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DISCRETE GREEN'S FUNCTION AND MAXIMUM PRINCIPLES*

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Abstract

In this paper the discrete Green's function (DGF) is introduced and its fundamental properties are proven. Further it is indicated how to use these results to prove the discrete maximum principle for 1D Poisson equation discretized by the *hp*-FEM with pure Dirichlet or with mixed Dirichlet-Neumann boundary conditions and with piecewise constant coefficient.

1. Introduction

The topic of discrete maximum principles (DMP) is already studied for several decades [1]. The problematics of DMP can be simplified to the question under what conditions a numerical method produces nonnegative solution in situations when the exact solution is known to be nonnegative. Numerical methods that satisfies DMP are useful and desirable for problems where naturally nonnegative quantities like temperature, concentration, or density are computed.

Results for the finite element methods (FEM) and for various problems are well known, see e.g. [2, 4, 5, 6] and references therein. These works, however, deal with piecewise linear approximations only. The results about higher order approximations are much scarce, see [3, 11] and recent works of the authors [10, 7, 8, 9]. The reason is that the condition for a piecewise linear function to be nonnegative is trivial but suitable condition for piecewise polynomial function is very difficult to obtain.

In this point of view the discrete Green's function turned out to be a very useful tool for investigation of DMP for higher order finite element methods.

2. Model problem

Although the theory is applicable for very general class of problems, we restrict ourselves for the clarity of explanation to relatively simple linear elliptic problem. The model problem is formulated in the classical way as follows

$$\begin{aligned} -\operatorname{div}(\mathcal{A}\nabla u) + cu &= f \quad \text{in } \Omega \\ u &= 0 \quad \text{on } \Gamma_{\mathrm{D}} \\ \alpha u + (\mathcal{A}\nabla u)\cdot\nu &= g \quad \text{on } \Gamma_{\mathrm{N}}. \end{aligned} \tag{1}$$

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Here Ω is a domain with Lipschitz continues boundary in $\mathbb{R}^d$. The boundary $\partial\Omega$ is split into two disjoint parts Γ_D and Γ_N. The matrix $\mathcal{A} = \mathcal{A}(x) \in \mathbb{R}^{d\times d}$ is uniformly positive definite and the coefficients $c = c(x)$ and $\alpha = \alpha(x)$ are nonnegative. The unit outward normal to $\partial\Omega$ is denoted by ν.

To give rigorous meaning to the model problem, we introduce the concept of weak solution. For that reason we define the space

$$V = \{u \in H^1(\Omega) : u = 0 \text{ on } \Gamma_\mathrm{D}\},$$

where the values on $\partial\Omega$ are understood in the sense of traces. The weak solution $u \in V$ of (1) is defined by identity

$$a(u, v) = F(v) \quad \forall v \in V. \tag{2}$$

The bilinear form $a : V \times V \mapsto \mathbb{R}$ and the linear functional $F : V \mapsto \mathbb{R}$ are given by

$$\begin{aligned} a(u, v) &= \int_\Omega (\mathcal{A}\nabla u) \cdot \nabla v \,\mathrm{d}x + \int_\Omega cuv \,\mathrm{d}x + \int_{\Gamma_\mathrm{N}} \alpha uv \,\mathrm{d}s, \\ F(v) &= \int_\Omega fv \,\mathrm{d}x + \int_{\Gamma_\mathrm{N}} gv \,\mathrm{d}s. \end{aligned}$$

These integrals are well defined if $\mathcal{A} \in \left[L^\infty(\Omega)\right]^{d\times d}$, $c \in L^\infty(\Omega)$, $\alpha \in L^\infty(\Gamma_\mathrm{N})$, $f \in L^2(\Omega)$, and $g \in L^2(\Gamma_\mathrm{N})$. If $\operatorname{meas}\Gamma_\mathrm{D} \neq 0$ or $c \not\equiv 0$ or $\alpha \not\equiv 0$ then by Lax-Milgram lemma the weak solution exists and is unique.

