

Nonlinear approximations, multi-linear tools and algorithms with finite but arbitrary accuracy

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Future Directions in Tensor-Based Computation and Modeling
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Some observations

- Success of Matlab or LAPACK is due (in a very significant way) to a (simple) data structure of a dense matrix
- Matrix algebra flourished perhaps because it is relatively easy to split a great variety of considerations leading to matrix formulations from the development of algorithms for matrices
- Numerical computing with tensors has a different flavor:
 - special data structures are a must from the beginning
 - analysis (i.e., use of approximation tools) is critical since purely algebraic approach (although useful) is limited in scope
 - tensor manipulations (i.e., numerical multilinear algebra) are neither “linear” nor “algebraic”

The future ain't what it used to be. Yogi Berra

Tensors and functions of many variables

- Formally, we may write $t_{ijklmn\dots}$ or $f(x_1, x_2, \dots, x_n)$ but neither has a dense form (as a collection of numbers) due to *the curse of dimensionality*
- Physics “painted” itself into a corner: many theories defy direct computation as they rely on the ordinary notion of functions of many variables
- Methods to integrate a function of many variables using random sampling implicitly assume that random sampling is capable of collecting information about the function

This points to importance of identifying useful subclasses of functions of many variables

Non-linear approximations

Linear approximation of functions (i.e., expressing solutions as a linear combination of pre-selected functions) does not extend well to high dimensions.

An alternative is the so-called nonlinear approximation of functions or operators that selects the best approximation (in some norm) for a given accuracy or number of terms from a wide class of functions, typically much wider than a basis set.

Nonlinear approximations are not new either from analytic point of view nor as a numerical tool:

Since the 1960's chemists used products of Gaussians (with unknown exponents) and polynomials (with unknown coefficients) to represent wave functions, see S.F. Boys; K. Singer and J.V.L. Longstaff, Proceedings of the Royal Society of London, v. 258, 1960 (later chemists switched to linear approximations).

Gaussians in Quantum Chemistry and Computing

- Besides using products of Gaussians and polynomials to represent wave functions, Gaussians were used to represent Coulomb potential, see W. Kutzelnigg, *Internat. J. Quantum Chem.* 51, 1994.
- We are using Gaussians to approximate non-oscillatory Green's functions, see R.J. Harrison, G.I. Fann, T. Yanai, Z. Gan and G. Beylkin, *J. Chem. Phys.* v. 121, n. 23, 14, 7, 2004 and, recently, oscillatory Green's functions, see G. Beylkin, C. Kurcz and L. Monzon, *Fast algorithms for Helmholtz Green's functions*, *Proceedings of the Royal Society A*, 464, 2008 and *Fast convolution with the free space Helmholtz Green's function* (*J. Comp. Phys.*, to appear) and multiparticle Green's functions, see G. Beylkin, M.J. Mohlenkamp, and Fernando Pérez, *Approximating a wavefunction as an unconstrained sum of Slater determinants*, *J. Math. Phys.* 49, no. 3, 2008.

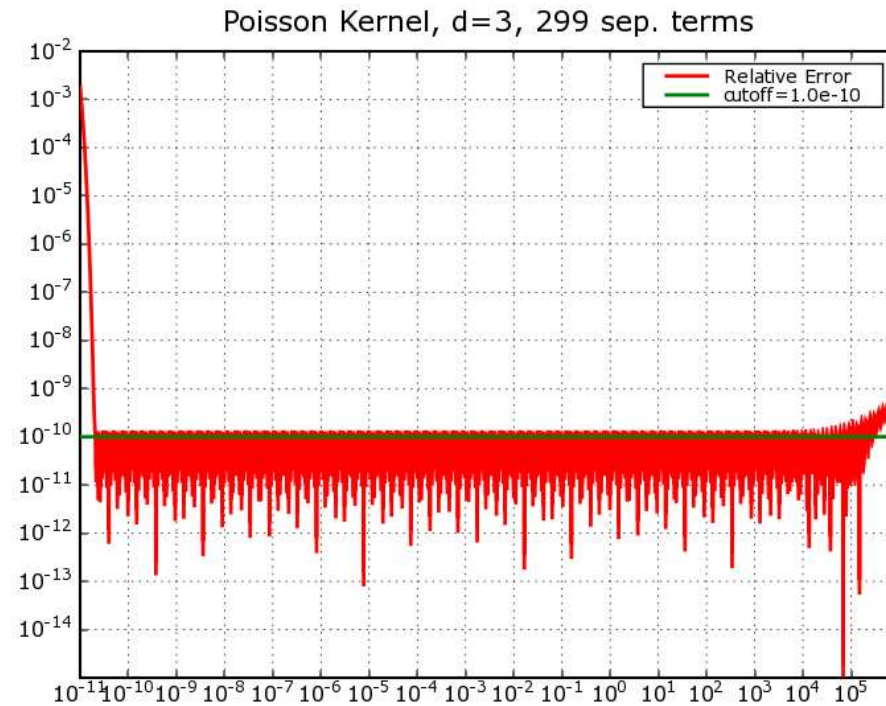
These are examples of nonlinear approximation of operators

The Poisson kernel via Gaussians

We have

$$\left| \frac{1}{\|r\|} - \sum_{m=1}^M w_m e^{-\tau_m \|r\|^2} \right| \leq \frac{\epsilon}{\|r\|},$$

for $\delta \leq \|r\| \leq R$, where $\tau_m, w_m > 0$ and $M = \mathcal{O}(-\log \delta)$.



Radial functions as sum of separable functions

Write

$$f(x) = h(\|x\|) = h(\sqrt{x_1^2 + \cdots + x_d^2}).$$

Approximate (in a single variable) $h(r) \approx \sum_{m=1}^M c_m e^{-\tau_m r^2}$ as a sum of Gaussians.

