Mastodon Theorem - 20 Years in the Making

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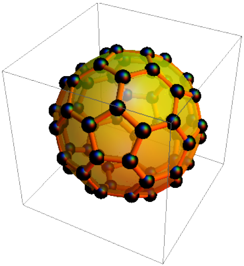
Optimal *s*-energy and Log-optimal codes

Thomson Problem (1904) -
("plum pudding" model of an atom)

Find the (most) stable (ground state) energy configuration (**code**) of N classical electrons (Coulomb law) constrained to move on the sphere $\mathbb{S}^2$.



Generalized Thomson Problem ($1/r^s$ potentials and $\log(1/r)$)

A code $C := \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^2$ that minimizes **Riesz *s*-energy**

$$E_s(C) := \sum_{j \neq k} \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|^s}, \quad s > 0, \qquad E_{\log}(\omega_N) := \sum_{j \neq k} \log \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|}$$

is called an **optimal *s*-energy code** (**log-optimal** for $s = 0$)

Optimal s-energy codes on $\mathbb{S}^2$

Known optimal s-energy codes on $\mathbb{S}^2$

- $s = \log$, Whyte's problem (1952, Monthly) ($N = 2-6,\ 12$);
- $s = 1$, Thomson Problem (known for $N = 2-6,\ 12$)
- $s = -1$, Fejes-Toth Problem (known for $N = 2-6,\ 12$)
- $s \to \infty$, Tammes Problem (known for $N = 1-12,\ 13, 14,\ 24$)

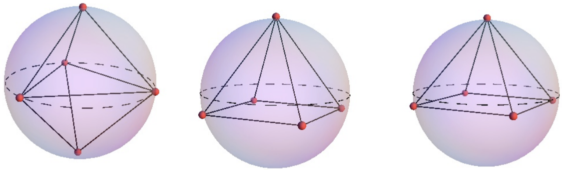
Limiting case - Best packing

For fixed N, any limit as $s \to \infty$ of optimal s-energy codes is an optimal (maximal) code.

Universally optimal codes

The codes with cardinality $N = 2, 3, 4, 6, 12$ are special (*sharp codes*) and minimize large class of potential energies. First "non-sharp" is $N = 5$ and very little is rigorously proven.

Optimal five point log and Riesz s-energy code on $\mathbb{S}^2$

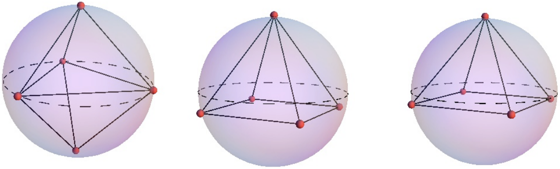


(a) (b) (c)

Figure: 'Optimal' 5-point codes on $\mathbb{S}^2$: (a) bipyramid BP, (b) optimal square-base pyramid SBP ($s = 1$) , (c) 'optimal' SBP ($s = 16$).

- $s = 0$: P. Dragnev, D. Legg, and D. Townsend, (2002) **(referred to by Ed Saff as "Mastodon" theorem)**;
- $s = -1$: X. Hou, J. Shao, (2011), computer-aided proof;
- $s = 1, 2$: R. E. Schwartz (2013), computer-aided proof;
- Bondarenko-Hardin-Saff (2014), As $s \to \infty$, any optimal s-energy codes of 5 limit is a square pyramid with base in the Equator;
- $0 < s < 15.04..$: R. E. Schwartz (2018).

Optimal five point log and Riesz s-energy code on $\mathbb{S}^2$



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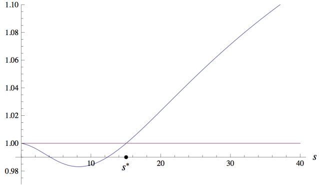

Melnik et.el. 1977 $s^* = 15.04\ldots$?

Figure: 5 points energy ratio

“Mastodon” Theorem on $\mathbb{S}^3$ and $\mathbb{S}^4$ (Dragnev - 2016)

Definition

Two vertices $\mathbf{x}_i$ and $\mathbf{x}_j$ are called *mirror related* (we write $\mathbf{x}_i \sim \mathbf{x}_j$), if $|\mathbf{x}_i - \mathbf{x}_k| = |\mathbf{x}_j - \mathbf{x}_k|$, for every $k \neq i, j$.

