Generalized Green’s functions for second-order
discrete boundary-value problems with nonlocal boundary conditions

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Abstract. In this paper, generalized Green’s functions for second-order discrete boundary-value problems with nonlocal boundary conditions are investigated, where the necessary and sufficient existence condition of discrete Green’s function is not satisfied and nonlocal boundary conditions are described by linear functionals.

Keywords: discrete boundary-value problem, generalized Green function, Moore–Penrose inverse, nonlocal boundary conditions.

Introduction

In practice, problems often arise where we cannot measure data directly at the boundary. Then nonlocal boundary conditions (NBCs) instead of classical boundary conditions (BCs) are often formulated. During the last decade there has been a great interest in solving problems with NBCs by numerical methods.

Let $X_n := \{0, 1, 2, \ldots, n\}$ and $F(X_n) := \{u | u : X_n \to \mathbb{C}\}$ denote the space of complex linear functions. We consider the space $F^*(X_n)$ of linear functionals in the space $F(X_n)$. Let $\langle \delta^j, u \rangle = u(i)$. Let us consider the second-order discrete problem with NBCs

$$Lu := a^2_i u_{i+2} + a^1_i u_{i+1} + a^0_i u_i = f_i, \quad i \in X_{n-2},$$

$$(L_j, u) := (\kappa_j, u) - \gamma_j (\zeta_j, u) = 0, \quad j = 1, 2,$$

where $L : F(X_n) \to F(X_{n-2}) = \text{im } L$ is a linear operator and $L_1, L_2$ are linear functionals, let $L = (L_1, L_2)$. Many NBCs can be written in the form (2), where $\langle \kappa_j, u \rangle, j = 1, 2$, are classical parts and $\langle \zeta_j, u \rangle, j = 1, 2$, are nonlocal parts of BCs. If the unique solution of the problem (1)–(2) can be given by

$$u_i = \sum_{j=0}^{n-2} G_{ij} f_j = (G_{ij}, f_j)_{X_{n-2}}, \quad i \in X_n,$$

where $(v_j, w_j)_{X_n} := \sum_{j=0}^{n} v_j w_j$, $v, w \in F(X_n)$, then the function $G \in F(X_n \times X_{n-2})$ is called discrete Green’s function of operator $L$ with NBCs (2). According to S. Ro-
man [2], the necessary and sufficient existence condition of discrete Green’s function is

\[ D(L)[u] = \begin{vmatrix} \langle L_1, u^1 \rangle & \langle L_2, u^1 \rangle \\ \langle L_1, u^2 \rangle & \langle L_2, u^2 \rangle \end{vmatrix} \neq 0, \]

where \( \{u^1, u^2\} \) is a fundamental system of homogeneous equation (1).

In this paper we consider the problem (1)–(2) and generalize its discrete Green function when \( D(L)[u] = 0 \).

1 Moore–Penrose inverse

The problem (1)–(2) is equivalent to the linear system of equations

\[ \tilde{A}u = \tilde{f}. \]

Then the existence condition of discrete Green’s function is equivalent to the condition \( \det \tilde{A} \neq 0 \). Therefore, discrete Green’s function can be constructed by

\[ G_{ij} = g_{ij}, \quad i \in X_n, \quad j \in X_{n-2}, \quad \text{if} \quad \tilde{A}^{-1} = (g_{ij}). \]

If \( \det \tilde{A} = 0 \), then discrete Green’s function doesn’t exist.

Definition 1. A matrix \( X \in \mathbb{C}^{m \times n} \) is called the Moore–Penrose inverse of \( A \in \mathbb{C}^{m \times n} \) and denoted by \( A^\dagger \), if it satisfies all Penrose equations

\[ AXA = A, \quad XAX = X, \quad (AX)^* = AX, \quad (XA)^* =XA, \]

where \( A^* \) denotes the adjoint matrix of \( A \), \( \mathbb{C}^{m \times n} - m \times n \) complex matrices.

The existence and uniqueness of the Moore–Penrose inverse was proved by Urquhart and Penrose, respectively [1]. It follows that the Moore–Penrose inverse of nonsingular matrix coincides with the ordinary inverse. According to this, we define generalized discrete Green’s function of operator \( L \) with NBCs (2) by

\[ \tilde{G}_{ij} = g_{ij}, \quad i \in X_n, \quad j \in X_{n-2}, \quad \text{where} \quad \tilde{A}^\dagger = (g_{ij}). \]

Corollary 1. Let \( A \in \mathbb{C}^{m \times n}, \; b \in \mathbb{C}^m \). The general solution of consistent system \( Ax = b \) is

\[ x_0 = A^\dagger b + P_{\ker A}c, \]

for arbitrary \( c \in \mathbb{C}^n \). Here \( P_{\ker A} \) is the orthogonal projector on \( \ker A \).

