Spectral Graph Theory May 26, 2021

The Quadratic Form and Standard Random Walk

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1 The Labelling Function

We consider the undirected graph $G = (V, E)$ and it satisfies the following properties:

- The graph is finite.
- Multiple parallel edges and self-loops are allowed.
- vertices of degree 0 are not allowed.

For simplicity, maybe we assume G is regular.

We can label the vertice set V by real numbers:

$$f : V \to \mathbb{R} \equiv \begin{bmatrix} f(v_1) \\ f(v_2) \\ \vdots \\ f(v_n) \end{bmatrix}$$

For example, f can be temperature, voltage, coordinate or $0-1$ indicator of $S \subseteq V$.

Remark that we can add or scalar multiply this function.

$$(f+g)(x) = f(x) + g(x),$$

$$c \cdot f(x) = f(c \cdot x).$$

So, $\{f : V \to \mathbb{R}\}$ is a vector space with dimension $n = |V|$.

2 Key to SGT: The Quadratic Form

Definition 1 *The quadratic form is defined to be*

$$\mathcal{E}[f] := \frac{1}{2} \mathop{\mathbb{E}}_{u \sim v} \left[(f(\boldsymbol{u}) - f(\boldsymbol{v}))^2 \right]$$

Where $u \sim v$ denotes we choose a uniform random edge $(u, v) \in E$.

From the definition, we have some facts about the quadratic form.

- $\mathcal{E}[f] \geq 0$.
- $\mathcal{E}[c \cdot f] = c^2 \cdot \mathcal{E}[f]$.

- $\mathcal{E}[f+c] = \mathcal{E}[f]$.

Intuitively, The quadratic form is small if and only if f's value don't vary much along edges.

For example, if we take $S \subseteq V$ and $f = 1_S$ (the indicator function):

$$f(v) = \begin{cases} 1, & \text{if } v \in S \\ 0, & \text{if } v \notin S \end{cases}$$

Then we have:

$$\begin{aligned}
\mathcal{E}[f] &= \frac{1}{2} \cdot \mathop{\mathbb{E}}_{u \sim v}[(1_s(u) - 1_s(v))^2] \\
&= \frac{1}{2} \cdot \mathop{\mathbb{E}}_{u \sim v}[1_{\{(u,v) \text{ cross the cut } (S,\bar{S})\}}] \\
&= \frac{1}{2} \cdot \{\text{fraction of edges on } \partial S\} \\
&= \Pr_{u \sim v}[u \to v \text{ is stepping out of } S]
\end{aligned}$$

3 Standard Random Walk

Next, we define a distribution over V. To choose a random vertex

- choose a uniform random edge (u, v) (direct).
- output u.

We denote this distribution by π.

Fact 2 $\pi[u]$ *is proportional to deg(u) and*

$$\pi(u) = \frac{deg(u)}{2|E|}.$$

If G is regular, π is a uniform distribution on V.

Fact 3 *If we draw a vertice $u \sim \pi$, and let v be a uniform random neighbor of u, then the distribution of (u, v) is identical to draw a uniform random edge (u^{prime}, v^{prime}), and v is also distributed according to π.*

Proof: The probability of choosing a vertice u is $\pi(u) = \frac{\deg(u)}{2|E|}$.

$$\begin{aligned}
\Pr[\text{pick the edge } (u,v)] &= \Pr[\text{pick a random neighbor } v \text{ of } u | \text{pick a random vertice } u] \cdot \pi(u) \\
&= \frac{1}{\deg(u)} \cdot \frac{\deg(u)}{2|E|} \\
&= \frac{1}{2|E|}
\end{aligned}$$

$\square$

Corollary 4 *Let $t \in \mathbb{N}$, draw a vertice $u \sim \pi$ and do standard random walk for t steps, then v is also distributed according to π.*

We define π as a invariant distribution. But now we have a new question, say u_0 is not distributed according to π, do a t steps random walk from u_0, as $t \to \infty$, does the distribution of $v \to \pi$? The answer is not if G is disconnected or G is bipartite. Otherwise, the answer is **YES**.

but how fast does it converge? We should consider the spectral of the graph. For example, let $S \subseteq V$, if the $cut(S, \bar{S})$ is tiny, then the convergence time may be very large, but we have showed in this case $\mathcal{E}[1_S]$ is small. Intuitively, converge fastly if and only if $\mathcal{E}[f]$ never small.

4 Enter Linear Algebra

Let $f : V \to \mathbb{R}$ and $u \sim \pi$, then $f(u)$ is a real random variable. We can define the mean and variance of this random variable.

- Mean: $\mathbb{E}[f] := \mathop{\mathbb{E}}_{u\sim\pi}[f(u)]$. For example, if $S \subseteq V$, and $f = 1_s$, then $\mathbb{E}[f] = \mathop{\mathbb{E}}_{u\sim\pi}[1_s(u)] = \mathop{Pr}_{u\sim\pi}[u \in S]$. This is the "weight"/"volumn" of S.
- Variance: $Var[f(u)] = \mathop{\mathbb{E}}_{u\sim\pi}[(f(u)-\mu)^2] = \mathop{\mathbb{E}}_{u\sim\pi}[f(u)^2] - \mathop{\mathbb{E}}_{u\sim\pi}[f(u)]^2 = \frac{1}{2}\mathop{\mathbb{E}}_{u\sim\pi,v\sim\pi}[(f(u)-f(v))^2]$. Recall that $\mathcal{E}[f] := \frac{1}{2}\mathop{\mathbb{E}}_{u\sim v}\left[(f(\boldsymbol{u}) - f(\boldsymbol{v}))^2\right]$.

