Constrained Tensor Factorization with Accelerated AO-ADMM

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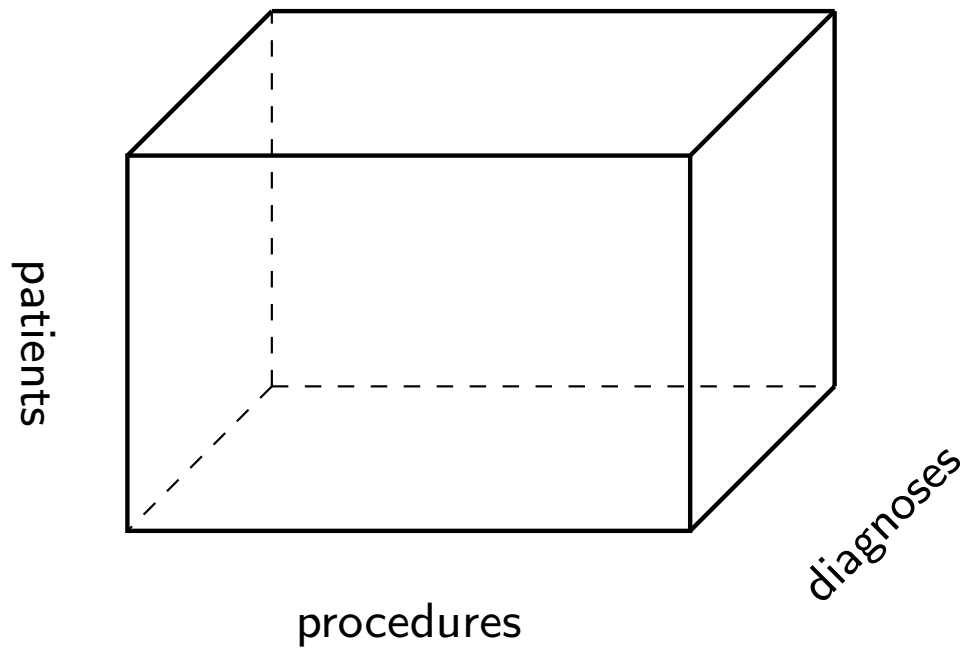
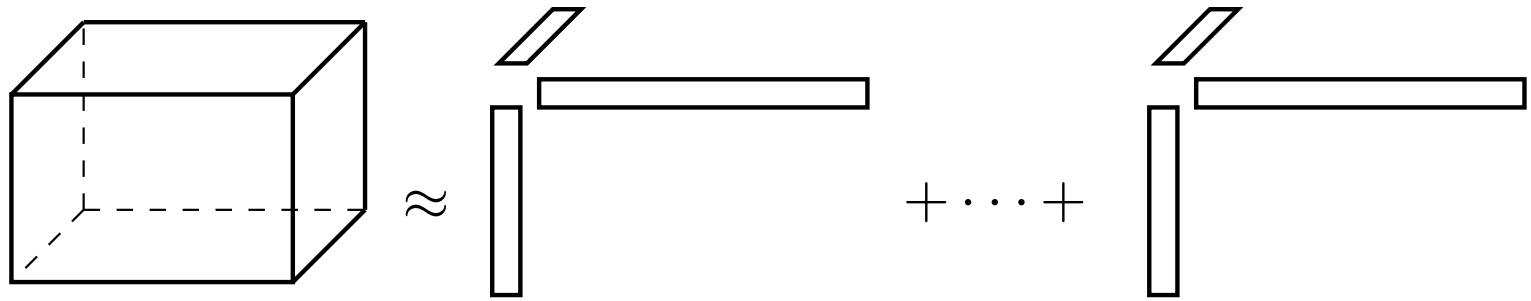
Tensor Introduction

- Tensors are the generalization of matrices to higher dimensions.
- Allow us to represent and analyze multi-dimensional data.
- Applications in precision healthcare, cybersecurity, recommender systems, ...



Canonical polyadic decomposition (CPD)

The CPD models a tensor as the summation of rank-1 tensors.



$$\underset{\mathbf{A},\mathbf{B},\mathbf{C}}{\text{minimize}} \quad \mathcal{L}(\boldsymbol{\mathcal{X}}, \mathbf{A}, \mathbf{B}, \mathbf{C}) = \left\| \boldsymbol{\mathcal{X}} - \sum_{f=1}^{F} \mathbf{A}(:, f) \circ \mathbf{B}(:, f) \circ \mathbf{C}(:, f) \right\|_F^2$$

Notation
$\mathbf{A} \in \mathbb{R}^{I \times F}$, $\mathbf{B} \in \mathbb{R}^{J \times F}$, and $\mathbf{C} \in \mathbb{R}^{K \times F}$ denote the factor matrices for a 3D tensor.

Alternating least squares (ALS)

The CPD is most commonly computed with ALS:

Algorithm 1 CPD-ALS

1: **while** not converged **do**

2: $\quad \mathbf{A}^T \leftarrow (\mathbf{C}^T\mathbf{C} * \mathbf{B}^T\mathbf{B})^{-1} \left(\mathbf{X}_{(1)}(\mathbf{C} \odot \mathbf{B})\right)^T$

3: $\quad \mathbf{B}^T \leftarrow (\mathbf{C}^T\mathbf{C} * \mathbf{A}^T\mathbf{A})^{-1} \left(\mathbf{X}_{(2)}(\mathbf{C} \odot \mathbf{A})\right)^T$

4: $\quad \mathbf{C}^T \leftarrow \underbrace{(\mathbf{B}^T\mathbf{B} * \mathbf{A}^T\mathbf{A})^{-1}}_{\text{Normal equations}} \underbrace{\left(\mathbf{X}_{(3)}(\mathbf{B} \odot \mathbf{A})\right)^T}_{\text{MTTKRP}}$

5: **end while**

Notation

$*$ denotes the Hadamard (elementwise) product.

Constrained factorization

We often want to impose some constraints or regularizations on the factorization:

$$\underset{\mathbf{A},\mathbf{B},\mathbf{C}}{\text{minimize}} \quad \underbrace{\mathcal{L}(\mathcal{X}, \mathbf{A}, \mathbf{B}, \mathbf{C})}_{\text{Loss}} + \underbrace{r(\mathbf{A}) + r(\mathbf{B}) + r(\mathbf{C})}_{\text{Constraints/Regularizations}}$$

Example

Non-negative factorizations use an indicator function for $\mathbb{R}_+$:

$$r(\mathbf{A}) = \begin{cases} 0 & \text{if } \mathbf{A} \geq \mathbf{0} \\ \infty & \text{otherwise} \end{cases}$$

AO-ADMM [Huang & Sidiropoulos '15]

AO-ADMM combines alternating optimization (AO) with alternating direction method of multipliers (ADMM).

