Generalizing the bottleneck matrix.

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Abstract

Given the Laplacian matrix associated to a weighted graph and given x a single vertex of it, the bottleneck matrix (related to x) is the inverse matrix of the sub matrix of the Laplacian obtained by eliminating the row and the column corresponding to x. The bottleneck matrix is used to calculate the group inverse of the initial Laplacian matrix, for instance.

In this work we have managed to generalize this situation twofold: in the sense of considering symmetric M–matrices related to Schrödinger operators acting on networks (doubly weighted graphs, where not only edges but also vertices are discriminated) and also by using sub-matrices of the initial one in which two, three or more rows and columns are erased, those corresponding to two, three or more vertices.

We conceive that every symmetric M–matrix corresponds to a network where both a conductance on the edges and a weight on the vertices are introduced. Solving boundary value problems for Schrödinger's operators throughout the whole network or just a part of it, we find the relation between the corresponding group inverse and inverse matrices respectively. Since the part of the network to be considered is arbitrary, the reduction in the order of the matrices is also arbitrary.

The work is finished by exposing the application of our result to the calculation of the Green function of a path.

Keywords: Bottleneck matrix, Schrodinger operator, Green's function, M-matrix, Group–inverse matrix.

1 Preliminaries

The triple $\Gamma = (V, E, c)$ denotes a finite *network;* that is, a finite connected graph without loops nor multiple edges. V is its vertex set, whose cardinality equals n, and E is the edge set in which each edge $\{x, y\}$ has been assigned a *conductance* $c(x, y) > 0$. So the conductance can be considered as a symmetric function $c\colon V \times V \longrightarrow [0, +\infty)$ satisfying $c(x, x) = 0$ for any $x \in V$ and moreover, vertex x is adjacent to vertex y, $x \sim y$, iff $c(x, y) > 0$. Whenever $c(x, y) > 0$, then the value $r(x, y) = c(x, y)^{-1}$ is called *resistance between x and y.*

The set of real functions on V is denoted by $\mathcal{C}(V)$. Once a labelling of V is given, then every $u \in \mathcal{C}(V)$ can be thought as a $n-$component real vector hence $\mathcal{C}(V)$ can be identified with $\mathbb{R}^n$. Moreover, for $u, v \in \mathcal{C}(V)$, the values $||u||_2 = \Big(\sum\limits_{x\in V} u(x)^2\Big)^{1/2}$ and $\langle u, v\rangle = \sum\limits_{x\in V} u(x)v(x)$, are conceived as a norm and its associated inner product, respectively.

Given $u \in \mathcal{C}(V)$ the set of functions that are orthogonal to u is denoted by $u^\perp$ and is a subspace of $\mathcal{C}(V)$. Also the *support* of $u \in \mathcal{C}(V)$ is $\mathsf{supp}(u) = \{x \in V : u(x) \neq 0\}$ and hence, $\mathsf{supp}(u) = \emptyset$ iff $u = 0$. A function $\omega \in \mathcal{C}(V)$ is a *weight* if $\omega(x) > 0$ for all $x \in V$ and moreover $\langle \omega, \omega\rangle = n$. The set of weight functions is denoted by $\Omega(V)$.

Given $F \subset V$, its *boundary* and its *closure* are the sets $\delta(F) = \{x \in V : c(x, y) > 0$ for some $y \in F\}$ and $\overline{F} = F \cup \delta(F)$, respectively. Clearly $\delta(F) \subset V \setminus F$ and F is a proper subset iff $\delta(F) \neq \emptyset$. If $u \in \mathcal{C}(V)$ and $F \subset V$, the notation $u \geq 0$ on F or $u > 0$ on F means that $u(x) \geq 0$ or $u(x) > 0$ respectively, for any $x \in F$. Also, $\mathcal{C}(F)$ is the subspace of real functions vanishing on $F^c = V \setminus F$ the complementary set of F. In the sequel we identify $\mathcal{C}(F)$ with the set of functions $u\colon F \longrightarrow \mathbb{R}$. Analogously, each function $h\colon F \times F \longrightarrow \mathbb{R}$ is identified with $h\colon V \times V \longrightarrow \mathbb{R}$ satisfying $h(x, y) = 0$ when $(x, y) \notin F \times F$.

