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Orthogonalization schemes in tensor train format

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Inria

Orthogonalization schemes in tensor train format

SIAM Conference on Applied Linear Algebra,
May 14, 2024, Paris

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joint work with Olivier Coulaud† and Luc Giraud†

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dell'Università
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Italiadomani
PIANO NAZIONALE
DI RIPRESA E RESILIENZA



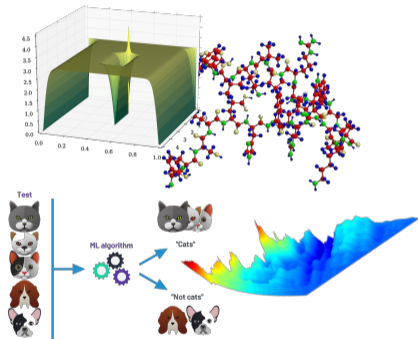
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Computing an orthogonal basis is a fundamental sub-problem for numerical simulations

Computing an orthogonal basis is a fundamental sub-problem for numerical simulations

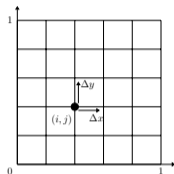
High-dimensional simulations arise in

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



Example

$$\begin{cases} \mathcal{L}(u) = f & \text{in } \Omega \\ u = f_0 & \text{in } \partial\Omega \end{cases} \quad \text{for } \Omega \subseteq \mathbb{R}^{n_1 \times \dots \times n_d}$$



$$\mathcal{A}\mathcal{X} = \mathcal{B}$$

where \mathcal{A} is a multilinear operator and \mathcal{B} is a tensor.

The curse of dimensionality

The storage cost increases **exponentially** with respect to the number of variables.



Several tensor decomposition techniques exist

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

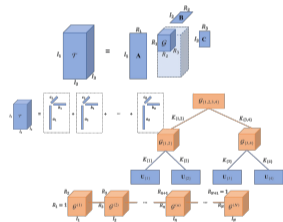


Figure: from [Bi et al. 2022]

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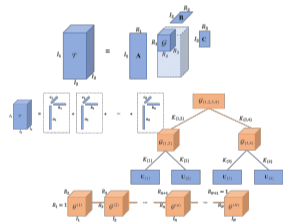




Figure: from [Bi et al. 2022]



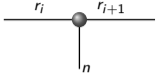
scalar



vector




matrix




order-3 tensor



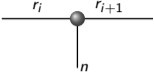
scalar



vector

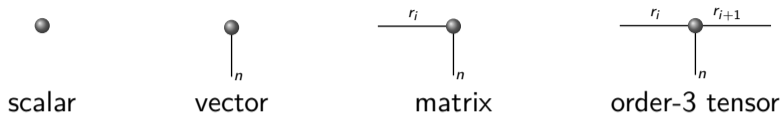


matrix

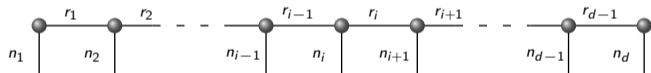


order-3 tensor

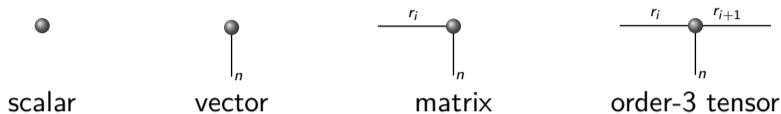
The TT-representation of \mathcal{X} an $(n_1 \times \dots \times n_d)$ tensor is



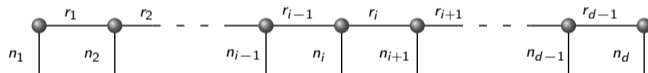
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+ The storage cost is $\mathcal{O}(dnr^2)$ with $r = \max\{r_i\}$, said **TT-ranks**



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

TT-rounding [Oseledets 2011]

If \mathcal{X} is a tensor in TT-format and $\delta \in (0, 1)$, then $\bar{\mathcal{X}} = \text{TT-rounding}(\mathcal{X}, \delta)$ such that

$$\|\mathcal{X} - \bar{\mathcal{X}}\| \leq \delta \|\mathcal{X}\|$$

where $\max(\text{TT-ranks}(\bar{\mathcal{X}})) < (\max \text{TT-ranks}(\mathcal{X}))$

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Question

How the introduction of compression steps affects the **loss of orthogonality**

$$\|\mathbb{I}_k - \mathcal{Q}_k^\top \mathcal{Q}_k\|$$

of computed basis \mathcal{Q}_k ?

