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An Introduction to Discrete Vector Calculus on Finite Networks

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We aim here at introducing the basic terminology and results on *discrete vector calculus on finite networks*. **After defining the tangent space at each vertex of a weighted network we introduce the basic difference operators that are the discrete counterpart of the differential operators. Specifically we define the derivative, gradient, divergence, curl and laplacian operators. Moreover we prove that the above defined operators satisfy properties that are analogues to those satisfied by their continuous counterpart.**

1. Preliminaries

Throughout these notes, $\Gamma = (V, E)$ denotes a simple connected and finite graph without loops, with vertex set V and edge set E. Two different vertices, $x, y \in V$, are called *adjacent*, which is represented by $x \sim y$, if $\{x, y\} \in E$. In this case, the edge $\{x, y\}$ is also denoted as e_{xy} and the vertices x and y are called incidents with e_{xy}. In addition, for any $x \in V$ the value $k(x)$ denote the number of vertices adjacent to x. When, $k(x) = k$ for any $x \in V$ we say that the graph is k-regular.

We denote by $\mathcal{C}(V)$ and $\mathcal{C}(V \times V)$, the vector spaces of real functions defined on the sets that appear between brackets. If $u \in \mathcal{C}(V)$ and $f \in \mathcal{C}(V \times V)$, uf denotes the function defined for any $x, y \in V$ as $(uf)(x, y) = u(x)f(x, y)$.

If $u \in \mathcal{C}(V)$, the *support of* u is the set $\mathsf{supp}(u) = \{x \in V : u(x) \neq 0\}$.

A function $\nu \in \mathcal{C}(V)$ is called a *weight on* V if $\nu(x) > 0$ for all $x \in V$. For each weight ν on V and any $u \in \mathcal{C}(V)$ we denote by $\displaystyle\int_V u\, d\nu$ the value $\displaystyle\sum_{x\in V} u(x)\,\nu(x)$. In particular, when $\nu(x) = 1$ for any $x \in V$, $\displaystyle\int_V u\, d\nu$ is simply denoted by $\displaystyle\int_V u\, dx$.

Throughout the paper we make use of the following subspace of $\mathcal{C}(V \times V)$:

$$\mathcal{C}(\Gamma) = \{f \in \mathcal{C}(V \times V) : f(x, y) = 0, \quad \text{if } x \not\sim y\}.$$

We call *conductance on* Γ a function $c \in \mathcal{C}(\Gamma)$ such that $c(x, y) > 0$ iff $x \sim y$. We call *network* any triple (Γ, c, ν), where ν is a weight and c is a conductance on Γ. In what follows we consider fixed the network (Γ, c) and we refer to it simply by Γ. The function $\kappa \in \mathcal{C}(V)$ defined as $\kappa(x) = \displaystyle\int_V c(x, y)\, dy$ for any $x \in V$ is called the *(generalized) degree of* Γ. Moreover we call *resistance of* Γ the function $r \in \mathcal{C}(\Gamma)$ defined as $r(x, y) = \dfrac{1}{c(x, y)}$ when $d(x, y) = 1$.

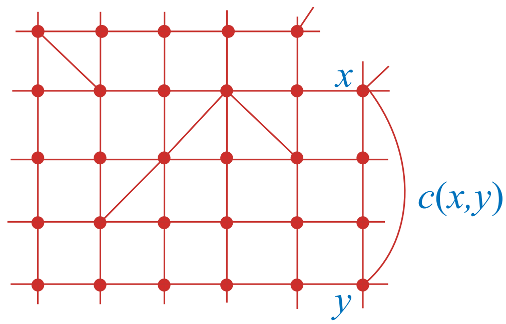

Figure 1. Weighted network

Next we define the tangent space at a vertex of a graph. Given $x \in V$, we call the real vector space of formal linear combinations of the edges incident with x, *tangent space at* x and we denote it by $T_x(\Gamma)$. So, the set of edges incident with x is a basis of $T_x(\Gamma)$, that is called *coordinate basis of* $T_x(\Gamma)$ and hence, $\dim T_x(\Gamma) = k(x)$. Note that, in the discrete setting, the dimension of the tangent space varies with each vertex except when the graph is regular.

