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A Fiedler center for graphs generalizing the characteristic set

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ABSTRACT

This work introduces a general concept of center for graphs, built on the model of the characteristic set ([12,14]) of trees. We define it as the set of cycles in a specific directed graph associated with the original graph G, and we let it depend on a function μ. In the case of trees we consider particular instances of μ given as weights of rooted subtrees, thus retrieving the characteristic set and, interestingly, the eccentricity-center. We investigate when the center of a graph G is *simple* – i.e., consisting of a unique cycle – and *quasi-simple* – i.e., inducing a connected subgraph of G. In particular, we prove that the center of a caterpillar tree associated with the so-called combinatorial Perron parameter ρ_c (studied in [2] and [3]) is always simple. We also make use of a discrete version of concavity to generate examples of simple and quasi-simple centers for graphs.

1. Introduction

One of the challenges in the fast-growing discipline of network science is to establish a rule to meaningfully associate a center – or a centrality distribution – with a given graph ([5,7,15]). Complex networks arising in this discipline, modeling phenomena from

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various fields such as social science ([18]), biology ([1,8]) or telecommunication ([16,17]), are typically large in size. Identifying a small set of vertices which are best suited to control the rest of the graph is then a step to gain insight into the structure of the graph itself.

A common way to define the center of a graph makes use of the *eccentricity* of its vertices (see for example [9, p. 35]). Let G be a connected graph having vertex set $V(G)$ and edge set $E(G)$. Given $v \in V(G)$, we let $ecc_G(v) := \max\{d_{u,v} \mid u \in V(G)\}$, where $d_{u,v}$ is the number of vertices in a shortest path connecting u to v in G.[1] The *eccentricity-center* of G – denoted by $\mathcal{EC}(G)$ – is the set of vertices in G attaining the minimum eccentricity.

In the case of trees there exists another classical notion of center, coming from the Fiedler theory ([4,12,14]). Consider an undirected tree U with n vertices labeled $1, \ldots, n$, and let $L \in \mathbb{R}^{n,n}$ be its Laplacian matrix ($L = D - A$, where D is the degree matrix and A is the adjacency matrix of U). Choosing a vertex $u \in V(U)$, let $L[u]$ be the principal submatrix of L obtained by deleting its u-th row and column. One can show that $L[u]$ is invertible; its inverse $B(u) = L[u]^{-1}$ is block-diagonal, and each block corresponds to a connected component (branch) T of $U \setminus \{u\}$. We call such a block the *bottleneck matrix* of T. Let us write it as $M = [m_{ij}]$. Its entries have a particularly simple description. If i, j are two vertices of T and r is the vertex of T adjacent to u in the original tree U, then m_{ij} is the number of vertices (in T) which simultaneously lie in the path joining i to r and in the path joining j to r ([11]). This description shows that the entries of M do not depend on the structure of $U \setminus T$. However, they do depend on which vertex in T is adjacent to u in U. For this reason, M is unambiguously associated with the pair (T, r), and we can refer to it as to the bottleneck matrix of the *rooted* tree (T, r). One can show that M is symmetric, positive definite and entrywise positive, so that it is possible to apply the Perron-Frobenius theory ([13]) to it. The *Perron value* $\rho((T, r))$ (hereafter abbreviated to $\rho(T)$) of the rooted tree (T, r) is defined as the spectral radius of M, while a corresponding positive eigenvector is called a *Perron vector*. Finally, a branch attaining the maximum Perron value among all the branches of U at the vertex u is called a *Perron branch* at u.

The following result, proved in [11], makes use of the Perron value of bottleneck matrices to classify unrooted trees in two disjoint sets.

Theorem 1.1. *Let U be an unrooted tree with more than one vertex. There are two possibilities:*

1. *There exists exactly one vertex z having $k \geq 2$ Perron branches $B_1, \ldots, B_k$ at z. U is said to be a type I tree and z is its characteristic vertex.*

[1] In the literature the distance between two vertices is usually defined as the number of *edges* in a shortest path connecting them. Here, and throughout the paper, we will adopt the less common definition given above in order to be consistent with [2] and [3].

2. *There exists exactly one edge pq such that the unique Perron branch B_p at p contains q and the unique Perron branch B_q at q contains p. U is said to be a type II tree and p, q are its characteristic vertices.*

The *characteristic set* of U is the set of its characteristic vertices, and it can be interpreted as a sort of "gravity center": it is the vertex or edge which best balances the Perron values of branches going out from it.

There is an important difference between the two notions of center introduced so far. To check whether a vertex v belongs to $\mathcal{EC}(G)$ one needs – in principle – to compare the eccentricity of v with the eccentricity of all the other vertices in G. In other words, one needs to verify that v is a *global* optimum for some function – namely, the function $ecc_G : V(G) \to \mathbb{R}$. On the other hand, to check whether a vertex v belongs to the characteristic set of a tree U, by virtue of Theorem 1.1 one only has to consider a *neighborhood* of v, and to compute the Perron value of branches whose roots lie in that neighborhood. This corresponds, intuitively, to verifying that v is a *local* optimum of a suitable function. Hence, checking whether a given vertex is central in the second case is virtually more efficient than in the first one (even though the actual computational efficiency of the various definitions of centers is affected by many other factors).

Keeping this idea in mind, in Section 2 we use the characteristic set of trees as a model to introduce a new notion of center for graphs. We let this depend on a real-valued function μ defined on the set of directed edges associated with the given graph. We investigate when this center is *simple* (consisting of a unique cycle) and *quasi-simple* (inducing a connected subgraph of the original graph). After proving in Section 3 a lower bound for the combinatorial Perron parameter ρ_c of a rooted tree ([2,3]), in Section 4 we adapt the new center concept to trees. Both the characteristic set (Proposition 4.4) and the eccentricity-center (Proposition 4.10) of a tree can be viewed as particular examples of the center notion given here, by letting μ be suitable weights – of algebraic or combinatorial nature – of rooted subtrees associated with the original tree. The function ρ_c is then used to provide an example of center which is simple in the case of caterpillar trees, as shown in Proposition 4.9. In Section 5 we present the results of a computational comparison of the various instances of center introduced thus far for trees, after giving a slightly modified definition of center – the *limit center* – which allows a more meaningful comparison. The idea introduced above of considering the center to be the result of the optimization of a function on the vertex set of a graph finally leads us to explore – in Section 6 – the notions of *discrete differential* and *discrete concavity* on graphs.

Notation: we use the word *graph* (resp. *tree*) to denote an undirected, unrooted graph (resp. tree). When we deal with directed or rooted graphs (trees) we specify it explicitly. For a directed graph, we use the word *connected* as a synonym of *weakly connected*, meaning that for every pair of distinct vertices i and j there exists an *undirected* path joining i and j. A *cycle* in a graph is a closed walk of at least three vertices with no repetitions of vertices other than the repetition of the first and last vertex. A *cycle* in a directed graph is a closed directed walk of at least one vertex with no repetitions of

vertices other than the repetition of the first and last vertex. A cycle of one vertex in a directed graph consists in a loop. In both the undirected and the directed case we usually denote a cycle of k vertices by $C = c_1c_2 \dots c_kc_1$. When the order of vertices is not important, we sometimes denote it by $C = \{c_1, c_2, \dots, c_k\}$, making no distinction between the cycle and the set of its vertices. A *rooted tree* consisting of the tree T and the root $r \in V(T)$ is denoted by (T, r) or just T whenever the root is considered known or not relevant in the context. The set of rooted trees is denoted by $\mathcal{T}$. We identify two rooted trees $(T_1, r_1), (T_2, r_2)$ in $\mathcal{T}$ when there exists a rooted tree isomorphism between them (i.e. a graph isomorphism mapping r_1 to r_2).

2. A new center concept

Inspired by Theorem 1.1, we introduce a general definition for the center of a connected graph (Definition 1) and we discuss some of its properties. In Section 4 we will prove that it is actually a generalization of the characteristic set of a tree (Proposition 4.4). Interestingly, also the eccentricity-center of a tree can be obtained from Definition 1 via a suitable choice of the function μ (as shown in Proposition 4.10).

Let G be a connected graph. We define the directed graph G_{dir} by replacing each undirected edge ij of G with the two directed edges $\overrightarrow{ij}$ and $\overrightarrow{ji}$ (where the symbol $\overrightarrow{ij}$ denotes the directed edge having i as tail and j as head). In other words, $V(G_{dir}) = V(G)$ and $E(G_{dir}) = \{\overrightarrow{ij} \mid i, j \in V(G),\ i \text{ and } j \text{ are adjacent in } G\}$. Consider now a function $\mu : E(G_{dir}) \to \mathbb{R}$. If $|V(G)| \geq 2$, then each vertex is adjacent to at least one other vertex (since G is assumed to be connected) and consequently it is the tail of at least one directed edge in G_{dir}. We can then define, for each $i \in V(G) = V(G_{dir})$, the set

$$\mathcal{A}_i := \left\{ \overrightarrow{ij} \in E(G_{dir}) \mid \mu(\overrightarrow{ij}) = \max_{\overrightarrow{ik} \in E(G_{dir})} \mu(\overrightarrow{ik}) \right\}.$$

That is, $\mathcal{A}_i$ is the set of all the directed edges in G_{dir} having i as tail that are maximal with respect to μ. The *optimality graph* of G w.r.t. μ is the directed graph G_μ defined by $V(G_\mu) = V(G)$ and

$$E(G_\mu) = \bigcup_{\substack{i \in V(G) \\ |\mathcal{A}_i| = 1}} \mathcal{A}_i \quad \bigcup \quad \left\{ \overrightarrow{ii} \mid i \in V(G), |\mathcal{A}_i| > 1 \right\}. \tag{1}$$

In other words, to obtain G_μ we start from the vertex set $V(G)$ and, for each vertex $i \in V(G)$, we draw the directed edge $\overrightarrow{ij}$ which maximizes μ among the edges in G_{dir} having i as tail; however, if this maximum is attained in more than one edge, we draw the loop $\overrightarrow{ii}$ instead. If $|V(G)| = 1$, letting v be the unique vertex of G, we define G_μ to be the directed graph having $\{v\}$ as vertex set and $\{\overrightarrow{vv}\}$ as edge set. Fig. 1 illustrates the procedure we have just described on a graph G with 8 vertices and a function $\mu : E(G_{dir}) \to \mathbb{R}$. G_μ has an interesting structure which we will now describe.

