Discrete Laplacian on Graphs, Dirichlet Problem, and Minimization of Energy

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Abstract

This report is primarily interested in discrete Laplacian on graphs and the Dirichlet problem. We investigate two cases of graphs, their Dirichlet problems, and the method of finding solutions to such problems by minimization of their corresponding energy functionals. In the case of an infinite, locally-finite, undirected, simple graph, we find that the minimization of its energy functional yields a solution to its Dirichlet or boundary-value problem. In the case of a finite, directed, locally-finite decision tree, we propose a type of such tree specified by a chosen vertex with no predecessors and by a chosen boundary set of vertices that have no successors. We then further consider a special case of such construction where all the paths of the tree terminate at the same *level*. We find that the minimization of such a special case's energy functional yields a solution to its Dirichlet problem only when some additional conditions *away from* the boundary (level of termination) are met.

1 Introduction

1.1 Motivation

In data science, regression and classification problems start with a given set of data. In the collection, some data are labeled and some are not labeled. In supervised learning, we train a model on data that have labels, learning a mapping between inputs and their corresponding labels, and then make prediction for unlabeled data. On the other hand, in semi-supervised learning, we train a model on both the labeled data and unlabeled data of a given data set. We use semi-supervised learning more often than supervised-learning when the data set contains a larger amount of unlabeled data than labeled data. There are various semi-supervised learning techniques, including graph-based methods. In this paper, we study special cases of the graph-based methods.

Let us consider a given data set V where $\partial V \subsetneq V$ are labeled and $V \setminus \partial V$ are unlabeled. Let $u: V \to \mathbb{R}$ be an unknown real-valued labeling function on the set. The data in $\partial V \subsetneq V$ are labeled, in other words, known by a real-valued function $f: \partial V \to \mathbb{R}$. From [2], we know that since there are arbitrarily many ways to extend the labels and the problem is ill-posed without some additional assumptions, it is standard to make *semi-supervising smoothness assumption*, which states that "the degree of smoothness should be locally proportional to the density of the graph." One approach is Laplacian regularization, which leads to energy minimization and the Dirichlet problem for discrete Laplacian on graphs, which are the primary interests in this paper.

1.2 Some definitions of graphs

Definition 1.1 (Undirected graph). An undirected graph $G \coloneqq \{V, E\}$ is a graph whose edges are a union of some subsets of the collection of all two-element subsets of the vertex set V, that is, for all $i \in I$, where I is an arbitrary index set,

$$E \coloneqq \bigcup_{i \in I} S_i,$$

where

$$S_i \subseteq \left\{ \{a, b\} \mid a, b \in V \right\}.$$

Definition 1.2 (Simple graph). A *simple graph* is a graph that contains at most one edge between any two vertices and no loops on any vertex itself.

Definition 1.3 (Directed graph, or Digraph). A directed graph $G := \{V, E\}$ is a graph whose edges are a union of some subsets of the collection of all ordered pairs of the vertex set V. Each edge is thought of having an initial vertex and a terminal vertex, that is, for all $i \in I$, where I is an arbitrary index set,

$$E \coloneqq \bigcup_{i \in I} S_i,$$

where

$$S_i \subseteq \Big\{ (a, b) \mid a, b \in V \Big\}.$$

Definition 1.4 (Infinite graph). An *infinite graph* is a graph with the set of vertices being countably infinite.

Definition 1.5 (Locally-finite graph). A graph is *locally finite* if all its vertices have finite degrees, that is, a finite number of neighbors.

2 Case of an infinite, locally-finite, undirected, simple graph

2.1 Graph setup

Let us consider an infinite, locally-finite, undirected, simple graph with a countably infinite set of vertices V and a proper, nonempty subset of V, which we call the *boundary* of V, denoted by $\partial V \subsetneq V$, and let us consider that for every element (vertex) v of V, there is a unique neighborhood consisting of $n_v \in \mathbb{N}^1$ adjacent, neighboring vertices (thus, locally finite), denoted by $S_v := \{v_i\}_{i=1}^{n_v}$, where $v'_i s$ are called the *successors* of the vertex v, with each v_i connecting to v by an edge. Let us denote the *cardinality* of S_v as n_v .

Proposition 2.1. Given a graph $G := \{V, E\}$ from Section 2.1, then for any $a, b \in V$, we have

$$a \in S_b \iff b \in S_a$$

Proof. For any $a, b \in V$, $a \in S_b \iff \{a, b\} \in E \iff b \in S_a$.

Proposition 2.1 implies the following.

Proposition 2.2. Let $a \in V$. Then for any $b \in S_a$, we have

$$b \in S_a \iff a \in S_b.$$

Proof. Given $a \in V$, by Proposition 2.1, there exists a unique neighborhood of a, which is S_a . For any $b \in S_a$, we have that $b \in V$ and that there exists a unique S_b by Proposition 2.1, and then $b \in S_a \iff a \in S_b$.

Let us define a function

$$u\colon V\to\mathbb{R}.\tag{1}$$

We definite the following discrete analogies, which we took inspirations from [6], to their corresponding continuous operations:

Definition 2.1. The gradient of function u(v) is

$$\nabla u(v) \coloneqq (u(v_i) - u(v))_{i=1}^{n_v}.$$
(2)

Definition 2.2. The *divergence* of $\nabla u(v)$ is

$$\operatorname{div}(\nabla u(v)) = \nabla \cdot \nabla u(v) = \Delta_2 u(v) = \Delta u(v) \coloneqq \sum_{i=1}^{n_v} \left(u(v_i) - u(v) \right).$$
(3)

Definition 2.3. The *integral* of u(v) is

$$\int_{V} u(v) \coloneqq \sum_{v \in V} u(v).$$
(4)

Definition 2.4. The L_2 -norm, or the Euclidean norm, is as usual, that is,

$$|\nabla u(v)|^2 := \sum_{i=1}^{n_v} (u(v_i) - u(v))^2.$$
(5)

¹Note: \mathbb{N} in this paper does not contain the element 0.

2.2 Dirichlet problem

2.2.1 Dirichlet problem on *p*-Laplacian

The Dirichlet problem is a concept in partial differential equations involving finding a solution to a given partial differential equation subject to some specified boundary conditions. In particular, the Dirichlet problem on p-Laplacian equation has the following setup, see [2]:

Find $u: U \subseteq \mathbb{R}^n \to \mathbb{R}$ such that for p where $\in 1 and for <math>f: \partial U \to \mathbb{R}$, we have that

$$\begin{cases} \operatorname{div}(|\nabla u|^{p-2}\nabla u) \coloneqq \Delta_p u = 0, & \text{in } U\\ u = f, & \text{on } \partial U \end{cases}$$
(6)

seeks to find a *p*-harmonic function subject to specified boundary conditions.