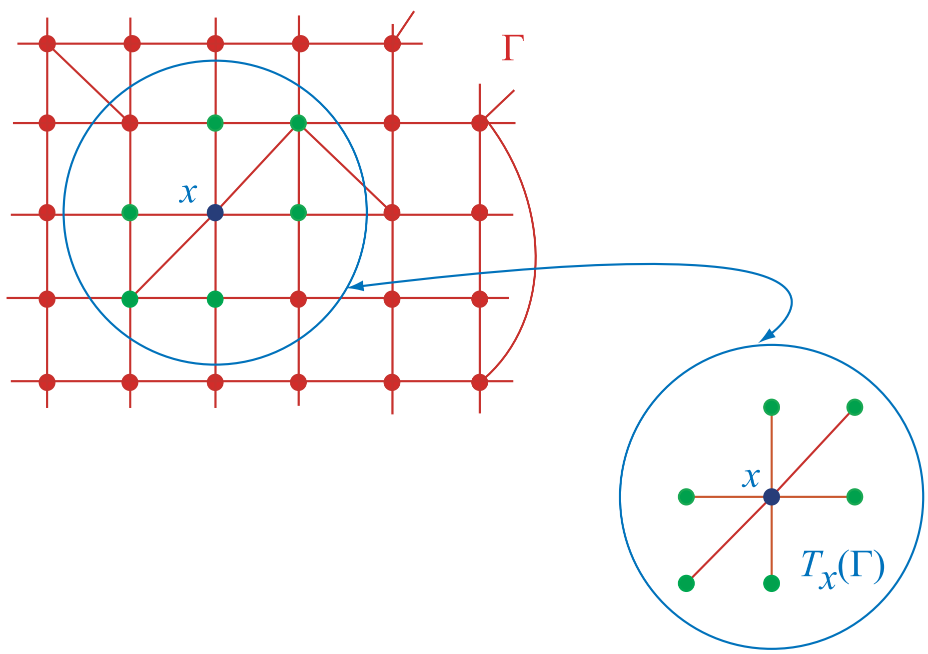

Figure 2. Tangent space at x

We call any application $\mathsf{f} : V \longrightarrow \bigcup\limits_{x \in V} T_x(\Gamma)$ such that $\mathsf{f}(x) \in T_x(\Gamma)$ for each $x \in V$, *vector field on* Γ. The *support of* f is defined as the set $\mathsf{supp}(\mathsf{f}) = \{x \in V : \mathsf{f}(x) \neq 0\}$. The space of vector fields on Γ is denoted by $\mathcal{X}(\Gamma)$.

If f is a vector field on Γ, then f is uniquely determined by its components in the coordinate basis. Therefore, we can associate with f the function $f \in \mathcal{C}(\Gamma)$ such that for each $x \in V$, $\mathsf{f}(x) = \sum\limits_{y\sim x} f(x,y)\, e_{xy}$ and hence $\mathcal{X}(\Gamma)$ can be identified with $\mathcal{C}(\Gamma)$.

A vector field f is called a *flow* when its component function satisfies that $f(x,y) = -f(y,x)$ for any $x, y \in V$, whereas f is called *symmetric* when its component function satisfies that $f(x,y) = f(y,x)$ for any $x, y \in V$. Given a vector field $\mathsf{f} \in \mathcal{X}(\Gamma)$, we consider two vector fields, *the symmetric and the antisymmetric fields associated with* f, denoted by f^s and f^a, respectively, that are defined as the fields whose component functions are given respectively by

$$f^s(x,y) = \frac{f(x,y) + f(y,x)}{2} \quad \text{and} \quad f^a(x,y) = \frac{f(x,y) - f(y,x)}{2}. \tag{1}$$

Observe that $\mathsf{f} = \mathsf{f}^s + \mathsf{f}^a$ for any $\mathsf{f} \in \mathcal{X}(\Gamma)$.

If $u \in \mathcal{C}(V)$ and $\mathsf{f} \in \mathcal{X}(\Gamma)$ has $f \in \mathcal{C}(\Gamma)$ as its component function, the field $u\mathsf{f}$ is defined as the field whose component function is uf.

If $\mathsf{f}, \mathsf{g} \in \mathcal{X}(\Gamma)$ and $f, g \in \mathcal{C}(\Gamma)$ are their component functions, the expression $\langle \mathsf{f}, \mathsf{g} \rangle$ denotes the function in $\mathcal{C}(V)$ given by

$$\langle \mathsf{f}, \mathsf{g} \rangle(x) = \sum_{y\sim x} f(x,y) g(x,y) r(x,y), \quad \text{for any } x \in V. \tag{2}$$

Clearly, for any $x \in V$, $\langle \cdot, \cdot \rangle(x)$ determines an inner product on $T_x(\Gamma)$.

