Enhanced negative type for finite metric trees

Ian Doust (UNSW) and Anthony Weston (Canisius)
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- Embed \((X, d)\) isometrically in a Hilbert space?
- Embed \((X, d)\) isometrically in \(L^p[0, 1]\)?
- Embed \((X, d)\) uniformly in one of the above spaces?

These types of questions arise in classification problems in functional analysis, and in more practical problems in theoretical computer science.
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Introduction
Metric Trees
The gap

Embeddings
Definitions

Typical problem

**Question (Smirnov < 1959)**

Is every separable metric space uniformly homeomorphic to a subset of a Hilbert space?

In answering this (negatively) Enflo (1969) introduced the concept of \textit{(generalized) roundness} for a metric space, which was a precursor of the Banach space notion of (Rademacher) type.

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Enhanced Negative Type
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In answering this (negatively) Enflo (1969) introduced the concept of *(generalized) roundness* for a metric space, which was a precursor of the Banach space notion of (Rademacher) type.
Theorem (Bretagnolle, Dacunha-Castelle, Krevine 1966)

A real normed space is linearly isometric to a subspace of some $L^p$ space ($0 < p \leq 2$) if and only if it has $p$-negative type.

So, what are these geometric conditions:
- generalized roundness
- $p$-negative type?
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Definition

Let \( p \geq 0 \) and let \((X, d)\) be a metric space. Then \((X, d)\) has **\( p \)-negative type** if for all natural numbers \( n \geq 2 \), all finite subsets \( \{x_1, \ldots, x_n\} \subseteq X \), and all choices of real numbers \( \eta_1, \ldots, \eta_n \) with \( \eta_1 + \cdots + \eta_n = 0 \), we have:

\[
\sum_{1 \leq i, j \leq n} d(x_i, x_j)^p \eta_i \eta_j \leq 0.
\]

i.e. the matrix \( (d(x_i, x_j)^p) \) is always ‘negative semidefinite on a hyperplane’.
Let $p \geq 0$ and let $(X, d)$ be a metric space. Then $(X, d)$ has $p$-negative type if for all natural numbers $n \geq 2$, all finite subsets $\{x_1, \ldots, x_n\} \subseteq X$, and all choices of real numbers $\eta_1, \ldots, \eta_n$ with $\eta_1 + \cdots + \eta_n = 0$, we have:

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Let $p \geq 0$ and let $(X, d)$ be a metric space. Then $(X, d)$ has **strict $p$-negative type** if for all natural numbers $n \geq 2$, all finite subsets $\{x_1, \ldots, x_n\} \subseteq X$, and all choices of real numbers $\eta_1, \ldots, \eta_n$ with $\eta_1 + \cdots + \eta_n = 0$ and $(\eta_1, \ldots, \eta_n) \neq \vec{0}$, we have:

$$\sum_{1 \leq i, j \leq n} d(x_i, x_j)^p \eta_i \eta_j < 0.$$ 

eg. If $X = \{x, y\}$ then $\eta_2 = -\eta_1$ and so

$$\sum_{1 \leq i, j \leq n} d(x_i, x_j)^p \eta_i \eta_j = -2d(x, y)^p \eta_1^2.$$ 

Thus $(X, d)$ has strict $p$-negative type for all $p \geq 0$. 

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**Definition**

Let $p \geq 0$ and let $(X, d)$ be a metric space. Then $(X, d)$ has **generalized roundness**-$p$ if for all natural numbers $n \in \mathbb{N}$, and all choices of points $a_1, \ldots, a_n, b_1, \ldots, b_n \in X$, we have:

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\sum_{1 \leq k < l \leq n} \{d(a_k, a_l)^p + d(b_k, b_l)^p\} \leq \sum_{1 \leq j, i \leq n} d(a_j, b_i)^p.
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n.b. Repetitions among the $a$’s and the $b$’s is allowed. However, one can assume that $a_j \neq b_i$ for all $j, i$. 
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These conditions are not easy to compute with! A big help is . . .

**Theorem (Lennard, Tonge, Weston 1997)**

Let \((X, d)\) be a metric space, and suppose that \(p \geq 0\). Then the following are equivalent:

1. \((X, d)\) has \(p\)-negative type.
2. \((X, d)\) has generalized roundness \(p\).
Some basic facts

**Theorem**

Let \((X, d)\) be a metric space.

