

# A GREEDY ALGORITHM FOR NUMERICAL METHODS IN HIGH DIMENSION

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# Motivation

- A. Ammar. B. Mokdad, F. Chinesta and R. Keunings. *A new family of solvers for some classes of multidimensional partial differential equations encountered in Kinetic Theory modelling Complex Fluids*, Journal of Non-Newtonian Fluid Mechanics, **139**, (2006), pp. 153-176.
- A. Ammar. B. Mokdad, F. Chinesta and R. Keunings. *A new family of solvers for some classes of multidimensional partial differential equations encountered in Kinetic Theory modelling Complex Fluids. Part II: Transient Simulations using Space-Time Separated Representations* Journal of Non-Newtonian Fluid Mechanics, **144**, (2007), pp. 98-121

# Heuristics (Part I)

- Consider a general linear boundary value problem  $L(u) = f$  with homogeneous boundary condition  $u|_{\partial\Omega} = 0$  and  $\Omega = [a, b]^d$ .
- We would to construct a solution step by step starting with a starting map given in separation of variables form:

$$u_0 = u_0^{(1)}(x_1) \cdots u_0^{(d)}(x_d) = u_0^{(1)} \otimes \cdots \otimes u_0^{(d)}$$

such that we would to minimize:

$$u_1^{(1)} \otimes \cdots \otimes u_1^{(d)} \in \arg \min_{u^{(1)} \otimes \cdots \otimes u^{(d)}} \|f - L(u_0 + u^{(1)} \otimes \cdots \otimes u^{(d)})\|$$

# Heuristics (Part II)

- Since  $L$  is a linear map, if we take the residual map

$$r_0 = f - L(u_0^{(1)} \otimes \cdots \otimes u_0^{(d)})$$

the above minimization program can be written as:

$$u_1^{(1)} \otimes \cdots \otimes u_1^{(d)} \in \arg \min_{u^{(1)} \otimes \cdots \otimes u^{(d)}} \|r_0 - L(u^{(1)} \otimes \cdots \otimes u^{(d)})\|$$

- They expect that

$$\|r_0 - L(u_1^{(1)} \otimes \cdots \otimes u_1^{(d)})\| < \|f - L(u_0^{(1)} \otimes \cdots \otimes u_0^{(d)})\|$$

# Heuristics (Part III)

- Proceeding inductively, if we denote by

$$u_n = \sum_{k=0}^n u_k^{(1)} \otimes \cdots \otimes u_k^{(d)}$$

and

$$\|f - L(u_{n+1})\| < \|f - L(u_n)\|$$

follows for all  $n = 0, 1, 2, \dots$ ,

- when

$$\|f - L(u_n)\| < \text{tol}$$

we stop the process and take  $u_n \sim u$ .

# Comments and Remarks

1. Is

$$\arg \min_{u^{(1)} \otimes \dots \otimes u^{(d)}} \|f - L(u^{(1)} \otimes \dots \otimes u^{(d)})\| \neq \emptyset?$$

Note that

$$\mathcal{M}_1 = \left\{ u : u = u^{(1)} \otimes \dots \otimes u^{(d)} \right\}$$

not is a linear space.

2. Is it true that

$$\|f - L(u_{n+1})\| < \|f - L(u_n)\|?$$

# Greedy Approximations

- Let  $X$  be a Banach space equipped with a norm  $\|\cdot\|_X$ . We say that a set  $\mathcal{D} \subset X$  is a *dictionary* if each  $g \in \mathcal{D}$  has norm one and the closure of  $\text{span } \mathcal{D}$  coincides with the whole  $X$ .
- Define  $G(f, \mathcal{D}, X) = \alpha(f)\alpha(g)$ , where  $\alpha(f) \in \mathbb{R}$  and  $\alpha(g) \in \mathcal{D}$  satisfy (we assume existence):

$$\min_{\alpha \in \mathbb{R}, g \in \mathcal{D}} \|f - \alpha g\| = \|f - G(f, \mathcal{D}, X)\| \quad (1)$$

# $X$ -Greedy Algorithm

- We define  $R_0(f, \mathcal{D}, X) := f$ ,  $G_0(f, \mathcal{D}, X) := 0$ . Then for each  $m \geq 1$  we inductively define

$$\begin{aligned}R_m(f, \mathcal{D}, X) &= R_{m-1}(f, \mathcal{D}, X) - G(R_{m-1}(f, \mathcal{D}, X)) \\G_m(f, \mathcal{D}, X) &= G_{m-1}(f, \mathcal{D}, X) + G(R_{m-1}(f, \mathcal{D}, X)).\end{aligned}$$

- Note that

$$R_m(f, \mathcal{D}, X) = f - G_m(f, \mathcal{D}, X) = f - \sum_{k=1}^m \alpha_k g_k,$$

where  $\alpha_k \in \mathbb{R}$  and  $g_k \in \mathcal{D}$ .