2.2.2 Variational method and minimization of energy functional

In calculus of variations, the first variation method minimizing an energy functional defined on all smooth functions u satisfying specified boundary conditions gives rise to some solutions to a given partial differential equation. In the context of the Dirichlet problem on regular, 2-Laplacian in Section 2.2.1, the energy functional has the following definition, see [3]:

Definition 2.5 (Energy functional). Given $f : \partial U \to \mathbb{R}$, the associated *energy functional* to the Dirichlet problem in Section 2.2.1 for p = 2 is defined as

$$I[w] \coloneqq \frac{1}{2} \int_{U} |\nabla u(x)|^2 dx, \tag{7}$$

where $w \in \mathcal{A} \coloneqq \{ w \in C^2(U) \mid w = f \text{ on } \partial U \}.$

Following, the minimization of energy has the following set up:

$$I[u] \coloneqq \min_{w \in \mathcal{A}} I[w].$$
(8)

There is a theorem for the Dirichlet problem on Laplacian equation pertaining to finding a harmonic solution that minimizes the energy functional:

Theorem 2.1. If $u \in A$ satisfies Eq. (8), then u solves the Dirichlet problem in Section 2.2.1 for p = 2, i.e., $\Delta u = 0$ in U.

In summary, by minimizing the energy functional associated with the Laplacian equation over all smooth functions satisfying specified boundary conditions, a function, if it exists, that minimizes the energy functional is a solution to the Laplace equation, and thus, a solution to the Dirichlet problem on the Laplacian equation.

2.2.3 Dirichlet problem on graph setup in Section 2.1

In the discrete analogy to regular, 2–Laplacian and specifically for the setup in Section 2.1, the Dirichlet problem becomes as such:

Find $u: V \to \mathbb{R}$ such that for $f: \partial V \to \mathbb{R}$, we have that

$$\begin{cases} \Delta u = 0, & \text{in } V \setminus \partial V \\ u = f, & \text{on } \partial V \end{cases}.$$
(9)

For the uniqueness and existence of general, p-harmonious functions on finite graphs, see [4]. For the uniqueness and existence and results related to connected, finite graphs with drift via games, see [5].

2.2.4 Minimization of energy on graph setup in Section 2.1

Given the setup for infinite, locally-finite, undirected, simple graphs in Section 2.1, let us first define the *energy functional* associated with its Dirichlet Problem defined in Section 2.2.3.

Definition 2.6 (Energy functional). Given $f: \partial V \to \mathbb{R}$, the associated *energy functional* of the graph setup in Section 2.1 to its Dirichlet problem (Section 2.2.3) is defined as

$$I[w] = \sum_{v \in V} |\nabla w(v)|^2, \tag{10}$$

where $w \in \mathcal{A} \coloneqq \{w \colon V \to \mathbb{R} \mid w = f \text{ on } \partial V\}.$

Consequently, the minimization of energy has the following setup:

$$I[u] \coloneqq \min_{w \in \mathcal{A}} I[w].$$
⁽¹¹⁾

The discrete version of Theorem 2.1 for the graph setup in Section 2.1 is similar. Let us first present a lemma and a proposition.

Lemma 2.2. Given $\phi: V \to \mathbb{R}$ such that there exists a support set $\operatorname{supp}(\phi) \coloneqq \{v \in V \mid \phi(v) \neq 0\}$ and given $u: V \to \mathbb{R}$, if $\operatorname{supp}(\phi) = \{v_0\}$, where $v_0 \in V \setminus \partial V$, then

$$\int_{V} \nabla u \cdot \nabla \phi = -2\phi(v_0)\Delta u(v_0).$$

Proof. We want to show that $\sum_{v \in V} \nabla u \cdot \nabla \phi = -2\phi(v_0)\Delta u(v_0)$.

We have

$$\sum_{v \in V} \nabla u \cdot \nabla \phi = \sum_{v \in V} \sum_{i=1}^{n_v} (u(v_i) - u(v))(\phi(v_i) - \phi(v)) :$$

We know that $(\phi(v_i) - \phi(v)) = 0$ for $v \in V$ such that $v_0 \notin \{v\} \cup S_v$ holds. Equivalently, $(\phi(v_i) - \phi(v)) \neq 0$ for $v \in V$ such that $v_0 \in \{v\} \cup S_v$. We also know that the statement that for all $v \in V$ such that $v_0 \in \{v\} \cup S_v$ is equivalent to the statement that for all $v \in V$ such that $v_0 = v$ or $v_0 \in S_v$, which is equivalent to $v = v_0$ or $v \in S_{v_0}$ by Proposition 2.1, which is equivalent to $v \in \{v_0\} \cup S_{v_0}$. Thus, we have

$$= \sum_{v \in v_0 \cup S_{v_0}} \sum_{i=1}^{n_v} (u(v_i) - u(v))(\phi(v_i) - \phi(v))$$

$$= \sum_{i=1}^{n_{v_0}} (u(v_{0_i}) - u(v_0)(\phi(v_{0_i}) - \phi(v_0)) + \sum_{v \in S_{v_0}} \sum_{i=1}^{n_v} (u(v_i) - u(v))(\phi(v_i) - \phi(v))$$

$$= -\phi(v_0)\Delta u(v_0) + \sum_{j=1}^{n_{v_0}} \sum_{i=1}^{n_{v_{0_j}}} (u(v_{0_ji}) - u(v_{0_j}))(\phi(v_{0_ji}) - \phi(v_{0_j})),$$

$$= \{v_0\}_{i=0}^{n_{v_0}} \text{ and } S_{v_0} := \{v_0\}_{i=0}^{n_{v_{0_j}}}$$

where $S_{v_0} \coloneqq \{v_{0j}\}_{j=1}^{n_{v_0}}$ and $S_{v_{0j}} \coloneqq \{v_{0j}\}_{i=1}^{n_{v_0j}}$: We have $\phi(v_{0i}) \equiv 0$ since v_{0i} are successors

