Journal of Combinatorial Optimization (2023) 45:107
https://doi.org/10.1007/s10878-023-01022-9

Tree-optimized labeled directed graphs

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Accepted: 24 March 2023

Abstract
For an additive submonoid $\mathcal{M}$ of $\mathbb{R}_{\ge 0}$, the weight of a finite $\mathcal{M}$-labeled directed graph is the sum of all of its edge labels, while the content is the product of the labels. Having fixed $\mathcal{M}$ and a directed tree E, we prove a general result on the shape of finite, acyclic, $\mathcal{M}$-labeled directed graphs Γ of weight $N \in \mathcal{M}$ maximizing the sum of the contents of all copies $E \subset \Gamma$. This specializes to recover a result of Hajac and the author's on the maximal number of length-k paths in an acyclic directed graph with N edges. It also applies to prove a conjecture by the same authors on the maximal sum of entries of A^k for a nilpotent $\mathbb{R}_{\ge 0}$-valued square matrix A whose entries add up to N. Finally, we apply the same techniques to obtain the maximal number of stars with α arms in a directed graph with N edges.

Keywords Acyclic directed graph · Labeled graph · Path · Star

Mathematics Subject Classification 05C35 · 05C20 · 05C30

1 Introduction

This note is motivated by (Hajac and Tobolski 2019, Theorem 1.10) and various ramifications thereof. The result in question gives a sharp upper bound for the number of length-k paths in an acyclic directed graph (henceforth ADG, for short) with N edges:

Theorem 1 *Let k and N be positive integers and $N = kq + r$ the decomposition of N modulo k. Then, an ADG with N edges contains at most $(q+1)^r q^{k-r}$ directed paths of length k.*

There is an alternative way to state the result, that is perhaps more conceptually expressive:

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Published online: 05 May 2023

Corollary 2 *Let N and k be two positive integers. The following numbers are then equal:*

(a) The maximal number of length-k paths in an N-edge ADG;
(b) The maximal product of k non-negative integers with sum N.

The fact that the maximum in point (b) is achieved for the "best-balanced" k-tuple

$$q+1,\ q+1,\ \cdots,\ q+1,\ q,\ q,\ \cdots,\ q$$

of positive integers can be seen easily, by noting for instance that if $a - b \geq 2$ then $ab < (a-1)(b+1)$ and replacing such pairs (a, b) of positive integers in the tuple with $(a-1, b+1)$ until the maximum is achieved.

(Hajac and Tobolski 2019, Conjecture 1.20) is an analogue of Theorem 1 obtained by relaxing the constraints on the adjacency matrix of the graph to allow for non-negative *real* (rather than integral) entries. To state it we introduce, for a matrix

$$A \in M_n(\mathbb{R}_{\geq 0})$$

with non-negative entries, the *weight*

$$|A| := \sum_{i,j=1}^{n} A_{ij}$$

(i.e. the sum of all of its entries). Then, (Hajac and Tobolski 2019, Conjecture 1.20) reads

Conjecture 3 *Let N be a non-negative real number, k a positive integer, and A a nilpotent square matrix of weight N with entries in $\mathbb{R}_{\geq 0}$. Then,*

$$|A^k| \leq \left(\frac{N}{k}\right)^k$$

and equality is achieved, e.g. by the $(k+1)\times(k+1)$ matrix with k entries $\frac{N}{k}$ immediately above the main diagonal and 0s elsewhere.

A finite directed graph will provide a non-negative adjacency matrix A as above, with rows and columns indexed by vertices and such that A_{ij} is the number of edges from i to j. The nilpotence encodes the fact that the graph is acyclic.

Remark 4 (Hajac and Tobolski 2019, Conjecture 1.20 also imposes the condition that the directed graph underlying the matrix A have no isolated vertices, i.e. that there be no i such that the i^{th} row and column are both zero. This condition seems unnecessary. □

We can restate the conjecture by analogy to Corollary 2.

Conjecture 5 *Let N be a non-negative real number and k a positive integer. The following numbers are then equal:*

- *The maximal weight of A^k, where A is a nilpotent square matrix of weight N with non-negative real entries;*
- *The maximal product of k non-negative real numbers with sum N;*
- $\left(\frac{N}{k}\right)^k$.

