Graph Laplacians and their continuum limit

Sangmin Park

CNA Working Group, CMU

October 6, 2020
Introduction: calculus on graphs
- Consistency: discrete to nonlocal
- Consistency: nonlocal to local
- Continuum limit of the solution to discrete Laplace’s equation[1]
Calculus on graphs

- Let $\mathcal{X}$ be the set of $n$ vertices and $W$ a $n \times n$ symmetric matrix with non-negative components. Let $d(x) = \sum_{y \in \mathcal{X}} w_{xy}$ be the degree of $x$.
- Let $\ell^2(\mathcal{X})$ denote the space of ‘square summable functions’ $u : \mathcal{X} \to \mathbb{R}$ with respect to the inner product

$$ (u, v)_{\ell^2(\mathcal{X})} = \sum_{x \in \mathcal{X}} u(x) v(x). $$

- Vector field is a function $V : \mathcal{X}^2 \to \mathbb{R}$ satisfying $V(x, y) = -V(y, x)$. The inner product between vector fields $V_1, V_2$ is

$$ (V_1, V_2)_{\ell^2(\mathcal{X}^2)} = \frac{1}{2} \sum_{x, y \in \mathcal{X}} w_{xy} V_1(x, y) V_2(x, y). $$
The gradient of a function $u \in \ell^2(\mathcal{X})$ is

$$\nabla u(x, y) = u(y) - u(x)$$

The divergence of a vector field is

$$\text{div } V(x) = \sum_{y \in \mathcal{X}} w_{xy} V(x, y).$$

Then we have the divergence formula

$$(\nabla u, V)_{\ell^2(\mathcal{X}^2)} = -(u, \text{div } V)_{\ell^2(\mathcal{X})}$$
Proof of the divergence formula

\[(\nabla u, V)_{\ell^2(\mathcal{X})} = \frac{1}{2} \sum_{x, y \in \mathcal{X}} w_{xy} (u(y) - u(x)) V(x, y)\]

\[= \frac{1}{2} \sum_{x, y \in \mathcal{X}} w_{xy} u(y) V(x, y) - \frac{1}{2} \sum_{x, y \in \mathcal{X}} W_{xy} u(x) V(x, y)\]

\[= \frac{1}{2} \sum_{x, y \in \mathcal{X}} w_{xy} u(x) V(y, x) - \frac{1}{2} \sum_{x, y \in \mathcal{X}} W_{xy} u(x) V(x, y)\]

\[= - \sum_{x, y \in \mathcal{X}} w_{xy} u(x) V(x, y) = -(u, \text{div } V)_{\ell^2(\mathcal{X})}\]
We define the graph Laplacian $\mathcal{L}$ by

$$\mathcal{L}u(x) = \text{div}(\nabla u) = \sum_{y \in \mathcal{X}} w_{xy}(u(y) - u(x)).$$

Note the connection to the mean value property by

$$\mathcal{L}u(x) = \sum_{y \in \mathcal{X}} w_{xy}(u(y) - u(x)) = \sum_{y \in \mathcal{X}} w_{xy}u(y) - d(x)u(x).$$

By the divergence formula we see that $\mathcal{L}$ is self-adjoint

$$(\mathcal{L}u, v)_{\ell^2(\mathcal{X})} = -(\nabla u, \nabla v)_{\ell^2(\mathcal{X}^2)} = (u, \mathcal{L}v)_{\ell^2(\mathcal{X})}$$

and that it is connected to the graph Dirichlet energy

$$(-\mathcal{L}u, u)_{\ell^2(\mathcal{X})} = (\nabla u, \nabla u)_{\ell^2(\mathcal{X}^2)} =: \mathcal{E}(u) \geq 0.$$
The maximum principle

Lemma 1

Let \( u \in \ell^2(\mathcal{X}) \) satisfying \( \mathcal{L}u(x) \geq 0 \) for all \( x \in \mathcal{X} \setminus \Gamma \). If the graph \((\mathcal{X}, W)\) is connected to \( \Gamma \), then

\[
\max_{x \in \mathcal{X}} u(x) = \max_{x \in \mathcal{X} \cap \Gamma} u(x).
\]

