Parallel Tensor Train Rounding using Gram SVD

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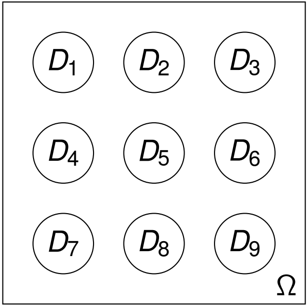
Tensor Train (TT) can make very high dimensional problems tractable



Consider the parameter-dependent PDE:

$$\begin{aligned} -\mathrm{div}(\sigma(x,y;\boldsymbol{\rho})\nabla(u(x,y;\boldsymbol{\rho}))) &= f(x,y) && \text{in } \Omega, \\ u(x,y;\boldsymbol{\rho}) &= 0 && \text{on } \partial\Omega, \end{aligned}$$

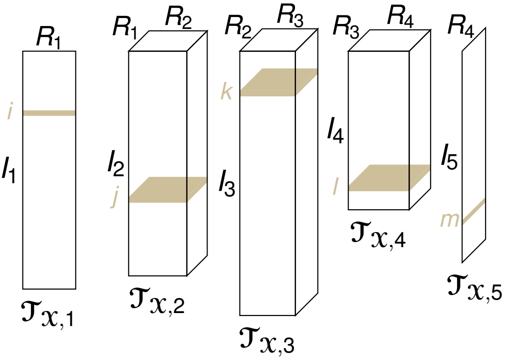
where σ is defined as:

$$\sigma(x,y;\boldsymbol{\rho}) = \begin{cases} 1+\rho_i & \text{if } (x,y) \in D_i \\ 1 & \text{elsewhere} \end{cases}$$

known as *cookies* problem [Tob12]

- Solving for all parameter values simultaneously, u is 11-D
- With mild assumptions, solution u has low TT ranks
- TT-based iterative linear solver exploits low-rank structure
  - can solve problem for high resolution [Dol13]

Tensor Train (TT) Notation



$\mathfrak{X} \approx \{\mathfrak{T}_{\mathfrak{X},n}\}, \mathfrak{X} \in \mathbb{R}^{I_1 \times I_2 \times I_3 \times I_4 \times I_5}$

$\mathfrak{T}_{\mathfrak{X},n} \in \mathbb{R}^{R_{n-1} \times I_n \times R_n}$ are *TT cores*

$$x_{ijklm} \approx \sum_{\alpha=1}^{R_1} \sum_{\beta=1}^{R_2} \sum_{\gamma=1}^{R_3} \sum_{\delta=1}^{R_4} \mathfrak{T}_{\mathfrak{X},1}(i,\alpha)\mathfrak{T}_{\mathfrak{X},2}(\alpha,j,\beta)\mathfrak{T}_{\mathfrak{X},3}(\beta,k,\gamma)\mathfrak{T}_{\mathfrak{X},4}(\gamma,l,\delta)\mathfrak{T}_{\mathfrak{X},5}(\delta,m)$$

TT-Rounding

Given a tensor in TT format, often need to compress the ranks

- algebraic operations on TT formats over-extend ranks
- recompression (rank truncation) subject to error threshold
  - or subject to target ranks
- analogous to floating point rounding

TT-Rounding

Given a tensor in TT format, often need to compress the ranks

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- analogous to floating point rounding

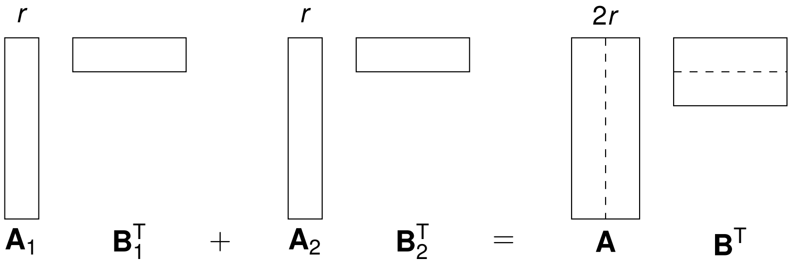
Goal: compute truncated SVDs of matricized TT-format tensors

