



Orthogonalization schemes in tensor train format

Martina Iannacito, Olivier Coulaud, Luc Giraud

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Orthogonalization schemes in tensor train format

29th Biennial Numerical Analysis Conference,
June 28th 2023, Glasgow

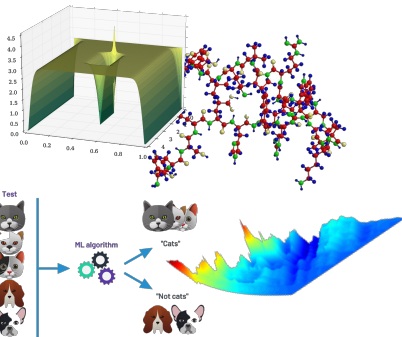
Martina Iannacito*
joint work with Olivier Coulaud[†] and Luc Giraud[†]

* KU Leuven

[†] Centre Inria at the University of Bordeaux

The context in matrix computation

- Stochastic equations
- Uncertainty quantification problems
- Quantum and vibration chemistry
- Optimization
- Machine learning



reduce their problems to

Least-squares

$$\min_{x \in S} \|b - Ax\|$$

Eigenpairs

$$Ax = \lambda x$$

Linear systems

$$Ax = b$$

Gram-Schmidt process [Leon et al. 2013]

Given $\{a_h\}_h$ linearly independent vectors, we construct an orthogonal basis $\{q_h\}$ such that

$$q_1 = a_1,$$

Gram-Schmidt process [Leon et al. 2013]

Given $\{a_h\}_h$ linearly independent vectors, we construct an orthogonal basis $\{q_h\}$ such that

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let $Q_k = [q_1, \dots, q_k]$ be a $n \times k$ matrix

All projections, then subtractions

Gram-Schmidt process [Leon et al. 2013]

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$$q_{k+1} \leftarrow (\mathbb{I}_n - Q_k Q_k^\top) a_{k+1}$$

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From theory to coding: an example I

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Are these versions equivalent in finite precision arithmetic?

Not equivalent in general

Classical Gram-Schmidt

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$$q_{k+1} \leftarrow (\mathbb{I}_n - Q_k Q_k^\top) a_{k+1}$$

Modified Gram-Schmidt

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From theory to coding: an example II

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$$A = \begin{bmatrix} 1 & 1 & 1 \\ \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{bmatrix} \quad \text{with} \quad \varepsilon = 1e-10 \quad \text{in fp64}$$

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$$Q_{\text{CGS}} = \begin{bmatrix} 1 & 0 & 0 \\ \varepsilon & -\varepsilon & -\varepsilon \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{bmatrix},$$

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This example was taken from [Björck 1996].

Loss of orthogonality

Let $Q_k = [q_1, \dots, q_k]$ be the computed orthogonal basis, then its **loss of orthogonality** is

$$\|\mathbb{I}_k - Q_k^\top Q_k\|.$$

It measures the quality in terms of orthogonality of the computed basis. It is linked with the computational precision u and the linearly dependency of the input vectors $A_k = [a_1, \dots, a_k]$, estimated through $\kappa(A_k)$.

Matrix		
Source	Algorithm	$\ \mathbb{I}_k - Q_k^\top Q_k\ $
[Stathopoulos et al. 2002]	Gram	$\mathcal{O}(u\kappa^2(A_k))$
[Giraud et al. 2005]	CGS	$\mathcal{O}(u\kappa^2(A_k))$
[Björck 1967]	MGS	$\mathcal{O}(u\kappa(A_k))$
[Giraud et al. 2005]	CGS2	$\mathcal{O}(u)$
[Giraud et al. 2005]	MGS2	$\mathcal{O}(u)$
[Wilkinson 1965]	Householder	$\mathcal{O}(u)$

