Tree-optimized directed graphs

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Abstract

For an additive submonoid $\mathcal{M}$ of $\mathbb{R}_{\geq 0}$, the weight of an $\mathcal{M}$-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 directed $\mathcal{M}$-labeled graphs $\Gamma$ 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 Tobolski on the maximal number of length-$k$ paths in a directed acyclic graph. It also applies to prove a conjecture by the same authors on the maximal sum of entries of $A^k$ for a nilpotent $\mathbb{R}_{\geq 0}$-valued square matrix $A$ whose entries add up to $N$. Finally, we apply the same techniques to obtain the maximal number of stars with $a$ arms in a directed graph with $N$ edges.

Key words: directed acyclic graph, labeled graph, path, star

MSC 2010: 05C35; 05C20; 05C30

Introduction

This note is motivated by [1, Theorem 1.10] and various ramifications thereof. The result in question gives a sharp upper bound for the number of length-$k$ paths in a directed acyclic graph (henceforth DAG, for short) with $N$ edges:

**Theorem 0.1** Let $k$ and $N$ be positive integer, with $N = kq + r$ be the decomposition of $N$ modulo $k$. Then, a DAG 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:

**Corollary 0.2** 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 DAG;

(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.

[1, Conjecture 1.20] is an analogue of Theorem 0.1 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 \textit{weight} 
\[ |A| := \sum_{i,j=1}^n A_{ij} \]
(i.e. the sum of all of its entries). Then, [1, Conjecture 1.20] reads

\textbf{Conjecture 0.3} Let \( N \) be a non-negative real and \( k \) a positive integer, and \( A \) a nilpotent square matrix with entries in \( \mathbb{R}_{\geq 0} \) of weight \( N \). Then,

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

and equality is achievable.

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.

\textbf{Remark 0.4} [1, 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 0.2.

\textbf{Conjecture 0.5} Let \( N \) be a non-negative real 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 reals 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 0.3 and 0.5 as a particular case of one of the main results of the present note (see Theorem 2.4 and corollary 2.5):

\textbf{Theorem 0.6} Conjecture 0.5 holds.

After a short introduction to the terminology and conventions in Section 1 we prove Theorem 2.2, stating that given a closed additive submonoid \( M \) of \( \mathbb{R} \) and a directed graph \( E \), the supremum of

\[ \sum \text{ product of labels of the edges of } E \]

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

This then recovers Theorem 0.1, proves Conjecture 0.5, and can be used to count the maximal number of \( a \)-arm stars in a directed graph with \( N \) edges (Corollary 2.10).
Acknowledgements

This work was partially supported by NSF grant DMS-1801011.
I am grateful for input from P.M. Hajac and M. Tobolski.

1 Preliminaries

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

Definition 1.1 Let $\mathcal{M}$ be a set with a distinguished symbol ‘0’. An $\mathcal{M}$-labeled directed graph is a simple directed graph (i.e. no repeated edges) for which every pair $(x, y)$ of vertices carries a label $\ell(x, y) \in \mathcal{M}$, with label 0 precisely when $(x, y)$ is not an 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 1.2 If $\mathcal{M} \subseteq \mathbb{R}_{\geq 0}$ the content of an $\mathcal{M}$-labeled graph $\Gamma$ is

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

and its weight is

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

Similarly, if $S$ is a set of edges in $\Gamma$, the $S$-exclusive content of $\Gamma$ is

$$\text{ct}_S \Gamma := \prod_{\text{edges } (x,y) \notin S} \ell(x, y).$$

With all of this in place, Theorem 0.1 and corollary 0.2 (which in turn paraphrase [1, Theorem 1.10 and Corollary 1.19]) can be conjoined as

Theorem 1.3 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 DAG;
- the sum
  $$\sum_{\text{length-$k$ paths in } \Gamma} \text{ct(path)}$$
  for $\mathbb{Z}_{\geq 0}$-labeled DAGs $\Gamma$;
- the weight of $A^k$, where $A$ is a square $\mathbb{Z}_{\geq 0}$-valued matrix of weight $N$;
- the product of $k$ non-negative integers with sum $N$. 