- **A**, **B**, and **C** are updated in sequence using ADMM.

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ADMM formulation for the update of $\mathbf{A}$:

$$\begin{aligned} \underset{\mathbf{A},\tilde{\mathbf{A}}}{\text{minimize}} \quad & \frac{1}{2}\left\|\mathbf{X}_{(1)} - \tilde{\mathbf{A}}^T(\mathbf{C}\odot\mathbf{B})^T\right\|_F^2 + r(\mathbf{A}) \\ \text{subject to} \quad & \mathbf{A} = \tilde{\mathbf{A}}^T. \end{aligned}$$

Alternating optimization step (outer iterations)

1: Initialize primal variables $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ randomly.
2: Initialize dual variables $\hat{\mathbf{A}}$, $\hat{\mathbf{B}}$, and $\hat{\mathbf{C}}$ with $\mathbf{0}$.
3: **repeat**
4: $\quad \mathbf{G} \leftarrow \mathbf{B}^T\mathbf{B} * \mathbf{C}^T\mathbf{C}$
5: $\quad \mathbf{K} \leftarrow \mathbf{X}_{(1)}(\mathbf{C} \odot \mathbf{B})$
6: $\quad \mathbf{A}, \hat{\mathbf{A}} \leftarrow \text{ADMM}(\mathbf{A}, \hat{\mathbf{A}}, \mathbf{K}, \mathbf{G})$
7:
8: $\quad \mathbf{G} \leftarrow \mathbf{A}^T\mathbf{A} * \mathbf{C}^T\mathbf{C}$
9: $\quad \mathbf{K} \leftarrow \mathbf{X}_{(2)}(\mathbf{C} \odot \mathbf{A})$
10: $\quad \mathbf{B}, \hat{\mathbf{B}} \leftarrow \text{ADMM}(\mathbf{B}, \hat{\mathbf{B}}, \mathbf{K}, \mathbf{G})$
11:
12: $\quad \mathbf{G} \leftarrow \mathbf{A}^T\mathbf{A} * \mathbf{B}^T\mathbf{B}$
13: $\quad \mathbf{K} \leftarrow \mathbf{X}_{(3)}(\mathbf{B} \odot \mathbf{A})$
14: $\quad \mathbf{C}, \hat{\mathbf{C}} \leftarrow \text{ADMM}(\mathbf{C}, \hat{\mathbf{C}}, \mathbf{K}, \mathbf{G})$
15: **until** $\mathcal{L}(\mathcal{X}, \mathbf{A}, \mathbf{B}, \mathbf{C})$ ceases to improve.

ADMM step (inner iterations)

ADMM to update one factor matrix:

1: **Input:** $\mathbf{H}$, $\mathbf{U}$, $\mathbf{K}$, $\mathbf{G}$
2: **Output:** $\mathbf{H}$, $\mathbf{U}$
3: $\rho \leftarrow \text{trace}(\mathbf{G})/F$
4: $\mathbf{L} \leftarrow \text{Cholesky}(\mathbf{G} + \rho\mathbf{I})$
5: **repeat**
6: $\quad \mathbf{H}_0 \leftarrow \mathbf{H}$
7: $\quad \tilde{\mathbf{H}} \leftarrow \mathbf{L}^{-T}\mathbf{L}^{-1}\left(\mathbf{K} + \rho(\mathbf{H} + \mathbf{U})\right)^T$
8: $\quad \mathbf{H} \leftarrow \text{argmin}_{\mathbf{H}}\, r(\mathbf{H}) + \frac{\rho}{2}||\mathbf{H} - \tilde{\mathbf{H}}^T + \mathbf{U}||_F^2$
9: $\quad \mathbf{U} \leftarrow \mathbf{U} + \mathbf{H} - \tilde{\mathbf{H}}^T$
10: $\quad r \leftarrow ||\mathbf{H} - \tilde{\mathbf{H}}^T||_F^2 / ||\mathbf{H}||_F^2$
11: $\quad s \leftarrow ||\mathbf{H} - \mathbf{H}_0||_F^2 / ||\mathbf{U}||_F^2$
12: **until** $r < \epsilon$ and $s < \epsilon$

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Parallelization opportunities

All steps but Line 8 are either element-wise or row-wise independent.

1: **Input:** $\mathbf{H}$, $\mathbf{U}$, $\mathbf{K}$, $\mathbf{G}$
2: **Output:** $\mathbf{H}$, $\mathbf{U}$
3: $\rho \leftarrow \text{trace}(\mathbf{G})/F$
4: $\mathbf{L} \leftarrow \text{Cholesky}(\mathbf{G} + \rho\mathbf{I})$
5: **repeat**
6: $\quad \mathbf{H}_0 \leftarrow \mathbf{H}$
7: $\quad \tilde{\mathbf{H}} \leftarrow \mathbf{L}^{-T}\mathbf{L}^{-1}\left(\mathbf{K} + \rho(\mathbf{H} + \mathbf{U})\right)^T$
8: $\quad \mathbf{H} \leftarrow \text{argmin}_{\mathbf{H}}\, r(\mathbf{H}) + \frac{\rho}{2}||\mathbf{H} - \tilde{\mathbf{H}}^T + \mathbf{U}||_F^2$
9: $\quad \mathbf{U} \leftarrow \mathbf{U} + \mathbf{H} - \tilde{\mathbf{H}}^T$
10: $\quad r \leftarrow ||\mathbf{H} - \tilde{\mathbf{H}}^T||_F^2 / ||\mathbf{H}||_F^2$
11: $\quad s \leftarrow ||\mathbf{H} - \mathbf{H}_0||_F^2 / ||\mathbf{U}||_F^2$
12: **until** $r < \epsilon$ and $s < \epsilon$

Performance opportunities

1. The factor matrices are tall-skinny (e.g., $10^6 \times 50$).
   - The ADMM step will be bound by memory bandwidth.
2. Real-world tensors have non-uniform distributions of non-zeros.
   - This may lead to non-uniform convergence of the factor rows during ADMM.
3. Many constraints and regularizations naturally invoke sparsity in the factors.
   - We can exploit this sparsity during MTTKRP (*in paper*).