- TT-ranks are ranks of unfoldings $\mathbf{X}_{(1:n)}$ for $1 \leq n \leq N$
- if $\mathcal{X}$ is $I_1 \times I_2 \times \cdots \times I_N$, then $\mathbf{X}_{(1:n)}$ is $(I_1 \cdots I_n) \times (I_{n+1} \cdots I_N)$
- $\mathbf{X}_{(1:n)}$ is generally a huge matrix, but it is highly structured

2D TT-Rounding (Matrix Case)

Low-rank matrix addition example

- consider $\mathbf{A}_1\mathbf{B}_1^T + \mathbf{A}_2\mathbf{B}_2^T$, where each factor has r columns
- can represent this in low-rank format $\begin{bmatrix}\mathbf{A}_1 & \mathbf{A}_2\end{bmatrix}\begin{bmatrix}\mathbf{B}_1 & \mathbf{B}_2\end{bmatrix}^T$ which now has rank $2r$
- goal is to compute low-rank approximation with rank $k < 2r$



Matrix Rounding via QR Decompositions

QR-based algorithm for rounding rank-r matrix $\mathbf{X} = \mathbf{A}\mathbf{B}^T$:

function $[\mathbf{U}, \mathbf{V}] = \text{QR-ROUNDING}(\mathbf{A}, \mathbf{B}, k)$

$[\mathbf{Q}_A, \mathbf{R}_A] = \text{QR}(\mathbf{A})$ ▷ (tall-skinny) QR decomposition

$[\mathbf{Q}_B, \mathbf{R}_B] = \text{QR}(\mathbf{B})$ ▷ (tall-skinny) QR decomposition

$[\hat{\mathbf{U}}_R, \hat{\Sigma}_R, \hat{\mathbf{V}}_R] = \text{TSVD}(\mathbf{R}_A \mathbf{R}_B^T, k)$ ▷ kth truncated SVD

$\mathbf{U} = \mathbf{Q}_A \hat{\mathbf{U}}_R$

$\mathbf{V} = \mathbf{Q}_B (\hat{\mathbf{V}}_R \hat{\Sigma}_R)$ ▷ $\mathbf{A}\mathbf{B}^T \approx \mathbf{U}\mathbf{V}^T$

Here's the algebra:

$$\mathbf{A}\mathbf{B}^\mathsf{T} = \underbrace{\mathbf{Q}_A \mathbf{R}_A}_{\mathbf{A}} \underbrace{\mathbf{R}_B^\mathsf{T} \mathbf{Q}_B^\mathsf{T}}_{\mathbf{B}^\mathsf{T}} \approx \mathbf{Q}_A \underbrace{\hat{\mathbf{U}}_R \hat{\Sigma}_R \hat{\mathbf{V}}_R^\mathsf{T}}_{\mathbf{R}_A \mathbf{R}_B^\mathsf{T}} \mathbf{Q}_B^\mathsf{T} = \underbrace{\mathbf{U}}_{\mathbf{Q}_A \hat{\mathbf{U}}_R} \underbrace{\mathbf{V}^\mathsf{T}}_{\hat{\Sigma}_R \hat{\mathbf{V}}_R^\mathsf{T} \mathbf{Q}_B^\mathsf{T}}$$

Matrix Rounding via Gram (1st attempt)

Gram SVD is a well-known method for computing singular values of rectangular matrices

- sing. values of $\mathbf{X}$ are square roots of eigenvalues of $\mathbf{X}^\mathsf{T}\mathbf{X}$
- if $\mathbf{X}$ is tall and skinny then $\mathbf{X}^\mathsf{T}\mathbf{X}$ is much smaller
- sacrifices some accuracy of singular values and vectors

If $\mathbf{X} = \mathbf{A}\mathbf{B}^\mathsf{T}$, then we can try direct application:

