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On the gap of finite metric spaces of p-negative type

Reinhard Wolf

Universität Salzburg, Fachbereich Mathematik, Austria

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ABSTRACT

Let (X, d) be a metric space of p-negative type. Recently I. Doust and A. Weston introduced a quantification of the p-negative type property, the so called gap Γ of X. This paper gives some formulas for the gap Γ of a finite metric space of strict p-negative type and applies them to evaluate Γ for some concrete finite metric spaces.

1. Introduction

Let (X, d) be a metric space and $p \geqslant 0$. Recall that (X, d) has p-negative type if for all natural numbers n, all $x_1, x_2, \ldots, x_n$ in X and all real numbers $\alpha_1, \alpha_2, \ldots, \alpha_n$ with $\alpha_1 + \alpha_2 + \cdots + \alpha_n = 0$ the inequality

$$\sum_{i,j=1}^{n} \alpha_i \alpha_j d(x_i, x_j)^p \leqslant 0$$

holds.

Moreover if (X, d) has p-negative type and

$$\sum_{i,j=1}^{n} \alpha_i \alpha_j d(x_i, x_j)^p = 0, \text{ together with } x_i \neq x_j, \text{ for all } i \neq j$$

implies $\alpha_1 = \alpha_2 = \cdots = \alpha_n = 0$, then (X, d) has strict p-negative type. ($(d(x, y)^0$ is defined to be 0 if $x = y$).

E-mail address: reinhard.wolf@sbg.ac.at

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Following [2,3] we define the p-negative type gap Γ_X^p (=Γ for short) of a p-negative type metric space (X, d) as the largest nonnegative constant, such that

$$\frac{\Gamma}{2}\left(\sum_{i=1}^{n}|\alpha_i|\right)^2 + \sum_{i,j=1}^{n}\alpha_i\alpha_j d(x_i, x_j)^p \leqslant 0$$

holds for all natural numbers n, all $x_1, x_2, \ldots, x_n$ in X with $x_i \neq x_j$, for all $i \neq j$, and all real numbers $\alpha_1, \alpha_2, \ldots, \alpha_n$ with $\alpha_1 + \alpha_2 + \cdots + \alpha_n = 0$.

The above defined p-negative type gap Γ_X^p can be used to enlarge the p-parameter, for which a given finite metric space is of strict p-negative type:

It is shown in [6] (Theorem 3.3) that a finite metric space X with cardinality $n = |X| \geqslant 3$ of strict p-negative type is of strict q-negative type for all $q \in [p, p + \xi)$ where

$$\xi = \frac{\ln\left(1 + \frac{\Gamma_X^p}{D(X)^p\cdot\gamma(n)}\right)}{\ln \mathfrak{D}(X)},$$

with $D(X) = \max_{x,y\in X} d(x, y)$, $\mathfrak{D}(X) = D(X)/\min_{x,y\in X, x\neq y} d(x, y)$ and $\gamma(n) = 1 - \frac{1}{2}\cdot(\lfloor\frac{n}{2}\rfloor^{-1} + \lceil\frac{n}{2}\rceil^{-1})$.

For basic information on p-negative type spaces (1-negative type spaces are also known as quasi-hypermetric spaces) see for example [2,4,6–11].

This paper explores formulas for the p-negative type gap of a finite p-negative type metric space. The main result is given in Theorem 3.5 (Section 3), which is itself a corollary of a more general result (Theorem 3.4, Section 3) concerning real symmetric matrices of strict negative type on certain subspaces of $\mathbb{R}^n$. Moreover we present a characterization of a finite metric space of p-negative type enjoying the additional property of being of strict p-negative type (Corollary 3.2).

In Section 4 we give some applications of the general results of Section 3. After calculating the 1-negative type gap Γ of a cycle graph with n vertices (considered as a finite metric space with the usual path length metric) we present short proofs for the evaluation of the 1-negative type gap of a finite discrete metric space, done by Weston in [11], and of a finite metric tree, done by Doust and Weston in [2]. I. Doust and A. Weston showed the surprising result, that the gap of a finite metric tree only depends on the weights associated to the edges of the tree.

2. Notation

For a given real $m \times n$ matrix A we denote by A^T the transposed matrix of A and by A^{-1} the inverse matrix of A, if it exists. Elements x in $\mathbb{R}^n$ are interpretated as column vectors, so $x^T = (x_1, x_2, \ldots, x_n)$. The canonical inner product of two elements x, y in $\mathbb{R}^n$ is given by $(x|y)$ and the canonical unit vectors are denoted by $e_1, e_2, \ldots, e_n$. The element $\underline{1}$ in $\mathbb{R}^n$ is defined as $\underline{1}^T = (1, 1, \ldots, 1)$. As usual we abbreviate $\{(\sigma_1, \sigma_2, \ldots, \sigma_n), \sigma_1, \ldots, \sigma_n \text{ in } \{-1, 1\}\}$ by $\{-1, 1\}^n$. The linear span and convex hull of a subset M in $\mathbb{R}^n$ are denoted by $[M]$ and conv M. Further let ker T be the kernel of a given linear map T.