The *combinatorial Laplacian,* or simply the *Laplacian,* of the network Γ is the endomorphism of $\mathcal{C}(V)$ that assigns to each $u \in \mathcal{C}(V)$ the function $\mathcal{L}(u)(x) = \sum\limits_{y\in V} c(x, y)\big(u(x) - u(y)\big)$, $x \in V$. It is well-known, that the Laplacian is a self-adjoint and positive semidefinite operator. Moreover, since Γ is connected, $\mathcal{L}(u) = 0$ iff u is a constant function.

Given a weight function $\omega \in \Omega(V)$ the *potential determinated by* ω is a function in $\mathcal{C}(V)$ defined such that $q_\omega(x) = -\dfrac{1}{\omega(x)}\mathcal{L}(\omega)(x)$, $x \in V$. Since it is $\langle \omega, q_\omega\rangle = 0$, the potential determinated by ω must take positive and negative values unless ω is a constant function in which case $q_\omega = 0$. Also if $\omega_1, \omega_2 \in \Omega(V)$ then $q_{\omega_1} = q_{\omega_2}$ iff $\omega_2 = a\omega_1,\ a > 0$.

The *Schrödinger operator* on Γ with *potential* q is the self–adjoint endomorphism $\mathcal{L}_q : \mathcal{C}(V) \to \mathcal{C}(V)$ that assigns to each $u \in \mathcal{C}(V)$ the function

$$\mathcal{L}_q(u)(x) = \mathcal{L}(u)(x) + q(x)u(x),$$

where $\mathcal{L}(u)(x)$ is the *Laplacian* of the network Γ and $q \in \mathcal{C}(V)$. Every potential $q \in \mathcal{C}(V)$ is closely related with a potential determinated by a weight q_ω as for every $q \in \mathcal{C}(V)$ there exist unique $\omega \in \Omega(V)$ and $\lambda \in \mathbb{R}$ such that $q = q_\omega + \lambda$. Moreover, λ is the lowest eigenvalue of $\mathcal{L}_q$ and ω is its correspondant positive eigenvector that satisfies $\langle \omega, \omega\rangle = n$.

The *Doob Transform (with respect to ω)* consists in the identity

$$\mathcal{L}_{q_\omega} u(x) = \frac{1}{\omega(x)} \sum_{y\in V} c(x, y)\omega(x)\omega(y)\left(\frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)}\right), \quad x \in V, \quad u \in \mathcal{C}(V). \tag{1}$$

Then $\langle u, \mathcal{L}_{q_\omega}(u)\rangle \geq 0$ so $\mathcal{L}_{q_\omega}$ is positive semidefinite and $\langle \mathcal{L}_{q_\omega}(u), \omega\rangle = 0$ so a property that generalizes the corresponding one for the combinatorial Laplacian is obtained: $\mathcal{L}_{q_\omega}(u) = 0$ iff $u = a\omega,\ a \in \mathbb{R}$. In particular, we conclude that $q_\sigma = q_\omega$ iff $\sigma = a\omega$ for some $a > 0$, and each potential of the form q_ω

characterizes its corresponding weight ω. Finally a Schrödinger operator $\mathcal{L}_q$ is positive definite iff $\lambda > 0$ and positive semidefinite iff $\lambda \geq 0$. Moreover, when $\lambda = 0$ then $\langle \mathcal{L}_{q_\omega}(v), v\rangle = 0$ iff $v = a\omega, a \in \mathbb{R}$.

For a non empty set $F \subseteq V$ and given a potential $q = q_\omega + \lambda$, $\lambda \geq 0$, and its corresponding Schrödinger operator $\mathcal{L}_q$, the *boundary value problem* consisting in

$$\text{Given } f \in \mathcal{C}(F), \text{ then find } u \in \mathcal{C}(F) \text{ such that } \mathcal{L}_q(u) = f \text{ on } F \tag{2}$$

is known as a *Poisson Equation* on V when $F = V$, and as a *Dirichlet Problem* on F when F is a proper subset of V. In this second case, as $\mathcal{C}(F) = \big\{u \in \mathcal{C}(\bar{F}) : u = 0 \text{ on } \delta(F)\big\}$, the Dirichlet problem can be rewritten in its most commonly used form as

$$\text{Given } f \in \mathcal{C}(F), \text{ then find } u \in \mathcal{C}(\bar{F}) \text{ such that } \mathcal{L}_q(u) = f \text{ on } F \text{ and } u = 0 \text{ on } \delta(F). \tag{3}$$

We remark that also in this latter case the linear operator is self–adjoint as $\langle \mathcal{L}_q(u), v\rangle_F = \langle u, \mathcal{L}_q(v)\rangle_F$ for any $u, v \in \mathcal{C}(F)$.