The exponential translates sums into products,

$$e^{-\tau_m \|x\|^2} = e^{-\tau_m (x_1^2 + \cdots + x_d^2)} = e^{-\tau_m x_1^2} \cdots e^{-\tau_m x_d^2}.$$

Then the radial function is approximated as

$$f(x) \approx \sum_{m=1}^M c_m \prod_{j=1}^d e^{-\tau_m x_j^2}$$

a separated representation (of Gaussians).

Estimates using Poisson summation

Serge Dubuc (“An approximation of the Gamma function”, 1990) derived a trapezoidal quadrature for $\int_{\mathbb{R}} f(t)dt$ (with an appropriate function f) using the following approach:

- For any $h > 0$ and real shift s , by Poisson summation, we have

$$h \sum_{n \in \mathbb{Z}} f(s + nh) = \sum_{n \in \mathbb{Z}} \hat{f}\left(\frac{n}{h}\right) e^{2\pi i s \frac{n}{h}}.$$

Since $\hat{f}(0) = \int_{\mathbb{R}} f(t)dt$,

$$\left| \int_{\mathbb{R}} f(t)dt - h \sum_{n \in \mathbb{Z}} f(s + nh) \right| \leq \sum_{n \neq 0} \left| \hat{f}\left(\frac{n}{h}\right) \right|.$$

- Fast decay of \hat{f} imply that we can choose h to achieve a small error.
- Fast decay of f yields a finite sum approximation.

Applying the idea to $r^{-\alpha}$

We have $r^{-\alpha} = \int_{-\infty}^{\infty} f(t)dt$ with

$$f(t) = \frac{e^{\alpha t}}{\Gamma(\alpha)} e^{-e^t r}, \quad \hat{f}(\xi) = \frac{\Gamma(\alpha - 2\pi i \xi)}{\Gamma(\alpha)} r^{2\pi i \xi - \alpha}$$

Both f and \hat{f} have exponential or super exponential decay at $\pm\infty$. A relative error estimate (independent of r) follows choosing h such that

$$\sum_{n \neq 0} \frac{|\Gamma(\alpha - 2\pi i \frac{n}{h})|}{\Gamma(\alpha)} < \epsilon.$$

The choice of h depends only on ϵ and α ,

$$h \leq \frac{2\pi}{\log 3 + \alpha \log(\cos 1)^{-1} + \log \epsilon^{-1}}.$$

Estimating the series' tails

Estimating the tails by integrals, lower (t_L) and upper (t_U) bounds are solutions of

$$1 - \frac{\Gamma(\alpha, e^{t_L})}{\Gamma(\alpha)} = \epsilon, \quad \frac{\Gamma(\alpha, \delta e^{t_U})}{\Gamma(\alpha)} = \epsilon.$$

which imply specific dependencies. Estimates:

$$t_L \leq \ln \Gamma(1 + \alpha)^{\frac{1}{\alpha}} + \frac{\ln \epsilon}{\alpha}$$

$$t_U \geq \ln \frac{e}{e-1} \delta^{-1} + \ln \ln [c(\alpha) \epsilon^{-1}],$$

for some explicit function $c(\alpha)$. We have

$$M = \frac{t_U - t_L}{h} = \log \epsilon^{-1} [c_0 + c_1 \log \delta^{-1} + c_2 \log \epsilon^{-1}].$$

Fast algorithms for applying operators

We develop numerical algorithms that

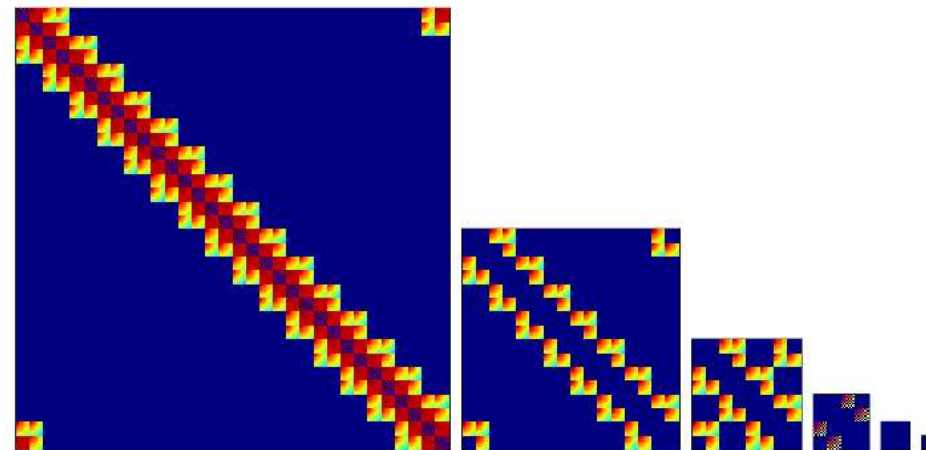
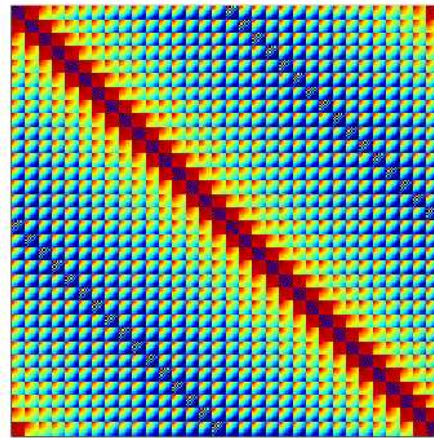
- yield finite but controlled precision
- are fast and fully adaptive
- address the “curse of dimensionality” in high dimensions

Approach: we use

- Separated representations to reduce the cost of dimensionality
- Multiresolution, sparse matrix representations for a large class of kernels

The modified ns-form

A graphical illustration of what we gain:

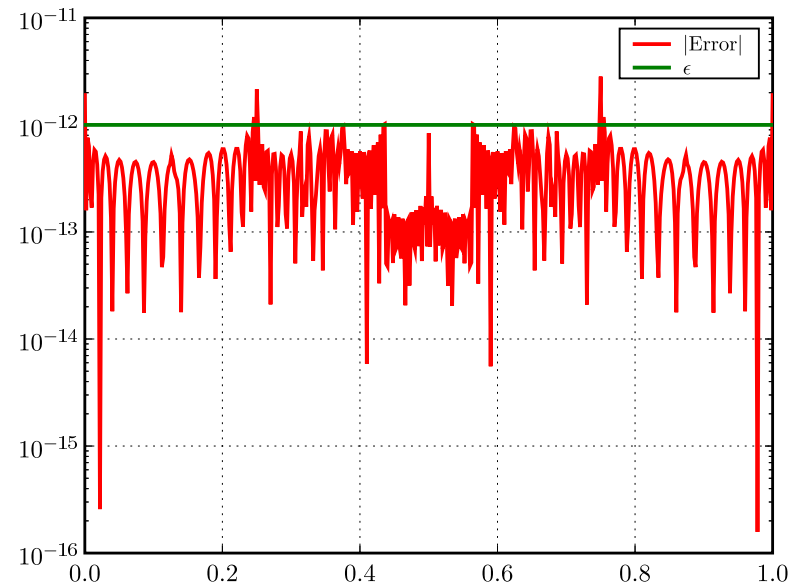
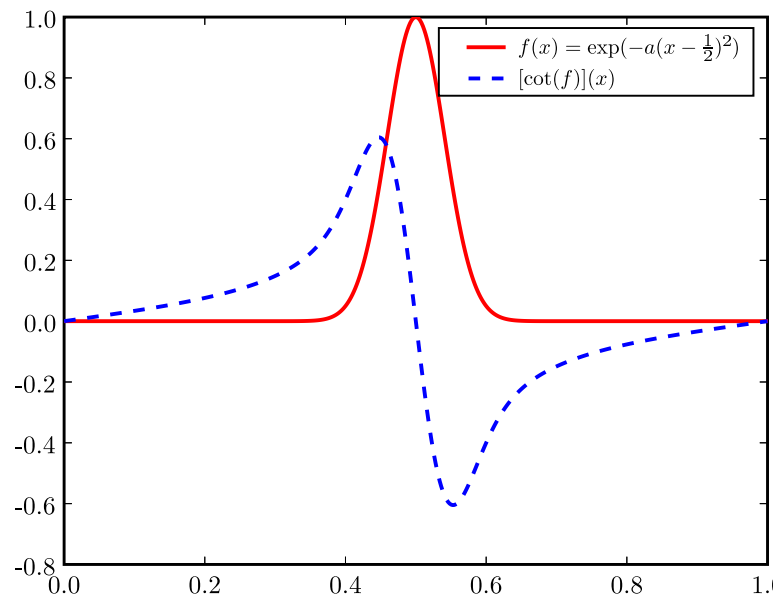


Example in 1D

The periodized Hilbert transform,

$$(Cf)(y) = \text{p.v.} \int_0^1 \cot(\pi(y-x)) f(x) dx,$$

$$f(x) = \sum_{k \in \mathbb{Z}} e^{-a(x+k-1/2)^2} \rightarrow (Cf)(y) = i\sqrt{\frac{\pi}{a}} \sum_{n \in \mathbb{Z}} \text{sign}(n) e^{-n^2\pi^2/a} e^{2\pi i n y}$$



The separated representation of the Poisson kernel

For the Poisson kernel in multiwavelet basis we need to compute $t_{ii',jj',kk'}^{n;1} = 2^{-2n} t_{ii',jj',kk'}^1$, where

$$t_{ii',jj',kk'}^1 = t_{ii',jj',kk'}^{l_1,l_2,l_3} = \frac{1}{4\pi} \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \frac{1}{\|\mathbf{x} + \mathbf{1}\|} \Phi_{ii'}(x_1) \Phi_{jj'}(x_2) \Phi_{kk'}(x_3) d\mathbf{x},$$

and $\Phi_{ii'}(x)$, $i, i' = 0, \dots, k-1$ are the cross-correlation functions of the scaling functions.

Theorem: For any $\epsilon > 0$ the coefficients $t_{ii',jj',kk'}^1$ have an approximation with a low separation rank,

$$r_{ii',jj',kk'}^1 = \sum_{m=1}^M \frac{w_m}{b} F_{ii'}^{m,l_1} F_{jj'}^{m,l_2} F_{kk'}^{m,l_3},$$

where

$$F_{ii'}^{m,l} = \int_{-1}^1 e^{-\tau_m(x+l)^2} \Phi_{ii'}(x) dx,$$

and $M = O(-\log \epsilon)$.

Functions of operators

Consider the problem of applying \mathcal{G}_μ^α , $0 < \alpha < 3/2$, $\mu \in \mathbb{R}$, where

$$\mathcal{G}_\mu^\alpha = \left(-\frac{1}{2}\nabla^2 + \mu^2\mathcal{I}\right)^{-\alpha}.$$

The kernel is a radial function,

$$\mathcal{G}_\mu^\alpha(\mathbf{x}) = \frac{2^{-\frac{1}{2}}}{\Gamma(\alpha)\pi^{\frac{3}{2}}}\left(\frac{\mu}{r}\right)^{\frac{3}{2}-\alpha}K_{\frac{3}{2}-\alpha}(\mu r),$$

where $r = \|\mathbf{x}\|$ and K is the modified Bessel function of the second kind.

If $\alpha = 1$, then $\mathcal{G}_\mu^1 = G_\mu$ is the Green's function; if $\alpha = 1/2$ then $\mathcal{G}_\mu^{1/2}(\mathbf{x})$ is the "inverse square root" (pseudodifferential) operator, etc.

