Scaling laws for intrinsic complexity: from random vectors and random fields to high frequency waves

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The intrinsic complexity of a set in a metric space

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- The dimension $\underline{N}^{\epsilon}$ of the best linear space $\mathcal{V} \subset \mathcal{W}$ that can approximate S to an ϵ error.

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- The Kolmogorov $\underline{N}^\epsilon$-width of S is ϵ.

Outline

Bounds and scaling laws for $\underline{N}^{\epsilon}$.

- Approximation of random vectors and random fields (Jennifer Bryson, Z., & Yimin Zhong, SIAM MMS).
- Approximation of high frequency wave fields (Bjorn Engquist & Z., CPAM).

Approximation of Random Vectors

Approximate embedding of vectors

$V = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n] \in R^{d\times n}$, $A = V^T V \in R^{n\times n}$, $a_{ij} =< \mathbf{v}_i, \mathbf{v}_j >$.
$\lambda_1 \geq \ldots \geq \lambda_n \geq 0$ e-values, $\mathbf{u}_i$ e-vectors of A, $\overline{S}_l = span\{\mathbf{u}_i\}_{i=1}^{l}$

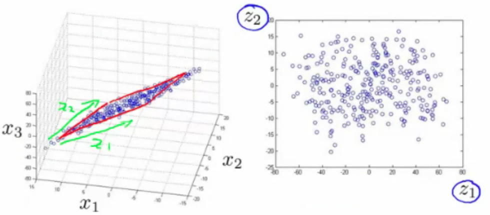
$$tr(A) = \sum_{m=1}^{n} \lambda_m = \sum_{m=1}^{n} \|\mathbf{v}_m\|_2^2$$

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

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

$$\Rightarrow \frac{\sum_{m=1}^{n} \|\mathbf{v}_m - P_{\overline{S}_{\underline{N}^{\epsilon}}}\mathbf{v}_m\|_2^2}{\sum_{m=1}^{n} \|\mathbf{v}_m\|_2^2} \leq \epsilon^2$$

$\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$ can be embedded into $\overline{S}_{\underline{N}^{\epsilon}} = span\{\mathbf{u}_i\}_{i=1}^{\underline{N}^{\epsilon}}$ with a relative r.m.s. error ϵ.



A general lower bound

Theorem 1

Given $\mathbf{v}_i \in R^d, i = 1, 2, \dots, n,$

$$\underline{N}^\epsilon \geq \frac{(\sum_{i=1}^n ||\mathbf{v}_i||_2^2)^2 (1-\epsilon^2)^2}{\sum_{i,j=1}^n (\mathbf{v}_i \cdot \mathbf{v}_j)^2}$$

Proof.

On one hand,

$$\sum_{i,j=1}^{n} (\mathbf{v}_i \cdot \mathbf{v}_j)^2 = tr(A^T A) = \sum_{i=1}^{n} \lambda_i^2 \geq \sum_{i=1}^{\underline{N}^\epsilon} \lambda_i^2 \geq \frac{1}{\underline{N}^\epsilon} \Big(\sum_{i=1}^{\underline{N}^\epsilon} \lambda_i \Big)^2.$$

On the other hand,

$$\sum_{i=1}^{\underline{N}^\epsilon} \lambda_i \geq (1-\epsilon^2) \sum_{i=1}^{n} \lambda_i = (1-\epsilon^2) \sum_{i=1}^{n} ||\mathbf{v}_i||_2^2.$$

□

An asymptotic lower bound

Theorem 2 (N. Alon)

Given $\mathbf{v}_i \in R^d, i = 1, 2, \ldots, n,\ \|\mathbf{v}_i\| = 1,\ | < \mathbf{v}_i, \mathbf{v}_j > | \leq \delta, i \neq j,$

$$\underline{N}^{\epsilon} \geq \frac{n(1-\epsilon^2)^2}{1+(n-1)\delta^2}.$$

1. *If* $\delta \leq O(n^{-\frac{1}{2}})$, $\underline{N}^{\epsilon} = O(n)$,
2. *If* $O(n^{-\frac{1}{2}}) \leq \delta < \frac{1}{2}$, $\underline{N}^{\epsilon} \geq O(\frac{1}{\delta^2 \log(\frac{1}{\delta})} \log n)$.

Remark

The asymptotic lower bound is sharp. The Johnson-Lindenstraus Lemma provides the upper bound.

Marčenko-Pastur law for random matrices

V: a $d \times n$ random matrix whose entries are i.i.d random variables with mean 0 and variance $\sigma^2 < \infty$.
Let $\hat{A} = \frac{1}{d} V^T V$ and $\hat{\lambda}_1 \geq \ldots \geq \hat{\lambda}_n$ be the eigenvalues of $\hat{A}$. Define

$$\mu_n(I) = \frac{1}{n} \#\{\hat{\lambda}_j \in I\}, \quad I \subset \mathbb{R}.$$

Assume $n, d \to \infty$ and $n/d \to \alpha \in (0, +\infty)$, then $\mu_n \to \mu$ weakly, where

$$\mu(I) = \begin{cases} (1 - \frac{1}{\alpha}) \mathbf{1}_{0 \in I} + \nu(I), & \text{if } \alpha > 1 \\ \nu(I), & \text{if } 0 \leq \alpha \leq 1 \end{cases}$$

and

$$d\nu(x) = \frac{1}{2\pi\sigma^2} \frac{\sqrt{(\hat{\lambda}_+ - x)(x - \hat{\lambda}_-)}}{\alpha x} \mathbf{1}_{[\hat{\lambda}_-, \hat{\lambda}_+]} \, dx$$

with

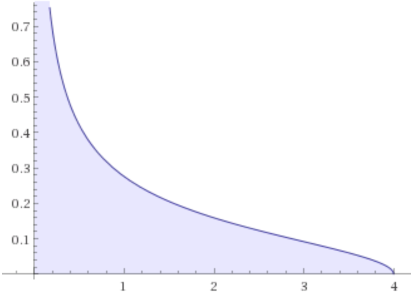
$$\hat{\lambda}_\pm = \sigma^2 (1 \pm \sqrt{\alpha})^2.$$