Corollary 2. Let \( A \in \mathbb{C}^{m \times n}, \; b \in \mathbb{C}^m \). A vector \( x \) is a least squares solution of \( Ax = b \) if and only if \( Ax = P_{\text{im} A}b = AA^{(1,3)}b \). Thus, the general least squares solution is

\[ x = A^{(1,3)}b + (I - A^{(1,3)}A)c, \]

where \( c \in \mathbb{C}^n \) is an arbitrary vector, \( I \) is the identity matrix, and \( A^{(1,3)} \) is any matrix, satisfying both Penrose equations \( AXA = A \), \( (AX)^* = AX \).
Remark 1. Because the Moore–Penrose inverse satisfies all four Penrose equations, it also satisfies the first and third Penrose equations. Thus, the vector (5) is always the general least squares solution for consistent or inconsistent linear system of equations, i.e., the vector (5) always minimizes the Euclidean norm of residual vector
\[ \|Ax_0 - b\| \leq \|Ax - b\|, \quad \forall x \in \mathbb{C}^n. \]

According to Remark 1, we define generalized discrete Green’s functions for consistent and inconsistent linear systems of equations by the same formula (4).

Theorem 1. Let \( A \) be a square singular matrix, let \( \{y_1, y_2, \ldots, y_n\} \) and \( \{x_1, x_2, \ldots, x_n\} \) be orthonormal bases of \( \ker A^* \) and \( \ker A \), respectively, and let \( \{\alpha_1, \alpha_2, \ldots, \alpha_n\} \) be non-zero scalars. Then the matrix
\[ A_0 = A + \sum_{i=1}^{n} \alpha_i y_i x_i^* \]
is non-singular and its inverse is
\[ A_0^{-1} = A^+ + \sum_{i=1}^{n} \frac{1}{\alpha_i} x_i y_i^*. \]

2 Applications to problems with NBCs

Let us denote
\[ \langle L_j, u \rangle := \sum_{k=0}^{n} b_j^k u_k, \quad j = 1, 2. \]

Then the system (3) can be written in the extended matrix form
\[
\begin{pmatrix}
    a_0^1 & a_0^2 & 0 & \ldots & 0 & 0 & 0 \\
    0 & a_1^1 & a_1^2 & \ldots & 0 & 0 & 0 \\
    \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots \\
    0 & 0 & 0 & \ldots & a_{n-3}^1 & a_{n-3}^2 & 0 \\
    0 & 0 & 0 & \ldots & a_{n-2}^0 & a_{n-2}^1 & a_{n-2}^2 \\
    b_1^n & b_1^{n-1} & b_1^{n-2} & \ldots & b_2^n & b_2^{n-1} & b_2^{n-2}
\end{pmatrix}
\begin{pmatrix}
    u_0 \\
    u_1 \\
    \vdots \\
    u_{n-3} \\
    u_{n-2} \\
    u_n
\end{pmatrix}
= \begin{pmatrix}
    f_0 \\
    f_1 \\
    \vdots \\
    f_{n-3} \\
    f_{n-2} \\
    0
\end{pmatrix}.
\]

Let \( \dim \ker \tilde{A} = \dim \ker \tilde{A}^* = r \in \{1, 2\} \). Then \( \det \tilde{A} = 0 \). Let us suppose that the basic \((n + 1 - r)\)-order minor of matrix \( \tilde{A} \in \mathbb{C}^{(n+1) \times (n+1)} \) satisfies \( M_{n+1-r} = \det A \neq 0 \), where \( A = (\tilde{A}_{ij}), i, j \in X_{n-r} \). Then the solution of \( \ker \tilde{A} = \{w \in \mathbb{C}^{n+1}; \tilde{A}w = 0\} \) basis is equivalent to the solution of the problem
\[ A\tilde{w} = g^1, \]
(6)
where \( \overline{w} = (w_0, w_1, \ldots, w_n)^T \), \( g^1_0 = 0 \), \( i \in X_{n-r-2} \), \( g^1_{n-r-1} = -a^2_{n-r-1}w_{n+1-r} \), \( g^1_{n-r} = -\delta^i_j(a^1_{n-r-2}w_{n-1} + a^2_{n-r-2}w_n) - \delta^i_jb^*_iw_n \). It is easy to see that (6) is a restriction of discrete problem