Approximation of \mathcal{G}_μ^α by Gaussians

We approximate the kernel $\mathcal{G}_\mu^\alpha(r)$ by Gaussians using

$$\mathcal{G}_\mu^\alpha(\mathbf{x} - \mathbf{y}) = -\frac{1}{2^{2\alpha-1}\Gamma(\alpha)\pi^{3/2}} \int_{-\infty}^{\infty} e^{-\|\mathbf{x}-\mathbf{y}\|^2 e^{2s}} e^{-\frac{1}{4}\mu^2 e^{-2s} + (3-2\alpha)s} ds.$$

For $\alpha = 1$ we obtain an integral representation for the bound state Helmholtz kernel,

$$\mathcal{G}_\mu^1(\mathbf{x} - \mathbf{y}) = -\frac{1}{2\pi^{3/2}} \int_{-\infty}^{\infty} e^{-\|\mathbf{x}-\mathbf{y}\|^2 e^{2s}} e^{-\frac{1}{4}\mu^2 e^{-2s} + s} ds,$$

and, for $\alpha = 1/2$,

$$\mathcal{G}_\mu^{1/2}(\mathbf{x} - \mathbf{y}) = -\frac{1}{\pi^2} \int_{-\infty}^{\infty} e^{-\|\mathbf{x}-\mathbf{y}\|^2 e^{2s}} e^{-\frac{1}{4}\mu^2 e^{-2s} + 2s} ds.$$

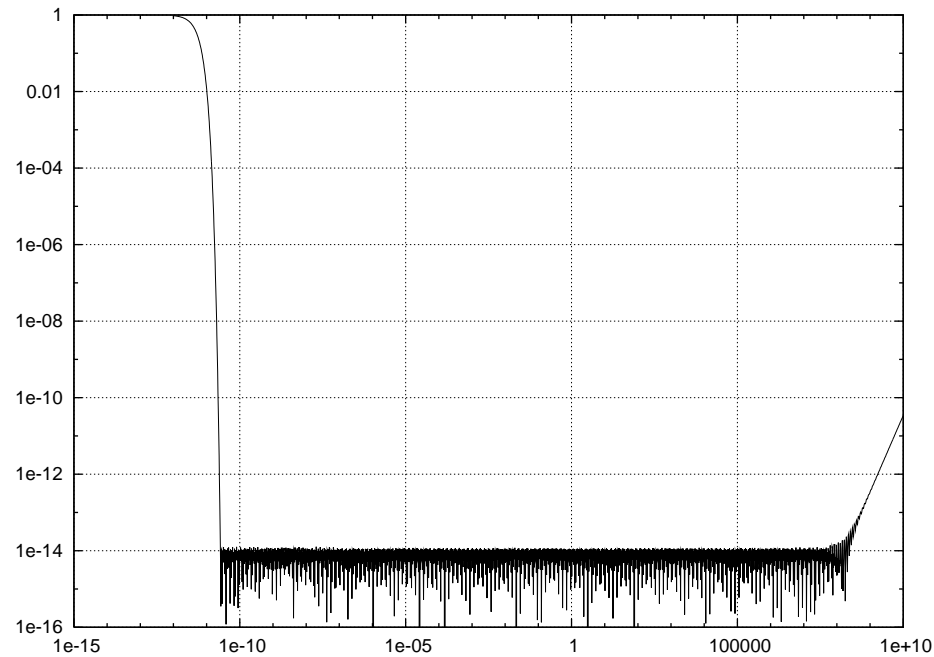
Discretization of these integrals leads to the desired representation via Gaussians.

Example

For a given accuracy ϵ , the operator is supplied as a set $\{w_m, p_m\}_{m=1}^M$, for example

$$\left| \mathcal{G}_\mu^{1/2}(\mathbf{x} - \mathbf{y}) - \sum_{m=1}^M w_m e^{-p_m \|\mathbf{x} - \mathbf{y}\|^2} \right| \leq \epsilon \left| \mathcal{G}_\mu^{1/2}(\mathbf{x} - \mathbf{y}) \right|,$$

for $\delta \leq \|\mathbf{x} - \mathbf{y}\| \leq 1$, where $p_m, w_m > 0$ and $M = \mathcal{O}(\log \delta^{-1})$.

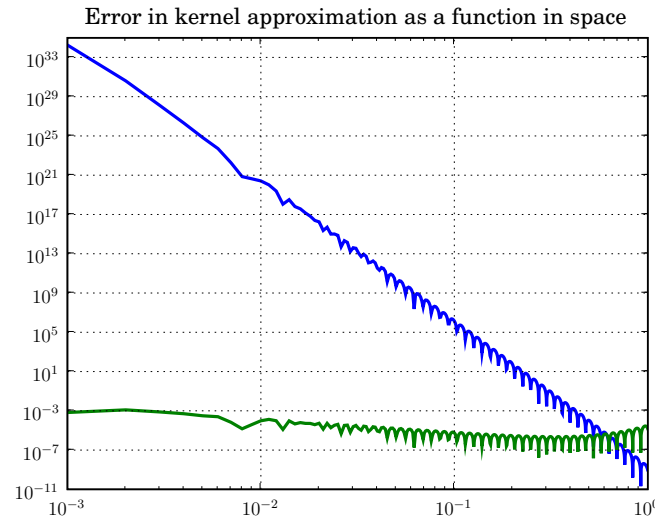


Error (\log_{10}) of approximating $\mathcal{G}_\mu^{1/2}(\mathbf{x} - \mathbf{y})$ for $10^{-10} \leq \|\mathbf{x} - \mathbf{y}\| \leq 10^8$, $M = 437$.

An estimate for the approximation

We prove

Theorem. For any $\epsilon > 0$, $\mu < 0$ and N , the N -particle Green's function \mathcal{G}_μ has a separated representation (via Gaussians) with the relative error ϵ in the *operator norm* and with the number of terms, $L = \mathcal{O}((\log \epsilon^{-1})^2)$, independent of μ and N .