We have $\phi(v_{0j}) \equiv 0$ since v_{0j} are successors of v_0 and the graph is simple, which has no loops. Thus, we have

$$= -\phi(v_0)\Delta u(v_0) + \sum_{j=1}^{n_{v_0}} \sum_{i=1}^{n_{v_0}} (u(v_{0ji}) - u(v_{0j}))(\phi(v_{0ji})) :$$

By Proposition 2.1, we know that for every j, there exists a unique (a simple graph has no duplicate edges) i such that $v_{0ji} = v_0 \in S_{v_{0j}}$, so we have

$$= -\phi(v_0)\Delta u(v_0) + \sum_{i=1}^{n_{v_0}} (u(v_0) - u(v_{0j}))(\phi(v_0))$$

$$= -\phi(v_0)\Delta u(v_0) - \sum_{i=1}^{n_{v_0}} (u(v_{0j}) - u(v_0))(\phi(v_0))$$

$$= -\phi(v_0)\Delta u(v_0) - \phi(v_0)\Delta u(v_0) = -2\phi(v_0)\Delta u(v_0).$$

We will see next that a similar result holds for the case when the support set is finite and nonempty.

Proposition 2.3. Given $\phi: V \to \mathbb{R}$ such that there exists a support set $\operatorname{supp}(\phi) \coloneqq \{v \in V \mid \phi(v) \neq 0\}$ and given $u: V \to \mathbb{R}$, if $\operatorname{supp}(\phi)$ is finite and nonempty, i.e., the cardinality

of $\operatorname{supp}(\phi) = n \in \mathbb{N}$, then

$$\int_V \nabla u \cdot \nabla \phi = -2 \int_V \phi \Delta u.$$

Proof. We want to show that $\sum_{v \in V} \nabla u(v) \cdot \nabla \phi(v) = -2 \sum_{v \in V} \phi(v) \Delta u(v)$.

We are given a finite support set, $\operatorname{supp}(\phi)$. Let $\operatorname{supp}(\phi) = \{v_1, v_2, v_3, \ldots, v_n\}$, where $n \in \mathbb{N}$. Note that $\operatorname{supp}(\phi) \subseteq V \setminus \partial V$ because $\phi(v) = 0$ for all $v \in \partial V$.

Let us define functions $\phi_i(v) \colon V \to \mathbb{R}$ as

$$\phi_i(v) = \begin{cases} \phi(v), & v = v_i \\ 0, & v \neq v_i \end{cases},$$

where $i \in \{1, 2, \ldots, n\}$ and $v_i \in \operatorname{supp}(\phi)$.

Thus, we can write the function ϕ as

$$\phi(v) = \begin{cases} \phi_i(v), & v = v_i \\ 0, & v \neq v_i \end{cases}$$

for all $i \in \{1, 2, ..., n\}$ and for all $v_i \in \operatorname{supp}(\phi)$.

Then we can also write $\phi(v) = \sum_{i=1}^{n} \phi_i(v)$. Let us show that $\nabla \phi(v) = \sum_{i=1}^{n} \nabla \phi_i(v)$. We have

$$\nabla \phi(v) = (\phi(v_j) - \phi(v))_{j=1,2,\dots,n_v}$$

= $\left(\sum_{i=1}^n \phi_i(v_j) - \sum_{i=1}^n \phi_i(v)\right)_{j=1,2,\dots,n_v}$
= $\sum_{i=1}^n (\phi_i(v_j) - \phi_i(v))_{j=1,2,\dots,n_v} = \sum_{i=1}^n \nabla \phi_i(v).$

Let us go back to the proof. We write

$$\int_{V} \nabla u \cdot \nabla \phi = \sum_{v \in V} \sum_{j=1}^{n_{v}} (u(v_{j}) - u(v))(\phi(v_{j}) - \phi(v))$$
$$= \sum_{v \in V} \sum_{j=1}^{n_{v}} (u(v_{j}) - u(v)) \sum_{i=1}^{n} (\phi_{i}(v_{j}) - \phi_{i}(v))$$
$$= \sum_{i=1}^{n} \left(\sum_{v \in V} \sum_{j=1}^{n_{v}} (u(v_{j}) - u(v))(\phi_{i}(v_{j}) - \phi_{i}(v)) \right)$$
$$= \sum_{i=1}^{n} \left(\int_{V} \nabla u \cdot \nabla \phi_{i} \right) :$$

Since $v_i \in V \setminus \partial V$ and $\operatorname{supp}(\phi_i) = \{v_i\}$, we can apply Lemma 2.2, and we obtain

$$=\sum_{i=1}^{n} (-2\phi_i(v_i)\Delta u(v_i)) = -2\sum_{i=1}^{n} \phi_i(v_i)\Delta u(v_i) = -2\sum_{i=1}^{n} \phi(v_i)\Delta u(v_i)$$
$$= -2\Big(\sum_{i=1}^{n} \phi(v_i)\Delta u(v_i) + \sum_{y\in V\setminus \text{supp}(\phi)} \phi(y)\Delta u(y)\Big)$$
$$= -2\Big(\sum_{v\in V} \phi(v)\Delta u(v)\Big) = -2\int_V \phi(v)\Delta u(v).$$

Theorem 2.3. Given a boundary condition $f : \partial V \to \mathbb{R}$, if $u \in \mathcal{A}$ satisfies

$$I[u] := \min_{w \in \mathcal{A}} I[w],$$

where $w \in \mathcal{A} \coloneqq \{w : V \to \mathbb{R} \mid w = f \text{ on } \partial V\}$, then

$$\Delta u = 0 \ in \ V \setminus \partial V.$$

In other words, u is then a solution to the Dirichlet problem on the graph setup in Section 2.1.

Proof. Suppose we are given a boundary condition $f: \partial V \to \mathbb{R}$, and suppose $u \in \mathcal{A}$ minimizes I[w] over all $w \in \mathcal{A}$, then for all $w \in \mathcal{A}$, we have $I[u] \leq I[w]$.