Marčenko-Pastur law for random matrices

Example: Let V be a $d \times n$ standard Gaussian matrix, and $\hat{A} = \frac{1}{d} V^T V$. Suppose $n/d \to 1$. Then $\mu_n(I) \to \mu$, where

$$d\mu(x) = \frac{1}{2\pi} \frac{\sqrt{(4-x)x}}{x} \mathbf{1}_{[0,4]}\, dx$$

The eigenvalue distribution of A looks like



Explicit formula for random vectors with i.i.d entries

Theorem 3

Given $V = [\mathbf{v}_1, \mathbf{v}_2, \ldots \mathbf{v}_n] \in \mathbb{R}^{d \times n}$ *where the entries of* V *are i.i.d with mean zero and variance* $= \sigma^2 < \infty$. *Let* $\mu(x)$ *be the eigenvalue distribution of* $\hat{A} = \frac{1}{d} V^T V$ *from Marčenko-Pastur law, then*

$$\frac{\underline{N}^{\epsilon}}{n} \overset{n \to \infty}{\longrightarrow} \int_{y}^{\hat{\lambda}_+} d\mu(x),$$

where y *satisfies* $\int_{\hat{\lambda}_-}^{y} x d\mu(x) = \sigma^2 \epsilon^2$.

Proof.

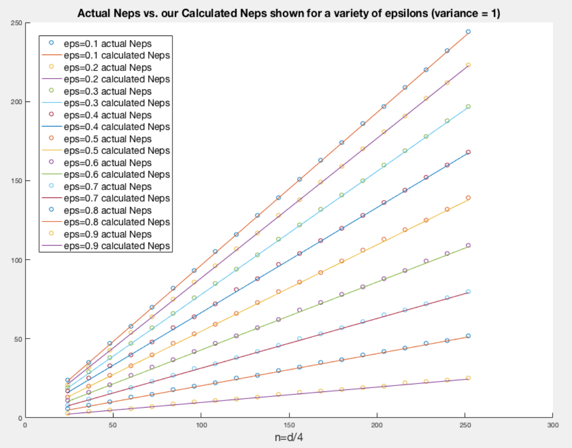
Key observation:

$$\frac{1}{n} \sum_{i=\underline{N}^{\epsilon}+1}^{n} \hat{\lambda}_i \to \int_{\hat{\lambda}_-}^{\hat{\lambda}_{N^{\epsilon}+1}} x d\mu(x)$$

Hence we need to find y such that $\int_{\hat{\lambda}_-}^{y} x d\mu(x) = \sigma^2 \epsilon^2$. □

Numerical test

V is a standard Gaussian matrix with $n = \frac{d}{4}$.



A dual question

Question: what is the minimal relative r.m.s error if $\mathbf{v}_1, \mathbf{v}_2, \ldots \mathbf{v}_n$ is embedded into a k dimensional space?

Corollary 4

Given a set of vectors $\{\mathbf{v}_i\}_{i=1}^n$ and k, $0 < k < \min d, n$, the relative r.m.s. error for the best k dimensional linear subspace is asymptotically given by

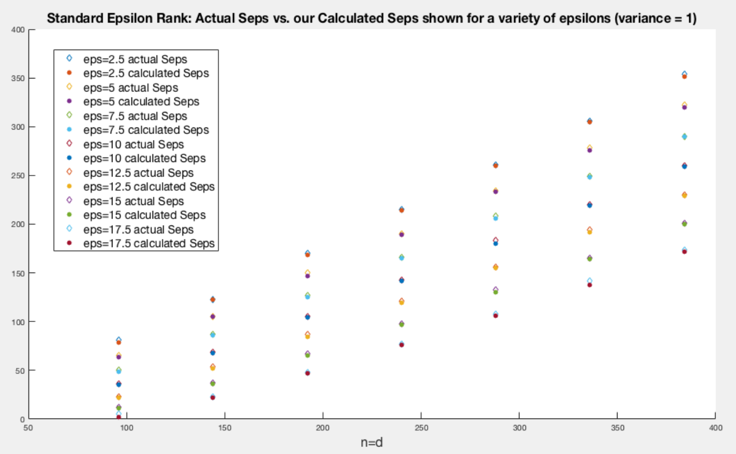
$$\sqrt{\frac{1}{\sigma^2}\int_{\hat{\lambda}_-}^{y} x d\mu(x)},$$

where y satisfies $\int_{\hat{\lambda}_-}^{y} d\mu(x) = \frac{n-k}{n}$.

ϵ rank approximation

Let R^ϵ be the the largest integer such that $\sqrt{\lambda_{R^\epsilon}} \geq \epsilon$. Under the same conditions in Marčenko-Pastur law

$$\frac{n - R^\epsilon + 1}{n} \to \int_{\hat{\lambda}_-}^{\frac{\epsilon^2}{d}} d\mu(x) \quad \text{or} \quad \frac{R^\epsilon}{n} \to 1 - \int_{\hat{\lambda}_-}^{\frac{\epsilon^2}{d}} d\mu(x) \quad \text{as } n \to \infty.$$



Random vectors with a given covariance structure

Let $\mathbf{v}_i \in \mathbb{R}^d$ be a sample of the random variable ξ_i, $i = 1, 2, \ldots, n$ with mean zero and covariance $C_{i,j} = cov(\xi_i, \xi_j) = \lim_{d\to\infty} \frac{1}{d}\mathbf{v}_i^T \mathbf{v}_j$.

If the covariance matrix is of the form $C_{i,j} = \exp(-\frac{|i-j|}{\sigma})$ and let $(\lambda_k, \mathbf{e}_k)$, $k = 1, 1, 2, \ldots n$ be the ordered eigen-pairs, it can be shown:

$$e_j^k = \cos(j\theta_k + \psi_k), \quad \lambda_k = \frac{\sinh\frac{1}{\sigma}}{\cosh\frac{1}{\sigma} - \cos(\theta_k)}$$

where $\tan(\psi_k) = \dfrac{\cos\theta_k - \exp(\frac{1}{\sigma})}{\sin\theta_k}$, $2\psi_k + (n+1)\theta_k = k\pi$, $\theta_k \in (\frac{k}{n}\pi, \frac{k+1}{n+1}\pi)$.