As the number of particles increases, the approximate and the exact multiparticle Green's functions differ significantly as *functions* but, when used as operators, produce results that differ only up to a fixed but arbitrary accuracy.

The Helmholtz kernel $G(r) = e^{i\kappa r}/r$

Consider

$$\hat{G}(\mathbf{p}) = \frac{1}{|\mathbf{p}|^2 - \kappa^2},$$

where $\mathbf{p} \in \mathbb{R}^d$. The inverse Fourier transform of \hat{G} is a singular integral and its usual regularization

$$G^\pm(\mathbf{x}) = \lim_{\lambda \rightarrow 0^+} \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{e^{i\mathbf{x} \cdot \mathbf{p}}}{|\mathbf{p}|^2 - \kappa^2 \mp i\lambda} d\mathbf{p},$$

yields the outgoing and incoming Green's functions

$$G^\pm(\mathbf{x}) = \frac{1}{4\pi} \frac{e^{\pm i\kappa|\mathbf{x}|}}{|\mathbf{x}|}$$

in dimension $d = 3$ and

$$G^\pm(\mathbf{x}) = \frac{i}{4} H_0^{(1)}(\pm\kappa|\mathbf{x}|) = -\frac{1}{4} Y_0(\pm\kappa|\mathbf{x}|) + \frac{i}{4} J_0(\pm\kappa|\mathbf{x}|)$$

in dimension $d = 2$.

Splitting between the spatial and Fourier domains

We approximate the real part of the Green's function

$$(\mathcal{R}e(G) * f)(\mathbf{x}) = \frac{1}{(2\pi)^d} \text{p.v.} \int_{\mathbb{R}^d} \hat{G}(\mathbf{p}) \hat{f}(\mathbf{p}) e^{i\mathbf{x} \cdot \mathbf{p}} d\mathbf{p}$$

by splitting this operator into two,

$$\hat{G}(\rho) = \hat{F}_{sing}(\rho) + \hat{F}_{oscill}(\rho),$$

where

$$\hat{F}_{sing}(\rho) = \frac{1 - e^{-\alpha^2(\rho^2 - \kappa^2)/\kappa^2}}{\rho^2 - \kappa^2},$$
$$\hat{F}_{oscill}(\rho) = \frac{e^{-\alpha^2(\rho^2 - \kappa^2)/\kappa^2}}{\rho^2 - \kappa^2},$$

and α is a real parameter. Approximation of both parts again involves Gaussians.

Estimate

Theorem. Let $D \subset \mathbb{R}^d$, $d = 2, 3$, be a bounded domain such that $\text{diam}(D) \leq 1$.

Given $\epsilon > 0$,

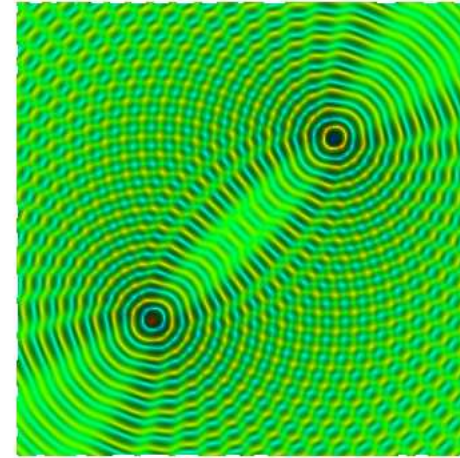
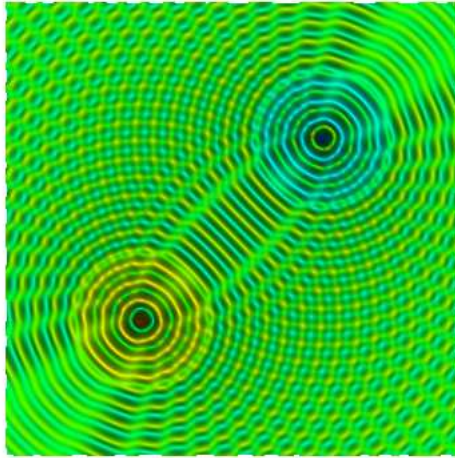
$$\tilde{G}_R(r) = S_{sing}(r) + S_{oscill}(r).$$

and $f \in L^p(D)$ for $1 \leq p \leq \infty$, we have

$$\left\| \left(\mathcal{R}e(G) - \tilde{G}_R \right) * f \right\|_{L^p(D)} \leq \epsilon \|f\|_{L^p(D)}.$$

Overall computational complexity: no worse than $\mathcal{O}(\kappa^d \log \kappa + C(\log \epsilon^{-1})^d)$.

Example



Convolution of a cylindrical “dipole” with the Green’s function where $k = 50\pi$ (real and imaginary parts). The algorithm involves splitting application of the operator between the spatial and Fourier domains.

Quasi-periodic Green's function

Let us consider the quasi-periodic Helmholtz Green's function to solve

$$\begin{aligned}(\Delta + \kappa^2) u(\mathbf{x}) &= -f(\mathbf{x}), \\ u(\mathbf{x} + \mathbf{l}) &= e^{-i\mathbf{k}\cdot\mathbf{l}} u(\mathbf{x}).\end{aligned}$$

