.2497	0.2264		0.1624
30	0.3441	0.2794	0.2430	0.2191		0.1524
60	0.3388	0.2732	0.2360	0.2114		0.1415
120	0.3361	0.2700	0.2323	0.2073		0.1355
180	0.3352	0.2689	0.2311	0.2060		0.1335
360	0.3343	0.2678	0.2298	0.2046		0.1314
500	0.3340	0.2675	0.2295	0.2042		0.1308
750	0.3338	0.2672	0.2292	0.2039		0.1303
1000	0.3337	0.2671	0.2290	0.2037		0.1300
1250	0.3336	0.2670	0.2289	0.2036		0.1299
1500	0.3336	0.2669	0.2289	0.2035		0.1298
2000	0.3335	0.2669	0.2288	0.2034		0.1296
10000	0.3334	0.2667	0.2286	0.2032		0.1293

6. Motivation from spectral graph theory

Given an undirected graph G with vertices $\{v_1, \cdots, v_m\}$ and k edges having no multiple edges or loops, one can form the Laplacian matrix $L_G = D_G - A_G$ where D_G is the diagonal matrix with the degree of vertex v_i in the i-th row and i-th column, while $A(G)$ is the adjacency matrix in which the entry in row i and column j is a one if v_i and v_j are joined by an edge, and zero otherwise.

The spectrum of L_G is of interest. We recommend the survey [Moh91a]. To begin, L_G is a positive semi-definite matrix. The multiplicity of the 0-eigenspace is equal to the number of connected components of G. Let the spectrum be denoted by:

$$0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_m.$$

The *algebraic connectivity* is given by λ_2. Intuitively, we expect "clustering" when λ_2 is small relative to the rest of the spectrum.

The results proved in [Moh91b] will be of interest here, which we now recall. First off the discrete Cheeger inequality asserts that the isoparametric number, $i(G)$, is intimately related to the spectrum of a graph. This number is defined as

$$i(G) := \min \left\{ \frac{|\delta X|}{|X|} : 0 < |X| < \frac{1}{2}|V(G)| \right\}$$

where $\delta(X)$ is defined to be the boundary of a set of vertices X (that is $v \in X$ iff v is in X but is joined to a vertex not in X). A deep result is

$$\frac{\lambda_2}{2} \le i(G) \le \sqrt{\lambda_2(2d_{max} - \lambda_2)} \tag{6.1}$$

where d_{max} is the maximum degree of a vertex in G. These results have their underpinnings in geometry and topology, see [Mém11], for example. Intuitively, the point here is that if G has two large subgraphs that are joined only by a small set of edges then the $i(G)$ is small. Unfortunately, computing $i(G)$ *exactly* is difficult.

Fortunately, the spectrum of G can be computed more effectively. In fact, let $\overline{\rho}(G)$ be the mean distance in G. We have

$$\frac{1}{m-1}\left(\frac{2}{\lambda_2} + \frac{m-2}{2}\right) \le \overline{\rho}(G) \le \frac{m}{m-1}\left[\frac{d_{max} - \lambda_2}{4\lambda_2}\ln(m-1)\right] \tag{6.2}$$

where m is the number of vertices in G.

From our point of view, we consider the graph G to be on the vertex set $\mathcal{C}(s,n)$ with two compositions joined exactly when the (unnormalized) Earth Mover's Distance is exactly 1. We call this graph the *Earth Mover's Graph*, denoted $G(s,n)$. In this case the distance between two vertices is the Earth Mover's Distance. The above inequalities then relate the spectrum of $G(s,n)$ to the coefficients of $H'_n(1,t)$.

7. Real world data

In this section, we will consider a real world data set coming from the Section Attrition and Grade Report published by the Office of Assessment and Institutional Research at the University of Wisconsin - Milwaukee for fall semesters of academic years 2013-2017. We selected data for courses with enrollments greater than 1,000. Analysis is done for the 12 grades A through F (with plus/minus grading). "W" grades were not reported by the University for the entire period and are not included.

Most universities collect and analyze similar types of retention and attrition data. Analysis of grade distribution data may be an as-yet untapped portal for self-examination that reveals patterns in large, multi-section courses, or allows for insight into cross-divisional course boundaries. Cluster analysis provides a visual reinforcement of the calculated EMD.

The data for 2013-2017 comprises a total of twenty one courses. In Fall 2013 there are five courses: English 101 and 102, Math 095 and 105, and Psychology 101. Math 095 was redesigned after Fall 2013 and enrollment dropped below 1,000; the other four courses were offered every year. Input data are sorted by division and year.

