Close evaluation of layer potentials in three dimensions*

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*Based on a paper by C. Carvalho, R. Cortez, S. Khatri, and A. D. Kim [in preparation].

Today's objective

Consider a three-dimensional domain D with boundary B.

The solution to Laplace's equation is given by

$$u(x) = \underbrace{-\frac{1}{4\pi}\int_B \frac{n(y)\cdot(x-y)}{|x-y|^3}u(y)\mathrm{d}\sigma_y}_{\text{double-layer potential}} + \underbrace{\frac{1}{4\pi}\int_B \frac{1}{|x-y|}\frac{\partial u}{\partial n}(y)\mathrm{d}\sigma_y}_{\text{single-layer potential}}, \quad x \in D.$$

We want a method to accurately compute the representation formula.

This requires numerical integration over two-dimensional surfaces.

Guiding principle for this talk

Numerical integration works really well for nearly constant functions[†].

[†] And, it does not work as well for less nearly constant functions.

Numerical integration on the sphere

Atkinson (1982) introduced the product Gaussian quadrature rule:

$$
\begin{aligned}
I(f) &= \int_0^{2\pi} \int_0^{\pi} f(\theta, \varphi) \sin\theta \mathrm{d}\theta \mathrm{d}\varphi \\
&= \int_0^{2\pi} \int_{-1}^{1} f(\arccos z, \varphi) \mathrm{d}z \mathrm{d}\varphi \quad \text{(substitute } z = \cos\theta\text{)} \\
&\approx I_M(f) \equiv \frac{\pi}{M} \sum_{j=1}^{2M} \sum_{i=1}^{M} w_i f(\arccos z_i, \varphi_j).
\end{aligned}
$$

- z_i and w_i for $i = 1, \cdots, M$ are the M-point Gauss-Legendre quadrature rule points and weights.
- $\varphi_j = (j-1)\pi/M$ are the $2M$-point periodic trapezoid rule points.

Why the substitution $z = \cos\theta$?

What happens when we substitute $z = \cos\theta$ into the integral below?

$$4\pi = \int_0^{2\pi} \int_0^{\pi} \sin\theta \mathrm{d}\theta \mathrm{d}\varphi$$

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We substitute $z = \cos\theta$ and $\mathrm{d}z = \sin\theta \mathrm{d}\theta$ and find that

$$4\pi = \int_0^{2\pi} \int_{-1}^{1} 1 \mathrm{d}z \mathrm{d}\varphi.$$

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$$4\pi = \int_0^{2\pi}\int_{-1}^{1} 1 \mathrm{d}z \mathrm{d}\varphi.$$

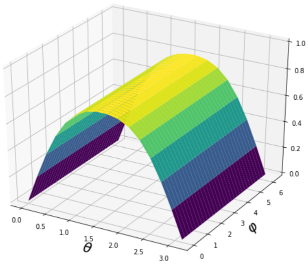
Since 1 is a constant, this substitution is *really good* for numerical integration!

Another example: Surface area of an oblate spheroid

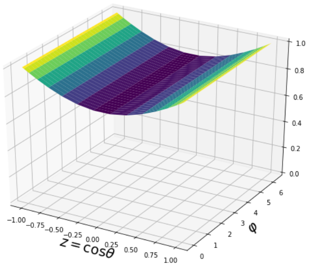
$$\int_0^{2\pi}\int_0^{\pi} \underbrace{\frac{a}{\sqrt{2}}\sqrt{a^2+c^2+(a^2-c^2)\cos 2\theta}}_{f(\theta,\varphi)} \sin\theta \mathrm{d}\theta\mathrm{d}\varphi = 2\pi a^2 + \pi\frac{c^2}{e}\log\left(\frac{1+e}{1-e}\right),$$

with $e^2 = 1 - c^2/a^2$ and $a \geq c$.