Theorem (Characterization of $(d+3)$ Log-stationary configurations)

A log-stationary configuration is either (a) degenerate; (b) there exists a vertex with all edges stemming out being equal; or (c) every vertex is mirror related to another vertex.

Remark

Mirror relation is equivalence relation and an equivalence class forms a regular simplex in the spanning affine hyperspace.

Theorem (Dragnev - 2016)

The $(d+3)$-Log-optimal configuration in $\mathbb{S}^1$, $\mathbb{S}^2$, $\mathbb{S}^3$, $\mathbb{S}^4$, is two orthogonal simplexes of type $\{2,2\}$, $\{2,3\}$, $\{3,3\}$, $\{3,4\}$ respectively.

“Mastodon” Theorem on $\mathbb{S}^{d-1}$ (Musin, D. - 2020)

Theorem (Main Theorem 1)

Up to orthogonal transform, every relative minimum of the logarithmic energy $E_{\log}(X)$ of $d+2$ points on $\mathbb{S}^{d-1}$ consists of two regular simplexes of cardinality $m \geq n > 1$, $m+n=d+2$, such that these simplexes are orthogonal to each other. The global minimum occurs when $m=n$ if d is even and $m=n+1$ otherwise.

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Remark

The only two other classes of minimal energy configurations are the regular simplex ($d+1$ points on $\mathbb{S}^{d-1}$) and the regular cross polytope ($2d$ points on $\mathbb{S}^{d-1}$), both of which are universally optimal.

Stationary Configurations of $d+2$ points on $\mathbb{S}^{d-1}$

Definition

A point configuration is called **degenerate** if it is contained in an affine hyperplane. (Ex. Pentagon on $\mathbb{S}^2$)

Theorem (Non-degenerate, non-equidistant case)

Let $N = d + 2$ *and* $X = \{x_1, \dots, x_N\}$ *be a non-degenerate stationary logarithmic configuration on* $\mathbb{S}^{d-1}$*. Suppose there is no point* $x \in X$ *that is equidistant to all other points in* X*. Then* X *can be split into two sets such that these sets are vertices of two regular orthogonal simplexes with the centers of mass in the center of* $\mathbb{S}^{d-1}$*.*

Remark

Strengthens 2016 Characterization theorem significantly.

Stationary Configurations of $d+2$ points on $\mathbb{S}^{d-1}$

Given potential interaction function $h : [-1,1] \to \overline{\mathbb{R}}$ *h-energy* is

$$E_h(X) := \sum_{1 \le i \ne j \le N} h(x_i \cdot x_j).$$

Theorem (Degenerate Case - h-energy)

Let X be any degenerate configuration, $N \geq d+2$, and $h : [-1,1] \to \mathbb{R}$ be a strictly convex potential function. Then there exists a continuous perturbation that decreases the h-energy $E_h(X)$.

Theorem (Equidistant case)

A non-degenerate stationary log-energy configuration of type $\{1,1,\dots,k,l\}$, where $1+1+\cdots+k+l = d+2$ is a saddle point. Moreover, there is a continuous perturbation that decreases the logarithmic energy of the $\{1,k,l\}$ part of the configuration to either $\{k+1,l\}$ or $\{k,l+1\}$. Sequence of such perturbations leads to relative minima as described in Main Theorem.

Auxiliary Results

Using Lagrange Multipliers method to *logarithmic energy*

$$E_{Log}(X) := -\frac{1}{2} \sum_{1 \leq i \neq j \leq N} \log(x_i \cdot x_i - 2x_i \cdot x_j + x_j \cdot x_j),$$

and differentiating yields

$$\sum_{j \neq i} \frac{x_i - x_j}{r_{i,j}} = \lambda_i x_i \quad i = 1, \ldots, N, \text{ where } r_{ij} := 1 - x_i \cdot x_j.$$

Taking inner product of both sides with x_i one obtains $\lambda_i = N - 1$, or

$$\sum_{j \neq i} \frac{x_i - x_j}{r_{i,j}} = (N-1)\, x_i, \quad i = 1, \ldots, N. \tag{1}$$

