Lower Bound of the Discrete Green Energy - Elkies Lemma

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Green Functions

Definition

A Green function $\mathcal{G}(x, y)$ for a linear differential operator L is given as the distributional solution, unique modulo *kern*(L), to

$$L_x \mathcal{G}(x, y) = \delta_{x-y},$$

where δ_z is the Dirac Delta. Put differently, if we want to solve

$$Lu(x) = f(x)$$

we set

$$u(x) = \int f(y) \mathcal{G}(x, y) \, \mathrm{d}y.$$

*It follows that

$$Lu(x) = \int f(y) L_x \mathcal{G}(x, y) \, \mathrm{d}y = \int f(y) \delta_{x-y} \, \mathrm{d}y = f(x).$$

Why Green Energy?

Theorem (C. Beltrán, N. Corral, J. G. Criado Del Rey (2017))

Let (M, g) be a compact Riemannian manifold of dimension $n > 1$. Let G be its normalized Green function for the Laplace-Beltrami operator, then the unique probability measure μ minimizing

$$\iint_M G(x, y)\, \mathrm{d}\mu(x)\, \mathrm{d}\mu(y),$$

is the uniform measure λ (via normalized volume element) on M. Moreover the minimizing point set for the Green energy interpreted as counting measure converges weak-$*$ to λ.

*" *Discrete and continuous Green energy on compact manifolds*". Journal of Approximation Theory (2019).

One of our Main Results

Let

$$\mathcal{E}_G(N) := \inf_{\{\alpha_1,\dots,\alpha_N \in \ \mathcal{SO}(3)\}} \sum_{j \neq k} G(\alpha_j, \alpha_k).$$

Theorem (C. Beltrán, DF (2019))

The discrete energy for the normalized Green function of the Laplace–Beltrami operator on $SO(3)$ *satisfies for all* $N \in \mathbb{N}$*:*

$$-3\pi^{1/3} N^{4/3} + O(N) \ \leq \ \mathcal{E}_G(N),$$

and for $N = \mathcal{C}_{2L}^{(2)}(1)$*, the Gegenbauer polynomials of degree* $2L$*, for* $L \in \mathbb{N}$*:*

$$\mathcal{E}_G(N) \ \leq \ -4\left(\frac{3}{4}\right)^{4/3} N^{4/3} + O(N).$$

*"*Approximation to uniform distribution in SO(3)*". arXiv (2019).

Other Results

Theorem (C. Beltrán, DF (2019))

For $s \in (0,3)$ *and* $N = \binom{2L+3}{3}$ *for* $L \in \mathbb{N}$, *we have*

$$\mathcal{E}_R^s(N) \ \leq \ \frac{2}{8^{s/2}\pi}\mathcal{B}\left(\frac{3-s}{2}, \frac{1}{2}\right)N^2 + O(N^{1+s/3}).$$

If $s \in \{1,2\}$, *we have more information on the term* $O(N^{1+s/3})$: *It is*

$$-\frac{\sqrt{2}}{\pi}\left(\frac{3}{4}\right)^{4/3}N^{4/3} + O(N) \quad \textit{and} \quad -\frac{4}{15}\left(\frac{3}{4}\right)^{5/3}N^{5/3} + O(N^{4/3}).$$

Theorem (C. Beltrán, DF (2019))

Let $N = \binom{2L+3}{3}$ *for* $L \in \mathbb{N}$, *then the Riesz 3-energy satisfies*

$$\mathcal{E}_R^3(N) \ \leq \ \frac{N^2\log(N)}{12\sqrt{2}\pi} + \frac{3\gamma + \log(8^2\cdot 6) - \frac{21}{4}}{12\sqrt{2}\pi}N^2 + O(N^{5/3}\log(N)).$$

*" *Approximation to uniform distribution in SO(3)*". arXiv (2019).

$\mathcal{SO}(3)$

Definition

The special orthogonal group $\mathcal{SO}(3)$ is the compact (Lie) group of 3 by 3 orthogonal matrices over $\mathbb{R}$ that represent rotations in $\mathbb{R}^3$, i.e. with determinant equal to one.

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Definition (Rotation Angle Distance)

For $\alpha, \beta \in \mathcal{SO}(3)$, we set

$$\omega(\alpha^{-1}\beta) = \text{arccos}\left(\frac{\textbf{Trace}(\alpha^{-1}\beta) - 1}{2}\right).$$

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Lemma

If $f \in L^1(\mathcal{SO}(3))$ *such that* $\exists\ \tilde{f} \in L^1([0,\pi])$ *with* $f(x) = \tilde{f}(\omega(x))$*, then*

$$\int_{\mathcal{SO}(3)} f(x)\,\mathrm{d}\mu(x) = \frac{2}{\pi}\int_0^\pi \tilde{f}(t)\sin^2\left(\frac{t}{2}\right)\,\mathrm{d}t.$$

Fredholm Theory

Theorem

Given a compact Riemannian manifold (M, g), then a system of orthonormal eigenfunctions $\{\phi_k\}_{k=1}^{\infty}$ of the Laplacian on M with corresponding eigenvalues $\{\lambda_k\}_{k=1}^{\infty}$ forms a basis for the Hilbert space $L^2(M)$; "the" Green function is given by

$$\mathcal{G}(x, y) = \sum_{k \geq 1} \frac{\phi_k(x)\overline{\phi_k(y)}}{\lambda_k}$$

Reference?