- $\mathbf{X}^\mathsf{T}\mathbf{X} = \mathbf{B}(\mathbf{A}^\mathsf{T}\mathbf{A})\mathbf{B}^\mathsf{T}$
- $\mathbf{X}\mathbf{X}^\mathsf{T} = \mathbf{A}(\mathbf{B}^\mathsf{T}\mathbf{B})\mathbf{A}^\mathsf{T}$

but we still have to orthogonalize one of the two factors in order to compute the eigendecomposition

Matrix Rounding via Gram SVD

Gram-based algorithm for rounding rank-r matrix $\mathbf{X} = \mathbf{A}\mathbf{B}^T$:

function $[\mathbf{U}, \mathbf{V}] = \textsc{Gram-Rounding}(\mathbf{A}, \mathbf{B}, k)$

$\mathbf{G}_A = \mathbf{A}^\mathsf{T}\mathbf{A}$ ▷ symmetric matrix multiplication

$\mathbf{G}_B = \mathbf{B}^\mathsf{T}\mathbf{B}$ ▷ symmetric matrix multiplication

$[\mathbf{V}_A, \mathbf{\Lambda}_A] = \textsc{Eig}(\mathbf{G}_A)$

$[\mathbf{V}_B, \mathbf{\Lambda}_B] = \textsc{Eig}(\mathbf{G}_B)$

$[\hat{\mathbf{U}}, \hat{\mathbf{\Sigma}}, \hat{\mathbf{V}}] = \textsc{tSVD}(\mathbf{\Lambda}_A^{1/2}\mathbf{V}_A^\mathsf{T}\mathbf{V}_B\mathbf{\Lambda}_B^{1/2}, k)$ ▷ kth truncated SVD

$\mathbf{U} = \mathbf{A}\left(\mathbf{V}_A\mathbf{\Lambda}_A^{-1/2}\hat{\mathbf{U}}\right)$

$\mathbf{V} = \mathbf{B}\left(\mathbf{V}_B\mathbf{\Lambda}_B^{-1/2}\hat{\mathbf{V}}\hat{\mathbf{\Sigma}}\right)$ ▷ $\mathbf{A}\mathbf{B}^T \approx \mathbf{U}\mathbf{V}^T$

Matrix Rounding via Gram SVD (continued)

Here's the algebra:

$$
\begin{aligned}
\mathbf{A}\mathbf{B}^{\mathsf{T}} &= \underbrace{\mathbf{U}_A \boldsymbol{\Sigma}_A \mathbf{V}_A^{\mathsf{T}}}_{\mathbf{A}} \underbrace{\mathbf{V}_B \boldsymbol{\Sigma}_B \mathbf{U}_B^{\mathsf{T}}}_{\mathbf{B}^{\mathsf{T}}} \\
&= \underbrace{\mathbf{A}\mathbf{V}_A \boldsymbol{\Lambda}_A^{-1/2} \boldsymbol{\Lambda}_A^{1/2} \mathbf{V}_A^{\mathsf{T}}}_{\mathbf{A}} \underbrace{\mathbf{V}_B \boldsymbol{\Lambda}_B^{1/2} \boldsymbol{\Lambda}_B^{-1/2} \mathbf{V}_B^{\mathsf{T}} \mathbf{B}^{\mathsf{T}}}_{\mathbf{B}^{\mathsf{T}}} \\
&= \underbrace{(\mathbf{A}\mathbf{V}_A \boldsymbol{\Lambda}_A^{-1/2})}_{\mathbf{U}_A} \underbrace{\boldsymbol{\Lambda}_A^{1/2} \mathbf{V}_A^{\mathsf{T}} \mathbf{V}_B \boldsymbol{\Lambda}_B^{1/2}}_{\mathbf{M}} \underbrace{(\mathbf{B}\mathbf{V}_B \boldsymbol{\Lambda}_B^{-1/2})}_{\mathbf{U}_B}{}^{\mathsf{T}} \\
&\approx \underbrace{(\mathbf{A}\mathbf{V}_A \boldsymbol{\Lambda}_A^{-1/2})}_{\mathbf{U}_A} \hat{\mathbf{U}} \hat{\boldsymbol{\Sigma}} \hat{\mathbf{V}}^{\mathsf{T}} \underbrace{(\mathbf{B}\mathbf{V}_B \boldsymbol{\Lambda}_B^{-1/2})}_{\mathbf{U}_B}{}^{\mathsf{T}} \\
&= \underbrace{\mathbf{A}(\mathbf{V}_A \boldsymbol{\Lambda}_A^{-1/2} \hat{\mathbf{U}})}_{\mathbf{U}} \underbrace{(\hat{\boldsymbol{\Sigma}} \hat{\mathbf{V}}^{\mathsf{T}} \boldsymbol{\Lambda}_B^{-1/2} \mathbf{V}_B^{\mathsf{T}}) \mathbf{B}^{\mathsf{T}}}_{\mathbf{V}^{\mathsf{T}}}
\end{aligned}
$$

