Algorithms of Scientific Computing

Hierarchical Methods and Sparse Grids

Michael Bader

Technische Universität München

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Part IV

Archimedes, *d*-Dimensional

Current State

One-dimensional quadrature

- One-dimensional functions f, interval $[a, b]$
- Compute approximation $F_1(f, a, b)$ of area:

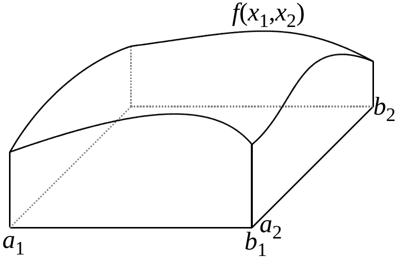
$$F_1(f, a, b) \approx \int_a^b f(x)\, dx$$

- Notation for appoximation of exact integral value in the following: $F_d(.)$, with d as the dimension
- One-dimensional quadrature rules:
  - Composite trapeziodal rule
  - Composite Simpson's rule
  - Archimedes' quadrature

Multi-Dimensional Quadrature

Consider multi-dimensional setting

$$F_d(f,\Omega) \approx \int_\Omega f(x_1,\dots,x_d)\,d\vec{x}, \qquad \Omega := \prod_{k=1}^{d}[a_k,b_k]$$



First Attempt

- remember theorem of Fubini:

$$F_d(f,\Omega) = \int_{a_d}^{b_d} \dots \int_{a_1}^{b_1} f(x_1,\dots,x_d)\, dx_1 \dots dx_d$$

- Use full-grid approach as before:

$$\begin{aligned}
G_0(x_1,x_2,x_3,\dots,x_d) &:= f(x_1,x_2,x_3,\dots,x_d) \\
G_1(x_2,x_3,\dots,x_d) &:= F_1(G_0(\bullet,x_2,x_3,\dots,x_d),a_1,b_1) \\
G_2(x_3,\dots,x_d) &:= F_1(G_1(\bullet,x_3,\dots,x_d),a_2,b_2) \\
&\vdots \\
G_d() &:= F_1(G_{d-1}(\bullet),a_d,b_d)
\end{aligned}$$

- We now consider the effect of Archimedes' quadrature as one-dimensional quadrature method for F_1

First Attempt: Employing Archimedes

- d nested loops $(x_1, x_2, \dots)$
- Summation of weighted function values
- No real advantages apart from adaptivity (which is not very useful this way)

Interplay of hierarchization and summation (integration)

- Consider setting with $d = 2$
- First, compute integrals in x_1-direction: $F_1(G_0(\bullet, x_2), a_1, b_1)$
  - Involves hierarchization in x_1-direction
  - But no impact on $G_1(x_2)$
- $G_1(x_2)$: no hierarchical values, thus all $G_1(x_2)$ of same order
- After summation (integration) in x_1-direction:
  - Hierarchization in x_2-direction
  - Finally summation in x_2-direction

Improved Version

- Consider computing $G_1(x_2)$
  - We are only interested in hierarchical surplus
  - Hierarchical surplus typically much smaller than function value

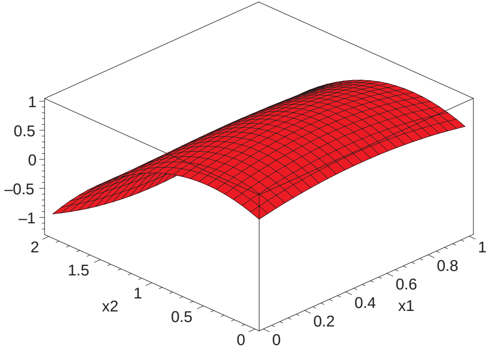
  $\Rightarrow$ Could be computed with much less grid points in x_1-direction
- We change the order of “integration in x_1-direction” and “hierarchization in x_2-direction”
  - Write hierarchical area elements of quadrature in x_2-direction (trapezoid, segments, triangles) as function of x_1
  - Integrate those in x_1-direction
- Now interplay of dimensions for integration much more complicated
- . . . but this will lead to much more efficient method

Example, $2d$

Consider

$$f(x_1, x_2) := \left(x_1 + \frac{1}{2}\right)\left(x_1 - \frac{3}{2}\right)\left(x_2 + \frac{1}{2}\right)\left(x_2 - \frac{3}{2}\right)$$

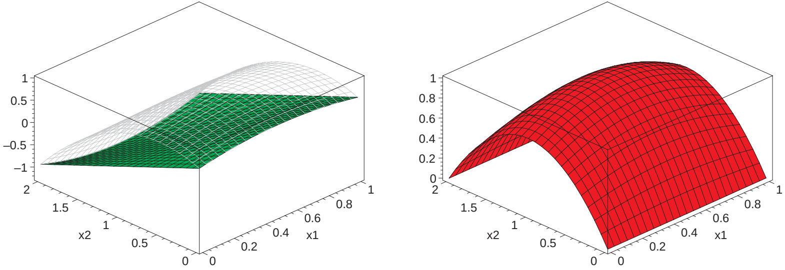
on $\Omega = [0, 1] \times [0, 2]$



Trapezoidal Volume and Remainder Segment

First step of the hierarchical decomposition

$$F_2(f,\Omega) = F_1(T_2, a_1, b_1) + S_2(f,\Omega)$$



“Green function” $\rightarrow$ linear interpolation of values at a_2, b_2:

$$\frac{f(x_1,a_2)(b_2-x_2)+f(x_1,b_2)(x_2-a_2)}{b_2-a_2} \qquad \text{for any } x_1$$