Let us recall the standard definition of Green's function for problem (2). For almost every $y \in \overline{\Omega}$, the Green's function $G_y \in V$ is given as a unique solution to

$$a(w, G_y) = \delta_y(w) \quad \forall w \in V. \tag{3}$$

The symbol δ_y stands for the Dirac functional. This δ_y is well defined for all continous function w by $\delta_y(w) = w(y)$. This definition can be augmented for w from V by the Hahn-Banach theorem.

By (2) and (3) we infer the fundamental Kirchhoff-Helmholtz representation formula

$$u(y) = \delta_y(u) = a(u, G_y) = F(G_y).$$

Hence for our model problem

$$u(y) = \int_\Omega f(x) G_y(x) \,\mathrm{d}x + \int_{\Gamma_\mathrm{N}} g(s) G_y(s) \,\mathrm{d}s.$$

3. Discretization by *hp*-FEM

In the *hp* version of the finite element method (*hp*-FEM) we vary both the sizes h and polynomial degrees p of elements. To discretize our model problem (2) by the

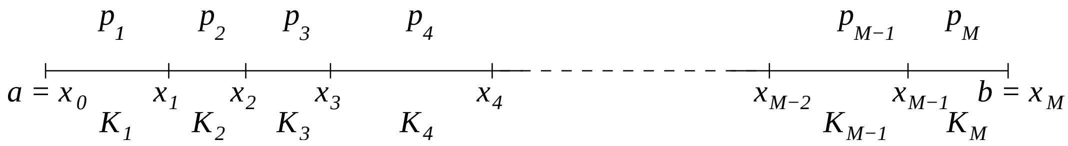

Fig. 1: *A 1D mesh $\mathcal{T}_{hp}$ with elements K_i of polynomial degrees p_i, $i = 1, 2, \dots, M$.*

hp-FEM we assume the domain Ω to be polytopic. We introduce simplicial partition $\mathcal{T}_{hp}$ of Ω into M elements and we endow each element $K_i \in \mathcal{T}_{hp}$, $i = 1, 2, \dots, M$, with an arbitrary polynomial degree $p_i \geq 1$. See Figure 1 for a 1D illustration.

The hp-FEM mesh $\mathcal{T}_{hp}$ defines the finite element space

$$V_{hp} = \{v_{hp} \in V : v_{hp}|_{K_i} \in P^{p_i}(K_i) \text{ for all } K_i \in \mathcal{T}_{hp}\},$$

where $P^{p_i}(K_i)$ stands for the space of polynomials on K_i of degree at most p_i. The hp-FEM solution $u_{hp} \in V_{hp}$ is then defined by identity

$$a(u_{hp}, v_{hp}) = F(v_{hp}) \quad \forall v_{hp} \in V_{hp}. \tag{4}$$

4. Discrete Green's function and its properties

The discrete Green's function (DGF) is defined in analogy with the continuous case, cf. (3). For all $y \in \overline{\Omega}$, define the discrete Green's function $G_{hp,y} \in V_{hp}$ by

$$a(w_{hp}, G_{hp,y}) = \delta_y(w_{hp}) \quad \forall w_{hp} \in V_{hp}. \tag{5}$$

It is convenient to put $G_{hp}(x, y) = G_{hp,y}(x)$. The combination of (4) and (5) gives again the representation formula

$$u_{hp}(y) = \delta_y(u_{hp}) = a(u_{hp}, G_{hp,y}) = F(G_{hp,y}).$$

For our model problem this becomes

$$u_{hp}(y) = \int_\Omega f(x) G_{hp}(x, y) \,\mathrm{d}x + \int_{\Gamma_\mathrm{N}} g(s) G_{hp}(s, y) \,\mathrm{d}s. \tag{6}$$

In contrast to the continuous case the DGF can be easily expressed through the inverse stiffness matrix, cf. [2].