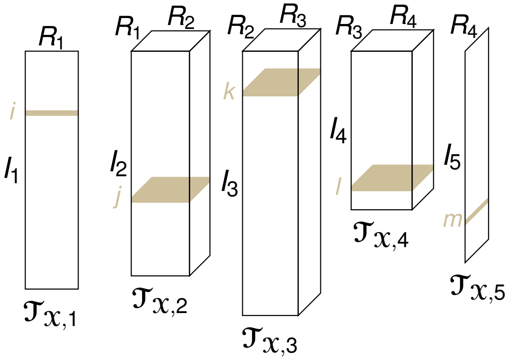
QR-Rounding vs Gram-Rounding

Gram-Rounding is at least twice as fast as QR-Rounding

- Gram-Rounding does half the flops of QR-Rounding
- Gram-Rounding dominated by matrix multiplication
- QR-Rounding dominated by computing QR and applying Q

QR-Rounding is more accurate than Gram-Rounding

- QR-Rounding computes singular values as small as $\sigma_1 \cdot \varepsilon$
- Gram-Rounding computes singular values only to $\sigma_1 \cdot \varepsilon^{1/2}$

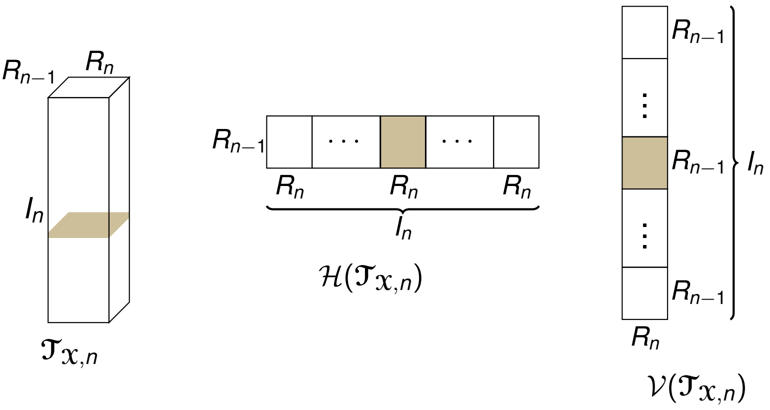


$\mathcal{X} \approx \{\mathcal{T}_{\mathcal{X},n}\}, \mathcal{X} \in \mathbb{R}^{I_1 \times I_2 \times I_3 \times I_4 \times I_5}$

$\mathcal{T}_{\mathcal{X},n} \in \mathbb{R}^{R_{n-1} \times I_n \times R_n}$ are *TT cores*

$$x_{ijklm} \approx \sum_{\alpha=1}^{R_1} \sum_{\beta=1}^{R_2} \sum_{\gamma=1}^{R_3} \sum_{\delta=1}^{R_4} \mathcal{T}_{\mathcal{X},1}(i,\alpha)\mathcal{T}_{\mathcal{X},2}(\alpha,j,\beta)\mathcal{T}_{\mathcal{X},3}(\beta,k,\gamma)\mathcal{T}_{\mathcal{X},4}(\gamma,l,\delta)\mathcal{T}_{\mathcal{X},5}(\delta,m)$$

