Graph Laplacians and their continuum limit

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October 6, 2020

Sangmin Park (CNA Working Group, CMU) Graph Laplacians and their continuum limit

- 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 X be the set of n vertices and W a n × n symmetric matrix with non-negative components. Let d(x) = ∑_{y∈X} w_{xy} be the degree of x.
- Let l²(X) denote the space of 'square summable functions'
 u : X → 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

$$(V_1, V_2)_{\ell^2(\mathcal{X}^2)} = \frac{1}{2} \sum_{x,y \in \mathcal{X}} w_{xy} V_1(x,y) V_2(x,y).$$

Calculus on graphs

• 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

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

• Then we have the divergence formula

$$(\nabla u, V)_{\ell^2(\mathcal{X}^2)} = -(u, \operatorname{div} V)_{\ell^2(\mathcal{X})}$$

Proof of the divergence formula

$$\begin{aligned} (\nabla u, V)_{\ell^2(\mathcal{X}^2)} &= \frac{1}{2} \sum_{x,y \in \mathcal{X}} w_{xy}(u(y) - u(x))V(x, y) \\ &= \frac{1}{2} \sum_{x,y \in \mathcal{X}} w_{xy}u(y)V(x, y) - \frac{1}{2} \sum_{x,y \in \mathcal{X}} W_{xy}u(x)V(x, y) \\ &= \frac{1}{2} \sum_{x,y \in \mathcal{X}} w_{xy}u(x)V(y, x) - \frac{1}{2} \sum_{x,y \in \mathcal{X}} W_{xy}u(x)V(x, y) \\ &= -\sum_{x,y \in \mathcal{X}} w_{xy}u(x)V(x, y) = -(u, \operatorname{div} V)_{\ell^2(\mathcal{X})} \end{aligned}$$

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Graph Laplacian

We define the graph Laplacian ${\mathcal L}$ by

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

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 $\ensuremath{\mathcal{L}}$ 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 $\mathcal{L}u(x) \ge 0$ for all $x \in \mathcal{X} \setminus \Gamma$. If the graph (\mathcal{X}, W) is connected to Γ , 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

$$u(x_0) \leq \frac{1}{d(x_0)} \sum_{y \in \mathcal{X}} w_{x_0y} u(y) \leq \frac{1}{d(x_0)} \sum_{y \in \mathcal{X}} w_{x_0y} u(x_0) = u(x_0).$$

• Thus if $w_{x_0y} > 0$ 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 $\mathcal{L}u(x) > 0$ 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 $u(x_0) \ge u(y)$ for each $y \in \mathcal{X}$ thus

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

which means $x_0 \in \Gamma$.

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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

$$\alpha \le \rho(\mathbf{x}) \le \alpha^{-1}$$

for some $\alpha > 0$.

- X_1, \dots, X_n a sequence of *i.i.d* r.v distributed according to ρ .
- $\mathcal{X} = \{X_1, \cdots, X_n\}$ the set of vertices
- η: [0,∞) → [0,∞) smooth and nonincreasing, supported on [0,1].
 η_ε(t) = ¹/_{ε^d}η(^t/_n).
- $\sigma_\eta = \int_{\mathbb{R}^d} |z_1|^2 \eta(|z|) \, dz$ 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 $abla_{n,\varepsilon} u$ and divergence $\operatorname{div}_{n,\varepsilon} V$ are

$$\nabla_{n,\varepsilon} u = \frac{1}{\varepsilon} (u(y) - u(x)), \quad \operatorname{div}_{n,\varepsilon} V = \frac{2}{\sigma_{\eta} n \varepsilon} \sum_{y \in \mathcal{X}} \eta_{\varepsilon} (|x - y|) V(x, y).$$

Unnormalized graph Laplacian

Definition 3 (Unnormalized graph Laplacian)

The unnormalized graph Laplacian is

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

Its corresponding nonlocal operator is

$$L_{\varepsilon}u(x) = \frac{2}{\sigma_{\eta}\varepsilon^2}\int_U \eta_{\varepsilon}(|x-y|)(u(y)-u(x))\rho(y)\,dy$$

and the corresponding local operator is

$$\Delta_{\rho} u = \rho^{-1} \operatorname{div}(\rho^2 \nabla u) = \rho \Delta u + 2 \nabla \rho \cdot \nabla u.$$

Symmetric normalized graph Laplacian

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

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

Its continuum (local) counterpart is the operator

$$u\mapsto rac{1}{
ho^{rac{3}{2}}}\operatorname{div}\left(
ho^2
abla\left(rac{u}{\sqrt{
ho}}
ight)
ight).$$

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] and as $\varepsilon \to 0$

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

Basic concentration inequalities

Theorem 5 (Bernstein's Inequality)

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

$$\mathbb{P}(S_n - \mu \ge t) \le \exp\left(-rac{nt^2}{2(\sigma^2 + rac{1}{3}bt)}
ight)$$

• Under the same assumptions, Hoeffding's inequality states

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

For Graph Laplacians, the variance is usually small, so Bernstein's inequality is preferred

Lemma 6 (Discrete to nonlocal)

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

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

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

Recall

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

and

$$\mathcal{L}_{\varepsilon}u(x) = rac{2}{\sigma_{\eta}\varepsilon^2}\int_U \eta_{\varepsilon}(|x-y|)(u(y)-u(x))\rho(y)\,dy.$$