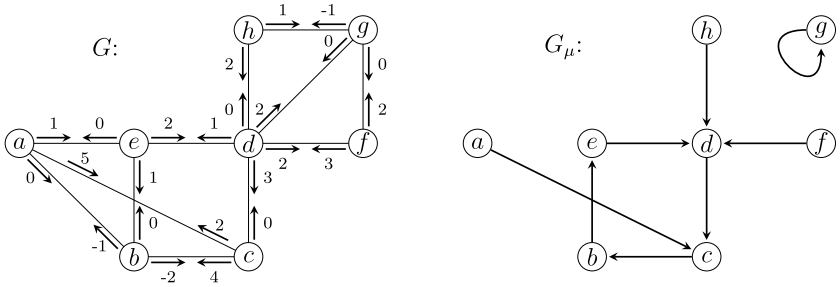


Fig. 1. On the left, an undirected graph G and a function $\mu : E(G_{dir}) \to \mathbb{R}$ (the number next to an arrow going out from a vertex i and pointing towards a vertex j is $\mu(\overrightarrow{ij})$). On the right, the optimality graph G_μ.

We say that a directed graph D is *deterministic* provided that for each $v \in V(D)$ there exists a unique directed edge e_v having v as tail. The name comes from the fact that, for such a graph, the route of a walker starting at any vertex and walking along directed edges according to their direction is uniquely determined. We notice that, if a graph D is deterministic, then $|E(D)| = |V(D)|$. It immediately follows from its construction that G_μ is deterministic. Furthermore, we define a *directed unicyclic graph* (Fig. 2) as a connected directed graph obtained by taking a directed cycle $C = c_1c_2 \dots c_kc_1$ with $k \geq 1$, and k rooted directed trees $T_1, \dots, T_k$ (where, given u and v adjacent vertices in T_i, the directed edge connecting them is $\overrightarrow{uv}$ if the path joining u to the root of T_i contains v, $\overrightarrow{vu}$ otherwise), and by identifying the root of T_i with c_i for each $i = 1, \dots, k$. (Notice that T_i can also be a trivial tree, with only one vertex.)

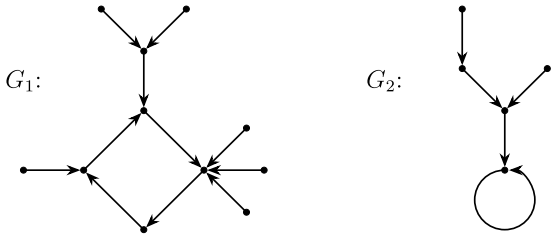


Fig. 2. Two directed unicyclic graphs. G_1 has a cycle of length 4, while G_2 has a cycle of length 1 (a loop).

Proposition 2.1. *A connected directed graph D is a directed unicyclic graph if and only if it is deterministic.*

Proof. Suppose first that D is a directed unicyclic graph, and let $C, T_1, \dots, T_k$ be as in the definition given above. Consider a vertex $v \in V(D)$. If v belongs to C, let w be the vertex coming immediately after v in C. If v does not belong to C, then it belongs to T_i for an $i \in \{1, \dots, k\}$. Moreover, v cannot be the root of T_i, since the latter is identified with a vertex in C. Let w be the vertex coming immediately after v in the unique path

joining v to the root of T_i. In both these situations, the only directed edge in D having v as tail is $\overrightarrow{vw}$, thus showing that D is deterministic.

Suppose now that D is deterministic. We show that D is a directed unicyclic graph by induction on the number n of vertices in D. If $n = 1$ the claim is clear. Suppose $n \geq 2$. If D is a directed cycle the claim holds, so assume that this is not the case. Label the vertices of D as $1, \ldots, n$, and let $A \in \mathbb{R}^{n,n}$ be the matrix whose (i, j)-th entry equals 1 if $\overrightarrow{ij} \in E(D)$, 0 otherwise. Let $R_1, \ldots, R_n$ and $C_1, \ldots, C_n$ be the row-sums and column-sums of A respectively. Since D is deterministic, $R_i = 1 \ \forall i = 1, \ldots, n$. We claim that there exists $j \in \{1, \ldots, n\}$ such that $C_j = 0$. This would imply that no edge of D has j as head. If the claim is not true, then $C_i \geq 1 \ \forall i = 1, \ldots, n$; since there are exactly n ones in A, we have that $C_i = 1 \ \forall i = 1, \ldots, n$. This shows that A is a permutation matrix, and hence – relabeling the vertices – it can be decomposed as a direct sum of diagonal blocks associated with cyclic permutations. Each block corresponds to a connected component of D. Being D connected, the permutation associated with A must then have a unique cycle. This means that D is a directed cycle, which contradicts our assumption. Summarizing, we can find a vertex j such that no edge of D has j as head. Let $\tilde{D}$ be the connected directed graph obtained by removing from D the vertex j and the unique directed edge having j as tail. $\tilde{D}$ is still deterministic, and by the inductive hypothesis it is a directed unicyclic graph. It follows that D is a directed unicyclic graph too, thus concluding the proof. □

The structure of an optimality graph is clear from Proposition 2.1.

Theorem 2.2. *Given a connected graph G and a function $\mu : E(G_{dir}) \to \mathbb{R}$, the optimality graph G_μ is a disjoint union of directed unicyclic graphs.*

We now define the main concept of the paper.

Definition 1. Consider a connected graph G and a function $\mu : E(G_{dir}) \to \mathbb{R}$. The *$\mu$-center* of G, denoted by $\mathcal{Z}_\mu(G)$, is the set of directed cycles in G_μ.

As an example, considering the graph G and the function μ illustrated in Fig. 1, we see that the μ-center of G consists of two directed cycles, one of which is a loop: $\mathcal{Z}_\mu(G) = \{bedcb\ ,\ gg\}$. We note, as anticipated in Section 1, that this notion of center is "local": to verify that a cycle C lies in $\mathcal{Z}_\mu(G)$ we only have to observe the values of the function μ in directed edges having tail in C, and we do not have to deal with the rest of the graph.

Note. The function μ we are considering here to build the μ-center of a graph is a generic real-valued function defined on $E(G_{dir})$. This general setting is already enough to obtain some properties for the center notion, as we shall see in the rest of this section. However, it will be clear why this construction actually generalizes the characteristic set of a tree only in Section 4, when we will focus on trees and we will consider a subset of functions

μ which can be viewed as weights – of algebraic or combinatorial nature – of rooted subtrees associated with the given tree. In Section 6, on the other hand, we will apply the results of this section to the different setting where the underlying graph is not required to be a tree and μ is given as the *discrete differential* of some function defined on the vertex set of the graph.

Given a set of vertices $W \subset V(G)$, we denote by $G[W]$ the subgraph of G induced by W – i.e., the vertex set of $G[W]$ is W, while the edge set of $G[W]$ is the set of edges of G having both endpoints in W. We define the *support* of $\mathcal{Z}_\mu(G)$ to be the set

$$\mathcal{SZ}_\mu(G) := \bigcup_{C \in \mathcal{Z}_\mu(G)} C.$$

In other words, $\mathcal{SZ}_\mu(G)$ is the set of vertices of G belonging to some cycle in $\mathcal{Z}_\mu(G)$. Given a connected graph G and a function $\mu : E(G_{dir}) \to \mathbb{R}$, we say that $\mathcal{Z}_\mu(G)$ is *simple* if $|\mathcal{Z}_\mu(G)| = 1$, and *quasi-simple* if $G[\mathcal{SZ}_\mu(G)]$ is a connected graph. Clearly a simple center is quasi-simple. From the structure of G_μ described in Theorem 2.2 we obtain some general properties of $\mathcal{Z}_\mu(G)$.

Proposition 2.3. *Consider a connected graph G and a function $\mu : E(G_{dir}) \to \mathbb{R}$. Then*

1. *$\mathcal{Z}_\mu(G) \neq \emptyset$.*
2. *The directed cycles in $\mathcal{Z}_\mu(G)$ are pairwise vertex-disjoint. Equivalently, every directed closed walk in G_μ is a directed cycle.*
3. *$\mathcal{Z}_\mu(G)$ is simple $\Leftrightarrow$ G_μ is connected.*

Proof. It directly follows from Theorem 2.2. □

We notice from the definition given above that the condition making a center simple puts a constraint on the number of cycles the center consists of, but not on the number of vertices in the cycles. However, in the case of trees there is an easy description of the size of the cycles belonging to the center.

Proposition 2.4. *Consider a tree U and a function $\mu : E(U_{dir}) \to \mathbb{R}$. Then each cycle in $\mathcal{Z}_\mu(U)$ has either one or two vertices.*

Proof. Let $C = c_1c_2 \dots c_kc_1 \in \mathcal{Z}_\mu(U)$, and suppose that $k \geq 3$. Since C is not a loop we can associate with each directed edge $\overrightarrow{ij}$ in C the corresponding undirected edge $ij \in E(U)$. Since $k \geq 3$, these undirected edges are all distinct, and they form an – undirected – cycle in the tree U, which is clearly impossible. □

In particular we see that, if the center of a tree is simple, then it consists of a directed cycle composed of either a single vertex or two adjacent vertices. We point out here that

in general the center of a tree is not quasi-simple and, a fortiori, not simple. Suppose, for example, that U is a path of $n \geq 5$ vertices labeled $p_1, \ldots, p_5$ in the natural way. Define the function $\mu : E(U_{dir}) \to \mathbb{R}$ to be constantly equal to 1 except for the directed edges $\overrightarrow{p_2p_1}$, $\overrightarrow{p_3p_4}$ and $\overrightarrow{p_4p_5}$, where its value is 2. Then, $\mathcal{Z}_\mu(G) = \{p_1p_2p_1\ ,\ p_4p_5p_4\}$, which is not simple nor quasi-simple.