(i) \(\{p : (X, d) \text{ has generalized roundness-} p\}\) is a closed subinterval of the form \([0, p_X]\). Thus it makes sense to talk about the maximal generalized roundness, \(\text{mgr}(X, d)\) of \((X, d)\).

(ii) \(\text{mgr}(X, d)\) can take on any values in \([0, \infty]\).

(iii) If \(|X| = N\), then \(\text{mgr}(X, d) \geq c_N > 0\).

(iv) If \(Y \subseteq X\), then \(\text{mgr}(X, d) \leq \text{mgr}(Y, d)\).

**Theorem (Enflo; Lennard, Tonge, Weston)**

(i) \(\text{mgr}(L^p[0, 1]) = p\) for \(1 \leq p \leq 2\).

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*If a Banach space $X$ has cotype infimum greater than 2, then $\text{mgr}(X) = 0$ and consequently $X$ does not isometrically embed in any $L^p(\mu)$ space with $p \leq 2$."

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Computation tutorial

GR: \[ \sum_{1 \leq k < l \leq n} \{d(a_k, a_l)^p + d(b_k, b_l)^p\} \leq \sum_{1 \leq j, i \leq n} d(a_j, b_i)^p. \]

Exercise 1: Let \((X, d)\) be

Necessarily, every \(a_k\) is at one node and every \(b_l\) at the other. Thus the LHS of GR is always 0, so \(\text{mgr}(X, d) = \infty\).
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**Exercise 2:** Let \((X, d)\) be

![Diagram](image)

Essentially two cases:

(i) \(a[k] - a[n - k] - b[n] \quad (0 \leq k \leq n)\)

(ii) \(a[k] - b[n] - a[n - k] \quad \text{(the extreme case!)}\).

For GR to hold in (ii) we need \(k(n - k)2^p \leq n^2\) for all \(n, k\).

A simple calculation shows that this requires \(p \leq 2\), ie \(\text{mgr}(X, d) = 2\).

*(Hence if \(E\) is a Banach space \(\text{mgr}(E) \leq 2\).*
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![Diagram of three points connected by lines with labels 1 and 1 between them]

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Exercise 3: Let \((X, d)\) be a space with \(0 < \alpha \leq 2\).

First: Find the extreme configuration:

This requires 3 steps:

**Enumeration:** how can you colour the vertices?

**Reduction:** which is the ‘optimal’ colouring?

**Calculus:** what is the best weighting?
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Exercise 3: Let \((X, d)\) be \(1 \sim 1 \sim \alpha \sim 1\) with \(0 < \alpha \leq 2\).

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Extreme configuration:

Here GR becomes $\alpha^p + 0 \leq 4$. This implies that

$$mgr(X, d) = \begin{cases} \frac{2}{\log_2 \alpha}, & 1 < \alpha \leq 2 \\ \infty, & 0 < \alpha \leq 1. \end{cases}$$

This gives examples with $mgr(X, d) \in [2, \infty]$. 
A **metric tree** is a tree with weighted edges and metric given by the edge-weighted path distance.
Some context

Low-distortion embeddings, especially of metric trees, are important in designing efficient algorithms in Computer Science. The **distortion** of an embedding \( \rho : (X, d) \rightarrow (E, \| \cdot \|) \) is the smallest \( c \) for which

\[
\frac{1}{c} \ d(x, y) \leq \| \rho(x) - \rho(y) \| \leq d(x, y).
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**Theorem (Bourgain 1985)**

Any \( n \)-point metric space \( (X, d) \) can be embedded into a Hilbert space of dimension at most \( \log n \) with distortion \( O(\log n) \).

**Theorem (Matoušek 1999)**

Any \( n \)-point metric tree embeds into \( \ell^p \) with distortion at most a constant times \( (\log \log n)^{\min(1/p, 1/2)} \).
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Some context

Low-distortion embeddings, especially of metric trees, are important in designing efficient algorithms in Computer Science. The distortion of an embedding \( \rho : (X, d) \rightarrow (E, \| \cdot \|) \) is the smallest \( c \) for which

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Theorem (Hjorth, Lisonek, Markvorsen and Thomassen 1998)

Every finite metric tree has strict 1-negative type.