If E is a linear subspace of $\mathbb{R}^n$ and $\|.\|$ is a norm on E we denote by $\|.\|^*$ the dual norm of $\|.\|$ on E with respect to the canonical inner product, i.e.

$$\|x\|^* = \sup_{y\in E, \|y\|\leqslant 1} |(x|y)|.$$

For $p \geqslant 1$ we let $\|x\|_p$ be the usual p-norm of some element x in $\mathbb{R}^n$. For a given real symmetric $n \times n$ matrix A which is positive semi-definite on a linear subspace E of $\mathbb{R}^n((Ax|x) \geqslant 0, \text{ for all } x \text{ in } E)$ we define the resulting semi-inner product on E by

$$(x|y)_A = (Ax|y); \quad x, y \text{ in } E.$$

Further the semi-norm $\|x\|_A$ of some element x in E is given by

$$\|x\|_A^2 = (Ax|x).$$

For a fixed $u \neq 0$ in $\mathbb{R}^n$ let

$$F_\alpha = \{x \in \mathbb{R}^n | (x|u) = \alpha\}, \quad \alpha \text{ in } \mathbb{R}.$$

For short let $F = F_0$.

3. General results

Let E be a linear subspace of $\mathbb{R}^n$ and A be a real symmetric $n \times n$ matrix of negative (strict negative) type on E, i.e.

$$(Ax|x) \leqslant 0, \quad \text{for all } x \text{ in } E \text{ and}$$
$$(Ax|x) < 0, \quad \text{for all } x \neq 0 \text{ in } E \text{ resp.}$$

For further discussion it is useful to define the negative type gap $\Gamma_{A,E}$ (=Γ for short) of A on E as the largest nonnegative constant, such that

$$\frac{\Gamma}{2}\|x\|_1^2 + (Ax|x) \leqslant 0$$

holds for all x in E. This is equivalent to

$$\left(\frac{\Gamma}{2}\right)^{\frac{1}{2}} \|x\|_1 \leqslant \|x\|_{-A}, \quad \text{for all } x \text{ in } E.$$

If A is of strict negative type on E, consider the identity operator i from the normed space $(E, \|\cdot\|_{-A})$ onto the normed space $(E, \|\cdot\|_1)$,

$$i : (E, \|\cdot\|_{-A}) \to (E, \|\cdot\|_1);\ i(x) = x, \quad \text{for all } x \text{ in } E.$$

Since E is of finite dimension, we obtain that i is bounded and by definition of $\|i\|$ we get

$$\|i\| = \inf\{c > 0 \mid \|x\|_1 \leqslant c\|x\|_{-A}, \text{ for all } x \text{ in } E\} = \sup_{x \in E, \|x\|_{-A} \leqslant 1} \|x\|_1.$$

It follows, that $\Gamma = \frac{2}{\|i\|^2} > 0$ and

$$(*) \quad \left(\frac{2}{\Gamma}\right)^{\frac{1}{2}} = \sup_{x \in E, \|x\|_{-A} \leqslant 1} \|x\|_1.$$

To continue, fix some $u \neq 0$ in $\mathbb{R}^n$ and recall

$$F_\alpha = \{x \in \mathbb{R}^n | (x|u) = \alpha\}, \quad \alpha \text{ in } \mathbb{R}$$

and $F = F_0$.

Furthermore let A be a real symmetric $n \times n$ matrix of negative type on F and not of negative type on $\mathbb{R}^n$ (note that this condition is equivalent to A is of negative type on F and there is some w in F_1 with $(Aw|w) > 0$). Following some ideas of [7–10] we define $M_{F_1}(A)(= M$ for short) as

$$M = \sup_{x \in F_1} (Ax|x) (> 0).$$

Theorem 3.1. *Let $u \neq 0$ in $\mathbb{R}^n$, $F = \{x \in \mathbb{R}^n | (x|u) = 0\}$ and $F_1 = \{x \in \mathbb{R}^n | (x|u) = 1\}$. Further let A be a real symmetric $n \times n$ matrix of negative type on F and not of negative type on $\mathbb{R}^n$. Let $M = \sup_{x \in F_1}$ $(Ax|x)$.*

We have

1. *A is of strict negative type on F if and only if A is nonsingular and* $(A^{-1}u|u) \neq 0$.
2. *If A is of strict negative type on F then we have*
   (a) *there is a unique (maximal) element z in* F_1 *such that* $M = (Az|z)$.
   (b) $Az = Mu$ *and* $M = (A^{-1}u|u)^{-1}$.

Proof. Assume first that A is of strict negative type on F and let $Ax = 0$ for some x in $\mathbb{R}^n$. Choose some w in F_1 with $(Aw|w) > 0$. If $(x|u) \neq 0$, we get $\left(A\left(w - \frac{x}{(x|u)}\right)|w - \frac{x}{(x|u)}\right) \leqslant 0$ and hence $(Aw|w) \leqslant 0$, a contradiction. Therefore we have x in F and so $x = 0$, which shows that A is nonsingular. Now let y in $\mathbb{R}^n$ be the unique element with $Ay = u$.