\[
\begin{align*}
L\omega & := a^2_i\omega_{i+2} + a^1_i\omega_{i+1} + a^0_i\omega_i + g^1_i, \quad i \in X_{n-2}, \\
\langle l_1, \omega \rangle & := \langle L^T_k, \omega_k \rangle = g^1_{n-1}, \quad \text{if } r = 1, \\
\langle l_{2-r+j}, \omega \rangle & := \omega_{n-r+j}, \quad j = 1, r,
\end{align*}
\]

where matrix determinant equals to \( M_{n+1-r} \neq 0 \). Therefore, \( D(l_1, l_2)[u] \neq 0 \). Then the solution of (6) is

\[
w_i = \sum_{j=0}^{n-2} G_{ij}g^1_j + g^1_{n-1-i}\delta^i_j = (G_{ij}, g^1_j)_{X_{n-r}}, \quad i \in X_{n-r},
\]

where \( G_{ij} \in F(X_n \times X_{n-2}) \) is discrete Green's function of operator \( L \) with NBCs \( \langle l_k, w \rangle = 0 \), \( k = 1, r \), and \( G_{i,n-1} := v^1_i = D(\delta, l_2)[u]/D(l_1, l_2)[u] \). Let \( e^i = (\delta^i_j) \), \( i, j \in X_n \), be the standard basis of \( \mathbb{R}^{n+1} \). Then the kernel of \( \tilde{A} \) is composed of the vector

\[
w = \sum_{i=0}^{n-r} (G_{ij}, g^1_j)_{X_{n-r}} e^i + \sum_{i=1}^r w_{n-1-i} e^{n+1-i}, \quad w_{n+1-k} \in \mathbb{C}, \quad k = 1, r.
\]

Taking \( w_{n+1-i}w_{n+1-j} = \delta^i_j, i, j = 1, r \), we get the concrete basis of ker \( \tilde{A} \).

The solution of ker \( \tilde{A}^* = \{ v \in \mathbb{C}^{n+1}; \tilde{A}^*v = 0 \} \) basis is equivalent to the solution of the problem

\[
\mathbb{A}^*\tilde{v} = g^2
\]

where \( \mathbb{A}^* \) is the adjoint matrix of (6) matrix \( \mathbb{A} \), \( \tilde{v} = (v_0, v_1, \ldots, v_{n-r})^T \), \( g^2_j = -\sum_{i=1}^r b^2_{ji}v_{n+1-k}, j \in X_{n-r}, \tilde{v} = x + iy = x - iy, x, y \in \mathbb{R}, \ i = \sqrt{-1} \). Similarly, we can show that the basis of ker \( \mathbb{A}^* \) is composed of vectors

\[
v^k = -\sum_{i=0}^{n-r} (G^2_{ji}, b^2_{ji-k})_{X_{n-r}} e^i + e^{n+1-k}, \quad k = 1, r.
\]

Let \( x'_1 = w^1 \), \( y'_1 = v^1 \). Then other vectors are orthogonalised by Gram–Schmidt orthogonalization process

\[
x'_2 = w^2 - \langle w^1, w^2 \rangle \frac{w^1}{||w^1||^2} - \langle v^1, v^2 \rangle \frac{v^1}{||v^1||^2},
\]

where \( \langle \cdot, \cdot \rangle \) denotes the standard inner product. Taking \( \alpha_i = ||x'_i|| \cdot ||y'_i||, i = 1, r \), and applying Theorem 1, we get that the Moore–Penrose inverse of \( \tilde{A} \) is

\[
\tilde{A}^+ = (\tilde{A} + \sum_{i=1}^{n-r} y'_i x'_{i}^*)^{-1} - \sum_{i=1}^{r} \frac{1}{||x'_i||^2 \cdot ||y'_i||^2} x'_i y'_{i}^*.
\]
Then generalized discrete Green’s function is
\[ \tilde{G}_{ij} = \tilde{A}_{ij}, \quad i \in X_n, \ j \in X_{n-2}, \]
and, according to (5), the general solution of (3) is given by
\[ u = Gf + \sum_{i=1}^{r} \frac{1}{\| \xi_i \|^2} X_i^* c, \]
for arbitrary \( c \in \mathbb{C}^{n+1}, \ G = (\tilde{G}_{ij}), \ f = (f_0, f_1, \ldots, f_{n-2})^T. \)

**Example 1.** Let us consider differential equation with Bitsadze–Samarskij NBC
\[ -u'' = f(x), \quad x \in (0, 1), \]
\[ u(0) = 0, \quad u(1) = \gamma u(\xi), \quad 0 < \xi < 1. \]