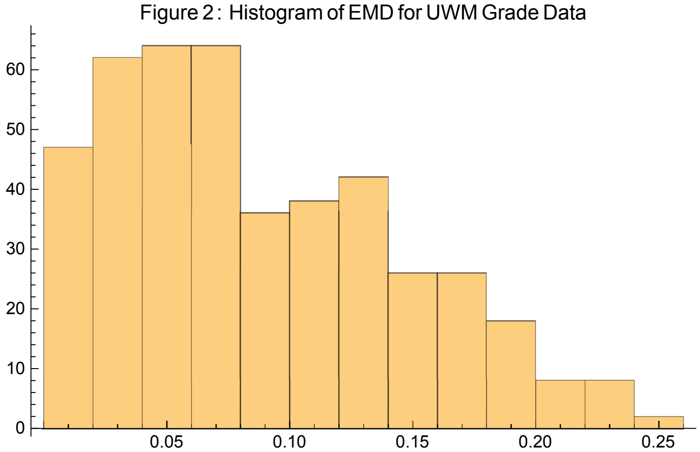
ID	*Division*	*Course*	*Year*	*Enrollment*
1	English	101	2013	1800
2	English	102	2013	1224
3	English	101	2014	1762
4	English	102	2014	1299
5	English	101	2015	1742
6	English	102	2015	1525
7	English	101	2016	1693
8	English	102	2016	1410
9	English	101	2017	1569
10	English	102	2017	1142
11	Math	95	2013	1166
12	Math	105	2013	1555
13	Math	105	2014	1701
14	Math	105	2015	1466
15	Math	105	2016	1604
16	Math	105	2017	1732
17	Psychology	101	2013	1507
18	Psychology	101	2014	1443
19	Psychology	101	2015	1337
20	Psychology	101	2016	1192
21	Psychology	101	2017	1333

7.1. **General remarks on clustering.** There are several "off the shelf" methods for clustering analysis. See [Mac03] Chapter 20 for some commentary, especially about the popular "k-means" algorithm. Here, we will focus on *spectral clustering* as it is related to the Theorem 1. However, the data that we consider in this article can and should be looked at from several points of view. In particular, unsupervised machine learning techniques are merited. See [HTF01] as a general reference.

7.2. **Histogram of EMD sample.** Following the algorithm presented above, the normalized EMD is calculated for each pair of courses. A histogram of the results is presented here. The structure definitely reflects the distribution of the theoretical case presented previously. It is interesting to note that below histogram shows maximal EMD between courses at around 0.25. Additionally, for each course one can compute the average EMD to all others. This course average has a minimum EMD of 0.067, mean 0.086, and maximum 0.129.

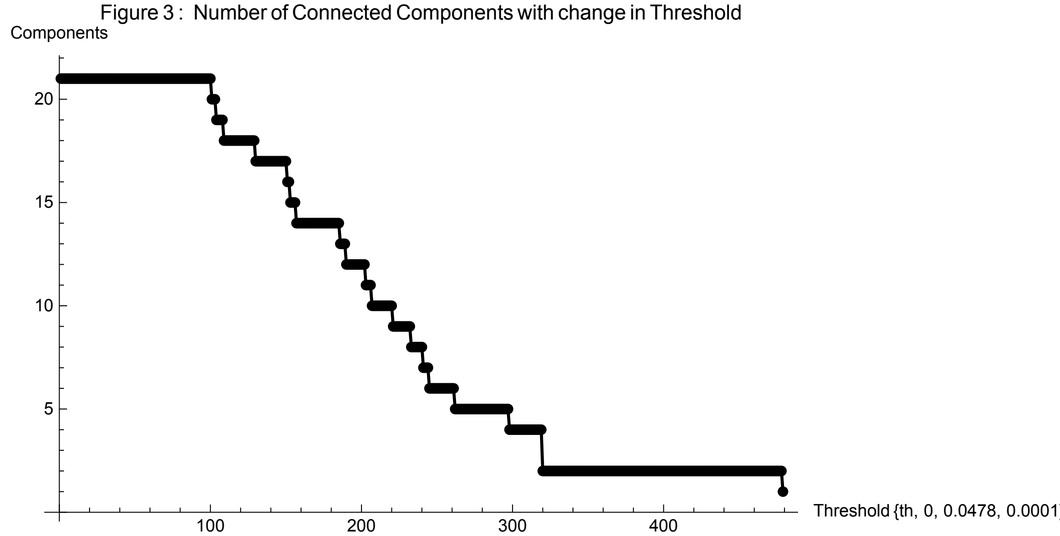
Under the assumption that all distributions are equally likely the predicted mean EMD is 0.1293 (unit normalized). For actual grade distribution data, not all grade distributions are equally likely. For this data set the maximum mean EMD corresponds to Psychology 101, Fall 2014.