Hence

$$\sum_{k=1}^{n} \lambda_k \to \int_0^{\pi} \frac{\sinh\frac{1}{\sigma}}{\cosh\frac{1}{\sigma} - \cos x}dx \quad \sum_{k=\underline{N}^\epsilon}^{n} \lambda_k \to \int_{\frac{\pi \underline{N}^\epsilon}{n}}^{\pi} \frac{\sinh\frac{1}{\sigma}}{\cosh\frac{1}{\sigma} - \cos x}dx.$$

and

$$\frac{\underline{N}^\epsilon}{n} \to \frac{2}{\pi}\arctan\left(\tanh\left(\frac{1}{2\sigma}\right)\tan\left(\frac{\pi}{2}(1-\epsilon^2)\right)\right) \quad \text{as } n\to\infty$$

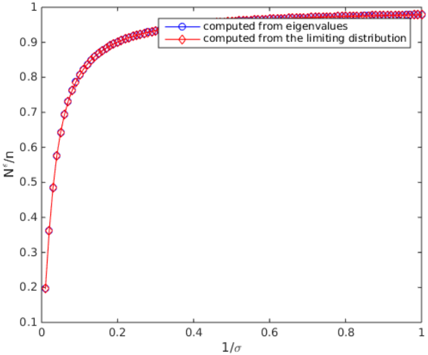
Numerical test

We use the following simple iterative method to solve θ_k, with $\theta_k^0 = \frac{k}{n}\pi$.

$$(n+1)\theta_k^n + 2\arctan\left(\frac{\cos\theta_k^{n-1} - \exp\tau}{\sin\theta_k^{n-1}}\right) = k\pi.$$

Then eigenvalue λ_k is computed through

$$\lambda_k = \frac{\sinh\tau}{\cosh\tau - \cos(\theta_k)}.$$



Approximation of Random Fields

Separable representation of a random field

Denote $a(x, \omega)$ a random field, where $\omega \in (\Omega, \Sigma, P)$ and $x \in D \subset R^d$. One can view $a(x, \omega)$

- $a(\cdot, \omega) : \Omega \to L^\infty(D)$, a set of functions on D parametrized by random variable $\omega \in \Omega$,

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Separable approximation of $a(x, \omega)$

$$a_N(x, \omega) \approx \sum_{n=1}^{N} \phi_n(x) Y_n(\omega),$$

Intrinsic complexity of $a(x, \omega)$

$$a_N(x, \omega) \approx \sum_{n=1}^{N} \phi_n(x) Y_n(\omega),$$

- what is the minimum number of terms needed in the expansion (by choosing the proper ϕ_n, Y_n) for a given tolerance?
- $a(x, \omega)$ as a set of random variables (functions) parametrized by $x \in D$ ($\omega \in \Omega$), what is the least dimension of a linear space that can approximate this set of random variables (functions) to a given tolerance.

Karhumen-Loéve (KL) expansion

Assume $a(x,\omega) \in L^2(D \times \Omega)$, *i.e.*, $\|a\|_2 < \infty$.
The mean field, $E_a(x)$, and covariance, $C_a(x,y)$:

$$E_a(x) = \int_\Omega a(x,\omega)dP(\omega), \;\; C_a(x,y) = \int_\Omega [a(x,\omega) - E_a(x)][a(y,\omega) - E_a(y)]dP(\omega)$$

$C_a(x,y)$ defines a compact, self-adjoint and non-negative operator $\mathcal{C}_a$:

$$(\mathcal{C}_a u)(x) = \int_D C_a(x,y)u(y)dy, \quad \forall u \in L^2(D)$$

Let $(\lambda_n, e_n(x)), n = 1, 2, \ldots$ be the eigen-pairs associated with $\mathcal{C}_a$, with $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n \cdots \to 0$. $e_n(x)$ form an orthonormal basis of $L^2(D)$.
KL expansion of the random field $a(x,w)$ is

$$a(x,w) = E_a(x) + \sum_{n=1}^{\infty} \sqrt{\lambda_n} e_n(x) Y_n(\omega),$$

and $Y_n(\omega)$ satisfy

$$Y_n(\omega) = \frac{1}{\sqrt{\lambda_n}} \int_D (a(x,\omega) - E_a(x)) e_n(x)dx, \quad E[Y_n] = 0, \quad E[Y_m Y_n] = \delta_{mn}.$$

KL approximation

For simplicity, assume $a(x,\omega)$ is centered, i.e., $E_a(x) = 0$.

- Truncated KL expansion is the best separable approximation of $a(x,\omega)$ in $L^2(D \times \Omega)$,

$$\|a - \sum_{n=1}^{N} \sqrt{\lambda_n} e_n(x) Y_n(\omega)\|_2^2 = \inf_{V \subset H, \dim V = N} \|a - P_{V \otimes S} a\|_2^2 = \sum_{n=N+1}^{\infty} \lambda_n,$$

  where $H = L^2(D), S = L^2(\Omega, dP)$ and $P_{V\otimes S} a$ denotes the L^2 projection of a in $V \otimes S$.

- $$\sum_{n=1}^{\infty} \lambda_n = \|a\|_2^2 = \int_D C_a(x,x) dx.$$

- Analogous to SVD of a matrix.

Lower bound and a scaling law for random fields

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

- $\underline{N}^{\epsilon}$ is the minimum number of terms needed in a separable approximation to achieve a relative r.m.s error ϵ in $L^2(D \times \Omega)$.
- If $V \subset L^2(D)$ is a linear space and $\frac{\|a - P_{V \otimes S} a\|_2}{\|a\|_2} \leq \epsilon$ then $\dim V \geq \underline{N}^{\epsilon}$.