- If maximum occurs at \( x_0 \), mean value property implies

\[
u(x_0) \leq \frac{1}{d(x_0)} \sum_{y \in \mathcal{X}} w_{x_0,y} u(y) \leq \frac{1}{d(x_0)} \sum_{y \in \mathcal{X}} w_{x_0,y} u(x_0) = u(x_0)\]

- Thus if \( w_{x_0,y} > 0 \) then

\[u(x_0) = u(y)\]

- By connectedness, we can find a connected ‘path’ reaching the boundary.
Lemma 2

Let $u \in \ell^2(\mathcal{X})$ such that $Lu(x) > 0$ for all $x \in \mathcal{X} \setminus \Gamma$. Then

$$\max_{x \in \mathcal{X}} u(x) = \max_{x \in \mathcal{X} \cap \Gamma} u(x).$$

- Suppose $x_0 \in \mathcal{X}$ such that $u(x_0) = \max_{x \in \mathcal{X}} u(x)$.
- Then $u(x_0) \geq u(y)$ for each $y \in \mathcal{X}$ thus

$$Lu(x_0) = \sum_{y \in \mathcal{X}} w_{xy} (u(y) - u(x_0)) \leq 0$$

which means $x_0 \in \Gamma$. 
Setting: Random geometric graphs

- $U \subset \mathbb{R}^d$ is an open connected bounded domain
- $\rho : U \to [0, \infty)$ a continuous probability density function, satisfying
  \[ \alpha \leq \rho(x) \leq \alpha^{-1} \]
  for some $\alpha > 0$.
- $X_1, \cdots, X_n$ a sequence of i.i.d r.v distributed according to $\rho$.
- $\mathcal{X} = \{X_1, \cdots, X_n\}$ the set of vertices
- $\eta : [0, \infty) \to [0, \infty)$ smooth and nonincreasing, supported on $[0,1]$.
- $\eta_{\varepsilon}(t) = \frac{1}{\varepsilon^d} \eta(\frac{t}{\eta})$.
- $\sigma_\eta = \int_{\mathbb{R}^d} |z_1|^2 \eta(|z|) \, dz$ could be interpreted as surface tension
Setting: Random geometric graphs

- The weight is given by $w_{xy} = \eta \varepsilon (|x - y|)$.
- The inner product between functions is given by
  \[
  (u, v)_{\ell^2(\mathcal{X})} = \frac{1}{n} \sum_{x \in \mathcal{X}} u(x)v(x)
  \]
- The inner product between vector fields is given by
  \[
  (V, W)_{\ell^2(\mathcal{X}^2)} = \frac{1}{\sigma \eta n^2} \sum_{x, y \in \mathcal{X}} \eta \varepsilon (|x - y|) V(x, y) W(x, y).
  \]
- The gradient $\nabla_{n,\varepsilon} u$ and divergence $\text{div}_{n,\varepsilon} V$ are
  \[
  \nabla_{n,\varepsilon} u = \frac{1}{\varepsilon} (u(y) - u(x)), \quad \text{div}_{n,\varepsilon} V = \frac{2}{\sigma \eta n^2} \sum_{y \in \mathcal{X}} \eta \varepsilon (|x - y|) V(x, y).
  \]
Definition 3 (Unnormalized graph Laplacian)

The unnormalized graph Laplacian is

$$\mathcal{L}_{n,\varepsilon} u(x) = \frac{2}{\sigma \eta n \varepsilon^2} \sum_{y \in X} \eta(x-y)(u(y) - u(x)).$$

Its corresponding nonlocal operator is

$$L_{\varepsilon} u(x) = \frac{2}{\sigma \eta \varepsilon^2} \int_{U} \eta(x-y)(u(y) - u(x))\rho(y) \, dy$$

and the corresponding local operator is

$$\Delta_{\rho} u = \rho^{-1} \text{div}(\rho^2 \nabla u) = \rho \Delta u + 2 \nabla \rho \cdot \nabla u.$$
Definition 4 (Symmetric normalized graph Laplacian)

Let $D$ be the diagonal matrix with entries $D_{ii} = d(x_i)$. We define the symmetric normalized graph Laplacian by

$$\mathcal{N} = D^{-\frac{1}{2}} \mathcal{L}_{n, \varepsilon} D^{-\frac{1}{2}}.$$ 