Let us fix a function $\phi: V \to \mathbb{R}$ such that $\phi = 0$ on ∂V . Thus, for all $t \in \mathbb{R}$, we have $(u + t\phi): V \to \mathbb{R}$ given by $(u + t\phi)(v) = u(v) + t\phi(v)$ for all $v \in V$, and we have $u + t\phi = u = f$ on ∂V . Thus, for all $t \in \mathbb{R}$, we have $u + t\phi \in \mathcal{A}$. In consequence, we have

$$I[u] \le I[u+t\phi] \quad \text{for all } t \in \mathbb{R}.$$

Let $i(t) \coloneqq I[u + t\phi]$ for all $t \in \mathbb{R}$. Then

$$I[u] = i(0) \le I[u + t\phi] = i(t) \quad \text{for all } t \in \mathbb{R}$$

Thus, we see that 0 is the point of absolute minimum for i(t) and that i'(0) = 0. Let us further restrict ϕ to be a function such that there exists a finite support set $\operatorname{supp}(\phi) := \{v \in V \mid \phi(v) \neq 0\} = \{v_0\}$, where $v_0 \in V \setminus \partial V$. Then

$$i(t) = I[u + t\phi] = \sum_{v \in V} |\nabla(u + t\phi)(v)|^2 = \sum_{v \in V} \sum_{i=1}^{n_v} [(u + t\phi)(v_i) - (u + t\phi)(v)]^2$$
$$= \sum_{v \in V} \sum_{i=1}^{n_v} [(u(v_i) - u(v)) + t(\phi(v_i) - \phi(v))]^2 = \sum_{v \in V} \sum_{i=1}^{n_v} |\nabla u + t\nabla \phi|^2.$$

We then have

$$\begin{aligned} i'(t) &= \frac{d}{dt} \left[\sum_{v \in V} \sum_{i=1}^{n_v} (u(v_i) - u(v))^2 + \sum_{v \in V} \sum_{i=1}^{n_v} 2t(u(v_i) - u(v))(\phi(v_i) - \phi(v)) + \sum_{v \in V} \sum_{i=1}^{n_v} t^2(\phi(v_i) - \phi(v))^2 \right] \\ &= \sum_{v \in V} \sum_{i=1}^{n_v} 2(u(v_i) - u(v))(\phi(v_i) - \phi(v)) + \sum_{v \in V} \sum_{i=1}^{n_v} 2t(\phi(v_i) - \phi(v))^2. \end{aligned}$$

We evaluate it at t = 0:

$$i'(t)|_{t=0} = \sum_{v \in V} \sum_{i=1}^{n_v} 2(u(v_i) - u(v))(\phi(v_i) - \phi(v))$$

Set i'(0) = 0:

$$i'(0) = \sum_{v \in V} \sum_{i=1}^{n_v} (u(v_i) - u(v))(\phi(v_i) - \phi(v)) = \sum_{v \in V} \nabla u \cdot \nabla \phi = 0 = \int_V \nabla u \cdot \nabla \phi = 0.$$

By Lemma 2.2, we know that

$$\int_{V} \nabla u \cdot \nabla \phi = -2\phi(v_0)\Delta u(v_0).$$

Thus,

$$-2\phi(v_0)\Delta u(v_0) = 0.$$

Let us choose the function ϕ to be as such:

Given $v_0 \in V \setminus \partial V$,

$$\phi(v_0) = \begin{cases} 1, & v = v_0 \\ 0, & v \neq v_0 \end{cases}.$$

Then

$$\Delta u(v_0) = 0 \quad \text{for all } v_0 \in V \setminus \partial V.$$

Thus, u restricted to $V \setminus \partial V$, that is, $u|_{V \setminus \partial V}$, is harmonic, and u is a solution to the Dirichlet problem (Section 2.2.3).

To summarize, by considering the case of infinite, locally-finite, undirected simple graph, we can show that given a boundary condition on the graph, the minimizer to the graph's associated energy functional is a solution to the graph's Dirichlet problem.

3 Case of a finite, directed, locally-finite decision tree

3.1 Tree setup

We will begin the setup with several similar definitions in graph theory. For general reference to the subject, see [1].

Definition 3.1 (Walk in a simple, undirected graph). In a simple, undirected graph $G := \{V, E\}$, a walk from vertex v_0 to vertex v_n is a sequence

$$W \coloneqq (v_0, v_1, v_2, \dots, v_n),$$

where for all i with $0 \leq i \leq n-1$, we have that v_i, v_{i+1} in the walk are such that $\{v_i, v_{i+1}\} \in E$. An undirected walk W from vertex u to vertex v is also called a u - v walk.

Definition 3.2 (Walk in a simple, directed graph). In a simple, directed graph $G := \{V, E\}$, a walk from vertex v_0 to vertex v_n is a sequence

$$W \coloneqq (v_0, v_1, v_2, \dots, v_n),$$

where given a fixed *i* with $0 \le i \le n-1$, we have that v_i, v_{i+1} in the walk satisfy either $(v_i, v_{i+1}) \in E$ or $(v_{i+1}, v_i) \in E$, but not both. A directed walk *W* from vertex *u* to vertex *v* is also called a u - v directed walk.

Remark. Note that this is not the standard definition in graph theory. We allow the possibility that such a walk has a direction for some i and an opposite direction for some i.

Definition 3.3 (Connected graph). A graph $G := \{V, E\}$ is connected if for all $u, v \in V$, there is a u - v walk.

Definition 3.4 (Path). A path is a walk with no repeated edges and no repeated vertices.

Definition 3.5 (Cycle). A cycle is a path with the same initial and end vertices.

Definition 3.6 (Tree). A graph $G := \{V, E\}$ is a tree if it is a connected, simple graph with no cycle.

Definition 3.7 (Directed tree). A tree is a directed tree if its underlying graph is a directed graph.

An equivalent definition for Definition 3.7 is as follows in Proposition 3.1:

Proposition 3.1. A directed tree is equivalent to a simple graph such that for any u, v vertices, there exists a u - v directed walk, and any u - v directed walk is either not a path or is a path with different initial and end vertices.

Definition 3.8 (Finite tree). A finite tree is a tree with a finite set of vertices.

Definition 3.9 (Locally-finite decision tree). A locally-finite decision tree is a directed tree such that for $v \in A \subseteq V$ (A is nonempty), there exists a unique neighborhood (thus, decision) consisted of $n_v \in \mathbb{N}$ adjacent, neighboring vertices in V (thus, locally finite), denoted by $S_v \coloneqq \{v_i\}_{i=1}^{n_v}$, such that $v_i \in S_v$ satisfies $(v, v_i) \in E$. We call v'_i s the successors of the vertex v.

Remark. Let us denote the *cardinality* of S_v as n_v . Note the construction that for any $v_i \in S_v$, $(v, v_i) \in E$, is so that there is a sense of direction flowing from v towards its successors $v'_i s$.