Theorem 5

$$\underline{N}^{\epsilon} \geq (1-\epsilon^2)^2 \frac{\left(\int_D C_a(x,x)dx\right)^2}{\iint_{D\times D} C_a^2(x,y)dxdy} = (1-\epsilon^2)^2 \frac{\|a\|_2^4}{\iint_{D\times D} C_a^2(x,y)dxdy}$$

Theorem 6

For a stationary random field $a(x,\omega)$, $x \in D \subset \mathbb{R}^d$, *D compact, with* $C_a(x,y) = f(\frac{x-y}{\sigma})$ *and* $\int_{\mathbb{R}^d} f^2(x)dx < \infty$, *then* $\exists c(D,f,\epsilon) > 0$

$$\underline{N}^{\epsilon} \geq c(D,f,\epsilon)\sigma^{-d}, \quad \text{as } \sigma \to 0. \tag{1}$$

Asymptotic bound as $\epsilon \to 0$

- Another interesting question: given a random field $a(x, \omega)$, the number of terms needed in a separable approximation as the tolerance $\epsilon \to 0$.
- A typical constructive approach to show high separability as $\epsilon \to 0$ is based on smoothness assumption: use polynomial basis for separable approximation and show an upper bound of polylog of ϵ^{-1} type. $\Rightarrow$ low rank strucutes can be exploited in the discretized linear system.
- For example, by assuming certain smoothness (or regularity) of the covariance matrix, $Ca(x, y)$, a decay rate of the eigenvalues of KL expansion was shown by C. Schwab and R. A. Todor (2006) and generalized multipole methods were developed.

Approximation theory

Lemma Let H be a Hilbert space and $\mathcal{C}$ be a symmetric, non-negative and compact operator whose eigenpair sequence is $(\lambda_m, \phi_m)_{m\geq 1}$. if $\mathcal{C}_m$ is an operator of rank at most m, then

$$\lambda_{m+1} \leq \|\mathcal{C} - \mathcal{C}_m\|$$

Approximation theory. Let S_h^p denote the space of piecewise polynomial functions of degree p on a quasi-uniform triangulation $\mathcal{T}_h$ of mesh size h for D. Denote by $n = dim S_h^p = O(h^{-d})$ its dimension. Let $\mathcal{P}_h : L^2(D) \to S_h^p(D)$ be the $L^2(D)$ projection.

- If $f \in H^p(D)$

$$\|f - \mathcal{P}_h f\|_{L^2(D)} \leq Cn^{-\frac{p}{d}} \quad \text{as } h \to 0,$$

- if f is analytic, there are $c, C > 0$ on a fixed triangulation $\mathcal{T}_h$ of D,

$$\|f - \mathcal{P}_h f\|_{L^2(D)} \leq C \exp(-cn^{\frac{1}{d}}), \quad \text{as } p \to \infty.$$

Decay rate for the eigenvalues of KL expansion based on the smoothness of the covariance function

$$\text{Approximate} \quad (\mathcal{C}_a u)(x) = \int_D C_a(x,y)u(y)dy \quad \forall u \in L^2(D)$$

$$\text{by} \quad (\mathcal{P}_h \mathcal{C}_a)u : L^2(D) \to S_h^p(D)$$

$\Rightarrow$ the rank of $\mathcal{P}_h \mathcal{C}_a$ is the dimension of $S_h^p(D)$,

- if $C_a(x,y)$ is analytic, $0 \leq \lambda_n \leq C_1 \exp(-c_1 n^{\frac{1}{d}})$.
- if $C_a(x,y)$ is H^p, $0 \leq \lambda_n \leq C_3 n^{-\frac{p}{d}}$.

cf: Schwab & Todor 06

Upper bound and its scaling law

Theorem 7

For a stationary random field $a(x,\omega)$, $x \in D \subset \mathbb{R}^d$, D compact, with $C_a(x,y) = f(\frac{x-y}{\sigma})$, we have upper bounds for $\underline{N}^{\epsilon}$, as $\sigma \to 0$,

1. *if $f \in H^p(\mathbb{R}^d), p > d$: $\underline{N}^{\epsilon} \leq C(D,f,d,\epsilon)\sigma^{-(1+\frac{d}{2(p-d)})d}$.*
2. *if f is analytic in $\mathbb{R}^d$: $\underline{N}^{\epsilon} \leq C(D,f,d,\epsilon)\sigma^{-d}|\log\sigma|^d$.*

Remarks

- For f analytic in $\mathbb{R}^d \Rightarrow 0 \leq \lambda_n \leq C_1 \exp(-c_1 n^{\frac{1}{d}})$, the key is to show $c_1 = O(\sigma)$, which needs the fact that f is a positive function $\Rightarrow \; f(t) = \int_{\mathbb{R}^d} e^{i\xi\cdot t} d\mu(\xi)$ for some $\mu(\xi) > 0$ with exponential decay.
- For f analytic, both upper and lower bounds for $\underline{N}^{\epsilon}$ are sharp.

Upper bound in terms of approximation error

Theorem 8
For a stationary random field $a(x,\omega)$, $x \in D \subset \mathbb{R}^d$, D compact, with $C_a(x,y) = f(x-y)$, we have upper bounds for $\underline{N}^\epsilon$, as $\epsilon \to 0$,

1. *if f is H^p and $p > d$: $\underline{N}^\epsilon \leq C(D,f,d)\epsilon^{\frac{2d}{d-p}}$.*
2. *if f is analytic: $\underline{N}^\epsilon \leq C(D,f,d)|\log \epsilon|^d$.*

Numerical tests

We study the eigenvalue behavior for the two often-used covariance function for random fields:

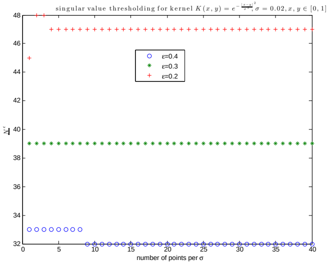
$$\tilde{C}_\sigma = \exp(-\frac{|x-y|^2}{\sigma^2}), \qquad \hat{C}_\sigma = \exp(-\frac{|x-y|}{\sigma})$$

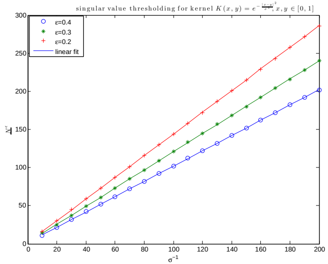
The covariance matrix is discretized on regular grids with a grid size $h = \frac{\sigma}{r}$, i.e., r grid points per σ.