so that

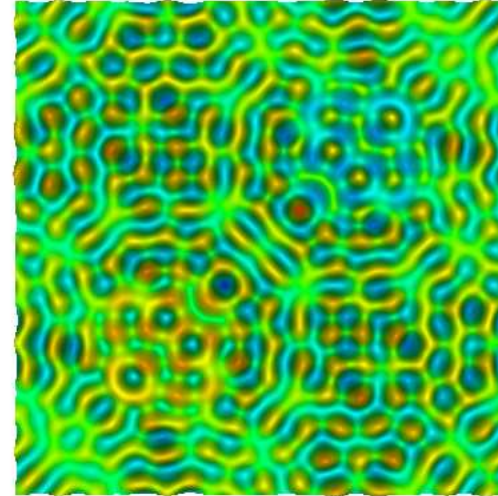
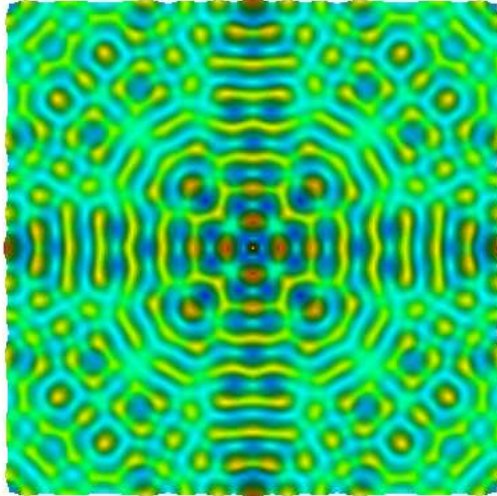
$$u(\mathbf{x}) = \int_D G_q(\mathbf{x} - \mathbf{y}) f(\mathbf{y}) d\mathbf{y},$$

for functions $f \in L^p(D)$, where D is the primitive cell of a Bravais lattice Λ defined by d linearly independent vectors in dimension $d \geq 2$. The Green's function G_q satisfies

$$\begin{aligned}(\Delta + \kappa^2) G_q(\mathbf{x}) &= -\delta(\mathbf{x}) \\ G_q(\mathbf{x} + \mathbf{l}) &= e^{-i\mathbf{k}\cdot\mathbf{l}} G_q(\mathbf{x}),\end{aligned}$$

where $\kappa > 0$, $\mathbf{l} \in \Lambda$, $\mathbf{x} \in D$, and $\mathbf{k} \in \mathbb{R}^d$ is a quasi-periodicity vector, sometimes referred to as Bloch or crystal momentum vector.

Quasi-Periodic Helmholtz Green's functions on a lattice



Convolution of a cylindrical "dipole" with the periodic Green's function on a cubic lattice

Green's function satisfying boundary conditions

For ease of notation let consider the two dimensional case with Dirichlet boundary conditions on the primitive cell $D = [-1/2, 1/2] \times [-1/2, 1/2]$. We construct this Green's function using the periodic Green's function (with 2κ instead of κ), satisfying

$$(\Delta + 4\kappa^2)G_p(\mathbf{x}) = -\delta(\mathbf{x}),$$

and periodic b.c. (i.e., quasi-periodic with $\mathbf{k} = 0$). We obtain the Green's function with Dirichlet boundary conditions on D as

$$G^D(x_1, x_2, y_1, y_2) = G_p\left(\frac{x_1 - y_1}{2}, \frac{x_2 - y_2}{2}\right) - G_p\left(\frac{x_1 + y_1 + 1}{2}, \frac{x_2 - y_2}{2}\right) - G_p\left(\frac{x_1 - y_1}{2}, \frac{x_2 + y_2 + 1}{2}\right) + G_p\left(\frac{x_1 + y_1 + 1}{2}, \frac{x_2 + y_2 + 1}{2}\right).$$

In 3D we have 9 terms, etc.

Approximation of Green's functions satisfying b. c.

For a desired accuracy ϵ , we construct q_j and σ_j for $j = 1, \dots, N$ to obtain the separated representation

$$\tilde{G}_{spatial}^D(x_1, x_2, y_1, y_2) = \sum_{\sqrt{n_1^2 + n_2^2} \leq a} \sum_{j=1}^N q_j S_{j,n_1}(x_1, y_1) S_{j,n_2}(x_2, y_2),$$

where $S_{j,n}(x, y) = e^{-\frac{\sigma_j}{4}(x-y+2n)^2} - e^{-\frac{\sigma_j}{4}(x+y+1+2n)^2}$. In the Fourier domain, we obtain

$$\tilde{G}_{fourier}^D(x_1, x_2, y_1, y_2) = \sum_{2\pi\sqrt{m_1^2 + m_2^2} \leq \kappa b} \frac{e^{\frac{-\pi^2(m_1^2 + m_2^2) + \kappa^2}{\eta^2}}}{4(\pi^2(m_1^2 + m_2^2) - \kappa^2)} e^{i\pi(m_1 x_1 + m_2 x_2)} \times \\ \left(e^{-i\pi m_1 y_1} - e^{i\pi m_1 (y_1 + 1)} \right) \left(e^{-i\pi m_2 y_2} - e^{i\pi m_2 (y_2 + 1)} \right).$$

The Green's Function for N-particle confining harmonic potential

Let us consider the Hamiltonian for the confining harmonic potential in 1D,

$$\mathcal{H} = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{x^2}{2}.$$

The operator \mathcal{H} has discrete spectrum $\lambda_n = n + \frac{1}{2}$, $n = 0, 1, \dots$, and its eigenfunctions are well-known so that

$$K_{\mathcal{H}}(x, y) = e^{-(x^2+y^2)/2} \sum_{n=0}^{\infty} \frac{\lambda_n}{\sqrt{\pi} 2^n n!} H_n(x) H_n(y),$$

where H_n are the Hermite polynomials.

The kernel of $e^{-t\mathcal{H}}$

For the kernel of $e^{-t\mathcal{H}}$, we have

$$K_{e^{-t\mathcal{H}}}(x, y) = e^{-(x^2+y^2)/2} \sum_{n=0}^{\infty} \frac{e^{-t\lambda_n}}{\sqrt{\pi} 2^n n!} H_n(x) H_n(y),$$

and (with a little bit of work)

$$K_{e^{-t\mathcal{H}}}(x, y) = \frac{1}{\sqrt{2\pi \sinh(2t)}} e^{-(x-y)^2/(2 \sinh(2t))} e^{-\tanh(t) (x^2+y^2)/2}.$$

Separated approximation of \mathcal{H}^{-1} .