Its continuum (local) counterpart is the operator

$$u \mapsto \frac{1}{\rho^\frac{3}{2}} \text{div} \left( \rho^2 \nabla \left( \frac{u}{\sqrt{\rho}} \right) \right).$$

This follows from the unnormalized case as

$$\mathcal{N} u(x) = \frac{1}{\sqrt{d(x)}} \mathcal{L}_{n, \varepsilon} \left( \frac{u}{\sqrt{d(x)}} \right)[3] \text{ and as } \varepsilon \to 0$$

$$\mathbb{E} d(x) = \int_U \eta_\varepsilon(|x - y|) \rho(y) \, dy \to \rho(x) \int \eta(|z|) \, dz.$$
Basic concentration inequalities

**Theorem 5 (Bernstein’s Inequality)**

Let $X_1, \cdots, X_n$ be a sequence of i.i.d. real valued r.v. with $\mathbb{E}[X_1] = \mu < \infty$, and $\sigma^2 = \text{Var}(X_i) < \infty$. Suppose $|X - \mu| \leq b$ almost surely. Letting $S_n = \frac{1}{n} \sum_{i=1}^{n} X_i$, we have for each $t > 0$

$$\mathbb{P}(S_n - \mu \geq t) \leq \exp \left( -\frac{nt^2}{2(\sigma^2 + \frac{1}{3}bt)} \right)$$

- Under the same assumptions, Hoeffding’s inequality states

  $$\mathbb{P}(S_n - \mu \geq t) \leq \exp \left( -\frac{nt^2}{2b^2} \right)$$

- For Graph Laplacians, the variance is usually small, so Bernstein’s inequality is preferred
Lemma 6 (Discrete to nonlocal)

Let $u : U \rightarrow \mathbb{R}$ be Lipschitz continuous, and $\varepsilon > 0$. Then for any $0 < \lambda \leq \varepsilon^{-1}$

$$\max_{x \in X} |\mathcal{L}_{n,\varepsilon} u(x) - \mathcal{L}_{\varepsilon} u(x)| \leq C \text{Lip}(u) \lambda$$

with probability at least $1 - C \exp(-cn\varepsilon^{d+2} \lambda^2 + \log(n))$.

Recall

$$\mathcal{L}_{n,\varepsilon} u(x) = \frac{2}{\sigma_\eta \varepsilon^2} \sum_{y \in X} \eta_\varepsilon(|x - y|)(u(y) - u(x))$$

and

$$\mathcal{L}_{\varepsilon} u(x) = \frac{2}{\sigma_\eta \varepsilon^2} \int_U \eta_\varepsilon(|x - y|)(u(y) - u(x))\rho(y) \, dy.$$
The proof is a direct application of Bernstein’s inequality. We first compute our $\mu, b, \sigma^2$

Fix $x \in U$ and let $Y_i = \eta_\varepsilon(|X_i - x|)(u(X_i) - u(x))$ such that

$$\mathcal{L}_{n, \varepsilon} u(x) = \frac{2}{\sigma \eta \varepsilon^2} \frac{1}{n} \sum_{i=1}^{n} Y_i.$$ 

Then our $\mu = \mathbb{E}[Y_i]$ is

$$\int_{U} \eta_\varepsilon(|y - x|)(u(y) - u(x))\rho(y)dy$$
Consistency: discrete to nonlocal

- Our $b$ is

$$|Y_i| = \eta_\varepsilon(|X_i - x|)|u(X_i) - u(x)| \leq \varepsilon^{-d} \|\eta\|_\infty \text{Lip}(u) \varepsilon = C \varepsilon^{1-d} \text{Lip}(u)$$

- Finally our $\sigma^2$ satisfies

$$\text{Var}(Y_i) \leq \mathbb{E}[Y_i^2] = \int_{B(x,\varepsilon) \cap U} \eta_\varepsilon(|x - y|)^2(u(y) - u(x))^2 \rho(y) \, dy$$

$$\leq \|\rho\|_\infty \text{Lip}(u)^2 \varepsilon^2 \int_{B(x,\varepsilon) \cap U} \varepsilon^{-2d} \eta(\varepsilon^{-1}|x - y|)^2 \, dy$$

$$\leq C \text{Lip}(u)^2 \varepsilon^2 \varepsilon^{-d} \int_{B(0,1)} \eta(|z|)^2 \, dz \leq C \text{Lip}(u)^2 \varepsilon^{2-d}$$