$\mathcal{H}(\mathfrak{T}_{\mathcal{X},n}) \in \mathbb{R}^{R_{n-1} \times I_n R_n}$ and $\mathcal{V}(\mathfrak{T}_{\mathcal{X},n}) \in \mathbb{R}^{R_{n-1} I_n \times R_n}$ are horizontal and vertical unfoldings of nth core



QR-Based TT Rounding Algorithm [Ose11]

function $\{\mathcal{T}_{\mathcal{Z},n}\} = \text{TT-ROUNDING}(\{\mathcal{T}_{\mathcal{X},n}\})$

$\triangleright$ Orthogonalization Phase

for $n = N$ down to 2 **do**

$[\mathbf{Y}_n, \mathbf{R}_n] = \text{QR}(\mathcal{H}(\mathcal{T}_{\mathcal{X},n})^T)$ $\triangleright$ (tall-skinny) QR factorization

$\mathcal{V}(\mathcal{T}_{\mathcal{X},n-1}) = \mathcal{V}(\mathcal{T}_{\mathcal{X},n-1}) \cdot \mathbf{R}^\mathsf{T}$ $\triangleright$ Apply **R** to previous core

$\triangleright$ Truncation Phase

$\mathcal{Z} = \mathcal{X}$

for $n = 1$ to $N - 1$ **do**

$[\mathbf{Y}_n, \mathbf{R}_n] = \text{QR}(\mathcal{V}(\mathcal{T}_{\mathcal{Z},n}))$ $\triangleright$ (tall-skinny) QR factorization

$[\hat{\mathbf{U}}_R, \hat{\Sigma}, \hat{\mathbf{V}}] \approx \text{TSVD}(\mathbf{R}_n)$ $\triangleright$ Truncated SVD of **R**

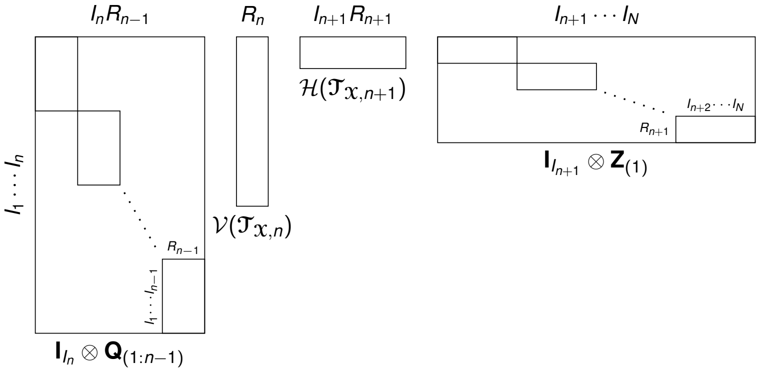
$\mathcal{V}(\mathcal{T}_{\mathcal{Z},n}) = \text{APPLY-Q}(\mathbf{Y}_n, \hat{\mathbf{U}}_R)$ $\triangleright$ Form explicit $\hat{\mathbf{U}}$

$\mathcal{H}(\mathcal{T}_{\mathcal{Z},n+1})^T = \text{APPLY-Q}(\mathbf{Y}_{n+1}, \hat{\mathbf{V}}\hat{\Sigma})$ $\triangleright$ Apply $\hat{\Sigma}\hat{\mathbf{V}}^\mathsf{T}$ to next core

We have parallelized this QR-based algorithm [DBB22] using the parallel TSQR algorithm [DGHL12]

TT-Rounding does truncated SVDs on $\mathbf{X}_{(1)}$, $\mathbf{X}_{(1:2)}$, $\mathbf{X}_{(1:3)}$, etc., and here is the matrix expression of each unfolding [DBB22]:

$$\mathbf{X}_{(1:n)} = (\mathbf{I}_{I_n} \otimes \mathbf{Q}_{(1:n-1)}) \cdot \mathcal{V}(\mathfrak{T}_{\mathcal{X},n}) \cdot \mathcal{H}(\mathfrak{T}_{\mathcal{X},n+1}) \cdot (\mathbf{I}_{I_{n+1}} \otimes \mathbf{Z}_{(1)})$$