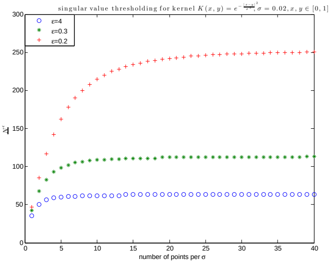
Def. $\underline{N}^\epsilon = \min n,\ s.t.\ \sum_{m=n+1}^{\infty} \lambda_m \le \epsilon^2 \sum_{m=1}^{\infty} \lambda_m.$

We show $\underline{N}^\epsilon$ for (1) different r with a fixed σ, and (2) different σ with fixed r, with $D=$ unit interval, unit square, and unit sphere.

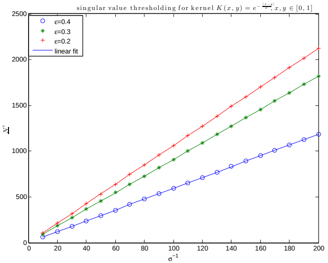
1D example: $x, y \in [0, 1]$





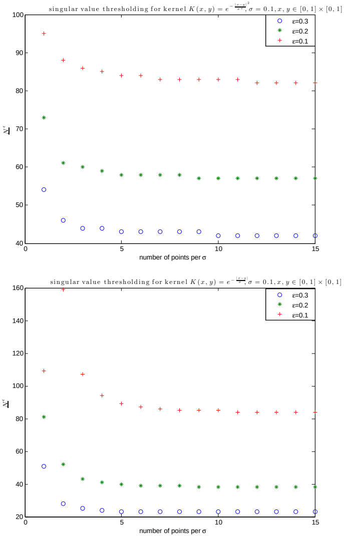


N^{ϵ} vs r with fixed σ

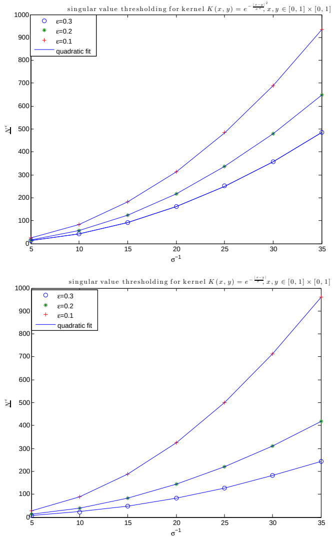


N^{ϵ} vs σ

2D example: $x, y \in [0,1] \times [0,1]$

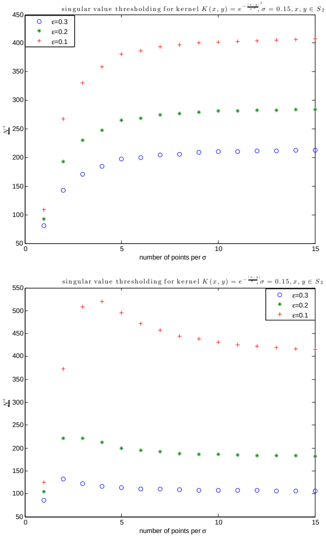


N^ϵ vs r with fixed σ

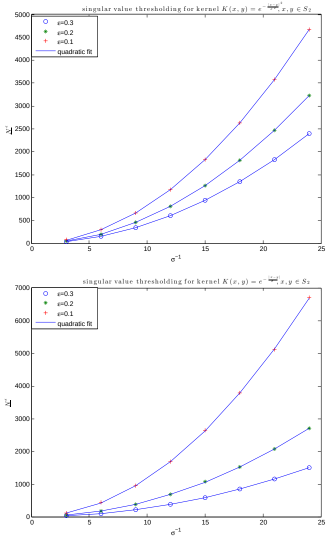


N^ϵ vs σ

2D example: $x, y \in S_2$



N^{ϵ} vs r with fixed σ



N^{ϵ} vs σ

Intrinsic Complexity for High Frequency Wave Fields

Approximate separability of the Green's function

Let $G(\mathbf{x}, \mathbf{y})$ be the Green's function of a linear PDE

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

Approximate separability of $G(\mathbf{x}, \mathbf{y})$: given two disjoint domains $X, Y \subseteq \Omega \subset R^d$, $\forall \epsilon > 0$, there is a smallest $\underline{N}^\epsilon$ and $f_l(\mathbf{x}), g_l(\mathbf{y}), l = 1, 2, \ldots, \underline{N}^\epsilon$, s.t.

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

Approximate separability of the Green's function

Let $G(\mathbf{x},\mathbf{y})$ be the Green's function of a linear PDE

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

Approximate separability of $G(\mathbf{x},\mathbf{y})$: given two disjoint domains $X, Y \subseteq \Omega \subset R^d$, $\forall \epsilon > 0$, there is a smallest $\underline{N}^\epsilon$ and $f_l(\mathbf{x}), g_l(\mathbf{y}), l = 1, 2, \ldots, \underline{N}^\epsilon$, s.t.

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

- $V = span\{f_l(\cdot)\}$ is a linear space of the least dimension $\underline{N}^\epsilon$ that approximates the family of functions $G(\cdot,\mathbf{y})$ on X $\forall \mathbf{y} \in Y$ to ϵ error.
- N^ϵ manifests the intrinsic complexity of the PDE.

$$L_x u = h \;\Rightarrow\; u(\mathbf{x}) = \int_\Omega G(\mathbf{x},\mathbf{y}) h(\mathbf{y}) d\mathbf{y} = \sum_{l=1}^{\underline{N}^\epsilon} f_l(\mathbf{x}) \int_\Omega g_l(\mathbf{y}) h(\mathbf{y}) d\mathbf{y} + O(\epsilon)$$

Implication to developing fast algorithms

High separability $\Rightarrow$ existence of low rank approximation for the discretized linear system.

