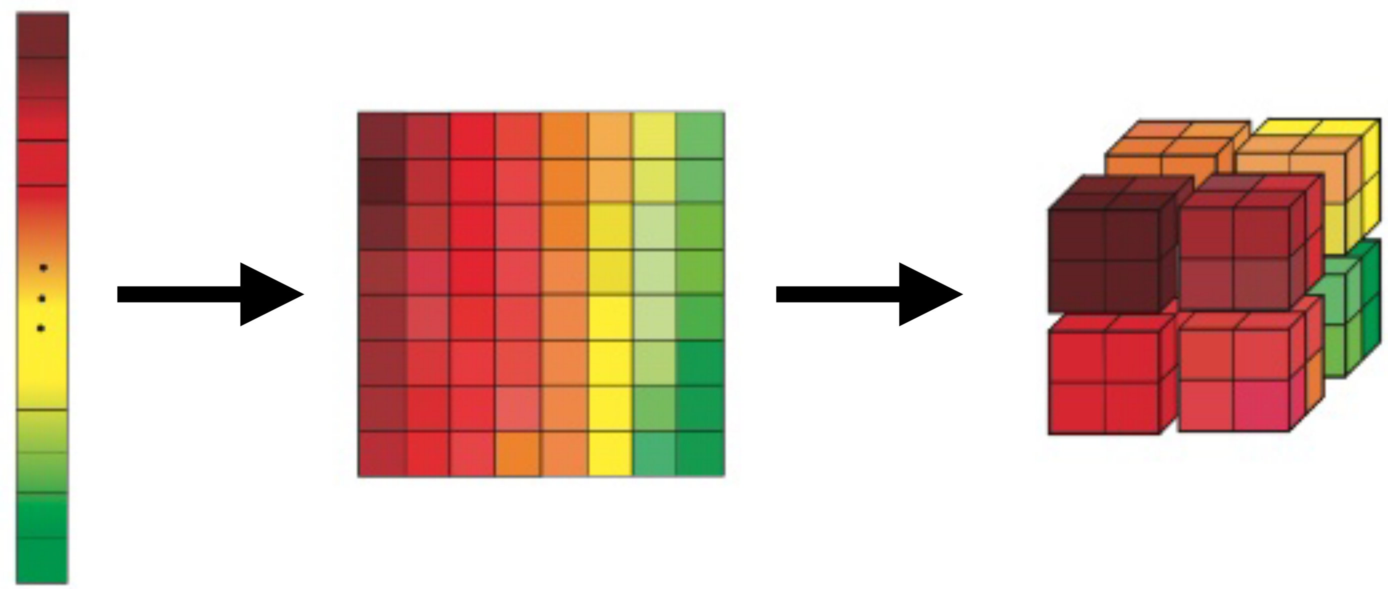


Parallel Sparse Tensor Decompositions using HiCOO Format

Jiajia Li, Jee Choi, Richard Vuduc

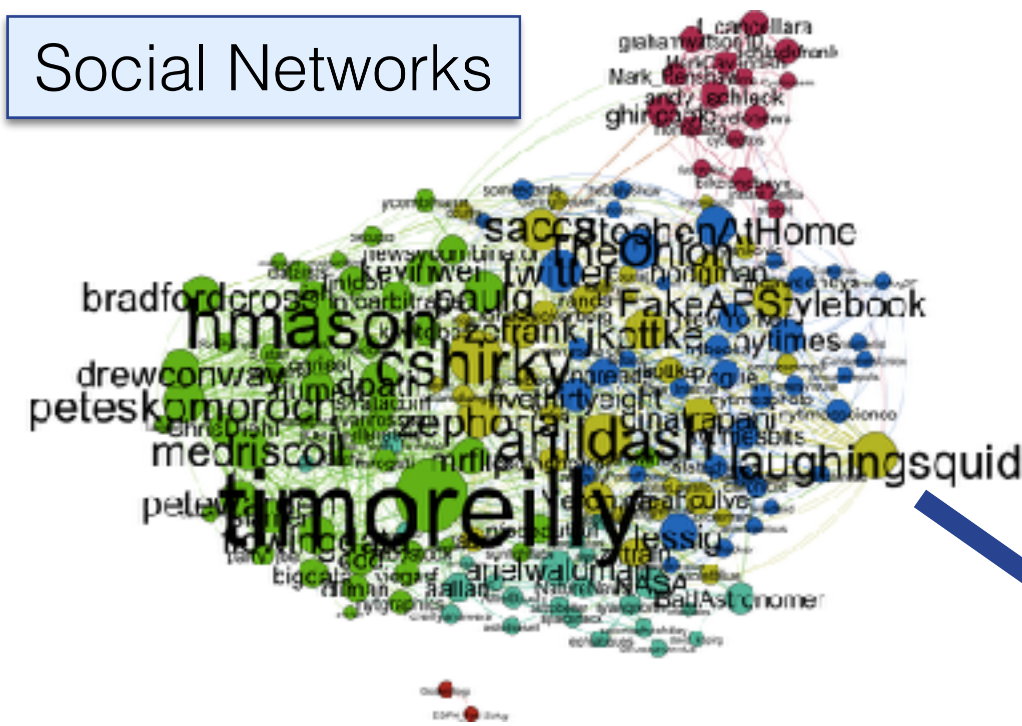
May 08, 2018 @ SIAM ALA'18

Outline

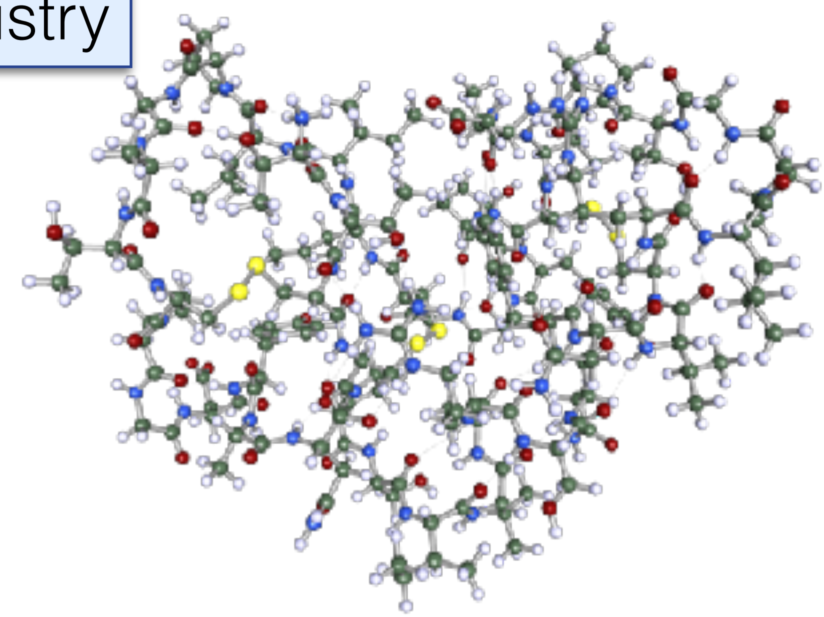
- Background