Of course, the fact that the last two items are equal is nothing but the arithmetic–geometric-mean inequality. We confirm Conjectures 3 and 5 as a particular case of one of the main results of the present note (see Theorem 3.4 and Corollary 3.5):

Theorem 6 *Conjectures 5 holds.* ■

After a short introduction to the terminology and conventions in Sect. 2 we prove Theorem 3.2, stating that given an additive submonoid $\mathcal{M}$ of $\mathbb{R}$ and a directed graph E, the supremum of

$$\sum_{\text{copies of } E \text{ contained in } \Gamma} \text{product of labels of the edges of } E$$

as Γ ranges over the $\mathcal{M}$-labeled directed graphs equals the analogous supremum over only those Γ for which every two edges lie on a common copy of $E \subset \Gamma$.

This then recovers Theorem 1, proves Conjectures 5, and can be used to count the maximal number of a-arm stars in a directed graph with N edges (Corollary 3.10).

2 Preliminaries

All graphs under discussion are finite and directed, so we often drop these adjectives. As in the Introduction, we abbreviate the phrase 'acyclic directed graph' (i.e. one without oriented cycles of any length, including single-edge loops) as 'ADG'.

Definition 2.1 Let $\mathcal{M}$ be a set with a distinguished symbol '0'. An $\mathcal{M}$-*labeled* directed graph is a directed graph without repeated edges for which every pair (x, y) of vertices carries a label $\ell(x, y) \in M$, with label 0 precisely when (x, y) is not and edge.

Plain directed graphs, possibly with repeated edges, can be alternatively regarded as $\mathbb{Z}_{\geq 0}$-labeled directed graphs *without* repeated edges, with (x, y) carrying the label $m \in \mathbb{Z}_{\geq 0}$ if there are m edges $x \to y$.

The *adjacency matrix* of an $\mathcal{M}$-labeled graph on the vertex set I is the $\mathcal{M}$-valued matrix whose (i, j) entry (for $i, j \in I$) is $\ell(x, y)$.

Definition 2.2 If $\mathcal{M} \subseteq \mathbb{R}_{\geq 0}$, the *content* of an $\mathcal{M}$-labeled graph Γ is

$$\operatorname{ct} \Gamma := \prod_{\text{edges } (x,y)} \ell(x, y)$$

and its *weight* is

$$\mathrm{wt}\,\Gamma := \sum_{\text{edges }(x,y)} \ell(x, y)$$

Similarly, if S is a set of edges in Γ, the S-*exclusive content* of Γ is

$$\mathrm{ct}_{\not S}\,\Gamma := \prod_{\text{edges }(x,y)\notin S} \ell(x, y).$$

With all of this in place, Theorem 1 and Corollary 2 (which in turn paraphrase (Hajac and Tobolski Hajac and Tobolski (2019), Theorem 1.10 and Corollary 1.19)) can be conjoined as

Theorem 2.3 *Let N and k be two positive integers, and $N = kq + r$ be the decomposition of N modulo k. The following quantities all admit the same maximal value $(q + 1)^r q^{k-r}$.*

- *The number of length-k paths in an N-edge ADG;*
- *The sum*

$$\sum_{\textit{length-}k\textit{ paths in }\Gamma} \mathrm{ct}(\textit{path})$$

  for $\mathbb{Z}_{\geq 0}$-labeled ADGs Γ;
- *The weight of A^k, where A is a square $\mathbb{Z}_{\geq 0}$-valued nilpotent matrix of weight N;*
- *The product of k non-negative integers with sum N.* ■

The fact that the first two optimization problems are identical follows immediately by recasting plain ADGs as labeled ADGs as in Definition 2.1. On the other hand, translating this into the language of the third item is simply passing between an ADG and its adjacency matrix.

With this phrasing, Theorem 3.4 below provides a direct generalization of Theorem 2.3.

3 Optimizing labeled graphs

Theorem 2.3 and the results mentioned in the discussion preceding it are concerned with counting *paths* in a directed graph. We will first prove a general principle applicable to optimization problems, with general directed graphs in place of paths.

Specifically, let E be a fixed finite *simple* directed graph (i.e. without repeated edges or loops), that will play the same role as a length-k path did above. Let also $(\mathcal{M}, +)$ be a submonoid of $(\mathbb{R}_{\geq 0}, +)$.

Definition 3.1 Let Γ be an $\mathcal{M}$-labeled directed graph. We define

$$\mathrm{ct}^E(\Gamma) = \mathrm{ct}^E_{\mathcal{M}}(\Gamma) := \sum_{\alpha} \mathrm{ct}(\alpha),$$

with α ranging over the subgraphs of Γ isomorphic to E, with the $\mathcal{M}$-labeling inherited from Γ. □

We then have

Theorem 3.2 *Let*

- E *be a directed graph with no repeated edges;*
- $(\mathcal{M}, +)$ *a submonoid of* $(\mathbb{R}_{\geq 0}, +)$*;*
- $N \in \mathcal{M}$ *an element.*

Then, $\sup\ \mathrm{ct}^E_{\mathcal{M}}(\Gamma)$ *for* $\mathcal{M}$*-labeled* Γ *of weight* N *is achieved over graphs* Γ *with the following property:*

$$\textit{Every vertex, edge or pair of edges of } \Gamma \textit{ belongs to some embedded copy } E \subset \Gamma. \tag{3.1}$$

Proof We have to prove that given an $\mathcal{M}$-labeled Γ of weight N, $\mathrm{ct}^E_{\mathcal{M}}$ can be improved by altering Γ progressively until we achieve 3.1.