We have $\mathcal{H}^{-1} = \int_0^\infty e^{-t\mathcal{H}} dt$. Since $1/\lambda_n = \int_0^\infty e^{-t\lambda_n} dt$ and $1/2 \leq \lambda_n$ for $n = 0, 1, \dots$, we approximate

$$\left| \int_0^\infty e^{-t\lambda_n} dt - \sum_{m=0}^M w_m e^{-t_m \lambda_n} \right| \leq \epsilon,$$

with $M = \mathcal{O}(\log \epsilon^{-1})$ and arrive at the representation

$$\mathcal{H}^{-1} = \sum_{m=1}^M w_m e^{-t_m \mathcal{H}}$$

or

$$\mathcal{H}^{-1}(x, y) = \sum_{m=1}^M w_m K_{e^{-t_m \mathcal{H}}}(x, y).$$

Importance of this example

Generalizing to multi-particle/multi-dimensional case, we have

$$\mathcal{H}^{-1}(\mathbf{x}, \mathbf{y}) = \frac{1}{\sqrt{2\pi}} \sum_{m=1}^M \frac{w_m}{\sqrt{\sinh(2t_m)}} e^{-\tanh(t_m) \|\mathbf{x}\|^2/2 - \|\mathbf{x}-\mathbf{y}\|^2/(2 \sinh(2t_m)) - \tanh(t_m) \|\mathbf{y}\|^2/2}$$

or

$$\mathcal{H}^{-1}(\mathbf{x}_1, \mathbf{y}_1, \dots, \mathbf{x}_N, \mathbf{y}_N) = \sum_{m=1}^M \tilde{w}_m \prod_{j=1}^N e^{-\tau_m \|\mathbf{x}_j\|^2} e^{-\sigma_m \|\mathbf{x}_j - \mathbf{y}_j\|^2} e^{-\tau_m \|\mathbf{y}_j\|^2}.$$

Conjecture:

The Green's functions (!restricted to subspaces spanned by bound states!) of other confining potentials have short representations of this form, where the exponents and coefficients are determined numerically.

Numerical experiments several years ago appear to confirm this conjecture.

Reduction problem in higher dimensions

Given a function

$$f(x_1, x_2, \dots, x_N) = \sum_{m=1}^M w_m e^{-\sum_{j=1}^N \tau_{m,j} x_j},$$

where $x_j \in [0, 1]$, $\tau_{m,j} > 0$, and $w_m > 0$, find for a given accuracy ϵ a function

$$g(x_1, x_2, \dots, x_N) = \sum_{m=1}^{\hat{M}} \hat{w}_m e^{-\sum_{j=1}^N \hat{\tau}_{m,j} x_j},$$

such that $\hat{M} < M$ and $\|f - g\| \leq \epsilon$.

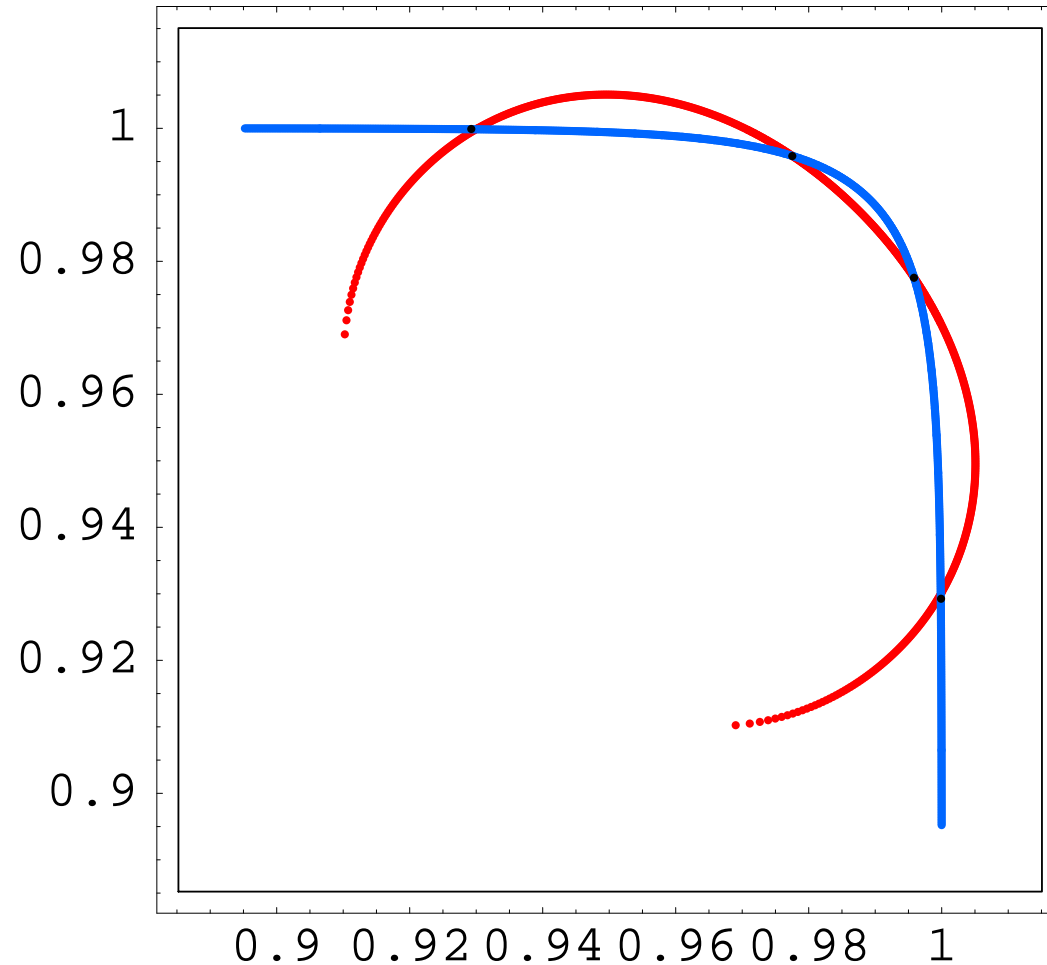
We know how to solve this problem for $N = 1$ (in a much more general setting) and have preliminary results for $N=2$. We are working on algorithms for $N \geq 3$.