The advent of tensors

matrix

$$\begin{bmatrix} 1 & 8 & 4 \\ 9 & 2 & 2 \\ 7 & 1 & 6 \end{bmatrix}$$

since the last century



tensor

$$\begin{bmatrix} 1 & 8 & 4 \\ 9 & 2 & 5 & 3 & 1 \\ 7 & 1 & 2 & 6 & 4 & 9 \\ & & 6 & 8 & 7 \end{bmatrix}$$

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Approximation techniques were proposed

- Canonical Polyadic
- Tucker
- Hierarchical Tucker
- Tensor-Train

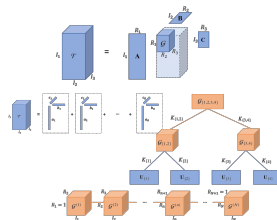


Figure: from [Bi et al. 2022]

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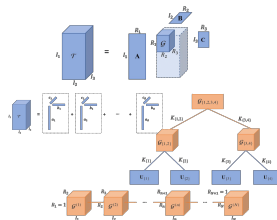


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Approximation techniques introduce **norm-wise** compression errors

Tensor Train formalism



scalar

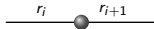


n

vector



matrix



order-3 tensor

Tensor Train formalism



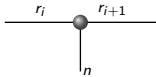
scalar



vector



matrix



order-3 tensor

Let $\mathbf{x} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ be order- d tensor, its TT-representation is

Tensor Train formalism



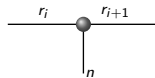
scalar



vector

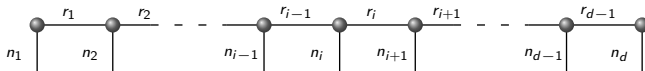


matrix



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+ The storage cost is $\mathcal{O}(dnr^2)$ with $r = \max\{r_i\}$, said **TT-ranks**

Tensor Train formalism



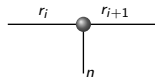
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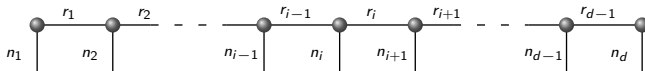


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- Linear combinations increase the TT-ranks

Tensor Train formalism



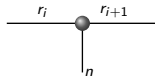
scalar



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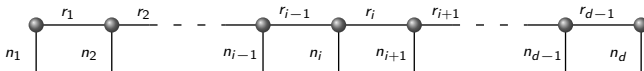


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- Linear combinations increase the TT-ranks

TT-rounding [Oseledets 2011]

If $\mathbf{z}$ is an order- d tensor in TT-format and $\delta \in (0, 1)$, then $\bar{\mathbf{z}} = \text{TT-rounding}(\mathbf{z}, \delta)$ such that

$$\|\mathbf{z} - \bar{\mathbf{z}}\| \leq \delta \|\mathbf{z}\|$$

In the Tensor-Train framework

compression precision δ

- norm-wise perturbation
- TT-model [Oseledets 2011]

computational precision u

- component-wise perturbation
- IEEE model [Higham 2002]

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- How to design orthogonalization kernels for tensor subspace?
- Does compression affect the loss of orthogonality?
- Are tensor results related with the known linear algebra ones?

Classical and Modified Gram-Schmidt

$$\mathcal{Q}, R = \text{CGS}(\mathcal{A}, \delta)$$

Input: $\mathcal{A} = \{\mathbf{a}_1, \dots, \mathbf{a}_m\}$, $\delta \in \mathbb{R}_+$

```
1 for  $i = 1, \dots, m$  do
2    $\mathbf{p} = \mathbf{a}_i$ 
3   for  $j = 1, \dots, i - 1$  do
4      $R(i, j) = \langle \mathbf{a}_i, \mathbf{q}_j \rangle$ 
5      $\mathbf{p} = \mathbf{p} - R(i, j)\mathbf{q}_j$ 
6   end
7    $\mathbf{p} = \text{TT-rounding}(\mathbf{p}, \delta)$ 
8    $R(i, i) = \|\mathbf{p}\|$ 
9    $\mathbf{q}_i = 1/R(i, i) \mathbf{p}$ 
10 end
```