First, as long as there are edges e belonging to no embedded $E \subset \Gamma$, we can erase them and transfer their labels to other edges by changing some $\ell(f)$ to $\ell(f) + \ell(e)$. Having exhausted the problematic edges, we can then delete vertices not belonging to any embedded copies of E, and so forth. This process will eventually stop, since we have finitely many vertices/edges to drop.

Next, suppose the edges e and f of Γ do *not* belong to a common copy $E \subset \Gamma$. Then, the sets $\mathcal{S}_e$ and $\mathcal{S}_f$ of E-subgraphs of Γ containing e and f respectively are disjoint. For each E-subgraph $\alpha \in \mathcal{S}_e$ containing e, consider the e-exclusive content $\mathrm{ct}_{\not e}\ \alpha$ as in Definition 2.2, and similarly for f. Without loss of generality, suppose

$$\Sigma_e := \sum_{\alpha \in \mathcal{S}_e} \mathrm{ct}_{\not e}\ \alpha$$

is at least as large as its counterpart

$$\Sigma_f := \sum_{\beta \in \mathcal{S}_f} \mathrm{ct}_{\not f}\ \beta.$$

We can then eliminate edge f and recycle its label into e, updating $\ell(e)$ to $\ell(e)+\ell(f)$. This modification of the graph will

- Not decrease $\mathrm{ct}^E_{\mathcal{M}}$; indeed, the latter is incremented by

$$\ell(f)\left(\Sigma_e - \Sigma_f\right) \geq 0,$$

  since we lose the terms of $\mathrm{ct}^E_{\mathcal{M}}$ corresponding to graphs containing f, making for an initial decrement of $\ell(f)\Sigma_f$, but boost the terms corresponding to graphs containing e by promoting the latter's label to $\ell(e) + \ell(f)$, giving an *increment* of $\ell(f)\Sigma_e$.

- Decrease the number of pairs of edges that do *not* belong to the same $E \subset \Gamma$.

We can continue the process so long as there are such pairs of edges, so the procedure concludes precisely when we have obtained a graph satisfying 3.1. This finishes the proof. □

3.1 Paths

Theorem 3.2 has a number of consequences germane to the problems discussed in the introduction. The present subsection focuses on the case where the graph E is a(n oriented) *path*: a graph of the form

$$\bullet \longrightarrow \bullet \longrightarrow \cdots \longrightarrow \bullet,$$

where the vertices are distinct (so the term entails acyclicity). The *length* of the path is the number of edges (possibly 0). One simple observation:

Lemma 3.3 *Let k be a positive integer and E a length-k oriented path. The only directed graphs Γ satisfying 3.1 are length-k paths and cycles any of the lengths $k+1$ up to $2k-1$.*

Proof Every vertex is incident to at least one edge (being contained in a length-k path). Since edges incident to two distinct vertices are contained in common paths, the graph Γ is connected.

Furthermore, a vertex cannot act as a source (or target) for more than one edge: two incident edges with the same source or target could not belong to a single path. It follows, then, that either vertex is

- Incident to precisely one edge (either as a source or target);
- Or a source for exactly one edge and a target for exactly one other.

One direction is simpler: if Γ is of the stated form, checking that it has property 3.1 is immediate. For the converse, there are a few cases to consider:

(a) *There is a vertex v_0*, source of the unique edge e_1 containing it There must then be a length-k path

$$v_0 \xrightarrow{e_1} v_1 \xrightarrow{e_2} \cdots \xrightarrow{e_k} v_k, \tag{3.2}$$

unique among those containing v_0. But then there can be no edge $v_k \xrightarrow{e_{k+1}} \bullet$, for it would not be contained in a length-k path together with e_1. It follows that the only edges incident to any of the v_i are the e_j depicted in 3.2, so that this must be the totality of Γ by the aforementioned connectedness.

(b) *There is a vertex v_0*, target of the unique edge e_1 containing it This is essentially the same argument: simply interchange the roles of sources and targets.