Lemma 4.1. *Let $\{\varphi_1, \varphi_2, \dots, \varphi_N\}$ be a basis in V_{hp}. If $A \in \mathbb{R}^{N\times N}$ be a matrix with entries $A_{ij} = a(\varphi_j, \varphi_i)$, $1 \leq i, j \leq N$, then*

$$G_{hp}(x, y) = \sum_{j=1}^{N} \sum_{k=1}^{N} A^{-1}_{jk} \varphi_k(x) \varphi_j(y), \tag{7}$$

where A^{-1}_{jk} are entries of A^{-1}, i.e., $\sum_{j=1}^{N} A_{ij} A^{-1}_{jk} = \delta_{ik}$ (Kronecker symbol).

Proof. The proof follows from (5) and can be found in [8]. □

The following two corollaries follow directly from Lemma 4.1.

Corollary 4.1. *If* $a(\cdot,\cdot)$ *is symmetric then* $G_{hp}(x,y) = G_{hp}(y,x)$.

Corollary 4.2. *Let* $\{l_1, l_2, \dots, l_N\}$ *be a basis of* V_{hp} *such that* $a(l_i, l_j) = \delta_{ij}$. *Then*

$$G_{hp}(x,y) = \sum_{i=1}^{N} l_i(x) l_i(y).$$

Since the nonnegativity of DGF is fundamental for discrete maximum principles, see Theorem 5.1 below, the following lemma is of particular interest.

Lemma 4.2. *If the bilinear form* $a(\cdot,\cdot)$ *is symmetric and if* $a(v_{hp}, v_{hp}) > 0$ *for all* $0 \neq v_{hp} \in V_{hp}$ *then* $G_{hp}(x,x) > 0$ *for all* $x \in \Omega$.

Proof. Let $\{\varphi_1, \varphi_2, \dots, \varphi_N\}$ be a basis in V_{hp}. By the assumptions the stiffness matrix $A_{ij} = a(\varphi_j, \varphi_i)$, $1 \leq i,j \leq N$, is symmetric and positive definite as well as its invers matrix. Thus, by Lemma 4.1, $G_{hp}(x,x) = \boldsymbol{\varphi}(x)^T A^{-1} \boldsymbol{\varphi}(x) > 0$, where $\boldsymbol{\varphi}(x) = (\varphi_1(x), \varphi_2(x), \dots, \varphi_N(x))^T$. Notice that $\boldsymbol{\varphi}(x) \neq \mathbf{0}$ for all $x \in \Omega$ since $\{\varphi_i(x)\}$ is a basis in V_{hp}. □

5. Application to the discrete maximum principles

These results about DGF can be used to proof certain qualitative properties of the discrete solution. Let us start with the comparison principle for our model problem.

Definition 5.1. *The problem* (4) *satisfies the discrete comparison principle if*

$$f \geq 0 \text{ and } g \geq 0 \quad \Rightarrow \quad u_{hp} \geq 0.$$

The following theorem is crucial for the analysis of discrete comparison principle via DGF.

Theorem 5.1. *Problem* (4) *satisfies the discrete comparison principle if and only if the corresponding discrete Green's function* $G_{hp}(x,y)$ *defined by* (5) *is nonnegative in* Ω^2.

Proof. By (7), the discrete Green's function $G_{hp}(x,z)$ is continuous up to the boundary of Ω^2. The rest follows immediately from representation formula (6). □

For certain problems the DGF can be explicitly expressed and its nonnegativity can be analyzed. We mention two of our results about discrete maximum principle. Both are based on Theorem 5.1. A crucial role in these results plays quantity

$$H^*_{\mathrm{rel}}(p) = 1, \quad \text{for } p = 1,$$
$$H^*_{\mathrm{rel}}(p) = 1 + \frac{1}{2} \min_{(\xi,\eta)\in[-1,1]^2} l_0(\xi) l_0(\eta) \sum_{k=2}^{p} \kappa_k(\xi)\kappa_k(\eta), \quad \text{for } p \geq 2.$$

Here, $l_0(\xi) = (1-\xi)/2$ and $\kappa_k(\xi) = \sqrt{\frac{2k-1}{2}}\frac{4}{k(1-k)}P'_{k-1}(\xi)$, where $P_k(\xi)$ stand for the Legendre polynomials of degree k and prime denotes the derivative.

