Approximate Separability of Green's Function for Helmholtz Equation in High Frequency Limit

Hongkai Zhao
University of California, Irvine

Joint work with Björn Engquist

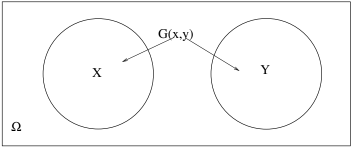
Approximate separability of Green's function

Green's function: given a linear differential operator L, $G(\mathbf{x}, \mathbf{y})$ is the fundamental solution to

$$\begin{cases} L_x G(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y}), & \mathbf{x}, \mathbf{y} \in \Omega \subseteq R^n \\ + \text{ boundary condition} \end{cases}$$

Approximate separability of $G(\mathbf{x}, \mathbf{y})$: given two domains $X, Y \subseteq \Omega \subset R^n$, $\forall \epsilon > 0$, there is a smallest N^ϵ s.t. there are $f_p(\mathbf{x}), g_p(\mathbf{y}), p = 1, 2, \ldots, N^\epsilon$

$$\left\| G(\mathbf{x}, \mathbf{y}) - \sum_{p=1}^{N^\epsilon} f_p(\mathbf{x}) g_p(\mathbf{y}) \right\|_{X \times Y} \leq \epsilon, \quad \mathbf{x} \in X, \mathbf{y} \in Y.$$



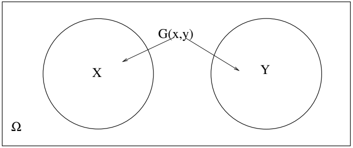
Approximate separability of Green's function

Green's function: given a linear differential operator L, $G(\mathbf{x},\mathbf{y})$ is the fundamental solution to

$$\begin{cases} L_x G(\mathbf{x},\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y}), \quad \mathbf{x},\mathbf{y} \in \Omega \subseteq R^n \\ + \text{ boundary condition} \end{cases}$$

Approximate separability of $G(\mathbf{x},\mathbf{y})$: given two domains $X, Y \subseteq \Omega \subset R^n$, $\forall \epsilon > 0$, there is a smallest N^ϵ s.t. there are $f_p(\mathbf{x}), g_p(\mathbf{y}), p = 1, 2, \ldots, N^\epsilon$

$$\left\| G(\mathbf{x},\mathbf{y}) - \sum_{p=1}^{N^\epsilon} f_p(\mathbf{x}) g_p(\mathbf{y}) \right\|_{X\times Y} \le \epsilon, \quad \mathbf{x} \in X, \mathbf{y} \in Y.$$



The key issue: How does N^ϵ depend on ϵ?

Implication of approximate separability

- The dependence of N^ϵ on ϵ manifests the complexity of the PDE within ϵ-approximation

$$L_x u = h \;\Rightarrow\; u(\mathbf{x}) = \int_\Omega G(\mathbf{x},\mathbf{y})h(\mathbf{y})d\mathbf{y} \approx \sum_{p=1}^{N^\epsilon} f_p(\mathbf{x}) \int_\Omega g_p(\mathbf{y})h(\mathbf{y})d\mathbf{y}$$

- View $G(\mathbf{x},\mathbf{y})$ as a family of functions on X parametrized by $\mathbf{y} \in Y$, the Kolmogorov n-width [1] is ϵ when $n = N^\epsilon$.

$$d(G(\cdot,\mathbf{y}), L_n) \le \epsilon,\; \mathbf{y} \in Y, \qquad L_n = span\{f_p(\cdot)\}_{p=1}^{N^\epsilon}$$

[1] Let W be a set in a normed space S, the Kolmogorov n-width $d_n(W,S)$ is

$$d_n(W,S) := \inf_{L_n} d(W, L_n)$$

where $L_n \subset S$ is a linear subspace of dimension n

Importance for developing fast algorithms

High separability $\Rightarrow$ existence of low rank approximation for the discretized system which is crucial for developing fast numerical algorithms.

- Fast (dense) matrix vector multiplication, e.g., for fast multipole methods, boundary integral methods, Fourier integral operators, ...
- $$Lu = f \quad \overset{\text{after discretization}}{\Longrightarrow} \quad Ax = b$$

  Each columns of A^{-1} is a numerical approximation of Green's function. Low rank structure for off-diagonal submatrices of A^{-1} can be explored to develop efficient numerical for solving the linear system such as hierarchical matrix method and structured inverse method.

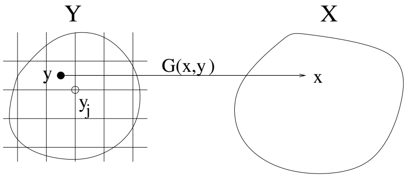
Some intuition for approximate separability

- X, Y are separated and compact, $G(\mathbf{x}, \mathbf{y})$ is continuous. There exist polynomial approximations by Weierstrass Theorem.
- Fourier series type of expansion of $G(\mathbf{x}, \mathbf{y})$.
- X, Y are separated and compact, $\dim(X) \geq \dim(Y) = d$. If $G(\mathbf{x}, \mathbf{y})$ is $C^m(X \times Y)$

$$N^\epsilon \leq O(\epsilon^{-\frac{d}{m}})$$

Proof: Lay down a grid $\mathbf{y}_j, j = 1, 2, \ldots J = O(\epsilon^{-\frac{d}{m}})$ with grid size $h = O(\epsilon^{\frac{1}{m}})$. Use interpolation of $m-1$ order.

$$|G(\mathbf{x}, \mathbf{y}) - \sum a_j(\mathbf{y}) G(\mathbf{x}, \mathbf{y}_j)| \leq C \| D_y^m G(\mathbf{x}, \mathbf{y}) \| h^m$$



Previous work on approximate separability

Mostly about showing upper bounds $N^{\epsilon} \leq O(|\log \epsilon|^q)$ for high separable cases due to regularity or special setup of X, Y.