If y is in F we obtain $(Ay|y) = 0$ and hence $y = 0$, a contradiction. Therefore we have $(A^{-1}u|u) = (y|u) \neq 0$. Let $z = \frac{1}{(y|u)}y$, z in F_1. So $Az = \frac{1}{(y|u)}u$ and it follows that for all x in F_1, $x \neq z$ we get $(A(x-z)|x-z) < 0$ and hence $(Ax|x) < \frac{1}{(y|u)}$. Since $(Az|z) = \frac{1}{(y|u)}$ we get $M = \frac{1}{(y|u)} = \frac{1}{(A^{-1}u|u)}$ and $Az = Mu$.

It remains to show that A nonsingular and $(A^{-1}u|u) \neq 0$ implies that A is of strict negative type on F.

Let $(Ax|x) = 0$ for some x in F. Since $|(Ax|y)|^2 \leqslant (Ax|x)(Ay|y)$ for all y in F we get

$$Ax = \lambda u, \quad \text{for some } \lambda \text{ in } \mathbb{R}.$$

Hence $0 = (x|u) = \lambda(A^{-1}u|u)$ and therefore $\lambda = 0$, which implies $Ax = 0$ and so $x = 0$. □

The following application was done in [10] (Theorem 2.11) for finite metric spaces of 1-negative type (finite quasihypermetric spaces).

Corollary 3.2. *Let* (X, d) *with* $X = \{x_1, x_2, \ldots, x_n\}$ *be a finite metric space of p-negative type of at least two points and let* $\underline{1} = (1, 1, \ldots, 1)$. (X, d) *is of strict p-negative type if and only if*

$$A = \left(d(x_i, x_j)^p\right)_{i,j=1}^n$$

is nonsingular and $(A^{-1}\underline{1}|\underline{1}) \neq 0$.

Proof. Take $u = \underline{1}$, and note that $(Aw|w) = \frac{d(x_i, x_j)^p}{2} > 0$, for $w = \frac{e_i + e_j}{2}$ in F_1 and $x_i \neq x_j$ and so we are done by Theorem 3.1, part 1. □

Now let A be of strict negative type on

$$F = \{x \in \mathbb{R}^n | (x|u) = 0\}, \quad u \neq 0 \text{ in } \mathbb{R}^n.$$

By Theorem 3.1 we know that $M = \sup_{x \in F_1}(Ax|x)$ is finite and there is a unique (maximal) element z in F_1, such that $M = (Az|z)$ and $Az = Mu$.

Define

$$C = Muu^T - A.$$

Again by Theorem 3.1, C is positive semi-definite on $\mathbb{R}^n$ with $\ker C = [z]$. Therefore we can extend the inner product $(.|.)_{-A}$ defined on F to a semi-inner product on $\mathbb{R}^n$ given by

$$(x|y)_C = (Cx|y), \quad \text{for } x, y \text{ in } \mathbb{R}^n.$$

Furthermore we define

$$B = \frac{1}{M} zz^T - A^{-1}.$$

Since $(BAx|Ax) = (Cx|x)$, for all x in $\mathbb{R}^n$, it follows that B is positive semi-definite on $\mathbb{R}^n$ with $\ker B = [u]$.

Before formulating the next lemma, dealing with dual norms on F, we define for $x^T = (x_1, x_2, \ldots, x_n)$ in $\mathbb{R}^n$ and a given (fixed) $u \neq 0$ in $\mathbb{R}^n$

$$o(x) = \max\left(\max_{i,j \in \text{ supp } u} \frac{|u_i x_j - u_j x_i|}{|u_i| + |u_j|}, \max_{i \notin \text{ supp } u} |x_i| \right),$$

where

$$\text{supp } u = \{1 \leqslant i \leqslant n | u_i \neq 0\}.$$

Note that $o(x + \lambda u) = o(x)$, for all x in $\mathbb{R}^n$ and λ in $\mathbb{R}$ (this follows immediately from the definition of $o(.)$ and the definition of supp u). Moreover it is easy to see, that $o(.)$ defines a semi-norm on $\mathbb{R}^n$ and $o(x) = 0$ if and only if x is in $[u]$.

Lemma 3.3. *We have*

1. *The dual norm of* $\|.\|_1$ *on F is given by* $\|x\|_1^* = o(x)$*, for all x in F.*
2. *The dual norm of* $\|.\|_{-A}$ *on F is given by* $\|x\|_{-A}^* = \|x\|_B$*, for all x in F.*
3. $\{x \in F | \|x\|_1^* \leqslant 1\} =$ conv *E, where*

$$E = \left\{ x - \frac{(x|u)}{\|u\|_2^2} u, x \in \{-1, 1\}^n \right\}.$$

Proof. ad 1. It is clear, that the set A of extreme points of $\{x \in F | \|x\|_1 \leqslant 1\}$ is obtained by intersecting F with the edges conv $\{\pm e_i, \pm e_j\}(1 \leqslant i \neq j \leqslant n)$ of the cross-polytope conv $\{\pm e_i, 1 \leqslant i \leqslant n\} = \{x \in \mathbb{R}^n | \|x\|_1 \leqslant 1\}$.