Blocked ADMM

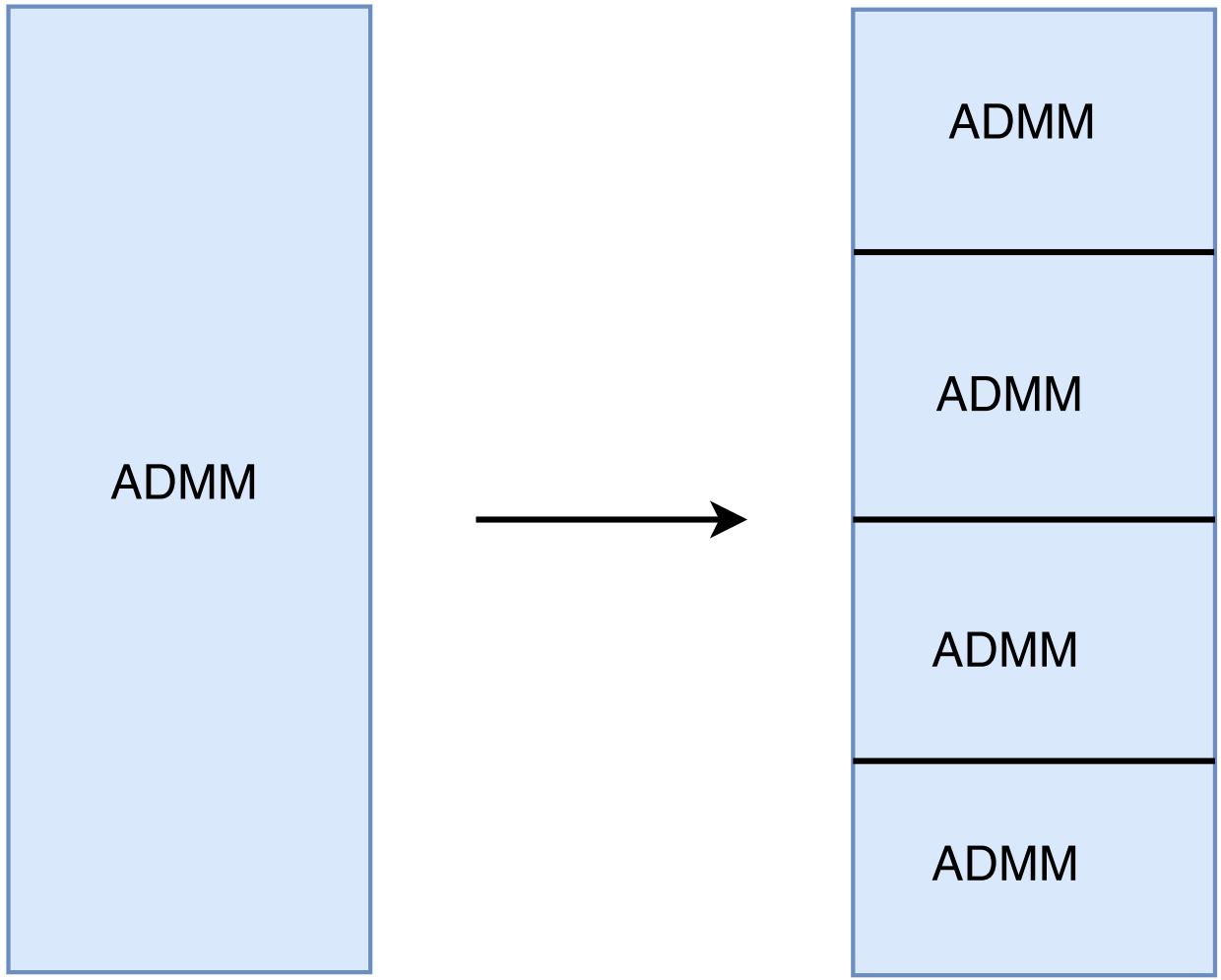
If the proximity operator coming from $r(\cdot)$ is row-separable, reformulate the ADMM problem to work on B blocks of rows:

$$\begin{aligned} \underset{(\mathbf{A}_1,\tilde{\mathbf{A}}_1),\ldots,(\mathbf{A}_B,\tilde{\mathbf{A}}_B)}{\text{minimize}} \quad & \sum_{b=1}^{B} \frac{1}{2} \left\| (\mathbf{X}_{(1)})_b - \tilde{\mathbf{A}}_b^T (\mathbf{C} \odot \mathbf{B})_b^T \right\|_F^2 + r(\mathbf{A}_b) \\ \text{subject to} \quad & \mathbf{A}_1 = \tilde{\mathbf{A}}_1, \ldots, \mathbf{A}_B = \tilde{\mathbf{A}}_B. \end{aligned}$$

Optimizing each block separately allows for them to converge at different rates, while acting as a form of cache tiling.

Blocked ADMM

More simply:



Effects of block size

The block size affects both convergence rate and computational efficiency:

- A block size of 1 optimizes each row of $\mathbf{H}$ independently.
- Larger block sizes better utilize hardware resources, but should be chosen to fit in cache.

Our evaluation uses $F{=}50$, and we experimentally found a block size of 50 rows to be a good balance between convergence rate and performance.

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Experimental Setup

Source code:

- Modified from SPLATT [1]
- Written in C and parallelized with OpenMP
- Compiled with `icc` v17.0.1 and linked with Intel MKL

Machine specifications:

- 2× 10-core Intel Xeon E5-2650v3 (Haswell)
- 396GB RAM

[1] `https://github.com/ShadenSmith/splatt`

Convergence measurement

We measure convergence based on the relative reconstruction error:

$$\text{relative error} = \frac{\mathcal{L}(\boldsymbol{\mathcal{X}}, \mathbf{A}, \mathbf{B}, \mathbf{C})}{\|\boldsymbol{\mathcal{X}}\|_F^2}.$$

Termination:

- Convergence is detected when the relative error improves less than 10^{-6} or if we exceed 200 outer iterations.
- ADMM is limited to 50 iterations and $\epsilon = 10^{-2}$.

