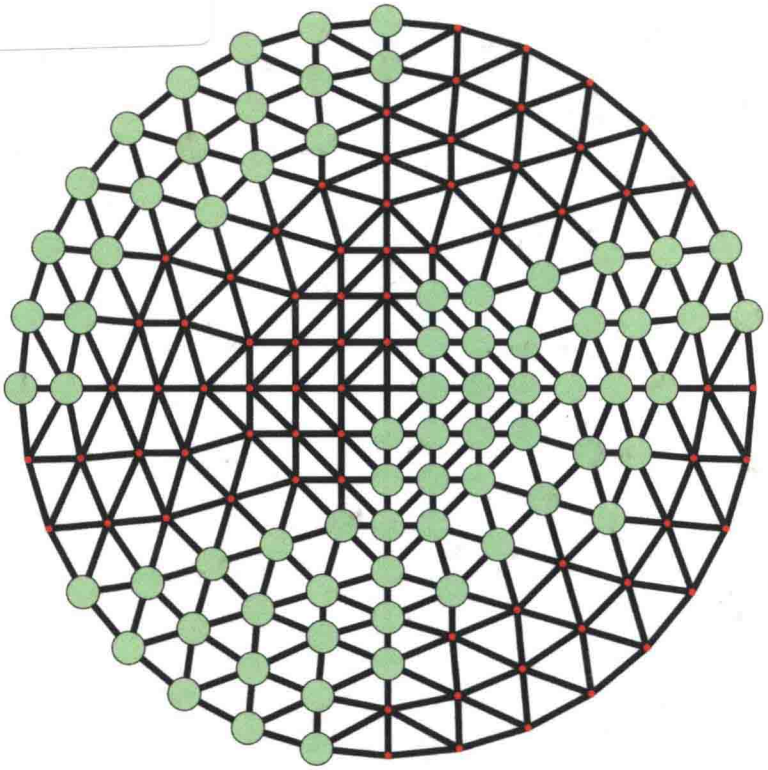
C. POZRIKIDIS



AN INTRODUCTION TO GRIDS, GRAPHS, AND NETWORKS

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PREFACE

Cartesian, curvilinear, and other unstructured grids are used for the numerical solution of ordinary and partial differential equations using finite difference, finite element, finite volume, and related methods. Graphs are broadly defined as finite or infinite sets of vertices connected by edges in structured or unstructured configurations. Infinite lattices and tiled surfaces are described by highly ordered graphs parametrized by an appropriate number of indices. Networks consist of nodes connected by physical or abstract links with an assigned conductance in spontaneous or engineered configurations. In physical and engineering applications, networks are venues for conducting or convecting a transported entity, such as heat, mass, or digitized information according to a prevailing transport law. The performance of networks is an important topic in the study of complex systems with applications in energy, material, and information transport.

The analysis of grids, graphs, and networks involves overlapping and complementary topics that benefit from a unified discussion. For example, finite difference and finite element grids can be regarded as networks whose link conductance is determined by the differential equation whose solution is sought as well as by the chosen finite difference or finite element approximation. Particular topics of interest include the properties of the node adjacency, Laplacian, and Kirchhoff matrices; the evaluation of percolation thresholds for infinite, periodic, and finite systems; the computation of the regular and generalized lattice Green's function describing the response to a nodal source; the pairwise resistance of any two nodes; the overall characterization of the network robustness; and the performance of damaged networks with reference to operational and percolation thresholds.

My goal in this text is to provide a concise and unified introduction to grids, graphs, and networks to a broad audience in the engineering, physical, biological, and social sciences. The approach is practical, in that only the necessary theoretical and mathematical concepts are introduced. Theory and computation are discussed alongside, and formulas amenable to computer programming are provided. The prerequisite is familiarity with college-level linear algebra, calculus, and elementary numerical methods.

One important new concept is the distinction between isolated and embedded networks. The former stand in isolation as though they were suspended in vacuum,

whereas the latter are connected to exterior nodes where a nodal potential, such as temperature, pressure, or electrical voltage, is specified. Regular Green's functions describing the discrete field due to a nodal impulse are available in the case of embedded or infinite networks, whereas generalized Green's functions describing the discrete field due to a nodal impulse in the presence of distributed sinks are available in the case of isolated networks. Discrete Green's functions can be used as building blocks for computing general solutions subject to given constraints.