Example: Note that the non-tree graph

![Graph](image)

with all edges of length 1 has

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Our work makes the extent of this strictness quantitative, and allows us to improve on the value of $p$ in the above theorem.

How negative is $\sum_{1 \leq i, j \leq n} d(x_i, x_j) \eta_i \eta_j$?
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How negative is $\sum_{1 \leq i, j \leq n} d(x_i, x_j) \eta_i \eta_j$?
From now on, $p = 1$.

Our aim is to quantify the difference between the LHS and the RHS of the generalized roundness inequality, i.e., between

$$\sum_{1 \leq k < l \leq n} \{d(a_k, a_l) + d(b_k, b_l)\}$$

and

$$\sum_{1 \leq j, i \leq n} d(a_j, b_i).$$

Recall that the points $a_j$ and $b_i$ may contain repetitions, so you need to normalize this to get something sensible. You can achieve this by replacing repetitions of the vertices with normalized weighting of the vertices.
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Definition

A normalized \((q, t)\)-simplex is a list of distinct vertices
\(D = [a_1, \ldots, a_q; b_1, \ldots, b_t] \subseteq X\), with associated positive vertex weights \(\omega = (m_1, \ldots, m_q; n_1, \ldots, n_t)\) which satisfy the normalizations

\[ m_1 + \cdots + m_q = n_1 + \cdots + n_t = 1. \]

Denote the normalized \((q, t)\)-simplex by \(D^\omega\).

Think of \(m_i\) as being the proportion of the time that vertex \(a_i\) is repeated.
A normalized $(2, 3)$-simplex

Consider the tree (with all edge weights 1)
A normalized \((2, 3)\)-simplex requires that we colour 2 vertices red and 3 vertices blue, and apply weights to each vertex.
The gap

The gap associated with $D^ω$ is the quantity

$$\gamma(D^ω) = \sum_{j,i=1}^{q,t} m_j n_i d(a_j, b_i)$$

$$- \sum_{1 \leq j_1 < j_2 \leq q} m_{j_1} m_{j_2} d(a_{j_1}, a_{j_2}) - \sum_{1 \leq i_1 < i_2 \leq t} n_{i_1} n_{i_2} d(b_{i_1}, b_{i_2}).$$

The 1-GR gap of $(X, d)$ is the quantity

$$\Gamma_X = \inf_{D^ω} \gamma(D^ω).$$

Notes: 1. If $(X, d)$ has 1-negative type then $\Gamma_X \geq 0$.
2. If $\Gamma_X > 0$ then $(X, d)$ has strict 1-negative type.
3. There exists $(X, d)$ with strict 1-negative type and $\Gamma_X = 0$.
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$$- \sum_{1 \leq j_1 < j_2 \leq q} m_{j_1} m_{j_2} d(a_{j_1}, a_{j_2}) - \sum_{1 \leq i_1 < i_2 \leq t} n_{i_1} n_{i_2} d(b_{i_1}, b_{i_2}).$$

The $1$-GR gap of $(X, d)$ is the quantity

$$\Gamma_X = \inf_{D^\omega} \gamma(D^\omega).$$

Notes: 1. If $(X, d)$ has 1-negative type then $\Gamma_X \geq 0$.
2. If $\Gamma_X > 0$ then $(X, d)$ has strict 1-negative type.
3. There exists $(X, d)$ with strict 1-negative type and $\Gamma_X = 0$. 
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Ian Doust (UNSW) and Anthony Weston (Canisius)
Our example

For the normalized \((2, 3)\)-simplex we just looked at

\[
\gamma(D^\omega) = \sum_{j=1}^{2} \sum_{i=1}^{3} m_j n_i d(a_j, b_i) - m_1 m_2 d(a_1, a_2) - \sum_{1 \leq i_1 < i_2 \leq 3} n_{i_1} n_{i_2} d(b_{i_1}, b_{i_2}).
\]

so

\[
\gamma(D^\omega) = \frac{2}{9} + \frac{2}{9} + \frac{4}{9} + \frac{2}{9} + \frac{2}{9} + \frac{1}{9} - \frac{2}{9} - \frac{2}{9} - \frac{3}{9} - \frac{3}{9} = \frac{1}{3}
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Main Theorem

Let \((T, d)\) be a metric tree with edge set \(E\).
Let \(|e|\) denote the length of edge \(e \in E\).