- Dense matrix vector multiplications, e.g., fast multipole methods, convolution, boundary integral methods, Fourier integral operators, ...
-
$$\text{PDE} \quad Lu = f \quad \stackrel{\text{after discretization}}{\Longrightarrow} \quad Ax = b$$
  - Each columns of A^{-1} is $\approx$ a Green's function.
  - Low rank structure for off-diagonal blocks of A^{-1} can be explored to develop fast algorithms for solving the linear system such as hierarchical matrix method and structured inverse method.

Previous work on approximate separability

Show upper bounds for high separability $\underline{N}^{\epsilon} \leq O(|\log \epsilon|^q)$.

- Construct separable approximation using explicit expression of $G(\mathbf{x}, \mathbf{y})$ and asymptotic expansions with fast convergence, e.g. fast multipole method, butterfly algorithm, ...
- M. Bebendorf and W. Hackbusch'03 proved approximate separability in L_2 norm for Green's function of strict elliptic operator

$$Lu = \sum_{i,j=1}^{d} \partial_j (a_{ij} \partial_i u)$$

with L_∞ coefficients on two disjoint compact sets X, Y

$$\underline{N}_{\epsilon} \lesssim |\log \epsilon|^{d+1}$$

Key point: Caccioppoli inequality for $\|\nabla u\|_2$ in term of $\|u\|_2$.

Helmholtz equation in high frequency limit

Helmholtz equation (HE):

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

3D 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 ($k \gg 1$), we show

- the Green's function is far from highly separable $\Rightarrow$ the intrinsic degree of freedom is large!

Approximate separability of the Green's function for HE in the high frequency limit

Main results

- An explicit characterization of the relation between two Green's functions.

$$\left|< \hat{G}(\cdot,\mathbf{y}_1), \hat{G}(\cdot,\mathbf{y}_2) >_X\right| \lesssim (k|\mathbf{y}_1 - \mathbf{y}_2|)^{-\alpha}, \quad \alpha = \frac{d \pm 1}{2}, d = \dim(X)$$

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

- Lower and upper bound estimates.
  For two compact manifolds X and Y with $\dim(X) \geq \dim(Y) = d$

$$k^{d+\delta} \gtrsim \underline{N}_k^{\epsilon} \gtrsim \begin{cases} k^{2\alpha}, & \alpha < \frac{d}{2}, \\ k^{d-\delta}, & \alpha \geq \frac{d}{2}, \ \forall \delta > 0 \end{cases} \qquad k \to \infty$$

- Explicit estimates and their sharpness for setups that are commonly used in practice.

Relation between two Green's functions

Due to fast oscillations, two Green's functions with sources separated more than one wavelength are almost orthogonal/decorrelated.

Relation between two Green's functions

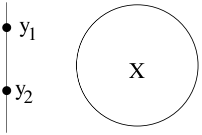
Due to fast oscillations, two Green's functions with sources separated more than one wavelength are almost orthogonal/decorrelated.

Theorem 9

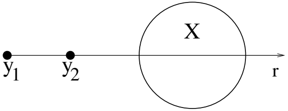
Assume $X \subset R^d, d = 2, 3$ is a compact domain. Depending on the positions of $\mathbf{y}_1, \mathbf{y}_2$ relative to X and its boundary, there is some $\alpha > 0$ such that

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

as $k|\mathbf{y}_1 - \mathbf{y}_2| \to \infty$. The constant in $\lesssim$ depends on X and the distances from $\mathbf{y}_1, \mathbf{y}_2$ to X.



case 1: ray through $\mathbf{y}_1, \mathbf{y}_2$ not intersecting X



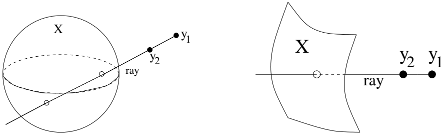
case 2: ray through $\mathbf{y}_1, \mathbf{y}_2$ intersecting X

Remarks

- Two Green's functions in heterogeneous media behave similarly based on geometric optics ansatz.
- X can be a compact embedded manifold. Generically,

$$\left| < \hat{G}(\cdot, \mathbf{y}_1), \hat{G}(\cdot, \mathbf{y}_2) >_X \right| \lesssim (k|\mathbf{y}_1 - \mathbf{y}_2|)^{-\alpha}, \quad \alpha \geq \frac{\dim(X)}{2},$$

  if the ray through $\mathbf{y}_1, \mathbf{y}_2$ intersects X a finite number of times.



- Scaling argument: if $\rho = \frac{|\mathbf{y}_1 - \mathbf{y}_2|}{dist(X, \mathbf{y}_i)} \ll 1$, k is rescaled to ρk (or $\rho^2 k$).
- Implication for imaging resolution from the decorrelation rate of two Green's functions: in plane resolution is better than range resolution.

Approximate embedding of a set of vectors

Denote $V = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N]$ and $A = V^T V$, $a_{mn} = < \mathbf{v}_m, \mathbf{v}_n >$.
Let $\lambda_1 \geq \ldots \geq \lambda_N \geq 0$ be the eigenvalues of A and $\mathbf{u}_i$ be the corresponding eigenvectors, then

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

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

where $P_{\overline{S}_l} \mathbf{v}$ denotes projection of $\mathbf{v}$ in $\overline{S}_l = span\{\mathbf{u}_i\}_{i=1}^{l}$.

