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‘Off-the-shelf’ ways to compute integrals

How do I compute an integral of a nasty singular kernel?
Symbolic integration

br'ttle

Why not Gaussian?

\[ \int_{\mathbb{R}^d} \log(|x-y|) \sigma(y) \, dy = \int_{\mathbb{R}^d} \log|x-y(1)| \sigma(y) \, dy \]

\[ = \int_{\mathbb{R}^d} \log|x-y(1)| \sigma(y) \, dy \]
Singular and Near-Singular Quadrature

Numerically distinct scenarios:

- Near-Singular quadrature
  - Integrand nonsingular
  - But may locally require lots of
  - Adaptive quadrature works, but...

- Singular quadrature
  - Integrand singular
  - Conventional quadrature fails
Kussmaul-Martensen quadrature

\[ \int_0^{\log(x-y(t))} \sigma(y(t)) \, dt \]

**Theorem (A special integral [Kress LIE Lemma 8.21])**

\[
\frac{1}{2\pi} \int_0^{2\pi} \log \left( \frac{4 \sin^2 \frac{t}{2}}{2} \right) e^{imt} \, dt = \begin{cases} 
0 & m = 0, \\
-\frac{1}{|m|} & m = \pm 1, \pm 2, \ldots 
\end{cases}
\]

Why is that exciting?

**Demo:** Kussmaul-Martensen quadrature
Singularity Subtraction

\[
\int \langle \text{Thing } X \text{ you would like to integrate} \rangle \\
= \int \langle \text{Thing } Y \text{ you } \textit{can} \text{ integrate} \rangle \\
+ \int \langle \text{Difference } X - Y \text{ which is easy to integrate (numerically)} \rangle
\]

Give a typical application.

Drawbacks?
High-Order Corrected Trapezoidal Quadrature

- Conditions for new nodes, weights
  (→ linear algebraic system, dep. on \( n \))
  to integrate
  \[
  \langle \text{smooth} \rangle \cdot \langle \text{singular} \rangle + \langle \text{smooth} \rangle
  \]
- Allowed singularities: \(|x|^\lambda\) (for \(|\lambda| < 1\)), \(\log |x|\)
- Generic nodes and weights for log singularity
- Nodes and weights copy-and-pasteable from paper
  [Kapur, Rokhlin ‘97]

Alpert ‘99 conceptually similar:
Generalized Gaussian

- "Gaussian":
  - Integrates $2n$ functions exactly with $n$ nodes
  - Positive weights
- Clarify assumptions on system of functions ("Chebyshev system") for which Gaussian quadratures exist
- When do (left/right) singular vectors of integral operators give rise to Chebyshev systems?
  - In many practical cases!
- Find nodes/weights by Newton’s method
  - With special starting point
- Very accurate
- Nodes and weights for download

[Yarvin/Rokhlin ‘98]
Singularity cancellation: Polar coordinate transform

\[ \int \int_{\partial \Omega} K(x, y) \phi(y) ds_y = \int_0^R \int_{x+r \in \partial \Omega \cap \partial B(x, r)} K(x, x+r) \phi(x+r) d\langle \text{angles} \rangle r \, dr \]

\[ = \int_0^R \int_{x+r \in \partial \Omega \cap \partial B(x, r)} \frac{K_{\text{less singular}}(x, x+r)}{r} \phi(x+r) d\langle \text{angles} \rangle r \, dr \]

where \( K_{\text{less singular}} = K \cdot r \).
Quadrature on Triangles

Problem: Singularity can sit anywhere in triangle → need lots of quadrature rules (one per target)
Quadrature on Triangles

Problem: Singularity can sit anywhere in triangle → need lots of quadrature rules (one per target)
Kernel regularization

Singularity makes integration troublesome: *Get rid of it!*

\[
\begin{align*}
\ldots \quad \frac{\cdot \cdot \cdot}{\sqrt{(x - y)^2}} & \quad \rightarrow \quad \frac{\cdot \cdot \cdot}{\sqrt{(x - y)^2 + \epsilon^2}} \\
\end{align*}
\]

Use Richardson extrapolation to recover limit as \( \epsilon \to 0 \).
(May also use geometric motivation: limit along line towards singular point.)

Primary drawbacks:

- Low-order accurate
- Need to make \( \epsilon \) smaller (i.e. kernel more singular) to get better accuracy

Can take many forms–for example:

- Convolve integrand to smooth it
  (\( \rightarrow \) remove/weaken singularity)
- Extrapolate towards no smoothing

Related: [Beale/Lai ‘01]
Acceleration and Quadature

\[\int_{x}^{x + \frac{\ell}{2\sigma}} \sigma(x) \, dx = \int_{\mathbb{R}} \sigma(x - y) \delta(y) \, dy\]

How can singular quadrature and FMM acceleration be made compatible?
FMMs and other Layer Potentials

How does an FMM evaluate a double layer?

compute poles of dip kernel

How does an FMM evaluate $S'$?

eval $\mathcal{D}$ of local expansions at the end

What effect does this have on accuracy?

