Milan J. Math. Vol. 87 (2019) 141–168
https://doi.org/10.1007/s00032-019-00296-1
Published online April 6, 2019

Milan Journal of Mathematics

Graph MBO on Star Graphs and Regular Trees. With Corrections to DOI 10.1007/s00032-014-0216-8

Yves van Gennip

Abstract. The graph Merriman–Bence–Osher scheme produces, starting from an initial node subset, a sequence of node sets obtained by iteratively applying graph diffusion and thresholding to the characteristic (or indicator) function of the node subsets. One result in [14] gives sufficient conditions on the diffusion time to ensure that the set membership of a given node changes in one iteration of the scheme. In particular, these conditions only depend on local information at the node (information about neighbors and neighbors of neighbors of the node in question). In this paper we show that there does not exist any graph which satisfies these conditions. To make up for this negative result, this paper also presents positive results regarding the Merriman–Bence–Osher dynamics on star graphs and regular trees. In particular, we present sufficient (and in some cases necessary) results for the set membership of a given node to change in one iteration.

Mathematics Subject Classification (2010). Primary 35R02, 49K15; Secondary 53C44, 35K05, 05C81.

Keywords. graph dynamics, Merriman–Bence–Osher scheme, threshold dynamics, star graph, regular tree graph.

1. Introduction

In this paper we present new results for the Merriman–Bence–Osher (MBO) scheme on graphs. This scheme, also known as threshold dynamics, consists of iteratively applying graph diffusion and a thresholding step. In [11, 12] this scheme was introduced in a continuum setting to approximate flow by mean curvature. In recent years the graph version of this process and variations thereof have been succesfully applied to data clustering and classifcation problems and other graph based problems, e.g. in [4, 5, 8, 9, 10, 7, 15, 3], which in turn has prompted further theoretical study of the MBO scheme on graphs [14, 1].

Birkhäuser

In particular, this paper is both a corrigendum and a direct sequel to [14]. The main correction which this paper provides concerns [14, Theorem 4.8]. That theorem gives a condition on the value of the diffusion parameter τ under which a given node changes its value in a single iteration of the graph MBO scheme. This paper shows that the condition from [14, Theorem 4.8] in fact cannot be satisfied (which also implies that the conditions derived from this Theorem that were given in [14, Lemma 4.9, Corollary 4.10, Remark 4.11] are wrong[1]).

As a consequence of this error, the star graph and regular tree examples that were given in [14, Sections 6.2–6.3] and which depended on the erroneous results of [14, Section 4.4 and Lemma 6.1] are also incorrect. In this paper we investigate these special graphs anew and prove various results about the behaviour of the MBO scheme on these graphs independent of [14, Theorem 4.8]. In particular we are interested in the question under which conditions the value at a given node does or does not change (the latter is called "pinning") in one iteration of the MBO scheme.

We also make use of this opportunity to address some secondary minor issues that relate to ambiguous statements and fixable small mistakes in the statements of some of the theorems and lemmas in [14] and their proofs. These corrections are included in the appendices to this paper.

In Section 2 we introduce the relevant graph concepts and notation, including the graph MBO algorithm, so that this paper can be read by itself without need for access to [14]. Section 3 recalls [14, Theorem 4.8] (and in the process addresses a definitional error that was present in [14, Section 4.4] leading up to Theorem 4.8) and through Theorem 3.1 shows that there are no graphs which satisfy the conditions of [14, Theorem 4.8]. In Section 4 and Section 5 we give various conditions under which pinning behaviour does or does not occur in star graphs and regular trees, respectively.

2. Set-up and the graph MBO algorithm

2.1. Set-up and notation

In this paper we mainly focus on star graphs and regular trees, but some results will hold for more general graphs. Whenever we do not specify a particular type of graph, we consider finite, simple (i.e. without multi-edges or self-loops), connected, undirected, positively edge-weighted graphs $G = (V, E, \omega)$, where V is the node (or vertex) set of the graph (with $n := |V| < \infty$), E the edge set, and $\omega : E \to \mathbb{R}$ an edge-weight function. We assume that ω takes positive values on E and we use the convention that the domain of ω is extended to $V \times V$, by setting $\omega(i, j) := 0$ for all $(i, j) \in V \times V \setminus E$. We will use the same convention for other edge functions[2]. For notational simplicity we write $\omega_{kl} := \omega(k, l)$ and similarly for other edge functions.

[1] Indeed, on further inspection errors were discovered in the computations of those conditions.

[2] We will find that our choice to give ω the value 0 outside of E means that the choice of value for other edge functions outside E becomes irrelevant, as those functions only appear in combinations with ω.

If $u : V \to \mathbb{R}$ is a node function, we write $u_i := u(i)$ for all $i \in V$. Note that by our assumption above self-loops are absent and thus, for all $i \in V$, $\omega_{ii} = 0$.

The degree of node i is $d_i := \sum_{j \in V} \omega_{ij}$ and, by our assumption of connectedness, for all $i \in V$, $d_i > 0$. We denote by $\mathcal{V}$ the set of all node functions $u : V \to \mathbb{R}$ and by $\mathcal{E}$ the set of all edge functions $\varphi : V \times V \to \mathbb{R}$ which are skew-symmetric (i.e., for all $i, j \in V$, $\varphi_{ij} = -\varphi_{ji}$). We turn these sets into inner product spaces by defining

$$\langle u, v \rangle_{\mathcal{V}} := \sum_{i \in V} d_i^r u_i v_i \quad \text{and} \quad \langle \varphi, \psi \rangle_{\mathcal{E}} := \frac{1}{2} \sum_{i,j \in V} \varphi_{ij} \psi_{ij} \omega_{ij}^{2q-1},$$

where $q \in [1/2, 1]$ and $r \in [0, 1]$ are parameters. We intepret ω_{ij}^0 to be 0 whenever $\omega_{ij} = 0$. These inner products give rise to norms $\| \cdot \|_{\mathcal{V}}$ and $\| \cdot \|_{\mathcal{E}}$ in the usual way. On $\mathcal{V}$ we also define the maximum norm $\|u\|_{\mathcal{V},\infty} := \max\{|u_i| : i \in V\}$.

We define the graph gradient to be

$$(\nabla u)_{ij} := \omega_{ij}^{1-q} (u_j - u_i).$$

With this choice of inner products and graph gradient, we define the graph divergence to be the adjoint of the graph gradient and the graph Laplacian to be the graph divergence of the graph gradient. This leads to

$$(\operatorname{div} \varphi)_i := d_i^{-r} \sum_{j \in V} \omega_{ij}^q \varphi_{ji} \quad \text{and} \quad (\Delta u)_i := d_i^{-r} \sum_{j \in V} \omega_{ij} (u_i - u_j).$$

It is easily checked that we indeed have

$$\langle \nabla u, \varphi \rangle_{\mathcal{E}} = \langle u, \operatorname{div} \varphi \rangle_{\mathcal{V}}.$$

Moreover, $\Delta u = \operatorname{div} \nabla u$ does not depend on the parameter q and thus neither does the MBO scheme.

We also recall the definition of graph curvature of the vertex set $S \subset V$ at node $i \in V$ from [14, Definition 3.2]:

$$(\kappa_S^{q,r})_i := d_i^{-r} \begin{cases} \sum_{j \in S^c} \omega_{ij}^q, & \text{if } i \in S, \\ -\sum_{j \in S} \omega_{ij}^q, & \text{if } i \in S^c. \end{cases} \tag{1}$$

Note that $S^c := V \setminus S$.

We denote the characteristic (or indicator) function of a node subset $S \subset V$ by χ_S, i.e.

$$(\chi_S)_i := \begin{cases} 1, & \text{if } i \in S, \\ 0, & \text{if } i \in S^c. \end{cases}$$

A quick computation then shows that

$$\Delta \chi_S = \kappa_S^{1,r}. \tag{2}$$

2.2. The graph MBO scheme

The graph MBO scheme or algorithm (which in [14] was called (MBO_τ)) is defined as follows. Given an initial node subset $S_0 \subset V$, a time step $\tau > 0$, and the number of time steps $N > 0$, the MBO algorithm produces a sequence of node subsets $\{S_k\}_{k=0}^N$ by iterating the following two steps N times for $k = 1$ to $k = N$:

1. **Diffusion step.** Let $v(\tau)$ be the solution at time τ of the initial value problem
$$\dot{v} = -\Delta v, \quad v(0) = \chi_{S_{k-1}}. \tag{3}$$
2. **Threshold step.** Define the set $S_k \subset V$ to be
$$S_k := \{i \in V : v_i(\tau) \geq \tfrac{1}{2}\}.$$

In practice the number of iterations N can be set a priori or can be determined adaptively by some S_k-dependent stopping condition. The graph MBO algorithm tends to converge quickly, such that in most applications after only a small number of iterations the sets S_k do not change anymore in subsequent iterations.

In this paper we are concerned with what happens at a given node in one iteration, so the value of N is of no importance to us here. We say that **pinning** occurs at node i in the k^{th} iteration of the MBO algorithm if $i \in S_{k-1} \cup S_k$ or $i \in S_{k-1}^c \cup S_k^c$.

We note that the solution to (3) is given by $v(\tau) = e^{-\tau\Delta}\chi_{S_{k-1}}$, where $e^{-\tau\Delta} := \sum_{j=0}^\infty \frac{1}{j!}(-\tau\Delta)^j$. If we now define the threshold operator $P : \mathcal{V} \to \mathcal{V}$ via
$$(Pu)_i := \begin{cases} 1, & \text{if } u_i \geq \frac{1}{2}, \\ 0, & \text{if } u_i < \frac{1}{2}, \end{cases}$$
then the k^{th} iteration of the MBO algorithm can be expressed as
$$S_k = \{i \in V : (Pe^{-\tau\Delta}\chi_{S_{k-1}})_i = 1\}.$$
As a consequence we have that $\chi_{S_k} = Pe^{-\tau\Delta}\chi_{S_{k-1}}$. In particular, pinning *does not* occur at node i in the k^{th} iteration if and only if $|(Pe^{-\tau\Delta}\chi_{S_{k-1}})_i - (\chi_{S_{k-1}})_i| = 1$. Equivalently, pinning *does* occur at node i in the k^{th} iteration if and only if $|(Pe^{-\tau\Delta}\chi_{S_{k-1}})_i - (\chi_{S_{k-1}})_i| = 0$. For more details about pinning in the graph MBO scheme we refer the reader to [14].

3. Corrections for [14, Section 4.4]

Our main result in this section is Theorem 3.1, which shows that there do not exist any graphs that satisfy the conditions of [14, Theorem 4.8]. To set the context for this result, we will first recall Theorem 4.8. This also offers the opportunity to address a definitional error from [14, Section 4.4] and clarify the proof of [14, Theorem 4.8][3].

[3]Note that [14, Theorem 4.8] is not incorrect, but rather it is a statement about the empty set. We hope that including a clearer proof of the theorem in the appendix might suggest alterations that can be made to turn the theorem into a nontrivial one.

For the reader's convenience we recall some of the notation needed for Theorem 4.8. The set of neighbors of a node $i \in V$ is $\mathcal{N}_i := \{j \in V : \omega_{ij} > 0\}$. Let $1 \in V$ be an arbitrary node in the graph G and let $S \subset V$. Define

$$S_1 := \begin{cases} \mathcal{N}_1 \cap S^c, & \text{if } 1 \in S, \\ \mathcal{N}_1 \cap S, & \text{if } 1 \in S^c, \end{cases} \quad \text{and} \quad \overline{S_1} := S_1 \cup \{1\}.$$

Thus $\overline{S_1}$ is the set containing node 1 and all its neighbors that belong to the set (S or S^c) that is complementary to the one to which node 1 belongs. We also define the reduced degrees, for $i \in V$, $d_i' := \sum_{j \in S_1} \omega_{ij}$.

