



# Orthogonalization schemes in tensor train format

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

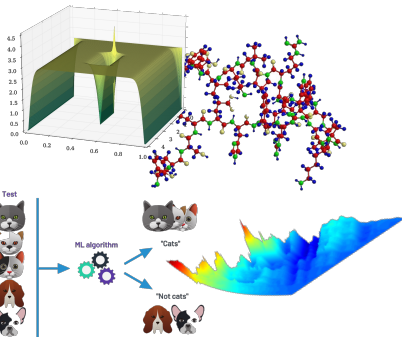
Martina Iannacito\*  
joint work with Olivier Coulaud<sup>†</sup> and Luc Giraud<sup>†</sup>

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# 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

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Are these versions equivalent in finite precision arithmetic?

Not equivalent in general

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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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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]	<b>Gram</b>	$\mathcal{O}(u\kappa^2(A_k))$
[Giraud et al. 2005]	<b>CGS</b>	$\mathcal{O}(u\kappa^2(A_k))$
[Björck 1967]	<b>MGS</b>	$\mathcal{O}(u\kappa(A_k))$
[Giraud et al. 2005]	<b>CGS2</b>	$\mathcal{O}(u)$
[Giraud et al. 2005]	<b>MGS2</b>	$\mathcal{O}(u)$
[Wilkinson 1965]	<b>Householder</b>	$\mathcal{O}(u)$

# 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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- + Better representation
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- Curse of dimensionality

Approximation techniques were proposed

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

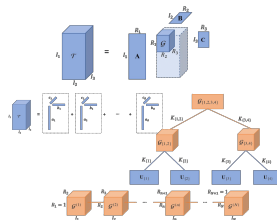


Figure: from [Bi et al. 2022]

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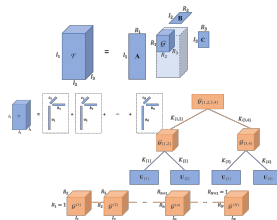


Figure: from [Bi et al. 2022]

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

# Tensor Train formalism



scalar



$n$

vector



$n$

matrix



$n$

order-3 tensor



# Tensor Train formalism



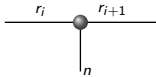
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order-3 tensor

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

# Tensor Train formalism



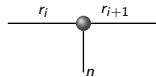
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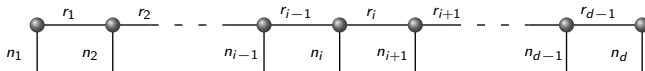


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+ The storage cost is  $\mathcal{O}(dnr^2)$  with  $r = \max\{r_i\}$ , said **TT-ranks**

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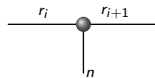
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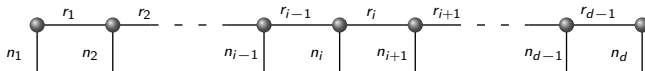


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- Linear combinations increase the TT-ranks

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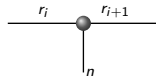
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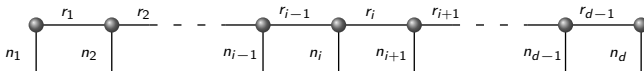


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## TT-rounding [Oseledets 2011]

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  $\delta$

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

computational precision  $u$

- component-wise perturbation
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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:**  $\mathcal{Q} = \{\mathbf{q}_1, \dots, \mathbf{q}_m\}$ ,  $R$

---

---

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

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

---

---

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

---

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**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

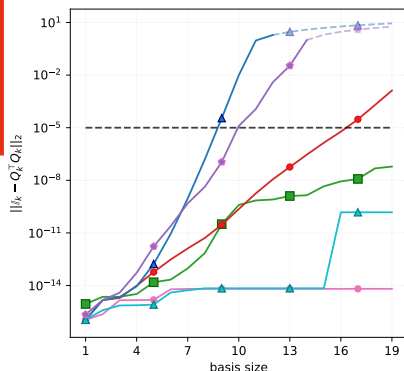
The Householder algorithm does **not** readily apply to tensor in TT-formats, because of the compressed nature of this format. It is described in [Iannacito 2022]

