2-WASSERSTEIN ON A GRAPH

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1. Gradient and divergence on a Graph

Let $G = (V, \omega)$ be a weighted simple connected graph, were ω is a zero-diagonal non-negative symmetric matrix. The adjacency matrix $E = [(\omega(x,y) > 0)]$ splits (in many ways) into the sum of two adjacency matrices of directed graphs on V in such a way that $E = \overrightarrow{E} + \overleftarrow{E}$. Let $M(G)$ be the vector space of matrices whose support is contained in the support of E. Similarly, we define the space of symmetric matrices $S(G)$ and the space of skew-symmetric matrices $A(G)$. Elements of $A(G)$ are also called *vector fields*. Both this special cases are uniquely characterised by their restriction on either $\overrightarrow{E}$ or $\overleftarrow{E}$.

For each given weight θ on G, that is, $\theta(x,y) \geq 0$ and $\theta(x,y) = 0$ if $\omega(x,y) = 0$, we define the *inner product* $\langle \cdot, \cdot \rangle_\theta$ for $a, b \in M(G)$ by

$$\langle a, b \rangle_\theta = \frac{1}{2} \sum_{x,y \in V} a(x,y)b(x,y)\theta(x,y) = \frac{1}{2} \sum_{E(x,y)=1} a(x,y)b(x,y)\theta(x,y) = \\ \sum_{\overrightarrow{E}(x,y)=1} \frac{1}{2}(a(x,y)b(x,y) + a(y,x)b(y,x))\theta(x,y) \ .$$

If a and b are either both symmetric, or both skew-symmetric, then

$$\langle a, b \rangle_\theta = \sum_{\overrightarrow{E}(x,y)=1} a(x,y)b(x,y)\theta(x,y) \ .$$

If a and b are one symmetric and the other skew-symmetric, then

$$\langle a, b \rangle_\theta = 0 \ .$$

Let us call *potential* a mapping $\Phi \colon V \to \mathbb{R}$. We can map potentials into vector fields by the operation of *G-gradient* ∇ defined by,

$$\nabla \phi(x,y) = \sqrt{\omega(x,y)}(\phi(x) - \phi(y)) \ , \quad x, y \in V \ .$$

The meaning of the square rooth will be explained later. As the graph G is connected, it holds $\ker \nabla = \mathbb{R}\mathbf{1}$.

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Let us compute the adjoint of the gradient operator. For all vector field $v \in A(G)$ it holds

$$\langle \nabla\phi, b\rangle_\theta = \frac{1}{2}\sum_{E(x,y)=1} \sqrt{\omega(x,y)}\theta(x,y)(\phi(x)-\phi(y))b(x,y) =$$

$$= \frac{1}{2}\sum_{x\in V}\sum_{y\in N(x)} \sqrt{\omega(x,y)}\theta(x,y)\phi(x)b(x,y) - \frac{1}{2}\sum_{x\in V}\sum_{y\in N(x)} \sqrt{\omega_{yx}}\theta_{yx}\phi(x)b(y,x) =$$

$$\sum_{x\in V}\left(\sum_{y\in N(x)} \sqrt{\omega(x,y)}\theta(x,y)b(x,y)\right)\phi(x) = \langle \phi, \operatorname{div}(\theta b)\rangle \ ,$$

where $N(x) = \{y \mid xy \in E\}$ and $\operatorname{div}\colon A(G) \to \mathbb{R}^V$ is defined by

$$\operatorname{div} w(x) = \sum_{y\in N(x)} \sqrt{\omega(x,y)}w(x,y) \ .$$

It holds $\operatorname{div}(\theta b) = 0$ if, and only if, b is θ-orthogonal to all vector fields of the form $\nabla\phi$.