$f(\theta,\varphi)\sin\theta$

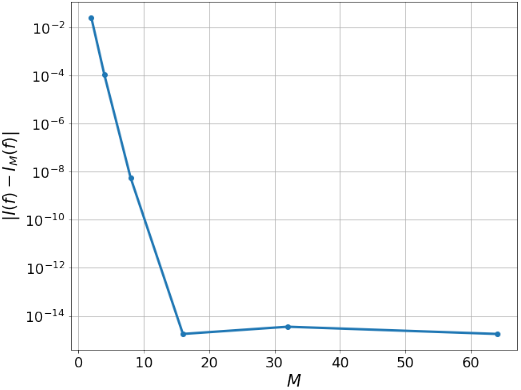


$f(\arccos z,\varphi)$



Another example: Surface area of an oblate spheroid

We apply the product Gaussian quadrature rule to the surface area integral for an oblate spheroid and obtain the following result.



Product Gaussian quadrature rule

- It is for numerical integration on the sphere.
- Substituting $z = \cos\theta$ makes the function to be integrated more nearly constant which is really good for numerical integratrion.
- It works very well!
- So why not use it for the representation formula?

Poisson's formula

The solution to Laplace's equation in the sphere $r < a$ with Dirichlet boundary data $u = f$ on $r = a$ is given by

$$u(x) = \frac{1}{4\pi} \int_{|y|=a} \frac{a^2 - |x|^2}{|x - y|^3} f(y) \mathrm{d}\sigma_y, \quad |x| < a.$$

In spherical coordinates, we have

$$u(r, \theta, \varphi) = \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} \frac{a(a^2 - r^2) f(s, t) \sin s \mathrm{d}s \mathrm{d}t}{\left[a^2 + r^2 - 2ar \left(\cos\theta \cos s + \sin\theta \sin s \cos(\varphi - t)\right)\right]^{3/2}}.$$

Poisson's formula along the $+z$-axis

To keep things simple, we focus on computing the solution along the $+z$-axis corresponding to $\theta = 0$:

$$u(r,0,\cdot) = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} \frac{a(a^2-r^2)f(s,t)\sin s\,\mathrm{d}s\mathrm{d}t}{\left(a^2+r^2-2ar\cos s\right)^{3/2}}.$$

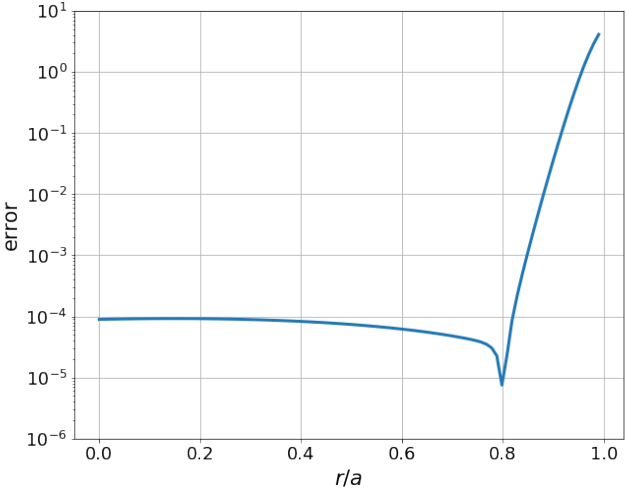
On $\theta = 0$, we have a so-called "coordinate singularity," so there is no sense of φ.

Working example. Substituting the harmonic function $u = (\cos x + \cos y)e^z$, we find

$$2e^r = a\frac{a^2-r^2}{4\pi}\int_0^{2\pi}\int_0^{\pi} \frac{\left[\cos(a\sin s\cos t)+\cos(a\sin s\sin t)\right]e^{a\cos s}}{\left(a^2+r^2-2ar\cos s\right)^{3/2}}\sin s\,\mathrm{d}s\mathrm{d}t.$$

Working example: error results

With $M = 32$, we obtain the following error results.