Datasets

We selected four tensors from the FROSTT [2] collection based on non-negative factorization performance:

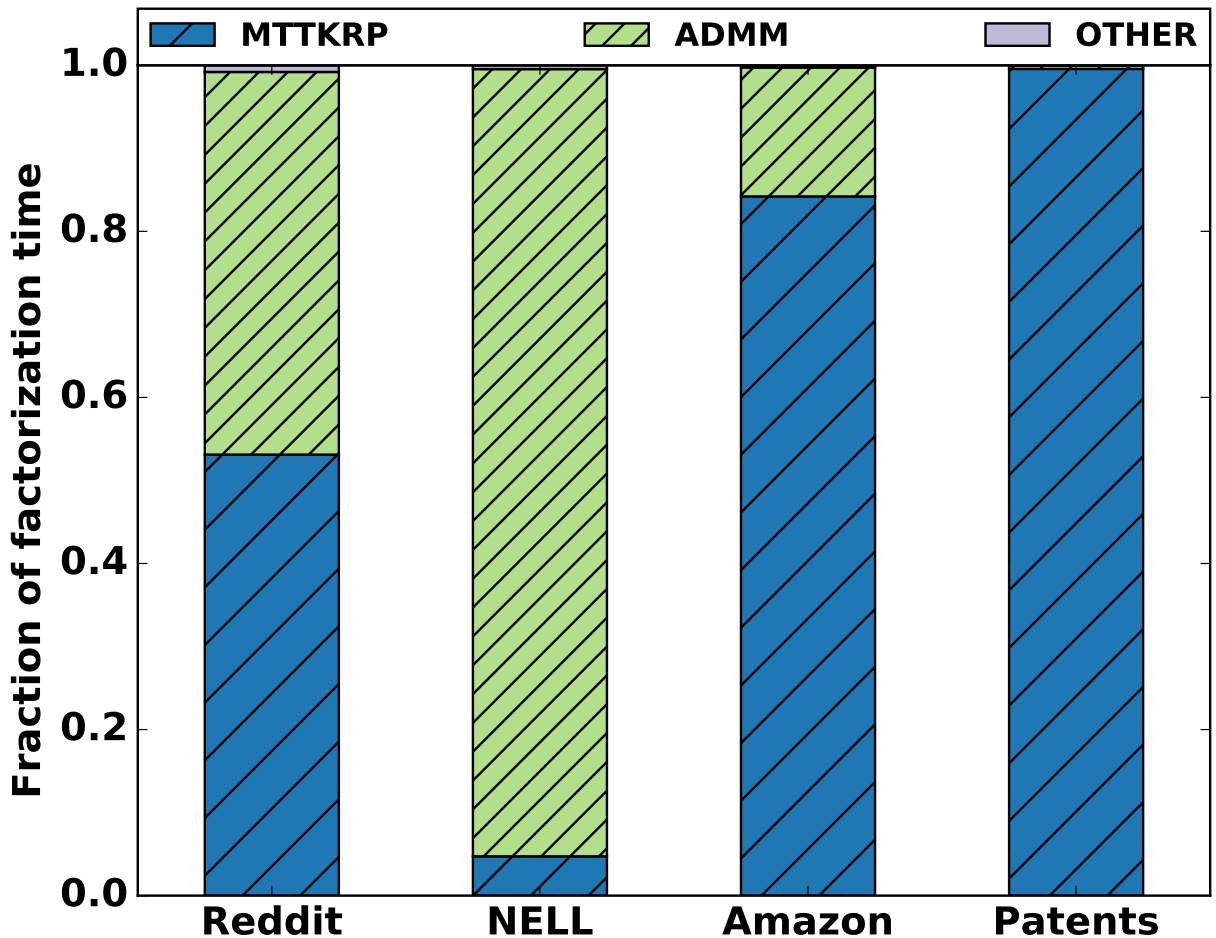
- require a non-trivial number of iterations
- have a factorization quality that suggests a non-negative CPD is appropriate

Dataset	NNZ	I	J	K
Reddit	95M	310K	6K	510K
NELL	143M	3M	2M	25M
Amazon	1.7B	5M	18M	2M
Patents	3.5B	46	240K	240K

[2] http://frostt.io/

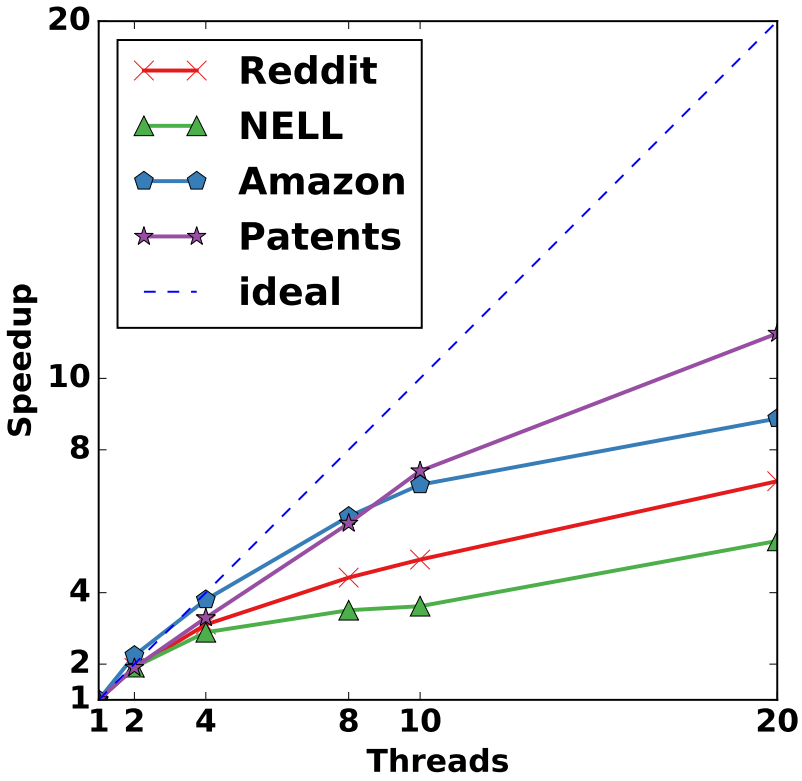
Relative Factorization Costs

Fraction of time spent in MTTKRP and ADMM during a rank-50 non-negative factorization:

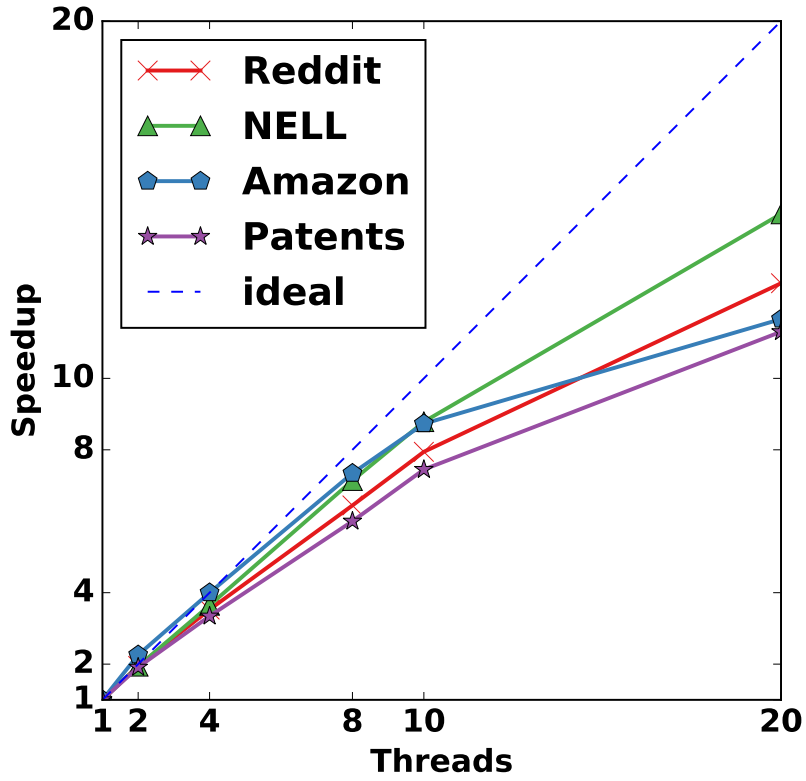


Parallel Scalability

Blocked ADMM improves speedup when the factorization is dominated by ADMM:



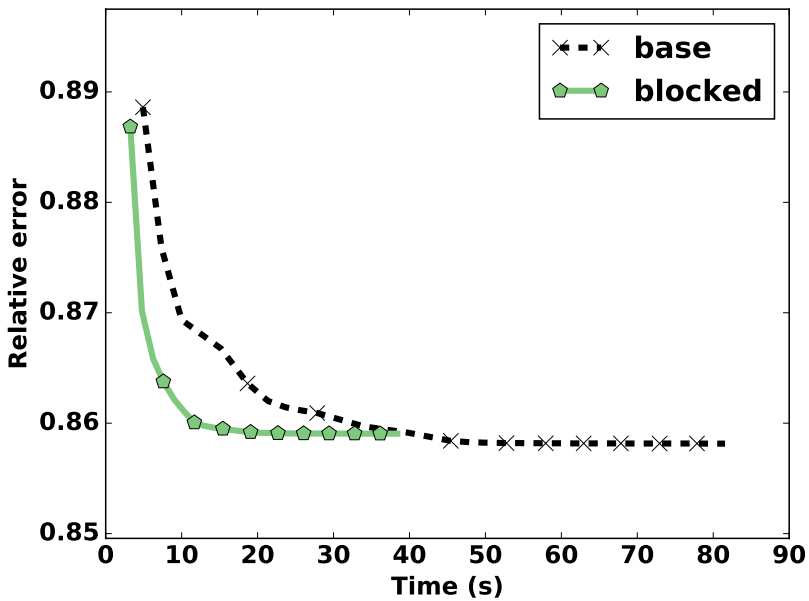
Baseline

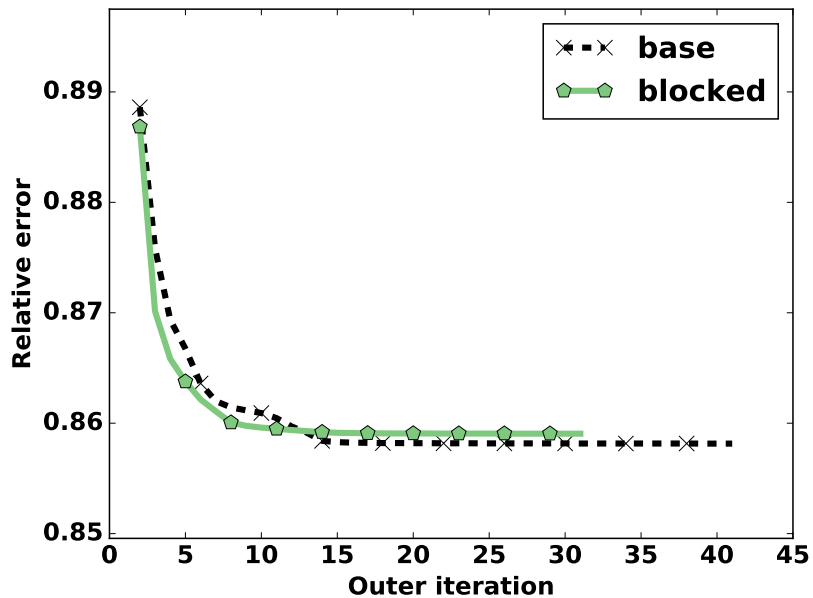


Blocked

Convergence: `Reddit`

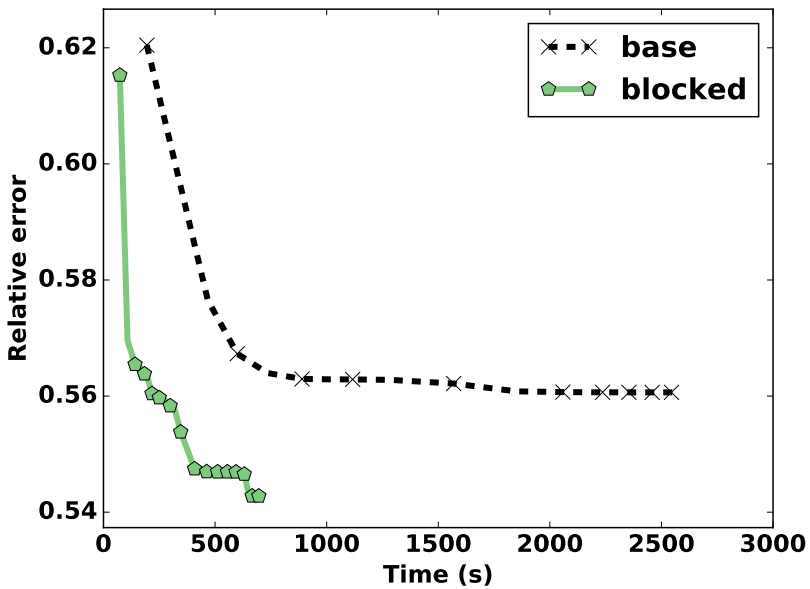
Blocking results in faster per-iteration runtimes and also converges in fewer iterations.