The paper [14] contained an incorrect definition of Δ'. The only property of Δ' which is explicitly used in the proof of Theorem 4.8 is the equality (5) below. This equality does not hold for the Δ' which was defined in the original paper[4]. To correct this mistake we need the set[5] $\overline{S_1}^* := \{1\} \cup \mathcal{N}(\overline{S_1})$, where $\mathcal{N}(\overline{S_1})$ is the set of neighbors of all nodes in $\overline{S_1}$:

$$\mathcal{N}(\overline{S_1}) := \{i \in V : \exists j \in \overline{S_1} \;\; i \in \mathcal{N}_j\}.$$

Note that, since $1 \in \overline{S_1}$, we have $S_1 \subset \mathcal{N}_1 \subset \mathcal{N}(\overline{S_1})$, and thus $\overline{S_1} \subset \overline{S_1}^*$. Moreover, if $S_1 \neq \emptyset$, then $1 \in \mathcal{N}(\overline{S_1})$, hence in that case $\overline{S_1}^* = \mathcal{N}(\overline{S_1})$. The correct definition of $\Delta' u$, for $u \in \mathcal{V}$, can now be given:

$$(\Delta' u)_i := \begin{cases} d_i^{-r} \sum_{j \in \overline{S_1}^*} \omega_{ij}(u_i - u_j), & \text{if } i \in \overline{S_1}, \\ 0, & \text{if } i \in \left(\overline{S_1}\right)^c. \end{cases} \tag{4}$$

If $v \in \mathcal{V}_1 := \{v \in \mathcal{V} : v = 0 \text{ on } \overline{S_1}^c\}$, then the following important equality holds:

$$(\Delta' v)_i = \begin{cases} (\Delta v)_i, & \text{if } i \in \overline{S_1}, \\ 0, & \text{if } i \in \left(\overline{S_1}\right)^c. \end{cases} \tag{5}$$

Through direct computation we can also verify the following useful identity, which is similar to (2):

$$(\Delta' \chi_{S_1})_i = \begin{cases} (\kappa_{S_1}^{1,r})_i, & \text{if } i \in \overline{S_1}, \\ 0, & \text{if } i \in \overline{S_1}^c. \end{cases} \tag{6}$$

Using (5) we obtain Theorem 4.8 as in the original paper:

Theorem 4.8 (from [14]**).** *Let $1 \in V$ be an arbitrary node and $S \subset V$ be such that $|(\kappa_S^{1,r})_1|^2 > \|(\Delta')^2 \chi_{S_1}\|_{\mathcal{V},\infty}$. If $\tau \in (\tau_1, \tau_2)$, where*

$$\tau_{1,2} := \frac{1}{\|(\Delta')^2 \chi_{S_1}\|_{\mathcal{V},\infty}} \left(|(\kappa_S^{1,r})_1| \pm \sqrt{|(\kappa_S^{1,r})_1|^2 - \|(\Delta')^2 \chi_{S_1}\|_{\mathcal{V},\infty}} \right) > 0,$$

then

$$|(Pe^{-\tau\Delta}\chi_S)_1 - (\chi_S)_1| = 1.$$

[4]In the original paper, however, the equality was —at the time mistakenly— assumed to hold for Δ', and therefore the actual proof of Theorem 4.8 did not suffer from the erroneous definition of Δ'.

[5]Note that $\overline{S_1}^* = \overline{S_1} \cup \partial(\overline{S_1}^c)$ where $\partial S := \{i \in S : \exists j \in V \; (\nabla \chi_S)_{ij} < 0\}$.

That is, the phase at node 1 *changes after one iteration of the MBO algorithm.*

For completeness, Appendix A provides an updated proof of this theorem (as the original proof was unclear in places and the updated proof might provide ideas for improving the theorem in future research). However, the main result of this section is that the condition $|(\kappa_S^{1,r})_1|^2 > \|(\Delta')^2\chi_{S_1}\|_{\mathcal{V},\infty}$ in Theorem 4.8 cannot be satisfied by any (finite, simple, connected, undirected, positively edge-weighted; see Section 2.1) graph. We state this as a theorem.

Theorem 3.1. *In the notation of Theorem* 4.8*, for all $S \subset V$ we have*

$$|(\kappa_S^{1,r})_1|^2 \le \|(\Delta')^2\chi_{S_1}\|_{\mathcal{V},\infty}.$$

Proof. First we note that $|(\kappa_S^{1,r})_1| = |(\kappa_{S_1}^{1,r})_1|$ (see for example the proof of Theorem 4.8). By (5) and (6) we have, for all $i \in \overline{S_1}$, $(\Delta'^2\chi_{S_1})_i = (\Delta' u)_i$, where $u_j = (\kappa_{S_1}^{1,r})_j$ if $j \in \overline{S_1}$ and $u_j = 0$ otherwise. Thus, for $i = 1$, we have

$$(\Delta'^2\chi_{S_1})_1 = d_1^{-r}\left(d_1(\kappa_{S_1}^{1,r})_1 - \sum_{k\in\overline{S_1}} \omega_{ik}(\kappa_{S_1}^{1,r})_k\right).$$

Since $1 \in S_1^c$, we have $d_1(\kappa_{S_1}^{1,r})_1 \le 0$ and since $\omega_{11} = 0$, we find

$$-\sum_{k\in\overline{S_1}} \omega_{ik}(\kappa_{S_1}^{1,r})_k = -\sum_{k\in S_1} \omega_{ik}(\kappa_{S_1}^{1,r})_k \le 0,$$

where we used that, for $k \in S_1$, $(\kappa_{S_1}^{1,r})_k \ge 0$. Hence

$$\|(\Delta')^2\chi_{S_1}\|_{\mathcal{V},\infty} \ge \left|(\Delta'^2\chi_{S_1})_1\right| = d_1^{-r}\left(\sum_{k\in S_1} \omega_{ik}(\kappa_{S_1}^{1,r})_k - d_1(\kappa_{S_1}^{1,r})_1\right).$$

Assume that $d_1^{-r}\left(\sum_{k\in S_1} \omega_{ik}(\kappa_{S_1}^{1,r})_k - d_1(\kappa_{S_1}^{1,r})_1\right) < |(\kappa_{S_1}^{1,r})_1|^2$, then

$$\begin{aligned}\sum_{k\in S_1} \omega_{ik}(\kappa_{S_1}^{1,r})_k &< d_1^r|(\kappa_{S_1}^{1,r})_1|^2 + d_1(\kappa_{S_1}^{1,r})_1 = d_1^{-r}d_1'^2 - d_1^{1-r}d_1' \\ &= \frac{d_1'}{d_1^r}(d_1' - d_1) \le 0,\end{aligned}$$

where we used $(\kappa_{S_1}^{1,r})_1 = -d_1^{-r}\sum_{j\in S_1}\omega_{1j} = -d_1^{-r}d_1'$, which follows from (1) and the definition of S_1. This is a contradiction and the result follows. □

Note that the inequality in Theorem 3.1 is optimal in the sense that equality can be achieved: If $S = V$ or $S = \emptyset$, then $(\kappa_S^{1,r})_1 = 0$ and, for all $i \in V$, $(\Delta'\chi_{S_1})_i = 0$, and thus $|(\kappa_S^{1,r})_1|^2 = 0 = \|(\Delta')^2\chi_{S_1}\|_{\mathcal{V},\infty}$. With these choices of S, of course, the MBO scheme is stationary and pinning occurs at every node.

The results in [14, Section 4.4] following Theorem 4.8 were aimed at providing examples of graphs that satisfiy the conditions of Theorem 4.8. These results are incompatible with Lemma 3.1 and indeed close inspection of those results revealed

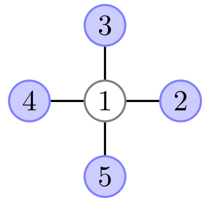


FIGURE 1. The star graph SG_5

seemingly minor, yet fatal, errors in one or two places that do render these results false.

Theorem 4.8 and its inadvertently false corollaries were used for some of the results in [14, Section 6], in particular for Lemma 6.1 and the resulting conclusions that were drawn for the star graph (Section 6.2) and regular tree graph (Section 6.3). Due to Lemma 3.1 these results are not correct. In Section 4 and Section 5 we provide extensive alternative results for the star graph and regular tree graph, respectively. These results are weaker than what Lemma 6.1 originally claimed to provide, but we have generalized some of the other computations in those sections.

4. Star graph

This section is partially based on and replaces [14, Section 6.2].

In this section we consider a star graph SG_n as in Figure 1 with $n \geq 3$ nodes[6]. We assume node 1 is the internal (or central) node, which is connected to all other nodes and the other $n-1$ nodes are only connected to the internall node. Hence, for all $i \in \{2, \ldots, n\}$, $\omega_{1i} = \omega_{i1} > 0$, and all the other ω_{jk} are zero.

Lemma 4.1. *If all the nonzero edge weights have the same value $\omega > 0$, then the eigenvalues of the graph Laplacian are $\lambda_1 = 0$, $\lambda_i = \omega^{1-r}$ for $i \in \{2, \ldots, n-1\}$, and $\lambda_n = \omega^{1-r}\left((n-1)^{1-r} + 1\right)$. A choice of corresponding ($\mathcal{V}$-normalized[7]) eigenfunctions (or eigenvectors) $\{v^i\}_{i=1}^n$ is given by*[8]

$$v^1 = (\text{vol } V)^{-\frac{1}{2}} \chi_V = \left((n-1)^r + n - 1\right)^{-\frac{1}{2}} \omega^{-\frac{r}{2}} \chi_V,$$

$$v_j^i = 2^{-\frac{1}{2}} \omega^{-\frac{r}{2}} \begin{cases} 1, & \text{if } j = i, \\ -1, & \text{if } j = i+1, \\ 0, & \text{else}, \end{cases} \qquad \text{for } i \in \{2, \ldots, n-1\},$$

$$v_j^n = \omega^{-\frac{r}{2}} \left((n-1)^{2-r} + n - 1\right)^{-\frac{1}{2}} \begin{cases} (n-1)^{1-r}, & \text{if } j = 1, \\ -1, & \text{if } j \neq 1. \end{cases}$$

---

[6]The assumption $n \geq 3$ might seem unnatural. Our main reason to exclude the case $n = 2$ is one of notation. See Remark 4.11 at the end of this section for more details.

[7]A function $u \in \mathcal{V}$ is $\mathcal{V}$-normalized if $\|u\|_{\mathcal{V}} = 1$.

[8]Here, subscripts j denote the components of the vectors.

Proof. It is instructive initially to keep the choice of ω_{1i} open. We will clearly indicate where we use the assumption that, for all $i \in \{2, \dots, n\}$, $\omega_{1i} = \omega$. We can explicitly compute the characteristic polynomial of the graph Laplacian:

$$p(\lambda) = \left(d_1^{1-r} - \lambda\right) \prod_{j=2}^{n} \left(d_j^{1-r} - \lambda\right) - d_1^{-r} \sum_{k=2}^{n} \omega_{1k}^2 d_k^{-r} \prod_{j \geq 2, j \neq k} \left(d_j^{1-r} - \lambda\right).$$

Via direct computation, we find

$$\begin{aligned} p(0) &= d_1^{1-r} \prod_{j=2}^{n} d_j^{1-r} - d_1^{-r} \sum_{k=2}^{n} \omega_{1k}^2 d_k^{-r} \prod_{j \geq 2, j \neq k} d_j^{1-r} \\ &= \left(\sum_{k=2}^{n} \omega_{1k}\right)^{1-r} \prod_{j=2}^{n} \omega_{1j}^{1-r} - \sum_{k=2}^{n} \omega_{1k}^{2-r} \left(\sum_{k=2}^{n} \omega_{1k}\right)^{-r} \prod_{j \geq 2, j \neq k} \omega_{1j}^{1-r} \\ &= \left(\sum_{k=2}^{n} \omega_{1k}\right)^{-r} \sum_{k=2}^{n} \omega_{1k} \left(\prod_{j=2}^{n} \omega_{1j}^{1-r} - \prod_{j=2} \omega_{1j}^{1-r}\right) = 0, \end{aligned}$$

where we used $d_1 = \sum_{j=2}^{n} \omega_{1j}$ and $d_i = \omega_{1i}$, for $i \in \{2, \dots, n\}$. Hence $\lambda = 0$ is one of the eigenvalues, as expected.

Using the assumption that all the nonzero edge weights have the same value $\omega > 0$, $p(\lambda)$ simplifies considerably to

$$\begin{aligned} p(\lambda) &= \left((n-1)^{1-r}\omega^{1-r} - \lambda\right)(\omega^{1-r} - \lambda)^{n-1} \\ &\qquad - (n-1)^{1-r}\omega^{2-2r}(\omega^{1-r} - \lambda)^{n-2} \\ &= \left(\omega^{1-r} - \lambda\right)^{n-2} \\ &\qquad \cdot \left[\left((n-1)^{1-r}\omega^{1-r} - \lambda\right)\left(\omega^{1-r} - \lambda\right) - (n-1)^{1-r}\omega^{2-2r}\right]. \end{aligned}$$

Direct computation shows that in this case the eigenvalues are $\lambda_1 = 0$, $\lambda_i = \omega^{1-r}$ for $i \in \{2, \dots, n-1\}$, and $\lambda_n = \omega^{1-r}\left((n-1)^{1-r} + 1\right)$, and a choice of corresponding ($\mathcal{V}$-normalized) eigenvectors is as given in the statement of the lemma. □

Note that, as expected, v^1 and v^n from Lemma 4.1 are $\mathcal{V}$-orthogonal to each other[9] and to the v^i ($i \in \{2, \dots, n-1\}$). These v^i, however, are not mutually $\mathcal{V}$-orthogonal. Of course a $\mathcal{V}$-orthogonal basis for the eigenspace spanned by those eigenvectors can be found if required.

