Bounds for the Green Energy on $\mathcal{SO}(3)$

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joint work with
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DOCTORAL PROGRAM DISCRETE MATHEMATICS
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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 to

$$L_x \mathcal{G}(x, y) = \delta_0(x - y);$$

or 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

$$Lu(x) = \int f(y) L_x \mathcal{G}(x, y) \, \mathrm{d}y = \int f(y) \delta_0(x - y) \, \mathrm{d}y = f(x).$$

f-Energies of N-Point Sets

Definition

Given a non-empty set X, $N \in \mathbb{N}$ and a function $f : X \times X \to \mathbb{R} \cup \{\pm\infty\}$; the (discrete) f-energy of X is given by

$$\mathcal{E}(f, N) = \inf_{\{x_1, \dots, x_N\} \subset X} \sum_{j \neq k}^{N} f(x_j, x_k).$$

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Example (Riesz potential)

Regard the unit sphere $S^2 \subset \mathbb{R}^3$ and for $s > 0$, let

$$f(x, y) = \frac{1}{\|x - y\|^s}.$$

For some $s < 0$ the problem also makes sense (Fejes-Toth potential). The case $s = 0$ sometimes refers to the logarithmic potential.

Why Care?

Theorem (Beltrán, Corral, Del Cray)

Let M be a compact Riemannian manifold of dimension $n > 1$ and let $\mathcal{G}$ be the (normalized) Green function for its Laplace-Beltrami operator. The unique probability measure minimizing the continuous Green energy

$$\mathcal{I}_{\mathcal{G}}[\mu] = \iint_M \mathcal{G}(x, y) \; \mathrm{d}\mu(x) \, \mathrm{d}\mu(y),$$

is the uniform measure on M.
Moreover, for each $N > 1$, let $w_N^* = \{x_1, \ldots, x_N\}$ be a set of minimizers for the Green energy, then

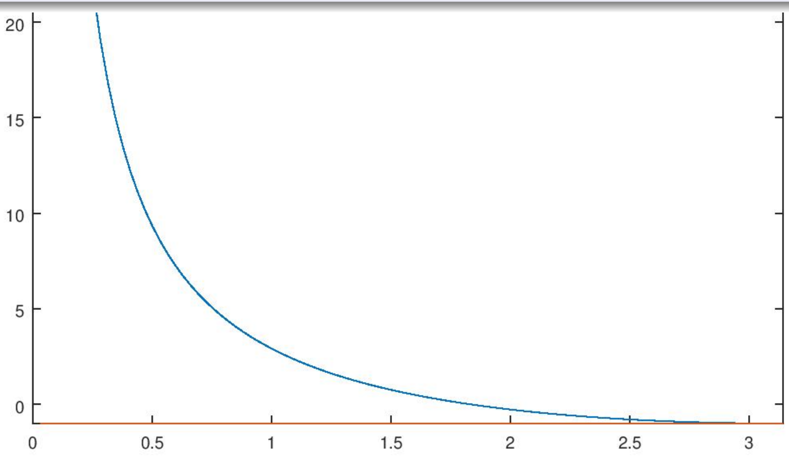
$$\frac{1}{N} \sum_{x \in w_N^*} \delta_x \xrightarrow{*} \lambda.$$

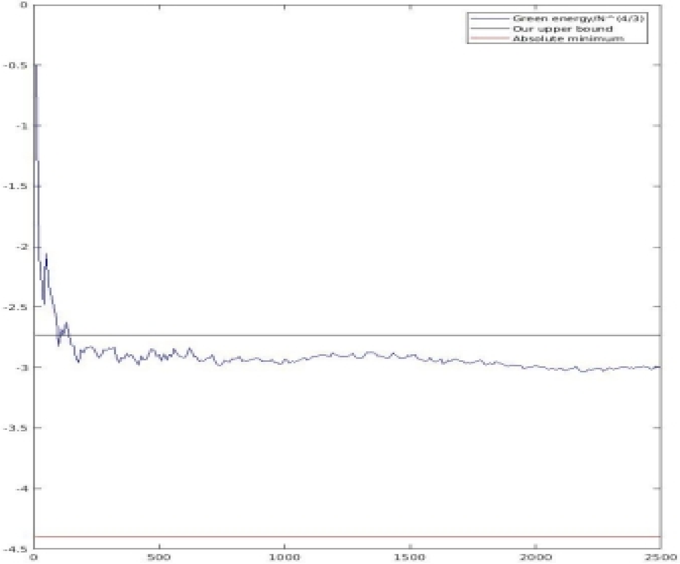
* "Discrete and Continuous Green Energy on Compact Manifolds" by C. Beltrn, N. Corral, and J. G. Criado Del Rey, (2017).