(c) *Every vertex is incident to precisely two edges* Together with connectedness, this condition ensures that the graph is a cycle. That the length is limited to the specified range is not difficult to see:

- Cycles of length $\leq k$ do not contain embedded copies of a length-k path at all;
- While cycles of length $\geq 2k$ contain pairs of edges too far apart to fit into a length-k path.

This concludes the proof. □

Theorem 3.4 *Let k be a positive integer, $(\mathcal{M}, +)$ a submonoid of $(\mathbb{R}_{\geq 0}, +)$ and $N \in \mathcal{M}$ an element. The following quantities all admit the same maximal value.*

(1) The sum

$$\sum_{\text{length-}k \text{ paths in } \Gamma} \mathrm{ct}(\textit{path})$$

for $\mathcal{M}$-labeled ADGs Γ of weight N;
(2) The weight of A^k, where A is a square $\mathcal{M}$-valued nilpotent matrix of weight N;
(3) The product of k non-negative elements of $\mathcal{M}$ with sum N.

Proof Given the bijective correspondence between adjacency matrices and graphs, we can argue that (1) and (2) have the same optimal value as follows: if A is the adjacency matrix of the labeled ADG Γ then the length-k paths in Γ are in bijection with the non-zero entries of A^k, and those entries are precisely the contents of the respective paths.

It thus remains to argue that the common maximal value of (1) and (2) also equals that of (3). This entails proving two inequalities:

$$\max\ (3) \leq \max\ (1) \tag{3.3}$$

and

$$\max\ (1) \leq \max\ (3). \tag{3.4}$$

3.3 is easier to prove: simply note that every k-tuple of elements in $\mathcal{M}$ can be realized as the k labels of a length-k path Γ.

As for 3.4, Theorem 3.2 applied to a k-path E and Lemma 3.3 imply that the maximum is achieved by an $\mathcal{M}$-labeled length-k path, and the labels of its k edges will be the k elements in (3). □

Corollary 3.5 *Conjectures 5 holds.*

Proof Simply take $\mathcal{M} = \mathbb{R}_{\geq 0}$ in Theorem 3.4 and observe, as in the Introduction, that the maximal value in (3) is achieved when all labels are equal to $\frac{N}{k}$ by the arithmetic–geometric-mean inequality. □

3.2 Stars

The following notion of oriented tree is fairly common in the literature (see e.g. (Knuth 1967, p.310).

Definition 3.6 An *oriented tree with root* v (or *rooted at* v) is an oriented graph with a distinguished vertex v such that for each vertex w there is a unique oriented path $w \to v$.

A *leaf* in such a rooted tree is a vertex attached to a single edge, for which it is a source.

The *arms* of a rooted oriented tree are its maximal oriented paths (so they all connect a leaf to the root).

In this section we focus on specific classes of rooted directed trees.

Definition 3.7 A rooted directed tree is ℓ-*equidistal* if all of its arms have the same length ℓ. It is a *star* if any two arms intersect only at their common target (i.e. the root of the tree).

Finally, a rooted directed tree is a ℓ-*star* if it is both a star and ℓ-equidistal.

The preceding discussion focused on k-paths, which are k-stars with one arm. At the other end of the spectrum, we can consider 1-stars with α arms instead. The analogue of Theorem 3.4 is

Theorem 3.8 *Let*

- E *be a* 1-*star with* α *arms;*
- $(\mathcal{M}, +)$ *a submonoid of* $(\mathbb{R}_{\geq 0}, +)$*;*
- $N \in \mathcal{M}$.

The following quantities all admit the same supremum.

(1) The sum

$$\mathrm{ct}^E_{\mathcal{M}}(\Gamma) = \sum_{1-stars\ with\ \alpha arms\ contained\ in\ \Gamma} \mathrm{ct}(star)$$

for $\mathcal{M}$*-labeled ADGs* Γ *of weight* N*, with stars* $\alpha \subseteq \Gamma$ *inheriting their labelings.*

(2) The α^{th} *elementary symmetric sum evaluated at some* t*-tuple of elements in* $\mathcal{M}$ *with sum* N *(for varying* t*):*

$$\sum_{1 \leq i_1 < \cdots < i_\alpha \leq t} \lambda_{i_1} \cdots \lambda_{i_\alpha}, \quad \lambda_i \in \mathcal{M}, \quad \sum \lambda_i = N. \tag{3.5}$$

Proof According to Theorem 3.2 it is enough to range over $\mathcal{M}$-labeled ADGs Γ for which every two edges lie in some common copy of $E \subset \Gamma$. In this case Γ itself is a 1-star with $t \geq \alpha$ arms.