Dirichlet problems as (3) are always compatible, as $\mathcal{L}_q$ establishes an automorphism on $\mathcal{C}(F)$. So are Poisson equations when $F = V$ and $\lambda > 0$. On the contrary, a problem (2) defined when $F = V$ and $\lambda = 0$ (i.e. $q = q_\omega$ for some $\omega \in \Omega(V)$) is compatible iff $f \in \omega^\perp$. In this case, there exists a unique solution $u \in \omega^\perp$ and $\{u + a\omega : a \in \mathbb{R}\}$ describes the set of all solutions to it.

The inverse of $\mathcal{L}_q$ on $\mathcal{C}(F)$ is called *Green's operator for* F and denoted by $\mathcal{G}_q^F$. The associated function $G_q^F : F \times F \longrightarrow \mathbb{R}$ defined for any $y \in F$ as $G_q^F(\cdot, y) = \mathcal{G}_q^F(\varepsilon_y)$[1], the unique solution of (3) corresponding to $f = \varepsilon_y$, is called the *Green function for* F. It turns out that the Green function for F is symmetrical and that, given $f \in \mathcal{C}(F)$, then $\mathcal{G}_q^F(f)(x) = \sum\limits_{y\in F} G_q^F(x, y)f(y)$, $x \in V$, is the unique solution of (3).

In the case of a positive semidefinite Poisson problem, as in (2), that is when $F = V$ and $\lambda = 0$, the Schrödinger operator $\mathcal{L}_{q_\omega}$ establishes an automorphism on $\omega^\perp$. The inverse of $\mathcal{L}_{q_\omega}$ on $\omega^\perp$ is called *orthogonal Green operator* and denoted by $\mathcal{G}_{q_\omega}$. We can extend $\mathcal{G}_{q_\omega}$ to a self-adjoint and positive semidefinite endomorphism on $\mathcal{C}(V)$ by defining $\mathcal{G}_{q_\omega}(f) = \mathcal{G}_{q_\omega}(f - \langle\omega,\omega\rangle^{-1}\langle f,\omega\rangle\omega)$ for any $f \in \mathcal{C}(V)$. The function $G_{q_\omega} : V \times V \longrightarrow \mathbb{R}$ defined for any $y \in V$ as $G_{q_\omega}(\cdot, y) = \mathcal{G}_{q_\omega}(\varepsilon_y) = \mathcal{G}_{q_\omega}(\varepsilon_y - \langle\omega,\omega\rangle^{-1}\omega(y)\omega)$, the unique solution of Problem (2) corresponding to $f = \varepsilon_y - \langle\omega,\omega\rangle^{-1}\omega(y)\omega$ is called the *orthogonal Green function*. Analogously to the preceeding paragraph, the orthogonal Green function is symmetrical and, given $f \in \omega^\perp$, the function defined as $\mathcal{G}_{q_\omega}(f)(x) = \sum\limits_{y\in V} G_{q_\omega}(x, y)f(y)$, $x \in V$, is the unique solution of Problem (2) belonging to $\omega^\perp$. In particular, $\mathcal{G}_{q_\omega}(f) = 0$ iff $f = a\omega$, $a \in \mathbb{R}$.