Summing (1) implies that the centroid lies at the origin, and hence

$$\sum_{j} r_{ij} = N, \quad i = 1, \ldots, N. \tag{2}$$

Auxiliary Results - Rank Lemma

Let

$$B = (b_{ij}), \quad b_{ij} := \frac{1}{r_{ij}}, \quad b_{ii} := N - 1 - \sum_{j \neq i} b_{ij},$$

$$A = (a_{ij}), \text{ where } a_{ij} := c - b_{ij}, \quad c := \frac{N-1}{N}.$$

Lemma

Let $\mathrm{X} = \{x_1, \ldots, x_N\}$ be a stationary logarithmic configuration on $\mathbb{S}^{d-1}$ that is non-degenerate. Then

$$\mathrm{rank}(A) \leq N - d - 1, \qquad \sum_{j=1}^{N} a_{ij} = 0, \quad i = 1, \ldots, N.$$

If $N = d + 2$, then $\mathrm{rank}(A) = 1$.

Proof of the Rank Lemma

Let $\mathrm{X} := [x_1, \ldots, x_N]^T$. The force equations (1) and (2) imply that

$$\sum_{j=1}^{N} b_{ij} x_j = 0, \quad \sum_{j=1}^{N} b_{ij} = N - 1.$$

In other words, $B\mathrm{X} = 0$ and $B\mathbf{1} = (N-1)\mathbf{1}$, where $\mathbf{1}$ denotes the N-dimensional column-vector of ones.

As X is non-degenerate, we have rank $\mathrm{X} = d$. Therefore, the column-vectors of X are linearly independent.

Since $\mathbf{1}$ is eigenvector of B with an eigenvalue of $N-1$, it is linearly independent to the columns of X (eigenvectors with eigenvalue 0).

The lemma follows from the rank-nullity theorem applied to $A[\mathrm{X}, \mathbf{1}] = 0$.

□

Auxiliary Results - $N = d + 2$

The following lemma elaborates on the case when $N = d + 2$.

Lemma

Let $N = d + 2$ and $X = \{x_1, \dots, x_N\}$ be a non-degenerate stationary logarithmic configuration on $\mathbb{S}^{d-1}$. Without loss of generality we may assume that $a_{1i} \geq 0$ for $i = 1, \dots k$ and $a_{1i} < 0$ for $i = k+1, \dots N$. Let

$$a_i = \sqrt{a_{ii}},\ i = 1, \dots k;\ \ a_i = -\sqrt{a_{ii}},\ i = k+1, \dots N.$$

Then

$$a_{ij} = a_i\, a_j, \quad a_1 + \dots + a_N = 0,$$

$$c - a_i a_j \geq \frac{1}{2}, \ \text{ for all } \ i \neq j,$$

$$\sum_{j \neq i} \frac{1}{c - a_i a_j} = N,\ i = 1, \dots, N. \tag{3}$$

Auxiliary Results - Supplemental Theorem

If $a_i = 0$ then the i-th row and i-th column in A are zero x_i is equidistant to all other points x_j. So, $a_i \neq 0$ for all $i = 1, \ldots, N$.

Theorem (Supplemental)

Let $a_1, \ldots, a_N$ be real numbers that satisfy the following assumptions

$$a_1 \geq \ldots \geq a_k > 0 > a_{k+1} \geq \ldots \geq a_N, \quad a_1 + \ldots, + a_N = 0,$$

$$\sum_{j \neq i} \frac{1}{c - a_i a_j} = N, \; i = 1, \ldots, N, \quad c - a_i a_j > 0, \; \textit{for all} \; i \neq j,$$

where $c := \frac{N-1}{N}$. Then

$$a_1 = ... = a_k, \quad a_{k+1} = ... = a_N.$$

Auxiliary Results - Technical Lemma

Lemma (Technical)

Suppose $a_1, \ldots, a_N$ are as in Supplemental Theorem. Then for all $i = 1, \ldots, N$ we have

$$T_i := \sum_{j \neq i} \frac{c - a_j^2}{c - a_i a_j} = N - 2. \tag{4}$$

and

$$|a_i| < \sqrt{c}, \quad i = 1, ..., N. \tag{5}$$

Proof of the Technical Lemma - Eq. (4)