Let us now give sufficient conditions for the μ-center of a graph to be simple and quasi-simple. Given a graph G, we say that a function $\mu : E(G_{dir}) \to \mathbb{R}$ is *weakly path-monotone* provided that $\mu(\overrightarrow{ij}) \geq \mu(\overrightarrow{jk})$ if $\overrightarrow{ij}, \overrightarrow{jk} \in E(G_{dir})$, $i \neq k$. We say that μ is *strongly path-monotone* if the inequality above is always strict.

Proposition 2.5. *Given a connected graph G and a function $\mu : E(G_{dir}) \to \mathbb{R}$,*

1. *μ is strongly path-monotone $\Rightarrow$ $\mathcal{Z}_\mu(G)$ is simple;*
2. *μ is weakly path-monotone $\Rightarrow$ $\mathcal{Z}_\mu(G)$ is quasi-simple.*

Proof. Let μ be strongly path-monotone and suppose that $\mathcal{Z}_\mu(G)$ is not simple, so that we can consider two distinct cycles $C, \tilde{C}$ in $\mathcal{Z}_\mu(G)$. We know by Proposition 2.3 that C and $\tilde{C}$ are vertex-disjoint. Choose a vertex c in C and a vertex $\tilde{c}$ in $\tilde{C}$ in such a way that $d(c, \tilde{c}) = \min\{d(c', \tilde{c}') \mid c' \in C, \tilde{c}' \in \tilde{C}\}$ (where the distances are computed in G), and let P be a shortest path connecting c to $\tilde{c}$. Clearly, no edge in P belongs to C or $\tilde{C}$. Since C and $\tilde{C}$ are vertex-disjoint, the number of edges in P is at least 1. Let us write $P = p_1p_2 \ldots p_k$, with $p_1 = c$, $p_k = \tilde{c}$ and $k \geq 2$. Since G_μ is deterministic, the directed edge $\overrightarrow{p_1p_2}$ does not belong to $E(G_\mu)$. This means that there exists a vertex $x \in V(G)$ such that $x \neq p_2$ and

$$\mu(\overrightarrow{p_1x}) \geq \mu(\overrightarrow{p_1p_2}). \tag{2}$$

Analogously, we can find a vertex $y \in V(G)$ such that $y \neq p_{k-1}$ and

$$\mu(\overrightarrow{p_ky}) \geq \mu(\overrightarrow{p_kp_{k-1}}). \tag{3}$$

Note that inequality (2) (resp. (3)) can be made strict if C (resp. $\tilde{C}$) is not a loop. Since μ is strongly path-monotone, then

$$\mu(\overrightarrow{p_1p_2}) > \mu(\overrightarrow{p_2p_3}) > \cdots > \mu(\overrightarrow{p_{k-1}p_k}) > \mu(\overrightarrow{p_ky}) \tag{4}$$

and

$$\mu(\overrightarrow{p_kp_{k-1}}) > \mu(\overrightarrow{p_{k-1}p_{k-2}}) > \cdots > \mu(\overrightarrow{p_2p_1}) > \mu(\overrightarrow{p_1x}). \tag{5}$$

Putting (2), (3), (4) and (5) together we obtain that

$$\mu(\overrightarrow{p_1p_2}) > \mu(\overrightarrow{p_ky}) \geq \mu(\overrightarrow{p_kp_{k-1}}) > \mu(\overrightarrow{p_1x}) \geq \mu(\overrightarrow{p_1p_2})$$

which is a contradiction. We conclude that $\mathcal{Z}_\mu(G)$ is simple, thus completing the proof of point (1) of the Proposition.

Suppose now that μ is weakly path-monotone and $\mathcal{Z}_\mu(G)$ is not quasi-simple. This means that $G[\mathcal{SZ}_\mu(G)]$ is not connected. Consider two cycles C and $\tilde{C}$ lying in two different connected components of $G[\mathcal{SZ}_\mu(G)]$. As above, choose c in C and $\tilde{c}$ in $\tilde{C}$ so that $d(c,\tilde{c}) = \min\{d(c',\tilde{c}') \mid c' \in C, \tilde{c}' \in \tilde{C}\}$, and let $P = p_1p_2\dots p_k$ be a shortest path connecting c to $\tilde{c}$; P has no edges in common with C or $\tilde{C}$. If $p_i \in \mathcal{SZ}_\mu(G)$ $\forall i = 2,\dots,k-1$, then C and $\tilde{C}$ would lie in the same connected component of $G[\mathcal{SZ}_\mu(G)]$. Hence, there exists j such that $2 \le j \le k-1$ and $p_j \notin \mathcal{SZ}_\mu(G)$. In particular, c, p_j and $\tilde{c}$ are all distinct vertices. As before, we can find two vertices x and y such that $x \neq p_2$, $y \neq p_{k-1}$, $\mu(\overrightarrow{p_1x}) \ge \mu(\overrightarrow{p_1p_2})$ and $\mu(\overrightarrow{p_ky}) \ge \mu(\overrightarrow{p_kp_{k-1}})$. Since μ is weakly path-monotone, we have

$$\mu(\overrightarrow{p_1p_2}) \ge \mu(\overrightarrow{p_2p_3}) \ge \cdots \ge \mu(\overrightarrow{p_{j-1}p_j}) \ge \mu(\overrightarrow{p_jp_{j+1}}) \ge \cdots \ge \mu(\overrightarrow{p_{k-1}p_k}) \ge \mu(\overrightarrow{p_ky})$$

and

$$\mu(\overrightarrow{p_kp_{k-1}}) \ge \mu(\overrightarrow{p_{k-1}p_{k-2}}) \ge \cdots \ge \mu(\overrightarrow{p_jp_{j-1}}) \ge \cdots \ge \mu(\overrightarrow{p_2p_1}) \ge \mu(\overrightarrow{p_1x}).$$

We obtain

$$\begin{aligned}\mu(\overrightarrow{p_1p_2}) \ge \mu(\overrightarrow{p_{j-1}p_j}) \ge \mu(\overrightarrow{p_jp_{j+1}}) \ge \mu(\overrightarrow{p_ky}) \ge \mu(\overrightarrow{p_kp_{k-1}}) \ge \mu(\overrightarrow{p_jp_{j-1}}) \ge \mu(\overrightarrow{p_1x})\\ \ge \mu(\overrightarrow{p_1p_2})\end{aligned}$$

which in particular implies that

$$\mu(\overrightarrow{p_{j-1}p_j}) = \mu(\overrightarrow{p_jp_{j+1}}) = \mu(\overrightarrow{p_jp_{j-1}}). \tag{6}$$

If v is a vertex in G adjacent to p_j other than p_{j-1}, weak path-monotonicity and (6) imply that

$$\mu(\overrightarrow{p_jv}) \le \mu(\overrightarrow{p_{j-1}p_j}) = \mu(\overrightarrow{p_jp_{j+1}}).$$

Therefore, $\overrightarrow{p_jp_{j+1}}$ and $\overrightarrow{p_jp_{j-1}}$ are both maximal w.r.t. μ among the directed edges in G_{dir} having p_j as tail. This means that $\overrightarrow{p_jp_j} \in E(G_\mu)$ so that the cycle $p_jp_j \in \mathcal{Z}_\mu(G)$ and hence $p_j \in \mathcal{SZ}_\mu(G)$, which is a contradiction. □

Strong path-monotonicity is a strict requirement for a function $\mu : E(G_{dir}) \to \mathbb{R}$. The next result shows that in fact it forces the graph G to be a tree.

Proposition 2.6. *Let G be a connected graph and let $\mu : E(G_{dir}) \to \mathbb{R}$ be a strongly path-monotone function. Then G is a tree.*

Proof. Suppose that G contains an undirected cycle $C = c_1c_2 \dots c_kc_1$ (where $k \geq 3$). The strong path-monotonicity of μ implies that $\mu(\overrightarrow{c_1c_2}) > \mu(\overrightarrow{c_2c_3}) > \dots > \mu(\overrightarrow{c_kc_1}) > \mu(\overrightarrow{c_1c_2})$ which is a contradiction. □

3. A lower bound for the combinatorial Perron parameter ρ_c of a rooted tree

The combinatorial Perron parameters, introduced in [2] and [3], are computationally-efficient approximations of the Perron value (see Section 1) of a given rooted tree. In this section we present a lower bound for the combinatorial Perron parameter ρ_c. Besides connecting to the study undertaken in [2] and [3], this result will be used in Section 4, where we will define a center for trees based on ρ_c.

Given a rooted tree (T, r) having n vertices labeled $1, \dots, n$, let $d = (d_1, \dots, d_n)^T \in \mathbb{R}^n$ be its distance vector, where d_i is the number of vertices in the path joining i to r. Let also $M = [m_{ij}] \in \mathbb{R}^{n,n}$ be the bottleneck matrix of (T, r), as defined in Section 1.

The parameter $\rho_c((T, r))$ (hereafter abbreviated to $\rho_c(T)$) is defined as the Rayleigh quotient of d with respect to M:

$$\rho_c(T) := \frac{d^T M d}{d^T d}. \tag{7}$$

We note that the Perron value $\rho(T)$ is an upper bound for $\rho_c(T)$; indeed, the former is the maximum Rayleigh quotient w.r.t. M over each nonzero vector $x \in \mathbb{C}^n$.

