On approximation of operators by Gaussians

Gregory Beylkin

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Plan of the talk

- A review of approximation of convolution operators and corresponding fast algorithms:
  - non-oscillatory kernels
  - multiparticle Green's function
  - oscillatory Green's function for Helmholtz operator
- Approximating non-convolutions (two examples):
  - Green's function satisfying boundary conditions on simple domains
  - Green's function for quantum harmonic oscillator
- Some comments on non-linear approximation by exponentials

Participants

- Gregory Beylkin, Lucas Monzón, University of Colorado
- Christopher Kurcz, National Cancer Institute
- Fernando Pérez, UC Berkeley
- Martin Mohlenkamp - Ohio University
- Robert Harrison and George Fann - Oak Ridge National Lab

Gaussians in Quantum Chemistry and Computing

- Since the 1960's chemists used products of Gaussians and polynomials 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.

- Gaussians were also used to represent Coulomb potential, see W. Kutzelnigg, Internat. J. Quantum Chem. 51, 1994.

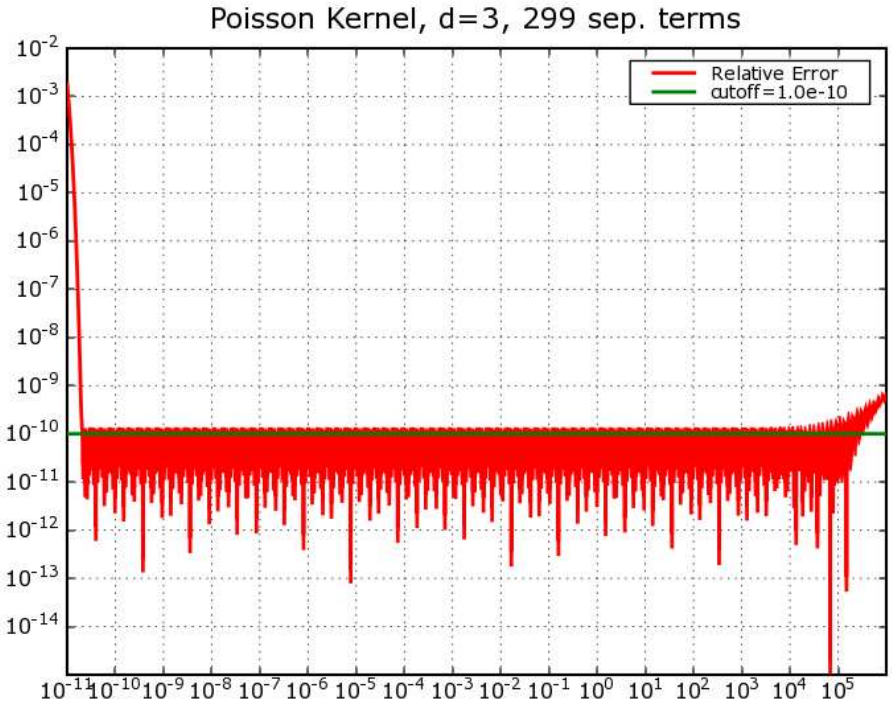
- We are using Gaussians to approximate non-oscillatory Green's functions, *see R.J. Harrison, G.I. Fann, T. Yanai, Z. Gan and G. Beylkin, J. Chem. Phys. v. 121, n. 23, 14, 7, 2004* and, recently, oscillatory Green's functions, *see G. Beylkin, C. Kurcz and L. Monzon, Fast algorithms for Helmholtz Green's 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*.

Example: the Poisson kernel

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 $M = \mathcal{O}(-\log \delta)$.



Approximating functions by linear combination of exponentials

- For $\epsilon > 0$ approximate f,

$$\left| f(r) - \sum_{m=1}^{M} w_m e^{-\tau_m r} \right| < \epsilon, \quad \forall r \in [0, b],$$

  with a small (minimal) number of **complex** coefficients w_m and exponents τ_m, with $\mathcal{R}e(\tau_m) \geq 0$.

- The smooth function f may be oscillatory, periodic, non-periodic, or singular.

- We observed (for non-singular),

$$M = \mathcal{O}(\log b) + \mathcal{O}(\log \epsilon^{-1}).$$

Approximation of power functions $r^{-\alpha}$ for $\alpha > 0$

Given $\epsilon > 0$, $\delta > 0$, we know how to obtain

$$\left| r^{-\alpha} - \sum_{m=1}^{M} w_m e^{-\tau_m \rho} \right| \leq \epsilon\, r^{-\alpha}, \quad \delta < r \leq 1,$$

with $w_m > 0$, $\tau_m > 0$ and small M.

- We now have a simpler and more revealing proof to show that

$$M = \log \epsilon^{-1} [c_0 + c_1 \log \delta^{-1} + c_2 \log \epsilon^{-1}],$$

  where c_k are constants that only depend on α.

- With additional reduction of terms, we observe

$$M = \log \epsilon^{-1} [\tilde{c}_0 + \tilde{c}_1 \log \delta^{-1}].$$

Exponential models (one-dimensional)

- Algorithm solves a non-linear approximation problem to find weights and exponents. Each representation is tailored to the function, interval and accuracy.
- In practice, we approximate uniform samples $f(\frac{bk}{N})$, $0 \leq k \leq N$, with N chosen to properly oversample f.
- The approximation is not unique since w_m and τ_m depend on ϵ, b, and N.
- Approximating $f(\sqrt{r})$ yields an approximation of $f(r)$ in terms of Gaussians.
- We may use relative or absolute error in our approximations.

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).

Approximating $r^{-\alpha}$

- We first obtain a sub-optimal exponential approximation and then use a variation of the algorithm (reduction) to find a shorter representation.

- Using

$$r^{-\alpha} = \frac{1}{\Gamma(\alpha)} \int_{-\infty}^{\infty} e^{-e^t r + \alpha t} dt$$

  and trapezoidal rule to discretize the integral yields an approximation (say M terms).