Now fix some $1 \leqslant i \neq j \leqslant n$. An element x is in $F \cap$ conv $\{\pm e_i, \pm e_j\}$ if and only if there exists some $0 \leqslant \lambda \leqslant 1$, such that $(x|u) = 0$ and $x = \pm(1 - \lambda)e_i \pm \lambda e_j$, which is equivalent to the equation $0 = \pm(1 - \lambda)u_i \pm \lambda u_j$, under the constraint $0 \leqslant \lambda \leqslant 1$.

The case $i, j \in$ supp u leads to $x = \pm \frac{u_i e_j - u_j e_i}{|u_i| + |u_j|}$.

If $i \in$ supp u, $j \notin$ supp u (resp. $i \notin$ supp u, $j \in$ supp u) we obtain $x = \pm e_j$ (resp. $x = \pm e_i$).

Finally $i, j \notin$ supp u leads to $F \cap$ conv $\{\pm e_i, \pm e_j\} =$ conv $\{\pm e_i, \pm e_j\}$ and hence the contribution to the set A of extreme points of $\{x \in F | \|x\|_1 \leqslant 1\}$ is given by $\pm e_i$ and $\pm e_j$. Summing up we get

$$A = \left\{ \pm \frac{u_i e_j - u_j e_i}{|u_i| + |u_j|}, i, j \in \text{ supp } u (i \neq j) \right\} \cup \{ \pm e_i, i \notin \text{supp } u\}$$

By convexity of the function $y \mapsto |(x|y)|$ (for some fixed x) we get

$$\|x\|_1^* = \sup_{y \in F, \|y\|_1 \leqslant 1} |(x|y)| = \sup_{y \in A} |(x|y)| = o(x), \text{ for all } x \in F.$$

ad 2. Let x, y be in F.
$(x|y)^2 = (A^{-1}x|Ay)^2 = (A^{-1}x|y)_{-A}^2 = (A^{-1}x|y)_C^2$, since $y \in F$ implies $Cy = -Ay$.

By Cauchy–Schwarz inequality, applied to the semi-inner product $(.|.)_C$, we get

$$(x|y)^2 = (A^{-1}x|y)_C^2 \leqslant (CA^{-1}x|A^{-1}x)(Cy|y) = (Bx|x)(y|y)_{-A} = (Bx|x)\|y\|_{-A}^2.$$

Hence $|(x|y)| \leqslant (Bx|x)^{\frac{1}{2}} \|y\|_{-A}$.

By definition of the dual norm $\|.\|_{-A}^{*}$ it follows that $\|x\|_{-A}^{*} \leqslant (Bx|x)^{\frac{1}{2}}$.

Let $y_0 = \dfrac{(x|z)}{M} z - A^{-1}x$. Note that y_0 in F, since $\ker B = [u]$, and $\|y_0\|_{-A}^{2} = (Bx|x)$ and so

$$\|x\|_{-A}^{*} \geqslant \left(x \Big| \frac{y_0}{(Bx|x)^{\frac{1}{2}}}\right) = (Bx|x)^{\frac{1}{2}}.$$

ad 3. Let x be in $\{-1, 1\}^n$. Now $o\left(x - \dfrac{(x|u)}{\|u\|_2^2} u\right) = o(x) \leqslant 1$ and hence $E \subseteq \{x \in F \,|\, \|x\|_1^{*} \leqslant 1\}$. It is well known, that $\operatorname{conv} E = \{x \in F \,|\, \|x\|_1^{*} \leqslant 1\}$ if and only if

$$\sup_{x \in E} (y|x) = \sup_{x \in F,\, \|x\|_1^{*} \leqslant 1} (y|x), \text{ for all } y \in F.$$

(For example see problem 16, page 347 in [5] and note that the bidual F^{**} of F is isometrically isomorphic to F). Since of course

$$\|y\|_1 = \sup_{x \in F,\, \|x\|_1^{*} \leqslant 1} (y|x)$$

we have to show that

$$\|y\|_1 = \sup_{x \in E} (y|x), \text{ for all } y \in F.$$

For a given y in F choose $\alpha^T = (\alpha_1, \alpha_2, \ldots, \alpha_n)$ in $\{-1, 1\}^n$ such that $\|y\|_1 = (y|\alpha)$. So $\left(y \Big| \alpha - \dfrac{(\alpha|u)u}{\|u\|_2^2}\right) = (y|\alpha) = \|y\|_1$ and hence

$$\|y\|_1 \leqslant \sup_{x \in E} (y|x).$$

Of course we have

$$\|y\|_1 \geqslant \sup_{x \in E} (y|x)$$

and hence

$$\|y\|_1 = \sup_{x \in E} (y|x). \quad \square$$

Theorem 3.4. *Let $u \neq 0$ be in $\mathbb{R}^n$ and $F = \{x \in \mathbb{R}^n | (x|u) = 0\}$. Further let A be a real symmetric $n \times n$ matrix of strict negative type on F, and not of negative type on $\mathbb{R}^n$.*