2 Contractions, null–extensions and bordered operators

From now on, we consider a fixed weight $\omega \in \Omega(V)$ and its correspondant Doob potential $q = q_\omega$ assuming $\lambda = 0$ so as the Schrödinger operator turns to be positive semidefinite. For any proper subset $F \subset V$, the inverse operator of $\mathcal{L}_{q_\omega}$ on $\mathcal{C}(F)$ will be called *Green's operator of* F *for the weight* ω, and will be denoted as $\mathcal{G}_{q_\omega}^F$. Then, the *Green function of* F *for* ω is the kernel associated with the Green operator of F for ω; that is, $G_{q_\omega}^F : F \times F \longrightarrow \mathbb{R}$ such that $G_{q_\omega}^F(x, y) = \mathcal{G}_{q_\omega}^F(\varepsilon_y)(x)$, for any $x, y \in F$. Therefore, $G_{q_\omega}^F$ is also symmetric and given $y \in F$, the function $u = G_{q_\omega}^F(\cdot, y)$ is the unique solution of the Dirichlet problem $\mathcal{L}_{q_\omega}(u) = \varepsilon_y$ on F, $u = 0$ on $\delta(F)$. In addition, $\mathcal{G}_{q_\omega}^F(f)(x) = \sum\limits_{y\in F} G_{q_\omega}^F(x, y)f(y)$ for any $f \in \mathcal{C}(F)$ and any $x \in F$.

2.1 Contractions and null–extensions

Let $\hat{x} \notin V$ be a new vertex and suppose that both ω and G_{q_ω}, are extended by 0 to $\widehat{V} = V \cup \{\hat{x}\}$ and $\widehat{V} \times \widehat{V}$ respectively; that is, let us assume that $\omega(\hat{x}) = 0$ and $G_{q_\omega}(\hat{x}, x) = G_{q_\omega}(x, \hat{x}) = G_{q_\omega}(\hat{x}, \hat{x}) = 0$ for any $x \in V$.

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We then take into account $\mathcal{G}_{q_\omega,\widehat{V}}$, the *null–extension* of $\mathcal{G}_{q_\omega}$ to $\mathcal{C}(\widehat{V})$ defined as $\mathcal{G}_{q_\omega,\widehat{V}}\colon \mathcal{C}(\widehat{V}) \to \mathcal{C}(\widehat{V})$

$$\mathcal{G}_{q_\omega,\widehat{V}}(u)(x) = \sum_{y\in\widehat{V}} G_{q_\omega}(x,y)u(y)$$

Evidently $\mathcal{G}_{q_\omega,\widehat{V}}(u)(x) = \mathcal{G}_{q_\omega}(u)(x) = \sum\limits_{y\in V} G_{q_\omega}(x,y)u(y)$, whenever $x \in V$, $u \in \mathcal{C}(V)$. We also notice that $\mathcal{G}_{q_\omega,\widehat{V}}(u)(\hat{x}) = 0$ for any $u \in \mathcal{C}(\widehat{V})$ and, in particular, that $\mathcal{G}_{q_\omega,\widehat{V}}(\varepsilon_{\hat{x}}) \equiv 0$.

Analogously for a proper $F \subset V$, let us consider $\widehat{F} = F \cup \{\hat{x}\}$ and let us define not only the *contraction to F of the Green operator* $\mathcal{G}_{q_\omega}$, denoted $\mathcal{G}_{q_\omega,F}\colon \mathcal{C}(F) \to \mathcal{C}(F)$ and such that

$$\mathcal{G}_{q_\omega,F}(u)(x) = \sum_{y\in F} G_{q_\omega}(x,y)u(y),\ x \in F,\ u \in \mathcal{C}(F),$$

but also the *null–extension to $\widehat{F}$ of* $\mathcal{G}_{q_\omega,F}$, noted as $\mathcal{G}_{q_\omega,\widehat{F}}\colon \mathcal{C}(\widehat{F}) \to \mathcal{C}(\widehat{F})$, and such that for any $u \in \mathcal{C}(\widehat{F})$ is $\mathcal{G}_{q_\omega,\widehat{F}}(u)(x) = \sum_{y\in\widehat{F}} G_{q_\omega}(x,y)u(y)$, while $x \in F$ and such that $\mathcal{G}_{q_\omega,\widehat{F}}(u)(\hat{x}) = 0$. Also it is $\mathcal{G}_{q_\omega,\widehat{F}}(u)(x) = \sum_{y\in F} G_{q_\omega}(x,y)u(y) = \mathcal{G}_{q_\omega,F}(u)(x)$ when $x \in F$.

2.2 Bordered and Host operators

[2] A critical role in our main result is devoted to two more operators (and their respective kernels) that are related to the operators we just come to define.