- Construct separable approximation using explicit expression of $G(\mathbf{x}, \mathbf{y})$ and asymptotic expansions with fast convergence.
- M. Bebendorf and W. Hackbusch'03 proved approximate separability in L_2 norm for Green's function of strict elliptic operator with L^{∞} coefficients, $Lu = \sum \partial_j (c_{ij} \partial_i u)$ ($+$ low order perturbation), on two separated compact sets X, Y

  $$N_{\epsilon} \leq C |\log \epsilon|^{d+1}$$

  Key estimate: Caccioppoli inequality for $\|\nabla u\|_2$ in term of $\|u\|_2$ on a little larger domain.
- Chandrasekaran'10 et al showed low rank estimate for off-diagonal blocks of matrices after finite difference discretization of elliptic operator.

Helmholtz equation in high frequency limit

Helmholtz equation (HE):

$$\Delta_x G(\mathbf{x}, \mathbf{y}) + k^2 n^2(\mathbf{x}) G(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y}) \quad + \text{ b.c.}$$

Free space ($n(\mathbf{x}) \equiv 1$) Green's function,

$$G_0(\mathbf{x}, \mathbf{y}) = \frac{1}{4\pi} \frac{e^{ik|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x} - \mathbf{y}|}$$

In high frequency regime, $k \gg 1$, HE is notoriously difficult to solve numerically.

- Solution is highly oscillatory $\Rightarrow$ derivatives are unbounded a.e. as $k \to \infty$.
- Singularity propagates along rays.
- Fine grids and large degrees of freedom are needed.
- The discretized system is indefinite. No effective iterative solvers.

Our main results

We give a sharp lower bound for the approximate separability for Green's function of the HE in high frequency limit

$$N_k^\epsilon \geq O(k^\rho), \quad \rho = \rho(d, X, Y) > 0, \quad \text{as } k \to \infty.$$

which characterizes intrinsic complexity for high frequency waves mathematically.
Key ideas:

- a geometric characterization of the relation between two Green's functions with sources separated in term of wavelength,

$$\left| < \hat{G}(\cdot, \mathbf{y}_1), \hat{G}(\cdot, \mathbf{y}_2) > \right| \lesssim (k|\mathbf{y}_1 - \mathbf{y}_2|)^{-\alpha}, \quad \alpha = \alpha(d, X, Y) > 0$$

  where $\quad \hat{G}(\mathbf{x}, \mathbf{y}) = \frac{G(\mathbf{x},\mathbf{y})}{\|G(\cdot,\mathbf{y})\|_{2(X)}}$.

- a sharp dimension estimate for approximating a set of almost orthogonal vectors

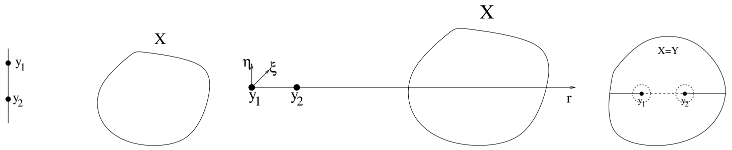
Almost orthogonality between two Green's functions

Theorem 1

Assume $X \subset R^n, n = 2, 3$ is a compact domain with piecewise smooth boundary. Depending on the positions of $\mathbf{y}_1, \mathbf{y}_2$ relative to X and its boundary, there is some $\alpha > 0$ such that

$$\left| < \hat{G}_0(\cdot, \mathbf{y}_1), \hat{G}_0(\cdot, \mathbf{y}_2) > \right| \lesssim (k|\mathbf{y}_1 - \mathbf{y}_2|)^{-\alpha}, \quad \min\{1, \frac{n-1}{2}\} \leq \alpha \leq \frac{n+1}{2}$$

as $k|\mathbf{y}_1 - \mathbf{y}_2| \to \infty$, where $\hat{G}_0(\mathbf{x}, \mathbf{y}) = \frac{G_0(\mathbf{x},\mathbf{y})}{\|G_0(\cdot,\mathbf{y})\|_{2(X)}}, \mathbf{x} \in X$.



case 1 case 2 case 3

Sketch of Proof

Case 1: no stationary point in X.

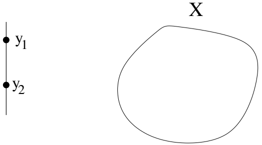
$$\tilde{k} = k|\mathbf{y}_1 - \mathbf{y}_2|, \quad \phi(\mathbf{x}) = |\mathbf{y}_1 - \mathbf{y}_2|^{-1}(|\mathbf{x} - \mathbf{y}_1| - |\mathbf{x} - \mathbf{y}_2|), \quad u(\mathbf{x}) = \frac{1}{|\mathbf{x}-\mathbf{y}_1||\mathbf{x}-\mathbf{y}_2|}$$

$\Rightarrow$

$$< \hat{G}_0(\cdot, \mathbf{y}_1), \hat{G}_0(\cdot, \mathbf{y}_2) >= \int_X e^{i\tilde{k}\phi(\mathbf{x})} u(\mathbf{x}) d\mathbf{x}$$

$$= O(\tilde{k}^{-\alpha}), \quad 1 \leq \alpha \leq \frac{n+1}{2}$$

by integration by part and using stationary phase theory to the boundary integral on ∂X.