**Theorem (Doust, Weston 2008)**

Let \((T, d)\) be a finite metric tree. Then

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\Gamma_T = \left\{ \sum_{e \in E} |e|^{-1} \right\}^{-1}.
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Thus the gap depends only on the unordered distribution of the tree's edge weights and not at all on the internal geometry of the tree.

Thus, if \(T\) is an unweighted (i.e. \(|e| = 1\) for all \(e\)) tree on \(n\) vertices, \(\Gamma_T = \frac{1}{n-1}\).
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The proof of our theorem is quite long! The main steps are:

1. Find (through extensive examination of examples) the extreme normalized \((q, t)\)-simplex, \(D^\omega_0\), for \((T, d)\).
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Sketch proof

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1. Find (through extensive examination of examples) the extreme normalized \((q, t)\)-simplex, \(D^\omega_0\), for \((T, d)\).
2. Show that the simplex gap for \(D^\omega_0\) is \(\left\{ \sum_{e \in E} |e|^{-1} \right\}^{-1}\).
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Ian Doust (UNSW) and Anthony Weston (Canisius)

Enhanced Negative Type
Sketch proof

The main steps are:

1. Find (through extensive examination of examples) the extreme normalized \((q, t)\)-simplex, \(D_{\omega_0}\), for \((T, d)\).

2. Show that the simplex gap for \(D_{\omega_0}\) is \(\left\{ \sum_{e \in E} |e|^{-1} \right\}^{-1}\).

3. Show that \(D_{\omega_0}\) is extreme among a certain class of normalized \((q, t)\)-simplexes.

4. Prove that the extreme gap must occur in the class in step 3.
Suppose that $T$ has been coloured into $q$ red and $t$ blue vertices.

The idea is to consider the extended gap function

$$
\gamma_D^{\times} : \mathbb{R}_+^{q+t} \rightarrow \mathbb{R},
$$

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\gamma_D^{\times}(m_1, \ldots, m_q, n_1, \ldots, n_t) = \sum_{j,i=1}^{q,t} m_j n_i d(a_j, b_i)
$$

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- \sum_{1 \leq j_1 < j_2 \leq q} m_{j_1} m_{j_2} d(a_{j_1}, a_{j_2}) - \sum_{1 \leq i_1 < i_2 \leq t} n_{i_1} n_{i_2} d(b_{i_1}, b_{i_2})
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and then to try to minimize $\gamma_D^{\times}(m_1, \ldots, m_q, n_1, \ldots, n_t)$ subject to $m_1 + \cdots + m_q = n_1 + \cdots + n_t = 1$ using Lagrange multipliers.

Unfortunately, this seems impossible for a general colouring!
Optimization

Suppose that $T$ has been coloured into $q$ red and $t$ blue vertices.
The idea is to consider the extended gap function
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\gamma_D^\times : \mathbb{R}^{q+t}_+ \to \mathbb{R},
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Transform the tree $(T, d)$ and normalized $(2, 2)$-simplex $D^\omega$

$$\gamma(D^\omega) = \frac{1}{4}(\alpha + (\alpha + \beta) + (\beta + \delta) + \delta - (\alpha + \beta + \delta) - \beta)$$

$$\gamma(D_1^\omega) = \frac{1}{4}(2\alpha + 2\delta - (\alpha + \delta)) = \gamma(D^\omega)$$
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$$\alpha \quad \beta \quad \delta$$

$a_1[\frac{1}{2}]$  $b_1[\frac{1}{2}]$  $b_2[\frac{1}{2}]$  $a_2[\frac{1}{2}]$

to the ‘pruned tree’ $(T_1, d_1)$ and normalized $(2, 1)$-simplex $D_1^{\omega_1}$

$$\alpha \quad \delta$$

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Ian Doust (UNSW) and Anthony Weston (Canisius)  Enhanced Negative Type
Transform the tree \((T, d)\) and normalized \((2, 2)\)-simplex \(D^\omega\)

![Diagram of a tree with vertices labeled \(a_1, b_1, b_2, a_2\) and edges labeled \(\alpha, \beta, \delta\).]