How to find the reduced set of nodes?

In contrast with the one dimensional case, we are not aware of *any* theoretical results to guide us.

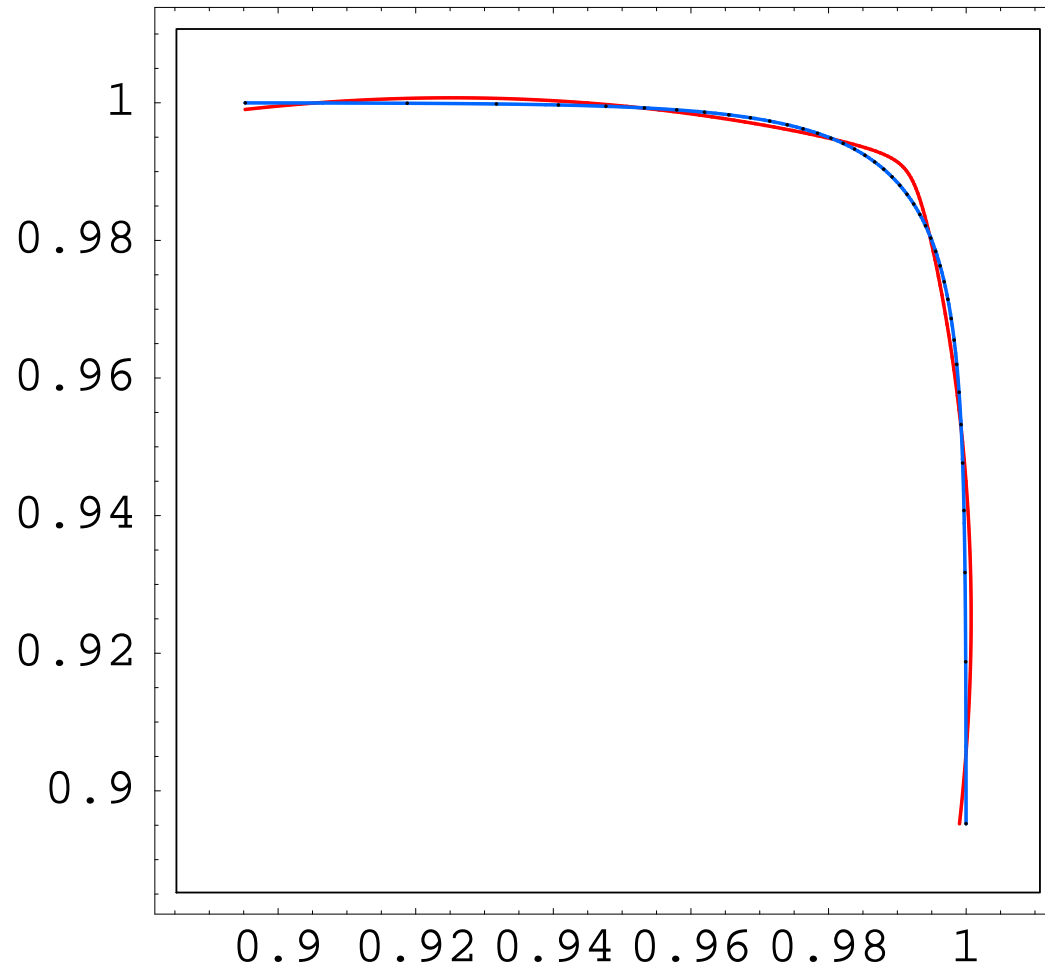
- We conjecture (and confirm by many examples) that the optimal nodes lie on the curve defined by the zeros of the c-eigenpolynomial (an **eigencurve** or **eigensurface**). We have a way of finding c-eigenpolynomials in any dimension.
- We use the “original curve” to select appropriate (initial) nodes on the eigencurve. We then optimize positions of these nodes (they move only slightly).
- Most of the theory still needs to be developed

Example: finding optimal nodes in 2D



Intersection between eigencurves with indices 4 (red) and 11 (blue). The 4 (optimal) nodes (vs. 41 original nodes) yield approximation with l_∞ error $1.6 \cdot 10^{-2}$.

Finding optimal nodes in 2D



Intersection between eigencurves with indices 6 (red) and 11 (blue). The black dots are the original 41 nodes.

Error of approximation vs. singular values

#of Terms=Index	Error	Normalized singular values
4	$1.6 \cdot 10^{-2}$	$7.8 \cdot 10^{-5}$
5	$1.6 \cdot 10^{-3}$	$1.6 \cdot 10^{-6}$
6	$1.5 \cdot 10^{-4}$	$3.5 \cdot 10^{-7}$
7	$9.2 \cdot 10^{-6}$	$3.7 \cdot 10^{-9}$
8	$7.5 \cdot 10^{-7}$	$2.2 \cdot 10^{-9}$
9	$5.7 \cdot 10^{-8}$	$2.0 \cdot 10^{-11}$
10	$1.7 \cdot 10^{-9}$	$5.2 \cdot 10^{-12}$

l_∞ error for different number of terms and their corresponding singular values (normalized by the first singular value).

Conclusions

Success consists of going from failure to failure without loss of enthusiasm.

Winston Churchill

- Nonlinear approximations of a wide class of important operators of mathematical physics lead to fast algorithms (with controlled accuracy)
- MADNESS (I anticipate more on this in Robert Harrison's talk)
- The approach uses data structures that are different (surprise!) than anticipated originally
- Future will see a fully developed operator calculus (computing approximations to functions of operators rather than just solving problems).
- Many difficult issues to address!