Lemma

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

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





Green energy/N^(4/3)
Our upper bound
Absolute minimum
0
-0.5
-1
-1.5
-2
-2.5
-3
-3.5
-4
-4.5
0
500
1000
1500
2000
2500

Enter Determinantal Point Processes

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

$$\mathbb{E}\left(\sum_{i \neq j} f(x_i, x_j)\right) = \iint_M f(x, y)\Big(\mathcal{K}_H(x, x)\mathcal{K}_H(y, y) - |\mathcal{K}_H(x, y)|^2\Big)\, \mathrm{d}\mu(x)\, \mathrm{d}\mu(y),$$

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

Let's Start Simple

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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

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

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

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

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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.

Class Functions and Integrals on $\mathcal{SO}(3)$

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 we are given a function $f \in L^1(\mathcal{SO}(3))$ such that we can find $\tilde{f} \in L^1([0,\pi])$ with $f(x) = \tilde{f}(\omega(x))$, then

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

*"Surface Spline Approximation on SO(3)" by T. Hangelbroek, D. Schmid; Appl. Comput. Harmon. Anal. Volume 31, Issue 2, 169-184 (2011).

Eigen- Values and Vectors for the Laplacian on $\mathcal{SO}(3)$

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.

It is known that

$$\sum_{m=-l}^{l} \sum_{n=-l}^{l} \mathcal{D}^l_{m,n}(\alpha)\overline{\mathcal{D}^l_{m,n}(\beta)} = \mathcal{U}_{2l}\Big(\cos\big(\tfrac{\omega(\alpha^{-1}\beta)}{2}\big)\Big),$$

where $\mathcal{U}_{2l}(x)$ is the Chebyshev polynomial of second kind.

Calculating the Projection Kernel for $\mathcal{SO}(3)$

Thus a projection kernel on the space $H_L = \oplus_{\ell=1}^{L} H_\ell$ is given by

$$\begin{aligned}
\mathcal{K}(\alpha,\beta) &= \sum_{l=0}^{L}(2l+1)\sum_{m=-l}^{l}\sum_{n=-l}^{l}\mathcal{D}_{m,n}^{l}(\alpha)\overline{\mathcal{D}_{m,n}^{l}(\beta)} \\
&= \sum_{l=0}^{L}(2l+1)\,\mathcal{U}_{2l}\Big(\cos\big(\tfrac{\omega(\alpha^{-1}\beta)}{2}\big)\Big) \\
&= \frac{d}{dx}\sum_{l=0}^{L}\ \mathcal{T}_{2l+1}(x)\Big|_{\cos(\ldots)} \\
&= \frac{d}{dx}\frac{1}{2}\mathcal{U}_{2L+1}(x)\Big|_{\cos(\ldots)} \\
&= \mathcal{C}_{2L}^{(2)}\Big(\cos\big(\tfrac{\omega(\alpha^{-1}\beta)}{2}\big)\Big).
\end{aligned}$$

Here, $\mathcal{C}_{2L}^{(2)}$, $L \geq 0$, is the sequence of Gegenbauer (ultraspherical) polynomials.