Figure 2 : Histogram of EMD for UWM Grade Data

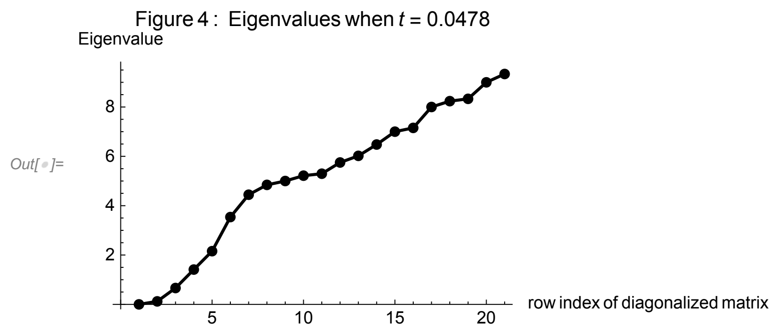


7.3. **The Laplacian Matrix.** A key component of spectral clustering is the construction of the Laplacian Matrix L_G as defined in Section 6. However for this data set it is not obvious how to define adjacent vertices, since every grade distribution has a calculated distance from every other distribution. In the next figure we step through various distance "threshold" values t and count the number of connected components. When t is small, the graph has 21 components. As t increases, the graph continues to connect, with the largest range of persistence for $t \in [0.0319, 0.0477]$ with two components. We set the threshold at 0.0478 when creating the Laplacian matrix.

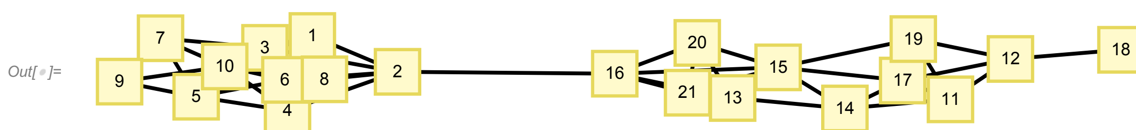
Figure 3 : Number of Connected Components with change in Threshold



7.4. **Algebraic Connectivity.** The second smallest eigenvalue of L_G gives the algebraic connectivity. For this data set $\lambda_2 = 0.121285$. The next figure presents a plot of the full spectrum. The associated eigenvector (the Fiedler vector) shows the partitioning of the data set through its positive and negative values.



We can verify the bounds on the isoparametric number (Equation 6.1) and the mean distance $\overline{\rho}(G)$ from Equation 6.2. In the case that the threshold $t = 0.0487$ we obtain the graph



For this 21 vertex graph, the algebraic connectivity is $\lambda_2 \cong 0.1213$, and the maximum degree is $d_{max} = 8$. It appears as if elements 2 and 16 create a tenuous bridge between the 2 components.

The bounds on the isoparametric number are

$$\frac{0.1213}{2} \leq i(G) \leq \sqrt{0.1213(2 \times 8 - 0.1213)}$$

$$.06065 \leq i(G) \leq 1.3878$$

with a computed value of $i(G) \cong 0.1$

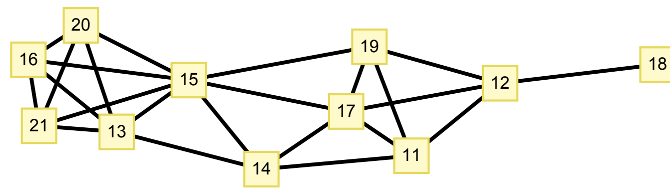
And the bounds on the mean distance are

$$\frac{1}{21-1}\left(\frac{2}{0.1213} + \frac{21-2}{2}\right) \leq \overline{\rho}(G) \leq \frac{21}{21-1}\left[\frac{8-0.1213}{4 \times 0.1213}\ln(21-1)\right]$$

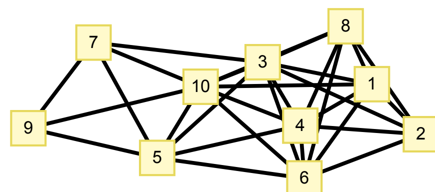
$$1.2995 \leq \overline{\rho}(G) \leq 51.08$$

and one can compute $\overline{\rho}(G) \cong 2.7710$.

The most curious part of this analysis appears in the plot of the 2 components. At threshold $t = 0.0477$ the algebraic connectivity goes to zero, and the EMD splits English off from Math and Psychology. Or equivalently, grade distributions in English courses are most similar to grade distributions in other English courses, and least similar to distributions in both Math and Psychology.



Out[∘]=



Although we see a clear partition of the data in the above illustration, one needs to be cautious about clustering algorithms. See the paper [Kle03] for a careful treatment of this topic.

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