Orthogonalization schemes in tensor train format

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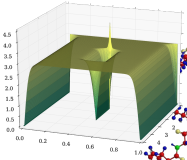
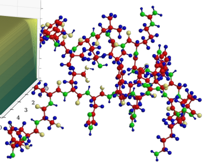
Martina Iannacito*
joint work with Olivier Coulaud† and Luc Giraud†

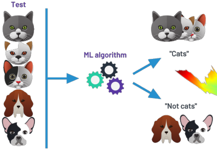
* KU Leuven
† Centre Inria at the University of Bordeaux

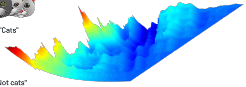
The context in matrix computation

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









reduce their problems to

Least-squares	Eigenpairs	Linear systems
$\min_{x \in \mathcal{S}} \|\|b - Ax\|\|$	$Ax = \lambda x$	$Ax = b$

From theory to coding: an example I

Gram-Schmidt process [Leon et al. 2013]

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

$$q_1 = a_1,$$

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All projections, then subtractions

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Are these versions equivalent in finite precision arithmetic?

From theory to coding: an example II

Not equivalent in general

Classical Gram-Schmidt	Modified Gram-Schmidt
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$$A = \begin{bmatrix} 1 & 1 & 1 \\ \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{bmatrix} \qquad \text{with} \qquad \varepsilon = 1e-10 \qquad \text{in fp64}$$

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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 $Q_k = [q_1, \ldots, q_k]$ 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 $A_k = [a_1, \ldots, a_k]$, estimated through $\kappa(A_k)$.

Matrix		
Source	*Algorithm*	$\left\|\mathbb{I}_k - Q_k^\top Q_k\right\|$
[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**	$\mathcal{O}(u)$

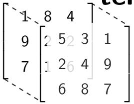
The advent of tensors

matrix

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

since the last century

tensor



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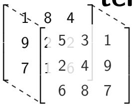

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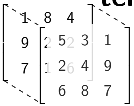

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Approximation techniques were proposed

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

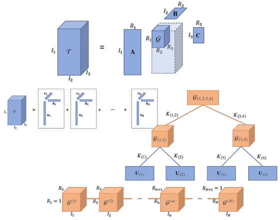

Figure: from [Bi et al. 2022]

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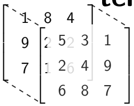

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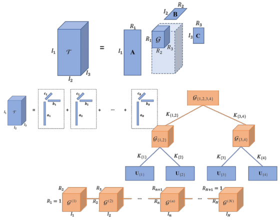

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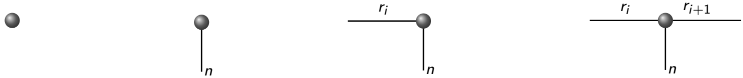
Approximation techniques introduce **norm-wise** compression errors

Tensor Train formalism



scalar vector matrix order-3 tensor

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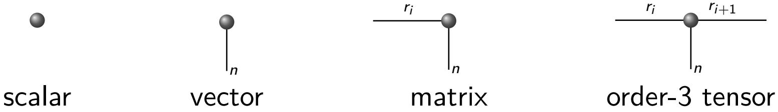

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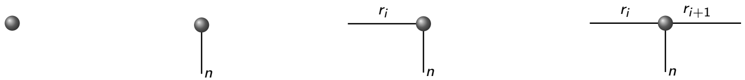

scalar | vector | matrix | order-3 tensor

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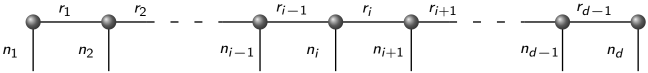

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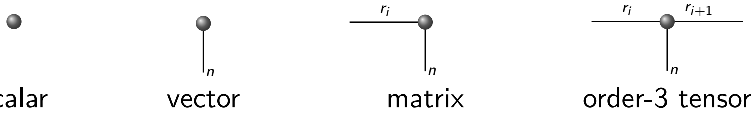

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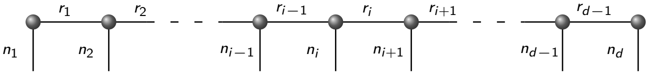

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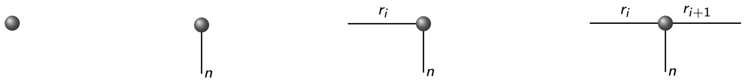

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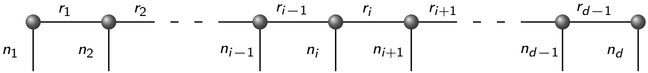

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TT-rounding [Oseledets 2011]

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

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

The questions

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]

The questions

In the Tensor-Train framework

compression precision δ	computational precision u
• norm-wise perturbation	• component-wise perturbation
• TT-model [Oseledets 2011]	• IEEE model [Higham 2002]

- 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

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

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

for $i = 1, \ldots, m$ **do**
- $\mathbf{p} = \mathbf{a}_i$
- **for** $j = 1, \ldots, i-1$ **do**
  - $R(i,j) = \langle \mathbf{a}_i, \mathbf{q}_j \rangle$
  - $\mathbf{p} = \mathbf{p} - R(i,j)\mathbf{q}_j$
- **end**
- $\mathbf{p} = \texttt{TT-rounding}(\mathbf{p}, \delta)$
- $R(i,i) = ||\mathbf{p}||$
- $\mathbf{q}_i = 1/R(i,i)\,\mathbf{p}$

end

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

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

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

for $i = 1, \ldots, m$ **do**
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They readily write in TT-format.