Denote

$$Q_i := \sum_{j\neq i} \frac{1}{c - a_i a_j}, \quad R_i := \sum_{j\neq i} \frac{a_j}{c - a_i a_j}, \quad S_i := \sum_{j\neq i} \frac{a_j^2 - a_j a_i}{c - a_i a_j}.$$

By the assumption $Q_i = N$ for all i, we get (recall $a_i \neq 0$)

$$N - 1 = \sum_{j\neq i} \frac{c - a_i a_j}{c - a_i a_j} = c\, Q_i - a_i R_i = N - 1 - a_i R_i,$$

or $R_i = 0$. Along with $a_i = -(a_1 + ... + a_{i-1} + a_{i+1} + ...a_N)$

$$a_i = (c - a_i^2) \sum_{j\neq i} \frac{a_j}{c - a_i a_j} - \sum_{j\neq i} a_j = a_i \sum_{j\neq i} \frac{a_j^2 - a_j a_i}{c - a_i a_j} = a_i S_i,$$

or $S_i = 1$ and subsequently

$$N - 2 = \sum_{j\neq i} \frac{c - a_i a_j}{c - a_i a_j} - S_i = \sum_{j\neq i} \frac{c - a_j^2}{c - a_i a_j} = T_i$$

Proof of the Technical Lemma - Ineq. (5)

W.l.g. $|a_1| \geq |a_i|$. From $S_i = 1$ we have

$$1 = \sum_{j \neq i} \frac{a_j^2 - a_i a_j}{c - a_i a_j} = \frac{a_1^2 - a_i a_1}{c - a_i a_1} + \sum_{2 \leq j \neq i} \frac{a_j^2 - a_i a_j}{c - a_i a_j}.$$

Then

$$\sum_{2 \leq j \neq i} \frac{a_j^2 - a_i a_j}{c - a_i a_j} = \frac{c - a_1^2}{c - a_i a_1}, \quad i = 2, \ldots, N.$$

Therefore,

$$\sum_{i=2}^{N} \sum_{2 \leq j \neq i} \frac{a_j^2 - a_i a_j}{c - a_i a_j} = \sum_{i>j=2}^{N} \frac{(a_i - a_j)^2}{c - a_i a_j} = (c - a_1^2) \sum_{i=2}^{N} \frac{1}{c - a_i a_1} = (c - a_1^2) Q_1.$$

Since $Q_1 = N$ and by the assumption $c - a_i a_j > 0$, we have

$$c - a_1^2 = \frac{1}{N} \sum_{i>j=2}^{N} \frac{(a_i - a_j)^2}{c - a_i a_j} > 0. \tag{6}$$

Thus, (6) implies $c - a_i^2 > 0$. $\square$

Proof of Supplemental Theorem

Let

$$F(t) := \sum_{j=1}^{N} \frac{c - a_j^2}{c - ta_j}.$$

Then Technical Lemma implies that for all $i = 1, \ldots, N$

$$F(a_i) = N - 1. \tag{7}$$

Since

$$F''(t) = 2 \sum_{j} \frac{\left(c - a_j^2\right) a_j^2}{(c - ta_j)^3},$$

by Technical Lemma again we have $F''(t) > 0$ for $t \in (-\sqrt{c}, \sqrt{c})$. Hence $F(t)$ is a convex function in this interval. Therefore, the equation $F(t) = N - 1$ has at most two solutions. By assumptions we have $a_i > 0$ for $i = 1, \ldots, k$ and $a_i < 0$, for $i = k + 1, \ldots, N$. Thus, (7) yields that all positive a_i are equal and all negative a_i are equal too. $\square$

Proofs of Degenerate, Equidistant, and Relative Minima cases

Even more complex and involved :-(

Degenerate case - *h*-energy

Theorem (Degenerate Case)

Let X be a degenerate configuration, $N \geq d+2$, and $h : [-1,1] \to \mathbb{R}$ be a strictly convex potential function. Then there exists a continuous perturbation that decreases the h-energy $E_h(X)$.