3.1.1 Proposed finite tree construction - finite tree with top

Let us construct a finite graph $\Pi \coloneqq (\mathcal{T}, E)$, from knowing just \mathcal{T} (the set of vertices), by first constructing the edge set E. E is such that for any $u \in \mathcal{T} \setminus \partial \mathcal{T}$, where $\partial \mathcal{T} \subsetneq \mathcal{T}$ and is nonempty, there exists a unique neighborhood consisted of $n_v \in \mathbb{N}$ adjacent, neighboring vertices in $\mathcal{T}, S_v \coloneqq \{v_i\}_{i=1}^{n_v}$, such that $v_i \in S_v$ satisfies $(v, v_i) \in E$. We again call v'_i s the successors of the vertex v. Let $\partial \mathcal{T} \coloneqq \{v \in \mathcal{T} \mid (v, q) \notin E \text{ for all } q \in \mathcal{T}\}$. Let us choose $\alpha \in \mathcal{T} \setminus \partial \mathcal{T}$ such that any $u \in \mathcal{T} \setminus \{\alpha\}$ is a successor of some $v \in \mathcal{T} \setminus \partial \mathcal{T}$ where $u \neq v$. We call v the predecessor of u. Note that v is unique by the construction of the graph.

Note also that α has no predecessor in \mathcal{T} . To see this, for any $u \in \mathcal{T} \setminus (\partial \mathcal{T} \cup \{\alpha\}) \subseteq \mathcal{T} \setminus \partial \mathcal{T}$ (and also, $\subseteq \mathcal{T} \setminus \{\alpha\}$), $u \in \mathcal{T} \setminus \partial \mathcal{T}$ and u has some predecessor $v \in \mathcal{T} \setminus \partial \mathcal{T}$. Thus, we have that for any $u \in \mathcal{T} \setminus \partial \mathcal{T}$ such that $u \notin \mathcal{T} \setminus (\partial \mathcal{T} \cup \{\alpha\})$, u has no predecessor in $\mathcal{T} \setminus \partial \mathcal{T}$. The only such $u \in \mathcal{T} \setminus \partial \mathcal{T}$ is α . Thus, α has no predecessor in $\mathcal{T} \setminus \partial \mathcal{T}$. Since for any $b \in \partial \mathcal{T}$, b has no successor. Thus, α has no predecessor in $\partial \mathcal{T}$, then altogether has no predecessor in \mathcal{T} .

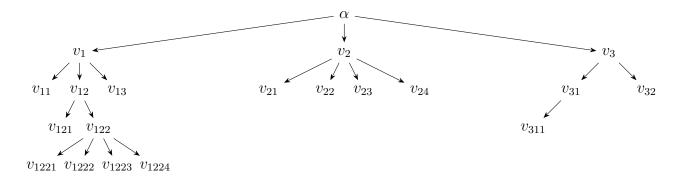


Figure 1: Example of proposed finite tree construction

We see that given a constructed E and a choice of $\alpha \in \mathcal{T} \setminus \partial \mathcal{T}$, the constructed finite graph is exactly $\Pi = \{(\alpha = a_0^0, a_1^1, \dots, a_i^i, \dots, a_k^k) \mid a_k^k \in \partial \mathcal{T}, k \in \mathbb{N} ; (a_i, a_{i+1}) \in E, 0 \leq i \leq k-1\}$, where k will be determined by a_k^k which will be determined by E and α . Let us call an element $p \in \Pi$ a path. We understand k as the number of successions a p has beginning going down from α ; let us call k the level of p, and we also say p has k levels, or p is with level k. We denote the subset of Π having all paths with $k \in \mathbb{N}$ levels to be $\Pi_k := \{p \in \Pi \mid p \text{ has } k \text{ levels}\}$; we denote an element from Π_k by p_k .

Proposition 3.2. The constructed graph $\Pi \coloneqq \{V, E\}$ is a directed, locally-finite decision tree as in Definition 3.7 and Definition 3.9, respectively.

In light of Proposition 3.2, we call the constructed finite graph $\Pi := \{V, E\}$ finite tree with top, and $p \in \Pi$ a path of the tree, and α the top.

Let us illustrate the finite tree construction with an example in Fig. 1. We see that given the constructed E based on the vertex set \mathcal{T} , and given the choice of α , we have a set of paths with different levels that end at the boundary

$$\partial \mathcal{T} = \{ v_{11}, v_{121}, v_{1221}, v_{1222}, v_{1223}, v_{1224}, v_{21}, v_{22}, v_{23}, v_{24}, v_{311}, v_{32} \}.$$

 α has no predecessors, any element in the boundary $\partial \mathcal{T}$ has no successors, and the predecessor-successor relationship is unique.

3.1.2 Infinite tree construction - infinite tree with top

Since the tree is locally-finite, when the *level of* p := k satisfies $k \in \mathbb{N}$ for any $p \in \Pi$, the tree is *finite* as is the case with a *finite tree with top* in Section 3.1.1; when the *level of* p satisfies k is ∞ for some $p \in \Pi$, the tree is *infinite*. In this case, we call the *infinite* tree *infinite tree with top*.

3.1.3 Special case of a finite tree with top in Section 3.1.1 - with uniform base

In Section 3.1.1, we see that we can construct one type of finite, directed, locally-finite decision tree with a specified vertex α , which we call the top, and E, the edge set constructed from specified decisions for all vertices not on the boundary. The finite tree with top, Π , in Section 3.1.1 is fairly complicated to work with since it has the possibility of having different levels for all p. A simpler case would be if for any path p in the tree Π , its level is the same as the level of any other path. Let us denote the level of p as k. In this special case of Π of Section 3.1.1, we have that any path p reaches the boundary $\partial \mathcal{T}$ at $k = n \in \mathbb{N}$. We shall also define more notations for convenience. We call n the level of the tree. We denote $\mathcal{T}_{i,j}$ to be the set of all vertices from and including level i to and including level j, where $0 \leq i < j \leq n$, and \mathcal{T}_i the set of all vertices at level i with $0 \leq i \leq n$. Let us call this special case of a finite tree with top in Section 3.1.1 finite tree with top and uniform base. Let us return to the original finite tree construction in Section 3.1.1.

3.2 Dirichlet problem on a finite tree with top in Section 3.1.1

Let us define a function:

$$u: \mathcal{T} \to \mathbb{R}.$$
 (12)

The gradient of function u(v), the divergence of $\nabla u(v)$, the integral of u(v) and the L_2 norm are the same as Eq. (2), Eq. (3), Eq. (4) and Eq. (5), respectively, in the case of infinite, locally-finite, undirected, simple graphs.

