Fast summation for an evolution equation with memory

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Background

Panel clustering method for BEM, W. Hackbusch and Z. P. Nowak, *Numer. Math.*, 1989.

Convolution quadrature:

$$\int_0^{t_n} \beta(t-s)u(s)\,ds \approx \sum_{j=0}^{n} \beta_{n-j}u(t_j).$$

FFT: Hairer, Lubich and Schlichte, *SISC*, 1985.

Exponentially accurate quadrature for contour integrals: Schädle, Lopez-Fernández and Lubich, *SISC*, 2006.

Fractional diffusion

Density $u = u(x,t)$ of particles undergoing anomalous subdiffusion satisfies

$$\frac{\partial u}{\partial t} - \nabla \cdot \left(\frac{\partial}{\partial t} \int_0^t \frac{(t-s)^{\nu-1}}{\Gamma(\nu)} K \nabla u(s)\, ds \right) = f(x,t),$$

for $x \in \Omega \subseteq \mathbb{R}^d$ and $0 < t < T$.

Mean-square displacement of particles

$$\frac{2Kt^\nu}{\Gamma(1+\nu)}, \qquad 0 < \nu < 1.$$

Recover classical diffusion in the limit as $\nu \to 1$:

$$u_t - \nabla \cdot (K \nabla u) = f.$$

Finite element solution

Combine piecewise-constant DG in time (implicit Euler) with continuous piecewise-linear finite elements in space, to compute

$$U_q^n = u(x_q, t_n) + O(k + h^2), \qquad 1 \le q \le Q, \quad 0 \le n \le N,$$

where

$$\begin{aligned} x_q &= q\text{th free node of spatial mesh}, \\ t_n &= (n/N)^\gamma T, \quad \gamma > 1, \\ k_n &= t_n - t_{n-1}, \\ k &= \max_{1 \le n \le N} k_n, \\ h &= \text{max element diameter of spatial mesh}. \end{aligned}$$

Linear system

At nth time step, solve

$$(\mathbf{M} + \beta_{nn}\mathbf{S})U^n = \mathbf{M}U^{n-1} + k_n \bar{f}^n + \mathbf{S}\sum_{j=1}^{n-1} \beta_{nj} U^j,$$

where

$$\mathbf{M} = Q \times Q \text{ mass matrix}, \qquad \mathbf{S} = Q \times Q \text{ stiffness matrix},$$

$$\bar{f}^n = \frac{1}{k_n}\int_{t_{n-1}}^{t_n} f(t)\,dt,$$

$$\beta_{nn} = \int_{t_{n-1}}^{t_n} \frac{(t-s)^{\nu-1}}{\Gamma(\nu)}\,ds = \frac{k_n^\nu}{\Gamma(1+\nu)},$$

$$\beta_{nj} = \int_{t_{j-1}}^{t_j} \left(\frac{(t_{n-1}-s)^{\nu-1}}{\Gamma(\nu)} - \frac{(t_n-s)^{\nu-1}}{\Gamma(\nu)} \right) ds > 0, \quad j < n.$$

Notice

$$\beta_{nn} \to k_n \quad \text{and} \quad \beta_{nj} \to 0 \quad \text{as } \nu \to 1.$$

Computational cost

Computing the RHS costs $O(nQ)$ operations, after which an optimal solver requires $O(Q)$ operations to compute U^n.

If $k = h^2$ then condition number of $\mathbf{M} + \beta_{nn}\mathbf{S}$ is $O(k^\nu/h^2) = O(k^{-(1-\nu)}) = O(h^{-2(1-\nu)})$; not too large if ν close to 1.

Cost of N timesteps is $O(N^2 Q)$ operations vs $O(NQ)$ for classical diffusion.

Storage cost is $O(NQ)$ vs $O(Q)$ for classical diffusion.

The key idea

Suppose $[\beta_{nj}] \in \mathbb{R}^{N\times N}$ has rank $r \ll N$:

$$\beta_{nj} = \sum_{p=1}^{r} \phi_{pn}\psi_{pj}.$$

Then,

$$\sum_{j=1}^{n-1} \beta_{nj} U^j = \sum_{p=1}^{r} \phi_{pn} \Psi_p^{n-1}(U) \quad \text{where} \quad \Psi_p^{n-1}(U) = \sum_{j=1}^{n-1} \psi_{pj} U^j.$$

Since

$$\Psi_p^n(U) = \psi_{pn} U^n + \Psi_p^{n-1}(U),$$

cost of computing the RHS reduced from $O(nQ)$ to $O(rQ)$.