- Originally we used the Euler-Maclaurin formula to estimate M and endpoints in the integral truncation, in terms of ϵ, δ, and α (quite involved).

Simpler 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

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

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

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

- 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 $r^{-\alpha}$

Changing variables $s = e^t r$

$$\Gamma(\alpha) = \int_0^\infty e^{-s} s^{\alpha-1} ds = r^\alpha \int_{-\infty}^\infty e^{-e^t r + \alpha t} dt,$$

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

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

The choice of h depends only on ϵ and α.

Estimating the discretization step h

For positive y, we have

$$\frac{|\Gamma(\alpha - iy)|}{\Gamma(\alpha)} \leq (\cos 1)^{-\alpha} e^{-y}.$$

With $y = \frac{2\pi}{h}$, we obtain

$$\sum_{n \neq 0} \frac{|\Gamma(\alpha - iyn|}{\Gamma(\alpha)} \leq 2(\cos 1)^{-\alpha} \sum_{n \geq 1} e^{-yn} = \frac{2(\cos 1)^{-\alpha}}{e^y - 1} < \epsilon,$$

if

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

The "Poisson" series provides, in relative norm, a (uniform) exponential approximation for all positive r,

$$\left| r^{-\alpha} - h \sum_{n \in \mathbb{Z}} f(s + nh) \right| \leq \epsilon\, r^{-\alpha}, \quad r > 0.$$

Estimating the series' tails

Monotonicity of f and 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

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

much cleaner than the original approach via Euler-Mclaurin formula.

An alternative to the reduction algorithm

$$r^{-\alpha} = \int_{-\infty}^{\infty} \frac{e^{\alpha t}}{\Gamma(\alpha)} e^{-e^t r} dt$$

- The uniform grid is appropriate for the exponential decay of the integrand as $t \to +\infty$, but is excesive as $t \to -\infty$. In the redundant portion the exponents of the form $-e^{-hn}$ are very small.

- Instead of using the reduction algorithm (reduces number of terms in an exponential sum), we rewrite the problem using Taylor expansions and apply Prony's method to obtain a shorter sum.

Using Prony for small exponents

Approximate in $r \in [0,1]$ an exponential sum (with small exponents) by a shorter one. By Taylor approximation,

$$\sum_{m=1}^{M_0} \rho_m e^{\alpha_m r} \approx \sum_{k=0}^{2M-1} h_k \frac{r^k}{k!},$$

where

$$h_k = \sum_{m=1}^{M_0} \rho_m \alpha_m^k$$

is a fast decaying sequence and $M \ll M_0$.

Using Prony, the $2M$ coefficients h_k may be written using $2M$ new variables, M weights w_m and M nodes γ_m (assumed distinct and within the unit circle),

$$h_k = \sum_{m=1}^{M} w_m \gamma_m^k, \quad 0 \le k < 2M,$$

a representation which we use for all $k \ge 0$.

Using Prony for small exponents (continue)

The approximation is then

$$\sum_{m=1}^{M_0} \rho_m e^{\alpha_m r} \approx \sum_{k=0}^{\infty} h_k \frac{r^k}{k!} = \sum_{k=0}^{\infty} (\sum_{m=1}^{M} w_m \gamma_m^k) \frac{r^k}{k!} = \sum_{m=1}^{M} w_m e^{\gamma_m r},$$

Assumptions

- α_k are small enough as to warranty small M.
- The nodes γ_k are distinct and if α_k are real they are also real.

Prony (Gaspard Clair François Marie Riche de Prony)

Represent $(h_0, \ldots, h_{2M-1})$ as $h_k = \sum_{m=1}^{M} w_m \gamma_m^k$. To find γ_m, define the polynomial

$$Q(z) = \prod_{m=1}^{M} (z - \gamma_m) = \sum_{k=0}^{M} q_k z^k$$

and note that for all k with $0 \leq k < M$,

$$\sum_{l=0}^{M} h_{k+l} q_l = \sum_{m=1}^{M} w_m \gamma_m^k \sum_{l=0}^{M} q_l \gamma_m^l = 0,$$

and then

$$\sum_{l=0}^{M-1} h_{k+l}\, q_l = -h_{M+k} \equiv b_k.$$

Thus, the vector $q = (q_0, \cdots, q_{M-1})$ is the solution of the linear system $Hq = b$, where H is the (non-singular) $M \times M$ Hankel matrix h_{k+l}. With q, form the polynomial $Q(z)$ and find its roots γ_m. Weights are solutions of a Vandermonde system.

Fast algorithms for applying operators

Numerical algorithms we develop

- 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

A brief review: applying operator to a function $g = Tf$

We have

$$V_0 \subset V_1 \subset V_2 \subset \cdots \subset V_j \cdots$$

or, with $V_j \oplus W_j = V_{j+1}$, for each V_n, $V_n = V_0 \oplus W_0 \oplus W_1 \oplus \cdots \oplus W_{n-1}$.