Output: $\mathcal{Q} = \{\mathbf{q}_1, \dots, \mathbf{q}_m\}$, R

$$\mathcal{Q}, R = \text{MGS}(\mathcal{A}, \delta)$$

Input: $\mathcal{A} = \{\mathbf{a}_1, \dots, \mathbf{a}_m\}$, $\delta \in \mathbb{R}_+$

```
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Output: $\mathcal{Q} = \{\mathbf{q}_1, \dots, \mathbf{q}_m\}$, R

They readily write in TT-format.

CGS and MGS with reorthogonalization

 $Q, R = \text{CGS2}(\mathcal{A}, \delta)$

Input: $\mathcal{A} = \{\mathbf{a}_1, \dots, \mathbf{a}_m\}$, $\delta \in \mathbb{R}_+$

```
1 for  $i = 1, \dots, m$  do
2    $\mathbf{p}_k = \mathbf{a}_i$ 
3   for  $k = 1, 2$  do
4      $\mathbf{p}_k = \mathbf{p}_{k-1}$ 
5     for  $j = 1, \dots, i - 1$  do
6        $R(i, j) = \langle \mathbf{p}_{k-1}, \mathbf{q}_j \rangle$ 
7        $\mathbf{p}_k = \mathbf{p}_k - R(i, j)\mathbf{q}_j$ 
8     end
9      $\mathbf{p}_k = \text{TT-rounding}(\mathbf{p}_k, \delta)$ 
10  end
11   $R(i, i) = \|\mathbf{p}_2\|$ 
12   $\mathbf{q}_i = 1/R(i, i) \mathbf{p}_2$ 
13 end
```

Output: $Q = \{\mathbf{q}_1, \dots, \mathbf{q}_m\}$, R

 $Q, R = \text{MGS2}(\mathcal{A}, \delta)$

Input: $\mathcal{A} = \{\mathbf{a}_1, \dots, \mathbf{a}_m\}$, $\delta \in \mathbb{R}_+$

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12   $\mathbf{q}_i = 1/R(i, i) \mathbf{p}_2$ 
13 end
```

Output: $Q = \{\mathbf{q}_1, \dots, \mathbf{q}_m\}$, R

Let $A = [a_1, \dots, a_m]$, then we look for $A = QR$ with $Q^\top Q = \mathbb{I}_m$
compute the Gram matrix

$$A^\top A = (R^\top Q^\top)QR = R^\top R$$

this is (almost) the **Cholesky** factorization of $A^\top A$ that can be written as

$$A^\top A = R^\top R = LL^\top$$

with the Cholesky factor $L = R^\top$. Thus, it follows

$$A = QR = QL^\top$$

from which we obtain Q by solving a linear system.

$$\mathcal{Q}, R = \text{Gram}(\mathcal{A}, \delta)$$

Input: $\mathcal{A} = \{\mathbf{a}_1, \dots, \mathbf{a}_m\}$, $\delta \in \mathbb{R}_+$

1 G is $(m \times m)$ Gram matrix from $\mathcal{A}$

2 $L = \text{cholesky}(G)$

3 $\{\mathbf{p}_1, \dots, \mathbf{p}_m\}$ from $\mathcal{A}$ and $(L^\top)^{-1}$

4 **for** $i = 1, \dots, m$ **do**

5 | $\mathbf{q}_i = \text{TT-rounding}(\mathbf{p}_i, \delta)$

6 **end**

Output: $\mathcal{Q} = \{\mathbf{q}_1, \dots, \mathbf{q}_m\}$, R

In TT-format the following modifications occur

- $G(i, j)$ is the scalar product of $\mathbf{a}_i$ and $\mathbf{a}_j$
- The inverse of $L^\top$ is explicitly computed
- $\mathbf{p}_i$ is constructed as a linear combination of $\mathcal{A}$ elements