The gap $\Gamma_A(F)(= \Gamma)$ of A on F is given by $\Gamma = \dfrac{2}{\beta}$, where

1. $\beta = \sup_{x \in F,\, o(Ax) \leqslant 1} (-Ax|x)$,
2. $\beta = \max_{x \in \{-1,1\}^n} (Bx|x)$,
   where
   $$B = (A^{-1}u|u)^{-1}(A^{-1}u)(A^{-1}u)^T - A^{-1}.$$
3. $\beta = \|B\|$, *where B is defined as in 2. and viewed as a linear operator from $(\mathbb{R}^n, \|.\|_\infty)$ to $(\mathbb{R}^n, \|.\|_1)$.*

Proof. We have

ad. 1 By formula $(*)$ at the beginning of Section 3 we have $\Gamma = \frac{2}{\beta}$ with

$$\beta^{\frac{1}{2}} = \sup_{x \in F, \|x\|_{-A} \leqslant 1} \|x\|_1.$$

By Lemma 3.3, part 1,2 we get

$$\beta^{\frac{1}{2}} = \sup_{x \in F, \|x\|_{-A} \leqslant 1} \|x\|_1 = \sup_{x \in F, \|x\|_1^* \leqslant 1} \|x\|_{-A}^* = \sup_{x \in F, o(x) \leqslant 1} \|x\|_B.$$

Recall that $\ker B = [u]$ and $o(x + \lambda u) = o(x)$, for all x in $\mathbb{R}^n$ and λ in $\mathbb{R}$ (as mentioned after the definition of $o(.)$). Hence

$$\beta = \sup_{x \in F, o(x) \leqslant 1} \|x\|_B^2 = \sup_{x \in \mathbb{R}^n, o(x) \leqslant 1} \|x\|_B^2 = \sup_{y \in \mathbb{R}^n, o(Ay) \leqslant 1} \|Ay\|_B^2,$$

since A is nonsingular by Theorem 3.1, part 1. Since $\|Ay\|_B^2 = (Cy|y)$ where $C = Muu^T - A$, $Az = Mu$ (see Theorem 3.1, part 2) we get

$$\beta = \sup_{y \in \mathbb{R}^n, o(Ay) \leqslant 1} (Cy|y).$$

Since z is not in F, we can write each y in $\mathbb{R}^n$ as $y = f + \lambda z$, for some f in F and λ in $\mathbb{R}$. Recall that $\ker C = [z]$ and $o(Ay) = o(Af + \lambda Mu) = o(Af)$ and so

$$\beta = \sup_{y \in \mathbb{R}^n, o(Ay) \leqslant 1} (Cy|y) = \sup_{x \in F, o(Ax) \leqslant 1} (-Ax|x).$$

ad. 2 From above we have

$$\beta = \sup_{x \in F, \|x\|_1^* \leqslant 1} \|x\|_B^2 = \max_{x \in E} (Bx|x)$$

by Lemma 3.3, part 3, where

$$E = \left\{ x - \frac{(x|u)}{\|u\|_2^2} u, x \in \{-1, 1\}^n \right\}.$$

Again using the fact, that $\ker B = [u]$ we get

$$\beta = \max_{x \in \{-1,1\}^n} (Bx|x).$$

ad. 3 Recall that B is positive semi-definite on $\mathbb{R}^n$ and hence for all x, y in $\{-1, 1\}^n$ we get $(Bx|y)^2 \leqslant (Bx|x)(By|y)$ and so

$$\beta = \max_{x,y \in \{-1,1\}^n} (Bx|y) = \max_{x \in \{-1,1\}^n} \|Bx\|_1 = \|B\|. \quad \square$$

Now let (X, d) be a finite metric space of strict p-negative type, $X = \{x_1, x_2, \ldots, x_n\}$, $n \geqslant 2$. Let $A = \left(d(x_i, x_j)^p\right)_{i,j=1}^n$ and $u = \underline{1}$. By Corollary 3.2 we know that A is nonsingular and $(A^{-1}\underline{1}|\underline{1}) \neq 0$. Recall that $(Aw|w) = \frac{d(x_i, x_j)^p}{2} > 0$, for $w = \frac{e_i + e_j}{2}$, $i \neq j$. Further observe that $u = \underline{1}$ implies $o(x) = \max_{i,j} \frac{|x_i - x_j|}{2}$, for all $x \in \mathbb{R}^n$ and x is in $\{-1, 1\}^n$ if and only $x + \underline{1}$ is in $\{0, 2\}^n$ with $o(x) = o(x + \underline{1})$. Applying Theorem 3.4 we get