CGS and MGS with reorthogonalization

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

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

for $i = 1, \ldots, m$ **do**
  $\mathbf{p}_k = \mathbf{a}_i$
  for $k = 1, 2$ **do**
    $\mathbf{p}_k = \mathbf{p}_{k-1}$
    for $j = 1, \ldots, i-1$ **do**
      $R(i,j) = \langle \mathbf{p}_{k-1}, \mathbf{q}_j \rangle$
      $\mathbf{p}_k = \mathbf{p}_k - R(i,j)\mathbf{q}_j$
    end
    $\mathbf{p}_k = \texttt{TT-rounding}(\mathbf{p}_k, \delta)$
  end
  $R(i,i) = ||\mathbf{p}_2||$
  $\mathbf{q}_i = 1/R(i,i)\,\mathbf{p}_2$
end

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

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

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

for $i = 1, \ldots, m$ **do**
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Gram approach - matrix format

Let $A = [a_1, \ldots, a_m]$, 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.

Gram approach - TT-format

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

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

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

$L = \texttt{cholesky}(G)$

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

for $i = 1, \ldots, m$ **do**

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

end

Output: $\mathcal{Q} = \{\mathbf{q}_1, \ldots, \mathbf{q}_m\}$, 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.,

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

Thanks to its properties, H writes as

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

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 $\mathbf{\Delta}_d$ is be the TT-Laplacian, then $\{\mathbf{a}_k\}$ are ‘Krylov tensors’, i.e.,

$$\mathbf{a}_{k+1} = \texttt{TT-rounding}(\mathbf{\Delta}_d \mathbf{x}_k, \texttt{max\_rank} = 1) \quad \text{with} \quad \mathbf{x}_{k+1} = \frac{1}{\|\mathbf{a}_{k+1}\|}\mathbf{a}_{k+1}$$

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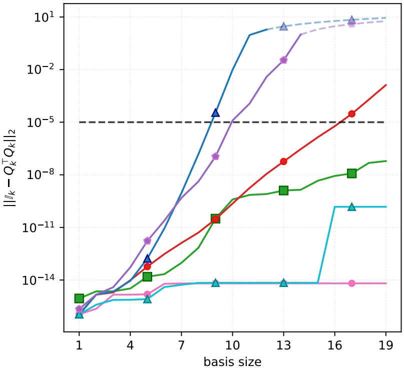
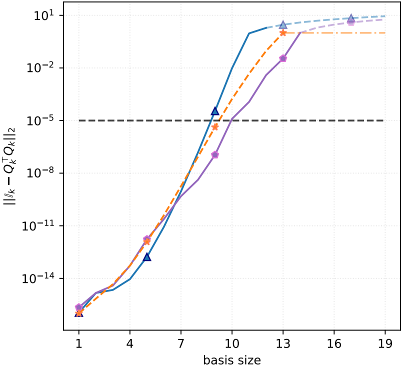


Figure: 20 tensors of order $d = 3$ and mode size $n = 15$, compression precision $\delta = 10^{-5}$, computational precision $u = \mathcal{O}(10^{-16})$

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

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



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- **Gram approach**
- **CGS**
- $\delta\kappa^2(A_k)$ with

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

then we conjecture

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

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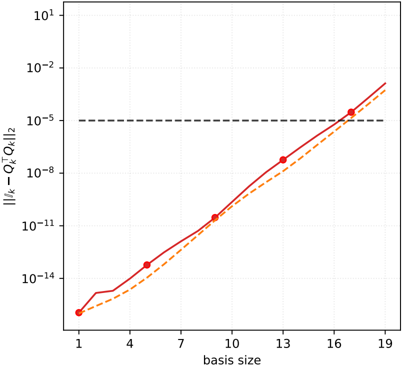

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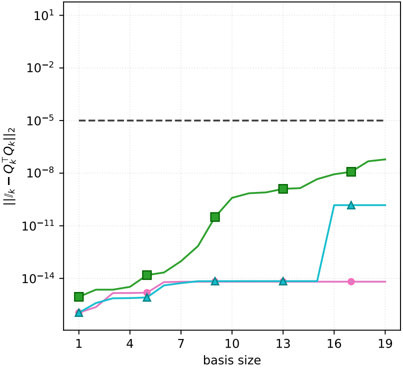

Figure: 20 tensors of order $d = 3$ and mode size $n = 15$, compression precision $\delta = 10^{-5}$, computational precision $u = \mathcal{O}(10^{-16})$

- **CGS2**
- **MGS2**
- **Householder transformation**

then we conjecture

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

Loss of orthogonality: matrix vs tensor

Algorithm	Matrix, theoretical $\left\lVert \mathbb{I}_k - Q_k^\top Q_k \right\rVert$	TT-format, conjecture $\left\lVert \mathbb{I}_k - \mathcal{Q}_k^\top \mathcal{Q}_k \right\rVert$
Gram	$\mathcal{O}(u\kappa^2(A_k))$	$\mathcal{O}(\delta\kappa^2(\mathcal{A}_k))$
CGS	$\mathcal{O}(u\kappa^2(A_k))$	$\mathcal{O}(\delta\kappa^2(\mathcal{A}_k))$
MGS	$\mathcal{O}(u\kappa(A_k))$	$\mathcal{O}(\delta\kappa(\mathcal{A}_k))$
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 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

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

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Thanks for the attention.

Questions?