What’s the problem?

What is the cause this large error as $r \to a^-$?

$$\int_0^{2\pi} \int_0^{\pi} \frac{[\cos(a \sin s \cos t) + \cos(a \sin s \sin t)]\, e^{a \cos s}}{\left(a^2 + r^2 - 2ar \cos s\right)^{3/2}} \sin s \mathrm{d}s \mathrm{d}t.$$

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What's the problem?

After substituting $z = \cos\theta$, we find that $\dfrac{1}{(a^2 + r^2 - 2arz)^{3/2}} \sim \dfrac{1}{(a-r)^3}$ as $z \to 1^-$ $(s \to 0^+)$.

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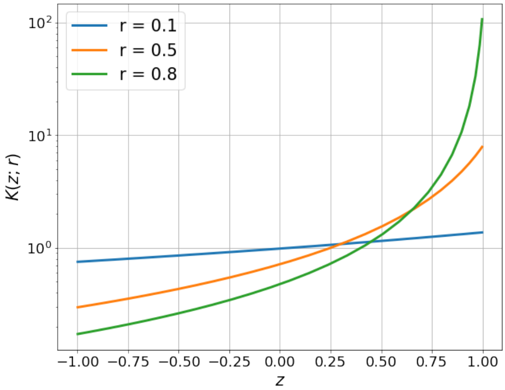

Since $r < a$ we never reach the singularity, but we are *nearly singular*!

This function is smooth, but far from nearly constant, so numerical integration does not work as well.

Product Gaussian quadrature rule for Poisson's formula

- It works well for points far from the boundary.
- The error becomes large as the point of evaluation approaches the boundary.
- We have identified the factor in Poisson's formula causing the problem – the function to be integrated rises rapidly on $z = 1$ ($s = 0$) as $r \to a$.
- Because of this nearly singular peak, the function to be integrated is far from nearly constant, so numerical integration does not work so well.

Look at Poisson's formula again

$$u(r,0,\cdot) = \frac{a(a^2-r^2)}{4\pi}\int_0^{2\pi}\int_0^{\pi}\frac{\sin s}{\left(a^2+r^2-2ar\cos s\right)^{3/2}}f(s,t)\mathrm{d}s\mathrm{d}t.$$

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If we do not make the substitution, $z = \cos s$, then we have

$$\frac{\sin s}{\left(a^2 + r^2 - 2ar\cos s\right)^{3/2}} \to 0 \quad \text{as } s \to 0 \text{ when } r < a.$$

So why not integrate with respect to s instead of z?

Modified product Gaussian quadrature rule

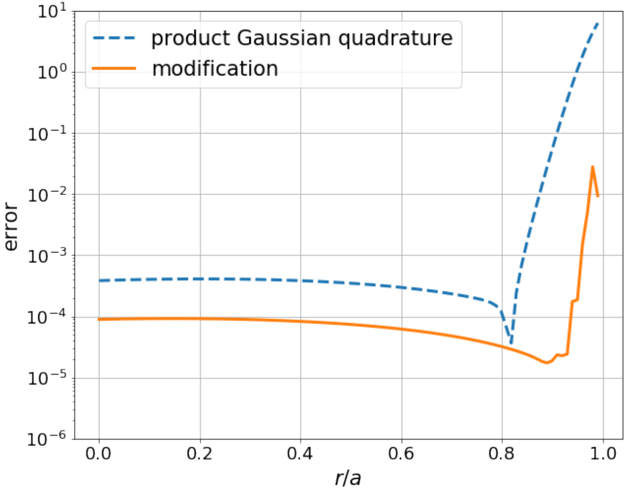
Instead of substituting $z = \cos\theta$, we map the Gauss-Legendre quadrature rule from $[-1, 1]$ to $[0, \pi]$ and obtain

$$I(f) = \int_0^{2\pi} \int_0^{\pi} f(\theta, \varphi) \sin\theta \mathrm{d}\theta \mathrm{d}\varphi$$
$$\approx \tilde{I}_M(f) \equiv \frac{\pi}{M} \sum_{j=1}^{2M} \sum_{i=1}^{M} \frac{\pi w_i}{2} f\left(\frac{\pi(z_i + 1)}{2}, \varphi_j\right) \sin\left(\frac{\pi(z_i + 1)}{2}\right).$$

Since $\sin s \sim s$ as $s \to 0$, this modification will kill the nearly singular growth on $s = 0$.