Theorem 3.1. *Let T be a rooted tree and d its distance vector. Then $\rho_c(T) \geq \|d\|_\infty$.*

Proof. Consider the function $\omega : \mathcal{T} \to \mathbb{R}$ defined by $\omega(T) = d_T^T M_T d_T - \|d_T\|_\infty d_T^T d_T$ for any $T \in \mathcal{T}$, where $\mathcal{T}$ is the set of rooted trees, M_T is the bottleneck matrix of T and d_T is its distance vector. To prove the Theorem we need to show that $\omega(T) \geq 0 \; \forall T \in \mathcal{T}$. We proceed by induction on the number n of vertices in T. If $n = 1$, the result is trivial since in this case $\omega(T) = 1 - 1 = 0$. Suppose now $n \geq 2$, and denote the distance vector d_T by $d = (d_i)$ and the bottleneck matrix M_T by $M = [m_{ij}]$ for the sake of simplicity. Let v be a vertex in T s.t. $d_v = \|d\|_\infty$. We note that v must be a leaf. Moreover, v cannot be the root of T, since $n \geq 2$. Let $\tilde{T}$ be the rooted tree obtained from T by removing the vertex v and the edge incident to it, and let $\tilde{d} = (\tilde{d}_i)$ and $\tilde{M} = [\tilde{m}_{ij}]$ be its distance vector and its bottleneck matrix respectively. Notice that $\tilde{d}_i = d_i$ and $\tilde{m}_{ij} = m_{ij}$ for each $i, j \neq v$. Hence,

- $\tilde{d}^T \tilde{d} = d^T d - d_v^2$
- $$\begin{aligned} \tilde{d}^T \tilde{M} \tilde{d} &= \sum_{i \neq v} \sum_{j \neq v} m_{ij} d_i d_j = \sum_{i=1}^{n} \sum_{j=1}^{n} m_{ij} d_i d_j - 2 \sum_{i=1}^{n} m_{iv} d_i d_v + m_{vv} d_v^2 \\ &= d^T M d - 2 \sum_{i=1}^{n} m_{iv} d_i d_v + d_v^3. \end{aligned}$$

Depending on whether v is the only vertex in T having distance d_v or not, we can have that $\|\tilde{d}\|_\infty = d_v - 1$ or $\|\tilde{d}\|_\infty = d_v$. In both cases, $\|\tilde{d}\|_\infty \geq d_v - 1$. Hence, we obtain

$$\begin{aligned}
\omega(T) - \omega(\tilde{T}) &= d^T M d - \|d\|_\infty d^T d - \tilde{d}^T \tilde{M} \tilde{d} + \|\tilde{d}\|_\infty \tilde{d}^T \tilde{d} \\
&\geq d^T M d - d_v d^T d - \tilde{d}^T \tilde{M} \tilde{d} + (d_v - 1)\tilde{d}^T \tilde{d} \\
&= d^T M d - d_v d^T d - d^T M d + 2\sum_{i=1}^{n} m_{iv} d_i d_v - d_v^3 + (d_v - 1)(d^T d - d_v^2) \\
&= 2\sum_{i=1}^{n} m_{iv} d_i d_v - 2d_v^3 + d_v^2 - d^T d \;\geq\; 2\sum_{i=1}^{n} m_{iv} d_i d_v - 2d_v^3 + d_v^2 - \sum_{i=1}^{n} d_v d_i \\
&= d_v \sum_{i=1}^{n} d_i (2m_{iv} - 1) - 2d_v^3 + d_v^2 \;\geq\; d_v^2 (2m_{vv} - 1) - 2d_v^3 + d_v^2 \\
&= 2d_v^3 - d_v^2 - 2d_v^3 + d_v^2 \;=\; 0
\end{aligned} \tag{8}$$

where, in the last inequality, we use that the term $2m_{iv} - 1$ is positive for any $i = 1, \ldots, n$ since the entries of M are ≥ 1. Given that $\tilde{T}$ has $n-1$ vertices, by the inductive hypothesis $\omega(\tilde{T}) \geq 0$. Combining this with (8) we conclude the proof. □

4. Application to trees

The aim of this section is to apply the theory developed in Section 2 to trees. Consider a function $R : \mathcal{T} \to \mathbb{R}$, where $\mathcal{T}$ is the set of rooted trees. Examples of such a function are the Perron value ρ and the combinatorial Perron parameters ρ_c, π_e and π_d described in [2] and [3]. Other natural choices for the function R are ϑ, ζ and λ defined as follows:

$$\begin{array}{lll}
\bullet\ \vartheta : \mathcal{T} \to \mathbb{R} & \bullet\ \zeta : \mathcal{T} \to \mathbb{R} & \bullet\ \lambda : \mathcal{T} \to \mathbb{R} \\
\quad T \mapsto |V(T)| & \quad T \mapsto \|d_T\|_\infty & \quad T \mapsto |\mathcal{L}(T)|
\end{array} \tag{9}$$

where d_T denotes the distance vector of T (the entry in d_T corresponding to a vertex v is the number of vertices in the path connecting v to the root of T) and $\mathcal{L}(T)$ denotes the set of leaves (pendant vertices) in T (if T is the rooted tree with one vertex, we consider that vertex to be a leaf).

Let U be a tree. Given a directed edge $\overrightarrow{ij} \in U_{dir}$, we define $U_{\overrightarrow{ij}}$ as the connected component of $U \setminus \{i\}$ containing j. We consider $U_{\overrightarrow{ij}}$ as a rooted tree having root j.

R induces a new function R^U as follows:

$$\begin{aligned}
R^U : E(U_{dir}) &\to \mathbb{R} \\
\overrightarrow{ij} &\mapsto R\left(U_{\overrightarrow{ij}}\right).
\end{aligned} \tag{10}$$

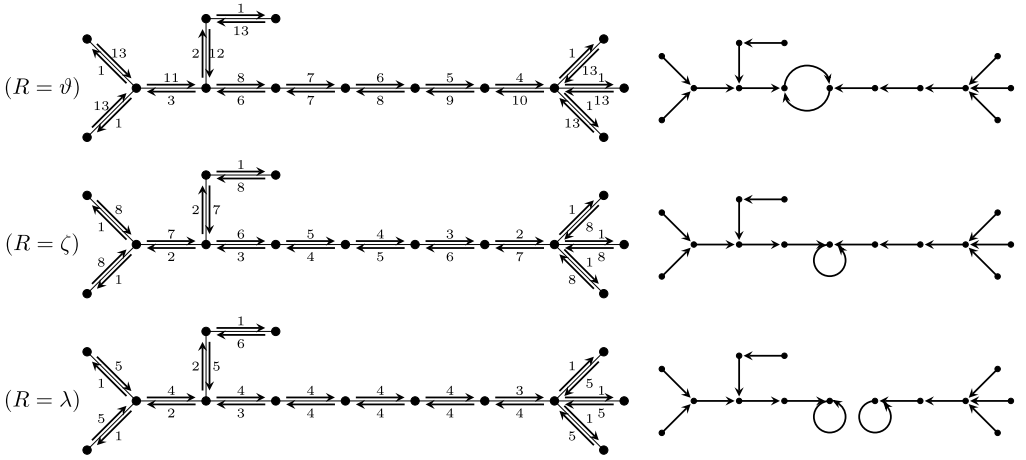


Fig. 3. On the left, the same undirected graph U is equipped with the function $R^U : E(U_{dir}) \to \mathbb{R}$, where R is ϑ (top), ζ (middle) or λ (bottom). The number next to an arrow $\overrightarrow{ij}$ is $R^U(\overrightarrow{ij}) = R(U_{\overrightarrow{ij}})$. On the right, the corresponding optimality graphs U_{R^U}.

For instance, given $\overrightarrow{ij} \in E(U_{dir})$, we have that $\vartheta^U(\overrightarrow{ij}) = |V(U_{\overrightarrow{ij}})|$, $\zeta^U(\overrightarrow{ij}) = \|d_{U_{\overrightarrow{ij}}}\|_\infty$ and $\lambda^U(\overrightarrow{ij}) = |\mathcal{L}(U_{\overrightarrow{ij}})|$.

Definition 2. Given a function $R : \mathcal{T} \to \mathbb{R}$ and a tree U we define the *R-center* of U as $\mathcal{Z}_R(U) := \mathcal{Z}_{R^U}(U)$ (with $\mathcal{Z}_{R^U}(U)$ as in Definition 1).

We can view the function R as the assignation of a *weight* $R(T)$ to any rooted tree $T \in \mathcal{T}$. Then, given $\overrightarrow{ij} \in E(U_{dir})$, $R^U(\overrightarrow{ij}) = R(U_{\overrightarrow{ij}})$ is the weight of the rooted subtree $U_{\overrightarrow{ij}}$ at i having root j. In this perspective, $\overrightarrow{ij}$ belongs to the optimality graph U_{R^U} if $U_{\overrightarrow{ij}}$ is the *heaviest* rooted subtree of the given tree U at i. Analogously, a loop $\overrightarrow{ii}$ in U_{R^U} means that there exist at least two rooted subtrees at i having maximum weight. A cycle $C \in \mathcal{Z}_R(U)$, then, corresponds to a set of vertices which best balance the weights of rooted subtrees of U. We denote by $\mathcal{SZ}_R(U)$ the support of $\mathcal{Z}_R(U)$:

$$\mathcal{SZ}_R(U) := \mathcal{SZ}_{R^U}(U) = \bigcup_{C \in \mathcal{Z}_R(U)} C. \tag{11}$$

Fig. 3 shows an instance of the construction described above on a tree U, using the three different weights ϑ, ζ and λ. We notice that $\mathcal{Z}_\vartheta(U)$ and $\mathcal{Z}_\zeta(U)$ are simple, while $\mathcal{Z}_\lambda(U)$ is quasi-simple but not simple. Sufficient conditions for the R-center of a tree to be simple or quasi-simple can be derived by transferring Proposition 2.5 to our new setting. Given three rooted trees T_1, T_2, T_3 we say that T_1 *extends* T_2 *via* T_3 *at* $v \in V(T_3)$ if v is not the root of T_3 and T_1 is obtained by considering T_2 and T_3, identifying the root of T_2 with v, and making the root of T_3 be the root of T_1. An example is shown in Fig. 4. We say that a function $R : \mathcal{T} \to \mathbb{R}$ is *weakly extension-monotone* if $R(T_1) \geq R(T_2)$

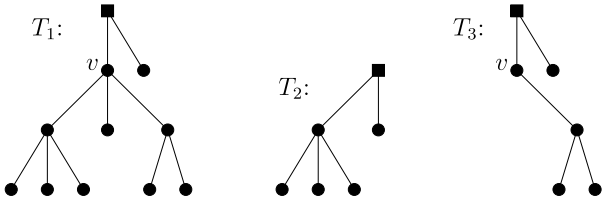


Fig. 4. Three rooted trees T_1, T_2, T_3 such that T_1 extends T_2 via T_3 at v. Root vertices are indicated by a square.

whenever $T_1, T_2 \in \mathcal{T}$ are such that T_1 extends T_2 via some rooted tree $T_3 \in \mathcal{T}$ at some vertex $v \in V(T_3)$. We say that R is *strongly extension-monotone* if the inequality above is always strict.