Proof.

$$x_1 = (r, \sqrt{1-r^2}, 0, \ldots, 0), x_2 = (r, -\sqrt{1-r^2}, 0, \ldots, 0)$$

$$x_j = (c_{j1}, c_{j2}, c_{j3}, \ldots, 0),\ j = 3, \ldots, N,$$

where $c_{32} \neq 0$. Preturb to $\widetilde{X}$

$$\tilde{x}_1 = (r, \sqrt{1-r^2}\cos\theta, 0, \ldots, \sqrt{1-r^2}\sin\theta),$$

$$\tilde{x}_2 = (r, -\sqrt{1-r^2}\cos\theta, 0, \ldots, -\sqrt{1-r^2}\sin\theta).$$

Then $E_h(X) > E_h(\widetilde{X})$ □

Equidistant case

Theorem (Equidistant case)

A non-degenerate stationary log-energy configuration of type $\{1, 1, \ldots, k, \ell\}$, where $1 + 1 + \cdots + k + \ell = d + 2$ is a saddle point. Moreover, there is a continuous perturbation that decreases the logarithmic energy of the $\{1, k, \ell\}$ part of the configuration to either $\{k + 1, \ell\}$ or $\{k, \ell + 1\}$. Sequence of such perturbations leads to relative minima as described in Main Theorem.

Equidistant case proof

Proof.

Let $X = \{1, k, \ell\}$ with $x_N \cdot x_i = -1/(N-1)$. Denote $x_i = (y_i, \frac{-1}{N-1})$, $z_i := (N-1)y_i/\sqrt{N(N-2)}$, $z_i \in \mathbb{S}^{d-2}$ satisfies force equation.

$$Y := \{(\sqrt{1-1/(k+m)^2}\, y_i, 0_{m-1}, -1/(k+m))\},$$

$$Z := \{(0_{k-1}, \sqrt{1-1/(k+m)^2}\, z_j, -1/(k+m))\}$$

Perturb to

$$\widetilde{Y}_t = \left\{ \left(\sqrt{1-(mt+1/(k+m))^2}\, y_i, 0_{m-1}, -1/(k+m) - mt \right) \right\}_{i=1}^{k}$$

$$\widetilde{Z}_t = \left\{ \left(0_{k-1}, \sqrt{1-(kt-1/(k+m))^2}\, z_j, -1/(k+m) + kt \right) \right\}_{j=1}^{m}.$$

Then $E_h(\widetilde{X}_t)$ has local max at $t=0$ and decreases to $\{k, \ell+1\}$ or $\{k+1, \ell\}$. □

Relative minima case

Theorem (Equidistant case)

Let $X = \{k, \ell\}$ a configuration of two orthogonal simplexes X_k and X_ℓ. Any perturbation will increase the energy locally.

We need two inequalities.

Relative minima case - Inequality 1

Lemma (H1)

Let $A = (a_{ij})$ be an $m \times m$ matrix, $m \geq 3$, such that
(a) $a_{ii} = 0, \quad i = 1, \ldots, m;$
(b) $\sum_{j=1}^{m} a_{ij} = 0.$
Then the following inequality holds

$$\sum_{1 \leq i < j \leq m} (a_{ij} + a_{ji})^2 \geq \frac{1}{m-2} \sum_{j=1}^{m} x_j^2, \quad \text{where} \quad x_j := \sum_{i=1}^{m} a_{ij}. \tag{8}$$

Proof of Inequality 1: part 1

For all $i, j = 1, \ldots, m$ define

$$\beta_{ij} := \frac{1}{m^2 - 2m} x_i + \frac{m-1}{m^2 - 2m} x_j, \quad i \neq j, \quad \text{and} \quad \beta_{ii} = 0.$$

Since $\sum_{j=1}^m x_j = 0$, we have $\sum_{j=1}^m \beta_{ij} = 0$ and $\sum_{i=1}^m \beta_{ij} = x_j$, i.e.

$$\sum_{j=1}^m \beta_{ij} = \sum_{j=1}^m a_{ij} \quad \text{and} \quad \sum_{i=1}^m \beta_{ij} = \sum_{i=1}^m a_{ij}.$$