Example: error results

With $M = 32$, we obtain the following error results.



Modified product Gaussian quadrature for Poisson's formula

- This modification is an improvement over the product Gaussian quadrature rule.
- The error still becomes large as the point of evaluation approaches the boundary, but the height and width of that region is greatly reduced compared with the product Gaussian quadrature rule.
- Keeping the factor of $\sin s$ helps, but if we can make the function to be integrated vanish more rapidly as $s \to 0$, that would be even better.

Subtraction method

A constant is harmonic, so

$$C = \frac{a(a^2 - r^2)}{4\pi} \int_0^{2\pi} \int_0^{\pi} \frac{C \sin s}{\left(a^2 + r^2 - 2ar \cos s\right)^{3/2}} \mathrm{d}s \mathrm{d}t$$

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We add and subtract the constant $f(0, \cdot)$ (the boundary data on $s = 0$) in Poisson's formula and obtain

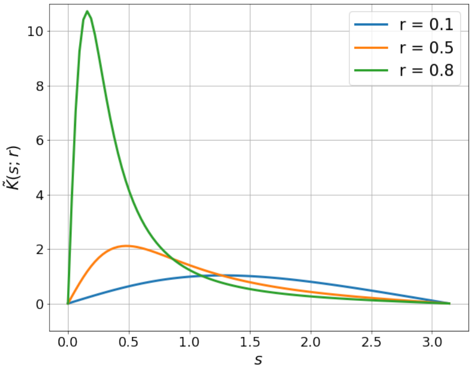
$$u(r, 0, \cdot) = f(0, \cdot) + \frac{a(a^2 - r^2)}{4\pi} \int_0^{2\pi} \int_0^{\pi} \frac{[f(s,t) - f(0,\cdot)] \sin s}{\left(a^2 + r^2 - 2ar\cos s\right)^{3/2}} \mathrm{d}s\mathrm{d}t.$$

For our example, $[f(s,t) - f(0,\cdot)] = O(s^2)$ as $s \to 0$.

Plots of the function

Let

$$\tilde{K}(s;r) = \frac{\sin s}{(a^2 + r^2 - 2ar\cos s)^{3/2}}.$$



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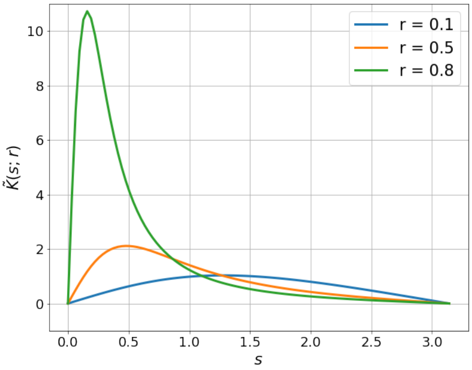
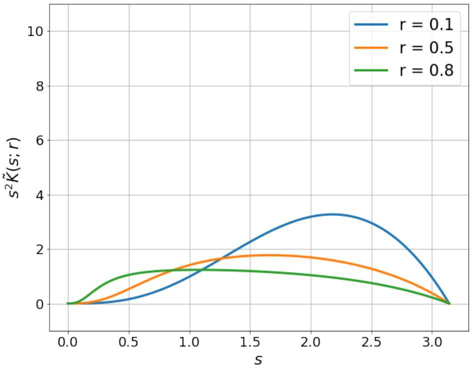
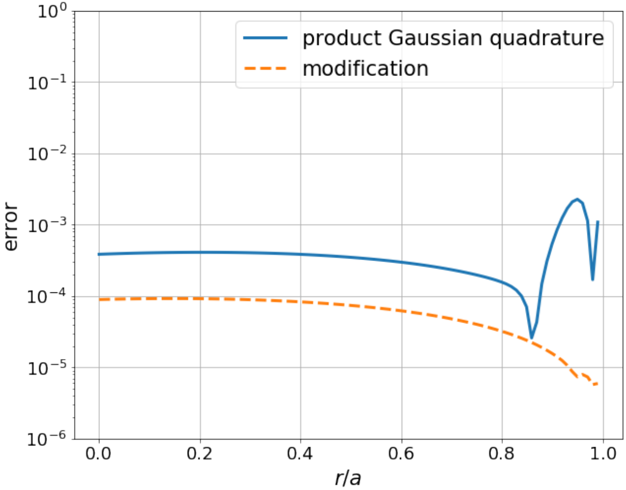