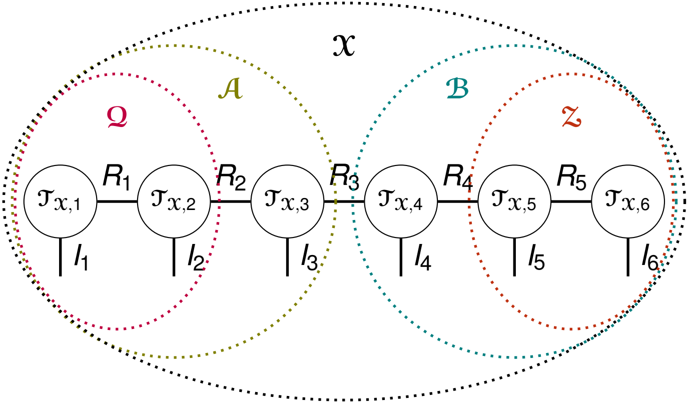
Main Ideas of Gram-Based TT-Rounding

Same matrix expression of nth unfolding:

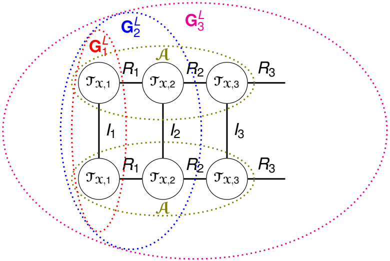
$$\mathbf{X}_{(1:n)} = \underbrace{(\mathbf{I}_{I_n} \otimes \mathbf{Q}_{(1:n-1)}) \cdot \mathcal{V}(\mathcal{T}_{\mathcal{X},n})}_{\mathbf{A}} \cdot \underbrace{\mathcal{H}(\mathcal{T}_{\mathcal{X},n+1}) \cdot (\mathbf{I}_{I_{n+1}} \otimes \mathbf{Z}_{(1)})}_{\mathbf{B}^{\mathsf{T}}}$$

- just like matrix case, we need to compute $\mathbf{A}^{\mathsf{T}}\mathbf{A}$ and $\mathbf{B}^{\mathsf{T}}\mathbf{B}$
- two key differences:
  - $\mathbf{A}$ and $\mathbf{B}$ are both highly structured
  - we need Gram matrices for all $1 \leq n \leq N$
- we obtain efficiency by exploiting structure and by exploiting the computational overlap across modes

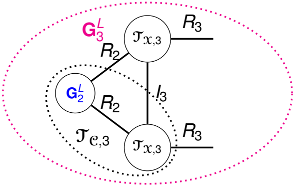
$$\mathbf{X}_{(1:n)} = \underbrace{(\mathbf{I}_{I_n} \otimes \mathbf{Q}_{(1:n-1)}) \cdot \mathcal{V}(\mathfrak{T}_{\mathfrak{X},n})}_{\mathbf{A}} \cdot \underbrace{\mathcal{H}(\mathfrak{T}_{\mathfrak{X},n+1}) \cdot (\mathbf{I}_{I_{n+1}} \otimes \mathbf{Z}_{(1)})}_{\mathbf{B}^\mathsf{T}}$$