We introduce the mesh \( \omega^h = \{x_i = ih: i \in X_n, \ nh = 1\}. \) Suppose \( \xi \) coincides with a mesh point, i.e., \( \xi = sh. \) We consider such an approximation problem
\[ Lu := -u_{i+1} + 2u_i - u_{i-1} = f_i h^2, \quad i = 1, n-1, \quad (9) \]
\[ u_0 = 0, \quad u_n = \gamma u_s, \quad (10) \]
where \( f_{i+1} = f(x_{i+1}), \ i \in X_{n-2}. \) The problem (9)–(10) has a unique solution and discrete Green’s function if \( \gamma \neq \frac{1}{2}. \) We consider the case, when discrete Green’s function doesn’t exist, i.e., \( \gamma = \frac{1}{2}. \) Firstly, discrete Green’s function of operator \( L \) with \( \langle l_1, u \rangle := u_0 = 0 \) and \( \langle l_2, u \rangle := u_n = 0 \) is
\[ G_{ij} = h \begin{cases} i(n-j-1), & i \leq j + 1, \\ (j+1)(n-i), & i \geq j + 1, \end{cases} \quad i \in X_n, \ j \in X_{n-2}. \]

Then it follows from (7) and (8) that
\[ w = \sum_{i=0}^{n-1} G_{i,n-2} e^i + e^n = h \sum_{i=0}^{n} ie^i + e^n = \frac{1}{n}(0, 1, 2, \ldots, n)^T, \]
\[ \| w \|^2 = \frac{1}{n^2} \sum_{k=0}^{n-1} k^2 = \frac{(n+1)(2n+1)}{6n}. \]
\[ v = \sum_{i=0}^{n-1} \gamma G_{ii}^2 e^i + e^n = \gamma \sum_{i=0}^{n-2} G_{ii}^2 e^i + \gamma v_1^1 e^{n-1} + e^n. \]

If we take \( u_1^1 = 1, \ u_2^1 = x_i, \) then \( v_1^1 = h(n-s) \) and
\[ v = \gamma h \left[ \sum_{s<i+1}^{n-2} (i+1)(n-s) e^i + \sum_{s<i+1}^{n-2} s(n-i-1) e^i + (n-s) e^{n-1} \right] + e^n. \]

We can show that
\[ \| v \|^2 = \frac{1}{6} \gamma^2 h^2 (n-s)(2(n-s)(ns^2 + 3) + ns) + 1, \quad s \in X_n. \]
Then
\[
\alpha = \left( \frac{(n+1)(2n+1)}{36n} \right)^{1/2} \left[ \gamma^2 h^2 (n-s) (2(n-s)(ns^2 + 3) + ns) + 1 \right]\biggl)^{1/2}.
\]

We calculate the orthogonal projector
\[
P_{\text{ker} \tilde{A}} = \frac{ww^T}{\|w\|^2} = \frac{6}{n(n+1)(2n+1)} \begin{pmatrix}
0 & 0 & 0 & \ldots & 0 \\
0 & 1 & 2 & \ldots & n \\
0 & 2 & 4 & \ldots & 2n \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & n & 2n & \ldots & n^2
\end{pmatrix}.
\]

Then the general discrete solution of (9)–(10) is given by
\[
u_i = h^2 \sum_{j=1}^{n-1} \tilde{G}_{i,j-1} f_j + \frac{6i}{n(n+1)(2n+1)} \sum_{j=0}^{n} j c_j, \quad c_j \in \mathbb{R}, \quad i, j \in X_n.
\]

3 Conclusion

1. Generalized discrete Green’s function always exists and is uniquely constructed.
2. If \(D(L)[u] \neq 0\), then generalized discrete Green’s function coincides with ordinary discrete Green’s function.
3. If \(M_{n+1-r} \neq 0\), then generalized discrete Green’s function can be described by the discrete Green function of the same discrete equation with simpler NBCs.

References

[1] A. Ben-Israel and T.N.E. Greville. Generalized Inverses. Theory and Applications. Springer-Verlag, New York, 2003.
[2] S. Roman. Green’s functions for boundary-value problems with nonlocal boundary conditions. Doctoral dissertation, Vilnius University, 2011.

REZIUMĖ

Apibendrintosios Gryno funkcijos antrosios eilės diskretiesiems uždaviniams su nelokaliosiomis kraštinėmis sąlygomis

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Straipsnyje yra nagrinėjamos apibendrintosios Gryno funkcijos antrosios eilės diskretiesiems uždaviniams su nelokaliosiomis kraštinėmis sąlygomis, kuomet yra nepatenkinta būtinoji ir pakankamoji diskrečiosios Gryno funkcijos egzistavimo sąlyga ir nelokaliosios kraštinės sąlygos yra užrašytos tiesinius funkcionalais.

Raktiniai žodžiai: diskretusis uždavinys, apibendrintoji Gryno funkcija, Moore ir Penrose atvirkštinė matrica, nelokaliosios kraštinės sąlygos.