Householder transformation

Given a vector $x \in \mathbb{R}^n$ and a direction $y \in \mathbb{R}^n$, the Householder reflector H reflects x along y , i.e.,

$$Hx = ||x||y \quad \text{with} \quad ||y|| = 1.$$

Thanks to its properties, H writes as

$$H = \mathbb{I}_n - \frac{2}{||z||^2} z \otimes z \quad \text{with} \quad z = (x - ||x||y).$$

The practical implementation of the Householder transformation kernel uses the components of the input vectors.

Remark

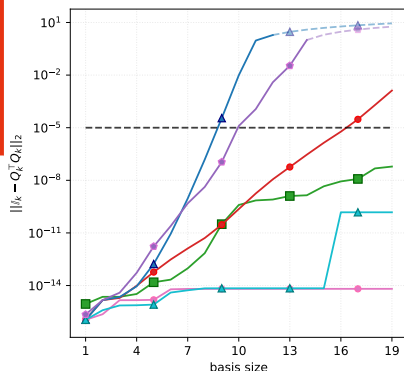
The Householder algorithm does **not** readily apply to tensor in TT-formats, because of the compressed nature of this format. It is described in [Iannacito 2022]

Numerical experiments in TT-format

Let Δ_d is be the TT-Laplacian, then $\{\mathbf{a}_k\}$ are 'Krylov tensors', i.e.,
 $\mathbf{a}_{k+1} = \text{TT-rounding}(\Delta_d \mathbf{x}_k, \text{max_rank} = 1)$ with $\mathbf{x}_{k+1} = \frac{1}{\|\mathbf{a}_{k+1}\|} \mathbf{a}_{k+1}$

Numerical experiments in TT-format

Let Δ_d is be the TT-Laplacian, then $\{\mathbf{a}_k\}$ are 'Krylov tensors', i.e.,
$$\mathbf{a}_{k+1} = \text{TT-rounding}(\Delta_d \mathbf{x}_k, \text{max_rank} = 1) \quad \text{with} \quad \mathbf{x}_{k+1} = \frac{1}{\|\mathbf{a}_{k+1}\|} \mathbf{a}_{k+1}$$

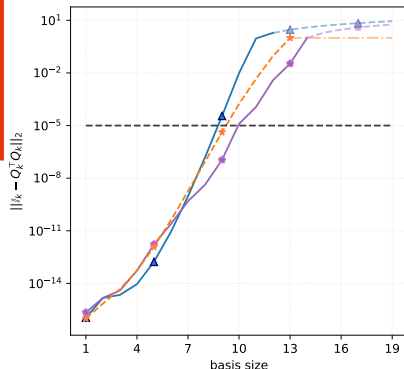


- Gram approach
- CGS
- MGS
- CGS2
- MGS2
- Householder transformation

Figure: 20 tensors of order $d = 3$ and mode size $n = 15$, compression precision $\delta = 10^{-5}$, computational precision $u = \mathcal{O}(10^{-16})$

Numerical experiments in TT-format

Loss of orthogonality for $\{\mathbf{a}_k\}$ 'Krylov tensors'



- Gram approach

- CGS

- $\delta\kappa^2(A_k)$ with

$$A_k = [\text{vec}(\mathbf{a}_1), \dots, \text{vec}(\mathbf{a}_k)]$$

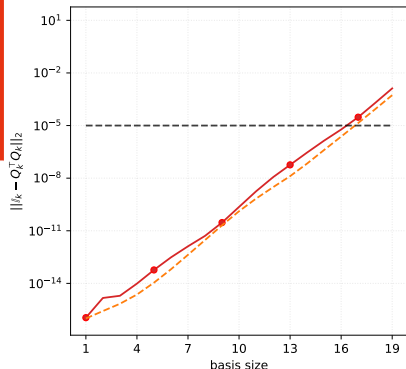
then we conjecture

$$\mathcal{O}(\delta\kappa^2(A_k))$$

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Numerical experiments in TT-format