Next we investigate the following question: If the initial node set $S_0 := S \subset V$ contains either only node 1 or all nodes except node 1, for which values of τ does pinning of the MBO evolution occur? Remember that we say that pinning occurs at node i (in the first iteration) if $(\chi_S)_i = \left(Pe^{-\tau\Delta}\chi_S\right)_i$, where P denotes the thresholding operator.

[9] I.e., $\langle v^1, v^n \rangle_{\mathcal{V}} = 0$.

Lemma 4.2. *Assume all the nonzero edge weights have the same value $\omega > 0$. First consider the case where $r \in [0,1)$. Define*

$$\tau_c := \frac{1}{\left((n-1)^{1-r}+1\right)\omega^{1-r}} \log\left(2\frac{(n-1)^r+n-1}{n-1-(n-1)^{2r-1}}\right).$$

First suppose that $S = \{1\}$. Then, for all $\tau \geq 0$ and for all $i \in \{2,\dots,n\}$, pinning occurs at node i. Pinning at node 1 occurs if and only if $\tau \leq \tau_c$.

Next suppose that $S = \{2,\dots,n\}$ instead. Then, for all $\tau \geq 0$ and for all $i \in \{2,\dots,n\}$, pinning occurs at node i. Pinning at node 1 occurs if and only if $\tau < \tau_c$.

If $r = 1$ instead, pinning occurs at every node in V for all $\tau \geq 0$.

Proof. First we consider $S = \{1\}$ and note that χ_S has an explicit expansion in terms of the eigenvectors,

$$\begin{aligned}\chi_S &= \omega^{-\frac{r}{2}}\left((n-1)^r+n-1\right)^{-\frac{1}{2}} d_1^r v^1 \\ &\qquad\qquad + \omega^{-\frac{r}{2}}(n-1)^{1-r}\left((n-1)^{2-r}+n-1\right) d_1^r v^n \\ &= d_1^r\omega^{-r}\left((n-1)^r+n-1\right)^{-1}\chi_V \\ &\quad + d_1^r\omega^{-r}(n-1)^{1-r}\left((n-1)^{2-r}+n-1\right)^{-1}\begin{pmatrix}(n-1)^{1-r}\\ -1\\ \vdots\\ -1\end{pmatrix}.\end{aligned}$$

We now consider the MBO iterates of χ_S. We compute

$$\begin{aligned}&\left(e^{-\tau\Delta}\chi_S\right)_1 \\ &= d_1^r\omega^{-r}\left((n-1)^r+n-1\right)^{-1} \\ &\quad + d_1^r\omega^{-r}(n-1)^{2-2r}\left((n-1)^{2-r}+n-1\right)^{-1} e^{-\left((n-1)^{1-r}+1\right)\omega^{1-r}\tau}.\end{aligned}$$

The value at node 1 remains unchanged in one MBO iteration if $\left(e^{-\tau\Delta}\chi_S\right)_1 \geq \frac{1}{2}$. Through a direct calculation we thus check that, if $r \in [0,1)$, pinning at node 1 occurs if $\tau \leq \tau_c$. This computation also shows that, if $\tau > \tau_c$, then $\left(Pe^{-\tau\Delta}\chi_S\right)_1 = 0$. If $r = 1$ instead, a similar calculation shows that[10], for all $\tau \geq 0$, $\left(e^{-\tau\Delta}\chi_S\right)_1 > \frac{1}{2}$, and therefore pinning occurs at node 1 for all $t \geq 0$.

Using a similar computation for[11] $i \in \{2,\dots,n\}$ and attempting to solve $\left(e^{-\tau\Delta}\chi_S\right)_i = \frac{1}{2}$, we find $e^{-\left((n-1)^{1-r}+1\right)\omega^{1-r}\tau} \leq 0$ (for any choice of $r \in [0,1]$). This is a contradiction. Moreover, when $\tau = 0$, $\left(e^{-\tau\Delta}\chi_S\right)_i = 0 < \frac{1}{2}$. Hence, for all $\tau \geq 0$ we

[10] Since $\left(e^{-\tau\Delta}\chi_S\right)_1 = \frac{1}{2}$ if and only if $e^{-\left((n-1)^{1-r}+1\right)\omega^{1-r}\tau} = 0$ (which has no solution), and for $\tau = 0$, $\left(e^{-\tau\Delta}\chi_S\right)_1 = 1 > \frac{1}{2}$.

[11] Using

$$\begin{aligned}\left(e^{-\tau\Delta}\chi_S\right)_i &= d_1^r\omega^{-r}\left((n-1)^r+n-1\right)^{-1} \\ &\quad - d_1^r\omega^{-r}(n-1)^{1-r}\left((n-1)^{2-r}+n-1\right)^{-1} e^{-\left((n-1)^{1-r}+1\right)\omega^{1-r}\tau}.\end{aligned}$$

have $\left(e^{-\tau\Delta}\chi_S\right)_i < \frac{1}{2}$, and thus pinning at node i occurs independent of the choice of $\tau \geq 0$ and independent of the choice of $r \in [0,1]$.

For the case where $S = \{2,\ldots,n\}$ we realize that $e^{-\tau\Delta}\chi_S = e^{-\tau\Delta}(\chi_V - \chi_{\{1\}}) = \chi_V - e^{-\tau\Delta}\chi_{\{1\}}$. Hence $\left(e^{-\tau\Delta}\chi_S\right)_1 \geq \frac{1}{2}$ if and only if $\left(e^{-\tau\Delta}\chi_{\{1\}}\right)_1 \leq \frac{1}{2}$. If $r \in [0,1)$, then by the computation above we know this is the case if and only if $\tau \geq \tau_c$. Hence pinning at node 1 occurs if and only if $\tau < \tau_c$. If $r = 1$, we know from above that, for all $\tau \geq 0$, $\left(e^{-\tau\Delta}\chi_{\{1\}}\right)_1 > \frac{1}{2}$, thus pinning at node 1 occurs for all $\tau \geq 0$ in this case.

If $i \in S$, we know that $\left(e^{-\tau\Delta}\chi_S\right)_i < \frac{1}{2}$ if and only if $\left(e^{-\tau\Delta}\chi_{\{1\}}\right)_1 > \frac{1}{2}$, which by the computation above does not have any solution $\tau \in [0,\infty)$, regardless of the choice of $r \in [0,1]$. Hence, for all $\tau \geq 0$ and for all $r \in [0,1]$, pinning occurs at node i.[12] □

Remark 4.3. In Lemma 4.2, note that $\tau_c \to \infty$ as $r \to 1$, which is consistent with our observation in the same lemma that for $r = 1$ pinning on the full graph[13] always occurs, independent of the choice of τ (if $S = \{1\}$ or $S = \{2,\ldots,n\}$). For $r = 0$, we have $\tau_c = \frac{1}{n\omega}\log\left(2\frac{n-1}{n-2}\right)$. Qualitatively, this latter example shows for the star graph (or perhaps also, in a more general setting, suggests) that it is easier for a solution to be pinned on nodes with smaller degree.

Remark 4.4. If $S = \{1\}$, the bound from [14, Theorem 4.2] states that pinning occurs on the full graph if

$$\tau < \tau_\rho(S) = \omega^{r-1}\left((n-1)^{1-r}+1\right)^{-1}\log\left(1+\frac{1}{2}(n-1)^{-\frac{r}{2}}\right).$$

The bound[14] in [14, Theorem 4.3] states that, for $r \in [0,1)$, if

$$\tau > \tau_t(S) = \omega^{r-1}\log\left(2\frac{\left((n-1)^r+n-1\right)^{\frac{1}{2}}(n-1)^{\frac{r}{2}}(n-1)^{\frac{1}{2}}}{(n-1-(n-1)^r)}\right), \tag{7}$$

[12]Instead of using that $\chi_S = \chi_V - \chi_{\{1\}}$, as we did above, we could also have done another explicit computation, as in the case $S = \{1\}$. For such a computation it is useful to know the expansions of χ_S (with $S = \{2,\ldots,n\}$ in terms of the eigenvectors:

$$\begin{aligned}\chi_S &= \left((n-1)^r+n-1\right)^{-\frac{1}{2}}(n-1)\omega^{\frac{r}{2}}v^1 \\ &\qquad - \left((n-1)^{2-r}+n-1\right)^{-\frac{1}{2}}(n-1)\omega^{\frac{r}{2}}v^n \\ &= (n-1)\left((n-1)^r+n-1\right)^{-1}\chi_V \\ &\quad - (n-1)\left((n-1)^{2-r}+n-1\right)^{-1}\begin{pmatrix}(n-1)^{1-r}\\ -1\\ \vdots\\ -1\end{pmatrix}.\end{aligned}$$

The rest of the computation now follows as in the first case.

[13]In this paper we use the terminology “pinning on the full graph” to mean “pinning at every node in the graph”. “Full graph” in this sense has no connection to the concept of “complete graph”, which does not occur in this paper (outside of this footnote).

[14]See also Appendix B.2 for some more information about τ_ρ and τ_t.

then, for all $i \in V$, $\left(Pe^{-\tau\Delta}\chi_S\right)_i = 0$. We also note that $\tau_t(S) \to \infty$ if $r \to 1$ as expected, since pinning at every node, and hence in particular no change in the value at node 1, occurs when $r = 1$. Note that $\tau_\rho(S)$ is not a sharp enough bound to fully describe this pinning behavior, since, for $r = 1$, $\tau_\rho(S) = \log\left(1 + \frac{1}{2}(n-1)^{-\frac{1}{2}}\right) < \infty$.

When $r = 0$ we find $\tau_\rho(S) = \frac{1}{n\omega}\log\frac{3}{2}$, which is (as expected) a less sharp bound than the exact bound τ_c from Lemma 4.2 (because $2\frac{n-1}{n-2} > 2 > \frac{3}{2}$). Furthermore, when $r = 0$, $\tau_t(S) = \frac{1}{\omega}\log\left(2\frac{n^{\frac{1}{2}}(n-1)^{\frac{1}{2}}}{n-2}\right)$.

Remark 4.5. If $S = \{2, \ldots, n\}$ we see again, from Lemma 4.2, that for $r = 1$ pinning occurs for any value of τ. In this case, the bound from [14, Theorem 4.2] states that pinning occurs if

$$\tau < \tau_\rho(S) = \omega^{r-1}\left((n-1)^{1-r} + 1\right)^{-1}\log\left(1 + \frac{1}{2}(n-1)^{-\frac{1}{2}}\right).$$

From [14, Theorem 4.3] we see that $\tau_t(S) = \tau_t(S^c)$, hence, if $r \in [0, 1)$ and $\tau > \tau_t(S)$, then, for all $i \in V$, $\left(Pe^{-\tau\Delta}\chi_S\right)_i = 1$, where $\tau_t(S)$ is as in (7).

For $r = 1$, $\tau_\rho(\{2, \ldots, n\})$ coincides with $\tau_\rho(\{1\})$. For $r = 0$, we have $\tau_\rho(S) = \frac{1}{n\omega}\log\left(1 + \frac{1}{2}(n-1)^{-\frac{1}{2}}\right)$. In this case we notice again that the bound $\tau_\rho(S)$ is less sharp than the exact bound τ_c from Lemma 4.2, because $1 + \frac{1}{2}(n-1)^{-\frac{1}{2}} < 2 < 2\frac{n-1}{n-2}$.

In the remainder of this section we consider the situation where G is any finite, simple, connected, undirected, positively edge-weighted graph and $S \subset V$ (and the labeling of the nodes) is such that the subgraph induced[15] by $\overline{S_1}$ is a star graph. This is certainly true for the case when the full graph G is itself a star graph with 1 being its internal node and $S = V \setminus \{1\}$. We denote by $\tilde{n} \geq 3$ the number of nodes[16] in the subgraph induced by $\overline{S_1}$. Note that $\tilde{n} \leq n$.