## Numerical experiments in TT-format

Let  $\Delta_d$  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

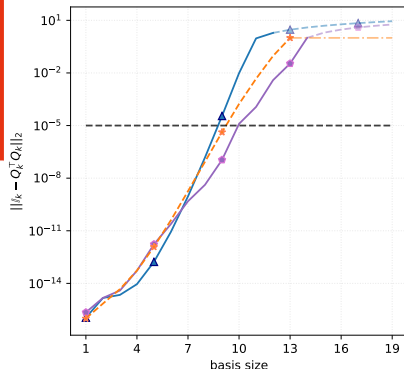
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- Gram approach
- CGS
- MGS
- CGS2
- MGS2
- Householder transformation

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

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



- Gram approach

- CGS

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

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

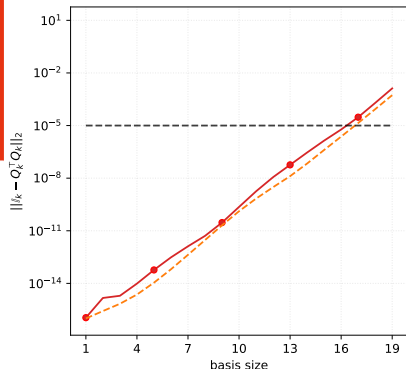
then we conjecture

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

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'



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

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

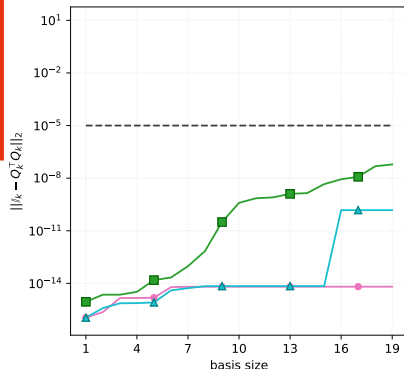
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Figure: 20 tensors of order  $d = 3$  and mode size  $n = 15$ , compression precision  $\delta = 10^{-5}$ , computational precision  $u = \mathcal{O}(10^{-16})$

# Numerical experiments in TT-format

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



- 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\ $
<b>Gram</b>	$\mathcal{O}(\mathbf{u}\kappa^2(A_k))$	$\mathcal{O}(\delta\kappa^2(\mathcal{A}_k))$
<b>CGS</b>	$\mathcal{O}(\mathbf{u}\kappa^2(A_k))$	$\mathcal{O}(\delta\kappa^2(\mathcal{A}_k))$
<b>MGS</b>	$\mathcal{O}(\mathbf{u}\kappa(A_k))$	$\mathcal{O}(\delta\kappa(\mathcal{A}_k))$
<b>CGS2</b>	$\mathcal{O}(\mathbf{u})$	$\mathcal{O}(\delta)$
<b>MGS2</b>	$\mathcal{O}(\mathbf{u})$	$\mathcal{O}(\delta)$
<b>Householder</b>	$\mathcal{O}(\mathbf{u})$	$\mathcal{O}(\delta)$

with  $\mathbf{u}$  the computational precision,  $\delta$  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  $\delta$  independent from the machine architecture
  - > the compression precision  $\delta$  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
<b>Gram</b>	$\mathcal{O}(2nm^2)$	$m$
<b>CGS</b>	$\mathcal{O}(2nm^2)$	$m$
<b>MGS</b>	$\mathcal{O}(2nm^2)$	$m$
<b>CGS2</b>	$\mathcal{O}(4nm^2)$	$2m$
<b>MGS2</b>	$\mathcal{O}(4nm^2)$	$2m$
<b>Householder</b>	$\mathcal{O}(2nm^2 - 2m^3/3)$	$4m$

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Thanks for the attention.

Questions?

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*Invia*