Proposition 4.1. *Consider a function $R : \mathcal{T} \to \mathbb{R}$. Then*

1. *R is strongly extension-monotone $\Rightarrow$ $\mathcal{Z}_R(U)$ is simple for any tree U;*
2. *R is weakly extension-monotone $\Rightarrow$ $\mathcal{Z}_R(U)$ is quasi-simple for any tree U.*

Note. Proposition 4.1 is similar to Proposition 2.5 except for one aspect: in this case the function R and its extension-monotonicity do not depend on the underlying graph U. Hence, contrary to the previous situation, we can check the monotonicity of R just once, and use it to deduce simpleness or quasi-simpleness for the R-center of any tree.

Proof. Assume that R is strongly extension-monotone, and consider a tree U. Let $i, j, k \in V(U)$ be distinct vertices such that i is adjacent to j and j is adjacent to k, and consider the rooted trees $U_{\overrightarrow{ij}}$ and $U_{\overrightarrow{jk}}$. Define $\tilde{V} := (V(U_{\overrightarrow{ij}}) \setminus V(U_{\overrightarrow{jk}})) \cup \{k\}$, and let $\tilde{T}$ be the rooted subtree of $U_{\overrightarrow{ij}}$ induced by vertices in $\tilde{V}$ and having j as root. We claim that $U_{\overrightarrow{ij}}$ extends $U_{\overrightarrow{jk}}$ via $\tilde{T}$ at k. Indeed, the root of $\tilde{T}$ is j and not k; moreover, $U_{\overrightarrow{ij}}$ is obtained by joining $U_{\overrightarrow{jk}}$ and $\tilde{T}$ in k, and its root j is the root of $\tilde{T}$. From strong extension-monotonicity and (10) we obtain that $R^U(\overrightarrow{ij}) = R(U_{\overrightarrow{ij}}) > R(U_{\overrightarrow{jk}}) = R^U(\overrightarrow{jk})$. This shows that the function $R^U : E(U_{dir}) \to \mathbb{R}$ is strongly path-monotone. If R is weakly extension-monotone we analogously obtain that R^U is weakly path-monotone. The result then follows from Proposition 2.5 and Definition 2. □

We now apply Proposition 4.1 to the functions ϑ, ζ and λ defined in (9).

Proposition 4.2. *Given a tree U, $\mathcal{Z}_\vartheta(U)$ and $\mathcal{Z}_\zeta(U)$ are simple, while $\mathcal{Z}_\lambda(U)$ is quasi-simple.*

Proof. By virtue of Proposition 4.1 it suffices to prove that ϑ and ζ are strongly extension-monotone, and that λ is weakly extension-monotone. The strong extension-monotonicity of ϑ and ζ follows directly from their definition. To prove the weak

extension-monotonicity of λ, consider three rooted trees $T_1, T_2, T_3 \in \mathcal{T}$ such that T_1 extends T_2 via T_3 at $v \in V(T_3)$, and let r_1 and r_2 be the roots of T_1 and T_2 respectively (in T_1 r_2 is identified with v). If $w \in V(T_2)$ is a pendant vertex in T_2 and $w \neq r_2$, then w is also pendant in T_1. Analogously, if $w \in V(T_3)$ is pendant in T_3 and $w \neq v$, then w is also pendant in T_1. Since $V(T_3)$ contains the distinct vertices v and r_1, $|V(T_3)| \geq 2$. Any tree with at least 2 vertices contains at least 2 pendant vertices, so that $|\mathcal{L}(T_3)| \geq 2$. We conclude that $\lambda(T_1) = |\mathcal{L}(T_1)| \geq |\mathcal{L}(T_2)| + |\mathcal{L}(T_3)| - 2 \geq |\mathcal{L}(T_2)| = \lambda(T_2)$. □

Let us now choose the Perron value ρ as the function R in Definition 2. In Proposition 4.4 we show that in this case the center we obtain is exactly the characteristic set, meaning that the center concept introduced here is indeed a generalization of the characteristic set coming from the Fiedler theory. Theorem 1.1 is hence enough to show that this center is simple. However, in Proposition 4.3 we prove its simpleness *a priori*, by using the machinery introduced so far.

Proposition 4.3. *Given a tree U, $\mathcal{Z}_\rho(U)$ is simple.*

Proof. We need to show that the function $\rho : \mathcal{T} \to \mathbb{R}$ is strongly extension-monotone. The result will then follow from Proposition 4.1. Let $T_1, T_2, T_3 \in \mathcal{T}$ be such that T_1 extends T_2 via T_3 at $v \in V(T_3)$. Notice that $V(T_2) \subset V(T_1)$, and the inclusion is strict since the root of T_1 does not belong to $V(T_2)$. Let $n_1 = |V(T_1)|$ and $n_2 = |V(T_2)|$, so that $n_1 > n_2$. Consider the bottleneck matrix $A = [a_{\alpha\beta}] \in \mathbb{R}^{n_1,n_1}$ associated with T_1, and the bottleneck matrix $B = [b_{\alpha\beta}] \in \mathbb{R}^{n_2,n_2}$ associated with T_2. Let also $C = [c_{\alpha\beta}] \in \mathbb{R}^{n_2,n_2}$ be the principal submatrix of A obtained by taking the rows and columns of A indexed by elements in $V(T_2)$. Denote by x the number of edges in the path (in T_1) joining v to the root of T_1, and notice that $x > 0$ since v is not the root of T_1. From the description of entries in bottleneck matrices we gave in Section 1

$$c_{\alpha\beta} = b_{\alpha\beta} + x > b_{\alpha\beta} \qquad \alpha, \beta \in \{1, \dots, n_2\}. \tag{12}$$

Let $sr(A)$ (resp. $sr(B)$, $sr(C)$) denote the spectral radius of A (resp. B, C). Recall that A, B and C are symmetric and entrywise positive matrices. Then, (12) implies by the Perron-Frobenius theory ([10, 8.2.P5]) that $sr(C) > sr(B)$. Moreover, the Cauchy's interlacing theorem ([10, Theorem 4.3.17]) shows that $sr(A) \geq sr(C)$. It follows that

$$\rho(T_1) = sr(A) \geq sr(C) > sr(B) = \rho(T_2)$$

thus showing that ρ is strongly extension-monotone. □

We now show that Definition 2 reduces to the characteristic set when we choose the Perron value ρ as the function R.

Proposition 4.4. *Let C be the characteristic set of a tree U with more than one vertex. Then $\mathcal{Z}_\rho(U) = \{C\}$.*

Proof. We know that $\mathcal{Z}_\rho(U) = \mathcal{Z}_{\rho^U}(U)$ is the set of directed cycles in the optimality graph U_{ρ^U}. The vertex set of U_{ρ^U} is $V(U)$; its edge set is $\{e(i) \mid i \in V(U)\}$, where

- $e(i) = \overrightarrow{ij}$ if the number n_i of directed edges maximizing $\rho^U(\overrightarrow{ik}) = \rho(U_{\overrightarrow{ik}})$ among all the directed edges $\overrightarrow{ik}$ in U_{dir} having i as tail is 1, and $\overrightarrow{ij}$ is the edge attaining the maximum;
- $e(i) = \overrightarrow{ii}$ if $n_i > 1$.

Proposition 4.3 shows that $\mathcal{Z}_\rho(U)$ contains a unique cycle D, while Proposition 2.4 tells us that D can either have one or two vertices. In the first case, D corresponds to a vertex v having more than one Perron branches. In the second case, D corresponds to two adjacent vertices u and v such that the unique Perron branch at u contains v and the unique Perron branch at v contains u. In either case, from Theorem 1.1 we see that D is the characteristic set of U. □

To find the characteristic set of a tree we ultimately need to compute the spectral radius of bottleneck matrices. As we will show in more detail in Section 5, this makes the computation of $\mathcal{Z}_\rho$ relatively expensive in terms of CPU time. A more computationally efficient choice consists in using a combinatorial Perron parameter as the function R, instead of the Perron value ρ. Among the various combinatorial Perron parameters described in [2] and [3] we focus here on ρ_c, defined in (7).