Sketch of Proof (continued)

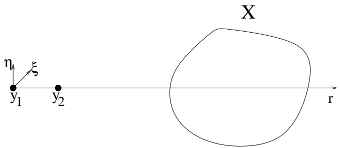
Case 2: all points on the line $l_{\mathbf{y}_1}^{\mathbf{y}_2}$ and inside X are stationary points.

$$< \hat{G}_0(\cdot, \mathbf{y}_1), \hat{G}_0(\cdot, \mathbf{y}_2) >= \int_{r_1}^{r_2} \int_{(\xi,\eta)} e^{i\tilde{k}\phi(r,\xi,\eta)} u(r,\xi,\eta) d\xi d\eta dr$$

$$= \int_{r_1}^{r_2} 2\pi i \tilde{k}^{-1} e^{i\tilde{k}} u(r,0,0)[1 + O(\tilde{k}^{-1})] dr \lesssim \tilde{k}^{-\frac{n-1}{2}}$$

by using stationary phase on $\xi - \eta$ plane for each r, since

$$\phi(r,0,0) = 1, \quad D^2_{\xi\eta}\phi(r,0,0) = \frac{1}{r(|\mathbf{y}_1 - \mathbf{y}_2| + r)} I,$$



Sketch of Proof (continued)

Case 3: $\mathbf{y}_1, \mathbf{y}_2$ are inside X. Main contributions come from stationary line and singularity. Let $I(k) = \int e^{ik\phi(\mathbf{x})}u(\mathbf{x})$, by applying a general stationary phase result

$$|I(k) - (\tfrac{2\pi}{k})^{d/2}\sum_{m=1}^{M}\frac{e^{ik\phi(\mathbf{x}_m)}}{|\det[D^2\phi(\mathbf{x}_m)]|^{1/2}}e^{\frac{i\pi}{4}\mathrm{sgn}(D^2\phi(\mathbf{x}_m))}u(\mathbf{x}_m)|$$

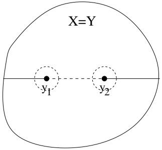
$$\leq Ck^{-d/2-1}|\det[D^2\phi(\mathbf{x}_m)]|^{-1/2}\|[D^2\phi(\mathbf{x}_m)]^{-1}\|\sum_{\beta\leq s+2}\|D^\beta u\|_{L^2},$$

where $s > d/2$ and C is a universal constant, to

$$\int_{\partial B(\mathbf{y}_1,r)} e^{i\tilde{k}\phi(\mathbf{x})}u(\mathbf{x})$$

$$= 2\pi i r^2\tilde{k}^{-\frac{n-1}{2}}[-e^{i\tilde{k}}u(r,\theta,0) + \frac{e^{i\tilde{k}|\mathbf{y}_1-\mathbf{y}_2|^{-1}(2r-|\mathbf{y}_1-\mathbf{y}_2|)}u(r,\theta,\pi)}{|\mathbf{y}_1-\mathbf{y}_2|-2r}] + O(\tilde{k}^{-\frac{n+1}{2}}r)$$

$$\Rightarrow \int_X e^{i\tilde{k}\phi(\mathbf{x})}u(\mathbf{x})d\mathbf{x} = \int_0^{r_0}\int_{\partial B(\mathbf{y}_1,r)} e^{i\tilde{k}\phi(\mathbf{x})}u(\mathbf{x})dsdr \lesssim \tilde{k}^{-\frac{n-1}{2}}$$



2D case

Green's function for 2D in free space is

$$G_0(\mathbf{x},\mathbf{y}) = -\frac{i}{4}H_0^{(1)}(k|\mathbf{x}-\mathbf{y}|) = -\frac{1}{2\pi}\int_0^{\infty} e^{ik|\mathbf{x}-\mathbf{y}|\cosh\theta}d\theta,$$

where $H_0^{(1)}(r)$ is the Hankel function which has the following asymptotic behavior

$$\lim_{r\to 0^+} H_0^{(1)}(r) = \frac{2i}{\pi}\log r,$$

and

$$H_0^{(1)}(r) = \sqrt{\tfrac{2}{\pi r}}\left[1 - \tfrac{8i}{r} - \tfrac{9}{128r^2} + \cdots + \tfrac{[(2n-1)!!]^2}{(8i)^n n!}\tfrac{1}{r^n} + \cdots\right] e^{i(r-\pi/4)}$$

$$= \sqrt{\tfrac{2}{\pi r}}e^{i(r-\pi/4)} + O(r^{-3/2}), \quad \text{if} \quad r \gg 1.$$

Green's function in heterogeneous medium

Use geometric optics ansatz $G(\mathbf{x},\mathbf{y}) = e^{ik\phi(\mathbf{x},\mathbf{y})}\sum_{m=0}^{\infty} a_m(\mathbf{x},\mathbf{y})(ik)^{-m}$.

$$< \hat{G}(\cdot,\mathbf{y}_1), \hat{G}(\cdot,\mathbf{y}_2) >= \int_X e^{i\tilde{k}\phi(\mathbf{x})} u(\mathbf{x}) d\mathbf{x} + O(k^{-(M+1)}),$$

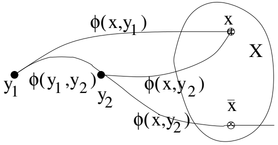
where

$$\tilde{k} = k\phi(\mathbf{y}_1,\mathbf{y}_2), \quad \phi(\mathbf{x}) = \phi^{-1}(\mathbf{y}_1,\mathbf{y}_2)(\phi(\mathbf{x},\mathbf{y}_1) - \phi(\mathbf{x},\mathbf{y}_2)).$$

If rays do not cross, i.e., no caustics, $\phi(\mathbf{x},\mathbf{y})$ is the shortest travel time along the unique ray connecting $\mathbf{x},\mathbf{y}$.

$$|\phi(\mathbf{x},\mathbf{y}_1) - \phi(\mathbf{x},\mathbf{y}_2)| \leq \phi(\mathbf{y}_2,\mathbf{y}_1)$$

The phase function $\phi(\mathbf{x};\mathbf{y}_1,\mathbf{y}_2)$ attains the global maximum or minimum ± 1 on the the ray $\Gamma_{\mathbf{y}_1}^{\mathbf{y}_2}$ outside the interval between $\mathbf{y}_1$ and $\mathbf{y}_2$.