If λ_i, $1 \leq i \leq t$, are the labels of the t arms of Γ so that

$$\sum_{i=1}^{t} \lambda_i = N,$$

then the content $\mathrm{ct}^E(\Gamma)$ is the α^{th} elementary symmetric function evaluated at the λ_i. This concludes the proof. □

The following consequence is a kind of continuous version of counting the maximal number such stars in an ADG with N edges.

Corollary 3.9 *Let*

- *E be a 1-star with α arms;*
- *$N \in \mathbb{R}_{\geq 0}$.*

The supremum

$$\sup_{\Gamma} \operatorname{ct}^{E}_{\mathbb{R}_{\geq 0}}(\Gamma), \quad \Gamma \textit{ an } \mathbb{R}_{\geq 0} - \textit{labeled directed graph of weight } N$$

is $\frac{N^\alpha}{\alpha!}$.

Proof According to Theorem 3.8, we want the supremum of 3.5 for $\lambda_i \in \mathbb{R}_{\geq 0}$ and varying t. For fixed t that expression is maximal when all λ_i are equal (to $\frac{N}{t}$), e.g. by *Maclaurin's inequality* (Zdravko 2012, Theorem 11.2). It follows that 3.5 is at most

$$\binom{t}{\alpha} \cdot \left(\frac{N}{t}\right)^\alpha = \frac{N^\alpha t(t-1)\cdots(t-\alpha+1)}{\alpha! t^\alpha}. \tag{3.6}$$

The t-dependent factors

$$\frac{t-m}{t} = 1 - \frac{m}{t}, \quad m = 0,\ 1,\ \cdots,\ \alpha - 1$$

are all non-decreasing in t and hence so is the expression 3.6. As $t \to \infty$ the right hand side converges to its supremum $\frac{N^\alpha}{\alpha!}$, hence the conclusion. □

As for the discrete version, it reads

Corollary 3.10 *Let N and α be two positive integers. The following quantities all have the same maximal value $\binom{N}{\alpha}$*

(1) The number of 1-stars with α arms contained in directed graph with N edges;
(2) The sum

$$\sum_{1-\textit{stars with } \alpha \textit{ arms contained in } \Gamma} \operatorname{ct}(star)$$

for $\mathbb{Z}_{\geq 0}$-labeled directed graphs Γ of weight N;
(3) The α^{th} elementary symmetric sum evaluated at some t-tuple of non-negative integers with sum N (for varying t):

$$\sum_{1 \leq i_1 < \cdots < i_\alpha \leq t} \lambda_{i_1} \cdots \lambda_{i_\alpha}, \quad \lambda_i \in \mathbb{Z}_{\geq 0}, \quad \sum \lambda_i = N. \tag{3.7}$$

Proof That (1) and (2) have the same optimal value follows as in the discussion following Theorem 2.3, by recasting repeated edges in a directed graph as $\mathbb{Z}_{\geq 0}$-labels. On the other hand, the fact that (1) and (2) have the same optimal value follows from Theorem 3.8 applied to $\mathcal{M} = \mathbb{Z}_{\geq 0}$ and E an a-arm 1-star. It thus remains to prove that the supremum is a maximum, and that that maximum is $\binom{N}{\alpha}$.

As in the proof of Theorem 3.8, we can assume Γ is a 1-star with t arms and respective labels $\lambda_i \in \mathbb{Z}_{>0}$, $1 \leq i \leq t$ (the labels can be assumed positive because 0 labels make no contribution to 3.7). In particular, $t \leq N$.

Having fixed t, we observed in the proof of Corollary 3.9 that the elementary symmetric function 3.7 is dominated by

$$\binom{t}{\alpha} \cdot \left(\frac{N}{t}\right)^{\alpha} = \frac{N^{\alpha} t(t-1)\cdots(t-\alpha+1)}{\alpha! t^{\alpha}}.$$

We saw in the proof of Corollary 3.9 why this expression is non-decreasing in t, so it reaches its maximum at $t = N$. That maximum is precisely

$$\binom{t}{\alpha} = \binom{N}{\alpha},$$

and is achievable by an $\mathbb{Z}_{\geq 0}$-labeled N-armed 1-star by simply assigning label $\lambda_i = 1$ to each of the N edges. □

Acknowledgements This work was partially supported by NSF grants DMS-1801011 and DMS-2001128, and is part of the project "Applications of graph algebras and higher-rank graph algebras in noncommutative geometry", partially supported by NCN grant UMO-2021/41/B/ST1/03387. I am grateful for input from P.M. Hajac and M. Tobolski, as well as the referees' insightful suggestions.

Data availability Not applicable.

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