Classical matrix results

The **loss of orthogonality** of the computed orthogonal basis \mathbf{Q}_k

- depends on the computational precision u
- may be affected by the collinearity of the input vectors $\mathbf{A}_k = [\mathbf{a}_1, \dots, \mathbf{a}_k]$, expressed by $\kappa(A_k)$

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<i>Source</i>	<i>Algorithm</i>	$\ \mathbb{I}_k - \mathbf{Q}_k^T \mathbf{Q}_k\ $
[Stathopoulos and Wu 2002]	Gram	$\mathcal{O}(u\kappa^2(\mathbf{A}_k))$
[Giraud, Langou, and Rozložník 2005]	CGS	$\mathcal{O}(u\kappa^2(\mathbf{A}_k))$
[Björck 1967]	MGS	$\mathcal{O}(u\kappa(\mathbf{A}_k))$
[Giraud, Langou, and Rozložník 2005]	CGS2	$\mathcal{O}(u)$
[Giraud, Langou, and Rozložník 2005]	MGS2	$\mathcal{O}(u)$
[Wilkinson 1965]	Householder	$\mathcal{O}(u)$

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TT-orthogonalization kernels

Classical and Modified Gram-Schmidt

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

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

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

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

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

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

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

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

They readily write in TT-format.

CGS and MGS with reorthogonalization

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

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

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

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

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

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

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

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

Gram approach - matrix format

Let $\mathbf{A} = [\mathbf{a}_1, \dots, \mathbf{a}_m]$, then we look for $\mathbf{A} = \mathbf{QR}$ with $\mathbf{Q}^\top \mathbf{Q} = \mathbb{I}_m$
compute the Gram matrix

$$\mathbf{A}^\top \mathbf{A} = (\mathbf{R}^\top \mathbf{Q}^\top) \mathbf{Q} \mathbf{R} = \mathbf{R}^\top \mathbf{R}$$

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

$$\mathbf{A}^\top \mathbf{A} = \mathbf{R}^\top \mathbf{R} = \mathbf{L} \mathbf{L}^\top$$

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

$$\mathbf{A} = \mathbf{QR} = \mathbf{QL}^\top$$

from which we obtain \mathbf{Q} by solving a linear system.

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

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

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

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

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

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

5 | $\mathcal{Q}_i = \text{TT-rounding}(\mathcal{P}_i, \delta)$

6 **end**

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

In TT-format the following modifications occur

- $\mathbf{G}(i, j) = \langle \mathcal{A}_i, \mathcal{A}_j \rangle$
- $(\mathbf{L}^\top)^{-1}$ is explicitly computed
- \mathcal{P}_i is constructed as a linear combination of \mathcal{A} elements

Householder transformation

Let \mathbf{x} and $\mathbf{y} \in \mathbb{R}^n$ be vectors with $\|\mathbf{y}\| = 1$, the Householder reflector \mathbf{H} reflects \mathbf{x} along \mathbf{y} , i.e., $\mathbf{H}\mathbf{x} = \|\mathbf{x}\|\mathbf{y}$. The Householder reflector \mathbf{H} is

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

Remark

- The Householder algorithm uses some of the components of the input vectors
- The Householder algorithm does **not** readily apply to tensor in TT-formats
- The approximation is applied to
 - * the tensor defining the Householder reflector
 - * the reflected tensors
 - * the tensor of the orthogonal basis

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Numerical experiments

Numerical experiments setting

We construct a set of 'Krylov TT-tensors', $\{\mathcal{A}_k\}$, such that

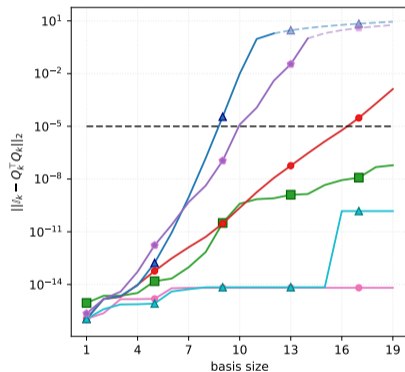
- \mathcal{A}_1 is randomly generated with $\max(\text{TT-rank}) = 1$
- $\mathcal{X}_k = 1/\|\mathcal{A}_k\| \mathcal{A}_k$
- $\mathcal{A}_{k+1} = \text{TT-rounding}(\Delta_d \mathcal{X}_k, \max_rank = 1)$ where Δ_d is be the TT-Laplacian