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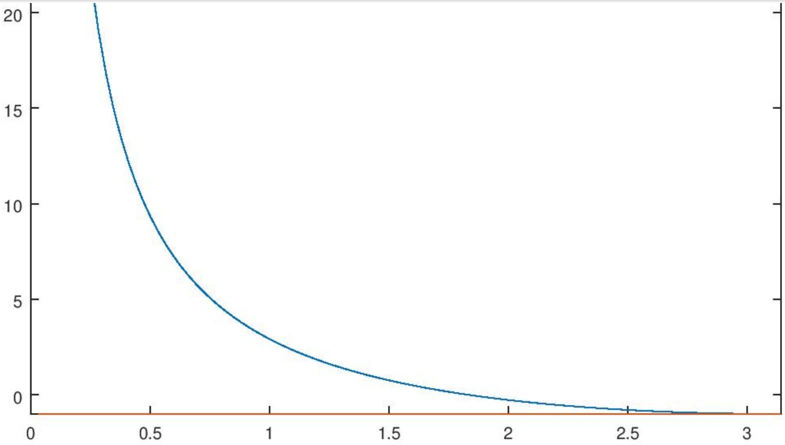
Lemma

The eigenvalues of Δ in $\mathcal{SO}(3)$ are $\lambda_\ell = \ell(\ell+1)$ for $\ell \geq 0$. Moreover, if H_ℓ is the eigenspace associated to λ_ℓ, then the dimension of H_ℓ is $(2\ell+1)^2$ and an orthonormal basis of H_ℓ is given by $\sqrt{2\ell+1}D^{\ell}_{m,n}$ where $-\ell \leq m, n \leq \ell$ and $D^{\ell}_{m,n}$ are Wigner's D–functions.

Lemma

The Green function for the Laplace-Beltrami operator on $\mathcal{SO}(3)$ *is*

$$\mathcal{G}(\alpha,\beta) = \left(\pi - \omega(\alpha^{-1}\beta)\right)\cot\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right) - 1.$$



Enter Determinantal Point Processes

We will have for any measurable function $f : M \times M \to [0, \infty]$,

$$\mathbb{E}\Big[\sum_{i \neq j} f(x_i, x_j)\Big] =$$

$$\iint_M f(x, y)\Big(\mathcal{K}_H(x, x)\mathcal{K}_H(y, y) - |\mathcal{K}_H(x, y)|^2\Big)\, \mathrm{d}\mu(x)\, \mathrm{d}\mu(y),$$

where $H \subseteq L^2(M)$ is any N–dimensional subspace in the set of square–integrable functions and $\mathcal{K}$ is the projection kernel onto H.

Let's Start Simple

A **simple point process** on a locally compact polish space Λ with reference measure μ is a positive Radon measure

$$\chi = \sum_{j=1} \delta_{x_j},$$

with $x_j \neq x_s$ for $j \neq s$. One usually identifies χ with a discrete subset of Λ. The **joint intensities** of χ w.r.t. μ, if they exist, are functions $\rho_k : \Lambda^k \to [0, \infty)$ for $k > 0$, such that for pairwise disjoint $\{D_s\}_{s=1}^k \subset \Lambda$

$$\mathbb{E}\left[\prod_{s=1}^k \chi(D_s)\right] = \int_{D_1 \times \ldots \times D_k} \rho_k(y_1, \ldots, y_k) \, \mathrm{d}\mu(y_1) \ldots \, \mathrm{d}\mu(y_k),$$

and $\rho_k(y_1, \ldots, y_k) = 0$ in case $y_j = y_s$ for some $j \neq s$.

Putting Determinant into Determinantal Point Processes

A simple point process is **determinantal** with kernel $\mathcal{K}$, iff for every $k \in \mathbb{N}$ and all y_j's

$$\rho_k(y_1, \ldots, y_k) = \det\Big(\mathcal{K}(y_j, y_s)\Big)_{1 \leq j,s \leq k}.$$

If the kernel is a projection kernel, then one speaks of a *determinantal projection process*. Hence if

$$\mathcal{K}(x, y) = \sum_{j=1}^{N} \phi_j(x)\bar{\phi}_j(y)$$

for some orthonormal system of ϕ_j's, then

$$\mathbb{E}\Big[\chi(\Lambda)\Big] = \int_\Lambda \mathcal{K}(y, y)\, \mathrm{d}\mu(y) = \sum_{j=1}^{N} \int_\Lambda |\phi_j(y)|^2\, \mathrm{d}\mu(y) = N.$$

It follows from the **Macchi–Soshnikov theorem** that a simple point process with N points, associated to the projection on a finite subspace exists in Λ.