Contrary to ρ, the function ρ_c is not strongly nor weakly extension-monotone, so that we cannot apply Proposition 4.1. Indeed, the ρ_c-center of a tree is in general not quasi-simple, even if it is quite laborious to find an example of this. Nevertheless, simpleness of the ρ_c-center can be achieved if we consider a specific class of trees – the so-called caterpillars – as we show in Proposition 4.9 after proving some technical results. Given a function $R : \mathcal{T} \to \mathbb{R}$, we say that R is *nontrivial* if

$$R(T) \geq 1 \quad \forall T \in \mathcal{T}, \tag{13a}$$

$$R(T) = 1 \quad \text{if and only if} \quad |V(T)| = 1. \tag{13b}$$

Proposition 4.5. *The functions ρ, ρ_c, ϑ, ζ and λ are nontrivial.*

Proof. The nontriviality of ϑ and ζ follows from their definition. To see that λ is nontrivial we use the known fact that every tree with at least two vertices has at least two leaves. To prove the nontriviality of ρ and ρ_c consider a rooted tree T. If $|V(T)| = 1$, then its bottleneck matrix is $M = [1]$ and its distance vector is $d = (1)$. Hence, both $\rho(T)$ and $\rho_c(T)$ are equal to 1. If $|V(T)| \geq 2$, then we have that

$$\rho(T) \geq \rho_c(T) \geq \|d\|_\infty = \zeta(T) > 1. \tag{14}$$

The first inequality in (14) is due to the fact that ρ_c is a lower bound for ρ; the second is Theorem 3.1; the last comes from the nontriviality of ζ proved above. □

Proposition 4.6. *Let U be a tree with $n > 2$ vertices, and let $R : \mathcal{T} \to \mathbb{R}$ be a nontrivial function. Then each cycle $C \in \mathcal{Z}_R(U)$ does not contain leaves.*

Proof. Denote by p the number of vertices in C. Let $v \in V(U)$ be a leaf, and suppose that $v \in C$. Since there is a unique (undirected) edge in U incident to v, there is a unique (directed) edge in U_{dir} having v as tail. This means that $\overrightarrow{vv} \notin E(U_{R^U})$, and hence $p > 1$. Applying Proposition 2.4, then, we conclude that $p = 2$. Let w be the vertex in C other than v. We have that $\overrightarrow{wv} \in E(U_{R^U})$, and therefore

$$R\left(U_{\overrightarrow{wv}}\right) > R\left(U_{\overrightarrow{wu}}\right) \qquad \forall\, u \text{ adjacent to } w, \quad u \neq v.$$

Since v is a leaf, the rooted tree $U_{\overrightarrow{wv}}$ has only one vertex. Using (13b) and (13a) we obtain that

$$1 = R\left(U_{\overrightarrow{wv}}\right) > R\left(U_{\overrightarrow{wu}}\right) \geq 1 \qquad \forall\, u \text{ adjacent to } w, \quad u \neq v.$$

This means that v is the only vertex in U adjacent to w, which in turn implies that U has exactly 2 vertices, contradicting the hypothesis of the Proposition. □

Combining Proposition 4.5 and Proposition 4.6 we obtain the following useful result.

Corollary 4.7. *Let U be a tree with $n > 2$ vertices, and let R be one of the functions $\rho, \rho_c, \vartheta, \zeta, \lambda$. Then each cycle $C \in \mathcal{Z}_R(U)$ does not contain leaves.*

We now focus on a class of trees called caterpillars. Given nonnegative integers $n_1, \ldots, n_k$, we define the *rooted caterpillar* $C(n_1, \ldots, n_k)$ to be the rooted tree consisting in a path P of k vertices, and n_i pendant vertices attached to the i-th vertex in P ($i \leq k$). We take the first vertex in P (associated with n_1) to be the root of $C(n_1, \ldots, n_k)$. We report here a result proved in [2] (Proposition 7.3), showing that the parameter ρ_c preserves the strict partial order defined by an extension relation in the set of rooted caterpillars.

Proposition 4.8 *([2]). Let C_1, C_2, C_3 be rooted caterpillars such that C_1 extends C_2 via C_3 at $v \in V(C_3)$ and suppose that v attains the maximum distance from the root of C_3 among the vertices of C_3. Then $\rho_c(C_1) > \rho_c(C_2)$.*

Finally, by *unrooted caterpillar* (or just *caterpillar*) we mean a rooted caterpillar where we ignore the root. Alternatively, an unrooted caterpillar can be characterized by being a tree such that there exists a path containing every non-pendant vertex.

Proposition 4.9. *Let U be a caterpillar. Then $\mathcal{Z}_{\rho_c}(U)$ is simple.*

Proof. Denote by n the number of vertices in U. If $n = 1$ or $n = 2$ the proof is trivial, so suppose $n \geq 3$. Among the possibly many paths in U containing every non-pendant vertex, choose one having maximum length, and denote it by P. Suppose that P has k vertices; since $n \geq 3$, then $k \geq 3$ too. Let C, D be two distinct cycles in $\mathcal{Z}_{\rho_c}(U)$, each of them containing either one or two vertices by virtue of Proposition 2.4. Corollary 4.7 shows that vertices in C and in D are non-pendant, and hence they must belong to P. We can label the vertices in P by $p_1, \ldots, p_k$ in such a way that the vertices in C have a smaller index than the vertices in D. Let $c = \max\{i \in \{1, \ldots, k\} \mid p_i \in C\}$ and $d = \min\{i \in \{1, \ldots, k\} \mid p_i \in D\}$. Using Corollary 4.7 and the second point of Proposition 2.3 we have that $1 < c < d < k$. Reasoning as in the proof of Proposition 2.5, we see that there must exist a vertex $x \in U$ adjacent to p_c such that $x \neq p_{c+1}$ and $\rho_c^U(\overrightarrow{p_c x}) \geq \rho_c^U(\overrightarrow{p_c p_{c+1}})$. If x is a leaf, then $\rho_c^U(\overrightarrow{p_c x}) = \rho_c(U_{\overrightarrow{p_c x}}) = 1$ by Proposition 4.5. Hence, $\rho_c^U(\overrightarrow{p_c p_{c-1}}) \geq 1 = \rho_c^U(\overrightarrow{p_c x}) \geq \rho_c^U(\overrightarrow{p_c p_{c+1}})$. If x is not a leaf, then $x = p_{c-1}$. In either case, we obtain that

$$\rho_c^U(\overrightarrow{p_c p_{c-1}}) \geq \rho_c^U(\overrightarrow{p_c p_{c+1}}). \tag{15}$$

Analogously, we find that

$$\rho_c^U(\overrightarrow{p_d p_{d+1}}) \geq \rho_c^U(\overrightarrow{p_d p_{d-1}}). \tag{16}$$

Define $\tilde{V} := (V(U_{\overrightarrow{p_c p_{c+1}}}) \setminus V(U_{\overrightarrow{p_d p_{d+1}}})) \cup \{p_{d+1}\}$, and let $\tilde{T}$ be the rooted subtree of $U_{\overrightarrow{p_c p_{c+1}}}$ induced by vertices in $\tilde{V}$ and having p_{c+1} as root. Note that $U_{\overrightarrow{p_c p_{c+1}}}$, $U_{\overrightarrow{p_d p_{d+1}}}$ and $\tilde{T}$ are rooted caterpillars, and that $U_{\overrightarrow{p_c p_{c+1}}}$ extends $U_{\overrightarrow{p_d p_{d+1}}}$ via $\tilde{T}$ at p_{d+1}. Moreover, p_{d+1} attains the maximum distance from the root p_{c+1} of $\tilde{T}$ among the vertices of $\tilde{T}$. Proposition 4.8 then shows that $\rho_c(U_{\overrightarrow{p_c p_{c+1}}}) > \rho_c(U_{\overrightarrow{p_d p_{d+1}}})$ or, equivalently,

$$\rho_c^U(\overrightarrow{p_c p_{c+1}}) > \rho_c^U(\overrightarrow{p_d p_{d+1}}). \tag{17}$$

Analogously,

$$\rho_c^U(\overrightarrow{p_d p_{d-1}}) > \rho_c^U(\overrightarrow{p_c p_{c-1}}). \tag{18}$$

Putting (15), (16), (17) and (18) together we find

$$\rho_c^U(\overrightarrow{p_c p_{c+1}}) > \rho_c^U(\overrightarrow{p_d p_{d+1}}) \geq \rho_c^U(\overrightarrow{p_d p_{d-1}}) > \rho_c^U(\overrightarrow{p_c p_{c-1}}) \geq \rho_c^U(\overrightarrow{p_c p_{c+1}})$$

which is a contradiction. □

Recall that by $\mathcal{EC}(G)$ we denote the eccentricity-center of a connected graph G, i.e., the set of vertices in G which minimize the eccentricity. Interestingly, the new notion of center that we have developed generalizes the eccentricity-center in the case of trees. This is obtained by choosing the function ζ as R in Definition 2.

Proposition 4.10. *Given a tree U, $\mathcal{Z}_\zeta(U) = \{\mathcal{EC}(U)\}$.*

Proof. If U has only one vertex the proof is trivial, so suppose that U has at least 2 vertices. Proposition 4.2 and Proposition 2.4 show that $\mathcal{Z}_\zeta(U)$ consists of a unique cycle X with either one or two vertices.

