

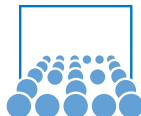
Algorithms of Scientific Computing

Hierarchical Methods and Sparse Grids

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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:

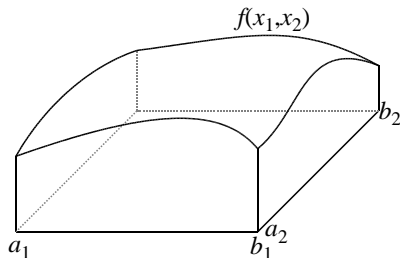
$$F_1(f, a, b) \approx \int_a^b f(x) dx$$

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

Multi-Dimensional Quadrature

Consider multi-dimensional setting

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



First Attempt

- 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

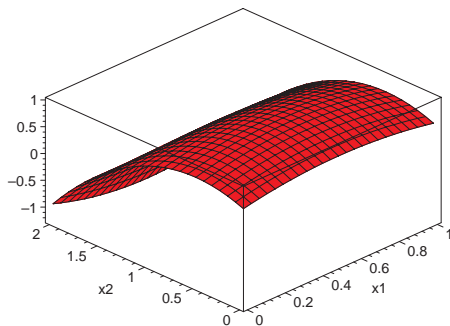
⇒ Could be computed with much less grid points in x_1 -direction
- We change the order of “integration in x_1 -direction” and “hierarchization in x_2 -direction”
 - Write hierarchical area elements of quadrature in x_2 -direction (trapezoid, segments, triangles) as function of x_1
 - Integrate those 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

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

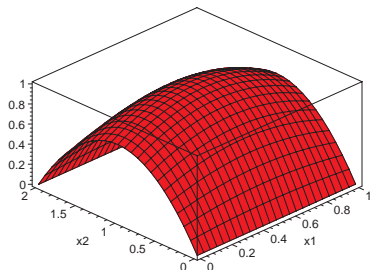
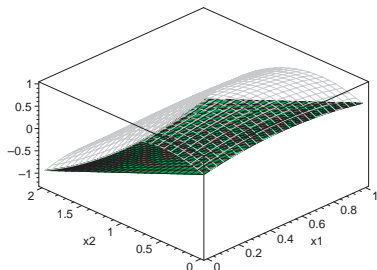
on $\Omega = [0, 1] \times [0, 2]$



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” → linear interpolation of values at a_2, b_2 :

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

Trapezoidal Volume and Remainder Segment (2)

Decompose volume into

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

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

→ will be integrated in x_1 -direction using quadrature rule F_1

- and remainder segment

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

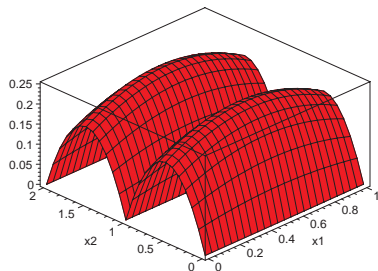
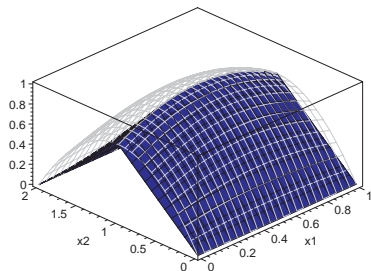
$$= \int_{a_2}^{b_2} \int_{a_1}^{b_1} \left(f(x_1, x_2) - \frac{f(x_1, a_2)(b_2 - x_2) + f(x_1, b_2)(x_2 - a_2)}{b_2 - a_2} \right) dx_1 dx_2$$

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

Triangular Volumes and Remainder Segments

Second step of the hierarchical decomposition

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



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

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

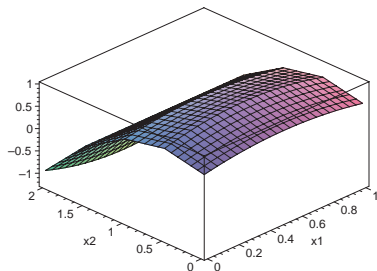
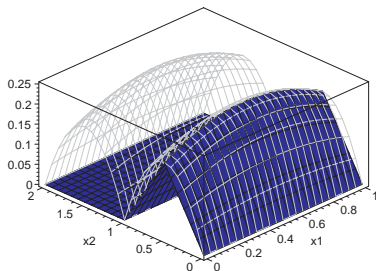
- and two remainder segments

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

Triangular Volumes and Remainder Segments (3)

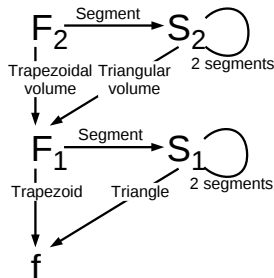
Recursive decomposition

- 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 worthwhile
 - In general much less than naive implementation
- Extend from composite trapezoidal rule to Simpsons' as in one-dimensional setting