The triple (Γ, c, ν), where ν is a weight on V, is called *weighted network*. So, on a weighted network we can consider the following inner products on $\mathcal{C}(V)$ and on $\mathcal{X}(\Gamma)$,

$$\int_V u\, v\, d\nu, \quad u, v \in \mathcal{C}(V) \quad \text{and} \quad \frac{1}{2}\int_V \langle \mathsf{f}, \mathsf{g} \rangle\, dx, \quad \mathsf{f}, \mathsf{g} \in \mathcal{X}(\Gamma), \tag{3}$$

where the factor $\frac{1}{2}$ is due to the fact that each edge is considered twice.

Lemma 1.1. *Given* $\mathsf{f}, \mathsf{g} \in \mathcal{X}(\Gamma)$ *such that* f *is symmetric and* g *is a flow, then* $\displaystyle\int_V \langle \mathsf{f}, \mathsf{g} \rangle\, dx = 0$.

2. Difference operators on weighted networks

Our objective in this section is to define the discrete analogues of the fundamental first and second order differential operators on Riemannian manifolds, specifically the derivative, gradient, divergence, curl and the laplacian. The last one is called *second order difference operator* whereas the former are generically called *first order difference operators*. From now on we suppose fixed the weighted network (Γ, c, ν) and also the associated inner products on $\mathcal{C}(V)$ and $\mathcal{X}(\Gamma)$.

We call *derivative operator* the linear map $\mathsf{d}\colon \mathcal{C}(V) \longrightarrow \mathcal{X}(\Gamma)$ that assigns to any $u \in \mathcal{C}(V)$ the flow $\mathsf{d}u$, called *derivative of* u, given by

$$\mathsf{d}u(x) = \sum_{y\sim x} \big(u(y) - u(x)\big)\, e_{xy}. \tag{4}$$

We call *gradient* the linear map $\nabla\colon \mathcal{C}(V) \longrightarrow \mathcal{X}(\Gamma)$ that assigns to any $u \in \mathcal{C}(V)$ the flow ∇u, called *gradient of* u, given by

$$\nabla u(x) = \sum_{y\sim x} c(x,y)\big(u(y) - u(x)\big)\, e_{xy}. \tag{5}$$

Clearly, it is verified that $\mathsf{d}u = \mathsf{0}$, or equivalently $\nabla u = \mathsf{0}$, iff u is a constant function.

We define the *divergence operator* as $\mathsf{div} = -\nabla^*$, that is the linear map $\mathsf{div}: \mathcal{X}(\Gamma) \longrightarrow \mathcal{C}(V)$ that assigns to any $\mathsf{f} \in \mathcal{X}(\Gamma)$ the function $\mathsf{div}\,\mathsf{f}$, called *divergence of* f, determined by the relation

$$\int_V u\, \mathsf{div}\,\mathsf{f}\, d\nu = -\frac{1}{2}\int_V \langle \nabla u, \mathsf{f} \rangle\, dx, \quad \text{for an } u \in \mathcal{C}(V). \tag{6}$$

Therefore, taking u constant in the above identity, we obtain that

$$\int_V \mathsf{div}\,\mathsf{f}\,d\nu = 0 \quad \text{for any } \mathsf{f} \in \mathcal{X}(\Gamma). \tag{7}$$

Proposition 2.1. *If* $\mathsf{f} \in \mathcal{X}(\Gamma)$, *for any* $x \in V$ *it holds*

$$\mathsf{div}\,\mathsf{f}(x) = \frac{1}{\nu(x)} \sum_{y\sim x} f^a(x,y).$$

Proof. For any $z \in V$ consider $u = \varepsilon_z$, the Dirac function at z. Then, from Identity (6) we get that

$$\mathsf{div}\,\mathsf{f}(z) = -\frac{1}{2\nu(z)} \int_V \langle \nabla\varepsilon_z, \mathsf{f}\rangle\, dx = -\frac{1}{2\nu(z)} \sum_{x\in V} \langle \nabla\varepsilon_z, \mathsf{f}\rangle(x)$$

Given $x \in V$, we get that

$$\begin{aligned}\langle \nabla\varepsilon_z, \mathsf{f}\rangle(x) &= \sum_{y\sim x} c(x,y)\big(\varepsilon_z(y) - \varepsilon_z(x)\big) f(x,y) r(x,y) = \sum_{y\in V} \big(\varepsilon_z(y) - \varepsilon_z(x)\big) f(x,y)\\ &= f(x,z) - \sum_{\substack{y\in V\\ y\neq z}} \varepsilon_z(x) f(x,y)\end{aligned}$$

and hence when $x \neq z$, then $\langle \nabla\varepsilon_z, \mathsf{f}\rangle(x) = f(x,z)$, whereas $\langle \nabla\varepsilon_z, \mathsf{f}\rangle(z) = -\sum\limits_{\substack{y\in V\\ y\neq z}} f(z,y)$. Therefore,

$$\mathsf{div}\,\mathsf{f}(z) = -\frac{1}{2\nu(z)} \sum_{x\in V} \langle \nabla\varepsilon_z, \mathsf{f}\rangle(x) = \frac{1}{2\nu(z)} \left[\sum_{\substack{y\in V\\ y\neq z}} f(z,y) - \sum_{\substack{x\in V\\ x\neq z}} f(x,z) \right] = \frac{1}{\nu(z)} \sum_{x\in V} f^a(z,x). \qquad \square$$