Let $\widetilde{a}_{ij} := a_{ij} - \beta_{ij}$. Then

$$\sum_i \widetilde{a}_{ij} = \sum_j \widetilde{a}_{ij} = 0.$$

Proof of Inequality 1: part 2

Consider $t_{ij} := a_{ij} + a_{ji} = w_{ij} + \beta_{ij} + \beta_{ji}$, where $w_{ij} = \widetilde{a}_{ij} + \widetilde{a}_{ji}$. Then $t_{ij} = w_{ij} + \frac{x_i}{m-2} + \frac{x_j}{m-2}$, $i \neq j$, where $\sum_i w_{ij} = \sum_j w_{ij} = 0$ (observe that $t_{ii} = 0$). Then

$$\sum_{i<j} t_{ij}^2 = \sum_{i<j} \left(w_{ij} + \frac{x_i}{m-2} + \frac{x_j}{m-2} \right)^2 = \sum_{i<j} w_{ij}^2 + \frac{1}{m-2} \sum_{i=1}^{m} x_i^2,$$

which implies (8).

Relative minima case - Inequality 2

Lemma (H2)

Given an $m \times n$ matrix $F = (f_{ij})$ and an $n \times m$ matrix $G = (g_{ij})$ such that $\sum_{j=1}^{n} f_{ij} = 0$ for all $i = 1, \ldots, m$ and $\sum_{j=1}^{m} g_{ij} = 0$ for all $i = 1, \ldots, n$. Then we have

$$\sum_{i=1}^{n} \sum_{j=1}^{m} (f_{ij} + g_{ji})^2 \geq \frac{1}{m} \sum_{j=1}^{n} y_j^2 + \frac{1}{n} \sum_{i=1}^{m} z_i^2,$$

$$y_j := \sum_{i=1}^{m} f_{ij}, \quad z_i := \sum_{j=1}^{n} g_{ji}.$$

Proof of Inequality 2

Let

$$\widetilde{f}_{ij} := f_{ij} - \frac{y_j}{m} \quad \text{and} \quad \widetilde{g}_{ij} := g_{ij} - \frac{z_i}{n}.$$

Since $\sum_j y_j = \sum_i z_i = 0$, we have $\sum_{i,j}(\widetilde{f}_{ij} + \widetilde{g}_{ji}) = 0$. Let $t_{ij} := \widetilde{f}_{ij} + \widetilde{g}_{ji}$. Observe that

$$\sum_{i=1}^{m} t_{ij} = \sum_{j=1}^{n} t_{ij} = 0.$$

From

$$f_{ij} + g_{ji} = \frac{y_j}{m} + \frac{z_i}{n} + t_{ij}.$$

one derives that

$$\sum_{i=1}^{m}\sum_{j=1}^{n}(f_{ij}+g_{ji})^2 = \sum_{i=1}^{m}\sum_{j=1}^{n}\left(\frac{y_j}{m} + \frac{z_i}{n} + t_{ij}\right)^2 = \sum_{i=1}^{m}\sum_{j=1}^{n} t_{ij}^2 + \frac{1}{m}\sum_{j=1}^{n} y_j^2 + \frac{1}{n}\sum_{i=1}^{m} z_i^2,$$

which completes the proof.

Relative minima case - Proof (part 1)

Perturb the two orthogonal simplexes ($k+\ell=d+2$)

$$X_k=\{x_1,x_2,\dots,x_k\},\quad X_\ell=\{x_{k+1},x_{m+2},\dots,x_{k+\ell}\},$$

to $Y=Y_k\cup Y_\ell$, where $y_i:=x_i+h_i$, $\|h_i\|<\epsilon$. Since $\|x_i\|=\|y_i\|=1$, we have $2x_i\cdot h_i=-\|h_i\|^2$, $1-y_i\cdot y_j=(1-x_i\cdot x_j)(1-z_{i,j})$, where

$$z_{i,j}:=\begin{cases}\frac{k-1}{k}(x_i\cdot h_j+x_j\cdot h_i+h_i\cdot h_j), & 1\le i\ne j\le k\\ x_i\cdot h_j+x_j\cdot h_i+h_i\cdot h_j, & i\le k<j \text{ or } j\le k<i\\ \frac{\ell-1}{\ell}(x_i\cdot h_j+x_j\cdot h_i+h_i\cdot h_j), & k<i\ne j\le k+\ell.\end{cases}\qquad (9)$$

Clearly $|z_{i,j}|<2\epsilon+O(\epsilon^2)$. We find

$$2\left[E_{\log}(Y)-E_{\log}(X)\right]=\sum_{1\le i\ne j\le k+\ell}\left(z_{i,j}+\frac{z_{i,j}^2}{2}\right)+O(\epsilon^3).\qquad (10)$$