Lemma 4.6. *Let $S \subset V$ be such that the subgraph induced by $\overline{S_1}$ is a star graph with node 1 being the internal node and nodes $2, \ldots, \tilde{n}$ the leaves. Let $r = 0$, assume that all nonzero edge weights in the graph[17] have the same value $\omega > 0$, and assume that there exists a $\theta \in \mathbb{N}$, such that, for all $j \in \{2, \ldots, \tilde{n}\}$, $d_j = d := \theta\omega$. Define*

[15] We remind the reader that the subgraph induced by a node subset $V' \subset V$ has node set V' and edge set $E' \subset E$ consisting of all edges from E that have both endpoints in V'. The edge weights on the edges in E' are the same as the ones on the corresponding edges from E.

[16] Similar to the situation addressed in footnote 6, we exclude the case $\tilde{n} = 2$ here mainly for notational reasons. See also Remark 4.11 at the end of this section.

[17] The assumption that *all* nonzero edge weights in the graph have the same value is in fact stronger than needed. It is sufficient for this condition to hold only for the weights of those edges who have one or both of their endpoints in $\overline{S_1}$.

$\theta_1 := d_1/\omega$ and

$$Q_\pm(\theta_1,\theta,\tilde n) := \frac{(\theta_1-\theta)\left(\theta_1-\theta\pm\sqrt{(\theta_1-\theta)^2+4(\tilde n-1)}\right)+2(\tilde n-1)}{(\theta_1-\theta)\left(\theta_1-\theta\pm\sqrt{(\theta_1-\theta)^2+4(\tilde n-1)}\right)+4(\tilde n-1)},$$
$$\gamma_\pm(\theta_1,\theta,\tilde n) := \theta_1-\theta\pm\sqrt{(\theta_1-\theta)^2+4(\tilde n-1)},$$
$$\lambda_\pm(\theta_1,\theta,\tilde n) := \frac{1}{2}\left(\theta_1+\theta\pm\sqrt{(\theta_1-\theta)^2+4(\tilde n-1)}\right)\omega.$$

If $\tau>0$ is such that

$$Q(\tau;\theta_1,\theta,\tilde n) := -\frac{2(\tilde n-1)}{\gamma_-(\theta_1,\theta,\tilde n)}Q_-(\theta_1,\theta,\tilde n)e^{-\lambda_-(\theta_1,\theta,\tilde n)\tau} - \frac{2(\tilde n-1)}{\gamma_+(\theta_1,\theta,\tilde n)}Q_+(\theta_1,\theta,\tilde n)e^{-\lambda_+(\theta_1,\theta,\tilde n)\tau} > \frac{1}{2}, \tag{8}$$

then $\left|P\left((e^{-\tau\Delta}\chi_S)_1\right)-(\chi_S)_1\right|=1$; that is, there is no pinning at node 1.

Proof. We start with some useful observations. Note by squaring the equation, that $\gamma_\pm(\theta_1,\theta,\tilde n)=0$ implies that $\tilde n=1$, which is ruled out by our assumption that $\tilde n\geq 3$[18]. Hence the divisions by $\gamma_\pm$ in the definition of Q are well-defined. It is a bit harder to see that the denominators of $Q_\pm(\theta_1,\theta,\tilde n)$ are nonzero, but later in this proof we will see that $Q_\pm$ are obtained as normalization factors of nonzero vectors and hence are well-defined as well.[19]

For future use, we will keep the calculations general at the start of the proof and we will only bring in the assumption that $r=0$ and the assumptions on the edge weights and node degrees when they are needed.

First we consider the situation where $1\in S^c$. We label the nodes such that $S_1=\{2,\dots,\tilde n\}$. Let Δ' be as defined in (4). Then, as in the proof of Theorem 4.8, we know that if

$$\left(e^{-\tau\Delta'}\chi_{S_1}\right)_1 \geq \frac{1}{2}, \tag{9}$$

then $\left(e^{-\tau\Delta}\chi_S\right)_1\geq\frac{1}{2}$ and thus the value at node 1 changes after one MBO iteration.

Since $\chi_{S_1}\in\mathcal V_1=\{v\in\mathcal V: v=0 \text{ on } \overline{S_1}^c\}$ (see also Section 3) we can represent $\Delta'\chi_{S_1}$ in matrix-vector form as

$$\begin{pmatrix} L' & 0\\ 0 & 0\end{pmatrix} v. \tag{10}$$

Here L' is the $\tilde n\times\tilde n$ matrix given by $L':=(D')^{-r}(D'-A')$, with D' being the diagonal matrix with the degrees d_i ($i\in\{1,\dots,\tilde n\}$) as diagonal entries and A' having entries $A'_{ij}:=\omega_{ij}$. Note that the degrees d_i are the degrees in the full graph, not in the

[18] Of course if we allow the case where $\tilde n=2$, this would also be ruled out.

[19] As a side note, we see that $\lambda_\pm(\theta_1,\theta,\tilde n)=0$ implies that $(\theta_1+\theta)^2=(\theta_1-\theta)^2+4(\tilde n-1)$ and thus $4\theta_1\theta=\tilde n-1$. However, substituting this condition back, we find $\lambda_\pm(\theta_1,\theta,1+4\theta_1\theta)=\theta_1+\theta\pm\sqrt{(\theta_1+\theta)^2+12\theta_1\theta}\geq 0$ with equality if and only if we consider λ_- (not λ_+) and $\theta_1=0$ or $\theta=0$. Those conditions are excluded by our assumption of connectedness of the graph. Hence $\lambda_\pm$ are nonzero.

S_1-induced subgraph. The vector $v \in \mathbb{R}^n$, has entries $v_i = 1$ for $i \in \{2, \ldots, \tilde{n}\}$ and $v_i = 0$ for $i \in \{1, \tilde{n}+1, \ldots, n\}$.

The characteristic polynomial of L' is

$$p(\lambda) := d_1^{-r} \left[(d_1 - d_1^r \lambda) \prod_{j=2}^{\tilde{n}} \left(d_j^{1-r} - \lambda \right) - \sum_{k=2}^{\tilde{n}} \omega_{1k}^2 d_k^{-r} \prod_{j=2, j\neq k}^{\tilde{n}} \left(d_j^{1-r} - \lambda \right) \right]. \quad (11)$$

Applying the assumptions from the current lemma to (11) we find that the characteristic polynomial of L' is

$$p(\lambda) = (d-\lambda)^{\tilde{n}-2} \left((d_1 - \lambda)(d-\lambda) - \omega^2(\tilde{n}-1) \right).$$

Hence the eigenvalues of L' are $\lambda_1 = \lambda_-$, $\lambda_i = d$, for $i \in \{2, \ldots, \tilde{n}-1\}$, and $\lambda_{\tilde{n}} = \lambda_+$. Via a direct computation we can find corresponding $\mathcal{V}$-normalized eigenvectors[20]:

$$v_j^1 = Q_-(\theta_1, \theta, \tilde{n})^{\frac{1}{2}} \begin{cases} -1, & \text{if } j = 1, \\ \frac{2}{\gamma_-(\theta_1,\theta,\tilde{n})}, & \text{if } j \in \{2, \ldots, \tilde{n}\}, \end{cases}$$

$$v_j^i = 2^{-\frac{1}{2}} \begin{cases} 1, & \text{if } j = i, \\ -1, & \text{if } j = i+1, \\ 0, & \text{otherwise}, \end{cases} \qquad \text{for } i \in \{2, \ldots, \tilde{n}-1\},$$

$$v_j^{\tilde{n}} = Q_+(\theta_1, \theta, \tilde{n})^{\frac{1}{2}} \begin{cases} -1, & \text{if } j = 1, \\ \frac{2}{\gamma_+(\theta_1,\theta,\tilde{n})}, & \text{if } j \in \{2, \ldots, \tilde{n}\}. \end{cases}$$

Note that v^1 and $v^{\tilde{n}}$ are $\mathcal{V}$-orthogonal to each other and to the v^i, for $i \in \{2, \ldots, \tilde{n}-1\}$ (but these v^i are not mutually $\mathcal{V}$-orthogonal). Hence, since $S_1 = \{2, \ldots, \tilde{n}\}$, we can expand $\chi := \chi_{S_1}|_{\overline{S_1}}$, i.e. the restriction of χ_{S_1} to $\overline{S_1}$, as

$$\chi = \frac{2(\tilde{n}-1)}{\gamma_-(\theta_1, \theta, \tilde{n})} Q_-(\theta_1, \theta, \tilde{n})^{\frac{1}{2}} v^1 + \frac{2(\tilde{n}-1)}{\gamma_+(\theta_1, \theta, \tilde{n})} Q_+(\theta_1, \theta, \tilde{n})^{\frac{1}{2}} v^{\tilde{n}},$$

and thus, by the representation in (10) (if we consider χ as a vector in $\mathbb{R}^{\tilde{n}}$),

$$\begin{aligned} \left(e^{-\tau\Delta'} \chi_{S_1} \right)_1 &= \left(e^{-\tau L'} \chi \right)_1 \\ &= -\frac{2(\tilde{n}-1)}{\gamma_-(\theta_1, \theta, \tilde{n})} Q_-(\theta_1, \theta, \tilde{n}) e^{-\lambda_-(\theta_1,\theta,\tilde{n})\tau} \\ &\quad - \frac{2(\tilde{n}-1)}{\gamma_+(\theta_1, \theta, \tilde{n})} Q_+(\theta_1, \theta, \tilde{n}) e^{-\lambda_+(\theta_1,\theta,\tilde{n})\tau}, \\ &= Q(\theta_1, \theta, \tilde{n}). \end{aligned}$$

which proves the result.

Finally, as at the end of the proof of Theorem 4.8, we argue that if $1 \in S$, the proof follows in a similar way: We have $\left(e^{-\tau\Delta}(\chi_S + \chi_{S^c}) \right)_1 = (\chi_V)_1 = 1$, so $\left(e^{-\tau\Delta}\chi_S \right)_1 < \frac{1}{2}$ if and only if $\left(e^{-\tau\Delta}\chi_{S^c} \right)_1 > \frac{1}{2}$. Now, as before in the proof of Theorem 4.8, we have that $\left(e^{-\tau\Delta}\chi_{S^c} \right)_1 \geq \left(e^{-\tau\Delta}\chi_{S_1} \right)_1 \geq \left(e^{-\tau\Delta'}\chi_{S_1} \right)_1$. The rest

[20] Again, subscripts j denote the components of the vectors.

of the proof then follows as before, if we note that now the inequality in (9) has to be a strict inequality, by our definition of the thresholding step of the MBO algorithm. $\square$

Note that in Lemma 4.6, $\tilde{n}$ is the number of nodes in the subgraph induced by $\overline{S_1}$, which is not equal to $n = |V|$, unless $\overline{S_1} = V$. In particular, under the assumptions in that lemma, we have $\left|\left(\kappa_S^{1,0}\right)_1\right| = (\tilde{n}-1)\omega$. The result from Lemma 4.6 will be illustrated for the example case of a regular tree in Section 5.

Remark 4.7. In Lemma 4.6 we used the fact that $\left(e^{-\tau\Delta'}\chi_{S_1}\right)_1 \geq \frac{1}{2}$ implies that $\left(e^{-\tau\Delta}\chi_S\right)_1 \geq \frac{1}{2}$ in order to localize our argument. Just as in the proof of Theorem 4.8 this allows us to only consider the neighbors of node 1 and (through Δ') their neighbors, instead of the whole graph. The price we pay for this is that the results of Lemma 4.6 (and similarly of Lemma 4.8 below) are only one-way implications and not equivalences as in Lemma 4.2 (where we used information from the full graph).

We end this section with results that show that the techniques that were used to prove Lemma 4.6 when $r = 0$ fail to provide useful results in the case when $r = 1$ (as is perhaps not surprising given Remark 4.3; that remark, however, refers only to the situation when the full graph is a star graph, not necessarily to the case when the subgraph induced by $\overline{S_1}$ is a star graph). We have chosen to include these results, as they do illustrate interesting behavior of the star graph and may lead to further future insight that could lead to positively formulated results for the case $r = 1$.

Lemma 4.8 and Corollary 4.10 mimic Lemma 4.6 for the case $r = 1$. Figure 2 shows why the result from Corollary 4.10 is not as useful as the analogous result from Lemma 4.6.

Lemma 4.8. *Let $S \subset V$ be such that the subgraph induced by $\overline{S_1}$ is a star graph with node 1 being the internal node and nodes $2, \ldots, \tilde{n}$ the leaves. Let $r = 1$ and define*

$$a := d_1^{-\frac{1}{2}} \left(\sum_{k=2}^{\tilde{n}} d_k^{-1}\omega_{1k}^2\right)^{\frac{1}{2}}. \tag{12}$$

Let $\tau \geq 0$ be such that

$$e^{-\tau}\left(e^{a\tau} - e^{-a\tau}\right) > \left|\left(\kappa_S^{1,1}\right)_1\right|^{-1} a, \tag{13}$$

then

$$\left|P\left((e^{-\tau\Delta}\chi_S)_1\right) - (\chi_S)_1\right| = 1;$$

that is, there is no pinning at node 1.