Our $[\beta_{nj}]$ has rank N, but sub-blocks are well approximated by matrices of low rank.

Fractional derivative

Recall

$$u_t + \mathcal{B}_\nu A u = f$$

where

$$Au = -\nabla \cdot (K \nabla u)$$

and

$$\mathcal{B}_\nu v(t) = \partial_t^{1-\nu} v = \frac{\partial}{\partial t} \int_0^t \frac{(t-s)^{\nu-1}}{\Gamma(\nu)} v(s)\, ds.$$

DG method involves discrete fractional derivative

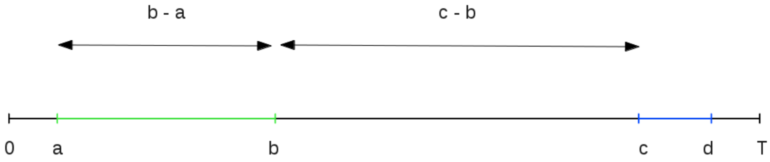
$$\bar{\mathcal{B}}_\nu^n V = \frac{1}{k_n} \int_{t_{n-1}}^{t_n} \mathcal{B}_\nu V(t)\, dt = \frac{1}{k_n} \left(\beta_{nn} V^n - \sum_{j=1}^{n-1} \beta_{nj} V^j \right).$$

Fast summation method introduces additional error from

$$\bar{\mathcal{B}}_\nu^n V \approx \widetilde{\mathcal{B}}_\nu^n V \equiv \frac{1}{k_n} \left(\beta_{nn} V^n - \sum_{j=1}^{n-1} \tilde{\beta}_{nj} V^j \right).$$

Well separated intervals

$$\frac{b-a}{c-b} \leq \eta \leq 1.$$



Taylor expansion

Let

$$I_n = (t_{n-1}, t_n] \quad \text{and} \quad B_\mu(t,k) = \int_{-k/2}^{k/2} \frac{(t+s)^{\mu-1}}{\Gamma(\mu)}\, ds.$$

Theorem

Suppose $0 \le a < b < c < d \le T$ *and* $0 < \eta \le 1$. *For*

$$I_j \subseteq [a,b], \quad I_n \subseteq [c,d], \quad \frac{b-a}{c-b} \le \eta, \quad \bar{s} = \tfrac{1}{2}(a+b),$$

put

$$\beta_{nj}^r = \sum_{p=1}^{r} \underbrace{(-1)^p B_{\nu-p}(t_{n-1/2} - \bar{s}, k_n)}_{\phi_{pn}} \underbrace{B_p(t_{j-1/2} - \bar{s}, k_j)}_{\psi_{pj}}.$$

Then

$$\left|\beta_{nj}^r - \beta_{nj}\right| \le 2^{2-\nu}(r+1)(\eta/2)^r \beta_{nj}.$$

Clusters

A cluster is a set of consecutive subintervals

$$I_{j,n} = \{I_j, I_{j+1}, \dots, I_n\} \quad \text{for } 1 \le j \le n \le N.$$

The diameter of a cluster $\mathrm{C} = I_{nj}$ is the diameter of its underlying point set $\bigcup \mathrm{C} = (t_{j-1}, t_n]$; thus,

$$\mathrm{diam}(\mathrm{C}) = t_n - t_{j-1} \quad \text{if } \mathrm{C} = I_{j,n}.$$

Likewise, the distance between two clusters is

$$\mathrm{dist}(\mathrm{C}_1, \mathrm{C}_2) = \mathrm{dist}\Big(\bigcup \mathrm{C}_1, \bigcup \mathrm{C}_2\Big).$$

The history of a cluster is the preceding half-open interval,

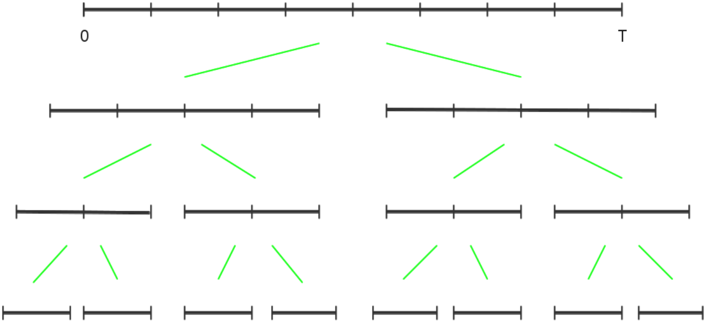
$$\mathrm{History}(\mathrm{C}) = (0, t_{j-1}] \quad \text{if } \mathrm{C} = I_{j,n}.$$