Relative minima case - Proof (part 2)

W.l.g. $x_i = (p_i, 0)$, $h_i = (a_i, b_i)$, $x_{k+j} = (0, q_j)$, $h_{k+j} = (c_j, d_j)$, where $p_i, a_i, c_j \in \mathbb{R}^{k-1}$ and $q_j, b_i, d_j \in \mathbb{R}^{\ell-1}$. Straight-forward calculations show that the linear in ϵ term in (10) vanishes. The quadratic term is

$$D := \sum_{1 \leq i \neq j \leq k+\ell} \frac{h_i \cdot h_j}{1 - x.x_j} + \frac{1}{2} \sum_{1 \leq i \neq j \leq k+\ell} \left(\frac{x_i \cdot h_j + x_j \cdot h_i}{1 - x.x_j} \right)^2$$

$$= \Big\| \sum_{i=1}^{k+\ell} h_i \Big\|^2 - \frac{1}{k} \left(\Big\| \sum_{i=1}^{k} a_i \Big\|^2 + \Big\| \sum_{i=1}^{k} b_i \Big\|^2 \right) - \frac{1}{\ell} \left(\Big\| \sum_{j=1}^{\ell} c_j \Big\|^2 + \Big\| \sum_{j=1}^{\ell} d_j \Big\|^2 \right)$$

$$+ \left(\frac{k-1}{k} \right)^2 \sum_{1 \leq i < j \leq k} (p_i \cdot a_j + p_j \cdot a_i)^2 + \left(\frac{\ell - 1}{\ell} \right)^2 \sum_{1 \leq i < j \leq \ell} (q_i \cdot d_j + q_j \cdot d_i)^2 \qquad (11)$$

$$+ \sum_{i=1}^{k} \sum_{j=1}^{\ell} (p_i \cdot c_j + q_j \cdot b_i)^2.$$

Relative minima case - Proof (part 3)

By extracting another $O(\epsilon^3)$ term we may reduce the condition $2x_i \cdot h_i = -\|h_i\|^2$ to $x_i \cdot h_i = 0$.
Thus, in this case we shall reduce the theorem to proving the inequalities

$$D_1 := \left(\frac{k-1}{k}\right)^2 \sum_{1\leq i<j\leq k} (p_i \cdot a_j + p_j \cdot a_i)^2 - \frac{1}{k}\Big\| \sum_{i=1}^{k} a_i \Big\|^2 \geq 0 \qquad (12)$$

$$D_2 := \left(\frac{\ell-1}{\ell}\right)^2 \sum_{1\leq i<j\leq \ell} (q_i \cdot d_j + q_j \cdot d_i)^2 - \frac{1}{\ell}\Big\| \sum_{j=1}^{\ell} d_j \Big\|^2 \geq 0 \qquad (13)$$

and

$$D_3 := \sum_{i=1}^{k} \sum_{j=1}^{\ell} (p_i \cdot c_j + q_j \cdot b_i)^2 - \frac{1}{k}\| \sum_{i=1}^{k} b_i \|^2 - \frac{1}{\ell}\Big\| \sum_{j=1}^{\ell} c_j \Big\|^2 \geq 0 \qquad (14)$$

provided $\{p_1, \ldots, p_k\}$ and $\{q_1, \ldots, q_\ell\}$ are orthogonal k- and ℓ-simplexes and $p_i \cdot a_i = 0$ and $q_j \cdot d_j = 0$.

Relative minima case - Proof (part 4)

Embed the first simplex $X_k = \{p_1, \dots, p_k\}$ in the hyperplane of $\mathbb{R}^k$ that is orthogonal to $(1, 1, \dots, 1)$. Similarly, we embed the second simplex $X_\ell = \{q_1, \dots, q_\ell\}$ in $\mathbb{R}^\ell$. Thus, we embed $X_k \cup X_\ell \subset \mathbb{R}^k \times \mathbb{R}^\ell$.