Tensor Network Diagram for Gram Matrix Computation

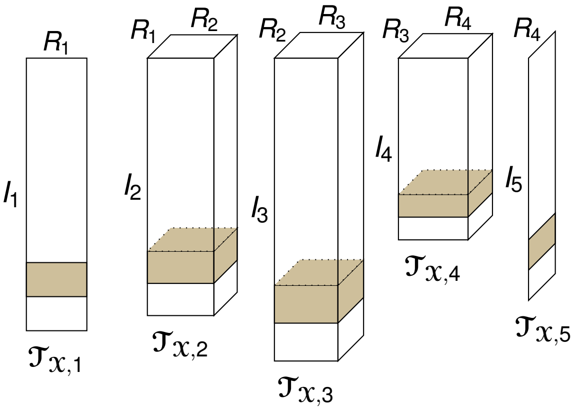


tensor network for $\mathbf{G}_3^L = \mathbf{A}^\mathsf{T}\mathbf{A}$



intermediate step,
computing $\mathbf{G}_3^L$ from $\mathbf{G}_2^L$

Parallel Distribution

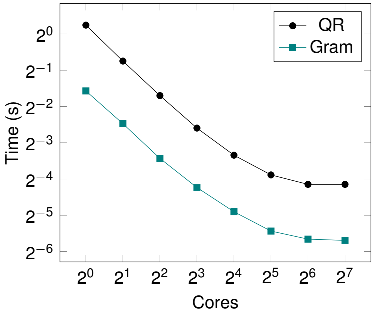


- Each core distributed across all P processors
- Local nth core dimensions are $R_{n-1} \times \frac{I_n}{P} \times R_n$
- Key: vertical and horizontal unfoldings are 1D-distributed

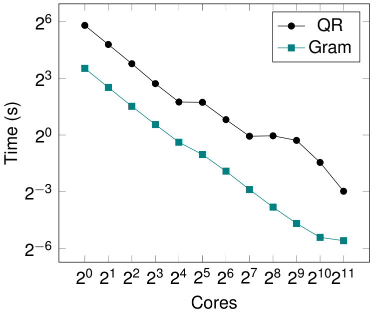
Strong Scaling Results for Synthetic Tensors

We round synthetic tensors with input TT-ranks $R = 20$ (all modes) down to $R = 10$, scaling up the number of processors

- results on Andes (ORNL), with 2 16-core AMD EPYC procs per node



N=50, $2K \times \cdots \times 2K$ (77 MB)

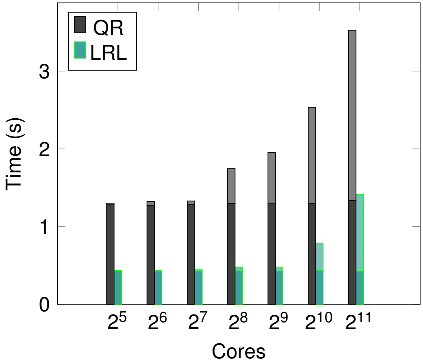


N=16, $100M \times 50K \times \cdots \times 50K \times 1M$ (8 GB)

Weak Scaling Results for Synthetic Tensor

We round the 50-mode synthetic tensor with input TT-ranks $R = 20$ down to $R = 10$, scaling up processors with fixed local data

- results on Andes (ORNL), with 2 16-core AMD EPYC procs per node

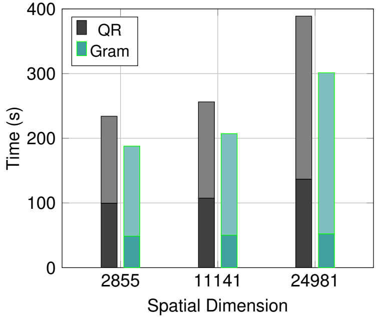


Dark signifies computation, light signifies communication

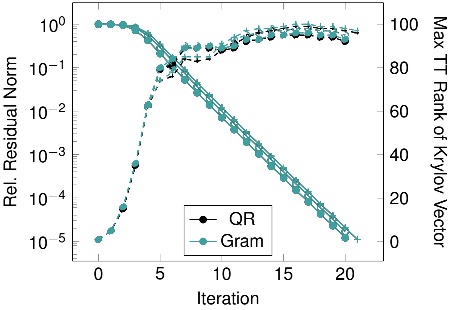
Results for Cookies Problem

We solve the Cookies problem with Matlab implementation of TT-GMRES [Dol13] and TT-Rounding (sequential)