- Thus $bt \leq C \sigma^2$ when $t \leq C \text{Lip}(u) \varepsilon$
Consistency: discrete to nonlocal

- By Bernstein’s inequality, if $bt \leq C\sigma^2$

  $$\mathbb{P}\left(\left|\frac{1}{n}\sum_{i=1}^{n} Y_i - \mathbb{E}[Y_1]\right| \geq t\right) = \mathbb{P}\left(\left|\frac{2}{\sigma \eta \varepsilon^2} \frac{1}{n} \sum_{i=1}^{n} Y_i - \frac{2\mathbb{E}[Y_1]}{\sigma \eta \varepsilon^2}\right| \geq \frac{2t}{\sigma \eta \varepsilon^2}\right) \leq 2 \exp\left(-c \text{Lip}(u)^{-2} n\varepsilon^{d-2} t^2\right)$$

- Choose $t = \frac{\sigma \eta}{2} \text{Lip}(u) \varepsilon^2 \lambda$ for $\lambda \leq \varepsilon^{-1}$

- Finally, condition on $X_i = x$ then the union bound gives

  $$\mathbb{P}\left(\max_{x \in \mathcal{X}} |\mathcal{L}_{n,\varepsilon} u(x) - \mathcal{L}_{\varepsilon} u(x)| \geq C \text{Lip}(u) \lambda\right) \leq 2 \exp(-cn\varepsilon^{d+2} \lambda^2 + \log n)$$

- The above bound is meaningful when $\varepsilon^{d+2} \gg n^{-1}$
Lemma 7 (Consistency: nonlocal to local)

Let $\rho \in C^2(\bar{U})$. Then there exists $C > 0$ such that for all $u \in C^3(\bar{U})$ and $x \in U$ with $\text{dist}(x, \partial U) \geq \varepsilon$ we have

$$|L_\varepsilon u(x) - \Delta \rho u(x)| \leq C\|u\|_{C^3(U)}\varepsilon.$$

- Extension of the consistency up to the boundary can be found in Calder, Slepcěv, and Thorpe’20.[2]
Consistency: nonlocal to local

- $B(x, \varepsilon) \cap U = B(x, \varepsilon)$ as $\text{dist}(x, \partial U) \geq \varepsilon$. Changing variable to $z = \frac{x-y}{\varepsilon}$ gives

$$\mathcal{L}_\varepsilon u(x) = \frac{2}{\sigma \eta \varepsilon^2} \int_{B(0,1)} \eta(|z|)(u(x + z\varepsilon) - u(x))\rho(x + z\varepsilon) \, dz$$

- Let $\beta := \|u\|_{C^3(U)}$. Taylor expanding, we have

$$u(x + z\varepsilon) - u(x) = \nabla u(x) \cdot z\varepsilon + \frac{\varepsilon^2}{2} z^T \nabla^2 u(x) z + O(\beta \varepsilon^3)$$

$$\rho(x + z\varepsilon) = \rho(x) + \nabla \rho(x) + O(\varepsilon^2)$$

- Plugging in, we have

$$\mathcal{L}_\varepsilon u(x) = \frac{2}{\sigma \eta} \int_{B(0,1)} \eta(|z|) \left( \rho(x) \nabla u(x) \cdot z^{-1} + \frac{1}{2} \rho(x) z^T \nabla^2 u(x) z \right. \left. + (\nabla u(x) \cdot z)(\nabla \rho(x) \cdot z) \right) \, dz + O(\beta \varepsilon).$$
Consistency: nonlocal to local

- $z \mapsto \eta(|z|) \rho(x) \nabla u(x) \cdot z \varepsilon^{-1}$ is odd, so its integral vanishes. Hence

$$L_\varepsilon u(x) = \frac{2}{\sigma_\eta} \int_{B(0,1)} \eta(|z|) \left( \frac{1}{2} \rho(x) z^T \nabla^2 u(x) z 
+ (\nabla u(x) \cdot z)(\nabla \rho(x) \cdot z) \, dz \right) + O(\beta \varepsilon) =: I + J + O(\beta \varepsilon)$$