Theorem 3.5. *Let (X, d) with $X = \{x_1, x_2, \ldots, x_n\}$ be a finite metric space of strict p-negative type of at least two points. Let*

$$A = \left(d(x_i, x_j)^p\right)_{i,j=1}^n .$$

The p-negative type gap Γ of X is given by $\Gamma = \dfrac{2}{\beta}$, where

1. $\beta = \sup\left\{(-Ay|y) | y_1 + y_2 + \cdots + y_n = 0 \text{ and } |(Ay|e_i - e_j)| \leqslant 2, \text{ for all } 1 \leqslant i, j \leqslant n\right\}$,
2. $\beta = \max\limits_{x \in \{-1,1\}^n} (Bx|x) = 4 \max\limits_{x \in \{0,1\}^n} (Bx|x)$, *where* $B = (A^{-1}\underline{1}|\underline{1})^{-1}(A^{-1}\underline{1})(A^{-1}\underline{1})^T - A^{-1}$,
3. $\beta = \|B\|$,
where B is defined as in 2. and viewed as a linear operator from $(\mathbb{R}^n, \|.\|_\infty)$ *to* $(\mathbb{R}^n, \|.\|_1)$.

The following easy example illustrates how Theorem 3.5 can be used to calculate the p-negative type gap Γ for a given finite metric space of strict p-negative type:

Example 3.6. Consider $\mathbb{R}^2$ equipped with the 1-norm induced metric and let X be the 4-point subspace given by

$$X = \left\{(0, 0), \left(\frac{1}{2}, 0\right), \left(-\frac{1}{2}, 0\right), \left(0, \frac{1}{2}\right)\right\}.$$

The distance matrix D of X is

$$D = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & 1 & 1 \\ \frac{1}{2} & 1 & 0 & 1 \\ \frac{1}{2} & 1 & 1 & 0 \end{pmatrix}.$$

For $p > 0$ the matrix A considered in Theorem 3.5 is given by

$$A = \begin{pmatrix} 0 & 2^{-p} & 2^{-p} & 2^{-p} \\ 2^{-p} & 0 & 1 & 1 \\ 2^{-p} & 1 & 0 & 1 \\ 2^{-p} & 1 & 1 & 0 \end{pmatrix}.$$

Now let $x = (x_1, x_2, x_3, x_4)$ in $\mathbb{R}^4$ with $x_1 + x_2 + x_3 + x_4 = 0$.
We have

$$(Ax|x) = -\left((2^{1-p} - 1)x_1^2 + x_2^2 + x_3^2 + x_4^2\right).$$

If $2^{-p} \geqslant \frac{1}{3}$ we get

$$\left(2^{1-p} - 1\right)x_1^2 + x_2^2 + x_3^2 + x_4^2 \geqslant -\frac{1}{3}(x_2 + x_3 + x_4)^2 + x_2^2 + x_3^2 + x_4^2 =$$
$$= \frac{1}{3}\left((x_2 - x_3)^2 + (x_2 - x_4)^2 + (x_3 - x_4)^2\right) \geqslant 0$$

and therefore

$$(Ax|x) \leqslant 0.$$

On the other hand if $2^{-p} < \frac{1}{3}$ we obtain for $x = (3, -1, -1, -1)$
$(Ax|x) = -6(3.2^{-p} - 1) > 0.$

Summing up the space X is of p-negative type if and only if $p \leqslant \frac{\ln 3}{\ln 2}$ and of strict p-negative type if and only if $p < \frac{\ln 3}{\ln 2}$.

For short let $\alpha = 2^{-p}$. We get

$$A = \begin{pmatrix} 0 & \alpha & \alpha & \alpha \\ \alpha & 0 & 1 & 1 \\ \alpha & 1 & 0 & 1 \\ \alpha & 1 & 1 & 0 \end{pmatrix},$$

$$A^{-1} = \frac{1}{3\alpha^2} \begin{pmatrix} -2 & \alpha & \alpha & \alpha \\ \alpha & -2\alpha^2 & \alpha^2 & \alpha^2 \\ \alpha & \alpha^2 & -2\alpha^2 & \alpha^2 \\ \alpha & \alpha^2 & \alpha^2 & -2\alpha^2 \end{pmatrix},$$

$$(A^{-1}\underline{1})^T = \frac{1}{3\alpha^2}(3\alpha - 2, \alpha, \alpha, \alpha),$$

$$(A^{-1}\underline{1}|\underline{1}) = \frac{2}{3}\alpha(3\alpha - 1),$$

$$(A^{-1}\underline{1})(A^{-1}\underline{1})^T = \frac{1}{9\alpha^4} \begin{pmatrix} (3\alpha-2)^2 & \alpha(3\alpha-2) & \alpha(3\alpha-2) & \alpha(3\alpha-2) \\ \alpha(3\alpha-2) & \alpha^2 & \alpha^2 & \alpha^2 \\ \alpha(3\alpha-2) & \alpha^2 & \alpha^2 & \alpha^2 \\ \alpha(3\alpha-2) & \alpha^2 & \alpha^2 & \alpha^2 \end{pmatrix}$$

and hence

$$B = \frac{1}{2(3\alpha - 1)} \begin{pmatrix} 3 & -1 & -1 & -1 \\ -1 & 4\alpha - 1 & 1 - 2\alpha & 1 - 2\alpha \\ -1 & 1 - 2\alpha & 4\alpha - 1 & 1 - 2\alpha \\ -1 & 1 - 2\alpha & 1 - 2\alpha & 4\alpha - 1 \end{pmatrix}$$