Proof. The proof follows along the same lines as the proof of Lemma 4.6 and we will use similar notation as in that proof. We have to find a sufficient condition for $\left(e^{-\tau\Delta'}\chi_{S_1}\right)_1 > \frac{1}{2}$ to hold.

First consider the case where $1 \in S^c$, then we arrive at the characteristic polynomial from (11) as before. Now assume $r = 1$, then

$$p(\lambda) = (1-\lambda)^{\tilde{n}-2} \left((1-\lambda)^2 - d_1^{-1} \sum_{k=2}^{\tilde{n}} d_k^{-1} \omega_{1k}^2 \right).$$

Computing the roots of p we find that the eigenvalues of L' (seen as linear operator on $\mathbb{R}^{\tilde{n}}$; see (10)) are $\lambda_1 = 1 - \sqrt{d_1^{-1} \sum_{k=2}^{\tilde{n}} d_k^{-1} \omega_{1k}^2}$, $\lambda_i = 1$, for $i \in \{2, \dots, \tilde{n}-1\}$, and $\lambda_{\tilde{n}} = 1 + \sqrt{d_1^{-1} \sum_{k=2}^{\tilde{n}} d_k^{-1} \omega_{1k}^2}$. Via direct computation we find corresponding $\mathcal{V}$-normalized eigenvectors:

$$v_j^1 = 2^{-\frac{1}{2}} \begin{cases} d_1^{-\frac{1}{2}}, & \text{if } j = 1, \\ \frac{\omega_{1j} d_j^{-1}}{\sqrt{\sum_{k=2}^{\tilde{n}} d_k^{-1} \omega_{1k}^2}}, & \text{if } j \in \{2, \dots, \tilde{n}\}, \end{cases}$$

$$v_j^i = \left(d_i \omega_{1i+1}^2 + d_{i+1} \omega_{1i}^2 \right)^{-\frac{1}{2}} \begin{cases} \omega_{1i+1}, & \text{if } j = i, \\ -\omega_{1i}, & \text{if } j = i+1, \\ 0, & \text{otherwise,} \end{cases} \qquad \text{for } i \in \{2, \dots, n-1\},$$

$$v_j^{\tilde{n}} = 2^{-\frac{1}{2}} \begin{cases} d_1^{-\frac{1}{2}}, & \text{if } j = 1, \\ -\frac{\omega_{1j} d_j^{-1}}{\sqrt{\sum_{k=2}^{\tilde{n}} d_k^{-1} \omega_{1k}^2}}, & \text{if } j \in \{2, \dots, \tilde{n}\}. \end{cases}$$

Note again that v^1 and $v^{\tilde{n}}$ are $\mathcal{V}$-orthogonal to each other and to the v^i, for $i \in \{2, \dots, \tilde{n}-1\}$ (but these v^i are not mutually $\mathcal{V}$-orthogonal). Let $\chi := \chi_{S_1}|_{\overline{S_1}}$, be the restriction of χ_{S_1} to $\overline{S_1}$, then we can expand χ on the basis of eigenvectors we just found:

$$\begin{aligned} \chi = {} & 2^{-\frac{1}{2}} \left(\sum_{k=2}^{\tilde{n}} d_k^{-1} \omega_{1k}^2 \right)^{-\frac{1}{2}} \left(\sum_{j=2}^{\tilde{n}} \omega_{1j} \right) \ v^1 \\ & + \sum_{i=2}^{\tilde{n}-1} \left(d_i \omega_{1i+1}^2 + d_{i+1} \omega_{1i}^2 \right)^{-\frac{1}{2}} \left(d_i \omega_{1i+1} - d_{i+1} \omega_{1i} \right) \ v^i \\ & - 2^{-\frac{1}{2}} \left(\sum_{k=2}^{\tilde{n}} d_k^{-1} \omega_{1k}^2 \right)^{-\frac{1}{2}} \left(\sum_{j=2}^{\tilde{n}} \omega_{1j} \right) \ v^{\tilde{n}}. \end{aligned}$$

Hence

$$\begin{aligned} \left(e^{-\tau \Delta'} \chi_{S_1} \right)_1 &= \left(e^{-\tau \Delta'} \chi \right)_1 \\ &= \left(d_1 \sum_{k=2}^{\tilde{n}} d_k^{-1} \omega_{1k}^2 \right)^{-\frac{1}{2}} \left(\sum_{j=2}^{\tilde{n}} \omega_{1j} \right) \ e^{-\tau} \ \sinh \left(d_1^{-\frac{1}{2}} \left(\sum_{k=2}^{\tilde{n}} d_k^{-1} \omega_{1k}^2 \right)^{\frac{1}{2}} \tau \right). \end{aligned}$$

So $\left(e^{-\tau\Delta'}\chi_{S_1}\right)_1 \geq \frac{1}{2}$ if and only if

$$e^{-\tau}\sinh\left(d_1^{-\frac{1}{2}}\left(\sum_{k=2}^{\tilde{n}} d_k^{-1}\omega_{1k}^2\right)^{\frac{1}{2}}\tau\right)$$
$$\geq \frac{1}{2}d_1^{-\frac{1}{2}}\left(\sum_{k=2}^{\tilde{n}} d_k^{-1}\omega_{1k}^2\right)^{\frac{1}{2}}\left|\left(\kappa_S^{1,1}\right)_1\right|^{-1}.$$

where we have used that $1 \in S^c$ and thus $\left(\kappa_S^{1,1}\right)_1 = \left(\kappa_{S_1}^{1,1}\right)_1 = -d_1^{-1}\sum_{j=2}^{\tilde{n}}\omega_{1j}$. Let a be as in (12), then $\left(e^{-\tau\Delta'}\chi_{S_1}\right)_1 \geq \frac{1}{2}$ if and only if

$$e^{-\tau}\left(e^{a\tau} - e^{-a\tau}\right) \geq \left|\left(\kappa_S^{1,1}\right)_1\right|^{-1} a.$$

As at the end of the proofs of Theorem 4.8 and Lemma 4.6, the proof for the case $1 \in S$ follows in a similar way. Note in particular that now $\left(\kappa_S^{1,1}\right)_1 = -\left(\kappa_{S_1}^{1,1}\right)_1 = d_1^{-1}\sum_{j=2}^{\tilde{n}}\omega_{1j}$. □

Remark 4.9. In the setting of Lemma 4.8, we note that

$$0 \leq \sum_{k=2}^{\tilde{n}} d_k^{-1}\omega_{1k}^2 \leq \sum_{k=2}^{\tilde{n}}\omega_{1k} \leq d_1,$$

hence from (12) it follows that $a \in [0,1]$. Moreover, equalities are attained in these inequalities if and only if, for all $k \in \{2,\ldots,\tilde{n}\}$, $\omega_{1k} = d_k$, and $d_1 = \sum_{k=2}^{\tilde{n}}\omega_{1k}$. These conditions are satisfied if and only if the only edges in the graph which have at least one endpoint in $\overline{S_1}$ are the edges connecting node 1 to each of the nodes in $\{2,\ldots,\tilde{n}\}$. By our assumption of connectedness, this is equivalent to the subgraph induced by $\overline{S_1}$ being the full graph. From Lemma 4.2 we already know that in that case, when $r = 1$, pinning occurs on the full graph for all $\tau \geq 0$ and so in particular at node 1.

On the other hand, $a = 0$ if and only if, for all $k \in \{2,\ldots,\tilde{n}\}$, $\omega_{1k} = 0$, which contradicts our assumption that the nodes in $\{2,\ldots,\tilde{n}\}$ form the leaves of a star graph induced by S_1. (We also see that condition (13) from Lemma 4.8 is not satisfied when $a = 0$.)

The following corollary deals with the remaining cases when $a \in (0,1)$.

Corollary 4.10. *Let the notation be as in Lemma* 4.8 *and assume* $a \in (0,1)$. *If*

$$\left|\left(\kappa_S^{1,1}\right)_1\right| a^{-1}\left(\left(\frac{1+a}{1-a}\right)^{\frac{a-1}{2a}} - \left(\frac{1-a}{1+a}\right)^{\frac{a+1}{2a}}\right) > 1, \tag{14}$$

then there exist a $\tau \in [0,\infty)$ *such that there is no pinning at node* 1 *for this* τ.

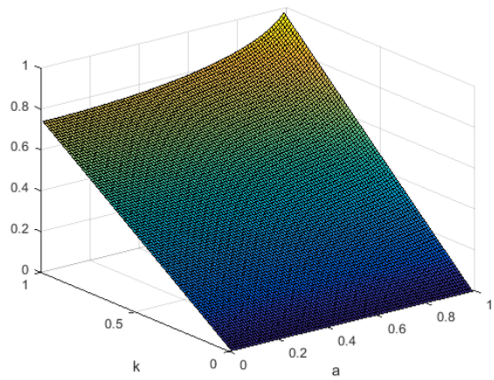


FIGURE 2. A plot of the left-hand side of the inequality in (14) as a function of a and $k := \left|\left(\kappa_S^{1,1}\right)_1\right|$.

Proof. A direct calculation[21] shows that the function given by $f(\tau) := e^{-\tau}\left(e^{a\tau} - e^{-a\tau}\right)$ achieves its maximum value $\left(\frac{1+a}{1-a}\right)^{\frac{a-1}{2a}} - \left(\frac{1-a}{1+a}\right)^{\frac{a+1}{2a}}$ when $\tau = \frac{1}{2a}\log\left(\frac{1+a}{1-a}\right)$. If the condition in (14) is satisfied, the maximum value of f is larger than $\left|\left(\kappa_S^{1,1}\right)_1\right|^{-1} a$ and hence, by continuity of f, there exists $\tau \in [0,\infty)$ such that condition (13) in Lemma 4.8 is satisfied. □

While the techniques employed in Lemma 4.8 and Corollary 4.10 appear to give promising results so far, Figure 2 shows a plot of the left-hand side of the inequality in (14). We see that no graph satisfies the condition in Corollary 4.10. It should be emphasized that this does *not* prove that, for all $\tau \geq 0$, pinning at node 1 does occur, but rather that our technique cannot be applied (in its present form) to arrive at a conclusion regarding pinning (see also Remark 4.7).

Remark 4.11. In this section we have assumed throughout that $n \geq 3$ and $\tilde{n} \geq 3$. We have done so mostly because it simplifies the notation. For example, alternatives for the notation $\{2,\dots,n-1\}$ would become cumbersome, and a result like the one in Lemma 4.1 would require a separate statement of essentially the same result for the case $n = 2$: The eigenvectors and eigenvalues v^1, v^n, λ_1, and λ_n, as given in the proof of the lemma, would remain and v^i and λ_i ($i \in \{2,\dots,n-1\}$), which are required in the case where $n \geq 3$, would be absent. In this remark we will point out a few other cosmetic changes which are required by the case $n = 2$ (or $\tilde{n} = 2$).

[21] Since $f'(\tau) = e^{-\tau}\left[(-1+a)e^{a\tau} + (1+a)e^{-a\tau}\right]$, we find that $f'(\tau) = 0$ if and only if $\tau = \tau_* := \frac{1}{2a}\log\left(\frac{1+a}{1-a}\right)$. Substituting this value into f gives $f(\tau_*) = \left(\frac{1+a}{1-a}\right)^{\frac{a-1}{2a}} - \left(\frac{1+a}{1-a}\right)^{-\frac{a+1}{2a}}$. Comparing the powers of these two terms, we find $\frac{a-1}{2a} - \left(-\frac{a+1}{2a}\right) = 1 > 0$. Moreover, since $a \in (0,1)$, we have $\frac{1+a}{1-a} > 1$, and thus we find $f(\tau_*) > 0$. Combined with the continuity of f and the facts that $f(0) = 0$ and $f(\tau) \to 0$ as $\tau \to \infty$ (since $-1+a < 0$ and $-1-a < 0$), we conclude that the value $f(\tau_*)$ is indeed the maximum value.

In Lemma 4.2 the denominator inside the logarithm in the definition of τ_c is zero if $n=2$ and thus pinning at each node occurs independent of the choice of τ (and, by symmetry, independent of whether $S=\{1\}$ or $S=\{2\}$). This can also be checked directly by computing $\left(e^{-\tau\Delta}\chi_S\right)_i$ (for $i\in V$) with $n=2$, based on the formulas given in the proof of the lemma (which are correct, also when $n=2$). We then see that $\left(e^{-\tau\Delta}\chi_S\right)_i=\frac{1}{2}$ is equivalent to the unsatisfiable condition that $e^{-2\omega^{1-r}\tau}=0$.