Working example: error results using the subtraction method

With $M = 32$, we obtain the following error results.



Generalizing the method

- Using subtraction and the modified product Gaussian quadrature rule appears to be a good method for evaluating Poisson's formula.
- The key to this method is evaluating Poisson's formula along the normal at the north pole of the sphere.
- We can *rotate* the coordinate system so that any boundary point is the north pole.

Moving on

Poisson's formula:

$$u(x) = \frac{1}{4\pi} \int_{|y|=a} \frac{a^2 - |x|^2}{|x-y|^3} f(y) \mathrm{d}\sigma_y, \quad |x| < a.$$

The representation formula:

$$u(x) = -\frac{1}{4\pi} \int_B \frac{n(y) \cdot (x-y)}{|x-y|^3} u(y) \mathrm{d}\sigma_y + \frac{1}{4\pi} \int_B \frac{1}{|x-y|} \frac{\partial u}{\partial n}(y) \mathrm{d}\sigma_y, \quad x \in D.$$

Assuming B can be mapped to the sphere, we can compute the double-layer potential just like we did for Poisson's formula.

Subtraction method for the double-layer potential

Gauss' theorem gives

$$-\frac{1}{4\pi}\int_B \frac{n(y)\cdot(x-y)}{|x-y|^3}1\mathrm{d}\sigma_y = \begin{cases} 1 & x \in D, \\ \frac{1}{2} & x \in B, \\ 0 & x \notin D \end{cases}$$

This allows us to write

$$-\frac{1}{4\pi}\int_B \frac{n(y)\cdot(x-y)}{|x-y|^3}u(y)\mathrm{d}\sigma_y = u(y^*) - \frac{1}{4\pi}\int_B \frac{n(y)\cdot(x-y)}{|x-y|^3}\left[u(y)-u(y^*)\right]\mathrm{d}\sigma_y,$$

since $x \in D$.

Close evaluation of the representation formula

When x is close to the boundary point y^*, we compute

$$u(x) = u(y^*) - \frac{1}{4\pi} \int_B \frac{n(y) \cdot (x - y)}{|x - y|^3} \left[u(y) - u(y^*) \right] \mathrm{d}\sigma_y + \frac{1}{4\pi} \int_B \frac{1}{|x - y|} \frac{\partial u}{\partial n}(y) \mathrm{d}\sigma_y$$

using our modified product Gaussian quadrature rule.