Cluster tree

A cluster tree for the mesh $0 = t_0 < t_1 < t_2 < \cdots < t_N = T$ is a tree T such that

1. each node of T is a cluster,
2. the root node of T is $I_{1,N}$,
3. if a node C is not a leaf, then C is the union of its children,
4. if $C_1, C_2 \in \text{Children}(C)$ for a node C, and if $C_1 \neq C_2$, then $C_1 \cap C_2 = \emptyset$.

Example — binary cluster tree



Admissible cover

Given a leaf L of T, and $\eta \in (0, 1]$, we say that a cluster C is (L, η)-admissible if

$$\bigcup \mathrm{C} \subseteq \mathrm{History}(\mathrm{L}) \quad \text{and} \quad \mathrm{diam}(\mathrm{C}) \leq \eta \, \mathrm{dist}(\mathrm{C}, \mathrm{L}).$$

In this case,

$$\left|\beta^r_{nj} - \beta_{nj}\right| \leq 2^{2-\nu}(r+1)(\eta/2)^r \beta_{nj} \quad \text{for } I_j \in \mathrm{C} \text{ and } I_n \in \mathrm{L}.$$

An (L, η)-admissible cover for T is a set $\mathcal{C}$ of clusters such that

1. each cluster $\mathrm{C} \in \mathcal{C}$ is a node of T,
2. $\bigcup \{\, I : I \in \mathrm{C} \in \mathcal{C} \,\} = \mathrm{History}(\mathrm{L})$,
3. if C_1, $\mathrm{C}_2 \in \mathcal{C}$ with $\mathrm{C}_1 \neq \mathrm{C}_2$, then $\mathrm{C}_1 \cap \mathrm{C}_2 = \emptyset$,
4. if $\mathrm{C} \in \mathcal{C}$ then either C is (L, η)-admissible or else C is a leaf of T.

Recursive subdivision

procedure *divide*$(\mathrm{C}, \mathcal{C}, \mathrm{L}, \mathrm{T}, \eta)$
Determine a, b, c, d such that $\bigcup \mathrm{C} = [a, b]$ and $\bigcup \mathrm{L} = [c, d]$
if $a \leq c$ **then**
  if $b \leq c$ **and** $b - a \leq \eta(c - b)$ **then**
    $\mathcal{C} = \mathcal{C} \cup \{\mathrm{C}\}$
  else if $b \leq c$ **and** C is a leaf **then**
    $\mathcal{C} = \mathcal{C} \cup \{\mathrm{C}\}$
  else
    for all $\mathrm{C}' \in \mathrm{Children}(\mathrm{C})$ **do**
      divide$(\mathrm{C}', \mathcal{C}, \mathrm{L}, \mathrm{T}, \eta)$
    end for
  end if
end if

Put $\mathcal{C} = \emptyset$ and call *divide*$(I_{1,N}, \mathcal{C}, \mathrm{L}, \mathrm{T}, \eta)$, then on return $\mathcal{C}$ is an (L, η)-admissible cover for T.

Near and far clusters

For each leaf L of T we obtain an (L,η)-admissible cover

$$\mathcal{C}(\mathsf{L}) = \mathrm{Near}(\mathsf{L}) \cup \mathrm{Far}(\mathsf{L}),$$

where

$$\begin{aligned}\mathrm{Near}(\mathsf{L}) &= \{\, \mathsf{C} \in \mathcal{C}(\mathsf{L}) : \mathsf{C} \text{ is not } (\mathsf{L},\eta)\text{-admissible} \,\},\\ \mathrm{Far}(\mathsf{L}) &= \{\, \mathsf{C} \in \mathcal{C}(\mathsf{L}) : \mathsf{C} \text{ is } (\mathsf{L},\eta)\text{-admissible} \,\}.\end{aligned}$$

Given $n \in \{1, 2, \ldots, N\}$ there is a unique leaf $\mathsf{L} = \mathsf{L}_n$ containing I_n.