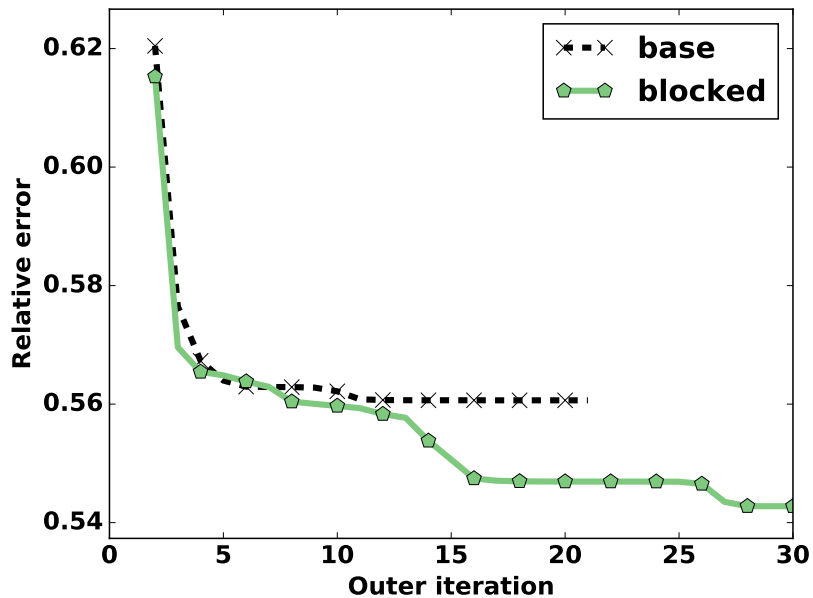




Convergence: NELL

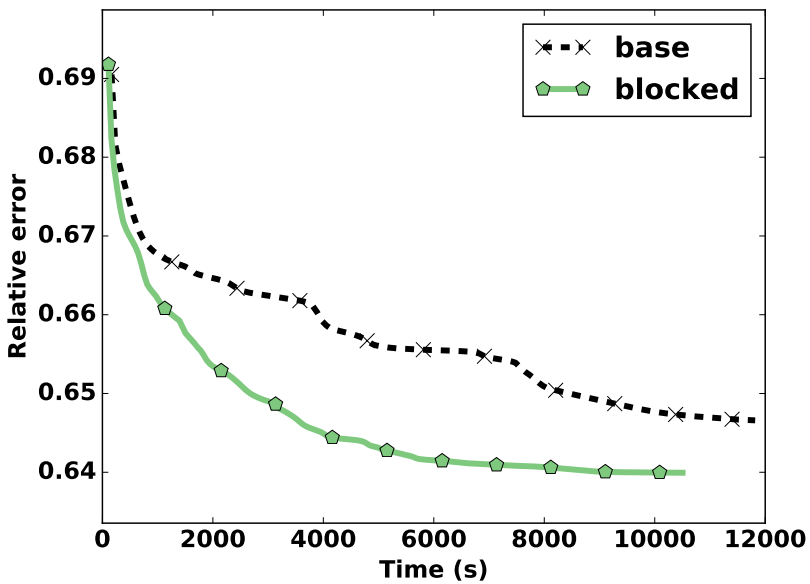
Convergence is 3.7× faster with blocking, despite using additional iterations to achieve a lower error.

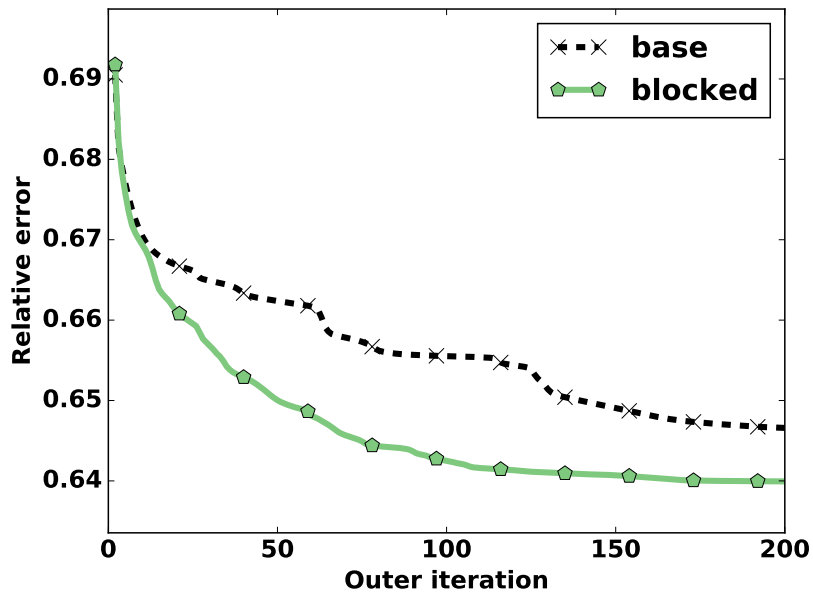




Convergence: Amazon

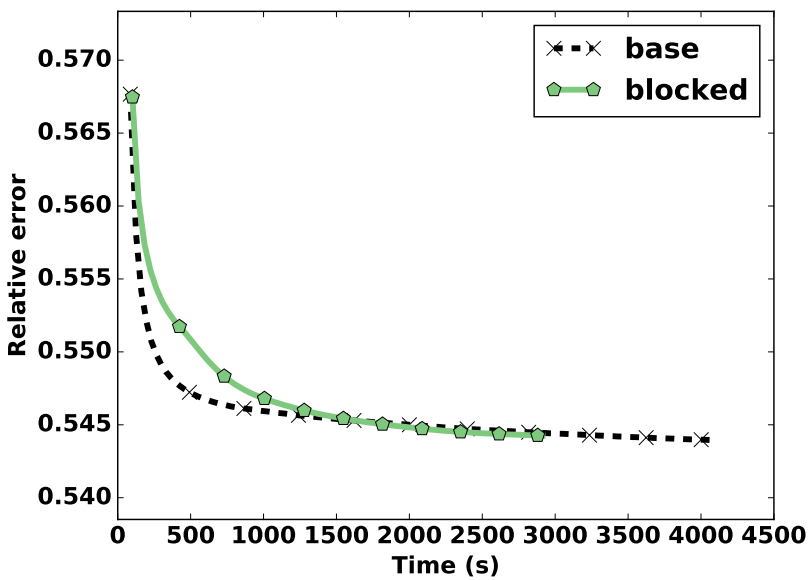
Both formulations exceed the maximum of 200 outer iterations, but the blocked formulation achieves a lower error in less time.