- By using (1) it is possible to show that

$$\|R_m(f, \mathcal{D}, X)\| \leq \|R_{m-1}(f, \mathcal{D}, X)\|.$$



# Bad (or Good ?) News

- There are not general results on convergence of  $X$ -Greedy Algorithms (V. N. Temlyakov).
- In particular there are not results for the sequence  $\{R_m(f, \mathcal{D}, X)\}$  to be strictly decreasing.
- Note that

$$\mathcal{D} = \{u \in \mathcal{M}_1 : \|u\| = 1\}$$

is a dictionary, and

$$\mathcal{M}_1 = \{\alpha u; \alpha \in \mathbb{R} \text{ and } u \in \mathcal{D}\}.$$

# Some related problems

1. Consider that  $L = I$  and  $f \in L_2(X \times Y)$ , then we would to find  $v_1, \dots, v_n \in L_2(X)$  and  $w_1, \dots, w_n \in L_2(Y)$  such that if

$$u_n = \sum_{k=1}^n v_k \otimes w_k$$

then

$$\|f - u_n\|_{L_2(X \times Y)},$$

is as small as possible. It was solved by Jaromir Simsa in 1992.

# Some related problems

2. Consider  $L = I$  and  $\mathbf{f} \in \mathbb{R}^{d_1 \times \dots \times d_k}$  then we would to construct a vector

$$\mathbf{u}_r = \sum_{j=1}^r \mathbf{v}_j^{(1)} \otimes \dots \otimes \mathbf{v}_j^{(k)}, \quad \mathbf{v}_j^{(i)} \in \mathbb{R}^{d_i}$$

that minimizes

$$\|\mathbf{f} - \mathbf{u}_r\|.$$

This problem is called the *best low-rank approximation problem*.

# Best low-rank approximation problem

- (a) For  $k = 2$  the problem is solved by using the SVD (Eckart-Young Theorem).
- (b) It has no solution in general for  $r = 2, \dots, \min\{d_1, d_2, \dots, d_k\}$  and  $k \geq 3$  (V. de Silva and L.H. Lim, 2008).
- (c) The set of tensors that fail to have best low-rank approximation has positive volume (V. de Silva and L.H. Lim, 2008).

# Introducing some notation

Recall the set

$$\mathcal{M}_1 = \left\{ u \in H : u = u^{(1)} \otimes \cdots \otimes u^{(d)}, u^{(i)} \in H_i \right\}$$

where  $H = H_1 \otimes \cdots \otimes H_d$  and  $H_i$  is a separable Hilbert space with norm given by

$$\| \cdot \|_H = \| \cdot \|_1 \cdots \| \cdot \|_d.$$

Note that

1.  $\alpha \mathcal{M}_1 = \mathcal{M}_1$  for all  $\alpha \in \mathbb{R} \setminus \{0\}$  and
2.  $0 \in \mathcal{M}_1$ .

# The problem in abstract setting

Let

$$\mathcal{M}_r = \overbrace{\mathcal{M}_1 + \cdots + \mathcal{M}_1}^{r\text{-times}}$$

and  $L : H \rightarrow H$  be a given linear operator. Then the  $r$ -best low-rank approximation problem for the initial problem can be stated as follows: For a given  $f \in H$  and is

$$\min_{u \in \mathcal{M}_r} \|f - L(u)\|$$

Unfortunately, for  $r \geq 2$  is ill-posed problem, because  $\mathcal{M}_r$  is not a closed set.

# A main result

**Theorem 1** *If  $L : H \rightarrow H$ , is bounded and has a bounded inverse then*

$$\arg \min_{u \in \mathcal{M}_1} \|f - L(u)\| \neq \emptyset.$$

**Lemma 2** *The set  $\mathcal{M}_1$  is closed in  $H$ .*

**Proof.** Let  $x_n \in \mathcal{M}_1 \rightarrow x$  in  $H$ , then  $x_n \in \mathcal{M}_1 \rightharpoonup x$  weakly,

Since  $x_n = \lambda_n u_n^1 \otimes \cdots \otimes u_n^d$  where  $\lambda_n = \|x_n\|_H$ , then

$\lambda_n \rightarrow \lambda = \|x\|$ . Since  $u_n^i$  belongs to the unit ball in  $H_i$ , then there exists a subsequence  $u_{n_k}^i \rightharpoonup u^i$  weakly. In

consequence  $x_{n_k} = \lambda_{n_k} u_{n_k}^1 \otimes \cdots \otimes u_{n_k}^d \rightharpoonup \lambda u^1 \otimes \cdots \otimes u^d$  weakly, and  $x = \lambda u^1 \otimes \cdots \otimes u^d \in \mathcal{M}_1$ . ■