2. Laplacian and Hodge decomposition

We define the following symmetric form on potentials:

$$\langle\langle \phi, \psi\rangle\rangle_\theta = \langle \nabla\phi, \nabla\Psi\rangle_\theta = \langle L\phi, \Psi\rangle \ ,$$

where $L(\theta)\phi = \operatorname{div}(\theta\nabla\phi)$ and $L(\theta)$ is the *Laplacian.*

The kernel of the gradient operator is charaterised by

$$0 = \langle\langle \phi, \phi\rangle\rangle_\theta = \frac{1}{2}\sum_{xy\in E} \omega(x,y)(\phi(x)-\phi(y))^2\theta(x,y) \ ,$$

that is, $\phi(x) = \phi(y)$ for all $x \in E$, that is, ϕ is constant. It follows that the symmetric form is a scalar product above on the space of sum-zero potentials, that is, on the affine space of the probability simplex on V.

Let us study the image of the gradient operator in the space of vector fields. The vector field w belongs to the orthogonal of the image of ∇ if, for all ϕ,

$$0 = \langle \nabla\phi, w\rangle_\theta = \langle \phi, \operatorname{div}(\theta w)\rangle \ ,$$

that is, if, and only if, $\operatorname{div}(\theta W) = 0$. The following statement follow easily. It is sometimes called *Hodge decomposition.*

Every vector field $v \in A(G)$ admits the θ-orthogonal decomposition $v = \nabla\phi + w$, where ϕ is a potential defined up to a constant and $\operatorname{div}(\theta w) = 0$

Clearly, the decomposition depends on θ

3. Continuity equation

Let θ be a smooth mapping from the probability simplex on V to the cone of positive $S(G)$, $\theta\colon \rho \mapsto \theta(\rho) \in S_+(G)$. Given a regular curve $[0,1] \ni t \mapsto \Phi(t)$ in the space of zero-sum potentials, the ordinary differential equation

$$\frac{d}{dt}\rho(t) + \operatorname{div}(\theta(\rho(t))\nabla\phi(t)) = 0 \ , \quad \rho(0) = \rho^0 \in \mathcal{P}_+(V) \ ,$$

has a local solution in $\mathcal{P}_+(V)$ because

$$\frac{d}{dt}\sum_x \rho(x;t) = \langle \dot\rho(t), \mathbf{1}\rangle = -\langle \operatorname{div}(\theta(\rho(t))\nabla\phi(t)), 1\rangle = \langle \nabla\Phi(t), \nabla 1\rangle_{\theta(\rho)} = 0 \ .$$

Given $\rho^0, \rho^1 \in \mathcal{P}_+(V)$, consider the value of the problem

$$\inf \int_0^1 \langle\!\langle \phi(t), \phi(t) \rangle\!\rangle_{\theta(\rho(t))} \, dt$$
$$\frac{d}{dt}\rho(t) + \operatorname{div}(\theta(\rho)\nabla\Phi(t)) = 0$$
$$\rho(0) = \rho^0 \ , \quad \rho(1) = \rho^1.$$

Let us write $L(\rho)\Phi = \operatorname{div}(\theta(\rho)\nabla\Phi)$ and consider that the conjugate of the quadratic form $\langle\!\langle \phi, \phi \rangle\!\rangle_{\theta(\rho)} = \frac{1}{2}\langle L(\rho)\phi, \psi \rangle$ is of the form

$$\frac{1}{2}\left\langle L(\rho)^\dagger \alpha, \alpha \right\rangle = \frac{1}{2} = \left\langle L(\rho)^\dagger L(\rho)\phi, L(\rho)(\phi) \right\rangle = \frac{1}{2} L(\rho)\phi\phi \ .$$

Writing now $\Phi = L(\rho)^\dagger \dot{\rho}$ in the problem above, we obtain the equivalent problem

$$\inf \int_0^1 \left\langle L(\rho(t))^\dagger \dot{\rho}(t), \dot{\rho}(t) \right\rangle \, dt$$
$$\rho(0) = \rho^0 \ , \quad \rho(1) = \rho^1 \ .$$

In conclusion, the value of the problem is a squared Riemannian distance for the metric whose tensor is $L(\rho)^\dagger$

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