The perturbations are due to

- the inexactness from the approximation at accuracy $\delta = 10^{-5}$
- the rounding error from the floating point system at precision $u = \mathcal{O}(10^{-16})$

Numerical experiments results

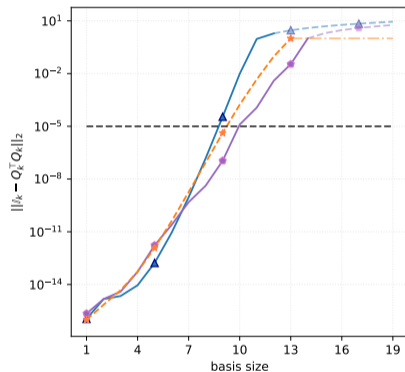
Loss of orthogonality for $\{\mathcal{A}_k\}$



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

Figure: 20 tensors of order $d = 3$ and mode size $n = 15$

Loss of orthogonality for $\{\mathcal{A}_k\}$

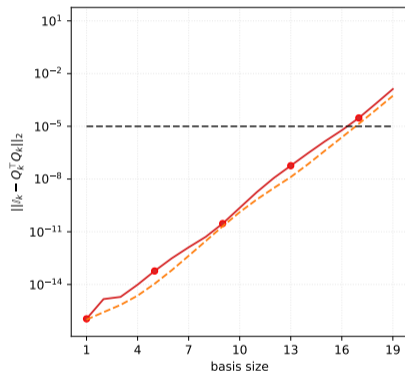


- Gram approach
- CGS
- $\delta\kappa^2(\mathbf{A}_k)$ with

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

Figure: 20 tensors of order $d = 3$ and mode size $n = 15$

Loss of orthogonality for $\{\mathcal{A}_k\}$



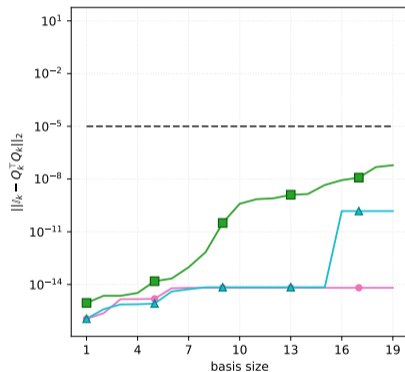
- **MGS**
- $\delta\kappa(\mathbf{A}_k)$ with

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

Figure: 20 tensors of order $d = 3$ and mode size $n = 15$

Numerical experiments results

Loss of orthogonality for $\{\mathcal{A}_k\}$



- CGS2
- MGS2
- Householder transformation

Figure: 20 tensors of order $d = 3$ and mode size $n = 15$

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

with u the computational precision, δ the compression accuracy

Computational costs: matrix vs tensor

	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	$\mathcal{O}(2nm^2 - 2m^3/3)$	$4m$

where m is the basis size and n is the length of each element

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Outlook

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 accuracy δ replacing the computational precision u
 - * the compression accuracy δ can be read as a computational precision with two peculiarities
 - > it is independent from the machine architecture
 - > it controls the perturbation norm-wise rather than component-wise

More detailed results can be found at [**Coulaud2022-Ortho**]

Conclusions and perspectives

- All the 6 kernels can be generalized to the TT-framework
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What is left out?

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

- [1] Y. Bi et al. "Chapter 1 - Tensor decompositions: computations, applications, and challenges". In: *Tensors for Data Processing*. Ed. by Y. Liu. Academic Press, 2022, pp. 1–30. ISBN: 978-0-12-824447-0. DOI: <https://doi.org/10.1016/B978-0-12-824447-0.00007-8>. URL: <https://www.sciencedirect.com/science/article/pii/B9780128244470000078>.
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