Series Representation of Green's Functions

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* $L^2(\ \mathcal{SO}(3))$*; "the" Green function is given by*

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

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

Lemma

The Green function for the Laplace-Beltrami operator on $\mathcal{SO}(3)$ can be written in terms of the metric ω:

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

An Upper Bound for the Green Energy

$$
\begin{aligned}
&\mathrm{E}\left(\sum_{i\neq j} f(x_i,x_j)\right)\\
&= \iint_M f(x,y)\Big(\mathcal{K}_H(x,x)\mathcal{K}_H(y,y) - |\mathcal{K}_H(x,y)|^2\Big)\,\mathrm{d}\mu(x)\,\mathrm{d}\mu(y)\\
&= \iint_{\mathcal{SO}(3)^2} \mathcal{G}(\alpha,\beta)\Big(\big[\mathcal{C}_{2L}^{(2)}(1)\big]^2 - \Big[\mathcal{C}_{2L}^{(2)}\Big(\cos\big(\tfrac{\omega(\alpha^{-1}\beta)}{2}\big)\Big)\Big]^2\Big)\,\mathrm{d}\mu(\alpha)\,\mathrm{d}\mu(\beta)\\
&= \int_{\mathcal{SO}(3)} \mathcal{G}(\alpha,1)\Big(\big[\mathcal{C}_{2L}^{(2)}(1)\big]^2 - \Big[\mathcal{C}_{2L}^{(2)}\Big(\cos\big(\tfrac{\omega(\alpha^{-1})}{2}\big)\Big)\Big]^2\Big)\,\mathrm{d}\mu(\alpha)\\
&= -\frac{2}{\pi}\int_0^\pi \Big((\pi-t)\cot(\tfrac{t}{2}) - 1\Big)\Big[\mathcal{C}_{2L}^{(2)}\Big(\cos\big(\tfrac{t}{2}\big)\Big)\Big]^2 \sin\left(\frac{t}{2}\right)^2\,\mathrm{d}t
\end{aligned}
$$

...some technicalities occur...

$$
= -4\left(\frac{3}{4}\right)^{\frac{4}{3}} N^{\frac{4}{3}} + O(N).
$$

Handling Technicalities

Lemma

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

$$\int_0^1 (x^2 - 1) \left[\mathcal{C}^{(2)}_{n-2}(x)\right]^2 \, \mathrm{d}x = \mathcal{O}(n^2 \log(n)).$$

Lemma

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

$$\int_0^1 \left[\mathcal{C}^{(2)}_{n-2}(x)\right]^2 \, \mathrm{d}x = \frac{n^4}{16} + \mathcal{O}(n^2 \log(n)).$$

Actually we have exact formulae.

A Lower Bound for the Green Energy

We define for $\alpha, \beta \in \mathcal{SO}(3)$ and $t > 0$:

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

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Lemma (N. Elkies)

For all $t > 0$ and $\alpha \neq \beta$ we have

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

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Lemma (N. Elkies)

For all $t > 0$ and $\alpha \neq \beta$ we have

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

Then for any collection of distinct points $\{\alpha_1, \ldots, \alpha_N\} \subset \mathcal{SO}(3)$

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

A Lower Bound for the Green Energy

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

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

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

A special choice for t yields

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

In Summary

Let $L \geq 0$ and let $H_L \subseteq L^2(\mathcal{SO}(3))$ be the span of the union of the eigenspaces of $\lambda_0, \ldots, \lambda_L$. Then, H_L has dimension

$$N = \dim(H_L) = \binom{2L+3}{3} = \mathcal{C}_{2L}^{(2)}(1) = \frac{(2L+3)(L+1)(2L+1)}{3}.$$

Theorem (Beltrán, F. (2018))

The minimal Green energy $\mathcal{E}(\mathcal{G}, N)$ in $\mathcal{SO}(3)$ for N as above satisfies

$$-3\sqrt[3]{\pi}N^{4/3} + O(N) \leq \mathcal{E}(\mathcal{G}, N) \leq -4\left(\frac{3}{4}\right)^{4/3} N^{4/3} + O(N).$$

The whole exposition can also be thought of as a blueprint for the same set of questions on various spaces.

Thank you for your Time

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