Theorem 5.2. *Let us consider simplified problem* (4) *in 1D setting with homogeneous Dirichlet boundary conditions, i.e.,* $\Omega = (\bar{a}, \bar{b})$, $\mathcal{A} = 1$, $c = 0$, $\alpha = 0$, $\Gamma_{\mathrm{D}} = \{\bar{a}, \bar{b}\}$, *and* $\Gamma_{\mathrm{N}} = \emptyset$. *Let* $\bar{a} = x_0 < x_1 < \ldots < x_M = \bar{b}$ *be a partition of the domain and let* $p_i \geq 1$ *be polynomial degrees assigned to elements* $K_i = [x_{i-1}, x_i]$, $i = 1, 2, \ldots, M$. *If*

$$\frac{x_i - x_{i-1}}{\bar{b} - \bar{a}} \leq H^*_{\mathrm{rel}}(p_i) \quad \textit{for all } i = 1, 2, \ldots, M, \tag{8}$$

then this problem satisfies the discrete comparison principle.

Theorem 5.3. *Let us consider simplified problem* (4) *in 1D setting with mixed boundary conditions, i.e.,* $\Omega = (\bar{a}, \bar{b})$, $\mathcal{A} = 1$, $c = 0$, $\alpha = 0$, $\Gamma_{\mathrm{D}} = \{\bar{a}\}$ *and* $\Gamma_{\mathrm{N}} = \{\bar{b}\}$. *Let* $\bar{a} = x_0 < x_1 < \ldots < x_M = \bar{b}$ *be a partition of the domain and let* $p_i \geq 1$ *be polynomial degrees assigned to elements* $K_i = [x_{i-1}, x_i]$, $i = 1, 2, \ldots, M$. *If*

$$H^*_{\mathrm{rel}}(p_i) \geq 0 \quad \textit{for all } i = 1, 2, \ldots, M, \tag{9}$$

then this problem satisfies the discrete comparison principle.

Proofs of Theorems 5.2 and 5.3 are given in [8] and [9], respectively. In the same papers we verified that $H_{\mathrm{rel}}(p) \geq 9/10$ for $1 \leq p \leq 100$. Thus, condition (9) is satisfied for these values of p and the condition (8) can be strengthened to $(x_i - x_{i-1})/(\bar{b} - \bar{a}) \leq 9/10$ which means that the discrete comparison principle is valid if all elements are shorter then 90 % of the length of the domain Ω.

Both the results from Theorems 5.2 and 5.3 can be generalized to the case of piecewise constant coefficient $\mathcal{A}$. The case of mixed boundary conditions (Theorem 5.3) remains valid even for piecewise constant $\mathcal{A}$, i.e., the comparison principle is guaranteed for all meshes with polynomial degrees not exceeding 100. The case of pure Dirichlet boundary conditions (Theorem 5.2) needs reformulation of condition (8) in the following way

$$\frac{\tilde{h}_i}{\sum_{k=1}^{M} \tilde{h}_k} \leq H^*_{\mathrm{rel}}(p_i) \quad \text{for all } i = 1, 2, \ldots, M. \tag{10}$$

Here $\tilde{h}_i = (x_i - x_{i-1})/\mathcal{A}_i$, $i = 1, 2, \ldots, M$, mean modified element lengths and $\mathcal{A}_i$ is the constant value of $\mathcal{A}(x)$ on the element K_i. Notice that the sum in the denominator in (10) can be interpretted as a length of a modified domain. More details about the case with piecewise constant coefficient can be found in [10].

Finally, let us recall that for problems treated in Theorems 5.2 and 5.3 the discrete comparison principle implies the discrete maximum principle. The discrete maximum principle states that in the case of nonpositive f and nonpositive g the maximum of u_{hp} is attained in the interior of Ω.

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