Let $w_k = (\frac{1}{k}, \frac{1}{k}, \dots, \frac{1}{k}) \in \mathbb{R}^k$, $\widetilde{p}_i := e_i - w_k$, so $p_i = \sqrt{\frac{k}{k-1}}\,\widetilde{p}_i$. Similarly, if $\widetilde{q}_j := e_j - w_\ell$, then $q_j = \sqrt{\frac{\ell}{\ell-1}}\,\widetilde{q}_j$.

For the perturbation vectors a_i, b_i, c_j, d_j, we have

$$\sum_{j=1}^{k} a_{ij} = 0, \quad \sum_{j=1}^{\ell} b_{ij} = 0, \quad \sum_{j=1}^{k} c_{ij} = 0, \quad \sum_{j=1}^{\ell} d_{ij} = 0.$$

$p_i \cdot a_i = 0 \Rightarrow a_{ii} = 0$, $q_j \cdot d_j = 0 \Rightarrow a_{ii} = 0$. Using $\widetilde{p}_i \cdot a_j = a_{ji}$ (12) is

$$\sum_{1 \le i < j \le k} (a_{ij} + a_{ji})^2 \ge \frac{1}{k-1} \sum_{j=1}^{k} \left(\sum_{i=1}^{k} a_{ij} \right)^2,$$

which follows from Lemma (H1). Similarly one gets (13).

Relative minima case - Proof (part 5)

Equality in (12) and (13) holds iff $a_{ij} + a_{ji} = 0$ and $d_{ij} + d_{ji} = 0$ respectively, which is equivalent to

$$p_i \cdot a_j + p_j \cdot a_i = 0, q_j \cdot d_i + q_i \cdot d_j = 0, \sum a_i = 0, \sum d_j = 0.$$

Lemma (H2) is used to derive the inequality (14). We have that

$$p_i \cdot c_j + q_j \cdot b_i = \sqrt{\frac{k}{k-1}} c_{ji} + \sqrt{\frac{\ell}{\ell-1}} b_{ij}$$

with the substitution $f_{ij} = \sqrt{\frac{\ell}{\ell-1}} b_{ij}$ and $g_{ji} = \sqrt{\frac{k}{k-1}} c_{ji}$ we re-write (14) as

$$\sum_{i=1}^{\ell} \sum_{j=1}^{k} (f_{ij} + g_{ij})^2 \geq \frac{1}{k} \frac{\ell-1}{\ell} \sum_{j=1}^{\ell} y_j^2 + \frac{1}{\ell} \frac{k-1}{k} \sum_{i=1}^{k} z_i^2,$$

which clearly follows from Lemma (H2). Moreover, equality occurs if and only if $p_i \cdot c_j + q_j \cdot b_i = 0$, $\sum c_i = 0$, and $\sum b_j = 0$.

Relative minima case - Proof (part 6)

So, the quadratic in ϵ term $D > 0$, or $E_{\log}(Y) - E_{\log}(X) > 0$, for any perturbation vectors $\{a_i, b_i, c_i, d_i\}$ ($p_i \cdot a_i = 0$, $q_j \cdot d_j = 0$), except when

$$p_i \cdot a_j + p_j \cdot a_i = 0, \quad q_j \cdot d_i + q_i \cdot d_j = 0, \quad p_i \cdot c_j + q_j \cdot b_i = 0,$$

$$\sum_{i=1}^{k} a_i = 0, \quad \sum_{i=1}^{k} b_i = 0, \sum_{j=1}^{\ell} c_i = 0, \quad \sum_{j=1}^{\ell} d_j = 0.$$

Utilizing (9) and these conditions, one simplifies (10) to

$$2\left[E_{\log}(Y) - E_{\log}(X)\right] = \frac{(k-1)^2}{2k^2} \sum_{1 \leq i \neq j \leq k} (a_i \cdot a_j)^2 + \frac{(\ell-1)^2}{2\ell^2} \sum_{1 \leq i \neq j \leq \ell} (d_i \cdot d_j)^2$$
$$+ \sum_{i=1}^{k} \sum_{j=1}^{\ell} (b_i \cdot c_j)^2 + O(\epsilon^5).$$

Clearly, the quartic term will be positive, unless all inner products vanish, in which case we easily derive that $a_i = c_j = 0$ and $b_i = d_j = 0$ for all $i = 1, \ldots, k$ and $j = 1, \ldots, \ell$. This completes the proof. $\square$

THANK YOU!