The Dirichlet problem on finite trees with top in Section 3.1.1 is the same as in the case of infinite, locally-finite, undirected, simple graphs in Section 2. In the context of the tree's setup, the version of Dirichlet problem with the analogous discrete Laplacian and its corresponding operations is as follows:

Find $u: \mathcal{T} \to \mathbb{R}$ such that for $f: \partial \mathcal{T} \to \mathbb{R}$

$$\begin{cases} \Delta u = 0, & \text{in } \mathcal{T} \setminus \partial \mathcal{T} \\ u = f, & \text{on } \partial \mathcal{T} \end{cases}.$$
(13)

Remark. $\partial \mathcal{T} = \mathcal{T}_n$, and $\mathcal{T} \setminus \partial \mathcal{T} = \mathcal{T}_{0,n-1}$. Since a finite tree with top and uniform base in Section 3.1.3 is a special case of a finite tree with top in Section 3.1.1. The Dirichlet problem works for the former as well.

3.3 Minimization of energy on a finite tree with top in Section 3.1.1

The minimization of energy here is similar to that in the case of infinite, locally-finite, undirected, simple graphs (Section 2.2.4). However, the boundary of the tree $\partial \mathcal{T}$ has no successors for the finite tree construction in Section 3.1.1. With its setup in mind, let us define the *energy functional* associated with its Dirichlet problem (Section 3.2).

Definition 3.10 (Energy functional). Given $f: \partial \mathcal{T} \to \mathbb{R}$, the associated *energy functional* of a finite tree with top to its Dirichlet problem (Section 3.2) is defined as

$$I[w] = \sum_{v \in \mathcal{T}_{0,n-1}} |\nabla w(v)|^2,$$
(14)

where $w \in \mathcal{A} \coloneqq \{ w \colon \mathcal{T} \to \mathbb{R} \mid w = f \text{ on } \partial \mathcal{T} \}.$

Following, the minimization of energy has the following setup:

$$I[u] \coloneqq \min_{w \in \mathcal{A}} I[w].$$
⁽¹⁵⁾

As in Theorem 2.1, we want to utilize the minimization of the corresponding energy functional to find a solution to the corresponding Dirichlet problem. Let us do a *finite tree with top and uniform base* in Section 3.1.3.

3.3.1 Minimization of energy on a finite tree with top and uniform base

In the case of a finite tree with top and uniform base, we do not have a straightforward theorem as in the case of an infinite, locally-finite, undirected, simple graph (Theorem 2.3), so let us proceed with a problem.

Problem 3.1. Given a boundary condition $f : \partial \mathcal{T} \to \mathbb{R}$, we want to know that if $u \in \mathcal{A}$ satisfies

$$I[u] := \min_{w \in \mathcal{A}} I[w],$$

where $w \in \mathcal{A} \coloneqq \{w : \mathcal{T} \to \mathbb{R} \mid w = f \text{ on } \partial \mathcal{T} \}$, then

$$\Delta u = 0 \ in \ \mathcal{T} \setminus \partial \mathcal{T};$$

in other words, is u a solution to the Dirichlet problem on a finite tree with top and uniform base?

Remark. Suppose we are given a boundary condition $f: \partial \mathcal{T} \to \mathbb{R}$, and suppose $u \in \mathcal{A}$ minimizes I[w] over all $w \in \mathcal{A}$, then for all $w \in \mathcal{A}$, we have $I[u] \leq I[w]$.

Let us fix a function $\phi \colon \mathcal{T} \to \mathbb{R}$ such that $\phi = 0$ on $\partial \mathcal{T}$. Thus, for all $t \in \mathbb{R}$, we have $(u + t\phi) \colon \mathcal{T} \to \mathbb{R}$ given by $(u + t\phi)(v) = u(v) + t\phi(v)$ for all $v \in \mathcal{T}$, and we have

 $u + t\phi = u = f$ on $\partial \mathcal{T}$. Thus, for all $t \in \mathbb{R}$, we have $u + t\phi \in \mathcal{A}$. In consequence,

$$I[u] \leq I[u+t\phi] \quad \text{for all } t \in \mathbb{R}.$$

Let $i(t) \coloneqq I[u + t\phi]$ for all $t \in \mathbb{R}$. Then

$$I[u] = i(0) \le I[u + t\phi] = i(t) \quad \text{for all } t \in \mathbb{R}.$$

Thus, we see that 0 is the point of absolute minimum for i(t) and that i'(0) = 0. We have

$$i(t) = I[u + t\phi] = \sum_{v \in \mathcal{T}_{0,n-1}} |\nabla(u + t\phi)(v)|^2 = \sum_{v \in \mathcal{T}_{0,n-1}} \sum_{i=1}^{n_v} [(u + t\phi)(v_i) - (u + t\phi)(v)]^2$$
$$= \sum_{v \in \mathcal{T}_{0,n-1}} \sum_{i=1}^{n_v} [(u(v_i) - u(v)) + t(\phi(v_i) - \phi(v))]^2 = \sum_{v \in \mathcal{T}_{0,n-1}} \sum_{i=1}^{n_v} |\nabla u + t\nabla \phi|^2.$$

Take the derivative:

$$\begin{split} i'(t) &= \frac{d}{dt} \left[\sum_{v \in \mathcal{T}_{0,n-1}} \sum_{i=1}^{n_v} (u(v_i) - u(v))^2 + \sum_{v \in \mathcal{T}_{0,n-1}} \sum_{i=1}^{n_v} 2t(u(v_i) - u(v))(\phi(v_i) - \phi(v)) \right. \\ &+ \sum_{v \in \mathcal{T}_{0,n-1}} \sum_{i=1}^{n_v} t^2 (\phi(v_i) - \phi(v))^2 \right] \\ &= \sum_{v \in \mathcal{T}_{0,n-1}} \sum_{i=1}^{n_v} 2(u(v_i) - u(v))(\phi(v_i) - \phi(v)) + \sum_{v \in \mathcal{T}_{0,n-1}} \sum_{i=1}^{n_v} 2t(\phi(v_i) - \phi(v))^2. \end{split}$$

Evaluate at t = 0:

$$i'(t)|_{t=0} = \sum_{v \in \mathcal{T}_{0,n-1}} \sum_{i=1}^{n_v} 2(u(v_i) - u(v))(\phi(v_i) - \phi(v)).$$