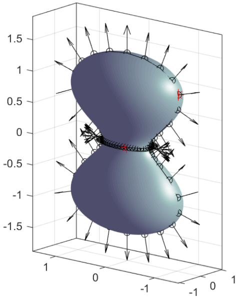
To evaluate x near y^*, we set

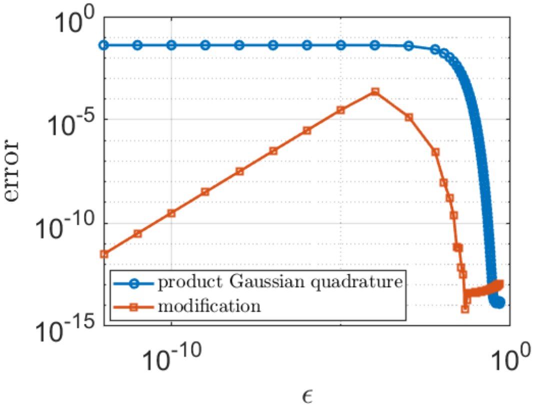
$$x = y^* - \epsilon n^*, \quad 0 < \epsilon \ll 1,$$

and study the error as a function of ϵ.

Example: peanut-shaped domain

For the harmonic function, $u = (\sin x + \sin y)e^z$, we use $M = 128$ and obtain the following results.





Some asymptotics

Using Gauss' theorem, we find that

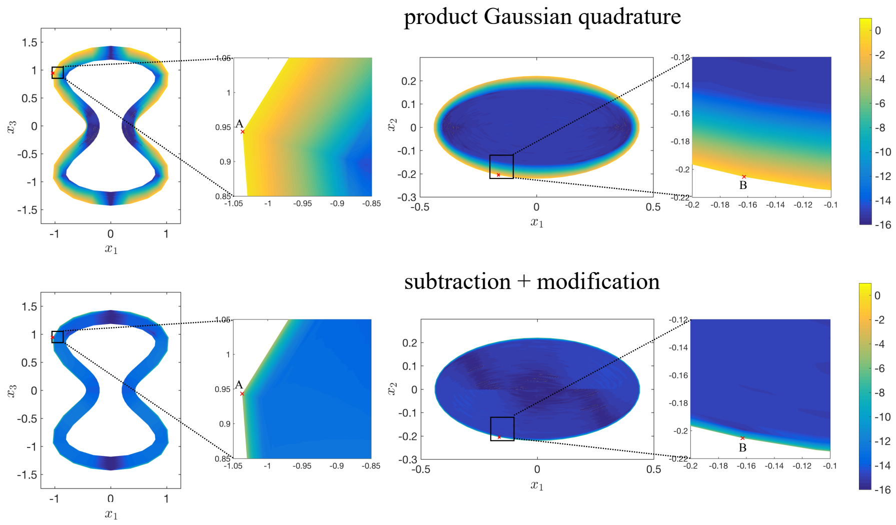
$$-\frac{1}{4\pi}\int_B \frac{n(y)\cdot(y^* - y - \epsilon n^*)}{|y^* - y - \epsilon n^*|^3} 1 \mathrm{d}\sigma_y = \begin{cases} 1 & \epsilon \neq 0, \\ \frac{1}{2} & \epsilon = 0 \end{cases}$$

This jump makes numerical integration of the double-layer potential challenging as $\epsilon \to 0^+$.

In contrast,

$$u(y^* - \epsilon n^*) - u(y^*) = -\frac{1}{4\pi}\int_B \frac{n(y)\cdot(y^* - y - \epsilon n^*)}{|y^* - y - \epsilon n^*|^3}\left[u(y) - u(y^*)\right] \mathrm{d}\sigma_y$$
$$+ \frac{1}{4\pi}\int_B \frac{1}{|y^* - y - \epsilon n^*|}\frac{\partial u}{\partial n}(y)\mathrm{d}\sigma_y = \mathcal{O}(\epsilon).$$

Some more peanut results



Summary

Numerical integration works really well for nearly constant functions.

- The function in the double-layer potential is far from nearly constant at close evaluation points.
- We introduced subtraction and a modification to the product Gaussian quadrature rule.
- Combining these two methods leads to a much more nearly constant function to integrate.
- That is why this method works better.