Consider orthogonal projectors

$$P_j : L^2([0,1]^d) \to V_j, \quad Q_j : L^2([0,1]^d) \to W_j$$

where $Q_j = P_{j+1} - P_j$. For an operator $T : L^2([0,1]^d) \to L^2([0,1]^d)$ we define

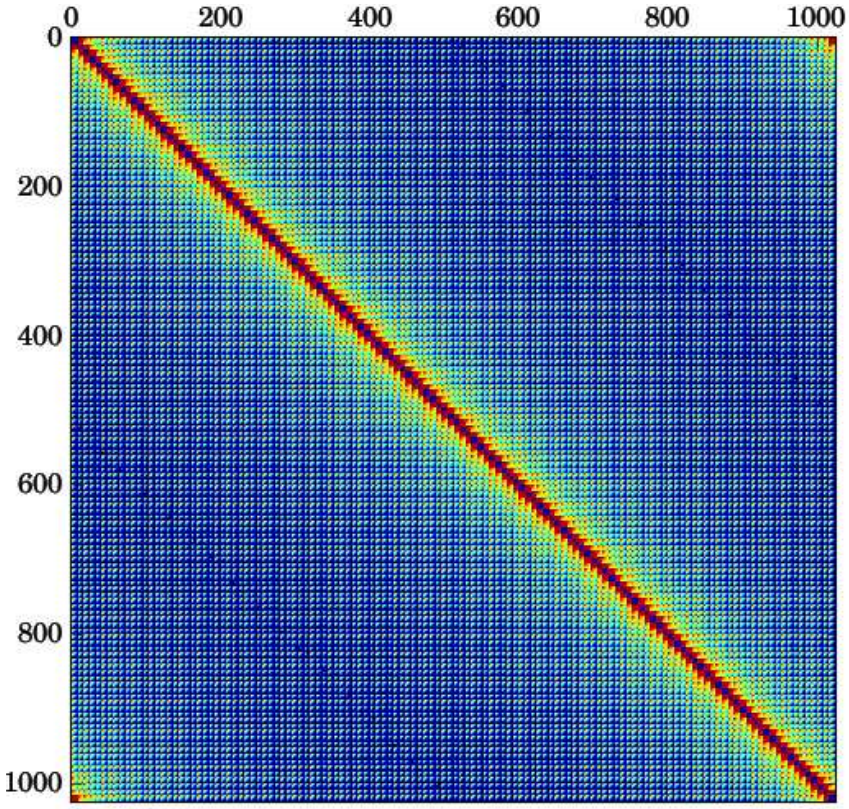
$$T_j = P_j T P_j, \quad T_j : V_j \to V_j$$

and use a telescopic expansion of T_n,

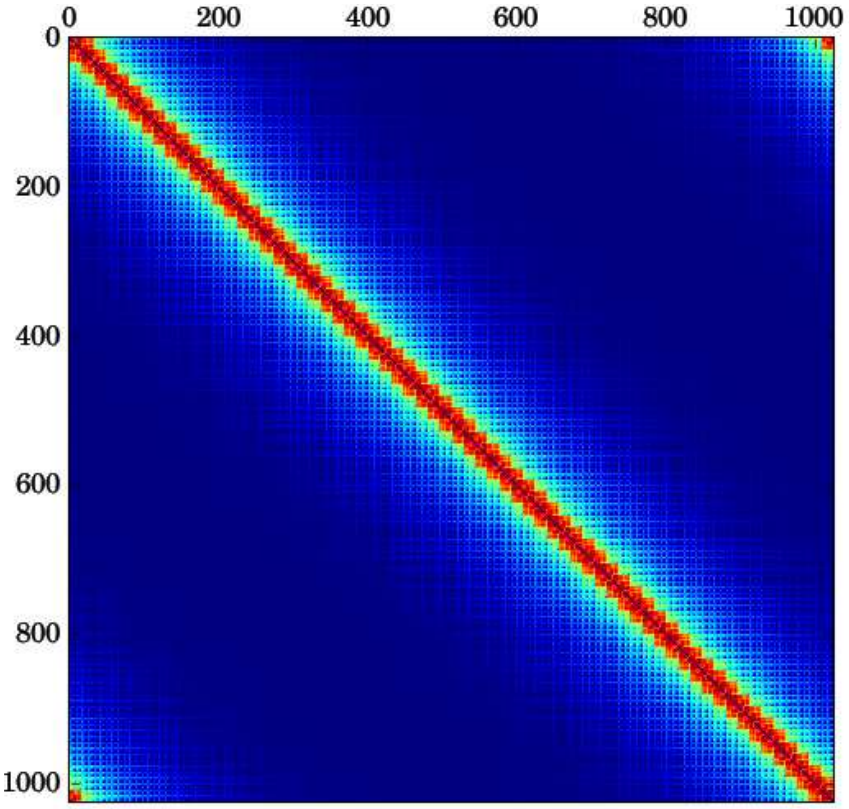
$$T_n = (T_n - T_{n-1}) + (T_{n-1} - T_{n-2}) + \cdots + (T_1 - T_0) + T_0.$$

An example

T_j



$T_j - T_{j-1}$



$j = 7$

The non-standard form

We compute $g = \mathbf{T} f$ using the telescopic expansion,

$$
\begin{aligned}
\hat{g}_0 &= \mathbf{T}_0 f_0 \\
\hat{g}_1 &= [\mathbf{T}_1 - \uparrow (\mathbf{T}_0)] f_1 \\
\hat{g}_2 &= [\mathbf{T}_2 - \uparrow (\mathbf{T}_1)] f_2 \\
\cdots \quad &\cdots \quad \cdots \\
\hat{g}_j &= [\mathbf{T}_j - \uparrow (\mathbf{T}_{j-1})] f_j \\
\cdots \quad &\cdots \quad \cdots
\end{aligned}
$$