...to the ‘pruned tree’ \((T_1, d_1)\) and normalized \((2, 1)\)-simplex \(D_1^\omega\)

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\]

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Pruning

It follows that if
\[ \gamma(D_1^{\omega^1}) \geq \left\{ \sum_{e \in E_1} |e|^{-1} \right\}^{-1}, \]
then \[ \gamma(D^{\omega}) \geq \left\{ \sum_{e \in E} |e|^{-1} \right\}^{-1}. \]

Similar analysis allows one to show that we need only look at a subclass of normalized simplexes.

Definition

Let \( T \) be a finite tree. Let \( D \) be a \((q, t)\)-simplex in \( T \). Then \( T \) is generically coloured if:

(a) Every vertex of \( T \) belongs to \( D \), and

(b) adjacent vertices have opposite simplex colour.

Obviously: There is essentially only one generic colouring of \( T \)!
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Enhanced Negative Type
Generically coloured simplexes admit identities not shared by general simplexes.

Note that trees can always be left-right oriented by fixing some leaf to be the leftmost point.

Given a \((q, t)\)-simplex \(D^\omega = [a_1, \ldots, a_q; b_1, \ldots, b_t]\) with weight vector \(\omega = (m_1, \ldots, m_q; n_1, \ldots, n_t)\), and an edge \(e\) in the tree define

\[
\alpha_L(\omega, e) = \sum m_j \quad \text{over all } j \text{ with vertices } a_j \text{ to the left of } e
\]

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\(\alpha_R(\omega, e)\) and \(\beta_R(\omega, e)\) are defined analogously.
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Lemma

Suppose that the finite metric tree \((T, d)\) is generically coloured with a \textbf{normalized} weight vector \(\omega = (m_1, \ldots, m_q; n_1, \ldots, n_t)\). Then

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\gamma(D^\omega) = \sum_{e \in E} \left\{ (\alpha_L(\omega, e) - \beta_L(\omega, e))^2 + (\alpha_R(\omega, e) - \beta_R(\omega, e))^2 \right\} \cdot \frac{|e|}{2}.
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Redefine \(\gamma^\times_D\) be the extension of this function to non-normalized weights \(\omega \in \mathbb{R}^{q+t}_{+}\). This new function turns out to allow the desired Lagrange multiplier computation to be completed.
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Theorem

Suppose that the finite metric tree \((T, d)\) is generically coloured. The minimum value of \(\gamma\times_D(\omega)\) (and hence \(\gamma(D^\omega)\)) subject to

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m_1 + \cdots + m_q = n_1 + \cdots + n_t = 1
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is

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\left\{ \sum_{e \in E} |e|^{-1} \right\}^{-1}.
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This completes the proof.
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This completes the proof.
The ‘Gap Theorem’ allows a quantitative improvement of the theorem of Hjorth et al.

Corollary

Let \((T, d)\) be a finite metric tree. Then for all natural numbers \(n \geq 2\), all finite subsets \(\{x_1, \ldots, x_n\} \subseteq X\), and all \(\eta \in \mathbb{R}^n\) with \(\eta_1 + \cdots + \eta_n = 0\) and \(\|\eta\|_1 = 1\), we have:

\[
\sum_{1 \leq i, j \leq n} d(x_i, x_j) \eta_i \eta_j \leq -\frac{\Gamma_T}{2}.
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... and this is sharp!

This obviously also holds for countable metric trees!
Consequences I

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This obviously also holds for *countable* metric trees!
A nice consequence of this is that one can show that finite metric trees have generalized roundness $p$ (or $p$-negative type) for some $p > 1$.

**Corollary**

Let $(T, d)$ be a finite unweighted tree with at $n \geq 3$ vertices. Then

$$
mgr(T, d) \geq 1 + \frac{\ln(1 + \frac{1}{(n-1)^3(n-2)})}{\ln(n - 1)}.
$$
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