$\blacksquare$
The fact that the first two optimization problems are identical follows immediately by recasting plain DAGs as labeled DAGs as in Definition 1.1. On the other hand, translating this into the language of the third item is simply passing between a DAG and its adjacency matrix.

With this phrasing, Theorem 2.4 below provides a direct generalization of Theorem 1.3.

2 Optimizing labeled graphs

Theorem 1.3 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 of this general form, 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 $(M, +)$ be a closed submonoid of $(\mathbb{R}_{\geq 0}, +)$.

**Definition 2.1** Let $\Gamma$ be an $M$-labeled directed graph. We define

$$ct^E(\Gamma) = ct^E_M(\Gamma) := \sum_\alpha ct(\alpha),$$

with $\alpha$ ranging over the subgraphs of $\Gamma$ isomorphic to $E$, with the $M$-labeling inherited from $\Gamma$. ♦

We then have

**Theorem 2.2** Let

- $E$ be a simple directed graph;
- $(M, +)$ a closed submonoid of $(\mathbb{R}_{\geq 0}, +)$;
- $N \in M$ an element.

Then, sup $ct^E_M(\Gamma)$ for $M$-labeled $\Gamma$ of weight $N$ is achieved over graphs $\Gamma$ with the following property:

$$\text{Every two edges of } \Gamma \text{ belong to some common embedded copy } E \subset \Gamma.$$  \hspace{1cm} (2-1)

**Proof** We have to prove that given an $M$-labeled $\Gamma$ of content $N$, $ct^E_M$ can be improved by altering $\Gamma$ progressively until we achieve (2-1).

Indeed, suppose the edges $e$ and $f$ of $\Gamma$ do not belong to a common copy $E \subset \Gamma$. Then, the sets $S_e$ and $S_f$ of $E$-subgraphs of $\Gamma$ containing $e$ and $f$ respectively are disjoint.

Now, for each path $\alpha \in S_e$ containing $e$, consider the $e$-exclusive content $ct_\varphi \alpha$ as in Definition 1.2, and similarly for $f$. Without loss of generality, suppose

$$\Sigma_e := \sum_{\alpha \in S_e} ct_\varphi \alpha$$

is at least as large as its counterpart

$$\Sigma_f := \sum_{\beta \in S_f} ct_f \beta.$$

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 $c_{\mathcal{M}}^E$; indeed, the latter is incremented by
\[ \ell(f) (\Sigma_e - \Sigma_f) \geq 0. \]
• 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 (2-1). This finishes the proof. □

2.1 Paths

Theorem 2.2 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 path, hence the relevance of the following simple observation.

**Lemma 2.3** Let $k$ be a positive integer and $E$ a length-$k$ oriented path. Then, the only directed graphs $\Gamma$ satisfying (2-1) are length-$k$ paths and cycles any of the lengths $k+1$ up to $2k-1$. □

**Theorem 2.4** Let $k$ be a positive integer, $(\mathcal{M}, +)$ a closed 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
\[ \sum_{\text{length-$k$ paths in } \Gamma} \text{ct(path)} \]
for $\mathcal{M}$-labeled DAGs $\Gamma$ of weight $N$;

(2) the weight of $A^k$, where $A$ is a square $\mathcal{M}$-valued matrix of weight $N$;

(3) the product of $k$ non-negative elements of $\mathcal{M}$ with sum $N$.

**Proof** The fact that (1) and (2) have the same optimal value follows by noting that if $A$ is the adjacency matrix of the labeled DAG $\Gamma$ then the length-$k$ paths in $\Gamma$ are in bijection with the non-zero entries of $A$, 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:

\[ \max (3) \leq \max (1) \] (2-2)
and
\[ \max (1) \leq \max (3). \] (2-3)

(2-2) 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 $\Gamma$.

As for (2-3), Theorem 2.2 applied to a $k$-path $E$ and Lemma 2.3 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 2.5** Conjecture 0.5 holds.

**Proof** Simply take $\mathcal{M} = \mathbb{R}_{\geq 0}$ in Theorem 2.4 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. □
2.2 Stars

The following notion of oriented tree is fairly common in the literature (see e.g. [2, p.310]).

Definition 2.6 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 \( w \rightarrow v \).