(Note that X is a simple example showing that A is nonsingular does not imply the strict p-negative type property: see Corollary 3.2 together with $(A^{-1}\underline{1}|\underline{1}) = 0$ for $p = \frac{\ln 3}{\ln 2}$.)

Routine calculations lead to

$$\beta = \max_{x \in \{-1,1\}^4} (Bx|x) = \begin{cases} \frac{6}{3\alpha - 1}, & \frac{1}{3} < \alpha \leqslant \frac{3}{4}, \\ \frac{8\alpha}{3\alpha - 1}, & \frac{3}{4} \leqslant \alpha. \end{cases}$$

Therefore the p-negative type gap $\Gamma = \frac{2}{\beta}$ of X is given by

$$\Gamma = \begin{cases} \frac{3}{4} - \frac{1}{4}2^{-p}, & p \leqslant 2 - \frac{\ln 3}{\ln 2}, \\ 2^{-p} - \frac{1}{3}, & 2 - \frac{\ln 3}{\ln 2} \leqslant p < \frac{\ln 3}{\ln 2} \end{cases}$$

4. Applications

Corollary 4.1. *Let n be a natural number greater or equal to 3 and let C_n be the cycle graph with n vertices, viewed as a finite metric space, equipped with the usual path metric. Then we have*

1. *C_n is of 1-negative type and of strict 1-negative type if and only if n is odd.*
2. *The 1-negative type gap Γ of C_n is given by*

$$\Gamma = \begin{cases} 0, & n \text{ even} \\ \frac{1}{2}\frac{n}{n^2-2n-1}, & n \text{ odd.} \end{cases}$$

Proof. Take the vertices $\{x_1, x_2, \ldots, x_n\}$ of a regular n-gon on a circle C of radius $r = \dfrac{n}{2\pi}$. It is evident, that C_n can be viewed as the subspace $\{x_1, x_2, \ldots, x_n\}$ of the metric space (C, d), where d is the arc-length metric on C. It is shown in [4] (see Theorem 4.3 and Theorem 9.1) that (C, d) is of 1-negative type and a finite subspace of (C, d) is of strict 1-negative type if and only if this subspace contains at most one pair of antipodal points. Hence part 1 follows at once. The definition of Γ implies that $\Gamma = 0$ if n is even, so let us assume that $n = 2k + 1$, for some k in $\mathbb{N}$.

Let A be the distance matrix of $C_n = C_{2k+1}$. It is shown in [1] (Theorem 3.1) that A^{-1} is given by

$$A^{-1} = -2I - C^k - C^{k+1} + \frac{2k+1}{k(k+1)}\underline{1}\,\underline{1}^T,$$

where I is the identity matrix and C is the matrix (with respect to the canonical bases) of the linear map on $\mathbb{R}^n$, which sends each $x^T = (x_1, x_2, \ldots, x_n)$ to $(x_2, x_3, \ldots, x_n, x_1)$. Now $A^{-1}\underline{1} = \dfrac{1}{k(k+1)}\underline{1}$ and so B (as defined in Theorem 3.5) is given by $B = 2I + C^k + C^{k+1} - \dfrac{4}{2k+1}\underline{1}\,\underline{1}^T$ and so

$$(Bx|x) = 2\|x\|_2^2 - \frac{4}{2k+1}(x|\underline{1})^2 + 2(x_1x_{k+1} + \cdots + x_{k+1}x_{2k+1} + x_{k+2}x_1 + \cdots + x_{2k+1}x_k),$$

for each $x^T = (x_1, x_2, \ldots, x_{2k+1})$ in $\mathbb{R}^{2k+1}$.