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

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

$$\sqrt{\frac{\sum_{m=1}^{N} \|\mathbf{v}_m - P_{S^\epsilon} \mathbf{v}_m\|_2^2}{N}} \leq c\epsilon \ \Rightarrow \frac{\sum_{m=M+1}^{N} \lambda_m}{\sum_{m=1}^{N} \lambda_m} \leq \frac{\sum_{m=1}^{N} \|\mathbf{v}_m - P_{S^\epsilon} \mathbf{v}_m\|_2^2}{\sum_{m=1}^{N} \|\mathbf{v}_m\|_2^2} \leq \epsilon^2$$

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

Approximation of Green's functions sampled on a grid

Lemma 10 (key lemma)

Let X, Y be two disjoint compact embedded manifolds. $\dim(X) \geq \dim(Y) = d$. *For any two points $\mathbf{y}_1, \mathbf{y}_2 \in Y$ assume*

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

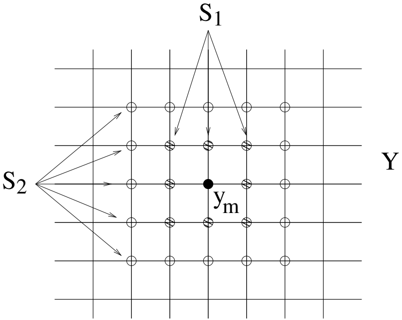
for some $\alpha > 0$, then there are points $\mathbf{y}_m \in Y, m = 1, 2, \ldots, N_\delta^s \sim k^{d-\delta}$ such that for the set of Green's functions $\{G(\mathbf{x}, \mathbf{y}_m)\}_{m=1}^{N_\delta^s} \subset L_2(X)$ and matrix $A = < \hat{G}(\cdot, \mathbf{y}_m), \hat{G}(\cdot, \mathbf{y}_n) >$

$$\underline{N}_k^\epsilon \gtrsim \begin{cases} (1-\epsilon^2)^2 k^{2\alpha}, & \alpha < \frac{d}{2}, \\ (1-\epsilon^2)^2 k^{d-\delta}, & \alpha \geq \frac{d}{2}, \end{cases} \tag{3}$$

for any $0 < \delta < 1$ and arbitrary close to 0, as $k \to \infty$, where the constants in $\lesssim$ and $\gtrsim$ only depend on X, Y.

Key idea of the proof

- Take $\mathbf{y}_m$ to be the grid points on a grid with grid size $\sim k^{-1+\frac{\delta}{d}}$.
- For a given point $\mathbf{y}_m$, divide all other points into groups according to their distances to $\mathbf{y}_m$.



Lower bound for approximate separability

Theorem 11 (main theorem)

Let X, Y be two compact embedded manifolds. $\dim(X) \geq \dim(Y) = d$. *For any two points* $\mathbf{y}_1, \mathbf{y}_2 \in Y$, *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 $f_l(\mathbf{x}) \in L_2(X), g_l(\mathbf{y}) \in L_2(Y), l = 1, 2, \ldots, N_k^\epsilon$ *such that*

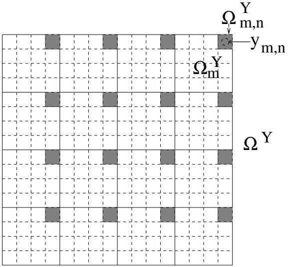
$$\left\| G(\mathbf{x}, \mathbf{y}) - \sum_{l=1}^{N_k^\epsilon} f_l(\mathbf{x}) g_l(\mathbf{y}) \right\|_{L_2(X \times Y)} \leq \epsilon,$$

then

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

for any δ *arbitrary close to 0 as* $k \to \infty$, *where* $c_\epsilon \geq c(1 - (C\epsilon)^2)^2$ *for some positive constants* c *and* C *that only depend on* X, Y *and* $n(\mathbf{x})$.

Proof based on a two grid approach



Upper bound for approximate separability

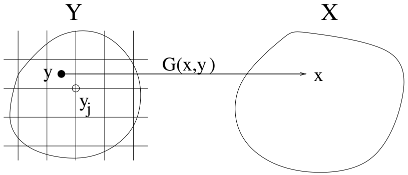
Theorem 12

Let X, Y be two compact embedded manifolds. $\dim(X) \geq \dim(Y) = d$. *For any* $\epsilon > 0$, $\exists\ f_l(\mathbf{x}) \in L_2(X), g_l(\mathbf{y}) \in L_2(Y), l = 1, 2, \ldots, N_k^\epsilon \lesssim k^{d+\delta}$ *such that*

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

for any $\delta > 0$ *and arbitrary close to 0 as* $k \to \infty$.

Proof: Use interpolation of Green's functions sampled on a grid with a grid size $h = k^{-1-\delta}$.



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

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

u_m is also the eigenfunction for the homogeneous Helmholtz operator with eigenvalue $\lambda_m + k^2$. Assuming Ω is not resonant

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

Lower and upper bounds in L_∞ for approximate separability

if X, Y are two disjoint compact embedded manifolds, the same lower and upper bounds in L_∞ for approximate separability hold.

Examples

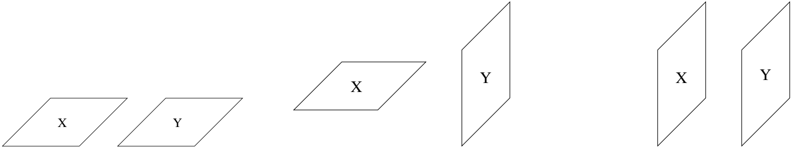
- X and Y are two disjoint compact 3D domains, $d = 3$. In general

$$|\langle \hat{G}(\cdot, \mathbf{y}_1), \hat{G}(\cdot, \mathbf{y}_2) \rangle| \lesssim (k|\mathbf{y}_1 - \mathbf{y}_2|)^{-1} \quad \Rightarrow \quad k^2 \lesssim \underline{N}_k^\epsilon \lesssim k^{3+\delta}.$$

- X and Y are two disjoint compact surfaces in 3D, $d = 2$, e.g., boundary integral method, multi-frontal method. In general

$$|\langle \hat{G}(\cdot, \mathbf{y}_1), \hat{G}(\cdot, \mathbf{y}_2) \rangle| \lesssim (k|\mathbf{y}_1 - \mathbf{y}_2|)^{-1} \quad \Rightarrow \quad k^{2-\delta} \lesssim \underline{N}_k^\epsilon \lesssim k^{2+\delta} \text{ (sharp!)}.$$

  Three examples for homogenous free space Green's functions:



(a) $k \lesssim \underline{N}_k^\epsilon \lesssim k^{2+\delta}$ (b) $k^{2-\delta} \lesssim \underline{N}_k^\epsilon \lesssim k^{2+\delta}$ (c) $k^{2-\delta} \lesssim \underline{N}_k^\epsilon \lesssim k^{2+\delta}$

k dependent special setups for high separability

Key: k dependent setup so fast osscilation 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

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

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

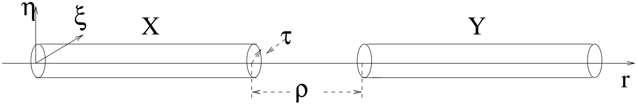
is a constant phase + bounded variation.