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 2.7 A rooted directed tree is \( \ell \)-equidistal if all of its arms have the same length \( \ell \). 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 \( \ell \)-star if it is both a star and \( \ell \)-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 \( a \) arms instead. The analogue of Theorem 2.4 is

Theorem 2.8 Let

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

The following quantities all admit the same supremum.

1. the sum

\[
\text{ct}^E_M(\Gamma) = \sum_{1 \text{-stars with } a \text{ arms contained in } \Gamma} \text{ct}(\text{star})
\]

for \( \mathcal{M} \)-labeled DAGs \( \Gamma \) of weight \( N \);

2. the \( a \)-th elementary symmetric sum evaluated at some \( t \)-tuple of elements in \( \mathcal{M} \) with sum \( N \) (for varying \( t \)):

\[
\sum_{1 \leq i_1 < \cdots < i_a \leq t} \lambda_{i_1} \cdots \lambda_{i_a}, \quad \lambda_i \in \mathcal{M}, \quad \sum \lambda_i = N.
\]

(2-4)

Proof According to Theorem 2.2 it is enough to range over \( \mathcal{M} \)-labeled DAGs \( \Gamma \) for which every two edges lie in some common copy of \( E \subset \Gamma \). This clearly implies that \( \Gamma \) itself must be a 1-star, with, say, \( t \) arms.

If \( \lambda_i, 1 \leq i \leq t \) are the labels of the \( t \) arms of \( \Gamma \) so that

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

then the content \( \text{ct}^E(\Gamma) \) is the \( a \)-th elementary symmetric function evaluated at the \( \lambda_i \). This concludes the proof.

The following consequence is a kind of continuous version of counting the maximal number such stars in a DAG with \( N \) edges.

Corollary 2.9 Let
• $E$ be a 1-star with $a$ arms;
• $N \in \mathbb{R}_{\geq 0}$.

The supremum

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

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

**Proof** According to Theorem 2.8, we want the supremum of (2-4) for $\lambda_i \in \mathbb{R}_{\geq 0}$ and varying $t$. For fixed $t$ that expression is maximal when all $\lambda_i$ are equal (to $\frac{N}{t}$), so (2-4) is at most

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

As $t \to \infty$ the right hand side converges to its supremum $\frac{N^a}{a!}$, hence the conclusion. ■

As for the discrete version, it reads

**Corollary 2.10** Let $N$ and $a$ be two positive integers. The following quantities all have the same maximal value $\left(\frac{N}{a}\right)$

1. the number of 1-stars with $a$ arms contained in directed graph with $N$ edges;
2. the sum

$$\sum_{\text{1-stars with a arms contained in } \Gamma} \text{ct}(\text{star})$$

for $\mathbb{N}_{\geq 0}$-labeled directed graphs $\Gamma$ of weight $N$;
3. the $a$th elementary symmetric sum evaluated at some $t$-tuple of non-negative integers with sum $N$ (for varying $t$):

$$\sum_{1 \leq i_1 < \cdots < i_a \leq t} \lambda_{i_1} \cdots \lambda_{i_a}, \quad \lambda_i \in \mathbb{N}_{\geq 0}, \quad \sum \lambda_i = N. \tag{2-5}$$

**Proof** That (1) and (2) have the same optimal value follows as in the discussion following Theorem 1.3, by recasting repeated edges in a directed graph as $\mathbb{N}_{\geq 0}$-labels. On the other hand, the fact that (2) and (3) have the same optimal value follows from Theorem 2.8 applied to $\mathcal{M} = \mathbb{N}_{\geq 0}$ and $E$ an $a$-arm 1-star. It thus remains to prove that the supremum is a maximum, and that that maximum is $\left(\frac{N}{a}\right)$.

As in the proof of Theorem 2.8, we can assume $\Gamma$ is a 1-star with $t$ arms and respective labels $\lambda_i \in \mathbb{N}_{\geq 0}, 1 \leq i \leq t$ (the labels can be assumed positive because 0 labels make no contribution to (2-5)). In particular, $t \leq N$.

Having fixed $t$, we observed in the proof of Corollary 2.9 that the elementary symmetric function (2-5) is dominated by

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

That expression is increasing in $t$, so reaches its maximum at $t = N$. That maximum is precisely

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

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

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