The *Bordered operator for $\widehat{F}$* is the linear operator $\mathcal{B}_{\widehat{F}}\colon \mathcal{C}(\widehat{F}) \longrightarrow \mathcal{C}(\widehat{F})$ defined for any $u \in \mathcal{C}(\widehat{F})$ as

$$\begin{cases} \mathcal{B}_{\widehat{F}}(u)(x) = \mathcal{G}_{q_\omega,\widehat{F}}(u)(x) + u(\hat{x})\omega(x) & x \in F,\\ \mathcal{B}_{\widehat{F}}(u)(\hat{x}) = \langle u,\omega\rangle_{\widehat{F}} \end{cases}$$

As $\omega(\hat{x}) = 0$, it turns out that $\mathcal{B}_{\widehat{F}}(u)(\hat{x}) = \langle u,\omega\rangle_F$.

Its corresponding kernel is called *bordered kernel for $\widehat{F}$*, is denoted by $B_{\widehat{F}}$ and is strongly related with the Green function defined on the initial whole vertex set V.

Proposition 2.1 *Given $F \subset V$, a proper subset, the bordered operator for $\widehat{F}$ is a non–singular and self–adjoint operator. In addition, the bordered kernel for $\widehat{F}$ is given by $B_{\widehat{F}}(x,y) = G_{q_\omega}(x,y)$, for any $x,y \in F$, $B_{\widehat{F}}(x,\hat{x}) = \omega(x)$, for any $x \in F$ and $B_{\widehat{F}}(\hat{x},\hat{x}) = 0$.*

Keeping in mind Proposition 2.1, for any proper subset $F \subset V$ we can define the so called *host operator for $\widehat{F}$* as the linear endomorphism on $\mathcal{C}(\widehat{F})$ that is the inverse of the previous bordered operator for $\widehat{F}$. Thus $\mathcal{H}_{\widehat{F}} = \big(\mathcal{B}_{\widehat{F}}\big)^{-1}$ and its associated kernel $H_{\widehat{F}}$ will be referred as the *host kernel for $\widehat{F}$*. Therefore, $H_{\widehat{F}}$ is also symmetric and it is characterized by the identities

$$\begin{aligned} \sum_{y\in F} G_{q_\omega}(x,y)H_{\widehat{F}}(y,z) + \omega(x)H_{\widehat{F}}(\hat{x},z) = \varepsilon_x(z), \quad x \in F,\ z \in \widehat{F}\\ \sum_{y\in F} \omega(y)H_{\widehat{F}}(y,z) = \varepsilon_{\hat{x}}(z), \quad z \in \widehat{F}. \end{aligned} \tag{4}$$

after applying $G_{q_\omega}(x,y) = G_{q_\omega,\hat{F}}(x,y)$ for $x,y \in F$ once again.

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3 A Poisson problem in connection with a Dirichlet problem

In this section we present our main result, that relates the solution of a Poisson equation as (2) on the whole V, with the solution of a related homogeneous Dirichlet problem as (3), on a proper $F \subset V$. Applying this idea to suitable Poisson equations and their related Dirichlet problems we are capable to relate their respective orthogonal Green kernel and Green kernel respectively.

Theorem 3.1 *Let $\Gamma = (V, E, c)$ be a network, let $\omega \in \Omega(V)$ be a weight, q_ω the potential determinated by ω and let $F \subset V$ be a proper subset. Consider the singular Schrödinger operator $\mathcal{L}_{q_\omega}$ on V and also $\mathcal{L}^F_{q_\omega}$ its nonsingular restriction to F. Then $G^F_{q_\omega}$ the Green function on F for ω is related with G_{q_ω} the orthogonal Green kernel on V for ω as follows: for every $x, y \in F$, it is*

$$\begin{aligned} G^F_{q_\omega}(x,y) = {} & G_{q_\omega}(x,y) - \sum_{z,t\in F^c} G_{q_\omega}(x,z) H_{\widehat{F^c}}(z,t) G_{q_\omega}(t,y) \\ & - \omega(y) \sum_{z\in F^c} H_{\widehat{F^c}}(\hat{x},z) G_{q_\omega}(z,x) - \omega(x) \sum_{z\in F^c} H_{\widehat{F^c}}(\hat{x},z) G_{q_\omega} v(z,y) - \omega(x)\omega(y) H_{\widehat{F^c}}(\hat{x},\hat{x}). \end{aligned}$$