Embedding a set of almost orthogonal unit vectors

The question: the minimum dimension d of a linear subspace that can contain a set of almost orthogonal unit vectors $\hat{\mathbf{v}}_n \in R^m, n = 1, 2, \ldots, N$.
Define $A = (a_{ij})_{n\times n}, \ a_{ij} =< \hat{v}_i, \hat{v}_j >$. Then $a_{ii} = 1, \ |a_{ij}| < \epsilon, i \neq j$, one has the following results (N. Alon'03).

$$d = rank(A) \geq \frac{N}{1 + (N-1)\epsilon^2}$$

Proof: Let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d > \lambda_{d+1} = \ldots = \lambda_N = 0$ be the eigenvalues of A.

$$N^2/d = d\left(\frac{\sum_{n=1}^N \lambda_n}{d}\right)^2 \leq \sum_{n=1}^N \lambda_n^2 = tr(A^T A) = \sum_{i,j=1}^N a_{ij}^2 \leq N + N(N-1)\epsilon^2.$$

If $|a_{ij}| < \epsilon, i \neq j$ for $\frac{1}{\sqrt{N}} \leq \epsilon < \frac{1}{2}$, then

$$d \gtrsim \frac{1}{\epsilon^2 |\log \epsilon|} \log N$$

- The above estimate shows sharpness of Johnson-Lindenstrauss Lemma.
- Direct application of the above results to our problem (1) renders suboptimal bounds, and (2) can not deal with approximate separability.

Approximation of a set of vectors

Denote $V = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N]$ and $A = [a_{mn}]_{N\times N} = V^T V$. Let $\lambda_1^2 \geq \ldots \geq \lambda_N^2$ be the eigenvalues of A, then

$$tr(A) = \sum_{m=1}^N \lambda_m^2 = \sum_m^N \|\mathbf{v}_m\|_2^2$$

$$\sum_m^N \|\mathbf{v}_m - P_{\overline{S}_l}\mathbf{v}_m\|_2^2 = \min_{S_l, \dim(S_l)=l} \sum_m^N \|\mathbf{v}_m - P_{S_l}\mathbf{v}_m\|_2^2 = \sum_{m=l+1}^N \lambda_m^2,$$

where $P_{S_l}\mathbf{v}$ denotes projection of $\mathbf{v}$ in S_l.

Def. Given $1 \geq \epsilon > 0$, $\underline{N}^\epsilon = \min M,\ s.t.\ \sum_{m=M+1}^N \lambda_m^2 \leq \epsilon^2 \sum_{m=1}^N \lambda_m^2$.

Assume $0 < c < \|\mathbf{v}_m\|_2 < C < \infty, \forall m$, if a linear subspace S^ϵ satisfies

$$\sqrt{\frac{\sum_m^N \|\mathbf{v}_m - P_{S^\epsilon}\mathbf{v}_m\|_2^2}{N}} \leq c\epsilon \quad \Rightarrow \frac{\sum_m^N \|\mathbf{v}_m - P_{S^\epsilon}\mathbf{v}_m\|_2^2}{\sum_m^N \|\mathbf{v}_m\|_2^2} \leq \epsilon^2$$

then $\dim(S^\epsilon) \geq N^\epsilon$.

Approximation of a set of Green's function as $k \to \infty$

Lemma 2 (key lemma)

Let X, Y be two compact manifolds in R^n and $\dim(X) \geq \dim(Y) = d$. For $\mathbf{y}_1, \mathbf{y}_2 \in Y$, assume

$$|< \hat{G}(\cdot, \mathbf{y}_1), \hat{G}(\cdot, \mathbf{y}_2) >| \lesssim (k|\mathbf{y}_1 - \mathbf{y}_2|)^{-\alpha} \quad \text{as } k|\mathbf{y}_1 - \mathbf{y}_2| \to \infty$$

there are points $\mathbf{y}_m \in Y, m = 1, 2, \ldots, N_\beta^d = O(k^{d\beta})$, such that for the set of Green's functions $\{G(\mathbf{x}, \mathbf{y}_m)\}_{m=1}^{N_\beta^d} \subset L_2(X)$ and matrix $A =< G(\cdot, \mathbf{y}_m), G(\cdot, \mathbf{y}_n) >$

$$\underline{N}_k^\epsilon \gtrsim \begin{cases} (1-\epsilon^2)^2 k^{2\alpha}, & \alpha < \frac{d}{2}, \\ (1-\epsilon^2)^2 k^{d\beta}, & \alpha \geq \frac{d}{2}, \end{cases} \quad \text{as } k \to \infty.$$

for any $\beta < 1$ and arbitrary close to 1,

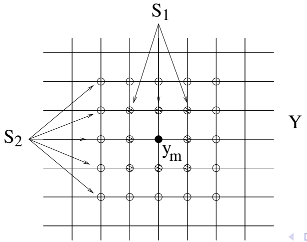
Sketch of proof

Lay down a uniform grid $\mathbf{y}_m, m = 1, 2, \ldots, n_k^h = O(k^{d\beta})$ with grid size $h = k^{-\beta}, 0 < \beta < 1$. Let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{n_k^h} \geq 0$ be the eigenvalues of $A =< \hat{G}(\cdot, \mathbf{y}_m), \hat{G}(\cdot, \mathbf{y}_n) >$.

$$\underline{N}_k^\epsilon = \min M, \ s.t. \ \sum_{m=M+1}^{n_k^h} \lambda_m \leq \epsilon^2 \sum_{m=1}^{n_k^h} \lambda_m = \epsilon^2 n_k^h$$

For each $\mathbf{y}_m$, divide all other points into 1st square neighbors, 2nd square neighbors, ..., j-th square neighbors S_j centered at $\mathbf{y}_m$ with length $2jh$, $j = 1, 2, \ldots, J = O(h^{-1} = k^\beta)$. Each S_j contains at most $8j$ grid points.

$$\Rightarrow a_{m,n_j} \lesssim (kjh)^{-\alpha} = j^{-\alpha} k^{\alpha(\beta-1)}, \quad \mathbf{y}_{n_j} \in S_j.$$