Trapezoidal Volume and Remainder Segment (2)

Decompose volume into

- trapezoidal (for constant x_1) cross-section with area

$$T_2(x_1) := \frac{b_2 - a_2}{2}\left(f(x_1, a_2) + f(x_1, b_2)\right),$$

$\rightarrow$ will be integrated in x_1-direction using quadrature rule F_1

- and remainder segment

$$S_2(f, \Omega) := F_2(f, \Omega) - F_1(T_2, a_1, b_1)$$

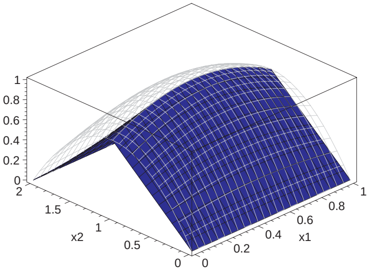
$$= \int_{a_2}^{b_2} \int_{a_1}^{b_1} \left(f(x_1, x_2) - \frac{f(x_1, a_2)(b_2 - x_2) + f(x_1, b_2)(x_2 - a_2)}{b_2 - a_2} \right) dx_1 \, dx_2$$

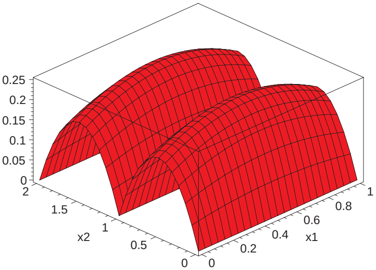
Note: T_2 is the integral over the linear interpolation (“green function”)

Triangular Volumes and Remainder Segments

Second step of the hierarchical decomposition

$$S_2(f,\Omega) = F_1(D_2, a_1, b_1) + S_2(f,\ldots) + S_2(f,\ldots)$$





again: hierarchization in x_2-direction; integrate in x_1-direction

Triangular Volumes and Remainder Segments (2)

Decompose remainder segment $S_2(f, \Omega)$ into

- triangular (for constant x_1) cross-section with area

$$D_2(x_1) := \frac{b_2 - a_2}{2} \left(f\left(x_1, \frac{a_2 + b_2}{2}\right) - \frac{f(x_1, a_2) + f(x_1, b_2)}{2} \right)$$

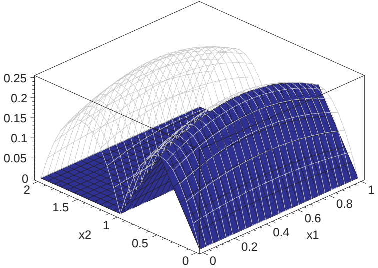
- and two remainder segments

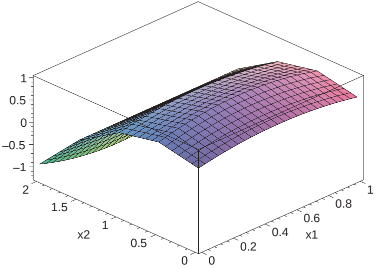
$$\begin{aligned} S_2(f, [a_1, b_1] \times [a_2, b_2]) &= F_1(D_2, a_1, b_1) \\ &+ S_2\left(f, [a_1, b_1] \times \left[a_2, \frac{a_2 + b_2}{2}\right]\right) \\ &+ S_2\left(f, [a_1, b_1] \times \left[\frac{a_2 + b_2}{2}, b_2\right]\right) \end{aligned}$$

Triangular Volumes and Remainder Segments (3)

Recursive decomposition

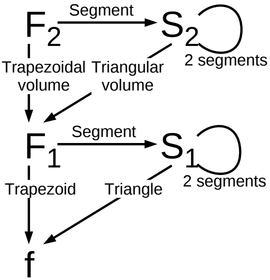
- Repeat last step for both remainder segments
- Decompose each into triangular sub-volume and two remainder segments
- Example for one of the two segments and sum of trapezoidal and first three triangular sub-volumes:





Recursive Structure of Function Calls

- Nested recursive structure of function calls
- For higher-dimensional problems: one more level (F_d and S_d) for each additional dimension



- Consider number of function evaluations for grid point inside of Ω
  - Straightforward: 3^d evaluations to compute surplus
  - All but one have already been computed!

Subvolumes

- F_1: the subvolumes (hierarchized in x_2-direction) are decomposed (in x_1-direction) into trapezoid and many triangles
- Integrand itself is area (one slice trapezoidal/triangular subareas)
- Subvolumes which are added in quadrature are pagodas (neglecting trapezoidals)
  - Height of pagodas: d-dimensional hierarchical surplus
  - Volume of pagodas: 2^{-d} times size of support times surplus (more in next part)
- Taking stopping criterion depending on surplus (d criteria: one in S_i each)
  - Find those grid points for which function evaluation is worthwile
  - In general much less than naive implementation
- Extend from composite trapezoidal rule to Simpsons' as in one-dimensional setting