The modified ns-form

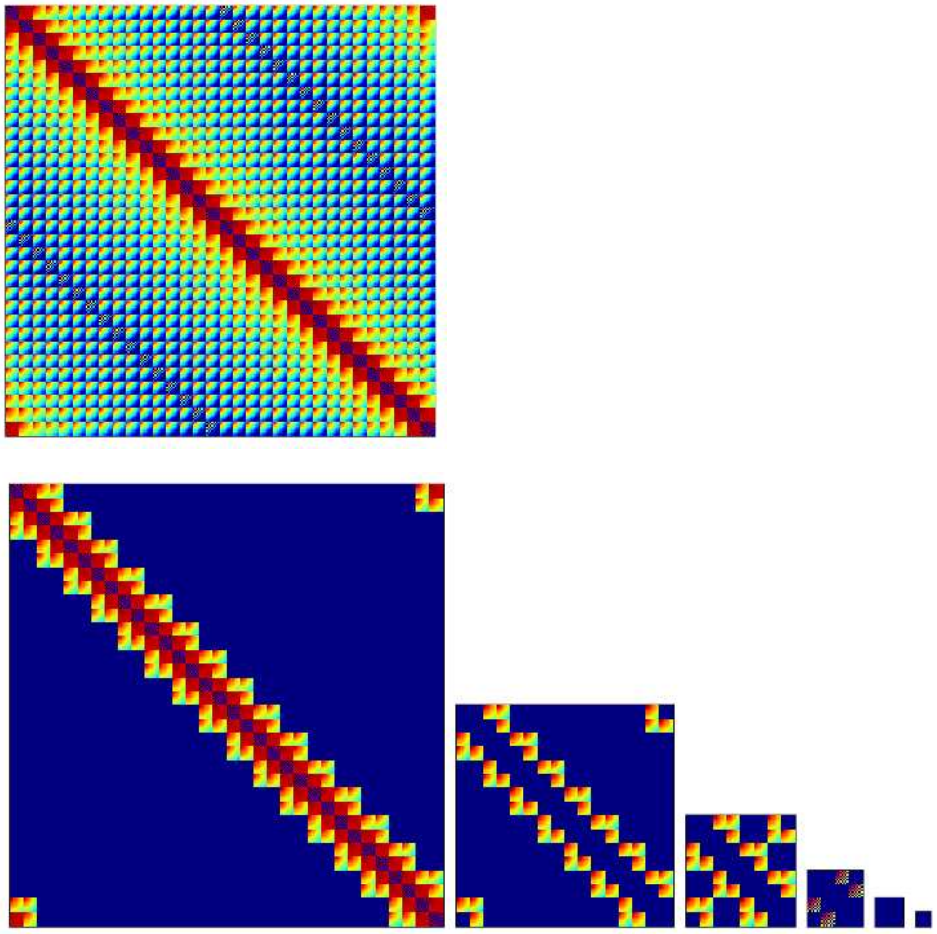
- We first truncate the bands on scale j for the *difference* $T_j - \uparrow T_{j-1}$.
- This defines a banded operator on scale j, $T_j^{b_j} - \uparrow T_{j-1}^{b_j}$, with the band b_j.
- We then bring $\uparrow T_{j-1}^{b_j}$ back to its natural scale, $j-1$

Fully assembled, the result on any given scale n is written as

$$g_n = \mathbf{T}_n^{b_n} f_n + \uparrow \left[\left(\mathbf{T}_{n-1}^{b_{n-1}} - \mathbf{T}_{n-1}^{\lfloor b_n/2 \rfloor} \right) f_{n-1} + \uparrow \left[\left(\mathbf{T}_{n-2}^{b_{n-2}} - \mathbf{T}_{n-2}^{\lfloor b_{n-1}/2 \rfloor} \right) f_{n-2} + \cdots \right. \right.$$
$$\left. \left. \cdots + \left[\uparrow \left[\left(\mathbf{T}_0 - \mathbf{T}_0^{\lfloor b_1/2 \rfloor} \right) f_0 \right] \right] \cdots \right] \right].$$

The modified ns-form

A graphical illustration of what we gain for T_j $(j = 5)$:

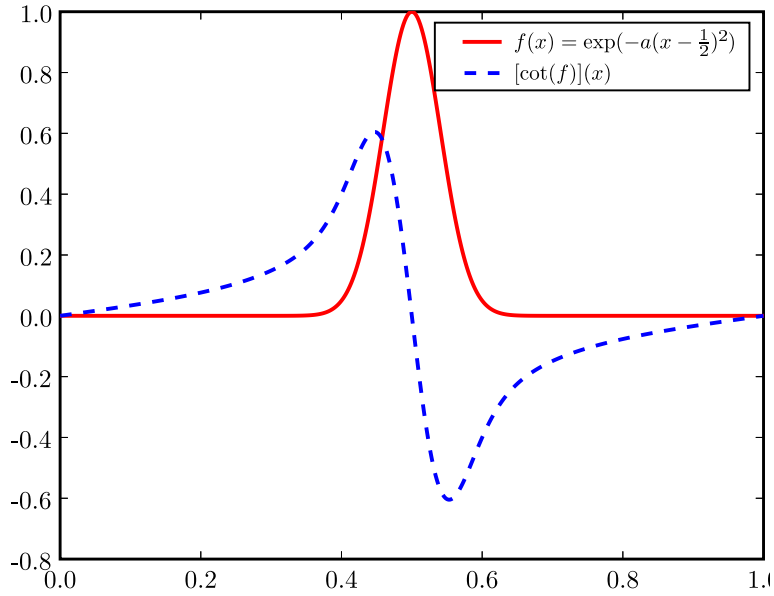


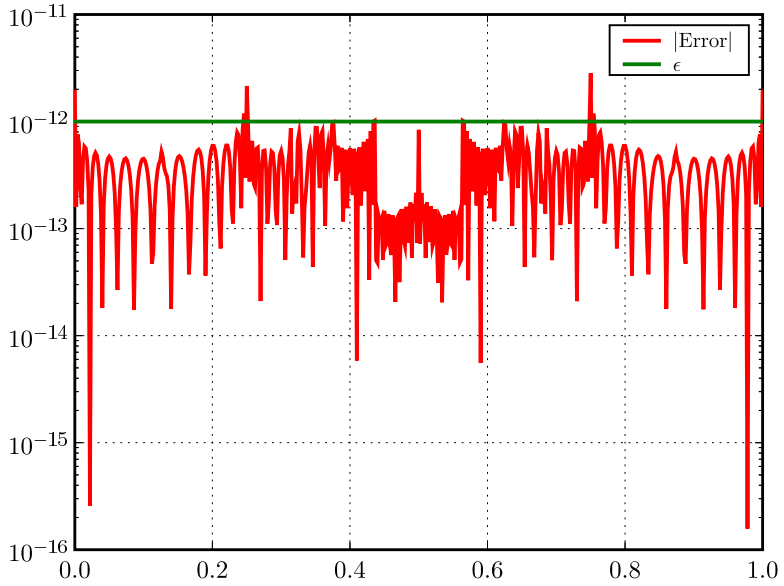
Example in 1D

The periodized Hilbert transform,

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

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





The Poisson kernel in a multiwavelet basis

Due to the homogeneity of the Poisson kernel, we have

$$t^{n;\mathbf{l}}_{ii',jj',kk'} = 2^{-2n}\, t^{\mathbf{l}}_{ii',jj',kk'} \ ,$$

where

$$t^{\mathbf{l}}_{ii',jj',kk'} = t^{l_1,l_2,l_3}_{ii',jj',kk'} = \frac{1}{4\pi}\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} \frac{1}{||\mathbf{x}+\mathbf{l}||}\, \Phi_{ii'}(x_1)\, \Phi_{jj'}(x_2)\, \Phi_{kk'}(x_3)\, d\mathbf{x},$$

and

$$\Phi_{ii'}(x) \ = \ \int_0^1 \phi_i(x+y)\, \phi_{i'}(y) dy \, , \quad i,i' = 0,\ldots,k-1 \, ,$$

are the cross-correlation functions of the scaling functions of the multiwavelet basis.

Gaussians to the rescue: separated representation of the Poisson kernel

Theorem: For any $\epsilon > 0$ the coefficients $t^{\mathbf{l}}_{ii',jj',kk'}$ have an approximation with a low separation rank,

$$r^{\mathbf{l}}_{ii',jj',kk'} = \sum_{m=1}^{M} \frac{w_m}{b} F^{m,l_1}_{ii'} F^{m,l_2}_{jj'} F^{m,l_3}_{kk'} ,$$

such that

$$\begin{aligned} |t^{\mathbf{l}}_{ii',jj',kk'} - r^{\mathbf{l}}_{ii',jj',kk'}| &\leq \frac{2\epsilon}{\pi} \qquad \max_i |l_i| \geq 2 \\ |t^{\mathbf{l}}_{ii',jj',kk'} - r^{\mathbf{l}}_{ii',jj',kk'}| &\leq C\delta^2 + \frac{2\epsilon}{\pi} \qquad \max_i |l_i| \leq 1 \end{aligned}$$

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

$b = \sqrt{3} + ||\mathbf{l}||$, and δ, $M = O(-\log \delta) + O(-\log \epsilon)$, τ_m, w_m, $m = 1, \ldots, M$ come from the separated representation of the kernel.

Outline of a multidimensional algorithm

- Use approximation via Gaussians to express the kernel in a separated form.
- Construct all one-dimensional sparse structures as for $d = 1$.
- Compute the norm estimates for the terms of the separated representation to keep only those above the threshold of accuracy
- Construct banded approximations to $\mathbf{T}_j^{\ell}- \uparrow (\mathbf{T}_{j-1}^{\ell})$
- Build all the necessary indexing tables
- Apply much like in the $d = 1$ case.

Note that if the function is in a separated form then the algorithm simplifies further

Poisson's equation in free space

Let's solve Poisson's equation:

$$\rho(\mathbf{r};\alpha) = \sum_{i=1}^{3}(6\alpha - 4\alpha^2 r_i^2)e^{-\alpha r_i^2} \Longrightarrow \phi(\mathbf{r};\alpha) = \sum_{i=1}^{3} e^{-\alpha r_i^2}, \quad \alpha = 300.$$

We compute

$$\phi(\mathbf{r}) = \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{\rho(\mathbf{r}')}{||\mathbf{r}-\mathbf{r}'||} d\mathbf{r}'.$$

Timings: done on a Pentium 4, 2.8 GHz

Tolerance	Resulting ϵ_{L^2}	Basis order	App. time (s)	MFLOPS
10^{-4}	2.3×10^{-5}	12	2.1	1770
10^{-6}	8.4×10^{-7}	12	12	1670
10^{-8}	2.0×10^{-9}	14	33	1880

Quantum Chemistry

With R. Harrison, G. Fann, T. Yanai and Z. Gan (ORNL)

- Complete elimination of the basis error
- Implementation for one-electron models (HF, DFT)
- Most accurate computations up to now (within these models)
- Correct scaling of cost with system size
- Much smaller computer code than "Gaussians" (<— R. Harrison)

Functions of operators

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

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

The kernel is a radial function,

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

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 $\mathcal{G}_\mu^\alpha$ 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 $\alpha = 1/2$,

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

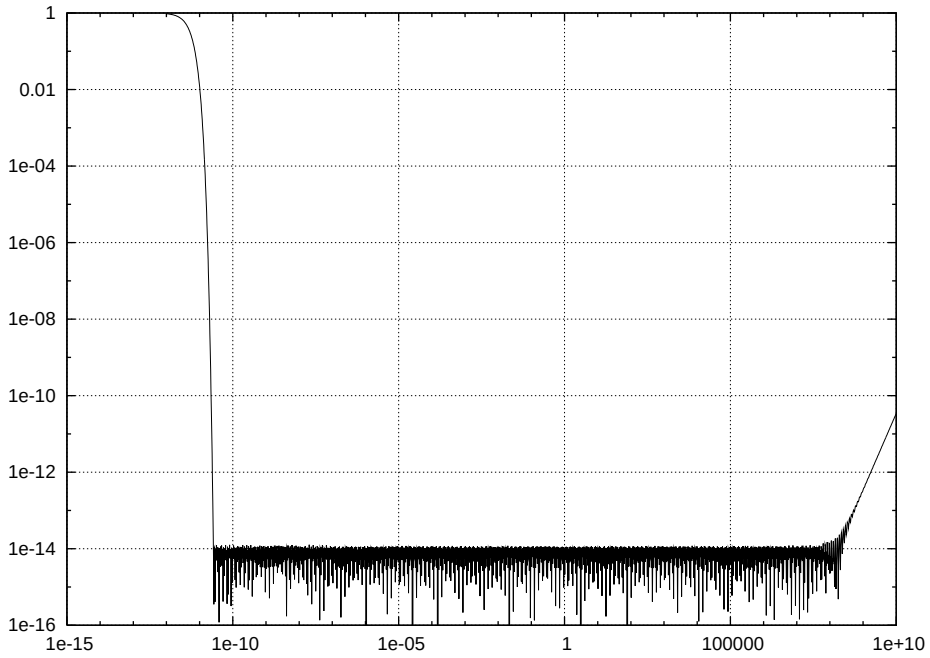
Discretization of these integrals leads to the desired representation via Gaussians.