- we use 4 parameters (cookies) and vary spatial discretization



Dark signifies time in TT-Rounding



Gram has negligible effect on GMRES behavior

Summary

- TT format efficiently approximates high-dim. tensors
  - TT arithmetic causes rank growth, TT-Rounding is key
  - enables solving problems like parameter-dependent PDEs
- TT-Rounding means truncated SVDs of unfoldings $\mathbf{X}_{(1:n)}$
  - QR-based approach most accurate but less efficient
  - Gram-based approach faster, can be accurate enough
- Gram-based computation exploits TT structure
  - efficient contraction of tensor network
  - par. distribution allows for comm.-efficient matrix multiplies

Thanks for your attention!

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MPI_ATTAC: Algorithms for Tensor Train Arithmetic and Computations

https://gitlab.com/aldaas/mpi_attac

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Parallel Algorithms for Tensor Train Arithmetic.
SIAM Journal on Scientific Computing 2022.
https://dx.doi.org/10.1137/20M1387158

More details on TT-Rounding...

TT-Rounding does SVDs on $\mathbf{X}_{(1)}$, $\mathbf{X}_{(1:2)}$, $\mathbf{X}_{(1:3)}$, etc., so we seek similar matrix expressions of those unfoldings

The unfolding of $\mathcal{X}$ that maps the first n tensor dimensions to rows can be expressed as a product of four matrices:

$$\mathbf{X}_{(1:n)} = (\mathbf{I}_{I_n} \otimes \mathbf{Q}_{(1:n-1)}) \cdot \mathcal{V}(\mathfrak{T}_{\mathcal{X},n}) \cdot \mathcal{H}(\mathfrak{T}_{\mathcal{X},n+1}) \cdot (\mathbf{I}_{I_{n+1}} \otimes \mathbf{Z}_{(1)})$$

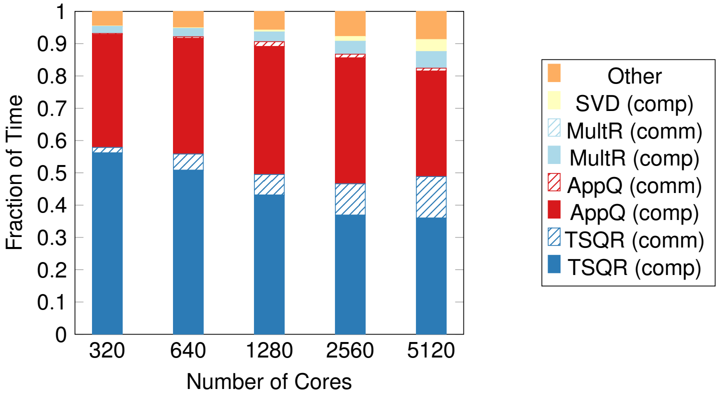
where $\mathfrak{Q}$ is $I_1 \times \cdots \times I_{n-1} \times R_{n-1}$ with

$$\mathfrak{Q}(i_1, \ldots, i_{n-1}, r_{n-1}) = \mathfrak{T}_{\mathcal{X},1}(i_1, :) \cdot \mathfrak{T}_{\mathcal{X},2}(:, i_2, :) \cdots \mathfrak{T}_{\mathcal{X},n-1}(:, i_{n-1}, r_{n-1}),$$

and $\mathfrak{Z}$ is $R_{n+1} \times I_{n+2} \times \cdots \times I_N$ with

$$\mathfrak{Z}(r_{n+1}, i_{n+2}, \ldots, i_N) = \mathfrak{T}_{\mathcal{X},n+2}(r_{n+1}, i_{n+2}, :) \cdot \mathfrak{T}_{\mathcal{X},n+3}(:, i_{n+3}, :) \cdots \mathfrak{T}_{\mathcal{X},N}(:, i_N).$$

Time Breakdown of Parallel QR-based TT-Rounding



- TT tensor: $I_n = 512K$, $R_n = 60 \to 30$, $N = 50$
- 70-80% of time spent in QR computations

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