Sketch of the proof

Let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{n_k^h} \geq 0$ be the eigenvalues of A. $n_k^h = O(k^{d\beta})$.
key inequality:

$$\sum_{m=1}^{n_k^h} \sum_{n=1}^{n_k^h} a_{mn}^2 = tr(A^T A) = \sum_{m=1}^{n_k^h} \lambda_m^2 > \sum_{m=1}^{\underline{N}_k^\epsilon} \lambda_m^2 \geq \underline{N}_k^\epsilon \left[\frac{(1-\epsilon^2) n_k^h}{\underline{N}_k^\epsilon} \right]^2 = \frac{[(1-\epsilon^2) n_k^h]^2}{\underline{N}_k^\epsilon}$$

key estimate:
sum of each row

$$\sum_{n=1}^{n_k^h} a_{mn}^2 = 1 + \sum_{j=1}^{J} \sum_{n_j} a_{m,n_j}^2 = \begin{cases} O(k^{d\beta - 2\alpha}) & \alpha < \frac{d}{2} \\ O(1) & \alpha \geq \frac{d}{2} \end{cases}$$

for β arbitrary close to 1

$$\Rightarrow \sum_{m=1}^{n_k^h} \sum_{n=1}^{n_k^h} a_{mn}^2 = \begin{cases} O(k^{2(d\beta - \alpha)}) & \alpha < \frac{d}{d} \\ O(k^{d\beta}) & \alpha \geq \frac{d}{2} \end{cases} \Rightarrow \underline{N}_k^\epsilon \gtrsim \begin{cases} (1-\epsilon^2)^2 k^{2\alpha} & \alpha < \frac{d}{2} \\ (1-\epsilon^2)^2 k^{d\beta} & \alpha \geq \frac{d}{2} \end{cases}$$

Lower bound estimate for approximate separability

Theorem 3 (main theorem)

Let X, Y be two compact manifolds in R^n and $\dim(X) \geq \dim(Y) = d$. *For* $\mathbf{y}_1, \mathbf{y}_2 \in Y$, *assume*

$$|<\hat{G}(\cdot, \mathbf{y}_1), \hat{G}(\cdot, \mathbf{y}_2)>| \lesssim (k|\mathbf{y}_1 - \mathbf{y}_2|)^{-\alpha}, \quad \textit{as } k|\mathbf{y}_1 - \mathbf{y}_2| \to \infty.$$

If there are $f_p(\mathbf{x}) \in L_2(X), g_p(\mathbf{y}) \in L_2(Y), p = 1, 2, \ldots, N_k^\epsilon$ *such that*

$$\left\| G(\mathbf{x}, \mathbf{y}) - \sum_{p=1}^{N_k^\epsilon} f_p(\mathbf{x}) g_p(\mathbf{y}) \right\|_{L_2(X \times Y)} \leq \epsilon,$$

then

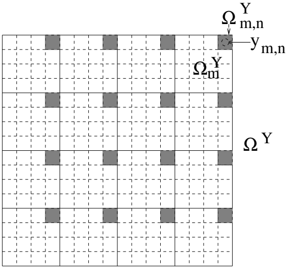
$$N_k^\epsilon \geq \begin{cases} c_\epsilon k^{2\alpha}, & \alpha < \frac{d}{2}, \\ c_\epsilon k^{d\beta}, & \alpha \geq \frac{d}{2}, \end{cases} \quad \textit{as } k \to \infty$$

for any $\beta < 1$ *and arbitrary close to 1, where* $c_\epsilon \geq c(1 - (C\epsilon)^2)^2$ *for some positive constants c and C that only depend on X, Y and* $n(\mathbf{x})$.

Sketch of the proof

Lay down a two scale grid with coarse cell Ω_m^Y, $m = 1, 2, \ldots N_k^{\overline{h}} = O(k^{d\beta})$ of size $\overline{h} = k^{-\beta}, 0 < \beta < 1$ and subdivide each coarse cell into finer cell $\Omega_{m,n}^Y$, $n = 1, 2, \ldots, N_k^{\underline{h}} = (\overline{h}/\underline{h})^d$ of size $\underline{h} < k^{-\gamma}, \gamma > 1$.
Define piecewise constant $G_{\underline{h}}(\mathbf{x}, \mathbf{y}) = G(\mathbf{x}, \mathbf{y}_{m,n})$ for $\mathbf{y} \in \Omega_{m,n}^Y$.
Given $\epsilon > 0$, choose $\underline{h}$ small enough

$$\int_Y \int_X |G(\mathbf{x}, \mathbf{y}) - G_{\underline{h}}(\mathbf{x}, \mathbf{y})|^2 = \sum_{m=1}^{N_k^{\overline{h}}} \sum_{n=1}^{N_k^{\underline{h}}} \int_{\Omega_{m,n}^Y} \int_X |G(\mathbf{x}, \mathbf{y}) - G(\mathbf{x}, \mathbf{y}_{m,n})|^2 \lesssim \epsilon^2$$



Sketch of the proof

Define $G_{\underline{h}}(\mathbf{x},\mathbf{y}) = G(\mathbf{x},\mathbf{y}_{m,n})$ for $\mathbf{y} \in \Omega^Y_{m,n}$. Given $\epsilon > 0$, choose $\underline{h}$ small enough

$$\int_Y \int_X |G(\mathbf{x},\mathbf{y}) - G_{\underline{h}}(\mathbf{x},\mathbf{y})|^2 = \sum_{m=1}^{N_k^{\overline{h}}} \sum_{n=1}^{N_k^{\underline{h}}} \int_{\Omega^Y_{m,n}} \int_X |G(\mathbf{x},\mathbf{y}) - G(\mathbf{x},\mathbf{y}_{m,n})|^2 \lesssim \epsilon^2$$

$$\Rightarrow \epsilon^2 \gtrsim \int_{\Omega^Y} \|(I - P_{S_X})G_{\underline{h}}(\mathbf{x},\mathbf{y})]\|^2_{L_2(X)}$$
$$\gtrsim \tfrac{1}{N_k^{\underline{h}}} \textstyle\sum_{n=1}^{N_k^{\underline{h}}} \tfrac{1}{N_k^{\overline{h}}} \textstyle\sum_{m=1}^{N_k^{\overline{h}}} \|G(\mathbf{x},\mathbf{y}_{m,n}) - P_{S_X} G(\mathbf{x},\mathbf{y}_{m,n})\|^2_{L_2(X)}$$

$$\Rightarrow \min_n \frac{1}{N_k^{\overline{h}}} \sum_{m=1}^{N_k^{\overline{h}}} \|G(\mathbf{x},\mathbf{y}_{m,n}) - P_{S_X} G(\mathbf{x},\mathbf{y}_{m,n})\|^2_{L_2(X)} \lesssim \epsilon^2,$$

where $S_X = span\{f_p(\mathbf{x})\}_{p=1}^{N_k^{\epsilon}}$.