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 $10^{-10} \leq ||\mathbf{x}-\mathbf{y}|| \leq 10^8$, $M = 437$.

Approximation of multiparticle Green's function

The kinetic energy operator is

$$\mathcal{T} = -\frac{1}{2}\sum_{i=1}^{N}\Delta_i, \quad \text{where} \quad \Delta_i = \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2}.$$

We approximate the multiparticle Green's function $\mathcal{G}_\mu = (\mathcal{T} - \mu)^{-1}$, $\mu < 0$ in the Fourier domain by discretizing the integral

$$\frac{1}{\|\mathbf{p}\|^2 - \mu} = \int_{-\infty}^{\infty} e^{-\|\mathbf{p}\|^2 e^s + \mu e^s + s} ds,$$

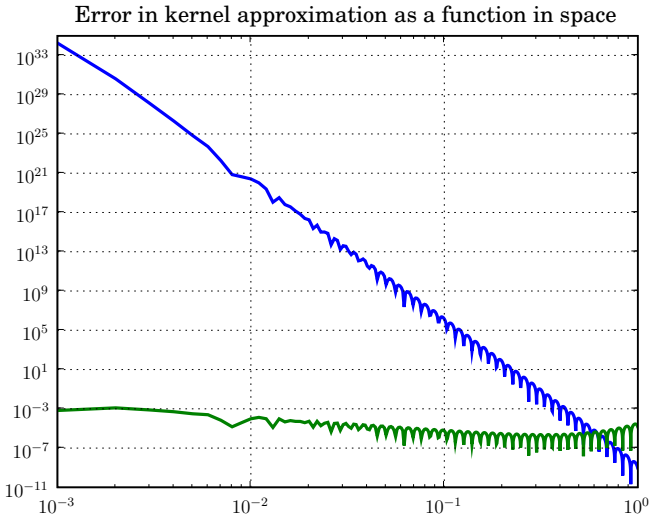
(using quadrature nodes τ_p and weights w_p) and obtain

$$\left\| \mathcal{G}_\mu - \sum_{p=1}^{L} \bigotimes_{i=1}^{N} \mathcal{F}_{\mathbf{r}_i}^p \right\| \leq \epsilon \left\| \mathcal{G}_\mu \right\|, \quad \left(\mathcal{F}_{\mathbf{r}_i}^p f\right)(..\mathbf{r}_i..) = w_p \int \exp\left(-\tau_p \|\mathbf{r}_i - \mathbf{r}_i'\|^2\right) f(..\mathbf{r}_i'..) d\mathbf{r}_i'.$$

An estimate for the approximation

We prove

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

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

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

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

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 in the spatial domain

We transform $\hat{F}_{sing}$ to the spatial domain

$$F_{sing}(r) = \frac{1}{2^{d-1}\pi^{d/2}} \int_{-\log\frac{\alpha}{\kappa}}^{\infty} e^{-r^2\frac{e^{2s}}{4}+\kappa^2 e^{-2s}+(d-2)s} ds,$$

discretize this integral and approximate F_{sing} in the region $r \geq \delta_0 > 0$ by a sum of decaying Gaussians with positive coefficients,

$$S_{sing}(r) = \sum_{n=1}^{N} q_n e^{-\sigma_n r^2}.$$

Approximation in the Fourier domain

Turning to $\hat{F}_{oscill}$, we define

$$\hat{S}_{oscill}(\rho) = \frac{e^{-\alpha^2(\rho^2-\kappa^2)/\kappa^2}}{2\rho} \sum_{m=1}^{M} w_m \left((\rho-\kappa) e^{-\tau_m(\rho-\kappa)^2} + (\rho+\kappa) e^{-\tau_m(\rho+\kappa)^2} \right)$$

for $0 \leq \rho \leq b\kappa$ and $\hat{S}_{oscill}(\rho) = 0$ for $b\kappa < \rho$, where $b > 1$ and $\delta > 0$ are parameters (chosen depending on the desired accuracy).

With a proper choice of these parameters, $\hat{S}_{oscill}$ accurately approximates $\hat{F}_{oscill}$ in the region $|\rho - \kappa| \geq \min\{\kappa\delta, \delta\}$.