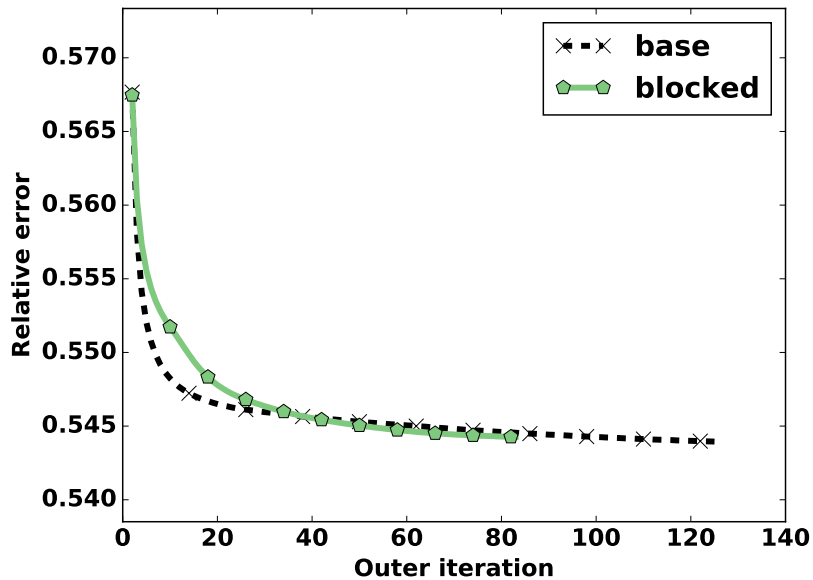




Convergence: Patents

Per-iteration runtimes are largely unaffected, as Patents is dominated by MTTKRP time. However, fewer iterations are required.





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Wrapping up

Blocked ADMM accelerates constrained tensor factorization in two ways:

- Optimizing blocks independently saves computation on the "simple" rows and better optimizes "hard" rows.
- Blocks can be kept in cache during ADMM, saving memory bandwidth.

Also in the paper:

- MTTKRP can be accelerated by exploiting the sparsity that dynamically evolves in the factors.
- An additional $\sim 2\times$ speedup is achieved.

Future work:

- Analytical model for selecting block sizes.
- Automatic runtime selection of data structure for sparse factors.

Reproducibility

All of our work is open source (in the `wip/ao-admm` branch for now):

`https://github.com/ShadenSmith/splatt`

Datasets are freely available:

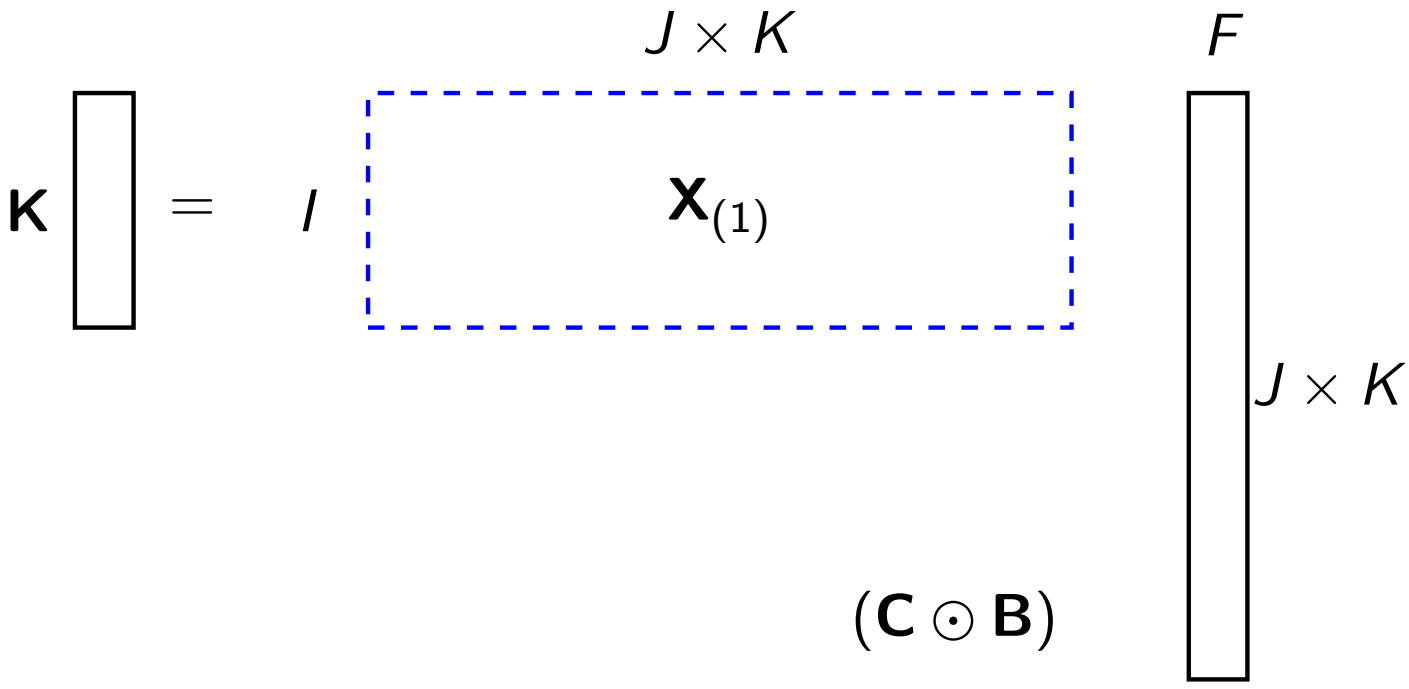
`http://frostt.io/`

Backup Slides

Matricized tensor times Khatri-Rao product

MTTKRP is a key kernel for computing the CPD:

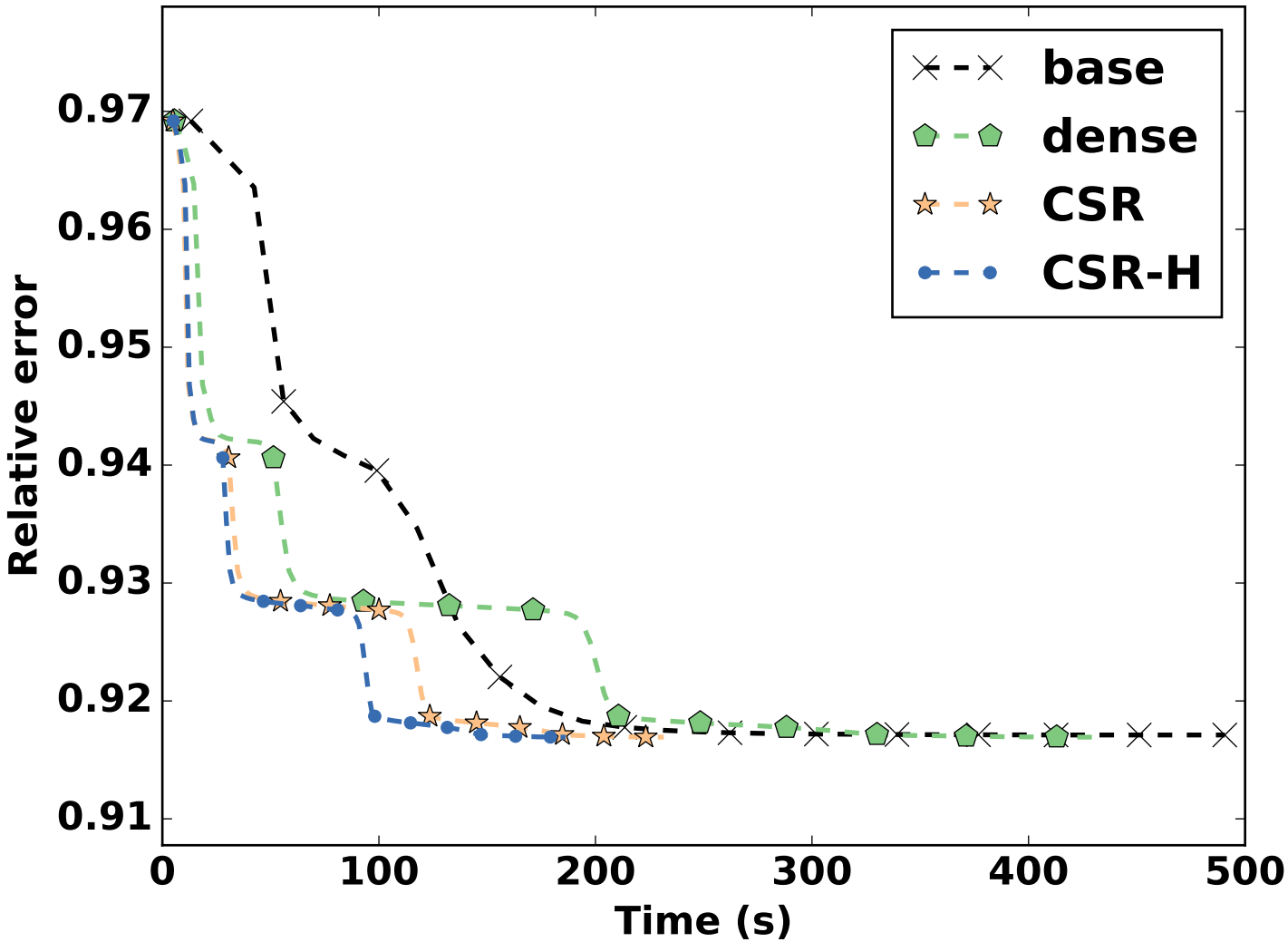
$$\mathbf{K} = \mathbf{X}_{(1)} (\mathbf{C} \odot \mathbf{B})$$



Notation
$\mathbf{X}_{(1)}$ *unfolds* a tensor.
$(\mathbf{C} \odot \mathbf{B})$ is the Khatri-Rao (columnwise Kronecker) product.

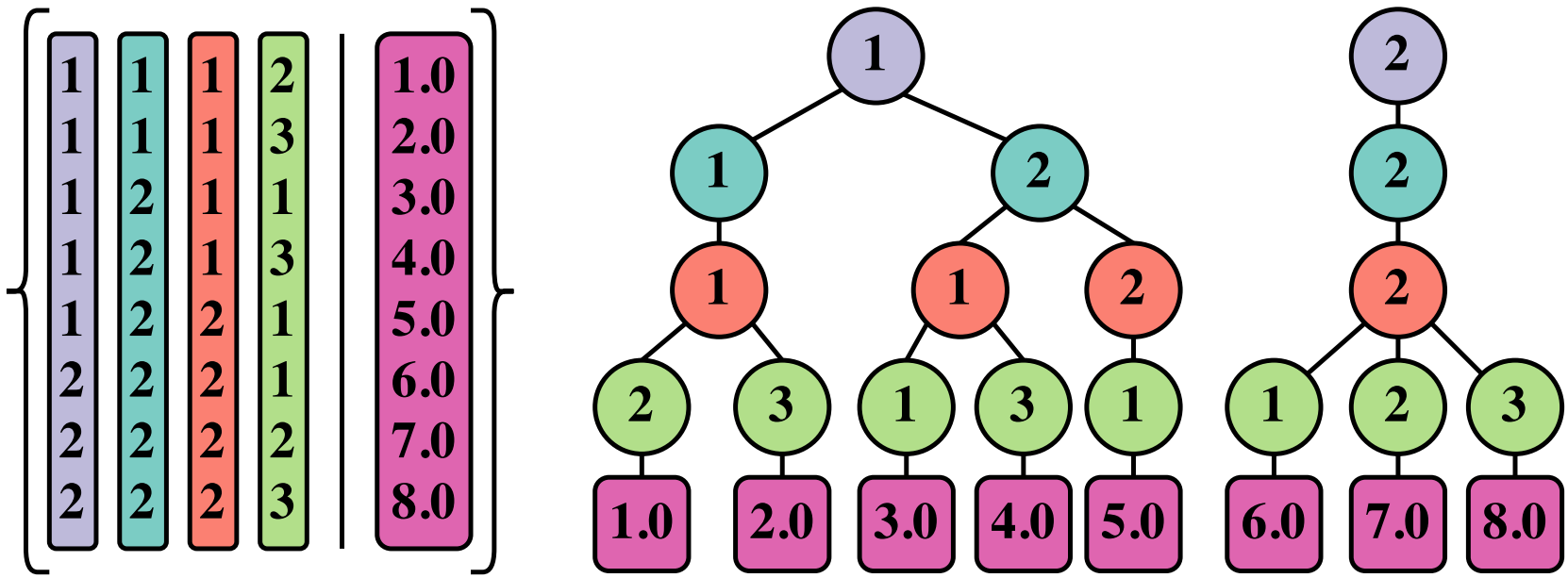
Sparse MTTKRP

Convergence on `Reddit` with $F = 100$ and $r(\cdot) = 10^{-1}||\cdot||_1$.



Compressed sparse fiber (CSF)

- Modes are recursively compressed.
- Paths from roots to leaves encode non-zeros.
- The tree structure encodes opportunities for savings.



MTTKRP with CSF

```
/* foreach outer slice */
for(int i=0; i < I; ++i) {
  /* foreach fiber in slice */
  for(int s = s_ptr[i]; s < s_ptr[i+1]; ++s) {
    accum[0:r] = 0;

    /* foreach  nnz in fiber */
    for(int nnz = f_ptr[s]; nnz < f_ptr[s+1]; ++nnz) {
      int k = f_ids[nnz];
      accum[0:r] += vals[nnz] * C[k][0:r];
    }

    int j = s_ids[s];
    A[i][0:r] += accum[0:r] * B[s][0:r];
  }
}
```