Upper bound for approximate separability

Theorem 4

Let X, Y be two compact manifolds embedded in R^n and $\dim(X) \geq \dim(Y) = d, d \leq n$. For any $\epsilon > 0$, there are $f_p(\mathbf{x}) \in L_2(X), g_p(\mathbf{y}) \in L_2(Y), p = 1, 2, \ldots, N_k^\epsilon \lesssim k^{d\gamma}$ such that

$$\left\| G(\mathbf{x}, \mathbf{y}) - \sum_{p=1}^{N_k^\epsilon} f_p(\mathbf{x}) g_p(\mathbf{y}) \right\|_{L_2(X \times Y)} \leq \epsilon$$

for any $\gamma > 1$ and arbitrary close to 1 as $k \to \infty$.

Sketch of proof

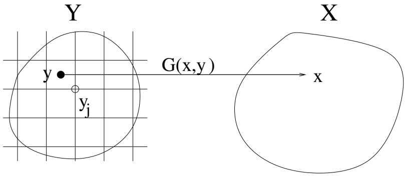
Denote $S_X = span\{G(\mathbf{x}, \mathbf{y}_m)\}_{m=1}^{N_k^h} \subset L_2(X)$.

- Lay down a uniform grid in R^3 that covers Y with grid size $h = k^{-\gamma}$.
- If X and Y are separated, uniformly in X and Y

$$|\nabla_{\mathbf{y}} G(\mathbf{x}, \mathbf{y})| \lesssim k, \quad \|D_{\mathbf{y}}^2 G(\mathbf{x}, \mathbf{y})\| \lesssim k^2.$$

- Use linear interpolation

$$\sqrt{\int_Y \|G(\mathbf{x}, \mathbf{y}) - P_{S_X} G(\mathbf{x}, \mathbf{y})\|_{L_2(X)}^2 d\mathbf{y}} \leq \epsilon$$



Lower bound in L_∞

Theorem 5

Let X, Y be two separated compact manifolds embedded in R^n and $\dim(X) \geq \dim(Y) = d, d \leq n$*.For $\mathbf{y}_1, \mathbf{y}_2 \in Y$, assume*

$$|<\hat{G}(\cdot,\mathbf{y}_1),\hat{G}(\cdot,\mathbf{y}_2)>| \lesssim (k|\mathbf{y}_1-\mathbf{y}_2|)^{-\alpha} \quad \text{as } k|\mathbf{y}_1-\mathbf{y}_2| \to \infty.$$

If there are $f_p(\mathbf{x}) \in L_\infty(X), g_p(\mathbf{y}) \in L_\infty(Y), p = 1,2,\ldots,N_k^\epsilon$ such that

$$\left\| G(\mathbf{x},\mathbf{y}) - \sum_{p=1}^{N_k^\epsilon} f_p(\mathbf{x}) g_p(\mathbf{y}) \right\|_{L_2(X\times Y)} \leq \epsilon,$$

then

$$N_k^\epsilon \geq \begin{cases} c_\epsilon k^{2\alpha}, & \alpha < \frac{d}{2}, \\ c_\epsilon k^{d\beta}, & \alpha \geq \frac{d}{2}, \end{cases} \quad \text{as } k \to \infty$$

for any $\beta < 1$ and arbitrary close to 1, where $c_\epsilon \geq c(1-(C\epsilon)^2)^2$ for some positive constants c and C that only depend on X, Y and $n(\mathbf{x})$.

Upper bound in L_∞

Theorem 6

Let X, Y be two separated compact manifolds embedded in R^n and $\dim(X) \geq \dim(Y) = d, d \leq n$. For any $\epsilon > 0$, there are $f_p(\mathbf{x}) \in L_\infty(X), g_p(\mathbf{y}) \in L_\infty(Y), p = 1, 2, \ldots, N_k^\epsilon \leq Ck^{d\gamma}$ such that

$$\left| G(\mathbf{x}, \mathbf{y}) - \sum_{p=1}^{N_k^\epsilon} f_p(\mathbf{x}) g_p(\mathbf{y}) \right| \leq \epsilon, \quad \forall \mathbf{x} \in X, \forall \mathbf{y} \in Y, \tag{1}$$

for any $\gamma > 1$ and arbitrary close to 1 as $k \to \infty$, where $C > 0$ is some constant that depends on X, Y and $n(\mathbf{x})$.

Upper bound using Weyl's formula

Let $u_m(\mathbf{x}), \|u_m\|_{L_2(\Omega)} = 1, m = 1, 2, \ldots$ be the eigenfunctions for

$$\Delta u_m(\mathbf{x}) = \lambda u_m(\mathbf{x}), \quad \mathbf{x} \in \Omega, \quad u_m(\mathbf{x}) = 0, \mathbf{x} \in \partial\Omega$$

with eigenvalues $0 > \lambda_1 \geq \lambda_2 \geq \ldots$. The Weyl's asymptotic formula

$$|\lambda_m| \approx \frac{4\pi^2 m^{2/d}}{(C_d|\Omega|)^{2/d}}$$

Then $u_m(\mathbf{x})$ are also the eigenfunctions for the homogeneous Helmholtz operator with eigenvalues $\lambda_m + k^2$. Assuming Ω is not resonant

$$G(\mathbf{x}, \mathbf{y}) = \sum_{m=1}^{\infty} (\lambda_m + k^2)^{-1} u_m(\mathbf{y}) u_m(\mathbf{x}).$$

Choose $N_k^\epsilon = M = O(k^{d+\delta}), \delta > 0$, so $|\lambda_m + k^2|^{-1} \lesssim |\lambda_m|^{-1}, m > M$,

$$\int_\Omega \int_\Omega |G(\mathbf{x}, \mathbf{y}) - \sum_{m=1}^{M} (\lambda_m + k^2)^{-1} u_m(\mathbf{y}) u_m(\mathbf{x})|^2 = O(\sum_{m=M+1}^{\infty} m^{-\frac{4}{d}}) = O(M^{1-\frac{4}{d}}) < \epsilon^2$$

for any $\epsilon > 0$ when k is large enough.