If we consider the case $\tilde{n}=2$ in Lemma 4.6, the computation in the proof of the lemma remains valid without requiring any changes, except that we only have the eigenvalues $\lambda_1=\lambda_-$ and $\lambda_{\tilde{n}}=\lambda_+$ with their corresponding eigenvectors v^1 and $v^{\tilde{n}}$ as given in the proof of the lemma. Since these are the only eigenvalues and eigenvectors which are used in the expansion of χ, the remainder of the proof —and thus the result of the lemma— remain unchanged.

Similarly, repeating the computations in the proof of Lemma 4.8 for $\tilde{n}=2$, we find the eigenvalues $\lambda_{1,\tilde{n}}=1\mp\sqrt{d_1^{-1}\sum_{k=2}^{\tilde{n}}d_k^{-1}\omega_{1k}}$ with corresponding eigenvectors $v^{1,\tilde{n}}$ as given in the proof. Even though in the case $\tilde{n}\geq 3$ the eigenvectors v^i ($i\in\{2,\dots,\tilde{n}-1\}$) were important in the expansion of χ, they did not play a role in the computation of $\left(e^{-\tau\Delta'}\chi_{S_1}\right)_1$, because their first coordinates v_1^i are zero. Hence, here too we find that the result of Lemma 4.8 —and thus also the result of Corollary 4.10— remain valid in the case $\tilde{n}=2$.

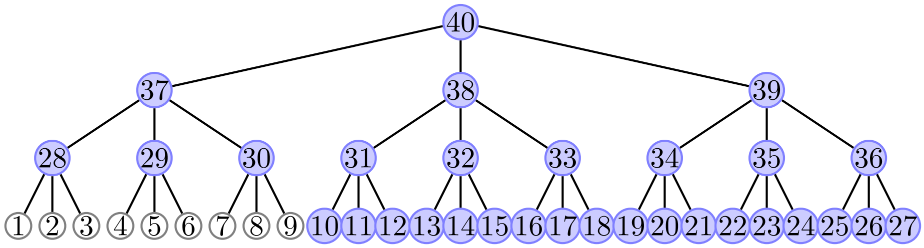
5. A regular tree

This section is partially based on and replaces [14, Section 6.3].

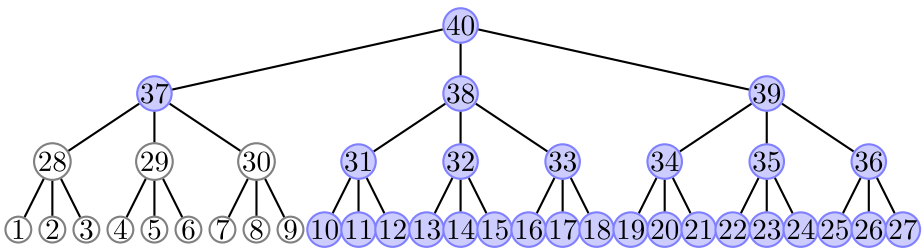
We consider the MBO iterations on a regular tree as in Figure 3. Let, for all $(i,j)\in E$, $\omega_{ij}=\omega>0$, and let $r=0$. As in Figure 3a, we consider the case where the initial set S consists of all the leaves of a single branch. We first observe, for all $j\in\{28,29,30\}$, that the subgraph induced by $\overline{S_j}$ is a star graph with node j as internal node and with three leaves (for an example of a star graph with four leaves, see Figure 1), so that the hypotheses of Lemma 4.6 are satisfied with nodes 28, 29, and 30 each playing the role of "node 1" in the lemma. Furthermore, in the notation of that lemma, $\tilde{n}=4$, $\theta_1=4$, and $\theta=1$. Figure 4a shows a plot of the quantity $Q(\tau;4,1,4)$ from (8) as a function of τ and we see that there exists a small range of τ-values for which $Q(\tau;4,1,4)>\frac{1}{2}$. For those values of τ, nodes 28, 29, and 30 will belong to S after one iteration of MBO and we end up with the situation as sketched in Figure 3b.

Generalizing the situation from Figure 3a we could leave $\tilde{n}$ as a free parameter (i.e. we consider a case where a given internal node that is in S^c, has $\tilde{n}-1$ neighbors in S and one neighbor in S^c), in which case $\theta_1=\tilde{n}-1$ and $\theta=1$. Figure 5a shows a plot of $Q(\tau;\tilde{n}-1,1,\tilde{n})$ as a function of both τ and $\tilde{n}$[22]. For larger $\tilde{n}$ the range of τ-values for which $Q(\tau;\tilde{n}-1,1,\tilde{n})>\frac{1}{2}$ gets larger. We should also note that for

[22]Even though we assumed $\tilde{n}\geq 3$, we can still plot Q for $\tilde{n}=2$. See also footnote 16.

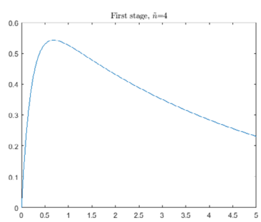


(A) Initial configuration (S: white nodes; S^c: purple nodes)

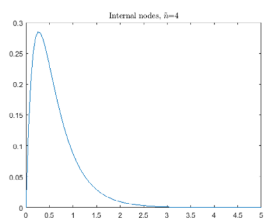


(B) Final configuration (S: white nodes; S^c: purple nodes)

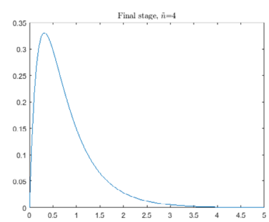
FIGURE 3. The initial and final configurations for one iteration of the MBO scheme on a tree graph; see Section 5.



(A) Plot of $Q(\tau; 4, 1, 4)$ from (8)



(B) Plot of $Q(\tau; 4, 4, 4)$ from (8)



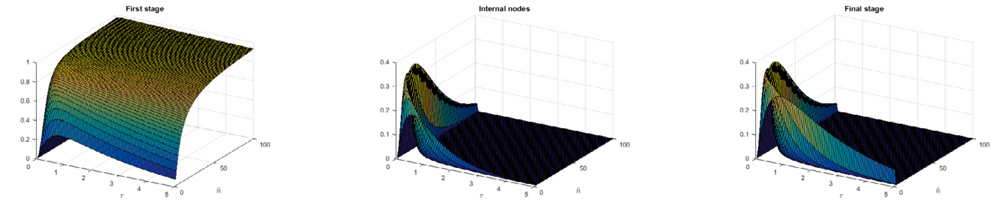
(C) Plot of $Q(\tau; 3, 4, 4)$ from (8)

FIGURE 4

$\tilde{n} = 2$ and $\tilde{n} = 3$ such a range does not exist, which means in those cases Lemma 4.6 cannot be used.

We can also ask the question what happens if we continue the MBO scheme beyond the first iteration. When, in Figure 3, the star graph induced by $\overline{S_{37}}$ is centered at node $37 \in S^c$ (with all children of 37 in S and its parent, node 40, not in S[23]), we have $\theta_1 = \theta = \tilde{n} = 4$. The plots in Figures 4b and 5b show that in this

[23] The use of the terms "children" and "parent" in this context is a slight abuse of terminology, as our graph is not directed. For ease of communication we intend these terms here to be interpreted in



(A) Plot of $Q(\tau; \tilde{n}, 1, \tilde{n})$ from (8)

(B) Plot of $Q(\tau; \tilde{n}, \tilde{n}, \tilde{n})$ from (8)

(C) Plot of $Q(\tau; \tilde{n}-1, \tilde{n}, \tilde{n})$ from (8)

FIGURE 5

case $Q(\tau; \tilde{n}, \tilde{n}, \tilde{n})$ does not exceed $\frac{1}{2}$ for any values of τ or $\tilde{n}$ in the plotted range (and further computations show that this is true for much larger ranges of τ and $\tilde{n}$). This does not necessarily mean that the value of node 37 does not change in the next MBO iteration, but rather that the method from Lemma 4.6 cannot be used to prove this is the case.

Similarly, if we consider the case in which the initial condition is $S = \{1, \ldots, n-1\}$ and $S^c = \{n\}$ where n is the parent node[24] of all other nodes (in the setting of Figure 3 this would mean $S = \{1, \ldots, 39\}$ and $S^c = \{40\}$), then $\theta_1 = \tilde{n} - 1$ and $\theta = \tilde{n}$ and Figures 4c and 5c show the relevant plots of $Q(\tau; \tilde{n}-1, \tilde{n}, \tilde{n})$. Again we see that in this case the method from Lemma 4.6 cannot be used to prove that the value of node 40 changes in the next MBO iteration.

6. Conclusions

In Theorem 3.1 we showed that the assumptions from [14, Theorem 4.8] cannot be satisfied by any graph. We then provided alternative results for the star graph and regular tree, which replace the wrong results from [14, Sections 6.2 and 6.3] which were based on [14, Theorem 4.8]. In particular, for those graphs we give conditions under which pinning occurs or does not occur at specific nodes.

It is an interesting question for future research if and how [14, Theorem 4.8] can be changed to provide a local (non-)pinning result for a large class of graphs, in the spirit in which the original theorem was intended.

In the appendices we provide a few minor corrections and clarifications to other parts of [14].

Acknowledgments. I would like to thank my coauthors from [14] for some discussions and feedback during the preparation of this paper.

---

the context of the directionality implied by the drawing in Figure 3, even though this directionality is not present in the mathematical description of the graph.

[24]In the sense of footnote 23.

A significant portion of the work for this paper was done by the author while he was a lecturer in the School of Mathematical Sciences of the University of Nottingham.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 777826.

Appendix A. Proof of Theorem 4.8

Before we give the updated proof of Theorem 4.8, we first give a helpful lemma, which is also interesting in its own right.

Lemma A.1. *Let v satisfy $\dot{v}_i = -(\Delta' v)_i$ with $v(0) = v_0$, where $v_0 \in \mathcal{V}_1$. Then for all $t \geq 0$, $v(t) = e^{-t\Delta'} v_0 \in \mathcal{V}_1$. Furthermore, if, for all $i \in V$, $(v_0)_i \geq 0$, then for all $t \geq 0$ and all $i \in V$, $v_i(t) \geq 0$.*

Proof. The first claim of this lemma follows directly from (5).

The remainder of the proof is very similar to the proof of the comparison principle in [14, Lemma 2.6(d)]. If, for all $i \in V$, $(v_0)_i = 0$, then for all $i \in V$ and all $t > 0$, $v_i(t) = 0$, by the uniqueness theorem for ordinary differential equations (ODEs). In this case there is nothing more to prove. By the first part of this lemma, we already know that for all $i \in \overline{S_1}^c$ and all $t \geq 0$ we have $v_i(t) = 0$. Hence we need to prove that for all $i \in \overline{S_1}$ we have $v_i(t) \geq 0$. Arguing by contradiction, suppose that $v_j(t^*) < 0$ for some $t^* \geq 0$ and some $j \in \overline{S_1}$. Define

$$t_0 := \sup\{\, t \geq 0 : \forall\, s \in (0,t)\ \forall l \in \overline{S_1}\ v_l(s) \geq 0\},$$

then $0 \leq t_0 \leq t^*$. By continuity of v_l for all $l \in \overline{S_1}$ (which follows from standard ODE theory) there is some $k \in \overline{S_1}$ such that $v_k(t_0) = 0$. Moreover, since $\dot{v}_k(t_0)$ exists (also by standard ODE theory), we have $\dot{v}_k(t_0) = \lim_{h\to 0} \frac{v_k(t_0) - v_k(t_0 - h)}{h} \leq 0$. Furthermore, $v_l(t_0) \geq 0$, for all $l \in \overline{S_1}$. This shows that if $v_i(t_0) > 0$ for some $i \in \overline{S_1} \cap \mathcal{N}_k$, then $(\Delta' v(t_0))_k < 0$ and $0 = \dot{v}_k(t_0) + (\Delta v(t_0))_k < 0$, which is a contradiction. We conclude that $v(t_0) = 0$ at all neighbors of k that are in $\overline{S_1}$. Since $\overline{S_1}$ is connected, by iterating the above argument we get in fact that $v(t_0) = 0$ at all nodes of $\overline{S_1}$ and thus at all nodes of V (since we already knew this to be the case at all nodes of $\overline{S_1}^c$). By the uniqueness theorem for ordinary differential equations we conclude that $v(t^*) = 0$ at all nodes, which gives a contradiction. □

Proof of Theorem 4.8. First we assume that $1 \in S^c$, so $S_1 = \mathcal{N}_1 \cap S$. By the comparison principle in [14, Lemma 2.6(d)], $\chi_{S_1} \leq \chi_S$ on V implies $(e^{-\tau\Delta}\chi_{S_1})_1 \leq (e^{-\tau\Delta}\chi_S)_1$. In particular, since $(\chi_{S_1})_1 = (\chi_S)_1 = 0$, we have $(e^{-\tau\Delta}\chi_S - \chi_S)_1 \geq (e^{-\tau\Delta}\chi_{S_1} - \chi_{S_1})_1$.