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- The proof is a direct application of Bernstein's inequality. We first compute our μ, b, σ²
- 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

$$\int_U \eta_{\varepsilon}(|y-x|)(u(y)-u(x))\rho(y)dy$$

• Our *b* is

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

• Finally our σ^2 satisfies

$$\begin{aligned} \operatorname{Var}(Y_i) &\leq \mathbb{E}[Y_i^2] = \int_{B(x,\varepsilon)\cap U} \eta_{\varepsilon} (|x-y|)^2 (u(y) - u(x))^2 \rho(y) \, dy \\ &\leq \|\rho\|_{\infty} \operatorname{Lip}(u)^2 \varepsilon^2 \int_{B(x,\varepsilon)\cap U} \varepsilon^{-2d} \eta(\varepsilon^{-1}|x-y|)^2 \, dy \\ &\leq C \operatorname{Lip}(u)^2 \varepsilon^2 \varepsilon^{-d} \int_{B(0,1)} \eta(|z|)^2 \, dz \leq C \operatorname{Lip}(u)^2 \varepsilon^{2-d} \end{aligned}$$

• Thus $bt \leq C\sigma^2$ when $t \leq C Lip(u)\varepsilon$

• By Bernstein's inequality, if $bt \leq C\sigma^2$

$$\mathbb{P}\left(\left|\frac{1}{n}\sum_{i=1}^{n}Y_{i}-\mathbb{E}[Y_{1}]\right|\geq t\right)=\mathbb{P}\left(\left|\frac{2}{\sigma_{\eta}\varepsilon^{2}}\frac{1}{n}\sum_{i=1}^{n}Y_{i}-\frac{2\mathbb{E}[Y_{1}]}{\sigma_{\eta}\varepsilon^{2}}\right|\geq\frac{2t}{\sigma_{\eta}\varepsilon^{2}}\right)\\\leq2\exp\left(-c\,\operatorname{Lip}(u)^{-2}n\varepsilon^{d-2}t^{2}\right)$$

• Choose
$$t = rac{\sigma_\eta}{2} Lip(u) arepsilon^2 \lambda$$
 for $\lambda \leq arepsilon^{-1}$

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

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

 $\bullet\,$ The above bound is meaningful when $\varepsilon^{d+2}\gg n^{-1}$

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Lemma 7 (Consistency: nonlocal to local)

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

$$|\mathcal{L}_{\varepsilon}u(x) - \Delta_{\rho}u(x)| \leq C ||u||_{C^{3}(U)} \varepsilon.$$

• 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 dist $(x,\partial U) \ge \varepsilon$. 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 $\beta := \|u\|_{C^3(\overline{U})}$. 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

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

Consistency: nonlocal to local

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

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

• 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

$$\mathcal{L}_{\varepsilon}u(x) = \rho(x)\Delta u(x) + 2\nabla\rho(x)\cdot\nabla u(x) + O(\beta\varepsilon)$$
$$= \rho^{-1}\operatorname{div}(\rho^{2}(x)\nabla u(x)) + O(\varepsilon ||u||_{C^{3}(\overline{U})})$$

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

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

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) $\begin{cases}
\mathcal{L}_{n,\varepsilon}u(x) = 0 & \text{if } x \in \mathcal{X} \setminus \partial_{\varepsilon}U \\
u(x) = g(x) & \text{if } x \in \mathcal{X} \cap \partial_{\varepsilon}U
\end{cases}$ (1) • (CBP) $\begin{cases}
\Delta_{\rho}u(x) = 0 & \text{if } x \in U \\
u(x) = g(x) & \text{if } x \in \partial U
\end{cases}$ (2)

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 $\lambda \in (0,1]$

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

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

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Let $\phi \in C^3(\overline{U})$ be the solution to

$$\begin{cases} -\Delta_{\rho}\phi = 1 \text{ in } U \\ \phi = 0 \text{ on } \partial U \end{cases}$$
(4)

• $\phi \geq 0$, as at its minimum $\Delta_{
ho}\phi(x) =
ho^{-1}\operatorname{div}(
ho^2
abla \phi(x)) \geq 0.$

• Goal is to show that $|u_{n,arepsilon}(x)-u(x)|\leq K\phi(x)$ for

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

Recall from the consistency results, that there exists some C_1 such that

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

and

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

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

$$|u_{n,\varepsilon}(x) - u(x)| \le 2 \|g\|_{\infty} \le 4C_1(\lambda + \varepsilon) \|u\|_{C^3(\overline{U})}$$

• 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 $\mathcal{X} \setminus \partial_{\varepsilon} U$

$$egin{aligned} \mathcal{L}_{n,arepsilon} w(x) &= \mathcal{L}_{n,arepsilon} u(x) - \mathcal{L}_{n,arepsilon} u_{n,arepsilon}(x) - \mathcal{K} \mathcal{L}_{n,arepsilon} \phi(x) \ &\geq rac{\mathcal{K}}{2} - C_1 \| u \|_{C^3(U)} (\lambda + arepsilon) > 0 \end{aligned}$$

if

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

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

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

So, on the boundary $w \leq -K\phi + \|u\|_{C^{3}(\overline{U})}\varepsilon \leq \|u\|_{C^{3}(\overline{U})}\varepsilon$

• The maximum principle applied to w we have $w(x) \le ||u||_{C^3(\overline{U})} \varepsilon$ on \mathcal{X} . Thus $\exists C > 0$ such that

$$u(x) - u_{n,\varepsilon}(x) \le ||u||_{C^{3}(\overline{U})}\varepsilon + K\phi(x)$$

= $||u||_{C^{3}(\overline{U})}\varepsilon + 2C_{1}||\phi||_{\infty}||u||_{C^{3}(\overline{U})}(\lambda + \varepsilon)$
=: $C||u||_{C^{3}(\overline{U})}(\lambda + \varepsilon)$

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

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

Connection to the graph Dirichlet energy

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 Γ . Then

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

Conclusion

Thank you!

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