Special setups for high separability: two thin cylinders

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 $\phi_1(\mathbf{x}) = -r_{\mathbf{x}}, \phi_2(\mathbf{y}) = r_{\mathbf{y}}$

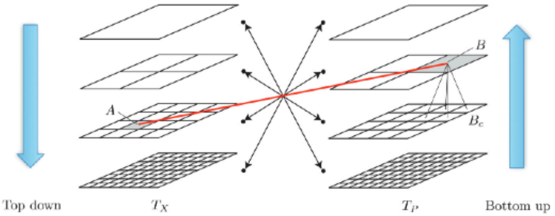
$$k|\phi(\mathbf{x},\mathbf{y}) - \phi_1(\mathbf{x}) - \phi_2(\mathbf{y})| = k(|\mathbf{x}-\mathbf{y}| - (r_{\mathbf{y}} - r_{\mathbf{x}})) < 2k\tau = 1$$

$$\Rightarrow \underline{N}_k^{\epsilon} \lesssim |\log \epsilon|^{12}$$



Special setups for high separability: butterfly algorithm

Butterfly algorithm setup is sharp! Butterfly algorithm for computing highly oscillatory Fourier integral operators (Candes, Demanet and Ying' 09) and boundary integrals for HE (Michielssen-Boag'96,Luo-Qian'14). A dyadic decomposition of X, Y and pairing of their subdomains, $A \subseteq X, B \subseteq Y$ such that $|A||B| \lesssim 1/k$.



Key observations

1: $k|\phi(\mathbf{x},\mathbf{y}) - \phi(\mathbf{x}_0,\mathbf{y}) - \phi(\mathbf{x},\mathbf{y}_0) + \phi(\mathbf{x}_0,\mathbf{y}_0)|$ 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 $O(|\log \epsilon|^4)$

2: scaling argument$\Rightarrow$ sharpness of the condition

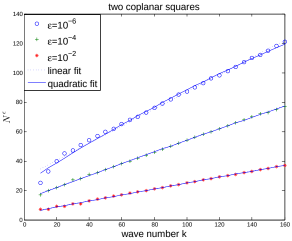
$$\left.\begin{array}{l} |A||B| \lesssim 1/k \Rightarrow r = \min(|A|,|B|) \lesssim k^{-\frac{1}{2}} \\ dist(X,Y) = O(1) \end{array}\right\} \Rightarrow k \text{ is scaled to } \frac{kr^2}{dist(X,Y)} = O(1).$$

Numerical test

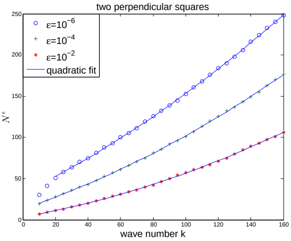
Let $\lambda_1 \geq \lambda_2, \ldots, \geq \lambda_N$ be the singular values of matrix $A_{N\times N}$ with $A_{ij} = G_0^k(\mathbf{x}_i, \mathbf{y}_j)$, where $\mathbf{x}_i \in X, \mathbf{y}_i \in Y$ are two discrete grids of X, Y respectively with a grid size h resolving the wavelength.

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

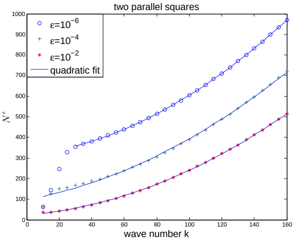
$\underline{N_k^\epsilon}$ vs. wave number k



(a) 2 coplanar squares



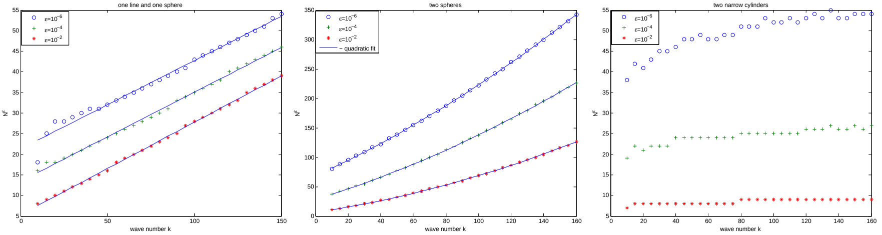
(b) 2 perpendicular squares



(c) 2 parallel squares

Numerical test

$\underline{N_k^\epsilon}$ vs. wave number k



(a) 1 line & 1 sphere (b) 2 shperes (c) 2 thin cylinders

What is the take so far?

- Green's functions of the Helmoholtz equation decorrelate fast when their sources are separated more than a wavelength in the high frequency limit.
- Lower bounds of the approximate separability of the Green's function $\Leftrightarrow$ the dimension of the best linear subspace to approximate a family of Green's function increases as some power of k as $k \to \infty$.
- Sharpness of the bounds: Let X, Y be two disjoint compact domains with $\dim(X) \geq \dim(Y) = d$. If two Green's functions decorrelate fast,

$$| < \hat{G}(\cdot, \mathbf{y}_1), \hat{G}(\cdot, \mathbf{y}_2) > | \lesssim (k|\mathbf{y}_1 - \mathbf{y}_2|)^{-\alpha}, \quad \alpha \geq \frac{d}{2},$$

then

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

Thank you!