Let v satisfy the heat equation with Dirichlet boundary data, i.e., for all $i \in V$, $\dot{v}_i = -(\Delta' v)_i$, with $v(0) = \chi_{S_1}$. Such a v exists by standard theory for ordinary differential equations. By Lemma A.1, for all $t \geq 0$, $v(t) \in \mathcal{V}_1$. Moreover, by the same lemma, for all $t \geq 0$, $v(t) \geq 0$. Hence $\Delta' v \geq \Delta v$ at all nodes and for all times $t \geq 0$. Thus v is subcaloric, *i.e.*, $\dot{v}_i(t) \leq -(\Delta v)_i(t)$ for all $i \in V$ and all $t \geq 0$, and

$v(0) \leq \chi_S$. In addition, if $i \in V$, then the Laplacian satisfies $-(\Delta u)_i \leq -(\Delta \tilde{u})_i$ if $u_i = \tilde{u}_i$ and $u_j \leq \tilde{u}_j$, for all $j \in V \setminus \{i\}$. Hence, by the theory of differential inequalities (see for example [13, Theorem 8.1(3)]),

$$v_i(t) \leq \left(e^{-t\Delta} v(0)\right)_i = \left(e^{-t\Delta} \chi_{S_1}\right)_i, \quad \text{for all } i \in V.$$

In particular,

$$\begin{aligned}\left(e^{-\tau\Delta}\chi_{S_1} - \chi_{S_1}\right)_1 \geq v_1(\tau) - v_1(0) &= \left(e^{-\tau\Delta'}\chi_{S_1} - \chi_{S_1}\right)_1 \\ &= -\tau\left(\Delta'\chi_{S_1}\right)_1 + \tau^2 r(\tau),\end{aligned}$$

where $|r(\tau)| \leq \frac{1}{2} \sup\limits_{t\in[0,\tau]} \left(e^{-t\Delta'}(\Delta')^2\chi_{S_1}\right)_1 \leq \frac{1}{2}\|(\Delta')^2\chi_{S_1}\|_{\mathcal{V},\infty}$. From (6), note that $-\left(\Delta'\chi_{S_1}\right)_1 = -(\kappa^{1,r}_{S_1})_1 = -(\kappa^{1,r}_S)_1 = |(\kappa^{1,r}_S)_1|$, where we have used that $1 \in S^c$. We conclude that

$$\begin{aligned}(e^{-\tau\Delta}\chi_S - \chi_S)_1 &\geq \left(e^{-\tau\Delta}\chi_{S_1} - \chi_{S_1}\right)_1 \\ &\geq |(\kappa^{1,r}_S)_1|\tau - \frac{1}{2}\|(\Delta')^2\chi_{S_1}\|_{\mathcal{V},\infty}\tau^2,\end{aligned}$$

hence $\tau \in [\tau_1, \tau_2] \Rightarrow (e^{-\tau\Delta}\chi_S - \chi_S)_1 \geq \frac{1}{2}$, which proves the result for the case in which $1 \in S^c$.

To prove the desired statement if $1 \in S$, we note that

$$(e^{-\tau\Delta} - 1)(\chi_S + \chi_{S^c}) = 0,$$

so the condition $(e^{-\tau\Delta}\chi_S - \chi_S)_1 < -\frac{1}{2}$ is equivalent to $(e^{-\tau\Delta}\chi_{S^c} - \chi_{S^c})_1 > \frac{1}{2}$. Recall that, in this case, $S_1 = \mathcal{N}_1 \cap S^c$, and the same derivation as above holds[25], since $1 \in S = (S^c)^c$, with the exception that the admissible range of τ becomes the open interval (τ_1, τ_2). This is because, by our definition of the MBO algorithm, the thresholding operator thresholds the $\frac{1}{2}$-level set to 1. □

Appendix B. Updates and corrections to [14, Sections 3.3 and 4.2]

In this section we make use of the opportunity that the current paper presents to give a few updates and corrections to results from [14, Sections 3.3 and 4.2]. These corrections are overall minor and the original errors they address mostly fall into the category “badly or ambiguously written, easily fixable, statements”.

B.1. Updates and corrections to [14, Section 3.3]

To sustain the self-containedness of this paper, we first recall a few definitions from [14], in particular the definition of (anisotropic) graph total variation $\mathrm{TV}^q_a \colon \mathcal{V} \to \mathbb{R}$,

$$\mathrm{TV}^q_{\mathrm{a}}(u) := \frac{1}{2} \sum_{i,j\in V} \omega^q_{ij}|u_i - u_j|,$$

[25]In particular, carefully note that now $-\left(\Delta'\chi_{S_1}\right)_1 = (\kappa^{1,r}_S)_1 = |(\kappa^{1,r}_S)_1|$ holds.

and the graph distance and graph mean curvature flow from [14, Definitions 2.3 and 3.8]:

Definition 2.3 (from [14]**).** *Let $i \in V$. For all $j \in \mathcal{N}_i$, define $d^G_{ij} := \omega_{ij}^{q-1}$, and set $d^G(i,i) := 0$.*

We say γ is a path on V from $j \in V$ to $k \in V$ if there exists an $m \in \mathbb{N}$ such that $\gamma = (i_1, i_2, ..., i_m) \in V^m$, $i_1 = j$, $i_m = k$, and, for each $l \in \{1, \ldots, m-1\}$, $i_{l+1} \in \mathcal{N}_{i_l}$. The length of such a path γ is $|\gamma| := \sum_{l=1}^{m-1} d^G_{i_l i_{l+1}}$.

If $i, j \in V$, then the graph distance between nodes i and j is $d^G_{ij} := \min_\gamma |\gamma|$, where the minimum is taken over all paths γ from i to j.

If $S \subset V$ is nonempty, the graph distance from $i \in V$ to S is $d^S_i := \min_{j \in S} d^G_{ij}$. If $S = \emptyset$ we set, for all $i \in V$, $d^S_i := +\infty$.

Note that the definition above allows paths to contain repeated nodes, but disallows infinite paths. Definitions in other sources may exclude repeated nodes or allow infinite paths, but for our purposes these distinctions will not be of importance.

Definition 3.8 (from [14]**).** *The mean curvature flow, for $n \in \mathbb{N}$, $S_n = S(n\eth t)$, with discrete time step $\eth t$ for an initial set $S_0 \subset V$, is recursively defined by*

$$S_{n+1} \in \arg\min_{\hat{S} \subset V} \mathcal{F}(\hat{S}, S_n), \tag{MCF$_{\eth t}$}$$

where

$$\mathcal{F}(\hat{S}, S_n) := TV_a^q(\chi_{\hat{S}}) - TV_a^q(\chi_{S_n}) + \frac{1}{\eth t}\langle \chi_{\hat{S}} - \chi_{S_n}, (\chi_{\hat{S}} - \chi_{S_n}) d^{\Sigma_n}\rangle_{\mathcal{V}} \tag{15}$$

and $\Sigma_n := \{i \in V : \exists\, (i,j) \in E\ \ (i \in S_n \wedge j \in S_n^c) \vee (i \in S_n^c \wedge j \in S_n)\}$.

In (15), d^{Σ_n} denotes the graph distance to the set Σ_n. In the original paper we did not address what happens when $\Sigma_n = \emptyset$. By the definition of the graph distance from a node to a node set in Definition 2.3, if $S_n = \emptyset$ or $S_n = V$, then $d^{\Sigma_n} = +\infty$, hence $\emptyset$ and V are stationary states of (MCF$_{\eth t}$). Equivalently it is often useful to implicitly assume that $\emptyset \neq S_n \neq V$ and consider (MCF$_{\eth t}$) to terminate when either the state $\emptyset$ or V is achieved. In order not to complicate notation, the original paper [14] can be read assuming this latter condition. In other words, in each iteration of MCF$_{\eth t}$, S_n is assumed to be such that $d^{\Sigma_n} < \infty$.

Using the signed graph distance $sd^{\Sigma_n} := (\chi_{S_n^c} - \chi_{S_n}) d^{\Sigma_n}$, in [14, Lemma 3.11] the minimization of $\mathcal{F}$ in (MCF$_{\eth t}$) was rewritten as a minimization of

$$\mathcal{F}'(\hat{S}, S_n) = \langle \kappa^{q,r}_{\hat{S}} + \kappa^{q,r}_{S_n}, \chi_{\hat{S}} - \chi_{S_n}\rangle_{\mathcal{V}} + \frac{1}{\eth t}\langle \chi_{\hat{S}}, sd^{\Sigma_n}\rangle_{\mathcal{V}} \tag{16}$$

over subsets $\hat{S} \subset V$. This rewrite includes a step in which the term $\langle \chi_{\hat{S}}(1 - 2\chi_{S_n}) + \chi_{S_n}, d^{\Sigma_n}\rangle_{\mathcal{V}}$ is split into $\langle \chi_{\hat{S}}, (\chi_{S_n^c} - \chi_{S_n}) d^{\Sigma_n}\rangle_{\mathcal{V}} + \langle \chi_{S_n}, d^{\Sigma_n}\rangle_{\mathcal{V}}$. This split of the inner product term into two terms is allowed because of our assumption that $d^{\Sigma_n} < \infty$, as explained above. In particular, this split is not valid if $S_n = V$. If we wanted to include this case, we could extend the definition of $\mathcal{F}'$ to cover that situation separately[26].

In the original paper, [14, Lemma 3.12 and Theorem 3.13] contained statements that were either ambiguous or false as given. We present clarified and corrected versions here.

Lemma 3.12 (from [14]). *Let $u \in \mathcal{V}$ and $E(t) := \{i \in V : u_i > t\}$, for $t \in \mathbb{R}$. Then $TV_a^q(u) = \int_{\mathbb{R}} TV_a^q(\chi_{E(s)})\, ds$. Suppose $u_-, u_+ \in \mathbb{R}$ are such that $u_- \leq \min_{i\in V} u_i$ and $\max_{i\in V} u_i \leq u_+$, then also*

$$TV_a^q(u) = \int_{u_-}^{\infty} TV_a^q(\chi_{E(s)})\, ds = \int_{-\infty}^{u_+} TV_a^q(\chi_{E(s)})\, ds$$
$$= \int_{u_-}^{u_+} TV_a^q(\chi_{E(s)})\, ds.$$

Proof. As also noted in [16] and [2], we have, for $i, j \in V$,

$$|u_i - u_j| = \int_{\mathbb{R}} \left| \left(\chi_{E(s)}\right)_i - \left(\chi_{E(s)}\right)_j \right| ds,$$

hence

$$\frac{1}{2} \sum_{i,j\in V} \omega_{ij}^q |u_i - u_j| = \int_{\mathbb{R}} \frac{1}{2} \sum_{i,j\in V} \omega_{ij}^q \left| \left(\chi_{E(s)}\right)_i - \left(\chi_{E(s)}\right)_j \right| ds.$$

The second result follows, since, for $i, j \in V$,

$$\int_{-\infty}^{u_-} \left| \left(\chi_{E(s)}\right)_i - \left(\chi_{E(s)}\right)_j \right| ds = \int_{u_+}^{\infty} \left| \left(\chi_{E(s)}\right)_i - \left(\chi_{E(s)}\right)_j \right| ds = 0.$$

□

Theorem 3.13 (from [14]). *Let $m \in \mathbb{R}$,*

$$\mathcal{V}_m := \{u \in \mathcal{V} : \forall i \in V \ -m \leq u_i \leq m\}^{27}, \tag{17}$$

and $F(u) := TV_a^q(u) + \frac{1}{\eth t}\langle u, sd^{\Sigma_n}\rangle_{\mathcal{V}}$. Then the convex minimization problem

$$\min_{u\in\mathcal{V}_m} F(u), \tag{18}$$

has a minimizer $u \in \mathcal{V}_m$. Furthermore, for all $s \in (-m, m)$, the superlevel set $E(s) := \{i \in V : u_i > s\}$ is a minimizer $\hat{S}$ of $\mathcal{F}(\cdot, S_n)$ from (15).