L^2-Norm of Gegenbauer Polynomials of Index 2

Lemma

The Gegenbauer polynomials $\mathcal{C}_{n-2}^{(2)}(x)$ satisfy

$$\int_0^1 (x^2-1)\left[\mathcal{C}_{n-2}^{(2)}(x)\right]^2 \mathrm{d}x = -\frac{2n^2-1}{8}\int_0^1 \left[\mathcal{U}_{n-1}(x)\right]^2 \mathrm{d}x + \frac{n^2}{8}$$
$$= -\frac{2n^2-1}{16}\Big(\psi(n+\tfrac{1}{2})+\gamma+\log(4)\Big)+\frac{n^2}{8}.$$

Lemma

The Gegenbauer polynomials $\mathcal{C}_{n-2}^{(2)}(x)$ satisfy

$$\int_0^1 \left[\mathcal{C}_{n-2}^{(2)}(x)\right]^2 \mathrm{d}x = \frac{n^4}{16}+\frac{4n^2-1}{64}\Big(\psi(n+\tfrac{1}{2})+\gamma+\log(4)\Big)-\frac{5}{32}n^2.$$

The Backbone of the Lower Bound

By Fredholm theory and some further details:

$$\mathcal{G}(\alpha,\beta)=\sum_{\ell=1}^{\infty}\frac{2\ell+1}{\ell(\ell+1)}\mathcal{U}_{2\ell}\Big(\cos\big(\tfrac{\omega(\alpha^{-1}\beta)}{2}\big)\Big).$$

Next we define for $0<t\ll 1$:

$$\mathcal{G}_t(\alpha,\beta)=\sum_{\ell=1}^{\infty}e^{-\ell(\ell+1)t}\frac{2\ell+1}{\ell(\ell+1)}\mathcal{U}_{2\ell}\Big(\cos\big(\tfrac{\omega(\alpha^{-1}\beta)}{2}\big)\Big).$$

Lemma (N. Elkies)

For $t>0$ and $\alpha,\beta\in\ \mathcal{SO}(3)$, with $\alpha\neq\beta$ we have

$$\mathcal{G}(\alpha,\beta)\geq\mathcal{G}_t(\alpha,\beta)-t.$$

Elkies Lemma in Action

Lemma (N. Elkies)

For $t > 0$ and $\alpha, \beta \in \mathcal{SO}(3)$, with $\alpha \neq \beta$ we have

$$\mathcal{G}(\alpha, \beta) \geq \mathcal{G}_t(\alpha, \beta) - t.$$

For distinct points $\{\alpha_1, \ldots, \alpha_N\} \subset \mathcal{SO}(3)$:

$$\sum_{s \neq k}^{N} \mathcal{G}(\alpha_s, \alpha_k) + N(N-1)2t \geq \sum_{s \neq k}^{N} \mathcal{G}_{2t}(\alpha_s, \alpha_k)$$

$$= \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} \sum_{s \neq k}^{N} e^{-\ell(\ell+1)\cdot 2t} \mathcal{D}^{\ell}_{m,n}(\alpha_s) \overline{\mathcal{D}^{\ell}_{m,n}(\alpha_k)} =$$

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$$\sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell^2+\ell} \sum_{m,n=-\ell}^{\ell} \left(\left| \sum_{k=1}^{N} e^{-\ell(\ell+1)\cdot t} \mathcal{D}^{\ell}_{m,n}(\alpha_k) \right|^2 - \sum_{k=1}^{N} e^{-\ell(\ell+1)\cdot 2t} \left| \mathcal{D}^{\ell}_{m,n}(\alpha_k) \right|^2 \right)$$

$$\geq - \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)} \sum_{m,n=-\ell}^{\ell} \sum_{k=1}^{N} e^{-\ell(\ell+1)\cdot 2t} \left| \mathcal{D}^{\ell}_{m,n}(\alpha_k) \right|^2 = -N\mathcal{G}_{2t}(\alpha, \alpha).$$

Last Part of the Puzzle

After some lengthy calculation, we obtain

$$\mathcal{G}_t(\alpha, \alpha) = 2\sqrt{\frac{\pi}{t}} + O(1);$$

and by choosing $t = \frac{\sqrt[3]{\pi}}{2N^{2/3}}$:

$$\mathcal{G}_{2t}(\alpha, \alpha) = 2\sqrt[3]{\pi}N^{\frac{1}{3}} + O(1).$$

Hence

$$\sum_{s \neq k}^{N} \mathcal{G}(\alpha_s, \alpha_k) \geq -3\sqrt[3]{\pi}N^{\frac{4}{3}} + O(N),$$

proving the lower bound.