Suppose that X has a unique vertex a. We want to prove that $\mathcal{EC}(U) = \{a\}$. Let $v_1, \dots, v_k$ be the vertices adjacent to a in U, where k is the degree of a. For each $i = 1, \dots, k$ let us denote by A_i the rooted tree $U_{\overrightarrow{av_i}}$ for the sake of simplicity; let also a_i be a vertex in A_i attaining the maximum distance from the root of A_i:

$$d_{A_i}(a_i) = \max\{d_{A_i}(v) \mid v \in V(A_i)\} = \zeta^U(\overrightarrow{av_i}).$$

Let

$$S = \{i \in \{1, \dots, k\} \mid \zeta^U(\overrightarrow{av_i}) = \max_{j=1,\dots,k} \zeta^U(\overrightarrow{av_j})\}.$$

Since a is the unique vertex in the cycle X, the optimality graph U_{ζ^U} contains the loop $\overrightarrow{aa}$. This means that ζ^U attains its maximum value among the directed edges in $E(U_{dir})$ having a as tail in at least two different edges (cfr. (1)). As a consequence, $\bar{k} := |S| \geq 2$. We can assume without loss of generality that $S = \{1, \dots, \bar{k}\}$, with $2 \leq \bar{k} \leq k$. For any $\alpha, \beta \in V(U)$ we denote by $d_{\alpha,\beta}$ the number of vertices in the path joining α and β in U. We have that

$$\begin{aligned} ecc_U(a) &= \max_{u \in V(U)} (d_{a,u}) = \max_{j=1,\dots,k} \left(1 + \max_{v \in V(A_j)} (d_{A_j}(v))\right) \\ &= 1 + \max_{j=1,\dots,k} \left(\max_{v \in V(A_j)} (d_{A_j}(v))\right) = 1 + \max_{j=1,\dots,k} \left(d_{A_j}(a_j)\right) \\ &= 1 + d_{A_i}(a_i) \quad \forall i = 1, \dots, \bar{k}. \end{aligned}$$

Given a vertex $w \in V(U)$, $w \neq a$, choose $h \in \{1, \dots, \bar{k}\}$ in such a way that $w \notin V(A_h)$. Then,

$$\begin{aligned} ecc_U(w) &\geq d_{w,a_h} = d_{w,a} - 1 + d_{a,a_h} = d_{w,a} - 1 + 1 + d_{A_h}(a_h) \\ &= d_{w,a} - 1 + ecc_U(a) > ecc_U(a), \end{aligned}$$

where the last inequality comes from the fact that $d_{w,a} \geq 2$ since $w \neq a$. This shows that $w \notin \mathcal{EC}(U)$ for each $w \in V(U) \setminus \{a\}$. Since $\mathcal{EC}(U) \neq \emptyset$, we conclude that $\mathcal{EC}(U) = \{a\}$.

Suppose now that X has two distinct vertices a and b. In this case the optimality graph U_{ζ^U} contains both the directed edges $\overrightarrow{ab}$ and $\overrightarrow{ba}$. Choose a vertex $\tilde{a} \in V(U_{\overrightarrow{ab}})$ in such a way that

$$d_{U_{\overrightarrow{ab}}}(\tilde{a}) = \max\left\{d_{U_{\overrightarrow{ab}}}(v) \mid v \in V\left(U_{\overrightarrow{ab}}\right)\right\} = \zeta^U(\overrightarrow{ab})$$

and analogously choose $\tilde{b} \in V(U_{\overrightarrow{ba}})$ in such a way that

$$d_{U_{\overrightarrow{ba}}}(\tilde{b}) = \max\left\{d_{U_{\overrightarrow{ba}}}(v) \mid v \in V\left(U_{\overrightarrow{ba}}\right)\right\} = \zeta^U(\overrightarrow{ba}).$$

Reasoning as before, we see that

$$ecc_U(a) = 1 + d_{U_{\overrightarrow{ab}}}(\tilde{a}) \qquad \text{and} \qquad ecc_U(b) = 1 + d_{U_{\overrightarrow{ba}}}(\tilde{b}). \tag{19}$$

Let $w \in V(U)$, $w \neq a, b$. If $w \notin V(U_{\overrightarrow{ab}})$, then

$$\begin{aligned} ecc_U(w) &\geq d_{w,\tilde{a}} = d_{w,a} - 1 + d_{a,\tilde{a}} = d_{w,a} - 1 + 1 + d_{U_{\overrightarrow{ab}}}(\tilde{a}) \\ &= d_{w,a} - 1 + ecc_U(a) > ecc_U(a). \end{aligned}$$

If $w \in V(U_{\overrightarrow{ab}})$, then $w \notin V(U_{\overrightarrow{ba}})$, and hence

$$\begin{aligned} ecc_U(w) &\geq d_{w,\tilde{b}} = d_{w,b} - 1 + d_{b,\tilde{b}} = d_{w,b} - 1 + 1 + d_{U_{\overrightarrow{ba}}}(\tilde{b}) \\ &= d_{w,b} - 1 + ecc_U(b) > ecc_U(b). \end{aligned}$$

This shows that $\mathcal{EC}(U) \subset \{a, b\}$. If we manage to prove that $ecc_U(a) = ecc_U(b)$ we can conclude that $\mathcal{EC}(U) = \{a, b\} = X$. Suppose $ecc_U(a) \neq ecc_U(b)$ and assume w.l.o.g. that $ecc_U(a) < ecc_U(b)$. From (19) we have that $d_{U_{\overrightarrow{ab}}}(\tilde{a}) < d_{U_{\overrightarrow{ba}}}(\tilde{b})$. This in particular implies that $d_{U_{\overrightarrow{ba}}}(\tilde{b}) > 1$, and hence $a \neq \tilde{b}$. Let c be the vertex adjacent to a lying on the path connecting a to $\tilde{b}$. We have that

$$d_{U_{\overrightarrow{ac}}}(\tilde{b}) = d_{U_{\overrightarrow{ba}}}(\tilde{b}) - 1 > d_{U_{\overrightarrow{ab}}}(\tilde{a}) - 1$$

and therefore, since we are dealing with integers, $d_{U_{\overrightarrow{ac}}}(\tilde{b}) \geq d_{U_{\overrightarrow{ab}}}(\tilde{a})$. We obtain that

$$\zeta^U(\overrightarrow{ac}) = \max\left\{d_{U_{\overrightarrow{ac}}}(v) \mid v \in V\left(U_{\overrightarrow{ac}}\right)\right\} \geq d_{U_{\overrightarrow{ac}}}(\tilde{b}) \geq d_{U_{\overrightarrow{ab}}}(\tilde{a}) = \zeta^U(\overrightarrow{ab})$$

which is impossible since $\overrightarrow{ab} \in E(U_{\zeta^U})$. This shows that $ecc_U(a) = ecc_U(b)$, thus concluding the proof. □

5. The limit center and a computational comparison

We have described so far five different center-instances for a given tree U, all of them coming from Definition 2: $\mathcal{Z}_\rho(U)$, $\mathcal{Z}_{\rho_c}(U)$, $\mathcal{Z}_\vartheta(U)$, $\mathcal{Z}_\zeta(U)$ and $\mathcal{Z}_\lambda(U)$. It is interesting to see how computationally efficient it is to find each one of these centers, and how "close" they are. By virtue of Proposition 4.2 and Proposition 4.3 we know that $\mathcal{Z}_\rho(U)$, $\mathcal{Z}_\vartheta(U)$ and $\mathcal{Z}_\zeta(U)$ are simple – which means, as shown in Proposition 2.4, that they consist of either one or two adjacent vertices. In order to make the comparison more meaningful,

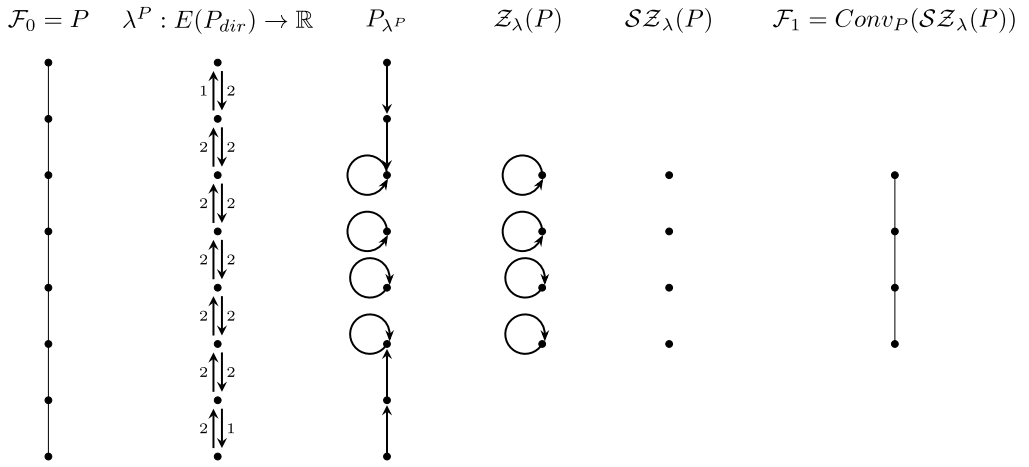


Fig. 5. One iteration of the "center" operator on a path P with 8 vertices, using the weight $R = \lambda$.

however, we would like each one of the five centers to be simple. This can be achieved by iterating the "center" operator for a sufficient number of times. We formalize this idea by defining the *limit center* of a tree.

Consider a set of vertices $S \subset V(U)$. The *convex hull* of S in U – denoted by $Conv_U(S)$ – is the smallest subtree of U containing all the vertices in S. Given a function $R : \mathcal{T} \to \mathbb{R}$, we recursively define the sequence of trees $(\mathcal{F}_i)_i$ as follows:

$$\begin{aligned} \mathcal{F}_0 &:= U; \\ \mathcal{F}_{i+1} &:= Conv_{\mathcal{F}_i}(\mathcal{SZ}_R(\mathcal{F}_i)), \quad i = 0, 1, 2, \dots \end{aligned} \tag{20}$$

where $\mathcal{SZ}_R$ was defined in (11) (see Fig. 5). Also, we let $\mathcal{V}_i := V(\mathcal{F}_i)$, $i = 0, 1, 2, \dots$, and we define the *limit R-center* of U to be

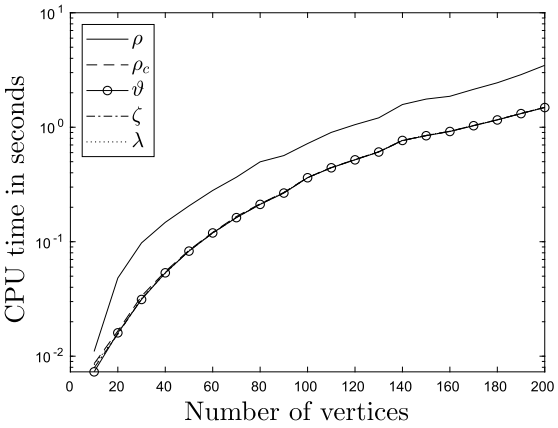
$$\mathcal{Z}_R^\infty(U) := \bigcap_{i \geq 0} \mathcal{V}_i.$$

Proposition 5.1. *Let U be a tree and let R be one of the functions $\rho, \rho_c, \vartheta, \zeta, \lambda$. Then $\mathcal{Z}_R^\infty(U)$ consists of either one or two adjacent vertices.*

Proof. Consider the three statements

1. $\mathcal{V}_{i+1} \subset \mathcal{V}_i, \quad i = 0, 1, 2, \dots;$
2. $|\mathcal{V}_i| > 0, \quad i = 0, 1, 2, \dots;$
3. $|\mathcal{V}_{i+1}| < |\mathcal{V}_i| \quad \text{if } |\mathcal{V}_i| > 2.$

They together imply the Proposition. Statement 1. directly follows from the recursive definition (20). Statement 2. is also clear by virtue of the first point of Proposition 2.3.