We can define inner product between two functions.

Definition 5 *Let $f, g : V \to \mathbb{R}$, the inner product of f, g is defines as $< f, g >_\pi := \mathop{\mathbb{E}}_{u\sim\pi}[f(u)g(u)]$*

Remark this is a vector space inner product.

- $\langle f, g\rangle_\pi = \langle g, f\rangle_\pi$.
- $\langle c \cdot f + g, h\rangle_\pi = c \cdot \langle f, h\rangle_\pi + \langle g, h\rangle_\pi$.
- $||f||_2^2 = \langle f, f\rangle_\pi = \mathop{\mathbb{E}}_{u\sim\pi}[f(u)^2] \geq 0$ and the equality holds if and only if $f \equiv 0$.

Let $S \subseteq V$, $f = 1_s$, then $||f||_1 := \mathop{\mathbb{E}}_{u\sim\pi}[|f(u)|] = \mathop{\mathbb{E}}_{u\sim\pi}[1_s(u)] = \mathop{Pr}_{u\sim\pi}[u \in S] =$ "volumn" of S. Notice that, $||f||_2^2 = \langle f, f\rangle = \mathop{\mathbb{E}}_{u\sim\pi}[f(u)^2] = \mathop{\mathbb{E}}_{u\sim\pi}[|f(u)|] = ||f||_1$.

5 Minimizing and Maxmizing the Quardratic Form

Now we have a question, how small can $\mathcal{E}[f]$ be? The answer is 0 if we take $f \equiv 0$. Is there a nontrival f with $\mathcal{E}[f] = 0$? Again, recall the definition of the quadratic form $\mathcal{E}[f] := \frac{1}{2}\mathop{\mathbb{E}}_{u\sim v}\left[(f(\boldsymbol{u}) - f(\boldsymbol{v}))^2\right]$.

Proposition 6 $\mathcal{E}[f] = 0$ *if and only if f is constant on each connected component of G and the number of connected component of G equals to the number of linear independent f with $\mathcal{E}[f] = 0$.*

If the components are $S_1, ..., S_l$, $1_{S_1}, 1_{S_2}, ..., 1_{S_l}$ are linear independent, the subspace $\{f : \mathcal{E}[f] = 0\} = \sum_{i=1}^{l} c_i \cdot 1_{S_i}$.

Next, we maxmize $\mathcal{E}[f]$. But recall we have $\mathcal{E}[c \cdot f] = c^2 \cdot \mathcal{E}[f]$, so our task is maxmizing $\mathcal{E}[f]$ subject to $Var[f] = 1(\leq 1)$. Remark this is identical to maxmize $\mathcal{E}[f]$ subject to $||f||_2^2 = \mathbb{E}[f^2] = 1(\leq 1)$, since $\mathbb{E}[f^2] = Ver[f] + \mathbb{E}[f]^2$.

Intuitively, the edge endpoints' value should be as far as possible. For what kind of G will you be most successful? The answer is bipartite graph. If G is bipartite, $V = (V_1, V_2)$, let $f = 1_{V_1} - 1_{V_2}$:

$$f(u) = \begin{cases} +1, & \text{if } u \in V_1 \\ -1, & \text{if } u \in V_2 \end{cases}$$

Now, we have

- $\underset{u \sim \pi}{\mathbb{E}}[f(u)^2] = \mathbb{E}[1] = 1.$
- $\mathcal{E}[f] = \frac{1}{2} \underset{u \sim v}{\mathbb{E}} \left[(f(\boldsymbol{u}) - f(\boldsymbol{v}))^2 \right] = 2.$

Proposition 7 $\mathcal{E}[f] \leq 2||f||_2^2 = 2\mathbb{E}[f^2]$.

Proof:

$$\begin{aligned}
\mathcal{E}[f] = \frac{1}{2} \underset{u \sim v}{\mathbb{E}} \left[(f(\boldsymbol{u}) - f(\boldsymbol{v}))^2 \right] &= \frac{1}{2} \underset{u \sim \pi}{\mathbb{E}}[f(u)^2] + \frac{1}{2} \underset{v \sim \pi}{\mathbb{E}}[f(v)^2] + \underset{u \sim v}{E}[f(u) \cdot f(v)] \\
&\leq \mathbb{E}[f^2] + \sqrt{\underset{u \sim v}{\mathbb{E}}[f(u)^2]} \cdot \sqrt{\underset{u \sim v}{\mathbb{E}}[f(v)^2]} \\
&= 2\mathbb{E}[f^2]
\end{aligned}$$

$\square$

Exercise: The equality $\mathcal{E}[f] = 2\mathbb{E}[f^2]$ is possible if and only if G is bipartite.