Set i'(0) = 0:

$$i'(0) = \sum_{v \in \mathcal{T}_{0,n-1}} \sum_{i=1}^{n_v} (u(v_i) - u(v))(\phi(v_i) - \phi(v)) = \sum_{v \in \mathcal{T}_{0,n-1}} \nabla u \cdot \nabla \phi = 0.$$

Thus, we have

$$\sum_{v \in \mathcal{T}_{0,n-1}} \nabla u \cdot \nabla v = \sum_{v \in \mathcal{T}_{0,n-1}} \sum_{i=1}^{n_v} (u(v_i) - u(v))\phi(v_i) - \sum_{v \in \mathcal{T}_{0,n-1}} \sum_{i=1}^{n_v} (u(v_i) - u(v))\phi(v) = 0,$$

and then

$$\sum_{v \in \mathcal{T}_{0,n-1}} \sum_{i=1}^{n_v} (u(v_i) - u(v))\phi(v_i) - \sum_{v \in \mathcal{T}_{0,n-1}} \phi(v)\Delta u = 0.$$
(16)

Theorem 3.1. From Problem 3.1, we obtain

$$\Delta u(v) = \begin{cases} 0, & v \in \mathcal{T}_0 \\ u(v) - u(\hat{v}), & v \in \mathcal{T}_k, \ 1 \le k \le n - 1 \end{cases},$$
(17)

where \hat{v} is the unique predecessor of v.

Proof. Continuing from Problem 3.1, let us utilize the function ϕ .

Given $\bar{v} \in \mathcal{T}_{0,n-1}$, let

$$\phi(v) = \begin{cases} 1, & v = \bar{v} \\ 0, & v \neq \bar{v} \end{cases}.$$
(18)

Let us investigate Eq. (16), which is

$$\sum_{v \in \mathcal{T}_{0,n-1}} \sum_{i=1}^{n_v} (u(v_i) - u(v))\phi(v_i) - \sum_{v \in \mathcal{T}_{0,n-1}} \phi(v)\Delta u = 0.$$

And denote

$$\mathbf{I} \coloneqq \sum_{v \in \mathcal{T}_{0,n-1}} \sum_{i=1}^{n_v} (u(v_i) - u(v))\phi(v_i)$$

and

$$II \coloneqq \sum_{v \in \mathcal{T}_{0,n-1}} \phi(v) \Delta u.$$

We break into cases:

Case $\bar{v} \in \mathcal{T}_0$:

Given $\bar{v} \in \mathcal{T}_0$, for $v \neq \bar{v}$, we have $\phi(v) = 0$. Since $v'_i s$ are successors of any $v \in \mathcal{T}_{0,n-1}$, they are from $\mathcal{T}_{1,n}$, so $v_i \notin \mathcal{T}_0$ and $\phi(v_i) \equiv 0$. Thus, I = 0. The element $\bar{v} \in \mathcal{T}_0$ is the only element in \mathcal{T}_0 and the only element in $\mathcal{T}_{0,n-1}$ such that $\phi(\bar{v}) = 1$, and for all $v \neq \bar{v}$, we have $\phi(v) = 0$. Then II = Δu . Thus, $\Delta u = 0$. **Case** $\bar{v} \in \mathcal{T}_{n-1}$:

We are given that $\bar{v} \in \mathcal{T}_{n-1}$, and for any $v \neq \bar{v}$, we have $\phi(v) = 0$. We know $\phi(v) = 0$ on \mathcal{T}_n , and we have the successors of \bar{v} to be in \mathcal{T}_n . Additionally, for all $v_i \in \mathcal{T}_{1,n-2}$, we have $v_i \neq \bar{v} \in \mathcal{T}_{n-1}$, so $\phi(v_i) = 0$. Any $v_i \in \mathcal{T}_{n-1}$ such that $v_i = \bar{v}$ satisfies $\phi(\bar{v}) = 1$, and any $v_i \in \mathcal{T}_{n-1}$ such that $v_i \neq \bar{v}$ satisfies $\phi(v_i) = 0$. Denote \hat{v} to be the predecessor of v. Thus, we have $I = u(\bar{v}) - u(\hat{v})$. Since for any $v \neq \bar{v}$, we have $\phi(v) = 0$. Then we have $II = \Delta u(\bar{v})$. Thus, $\Delta u(\bar{v}) = u(\bar{v}) - u(\hat{v})$. **Case** $\bar{v} \in \mathcal{T}_k$, $1 \leq k \leq n-2$:

The proof is the same as that for the case of $\bar{v} \in \mathcal{T}_{n-1}$. Note that when k = 1, we still obtain that $I = u(\bar{v}) - u(\bar{v})$ because $\hat{v} \in \mathcal{T}_0$ will still be in the tree. We get a similar result as the previous case.

We are now ready to investigate the possibility of the minimizer being harmonic.

Theorem 3.2. If the minimizer of the energy functional defined in Definition 3.10 is a solution to the Dirichlet problem of a finite tree with top and uniform base defined in Section 3.1.3, then u(v) is constant for all $v \in \mathcal{T}_{0,n-1}$.

Furthermore, denoting $C \coloneqq \frac{\sum_{i=1}^{n_v} f(v_i)}{n_v}$ for all $v \in \mathcal{T}_{n-1}$, we then have u(v) = C for all $v \in \mathcal{T}_{0,n-1}$.

Proof. Suppose the minimizer u is harmonic, that is, $\Delta u(v) = 0$ for all $v \in \mathcal{T}_{0,n-1}$. From Theorem 3.1, we know that $\Delta u(v) = u(v) - u(\hat{v})$ for all $v \in \mathcal{T}_{1,n-1}$. Thus, u is constant on any path in the tree from the top vertex to level n-1. Since every path starts at the top vertex, this yields that u is constant for all $v \in \mathcal{T}_{0,n-1}$. Additionally, $\Delta u(v) = 0$ for all $v \in \mathcal{T}_{n-1}$. Thus, we know that $u(v) = \frac{\sum_{i=1}^{n_v} f(v_i)}{n_v}$ for all $v \in \mathcal{T}_{n-1}$. Denoting $C \coloneqq \frac{\sum_{i=1}^{n_v} f(v_i)}{n_v}$ for all $v \in \mathcal{T}_{n-1}$, since u is constant in the whole tree except at the boundary, we have u(v) = C for all $v \in \mathcal{T}_{0,n-1}$.