Proof. We can identify $\mathcal{V}_m$ with a compact subset of $\mathbb{R}^n$ and, in that setting, F with a real-valued continuous function on this compact subset. Hence, a minimizer $u \in \mathcal{V}_m$ exists.

[26] This could be done by redefining $\mathcal{F}'$ to be equal to the expression in (16) when $\emptyset \neq S_n \neq V$, equal to 0 when $S = S_n = \emptyset$ or $S = S_n = V$, and equal to $+\infty$ otherwise.

[27] Note that, for $m = 1$, the set $\mathcal{V}_1$ introduced here is not the same as the set $\mathcal{V}_1$ that was defined in Section 3 and that was used in several instances in Sections 3, 4, and A.

Since $-m \leq \min_{i\in V} u_i$ and $m \geq \max_{i\in V} u_i$, we know from Lemma 3.12 that $\mathrm{TV}_{\mathrm{a}}^q(u) = \int_{-m}^m \mathrm{TV}_{\mathrm{a}}^q(\chi_{E(s)})\,ds$. Writing $u_i - m = \int_{-m}^m \left(\chi_{E(s)}\right)_i ds$, we get $\langle u - m, sd^{\Sigma_n}\rangle_{\mathcal{V}} = \int_{-m}^m \langle \chi_{E(s)}, sd^{\Sigma_n}\rangle_{\mathcal{V}}\, ds$. This gives

$$\begin{aligned} F(u) - \frac{1}{\eth t}\langle m, sd^{\Sigma_n}\rangle_{\mathcal{V}} &= \int_{-m}^m \left[\mathrm{TV}_{\mathrm{a}}^q(\chi_{E(s)}) + \frac{1}{\eth t}\langle \chi_{E(s)}, sd^{\Sigma_n}\rangle_{\mathcal{V}}\right] ds \\ &= \int_{-m}^m \mathcal{F}''(E(s), S_n)\, ds, \end{aligned}$$

where, for $\hat{S} \subset V$,

$$\mathcal{F}''(\hat{S}, S_n) := \mathcal{F}'(\hat{S}, S_n) + \mathrm{TV}_{\mathrm{a}}^q(S_n) = \mathrm{TV}_{\mathrm{a}}^q(\chi_{\hat{S}}) + \frac{1}{\eth t}\langle \chi_{\hat{S}}, sd^{\Sigma_n}\rangle_{\mathcal{V}}.$$

Hence, if u minimizes F, then for a.e. $s \in (-m, m)$, the superlevel set $E(s)$ minimizes $\mathcal{F}''(\cdot, S_n)$ and thus also $\mathcal{F}'(\cdot, S_n)$. Because u takes only finitely many values, the result holds for all $s \in (-m, m)$. Since the minimization of $\mathcal{F}$ in (MCF$_{\eth t}$) is equivalent to the minimization of $\mathcal{F}'$, the proof is complete. □

Lemma 3.12 and Theorem 3.13 above also hold if we define $E(t)$ in terms of a non-strict inequality instead: $E(t) := \{i \in V : u_i \geq t\}$.

Finally, we note that in light of the extra constraints put on the domain of minimization in (18) (compared to what was written in the original [14, Theorem 3.13]), the Euler-Langrange equation for solutions of the minimization problem (18) given in [14, Remark 3.14] becomes

$$\operatorname{div}\operatorname{sgn}(\nabla u) + \frac{1}{\eth t} sd^{\Sigma_n} + \mu_u - \mu_l = 0,$$

provided ∇u is never zero. Here $\mu_u, \mu_l \in \mathcal{V}$ are the nonnegative Lagrange multipliers associated to the upper bound and lower bound, respectively, which are imposed by u being restricted to $\mathcal{V}_m$ from (17). Whenever $(\nabla u)_{ij} = 0$ for some i, j, the above equation is replaced by a differential inclusion in terms of the subdifferential of the absolute value function. Concretely, since the subdifferential of the absolute value function at 0 is the interval $[-1, 1]$, there exists $\phi \in \mathcal{E}$ such that for all $i, j \in V$, $|\phi_{ij}| \leq 1$,

$$\operatorname{div}\phi + \frac{1}{\eth t} sd^{\Sigma_n} + +\mu_u - \mu_l = 0,$$

and if $(\nabla u)_{ij} \neq 0$, then $\phi_{ij} = \operatorname{sgn}((\nabla u)_{ij})$.

We end this section by noting a minor error earlier in [14, Section 3]. The formula for $|B_\delta(x) \cap S| - \frac{1}{2}|B_\delta(x)|$ in the continuum case at the bottom of [14, page 18], should have read [6]: the mean curvature $\kappa(x)$ at the point $x \in \partial S$ in the boundary of a set $S \in \mathbb{R}^d$ satisfies the property that, if S is smooth enough, then there is a constant C (depending on d) such that for any given ball $B_\delta(x)$ of radius δ and center $x \in \partial S$,

$$|B_\delta(x) \cap S| - \tfrac{1}{2}|B_\delta(x)| = C\kappa\delta|B_\delta(x)| + o(\delta|B_\delta(x)|).$$

B.2. A corrected proof for Theorem 4.4

In the original paper [14, Theorem 4.4] had errors in its proof, although the result as it was stated is correct. Below is the corrected version. We first need to recall some notation from [14]. The n eigenvalues (counted with multiplicity) of the graph Laplacian Δ are denoted by $0 = \lambda_1 < \lambda_2 \leq \ldots \leq \lambda_n$. The spectral radius ρ is, in this case, equal to the largest eigenvalue λ_n. The minimal degree in the graph is $d_- := \min_{i\in V} d_i$. For a subset $S \subset V$, define $R_S := \frac{\mathrm{vol}S}{\mathrm{vol}V}$, where $\mathrm{vol}S := \|\chi_S\|_{\mathcal{V}}^2$. Then, from [14, Theorems 4.2 and 4.3] we take the definitions, for $\emptyset \neq S \neq V$,

$$\tau_\rho(S) := \rho^{-1} \log\left(1 + \frac{1}{2} d_-^{\frac{r}{2}} (\mathrm{vol}S)^{-\frac{1}{2}}\right),$$

$$\tau_t(S) := \lambda_2^{-1} \log\left(\frac{(\mathrm{vol}S)^{\frac{1}{2}} (\mathrm{vol}S^c)^{\frac{1}{2}}}{(\mathrm{vol}V)^{\frac{1}{2}} \left|R_S - \frac{1}{2}\right| d_-^{\frac{r}{2}}}\right), \quad \text{if } R_S \neq \frac{1}{2}.$$

(Some of) the results from [14, Theorems 4.2 and 4.3] are that pinning occurs at all nodes of the graph (with MBO initial node set S) if $\tau < \tau_\rho(S)$ and that trivial dynamics occurs if $\tau > \tau_t(S)$, in the sense that $Pe^{-\tau\Delta}\chi_S = \chi_V$ if $R_S > \frac{1}{2}$ and $Pe^{-\tau\Delta}\chi_S = 0$ if $R_S < \frac{1}{2}$ (and thus after one iteration MBO has arrived at a stationary state from initial set S). The result in [14, Theorem 4.4] gives a sufficient condition on the spectrum of Δ (and thus on the graph) such that there is a gap between τ_ρ and τ_t in which potentially interesting dynamics could happen (note that the theorem does *not* guarantee that pinning and trivial dynamics are both absent for choices of τ in this gap).

Theorem 4.4 (From [14]**).** *Let $n \geq 2$ and let $S \subset V$ be such that $\emptyset \neq S \neq V$ and $R_S \neq \frac{1}{2}$. If $\frac{\lambda_2}{\lambda_n} < \frac{\log\sqrt{2}}{\log\frac{3}{2}} \approx 0.85$, then $\tau_\rho(S) < \tau_t(S)$.*

Proof. We have $\left|R_S - \frac{1}{2}\right| \leq \frac{1}{2}$ and $d_-^r \leq \mathrm{vol}S \leq \mathrm{vol}V - d_-^r$, since $\emptyset \neq S \neq V$. Thus, since $\mathrm{vol}S \mapsto \mathrm{vol}S\,(\mathrm{vol}V - \mathrm{vol}S) = (\mathrm{vol}S)\ (\mathrm{vol}S^c)$ is concave, we also find that $(\mathrm{vol}S)\ (\mathrm{vol}S^c) \geq d_-^r(\mathrm{vol}V - d_-^r)$. Therefore

$$\tau_\rho(S) = \lambda_n^{-1} \log\left(1 + \frac{1}{2}\ d_-^{\frac{r}{2}}\ (\mathrm{vol}\ S)^{-\frac{1}{2}}\right) \leq \lambda_n^{-1}\ \log\frac{3}{2},$$

$$\tau_t(S) \geq \lambda_2^{-1}\ \log\left(2\sqrt{1 - \frac{d_-^r}{\mathrm{vol}V}}\right) \geq \lambda_2^{-1}\ \log\sqrt{2},$$

where in the final inequality we have used that $\mathrm{vol}V \geq n d_-^r \geq 2 d_-^r$. The result follows. $\square$

Publishers Note. Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

References

[1] J. Budd and Y. van Gennip, *Deriving graph MBO as a semi-discrete implicit Euler scheme for graph Allen–Cahn, towards a potential link to graph mean curvature flow*, in preparation.

[2] A. Chambolle, Total variation minimization and a class of binary MRF models, in: *Energy Minimization Methods in Computer Vision and Pattern Recognition*, LNCS Vol. **3757**, pp. 136–152, Springer, 2005.

[3] M. Cucuringu, A. Pizzoferrato, and Y. van Gennip, it An MBO scheme for clustering and semi-supervised clustering of signed networks, in preparation; preprint arXiv:190103091.

[4] H. Hu, T. Laurent, M.A. Porter, and A.L. Bertozzi, A method based on total variation for network modularity optimization using the MBO scheme, *SIAM Journal on Applied Mathematics* **73** no. 6 (2013), 2224–2246.

[5] H. Hu, J. Sunu, and A.L. Bertozzi, Multi-class graph Mumford-Shah model for plume detection using the MBO scheme, in: *Energy Minimization Methods in Computer Vision and Pattern Recognition*, LNCS Vol. **8932**, pp. 209–225, Springer, 2015.

[6] D. Hulin and M. Troyanov, Mean curvature and asymptotic volume of small balls, *The American Mathematical Monthly* **110** no. 10 (2003), 947–950.

[7] B. Keetch and Y. van Gennip, *A Max-Cut approximation using a graph based MBO scheme*, to appear; preprint arXiv:1711.02419.

[8] E. Merkurjev, T. Kostic, and A.L. Bertozzi, An MBO scheme on graphs for segmentation and image processing, *SIAM Journal on Imaging Sciences* **6** no. 4 (2013), 1903–1930.

[9] E. Merkurjev, J. Sunu, and A.L. Bertozzi, Graph MBO method for multiclass segmentation of hyperspectral stand-off detection video, in: 2014 *IEEE International Conference on Image Processing (ICIP)*, pp. 689–693, IEEE, 2014.

[10] E. Merkurjev, A.L. Bertozzi, and F.R.K. Chung, *A semi-supervised heat kernel pagerank MBO algorithm for data classification*, Tech. report, University of California, Los Angeles, 2016.

[11] B. Merriman, J.K. Bence, and S. Osher, *Diffusion generated motion by mean curvature*, UCLA Department of Mathematics CAM report CAM 06–32, 1992.

[12] B. Merriman, J.K. Bence, and S. Osher, Diffusion generated motion by mean curvature, in: *AMS Selected Letters, Crystal Grower's Workshop*, pp. 73–83, AMS, 1993.

[13] J. Szarski, *Differential inequalities*, PWN Warsaw, 1965.

[14] Y. van Gennip, N. Guillen, B. Osting, and A.L. Bertozzi, Mean curvature, threshold dynamics, and phase field theory on finite graphs, *Milan J. Math.* **82** no. 1 (2014), 3–65.

[15] Y. van Gennip, An MBO scheme for Minimizing the Graph Ohta–Kawasaki Functional, *Journal of Nonlinear Science* (2018); `https://doi.org/10.1007/s00332-018-9468-8`.

[16] B.A. Zalesky, Network flow optimization for restoration of images, *Journal of Applied Mathematics* **2** no. 4 (2002), 199–218.

Yves van Gennip
Delft Institute of Applied Mathematics
Delft University of Technology
2628 XE Delft
The Netherlands
e-mail: y.vangennip@tudelft.nl

Received: April 16, 2018.
Accepted: February 20, 2019.