Define $\phi_{pn}(\mathsf{C})$ and $\psi_{pj}(\mathsf{C})$ using the formulae with $[a, b] = \bigcup \mathsf{C}$ and $[c, d] = \bigcup \mathsf{L}_n$.

Example — admissible cover

$N = 32$, $n = 30$ and $\eta = 1.0$ (top) or $\eta = 0.5$ (bottom).

Cluster sums

Define

$$\tilde{\beta}_{nj} = \begin{cases} \beta_{nj} & \text{if } I_j \in \mathsf{L}_n \text{ or } I_j \in \mathsf{C} \in \mathrm{Near}(\mathsf{L}_n), \\ \beta_{nj}^r & \text{if } I_j \in \mathsf{C} \in \mathrm{Far}(\mathsf{L}_n), \end{cases}$$

and

$$\Sigma_n(\mathsf{C}, V) = \sum_{\substack{I_j \in \mathsf{C} \\ j \le n-1}} \beta_{nj} V^j, \qquad \Psi_p(\mathsf{C}, V) = \sum_{I_j \in \mathsf{C}} \psi_{pj}(\mathsf{C}) V^j,$$

$$\widetilde{\Sigma}_n(\mathsf{C}, V) = \sum_{I_j \in \mathsf{C}} \tilde{\beta}_{nj} V^j = \sum_{p=1}^{r} \phi_{pn}(\mathsf{C}) \Psi_p(\mathsf{C}, V).$$

Fast summation:

$$\sum_{j=1}^{n-1} \tilde{\beta}_{nj} V^j = \Sigma_n(\mathsf{L}_n, V) + \sum_{\mathsf{C} \in \mathrm{Near}(\mathsf{L}_n)} \Sigma_n(\mathsf{C}, V) + \sum_{\mathsf{C} \in \mathrm{Far}(\mathsf{L}_n)} \widetilde{\Sigma}_n(\mathsf{C}, V).$$

Numerical example

$T = 6$, $N = 6144$, $Q = 3969$ (64×64 grid), up to 16 far-field clusters, $r = 5$ terms, $\eta = 1$.

CPU times (seconds):

	Fast	Slow
Setup	0.31	17.57
RHS	8.24	224.09
Solver	3.59	3.90
Total	12.14	245.56

$$\max_{\substack{1\le n\le N\\ 1\le q\le Q}} \left|\tilde{U}_q^n - u(x_q, t_n)\right| = 4.47 \times 10^{-4},$$

$$\max_{\substack{1\le n\le N\\ 1\le q\le Q}} \left|\tilde{U}_q^n - U_q^n\right| = 0.84 \times 10^{-4}.$$

Stability

Perturbed problem,

$$(\mathbf{M} + \beta_{nn}\mathbf{S})\tilde{U}^n = \mathbf{M}\tilde{U}^{n-1} + k_n \bar{f}^n + \mathbf{S}\sum_{j=1}^{n-1} \tilde{\beta}_{nj} U^j,$$

Write $\|v\| = \|v\|_{L_2(\Omega)}$.

Theorem

If, for every real-valued, piecewise-constant function V,

$$\sum_{n=1}^{N} k_n (\tilde{\mathcal{B}}_\nu^n V) V^n \geq 0,$$

then

$$\|\tilde{U}^n\| \leq \|U^0\| + 2\sum_{j=1}^{n} k_j \|\bar{f}^j\|, \qquad 1 \leq n \leq N.$$

Accuracy

Theorem

If the perturbed problem is stable, and if

$$\sum_{j=1}^{n} \sum_{l=1}^{j-1} |\tilde{\beta}_{jl} - \beta_{jl}| \leq \frac{\epsilon_n}{\lambda_{\max}(\mathbf{S})},$$

then

$$\|\tilde{U}^n - U^n\| \leq \epsilon_n \max_{1 \leq j \leq n-1} \|U^j\|.$$

Remark:

$$\sum_{n=1}^{N} k_n (\mathcal{B}_\nu^n V) V^n \geq \left(\frac{\pi}{T}\right)^{1-\nu} \frac{(1-\nu)^{1-\nu}}{(2-\nu)^{2-\nu}} \sin(\tfrac{1}{2}\pi\nu) \sum_{n=1}^{N} k_n (V^n)^2.$$