We call *curl* the linear map $\mathsf{curl} : \mathcal{X}(\Gamma) \longrightarrow \mathcal{X}(\Gamma)$ that assigns to any $\mathsf{f} \in \mathcal{X}(\Gamma)$ the symmetric vector field $\mathsf{curl}\,\mathsf{f}$, called *curl of* f, given by

$$\mathsf{curl}\,\mathsf{f}(x) = \sum_{y\sim x} r(x,y) f^s(x,y)\, e_{xy}. \tag{8}$$

In the following result we show that the above defined difference operators verify properties that are mimetic to the ones verified by their differential analogues.

Proposition 2.2. $\mathsf{curl}^* = \mathsf{curl}$, $\mathsf{div} \circ \mathsf{curl} = 0$ *and* $\mathsf{curl} \circ \nabla = 0$.

Now we introduce the fundamental second order difference operator on $\mathcal{C}(V)$ which is obtained by composition of two first order operators. Specifically, we consider the endomorphism of $\mathcal{C}(V)$ given by $\mathcal{L} = -\mathsf{div} \circ \nabla$, that we call the *Laplace-Beltrami operator or Laplacian of* Γ.

Proposition 2.3. *For any* $u \in \mathcal{C}(V)$ *and for any* $x \in V$ *we get that*

$$\mathcal{L}(u)(x) = \frac{1}{\nu(x)} \sum_{y\sim x} c(x,y)\big(u(x) - u(y)\big) = \frac{1}{\nu(x)} \int_V c(x,y)\big(u(x) - u(y)\big) dy.$$

Moreover, given $u, v \in \mathcal{C}(V)$, *the following properties hold:*

(i) First Green Identity

$$\int_V v\mathcal{L}(u) d\nu = \frac{1}{2} \int_V \langle \nabla u, \nabla v\rangle dx = \frac{1}{2} \int_{V\times V} c(x,y)\big(u(x) - u(y)\big)\big(v(x) - v(y)\big) dxdy.$$

(ii) Second Green Identity

$$\int_V v\mathcal{L}(u) d\nu = \int_V u\mathcal{L}(v) d\nu.$$

(iii) Gauss Theorem

$$\int_V \mathcal{L}(u) d\nu = 0.$$

Proof. The expression for the Laplacian of u follows from the expression of the divergence keeping in mind that ∇u is a flow. On the other hand, given $v \in \mathcal{C}(V)$ from the definition of divergence we get that

$$\int_V v\mathcal{L}(u)\, d\nu = -\int_V v \mathsf{div}\,(\nabla u)\, d\nu = \frac{1}{2}\int_V \langle \nabla u, \nabla v\rangle dx = \frac{1}{2}\int_{V\times V} c(x,y)\big(u(x)-u(y)\big)\big(v(x)-v(y)\big)dx\, dy$$

and the First Green Identity follows. The proof of the Second Green Identity and the Gauss Theorem are straightforward consequence of (i). □

Corollary 2.4. *The Laplacian of* Γ *is self-adjoint and positive semi–definite. Moreover* $\mathcal{L}(u) = 0$ *iff* u *is constant.*

Remark: Suppose that $V = \{x_1, \dots, x_n\}$, assume that $\nu = 1$ and consider $c_{ij} = c(x_i, x_j) = c_{ji}$. Then, each $u \in \mathcal{C}(V)$ is identified with $\big(u(x_1), \dots, u(x_n)\big)^T \in \mathbb{R}^n$ and the Laplacian of Γ is identified with the irreducible matrix

$$\mathsf{L} = \begin{bmatrix} k_1 & -c_{12} & \cdots & -c_{1n} \\ -c_{21} & k_2 & \cdots & -c_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ -c_{n1} & -c_{n2} & \cdots & k_n \end{bmatrix}$$

where $k_i = \sum_{j=1}^{n} c_{ij}$, $i = 1, \dots, n$. Clearly, this matrix is symmetric and diagonally dominant [1] and hence it is positive semi-definite. Moreover, it is singular and 0 is a simple eigenvalue whose associated eigenvectors are constant.

[1] `http://en.wikipedia.org/wiki/Diagonally_dominant_matrix`