$\mathcal{D}$ does not lose an order
$S'$ loses an order
Outline

Introduction

Dense Matrices and Computation

Tools for Low-Rank Linear Algebra

Rank and Smoothness

Near and Far: Separating out High-Rank Interactions

Outlook: Building a Fast PDE Solver

Going Infinite: Integral Operators and Functional Analysis

Singular Integrals and Potential Theory

Boundary Value Problems

Back from Infinity: Discretization

Computing Integrals: Approaches to Quadrature

A Bag of Quadrature Tricks

Quadrature by expansion ("QBX")

QBX Acceleration

Reducing Complexity through better Expansions

Results: Layer Potentials

Results: Poisson

Going General: More PDEs
Layer Potential Evaluation: Some Intuition
QBX: Idea

Expansion center

Potential from expansion

"Naive" potential

Target point $x$

Curve $\Gamma$

Source quad. nodes $x'$

$\log_{10}(\text{Error})$

-6.0

-5.4

-4.8

-4.2

-3.6

-3.0

-2.4

-1.8

-1.2

-0.6

0.0
QBX: An Experiment

$p = 3, N = 80$
QBX: An Experiment

\[ p = 3, \quad N = 80 \]

\[ p = 6, \quad N = 80 \]
QBX: An Experiment

\[ p = 3, \ N = 80 \]

\[ p = 6, \ N = 80 \]

\[ p = 12, \ N = 80 \]
QBX: An Experiment

\begin{align*}
p = 3, \ N = 80 \\
p = 6, \ N = 80 \\
p = 12, \ N = 80 \\
p = 12, \ N = 240
\end{align*}
QBX: Notation, Basics

Graf’s addition theorem
Requires: $|x - c| < |x' - c|$ ("local expansion")

\[
H_0^{(1)}(k|x - x'|) = \sum_{l=-\infty}^{\infty} H_l^{(1)}(k|x' - c|) e^{il\theta'} J_l(k|x - c|) e^{-il\theta}
\]
Compute layer potential on the disk as

\[ S_k \sigma(x) = \sum_{l=-\infty}^{\infty} \alpha_l J_l(k \rho) e^{-il\theta} \]

with

\[ \alpha_l = \left( -\frac{i}{4} \right) \oint H_l^{(1)}(k|x'| - c|) e^{i\theta'} \sigma(x') \, dx' \quad (l = -\infty, \ldots, \infty) \]

\( S \sigma \) is a smooth function up to \( \Gamma \).
QBX: Formulation, Discretization

\[ S_{QBx} = \mathcal{E} \int \mathcal{H}_e (\ldots ) \sigma (y) \, dy \]

Compute layer potential on the disk as

\[ S_k \sigma(x) = \sum_{l=-p}^{p} \alpha_l J_l(k\rho) e^{-il\theta} \]

with

\[ \alpha_l = \frac{i}{4} T_N \left( \int_{\Gamma} \mathcal{H}_l^{(1)}(k|x' - c|) e^{il\theta'} \sigma(x') \, dx' \right) \]

\( l = -\infty, \ldots, \infty \)

\( S\sigma \) is a smooth function up to \( \Gamma \).
Quadrature by Expansion (QBX)

\[ r \sim 1 \]
\[ r = \frac{1}{r} \]

\[
\text{Error} \leq \left( C + C \begin{pmatrix} \frac{h}{r} \end{pmatrix}^q \right) \left\| \sigma \right\|
\]

\[ (\frac{1}{r})^9 \]

[K, Barnett, Greengard, O’Neil JCP ‘13]
Achieving high order

\[
\text{Error } \leq \left( C r^{p+1} \underbrace{\text{Truncation error}}_{\text{Truncation error}} + C \underbrace{\left( \frac{h}{r} \right)^q}_{\text{Quadrature error}} \right) \| \sigma \|
\]

Two approaches:

- **Asymptotically convergent**: \( r = \sqrt{h} \)
  - \( \bigoplus \text{Error } \to 0 \text{ as } h \to 0 \)
  - \( \bigcirc \text{Low order: } h^{(p+1)/2} \)

- **Convergent with controlled precision**: \( r = 5h \)
  - \( \bigcirc \text{Error } \not\to 0 \text{ as } h \to 0 \)
  - \( \bigoplus \text{High order: } h^{p+1} \text{ to controlled precision } \epsilon := (1/5)^q \)
Other layer potentials

Can’t just do single-layer potentials:

\[ \alpha_i^D = \frac{i}{4} \int_{\Gamma} \frac{\partial}{\partial \hat{n}_{x'}} H_i^{(1)}(k|x' - c|) e^{i l \theta'} \mu(x') \, dx'. \]

Even easier for target derivatives (S’ et al.): Take derivative of local expansion.
Analysis says: Will lose an order.
Slight issue: QBX computes one-sided limits.
Fortunately: Jump relations are known—e.g.

\[ (PV) D^* \mu(x)|_\Gamma = \lim_{x^\pm \to x} D\mu(x^\pm) + \frac{1}{2} \mu(x). \]

Alternative: Two-sided average → Preferred because of conditioning