Thus, a convolution with F_{oscill} is approximated in the Fourier domain as

$$\left(S_{oscill} * f\right)(\mathbf{x}) = \frac{1}{(2\pi)^d} \int_{|\mathbf{p}| \leq b\kappa} \hat{S}_{oscill}(|\mathbf{p}|) \hat{f}(\mathbf{p}) e^{i\mathbf{x}\cdot\mathbf{p}} d\mathbf{p}.$$

Estimate

Theorem. Let $D \subset \mathbb{R}^d$, $d = 2, 3$, be a bounded domain such that $\mathrm{diam}(D) \leq 1$. Given $\epsilon > 0$,

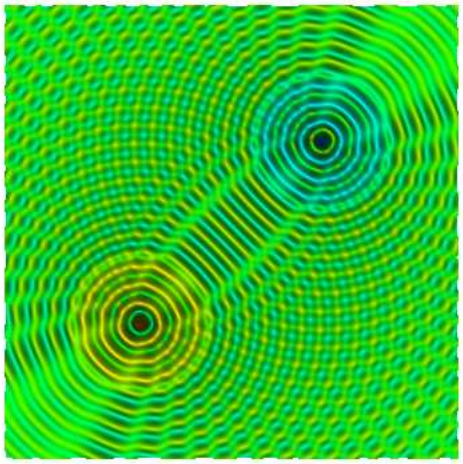
$$\tilde{G}_R(r) = S_{sing}(r) + S_{oscill}(r).$$

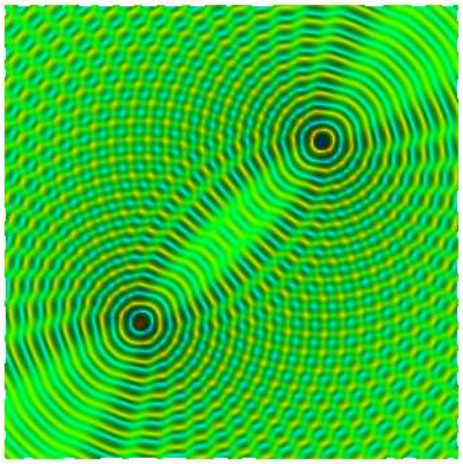
and $f \in L^p(D)$ for $1 \leq p \leq \infty$, we have

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

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

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

so that

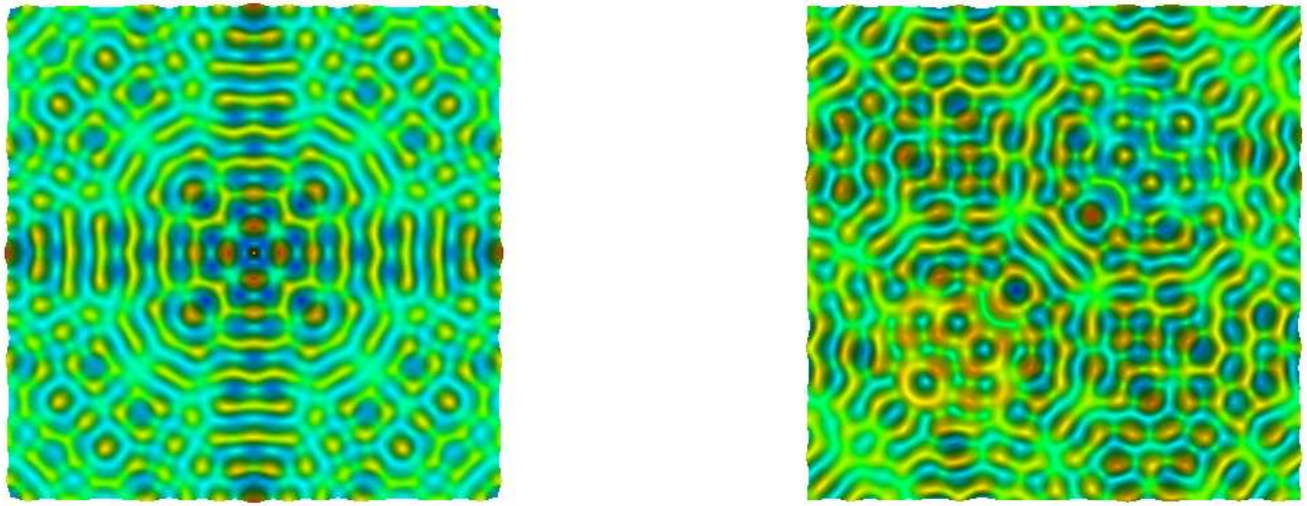
$$u(\mathbf{x}) = \int_D G_q(\mathbf{x}-\mathbf{y}) f(\mathbf{y}) d\mathbf{y},$$

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

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

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

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

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 $j = 1, \ldots, N$ to obtain the separated representation

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

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

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

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 $\lambda_n = n + \frac{1}{2}$, $n = 0, 1, \ldots$, 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 $n = 0, 1, \ldots,$ we approximate

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

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

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

or

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

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

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

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

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

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?