Sharpness of the bounds and its implication

Let X, Y be two separated compact manifolds embedded in R^n and $\dim(X) \geq \dim(Y) = d, d \leq n$.

- When Green's functions at two points become almost orthogonal or decorrelate fast, $|< G(\cdot, \mathbf{y}_1), G(\cdot, \mathbf{y}_2) >| \lesssim (k|\mathbf{y}_1 - \mathbf{y}_2|)^{-\alpha}$ with $\alpha \geq \frac{d}{2}$, Our estimates are sharp

$$k^{d-\delta} \lesssim N_k^\epsilon \lesssim k^{d+\delta}, \quad \forall \delta > 0.$$

- The sharpness of the lower bound implies sharpness of the following

$$\sum_{m=1}^{\underline{N}_k^\epsilon} \lambda_m^2 \geq \underline{N}_k^\epsilon \left[\frac{(1-\epsilon^2) n_k^h}{\underline{N}_k^\epsilon} \right]^2 = \frac{[(1-\epsilon^2) n_k^h]^2}{\underline{N}_k^\epsilon}$$

$\Rightarrow$ flatness of the leading spectrum of $A =< G(\cdot, \mathbf{y}_i), G(\cdot, \mathbf{y}_j) >$.

Practical cases when the bounds are sharp

Assume $| < G(\cdot, \mathbf{y}_1), G(\cdot, \mathbf{y}_2) > | \lesssim (k|\mathbf{y}_1 - \mathbf{y}_2|)^{-\alpha}$ for some $\alpha > 0$.

- X, Y are two surfaces in 3D, e.g.,(a) boundary of two scatterers, or (b) the case for multi-frontal type algorithms,

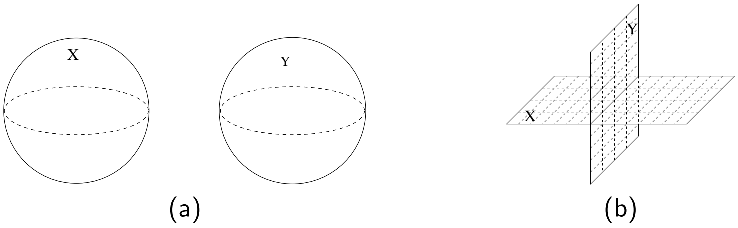
$$\alpha = 1 \quad \Rightarrow \quad k^{2-\delta} \lesssim N_k^{\epsilon} \lesssim k^{2+\delta}, \quad \forall \delta > 0.$$

- X, Y are two curves,

$$\alpha = \frac{1}{2} \quad \Rightarrow \quad k^{1-\delta} \lesssim N_k^{\epsilon} \lesssim k^{1+\delta}, \quad \forall \delta > 0.$$

- $\dim(X) = 3$, $\dim(Y) = d \leq 2$,

$$\alpha = 1 \quad \Rightarrow \quad k^{d-\delta} \lesssim N_k^{\epsilon} \lesssim k^{d+\delta}, \quad \forall \delta > 0.$$



Practical cases when the bounds are not sharp

Assume $| < G(\cdot, \mathbf{y}_1), G(\cdot, \mathbf{y}_2) > | \lesssim (k|\mathbf{y}_1 - \mathbf{y}_2|)^{-\alpha}$ for some $\alpha > 0$.

- Two domains in R^3 and $\dim(X) = \dim(Y) = 3$,

$$\alpha = 1 \quad \Rightarrow \quad k^2 \lesssim N_k^\epsilon \lesssim k^{3+\delta}, \quad \forall \delta > 0.$$

- Two domains in R^2 and $\dim(X) = \dim(Y) = 2$,

$$\alpha = \frac{1}{2} \quad \Rightarrow \quad k \lesssim N_k^\epsilon \lesssim k^{2+\delta}, \quad \forall \delta > 0.$$

Special setups where high separability can be achieved

Key: Fast oscilation in the phase is not felt.
Assume $G(\mathbf{x},\mathbf{y}) = A(\mathbf{x},\mathbf{y})e^{ik\phi(\mathbf{x},\mathbf{y})} \Rightarrow$ Find $\phi_1(\mathbf{x})$ and $\phi_2(\mathbf{y})$ s.t. $k(\phi(\mathbf{x},\mathbf{y})-\phi_1(\mathbf{x})-\phi_2(\mathbf{y}))$ is uniformly bounded with respect to $\mathbf{x}\in X, \mathbf{y}\in Y$ and k. So the phase difference

$$k(\phi(\mathbf{x},\mathbf{y}_1)-\phi(\mathbf{x},\mathbf{y}_2))$$

$$=k(\phi_2(\mathbf{y}_1)-\phi_2(\mathbf{y}_2))+k[(\phi(\mathbf{x},\mathbf{y}_1)-\phi_1(\mathbf{x})-\phi_2(\mathbf{y}_1))-(\phi(\mathbf{x},\mathbf{y}_2)-\phi_1(\mathbf{x})-\phi_2(\mathbf{y}_2))]$$