- By symmetry, $\int_{B(0,1)} \eta(|z|) z_i z_j \, dz = 0$ for $i \neq j$. Thus

$$I = \frac{1}{\sigma_\eta} \rho(x) \sum_{i, j=1}^d u_{x_i x_j}(x) \int_{B(0,1)} \eta(|z|) z_i z_j \, dz$$

$$= \frac{1}{\sigma_\eta} \rho(x) \sum_{i=1}^d u_{x_i x_i}(x) \int_{B(0,1)} \eta(|z|) z_i^2 \, dz = \rho(x) \Delta u(x).$$
Consistency: nonlocal to local

- Similarly

\[ J = \frac{2}{\sigma \eta} \rho(x) \sum_{i=1}^{d} u_{x_i}(x) \rho_{x_i}(x) \int_{B(0,1)} \eta(|z|) z_i^2 \, dz = 2 \nabla \rho(x) \cdot \nabla u(x). \]

- Finally, by product rule

\[
L_{\varepsilon} u(x) = \rho(x) \Delta u(x) + 2 \nabla \rho(x) \cdot \nabla u(x) + O(\beta \varepsilon) \\
= \rho^{-1} \text{div}(\rho^2(x) \nabla u(x)) + O(\varepsilon \| u \|_{C^3(\overline{U})})
\]

**Theorem 8 (Consistency of graph Laplacian)**

Let \( u \in C^3(\overline{U}), \rho \in C^2(\overline{U}) \). Then there exists \( C > 0 \) such that

\[
\max_{x \in \mathcal{X}} |L_{n,\varepsilon} u(x) - \Delta_{\rho} u(x)| \leq C(\lambda + \varepsilon) \| u \|_{C^3(\overline{U})}
\]

with probability at least \( 1 - C \exp(-cn\varepsilon^{d+2} \lambda^2 + \log(n)) \). 
Let $g : U \to \mathbb{R}$ be some Lipschitz function. We define the discrete boundary value problem

**(DBP)**

$\begin{cases}
\mathcal{L}_{n,\varepsilon} u(x) = 0 & \text{if } x \in \mathcal{X} \setminus \partial_{\varepsilon} U \\
u(x) = g(x) & \text{if } x \in \mathcal{X} \cap \partial_{\varepsilon} U
\end{cases}$

**(CBP)**

$\begin{cases}
\Delta_\rho u(x) = 0 & \text{if } x \in U \\
u(x) = g(x) & \text{if } x \in \partial U
\end{cases}$
Theorem 9 (Continuum limit of solutions to (DBP))

Let $\varepsilon \in (0, 1)$. Suppose $u_{n,\varepsilon} \in \ell^2(\mathcal{X})$, $u \in C^3(\overline{U})$ are solutions to (DBP) and (CBP) respectively. Then for any $\lambda \in (0, 1]$

$$\max_{x \in \mathcal{X}} |u_{n,\varepsilon}(x) - u(x)| \leq C\|u\|_{C^3(\overline{U})}(\lambda + \varepsilon)$$

(3)

with probability at least $1 - C \exp(-cn\varepsilon^d + 2\lambda^2 + \log(n))$. 
Let $\phi \in C^3(\overline{U})$ be the solution to

\[
\begin{align*}
-\Delta_\rho \phi &= 1 \text{ in } U \\
\phi &= 0 \text{ on } \partial U
\end{align*}
\]

(4)

- $\phi \geq 0$, as at its minimum $\Delta_\rho \phi(x) = \rho^{-1} \text{div}(\rho^2 \nabla \phi(x)) \geq 0$.
- Goal is to show that $|u_{n,\varepsilon}(x) - u(x)| \leq K\phi(x)$ for