	ρ	ρ_c	ϑ	ζ	λ
ρ	0	0.03	0.21	0.55	0.25
ρ_c		0	0.24	0.55	0.28
ϑ			0	0.72	0.06
ζ				0	0.73
λ					0

Fig. 6. Left: average CPU time to find the limit R-centers of randomly generated trees with increasing number of vertices. Right: average distance between the limit R-centers of randomly generated trees with 200 vertices (distances are computed here following the same procedure used in a similar analysis in [2, §7]). All the computations use algorithms written in MATLAB.

To prove statement 3., suppose that $|\mathcal{V}_i| = |V(\mathcal{F}_i)| > 2$ for some i, and let v be a pendant vertex of $\mathcal{F}_i$. Corollary 4.7 shows that v does not belong to any cycle in $\mathcal{Z}_R(\mathcal{F}_i)$; hence, $v \notin \mathcal{SZ}_R(\mathcal{F}_i)$. Since v is pendant in $\mathcal{F}_i$, then $v \notin Conv_{\mathcal{F}_i}(\mathcal{SZ}_R(\mathcal{F}_i)) = \mathcal{F}_{i+1}$. Hence, statement 3. holds and the Proposition is proved. □

We can give the limit R-center a more intuitive description. Start with a tree, take the convex hull of the support of its R-center and iterate this operation. After a finite number of iterations, this process stabilizes; moreover, if R is one of the five functions considered above, Proposition 5.1 shows that, when it stabilizes, we necessarily have one or two adjacent vertices. If $R = \rho$, ϑ or ζ, this result is not surprising; indeed, in this case $\mathcal{Z}_R(U)$ is already simple, so that the process stabilizes after just one iteration: $\mathcal{F}_1 = \mathcal{F}_2 = \mathcal{F}_3 = \dots$ (notice, in this regard, that if $\mathcal{F}_i$ is the tree of one or two vertices, then $\mathcal{F}_{i+1} = \mathcal{F}_i$ for any function R), and therefore $\mathcal{Z}_R^\infty(U) = \mathcal{V}_1 = \mathcal{SZ}_R(U)$. If $R = \rho_c$ or λ, however, more iterations may be necessary. For example, when $R = \lambda$ and the starting tree is $\mathcal{P}_{16}$ (we denote by $\mathcal{P}_n$ the path on n vertices), applying repeatedly the procedure outlined in Fig. 5 we obtain that the sequence $(\mathcal{F}_i)_i$ is given by

$$\mathcal{F}_0 = \mathcal{P}_{16}, \quad \mathcal{F}_1 = \mathcal{P}_{12}, \quad \mathcal{F}_2 = \mathcal{P}_8, \quad \mathcal{F}_3 = \mathcal{P}_4, \quad \mathcal{F}_4 = \mathcal{F}_5 = \mathcal{F}_6 = \dots = \mathcal{P}_2.$$

Fig. 6 shows the results of a computational comparison of the various limit R-centers. It emerges that computing $\mathcal{Z}_\rho^\infty$ (i.e. the characteristic set, see Proposition 4.4) is significantly more expensive than computing the other four centers. The reason behind this is that the former requires the calculation of spectral radii of matrices, while all the other centers only use algebraic and combinatorial expressions. On the other hand, the five centers are in general very close among each other; in particular, the average distance

between $\mathcal{Z}_{\rho}^{\infty}$ and $\mathcal{Z}_{\rho_c}^{\infty}$ is extremely small, which confirms the results presented in [2] and [3], showing that ρ_c is a good approximation of ρ.

In summary, the center concept presented in this work not only generalizes the characteristic set coming from the Fiedler theory, but it also provides – in the case of trees – very close approximations of it, which are significantly cheaper to compute in terms of CPU time.

6. Discrete differential and discrete concavity

In Section 4 and Section 5 we adapted the notion of μ-center (Definition 1) to make it fit the situation where the underlying graph is a tree and μ comes from a function R defined on rooted trees. Here we abandon the requirement of the graph being a tree, and we focus on a class of functions μ which can be viewed as "differentials" of functions defined on the vertex set of the given graph.

Consider a connected graph G and a function $f : V(G) \to \mathbb{R}$. We define the *discrete differential* of f to be the function

$$\begin{aligned} Df : E(G_{dir}) &\to \mathbb{R} \\ \overrightarrow{ij} &\mapsto f(j) - f(i). \end{aligned}$$

Note the similarity of this definition to that of the standard differential of a function $g : \mathbb{R}^n \to \mathbb{R}$ at a point $P \in \mathbb{R}^n$ along a vector $\mathbf{u} \in T_P\mathbb{R}^n$, where $T_P\mathbb{R}^n$ is the tangent space of $\mathbb{R}^n$ at P. In our setting, the vertex i represents the point P, while the directed edge $\overrightarrow{ij}$ has the role of $\mathbf{u}$. This new object allows us to define in a natural way a center of G associated with f.

Definition 3. Given a connected graph G and a function $f : V(G) \to \mathbb{R}$ we define the *f-center* of G as $\mathcal{Z}_f(G) := \mathcal{Z}_{Df}(G)$ (with $\mathcal{Z}_{Df}(G)$ as in Definition 1).

We now investigate some conditions making the center defined above simple or quasi-simple. It is useful, for this purpose, to find a more intuitive interpretation of $\mathcal{Z}_f(G)$. Consider the optimality graph G_{Df}. This is obtained by drawing, for each vertex $i \in V(G) = V(G_{Df})$, the directed edge $\overrightarrow{ij}$ maximizing Df among all the directed edges having i as tail (we only consider, for simplicity, the case where the maximum is unique). In other words, $\overrightarrow{ij}$ is the direction of maximum increase of f at i, so that we can consider it to be the *discrete gradient* of f at i, and G_{Df} to be the *discrete gradient map* of f. A cycle in G_{Df} corresponds to a change in direction of the gradient and would imply the existence – in the continuous case – of an attractor point in the gradient map, where the gradient is zero: a local maximum. We can then interpret $\mathcal{Z}_f(G)$ as the set of local maxima of f. In this perspective, $\mathcal{Z}_f(G)$ being simple corresponds to f having a unique local maximum in G. This suggests that the feature f should have to make $\mathcal{Z}_f(G)$ simple is *concavity*.

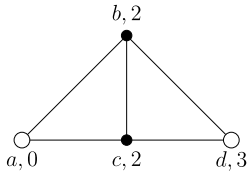


Fig. 7. The graph G. Next to each vertex there is its label and the corresponding value of f. The f-center of G consists of two 1-cycles corresponding to the two vertices in white.

Given two vertices $\alpha, \beta \in V(G)$, we let $\tilde{d}_{\alpha,\beta}$ denote the number of *edges* in a shortest path connecting α and β. Following [6], we say that the function $f : V(G) \to \mathbb{R}$ is *weakly concave* if the inequality

$$f(y) \geq \frac{\tilde{d}_{y,z}}{\tilde{d}_{x,z}} f(x) + \frac{\tilde{d}_{y,x}}{\tilde{d}_{x,z}} f(z) \tag{21}$$

holds for each triplet of distinct vertices $x, y, z \in V(G)$ such that y lies in some shortest path joining x to z. We say that f is *strongly concave* if inequality (21) is always strict.

Proposition 6.1. *Let G be a triangle-free connected graph. If $f : V(G) \to \mathbb{R}$ is strongly concave (resp. weakly concave), then $\mathcal{Z}_f(G)$ is simple (resp. quasi-simple).*

Proof. Suppose that f is strongly concave, and consider three distinct vertices $i, j, k \in V(G)$ such that i is adjacent to j and j is adjacent to k. Since G is triangle-free, i is not adjacent to k. This means that j lies in the shortest path $P = ijk$ connecting i to k. Using the concavity of f we obtain that $f(j) > \frac{1}{2}f(i) + \frac{1}{2}f(k)$, which can be rewritten as $f(j) - f(i) > f(k) - f(j)$ or, alternatively, as $Df(\overrightarrow{ij}) > Df(\overrightarrow{jk})$. The map Df is hence strongly path-monotone. If f is weakly concave we analogously obtain that Df is weakly path-monotone. The result then follows from Proposition 2.5. □

The requirement of the graph being triangle-free is necessary in Proposition 6.1. Consider for example the graph G in Fig. 7, and the function $f : V(G) \to \mathbb{R}$ defined by $f(a) = 0, f(b) = f(c) = 2, f(d) = 3$. One can check that f is strongly concave: the only triplets of vertices which need to be considered are abd and acd, and they both satisfy (21) with strict inequality. However, $\mathcal{Z}_f(G)$ consists of the two cycles aa and dd, so that it is not simple and not even quasi-simple.

Declaration of competing interest

The author declares that he has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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