3.1 The bottleneck, when $F^c = \{z\}$

$$\begin{aligned} G^F_q(x,y) &= G_q(x,y) - \frac{1}{\omega(z)} \Big[\omega(y) G_q(x,z) + \omega(x) G_q(y,z)\Big] + \frac{G_q(z,z)}{\omega(z)^2}\, \omega(x)\omega(y) \\ &= G_q(x,y) - \Big[\frac{G_q(x,z)}{\omega(x)\omega(z)} + \frac{G_q(y,z)}{\omega(y)\omega(z)} - \frac{G_q(z,z)}{\omega(z)^2}\Big]\, \omega(x)\omega(y), \qquad \text{for every } x, y \in F. \end{aligned}$$

3.2 Case $F^c = \{z_1, z_2\}$

$$\begin{aligned} G^F_q(x,y) = {} & G_q(x,y) \\ & - \frac{G_q(x,z_1)G_q(y,z_1)}{R(z_1,z_2)\omega(z_1)^2} + \frac{G_q(x,z_1)G_q(y,z_2) + G_q(x,z_2)G_q(y,z_1)}{R(z_1,z_2)\omega(z_1)\omega(z_2)} - \frac{G_q(x,z_2)G_q(y,z_2)}{R(z_1,z_2)\omega(z_2)^2} \\ & - \left[\frac{\omega(z_1)G_q(z_2,z_2) - \omega(z_2)G_q(z_1,z_2)}{R(z_1,z_2)\omega(z_1)^2\omega(z_2)^2}\right] \Big[\omega(y)G_q(x,z_1) + \omega(x)G_q(y,z_1)\Big] \\ & - \left[\frac{\omega(z_2)G_q(z_1,z_1) - \omega(z_1)G_q(z_1,z_2)}{R(z_1,z_2)\omega(z_1)^2\omega(z_2)^2}\right] \Big[\omega(y)G_q(x,z_2) + \omega(x)G_q(y,z_2)\Big] \\ & - \left[\frac{G_q(z_1,z_2)^2 - G_q(z_1,z_1)G_q(z_2,z_2)}{R(z_1,z_2)\omega(z_1)^2\omega(z_2)^2}\right] \omega(x)\omega(y), \qquad \text{for every } x, y \in F. \end{aligned}$$

4 Green function of a n–path

In the particular very important case of considering a path, when taking into account some propierties of the Green function of the path, then the next expressions are also fulfilled

Applying the very well known

Corollary 4.1 *If Γ is a weighted n–vertices path, then for any $\omega \in \Omega(V)$ the orthogonal Green kernel of $\mathcal{L}_{q_\omega}$ is given by*

$$G(x_i, x_j) = \omega(x_i)\omega(x_j) \left[\sum_{k=1}^{\min\{i,j\}-1} \frac{W_k^2}{C_k} + \sum_{k=\max\{i,j\}}^{n-1} \frac{(1-W_k)^2}{C_k} - \sum_{k=\min\{i,j\}}^{\max\{i,j\}-1} \frac{W_k(1-W_k)}{C_k} \right],$$

for any $i, j = 1, \dots, n$, *where* $W_k = \sum_{\ell=1}^{k} \omega^2(x_\ell)$ *and* $C_k = c(x_k, x_{k+1})\omega(x_k)\omega(x_{k+1})$, $k = 1, \dots, n-1$.

It tunrs out that

$$\frac{G_q^F(x_i, x_j)}{\omega(x_i)\omega(x_j)} = \frac{G_q(x_i, x_j}{\omega(x_i)\omega(x_j)} - \frac{R(x_i, x_n)R(x_j, x_n)}{R(x_1, x_n)} + \sum_{k=i}^{n-1} \frac{W_k}{C_k} + \sum_{k=j}^{n-1} \frac{W_k}{C_k} - \sum_{k=1}^{n-1} \frac{W_k^2}{C_k}$$

$$= \frac{R(x_j, x_n)R(x_1, x_i)}{R(x_1, x_n)} = \frac{R(x_1, x_{\min\{i,j\}})R(x_{\max\{i,j\}}, x_n)}{R(x_1, x_n)}.$$