Special setups where high separability can be achieved

Key: Fast oscilation in the phase is not felt.
Assume $G(\mathbf{x},\mathbf{y}) = A(\mathbf{x},\mathbf{y})e^{ik\phi(\mathbf{x},\mathbf{y})} \Rightarrow$ Find $\phi_1(\mathbf{x})$ and $\phi_2(\mathbf{y})$ s.t. $k(\phi(\mathbf{x},\mathbf{y})-\phi_1(\mathbf{x})-\phi_2(\mathbf{y}))$ is uniformly bounded with respect to $\mathbf{x}\in X, \mathbf{y}\in Y$ and k. So the phase difference

$$k(\phi(\mathbf{x},\mathbf{y}_1)-\phi(\mathbf{x},\mathbf{y}_2))$$

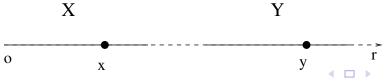
$$=k(\phi_2(\mathbf{y}_1)-\phi_2(\mathbf{y}_2))+k[(\phi(\mathbf{x},\mathbf{y}_1)-\phi_1(\mathbf{x})-\phi_2(\mathbf{y}_1))-(\phi(\mathbf{x},\mathbf{y}_2)-\phi_1(\mathbf{x})-\phi_2(\mathbf{y}_2))]$$

Example 1: Two collinear line segments, $\phi_1(\mathbf{x}) = -r_{\mathbf{x}}, \phi_2(\mathbf{y}) = r_{\mathbf{y}}$.

$$< G_0(\cdot,\mathbf{y}_1), G_0(\cdot,\mathbf{y}_2) >= e^{ik(\mathbf{y}_2-\mathbf{y}_1)}\int_X \frac{1}{|\mathbf{x}-\mathbf{y}_1||\mathbf{x}-\mathbf{y}_2|}d\mathbf{x} = O(1).$$

$$G_0(\mathbf{x},\mathbf{y}) = \frac{1}{4\pi}e^{-ikr_{\mathbf{x}}}e^{ikr_{\mathbf{y}}}\frac{1}{r_{\mathbf{y}}-r_{\mathbf{x}}} = \frac{1}{4\pi}e^{-ikr_{\mathbf{x}}}e^{ikr_{\mathbf{y}}}r_{\mathbf{y}}^{-1}\sum_{m=0}^{\infty}(\frac{r_{\mathbf{x}}}{r_{\mathbf{y}}})^m.$$

$$\Rightarrow N_k^{\epsilon} \le (\log\frac{l_X}{l_X+d})^{-1}\log(4\pi d\epsilon)$$

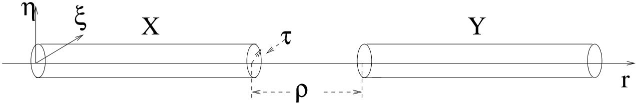


Special setups where high separability can be achieved

Example 2: X and Y are two collinear separated narrow tubes (similar to a 2D case by Martinsson-Rokhlin'07).
Let $\rho = \inf_{\mathbf{x}\in X, \mathbf{y}\in Y}(r_x - r_y)$ and $\tau = \sup_{\mathbf{x}\in X, \mathbf{y}\in Y} \sqrt{\xi^2 + \eta^2}$. Assume $k\tau < \frac{1}{2}, \mu = \frac{\tau}{\rho} < \frac{1}{2}$. Take $\phi_1(\mathbf{x}) = -r_{\mathbf{x}}, \phi_2(\mathbf{y}) = r_{\mathbf{y}}$

$$k|\phi(\mathbf{x},\mathbf{y}) - \phi_1(\mathbf{x}) - \phi_2(\mathbf{y})| = k(|\mathbf{x}-\mathbf{y}| - (r_{\mathbf{y}} - r_{\mathbf{x}})) < 2k\tau = 1$$

$$\Rightarrow N_k^\epsilon \lesssim |\log \epsilon|^{12}$$



Special setups where high separability can be achieved

Example 3: Fast butterfly algorithms for computing highly oscillatory Fourier integral operators (Candes et al' 09) and boundary integrals for HE (Luo-Qian'14). A hierarchical decomposition and pairing of domains, X, Y, $|X||Y| \leq 1/k$.

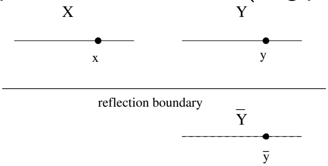
Key observation: $k|\phi(\mathbf{x},\mathbf{y}) - \phi(\mathbf{x}_0,\mathbf{y}) - \phi(\mathbf{x},\mathbf{y}_0) + \phi(\mathbf{x}_0,\mathbf{y}_0)|$ is uniformly bounded for all k, $\mathbf{x} \in X, \mathbf{y} \in Y$, where $\mathbf{x}_0, \mathbf{y}_0$ are the centers of X, Y respectively. $\Rightarrow$ low rank approximation $O(|\log \epsilon|^4)$

Special setups where high separability can be achieved

Example 3: Fast butterfly algorithms for computing highly oscillatory Fourier integral operators (Candes et al' 09) and boundary integrals for HE (Luo-Qian'14). A hierarchical decomposition and pairing of domains, X, Y, $|X||Y| \leq 1/k$.

Key observation: $k|\phi(\mathbf{x},\mathbf{y}) - \phi(\mathbf{x}_0,\mathbf{y}) - \phi(\mathbf{x},\mathbf{y}_0) + \phi(\mathbf{x}_0,\mathbf{y}_0)|$ is uniformly bounded for all k, $\mathbf{x} \in X, \mathbf{y} \in Y$, where $\mathbf{x}_0, \mathbf{y}_0$ are the centers of X, Y respectively. $\Rightarrow$ low rank approximation $O(|\log \epsilon|^4)$

Example 4: Sweeping preconditioner for HE (Engquist-Ying'11).



Then the Green's function in for half space $G_1(\mathbf{x},\mathbf{y}) = G_0(\mathbf{x},\mathbf{y}) - G_0(\mathbf{x},\bar{\mathbf{y}})$. If the distance to the boundary is $\leq 1/k$, $G_1(\mathbf{x},\mathbf{y})$ is highly separable as in Example 2.

Summary

We developed a general approach to study approximate separability of Green's function for Helmholtz equation in high frequency limit by

- showing a geometric characterization of relations between two Green's function,
- deriving sharp lower and upper bounds for approximate separability,
- studying various setups of practical interest.