This book is suitable for self-study and as a text in an upper-level undergraduate or entry-level graduate course in sciences, engineering, and applied mathematics. The material serves as a reference of terms and concepts and as a resource of topics for further study.

C. Pozrikidis

September, 2013

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CONTENTS

/// 1 /// ONE-DIMENSIONAL GRIDS

A finite difference grid for solving ordinary or partial differential equations consists of rectilinear or curvilinear grid lines that can be regarded as conveying links intersecting at nodes. This interpretation provides us with a point of departure for making an analogy between numerical grids, mathematical graphs, and physical or abstract networks. We begin in this chapter by developing finite difference equations for an elementary ordinary equation with the objective of identifying similarities between grids and graphs, and then we generalize the framework to higher dimensions.

1.1 POISSON EQUATION IN ONE DIMENSION

Consider the Poisson equation in one dimension for an unknown function of one variable, $f(x)$,

$$\frac{d^2f}{dx^2} + g(x) = 0, \tag{1.1.1}$$

to be solved in a finite domain, $[a, b]$, where $g(x)$ is a given source function. When $g(x) = 0$, the Poisson equation reduces to Laplace's equation. When $g(x) = \alpha f(x)$, the Poisson equation reduces to Helmholtz's equation, where α is a real or complex constant.

A numerical solution can be found on a uniform finite difference grid with K divisions defined by $K + 1$ nodes, as shown in Figure 1.1.1. Nodes numbered 0 and

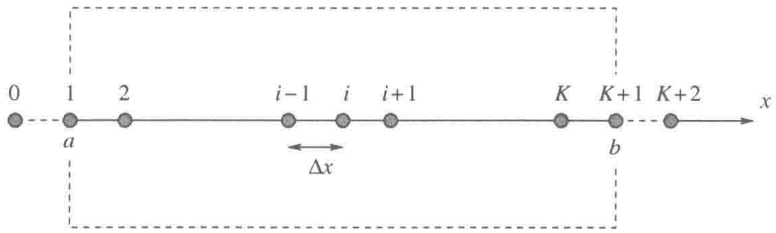

FIGURE 1.1.1 A finite difference with K uniform divisions along the x axis. Dirichlet or Neumann boundary conditions are specified at the two ends of the solution domain.

$K+2$ are phantom nodes, lying outside the solution domain, introduced to implement the Neumann boundary condition, when specified, as discussed later in this chapter.

Applying the Poisson equation at the ith node, approximating the second derivative with a central difference by setting

$$f''(x_i) \simeq \frac{f_{i-1} - 2f_i + f_{i+1}}{\Delta x^2} + O(\Delta x^2) \tag{1.1.2}$$

with an error of order Δx^2, and rearranging, we obtain the difference equation

$$-f_{i-1} + 2f_i - f_{i+1} = \Delta x^2 g_i \tag{1.1.3}$$

to be applied at an appropriate number of nodes. To simplify the notation, we have denoted

$$f_i \equiv f(x_i), \quad g_i \equiv g(x_i). \tag{1.1.4}$$

The signs on the left- and right-hand sides of (1.1.3) were chosen intentionally to conform with standard notation in graph theory regarding the Laplacian, as discussed in Section 1.7.

Collecting all available difference equations and implementing the boundary conditions provides us with a system of linear algebraic equations for a suitable number of unknown nodal values contained in a solution vector, $\boldsymbol{\psi}$,

$$\mathbf{L} \cdot \boldsymbol{\psi} = \mathbf{b}, \tag{1.1.5}$$

where the centered dot denotes the matrix–vector product. The size and specific form of the coefficient matrix, $\mathbf{L}$, solution vector, $\boldsymbol{\psi}$, and vector on the right-hand side, $\mathbf{b}$, depend on the choice of boundary conditions. Several possibilities are discussed in this chapter.

Factorization

We will see that, for any type of boundary conditions—Neumann, Dirichlet, or periodic—the coefficient matrix of the linear system admits the factorization

$$\mathbf{L} = \mathbf{R} \cdot \mathbf{R}^T, \tag{1.1.6}$$

where $\mathbf{R}$ is a square or rectangular matrix, the superscript T denotes the matrix transpose, and the centered dot denotes the usual matrix product (e.g., [35]). This factorization can be regarded as the discrete counterpart of the definition of the second derivative as the sequential application of the first derivative,

$$\frac{d^2}{dx^2} = \frac{d}{dx}\frac{d}{dx}. \tag{1.1.7}$$