Strong Maximum Principle for Manifolds

Remember

$$\mathcal{G}_t(\alpha,\beta)=\sum_{\ell=1}^{\infty} e^{-\ell(\ell+1)t}\,\frac{2\ell+1}{\ell(\ell+1)}\mathcal{U}_{2\ell}\Big(\cos\big(\tfrac{\omega(\alpha^{-1}\beta)}{2}\big)\Big).$$

Theorem

Let (M,g) be an n-dimensional compact Riemannian manifold, not necessarily connected, with or without boundary.
Suppose $u\in\mathcal{C}^2_1(M\times(0,T))\cap\mathcal{C}(M\times[0,T])$ for $T>0$, satisfies

$$\Delta_g u(x,t)+\frac{\partial}{\partial t}u(x,t)=0;$$

if the maximum or minimum is attained at $(x_0,t_0)\in M\times(0,T]$, then $u(x,t)\equiv u(x_0,t_0)$ for all $(x,t)\in M_{x_0}\times[0,t_0]$.
The maximum/minimum is in particular attained at the boundary.

How to Prove Elkies Lemma I

Using the ONB, any smooth test function ϕ can be written as $\sum \lambda_\ell \phi_\ell$. Set

$$u(\alpha, t) := -\int_{\mathcal{SO}(3)} \partial_t \mathcal{G}_t(\alpha, \beta)\phi(\beta) \, \mathrm{d}\mu(\beta) = \sum_{\ell=1}^{\infty} e^{-\ell(\ell+1)\cdot t} \lambda_\ell \phi_\ell(\alpha),$$

obtaining, uniformly

$$\lim_{t \to 0} u(\alpha, t) = \phi(\alpha) - \int_{\mathcal{SO}(3)} \phi(\beta) \, \mathrm{d}\mu(\beta) = \phi(\alpha) - \lambda_0.$$

For $t > 0$ fixed, we can interchange differentiation and integration yielding

$$\Delta_g u(\alpha, t) + \partial_t u(\alpha, t) = 0.$$

By the strong maximum principle, we have for every $t > 0$:

$$\min_{\alpha \in \mathcal{SO}(3)} u(\alpha, t) \geq \min_{\alpha \in \mathcal{SO}(3)} u(\alpha, 0).$$

How to Prove Elkies Lemma II

The same PDE and estimates hold for

$$v(\alpha, t) = u(\alpha, t) + \lambda_0.$$

If $\phi \geq 0$, then $v(\alpha, t) \geq 0$ for all $t > 0$ by the maximum principle as $v(\alpha, 0) = \phi(\alpha)$. Hence

$$u(\alpha, t) = v(\alpha, t) - \lambda_0 \geq -\lambda_0 \quad \text{for } \phi \geq 0.$$

We further set

$$\mathcal{I}(\alpha, t) := \int_{\mathcal{SO}(3)} \mathcal{G}_t(\alpha, \beta)\phi(\beta)\, \mathrm{d}\mu(\beta) = \sum_{\ell=1}^{\infty} e^{-\ell(\ell+1)\cdot t} \frac{\lambda_\ell \phi_\ell(\alpha)}{\ell(\ell+1)}.$$

Differentiating term-wise for $t > 0$ yields

$$\partial_t \mathcal{I}(\alpha, t) = -\sum_{\ell=1}^{\infty} e^{-\ell(\ell+1)\cdot t} \lambda_\ell \phi_\ell(\alpha) = -u(\alpha, t) \leq \lambda_0 \quad \text{for } \phi \geq 0.$$

How to Prove Elkies Lemma III

Finally, for fixed α let $t > \epsilon > 0$, then

$$\lim_{\epsilon \to 0} \mathcal{I}(\alpha, t) - \mathcal{I}(\alpha, \epsilon) = \lim_{\epsilon \to 0} \int_{\epsilon}^{t} -u(\alpha, t) \, \mathrm{d}t \leq \lambda_0 \cdot t$$

and thus, for all non-negative test functions ϕ

$$\int_{\mathcal{SO}(3)} \Big(\mathcal{G}_t(\alpha, \beta) - \mathcal{G}(\alpha, \beta) - t \cdot 1 \Big) \phi(\beta) \, \mathrm{d}\mu(\beta) \leq 0.$$

Since $\mathcal{G}(\alpha, \beta)$ is continuous and locally integrable in β away of α, this proves the lemma.

Thank You for Your Attention

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