Remark. One interesting observation one can see from the contrapositive of Theorem 3.2 is that if the given boundary condition f is such that $\frac{\sum_{i=1}^{n_v} f(v_i)}{n_v}$ is not constant for some $v \in \mathcal{T}_{n-1}$, then the minimizer is not a solution to the Dirichlet problem.

Lemma 3.3. The sufficient condition in Theorem 3.2 is true.

Proof. Let us prove by contradiction. Suppose that u(v) is constant for all $v \in \mathcal{T}_{0,n-1}$ and that $\Delta u(v) \neq 0$ for some $v \in \mathcal{T}_{0,n-1}$. We know that $\Delta u(v) = u(v) - u(\hat{v})$ for all $v \in \mathcal{T}_{1,n-1}$.

Since, by assumption, there is $v \in \mathcal{T}_{1,n-1}$ such that $\Delta u(v) \neq 0$, then there is the predecessor of v, which is $\hat{v} \in \mathcal{T}_{0,n-2}$, such that $u(\hat{v}) \neq u(v)$. Note that we are excluding the possibility that $\hat{v} \in \mathcal{T}_0$ because, if we recall Theorem 3.1, we have $\Delta u(v) = 0$ for $v \in \mathcal{T}_0$. We effectively have a contradiction with the assumption that u(v) is constant for all $\mathcal{T}_{0,n-1}$. Thus, the sufficient condition is true.

From Theorem 3.2 and Lemma 3.3, we obtain the following:

Corollary 3.3.1. The minimizer of the energy functional defined in Definition 3.10 is a solution to the Dirichlet problem of a finite tree with top and uniform base defined in Section 3.1.3 if and only if u(v) is constant for all $v \in \mathcal{T}_{0,n-1}$.

4 Uniqueness of solutions to Dirichlet problems

We investigate uniqueness of a solution, if it exists, for the Dirichlet problems in the case of an infinite, locally-finite, undirected, simple graph in Section 2, in the case of a finite tree with top, and in its special case, a finite tree with top and uniform base in Section 3. These cases share the same Dirichlet problem. **Lemma 4.1.** Let $u: V \to \mathbb{R}$. If the graph G := (V, E) is connected and

$$\begin{cases} \Delta u = 0, & in \ V \setminus \partial V \\ u = 0, & on \ \partial V \end{cases},$$
(19)

then $u \equiv 0$.

Proof. We do a proof by contradiction. Suppose there exists $v \in V$ such that u(v) > 0, then we have

$$M = \max\{u(v) \mid v \in V\} > 0.$$

Since u = 0 on ∂V , we have

$$M = u(v_{\star})$$
 for some $v_{\star} \in V \setminus \partial V$.

Since $\Delta u = 0$ on $V \setminus \partial V$, we have $\Delta u(v_{\star}) = 0$. Then

$$M = u(v_{\star}) = \frac{\sum_{i=1}^{n_{v_{\star}}} u(v_{\star_i})}{n_{v_{\star}}} \equiv$$
$$n_{v_{\star}}M = \sum_{i=1}^{n_{v_{\star}}} u(v_{\star_i}) \equiv$$
$$n_{v_{\star}}M - \sum_{i=1}^{n_{v_{\star}}} u(v_{\star_i}) = 0 \equiv$$
$$\sum_{i=1}^{n_{v_{\star}}} (M - u(v_{\star_i})) = 0.$$

Since $M - u(v_{\star_i}) \ge 0$, we have

$$M - u(v_{\star i}) = 0$$
 for all $i \in \{1 \dots n_{v_{\star}}\}.$

Then

$$u(v_{\star_i}) = M \quad \text{for all } i \in \{1 \dots n_{v_\star}\},\$$

that is,

$$u(v) = M$$
 for all $v \in S_{v_{\star}}$.

Because the graph is connected, we obtain

$$u(v) = M > 0$$
 for all $v \in V$.

However, u(v) = 0 on ∂V . Thus, we have a contradiction. The case where we suppose there exists $v \in V$ such that u(v) < 0 is similar.

Theorem 4.2 (Uniqueness of solutions). A solution to the Dirichlet problem on a connected graph, if it exists, is unique.

Proof. Suppose u_1 and u_2 are both solutions to the Dirichlet problem, then we have

$$\begin{cases} \Delta u_1 = 0, & \text{in } V \setminus \partial V \\ u_1 = f, & \text{on } \partial V \end{cases}, \quad \text{and} \quad \begin{cases} \Delta u_2 = 0, & \text{in } V \setminus \partial V \\ u_2 = f, & \text{on } \partial V \end{cases}.$$

This implies that $u_1 = u_2 = f$ on ∂V , which implies that $u_1 - u_2 = 0$ on ∂V . Let us consider $(u_1 - u_2)(v)$ as a function on V. Thus, the function $(u_1 - u_2) = 0$ on ∂V and that $\Delta u_1 - \Delta u_2 = 0$ on $V \setminus \partial V$, that is, $\Delta (u_1 - u_2) = 0$ on $V \setminus \partial V$. Thus, $(u_1 - u_2)$ is a solution to the Dirichlet problem with boundary condition $(u_1 - u_2) = 0$ on ∂V . Let us write it out explicitly. We have

$$\begin{cases} \Delta(u_1 - u_2) = 0, & \text{in } V \setminus \partial V \\ u_1 - u_2 = 0, & \text{on } \partial V \end{cases}$$

By Lemma 4.1, we know that $u_1 - u_2 = 0$ for all $v \in V$, that is, $u_1 \equiv u_2$. Thus, a solution, if it exists, is unique.

5 Conclusion

The distinction between directed and undirected graphs influences the ability of the method of minimizing energy functional to find a solution to their boundary-value problems. In the first case with an infinite, locally-finite, undirected simple graph, we are able to utilize in the minimization of the graph's energy functional the undirectness of two vertices to find a solution to its boundary-value problem. In the case of a finite, directed, locally-finite decision tree, we have no such tool. We are, however, able to find that the minimization of energy functional yields that, if restricted to only the top vertex of the tree, the minimizer is harmonic. In addition, we find that the minimization yields a solution to the tree's boundary value problem if and only if some additional conditions away from the boundary are satisfied. The conditions are satisfied through some combination of the given boundary condition and an unknown labeling function on the tree. Since both criteria are arbitrary, it is unlikely in practice that the minimizer is a solution to the tree's boundary value problem. It suggests that to understand the solutions to such a tree, one might solve it directly without energy minimization. Furthermore, we find that the solutions to the Dirichlet problems are unique for connected graphs.

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