# Proof of Theorem

Note that the map  $\Phi(u) = \|f - L(u)\|$  is bounded below and continuous from  $\mathcal{M}_1$  to  $\mathbb{R}$ . Let  $\alpha = \inf_{u \in \mathcal{M}_1} \Phi(u)$ . Then, there exists  $u_n \in \mathcal{M}_1$  be such that

$$\alpha + \frac{1}{n} \geq \Phi(u_n) \geq \alpha \text{ in } \mathbb{R}.$$

Thus,  $w_n = f - L(u_n)$  is a bounded sequence in  $H$ , thus there exists a subsequence  $w_{n_k} \rightharpoonup w^*$  weakly. Then, since  $L^{-1}$  exists and it is bounded  $u_{n_k} \rightharpoonup L^{-1}(f - w^*) = u^* \in \mathcal{M}_1$ . In consequence  $\Phi(u_{n_k}) \rightarrow \Phi(u^*) = \alpha$ , and

$$u^* \in \arg \min_{u \in \mathcal{M}_1} \|f - L(u)\|.$$



# The main result

**Theorem 3** *Assume that  $L : H \rightarrow H$ , is bounded and has a bounded inverse. Then there exists a sequence  $\{u_n\}_{n=0}^{\infty} \subset H$  such that  $u_0 = 0$ , and  $u_{n+1} \in \mathcal{M}_{n+1}$  for each  $n \geq 0$  satisfy the following optimal condition:*

$$\|f - L(u_{n+1})\| = \min_{x \in \mathcal{M}_1} \|f - L(x + u_n)\|. \quad (2)$$

*Moreover, if for some  $n \in \mathbb{N}$  it follows that*

$$\|f - L(u_n)\| = \|f - L(u_{n-1})\| \quad (3)$$

*then  $f = L(u_{n-1})$ .*

# Proof of main result I

Let  $u_0 = 0$ , then by using Theorem 1 inductively (2) follows. In order to prove the second part of theorem, we start with the case  $n = 1$ . Thus, assume that it follows

$$\|f - L(u_1)\| = \|f\| = \inf_{x \in \mathcal{M}_1} \|f - L(x)\|.$$

If  $x_i \in H_i$  for  $i = 1, 2, \dots, d$ , then

$$\lambda x_1 \otimes x_2 \otimes \dots \otimes x_d \in \mathcal{M}_1$$

for all  $\lambda \in \mathbb{R}$ . Consequently, we have

$$\|f - L(\lambda x_1 \otimes x_2 \otimes \dots \otimes x_d)\| \geq \|f\| \quad (4)$$

for every  $\lambda \in \mathbb{R}$ .

# Proof of main result II

This implies that  $f$  and  $L(x_1 \otimes x_2 \otimes \cdots \otimes x_d)$  are orthogonal. Since the vectors  $x_i \in H_i$  for  $i = 1, 2, \dots, d$ , are arbitrary and  $L$  has zero null space, this means that  $f = 0$ , which proves the second part of the theorem for  $n = 1$ . To prove it with  $n > 1$ , suppose that

$$\|f - L(u_n)\| = \inf_{x \in \mathcal{M}_1} \|f - L(u_{n-1}) - L(x)\| = \|f - L(u_{n-1})\|$$

which implies, by using a similar argument as above, that  $f - L(u_{n-1}) = 0$ .

# A Greedy Algorithm

```
1: procedure ( $\|f - L(u)\| < \varepsilon : u \in \mathcal{M}_{\text{rank\_max}}$ )
2:    $r_0 = f$ 
3:    $u = 0$ 
4:   for  $i = 0, 1, 2, \dots, \text{rank\_max}$  do
5:      $x =$  procedure ( $\min_{x \in \mathcal{M}_1} \|r_i - L(x)\|$ )
6:      $r_{i+1} = r_i - L(x)$ 
7:      $u \leftarrow u + x$ 
8:     if  $\|r_{i+1}\| < \varepsilon$  or  $\| \|r_{i+1}\| - \|r_i\| \| < \text{tol}$  then goto
13
9:       end if
10:    end for
11:    return  $u$  and  $\|r_{\text{rank\_max}}\|$ .
12:    break
13:    return  $u$  and  $\|r_{i+1}\|$ 
14: end procedure
```

# Some remarks

Note that in 6:

$$\|r_{i+1}\| = \|r_i - L(x)\| \leq \|r_i - L(y)\|$$

for all  $y \in \mathcal{M}_1$ , since  $0 \in \mathcal{M}_1$

$$\|r_{i+1}\| = \|r_i - L(x)\| \leq \|r_i\|$$

Theorem 2 implies that either  $\|r_i\| = 0$  or

$$\|r_{i+1}\| < \|r_i\|$$

# A numerical example

we compute for a given vector  $\mathbf{f} \in \mathbb{R}^{14 \times 14 \times 14}$  its approximation by a vector  $\sum_{j=1}^n \mathbf{f}_j^1 \otimes_K \mathbf{f}_j^2 \otimes_K \mathbf{f}_j^3$ , Here  $\otimes_K$  denotes the Kronecker product. To this end we consider

$$L = I$$

where  $I$  is the identity matrix. Then for a randomly choosed vector  $\mathbf{f}$  and for the parameter values `iter_max` = 10, `rank_max` = 1000 and  $\varepsilon = 0.001$ , we compute the sequence  $\|\mathbf{r}^n\| = \|\mathbf{f} - A\mathbf{z}_n\|$ . As can see in Figure 23 it is a strictly decreasing sequence. The algorithm stopped at  $n = 580$  after 46.13 seconds with a relative error equal to  $3.31590880125612e - 05$

# Figure