Now let x be in $\{0, 1\}^{2k+1}$ and let $s = |\{1 \leqslant i \leqslant 2k+1 | x_i = 1\}|$. In the case $s = 0$ and $s = 2k+1$ we get $(Bx|x) = 0$, so assume that $1 \leqslant s \leqslant 2k$. Since

$$x_1x_{k+1} + \cdots + x_{k+1}x_{2k+1} + x_{k+2}x_1 + \cdots + x_{2k+1}x_k < \|x\|_2^2 = s,$$

we get

$$(Bx|x) \leqslant 2s - \frac{4}{2k+1}s^2 + 2(s-1) = 2\left(2s - 1 - \frac{2}{2k+1}s^2\right).$$

It follows immediately, that

$$\max_{1\leqslant s\leqslant 2k}\left(2s - 1 - \frac{2}{2k+1}s^2\right) = \frac{2k^2-1}{2k+1}$$

and hence

$$\max_{x\in\{0,1\}^{2k+1}}(Bx|x) \leqslant \frac{4k^2-2}{2k+1}.$$

On the other hand define $\bar{x}$ in $\{0, 1\}^{2k+1}$ as $\bar{x}^T = (\alpha_1, \alpha_2, \ldots, \alpha_{2k+1})$, with $\alpha_i = 1$ if and only if $i \in \{1, 2, \ldots, m, 2m+1, 2m+2, \ldots 3m+1\}$ if $k = 2m$ and $\alpha_i = 1$ if and only if $i \in \{1, 2, \ldots, m,$

$2m+2, 2m+3, \ldots, 3m+2\}$ if $k = 2m+1$, m in $\mathbb{N}$. In each case ($k = 2m, 2m+1$) we get $(B\overline{x}|\overline{x}) = \frac{4k^2-2}{2k+1}$. Summing up we have $\max_{x\in\{0,1\}^{2k+1}}(Bx|x) = \frac{4k^2-2}{2k+1}$ and hence Theorem 3.5, part 2 implies $\Gamma = \frac{2k+1}{8k^2-4} = \frac{1}{2}\frac{n}{n^2-2n-1}$. □

Corollary 4.2 (= Theorem 3.2 of [11]). *Let (X, d) be a finite discrete space consisting of n points, $n \geqslant 2$. The 1-negative type gap Γ of X is given by*

$$\Gamma = \frac{1}{2}\left(\frac{1}{\lfloor\frac{n}{2}\rfloor} + \frac{1}{\lceil\frac{n}{2}\rceil}\right).$$

Proof. Let A be the distance matrix of X. We have $A = \underline{1}\,\underline{1}^T - I$ (I the identity matrix) and hence $A^{-1} = \frac{1}{n-1}\underline{1}\,\underline{1}^T - I$. So the matrix B defined as in Theorem 3.5 is given by $B = I - \frac{1}{n}\underline{1}\,\underline{1}^T$. Applying Theorem 3.5, part 2 we get

$$\beta = \max_{x\in\{-1,1\}^n}(Bx|x) = n - \frac{1}{n}\min_{x\in\{-1,1\}^n}(x|\underline{1})^2 = \begin{cases} n, & n \text{ even},\\ n-\frac{1}{n}, & n \text{ odd}\end{cases}$$

and so $\Gamma = \frac{2}{\beta} = \frac{1}{2}\left(\frac{1}{\lfloor\frac{n}{2}\rfloor} + \frac{1}{\lceil\frac{n}{2}\rceil}\right)$. □

Recall that for a given finite connected simple graph $G = (V, E)$ and a given collection $\{w(e), e \in E\}$ of positive weights associated to the edges of G, the graph G becomes a finite metric space, where the metric is given by the natural weighted path metric on G. A finite metric tree $T = (V, E)$ is a finite connected simple graph that has no cycles, endowed with the above given edge weighted path metric. It is shown in [4] (Corollary 7.2) that metric trees are of strict 1-negative type.

Corollary 4.3 (=Corollary 4.14 of [2]). *Let $T = (V, E)$ be a finite metric tree. The 1-negative type gap Γ of G is given by $\Gamma = \left(\sum_{e\in E}\frac{1}{w(e)}\right)^{-1}$, where $w(e)$ denotes the weight of the edge e.*

Proof. It is shown in [1] (Theorem 2.1) that the inverse matrix A^{-1} of the distance matrix A of a finite metric tree is given by

$$A^{-1} = -\frac{1}{2}L + \left(2\sum_{e\in E}w(e)\right)^{-1}\delta\delta^T,$$

where L denotes the Laplacian matrix for the weighting of T that arises by replacing each edge weight by its reciprocal and δ in $\mathbb{R}^n$ is given by $\delta^T = (\delta_1, \delta_2, \ldots, \delta_n)$ with $\delta_i = 2 - d(i)$, $d(i)$ denotes the degree of the vertex i. It follows easily that the matrix B defined as in Theorem 3.5 is given by $B = \frac{1}{2}L$. Routine calculations show, that

$$(Bx|x) \leqslant 2\sum_{e\in E}\frac{1}{w(e)}, \quad \text{for all } x \text{ in } \{-1, 1\}^n.$$

Moreover we get $(B\bar{x}|\bar{x}) = 2\sum_{e\in E}\frac{1}{w(e)}$, for $\bar{x}^T = (x_1, x_2, \ldots, x_n)$ in $\{-1, 1\}^n$, a 2-colouring of the vertices $1, 2, \ldots, n$. By Theorem 3.5, part 2 we get $\Gamma = \left(\sum_{e\in E}\frac{1}{w(e)}\right)^{-1}$. □

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