$K = 3C_1 \|u\|_{C^3(\overline{U})}(\lambda + \varepsilon)$
Recall from the consistency results, that there exists some $C_1$ such that

$$\max_{x \in \mathcal{X} \setminus \partial \varepsilon U} |\mathcal{L}_{n,\varepsilon} \phi(x) + 1| \leq C_1 (\lambda + \varepsilon) \quad (5)$$

and

$$\max_{x \in \mathcal{X} \setminus \partial \varepsilon U} |\mathcal{L}_{n,\varepsilon} u(x)| \leq C_1 \|u\|_{C^3(U)} (\lambda + \varepsilon) \quad (6)$$

**Trivial case:** if $C_1 (\lambda + \varepsilon) \geq \frac{1}{2}$ then by the maximum principle

$$|u_{n,\varepsilon}(x) - u(x)| \leq 2 \|g\|_{\infty} \leq 4 C_1 (\lambda + \varepsilon) \|u\|_{C^3(U)}$$
Continuum limit of the solution to (DBP)

- **Main case:** suppose $C_1(\lambda + \varepsilon) \leq \frac{1}{2}$. Then $\mathcal{L}_{n,\varepsilon}\phi \leq -\frac{1}{2}$.

- Let $w = u - u_{n,\varepsilon} - K\phi$. Then on $\mathcal{X} \setminus \partial_\varepsilon U$

  $$\mathcal{L}_{n,\varepsilon}w(x) = \mathcal{L}_{n,\varepsilon}u(x) - \mathcal{L}_{n,\varepsilon}u_{n,\varepsilon}(x) - K\mathcal{L}_{n,\varepsilon}\phi(x)$$

  $$\geq \frac{K}{2} - C_1\|u\|_{C^3_3(U)}(\lambda + \varepsilon) > 0$$

  if

  $$K = 3C_1\|u\|_{C^3_3(U)}(\lambda + \varepsilon).$$

- Observe that for $x \in \mathcal{X} \cap \partial_\varepsilon U$

  $$|u_{n,\varepsilon}(x) - u(x)| \leq \text{Lip}(g)\varepsilon \leq \|u\|_{C^3_3(U)}\varepsilon$$

So, on the boundary $w \leq -K\phi + \|u\|_{C^3_3(U)}\varepsilon \leq \|u\|_{C^3_3(U)}\varepsilon$
The maximum principle applied to \( w \) we have \( w(x) \leq \| u \|_{C^3(U)} \varepsilon \) on \( X \). Thus \( \exists C > 0 \) such that

\[
\begin{align*}
   u(x) - u_{n,\varepsilon}(x) &\leq \| u \|_{C^3(U)} \varepsilon + K\phi(x) \\
   &= \| u \|_{C^3(U)} \varepsilon + 2C_1\| \phi \|_{\infty} \| u \|_{C^3(U)}(\lambda + \varepsilon) \\
   &=: C\| u \|_{C^3(U)}(\lambda + \varepsilon)
\end{align*}
\]

The same argument could be applied to \( w = u_{n,\varepsilon} - u - K\phi \) to get

\[
   u_{n,\varepsilon}(x) - u(x) \leq C\| u \|_{C^3(U)}(\lambda + \varepsilon)
\]

Theorem 10

Let $\mathcal{E}(u) = (\nabla u, \nabla u)_{\ell^2(\mathcal{X}^2)}$ and $\mathcal{A} = \{u \in \ell^2(\mathcal{X}) : u(x) = g(x) \text{ on } \Gamma\}$. Suppose $u \in \mathcal{A}$ satisfies

$$\mathcal{E}(u) = \min_{w \in \mathcal{A}} \mathcal{E}(w).$$

Then $u$ solves (DBP).

Let $u \in \mathcal{A}$ and $v \in \ell^2(\mathcal{X})$ such that $v = 0$ on $\Gamma$. Then

$$0 = \left. \frac{d}{dt} \right|_{t=0} \mathcal{E}(u + tv) = \left. \frac{d}{dt} \right|_{t=0} (-\mathcal{L}(u + tv), u + tv)_{\ell^2(\mathcal{X})}$$

$$= \left. \frac{d}{dt} \right|_{t=0} ((-\mathcal{L}u, u) + t(-\mathcal{L}u, v) + t(u, 0\mathcal{L}v) + t^2(-\mathcal{L}v, v))$$

$$= (-\mathcal{L}u, v) + (u, -\mathcal{L}v) = 2(-\mathcal{L}u, v).$$
Thank you!
References