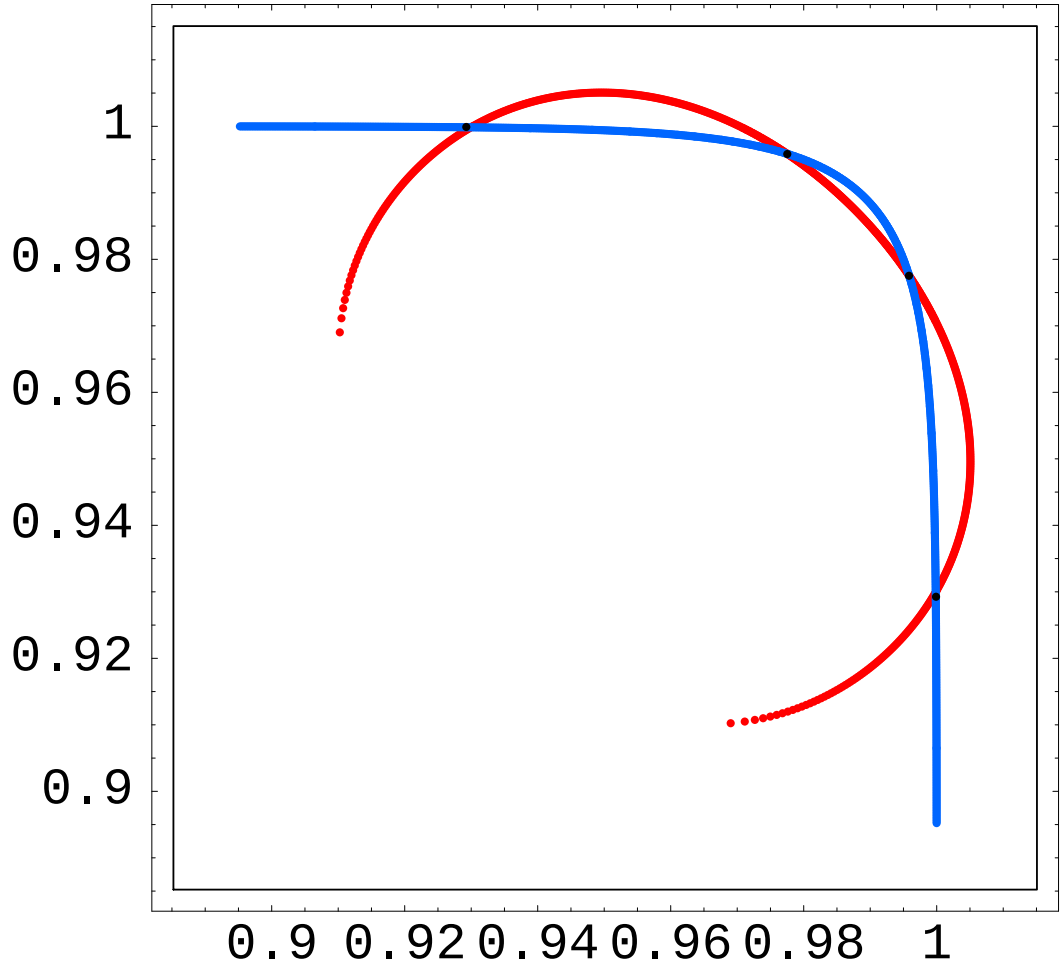
In contrast with the one dimensional case, we are not aware of *any* theoretical results to guide us.

- We conjecture (an 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).

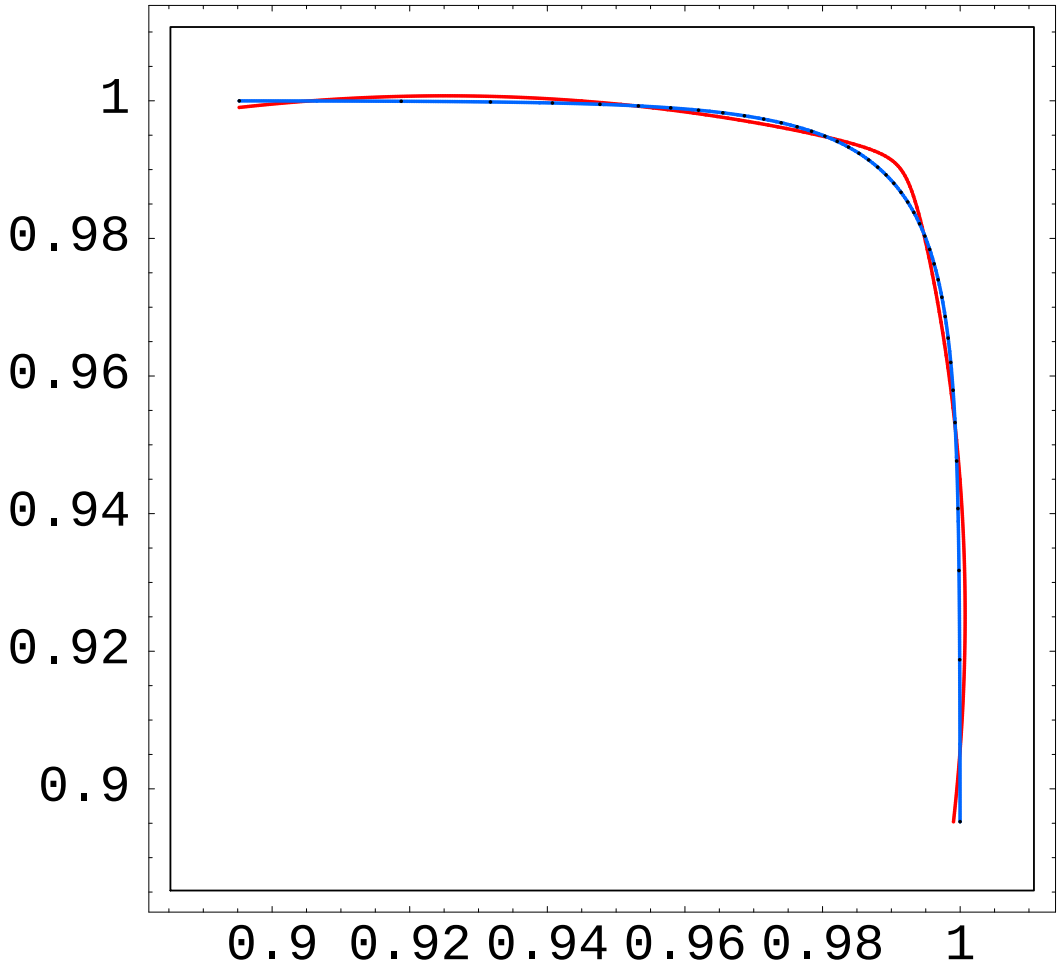
- Most of the theory still needs to be developed

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	$1.6\,10^{-2}$	$7.8\,10^{-5}$
5	$1.6\,10^{-3}$	$1.6\,10^{-6}$
6	$1.5\,10^{-4}$	$3.5\,10^{-7}$
7	$9.2\,10^{-6}$	$3.7\,10^{-9}$
8	$7.5\,10^{-7}$	$2.2\,10^{-9}$
9	$5.7\,10^{-8}$	$2.0\,10^{-11}$
10	$1.7\,10^{-9}$	$5.2\,10^{-12}$

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