Loss of orthogonality for $\{\mathbf{a}_k\}$ 'Krylov tensors'



- **MGS**
- $\delta\kappa(A_k)$ with

$$A_k = [\text{vec}(\mathbf{a}_1), \dots, \text{vec}(\mathbf{a}_k)]$$

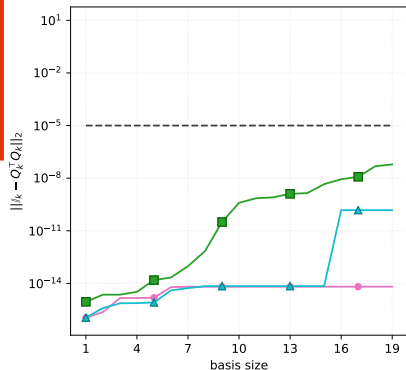
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Numerical experiments in TT-format

Loss of orthogonality for $\{\mathbf{a}_k\}$ 'Krylov tensors'



- CGS2
 - MGS2
 - Householder transformation
- then we conjecture

$$\mathcal{O}(\delta)$$

Figure: 20 tensors of order $d = 3$ and mode size $n = 15$, compression precision $\delta = 10^{-5}$, computational precision $u = \mathcal{O}(10^{-16})$

<i>Algorithm</i>	Matrix, theoretical	TT-format, conjecture
	$\ \mathbb{I}_k - Q_k^\top Q_k\ $	$\ \mathbb{I}_k - \mathcal{Q}_k^\top \mathcal{Q}_k\ $
Gram	$\mathcal{O}(\textcolor{red}{u}\kappa^2(A_k))$	$\mathcal{O}(\textcolor{red}{\delta}\kappa^2(\mathcal{A}_k))$
CGS	$\mathcal{O}(\textcolor{red}{u}\kappa^2(A_k))$	$\mathcal{O}(\textcolor{red}{\delta}\kappa^2(\mathcal{A}_k))$
MGS	$\mathcal{O}(\textcolor{red}{u}\kappa(A_k))$	$\mathcal{O}(\textcolor{red}{\delta}\kappa(\mathcal{A}_k))$
CGS2	$\mathcal{O}(\textcolor{red}{u})$	$\mathcal{O}(\textcolor{red}{\delta})$
MGS2	$\mathcal{O}(\textcolor{red}{u})$	$\mathcal{O}(\textcolor{red}{\delta})$
Householder	$\mathcal{O}(\textcolor{red}{u})$	$\mathcal{O}(\textcolor{red}{\delta})$

with $\textcolor{red}{u}$ the computational precision, $\textcolor{red}{\delta}$ the compression precision

Conclusions and perspectives

- All the 6 kernels can be generalized to the TT-framework
- Loss of orthogonality bounds appears to hold true with
 - > the compression precision δ independent from the machine architecture
 - > the compression precision δ replacing the computational one u
 - > the compression acting norm-wise rather than component-wise

More detailed results can be found at [Coulaud et al. 2022]

Conclusions and perspectives

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What is left out?

- Theoretical proof of the loss of orthogonality bounds
- Investigating the quality of the tensor subspace spanned by the orthogonal basis

	cost in fp operations	cost in TT-rounding
Gram	$\mathcal{O}(2nm^2)$	m
CGS	$\mathcal{O}(2nm^2)$	m
MGS	$\mathcal{O}(2nm^2)$	m
CGS2	$\mathcal{O}(4nm^2)$	$2m$
MGS2	$\mathcal{O}(4nm^2)$	$2m$
Householder	$\mathcal{O}(2nm^2 - 2m^3/3)$	$4m$

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Thanks for the attention.

Questions?

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