- HiCOO Format
- Multicore CP-ALS
- Distributed CPDs

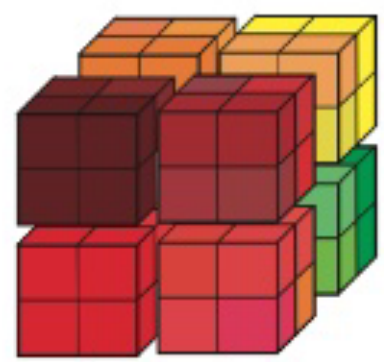
Tensors

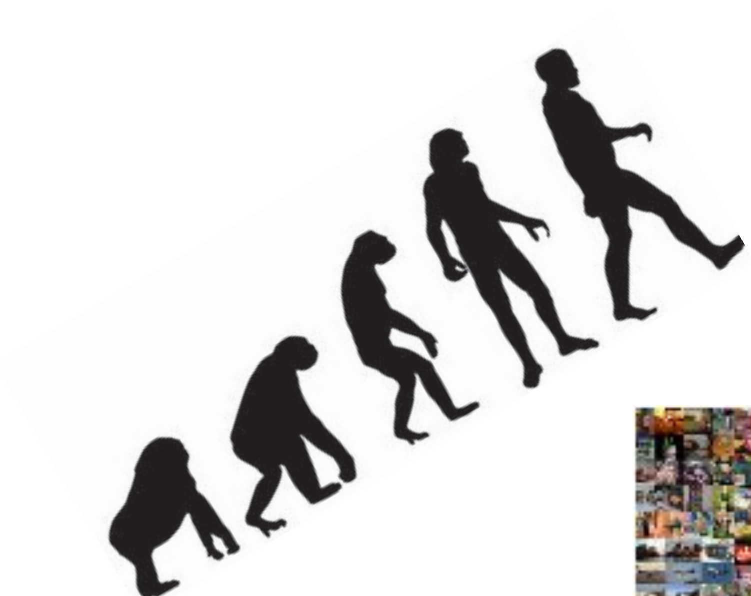
Social Networks

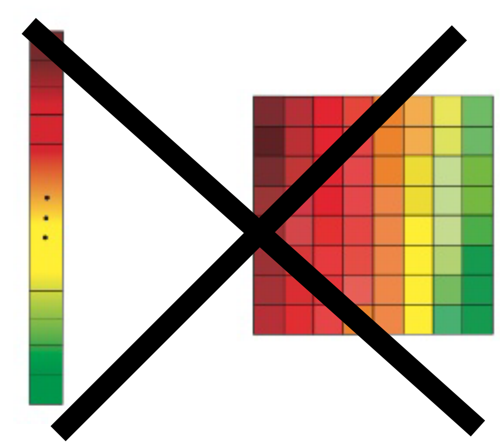


Quantum Chemistry







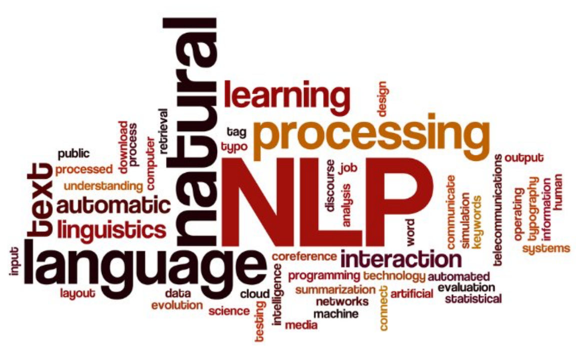


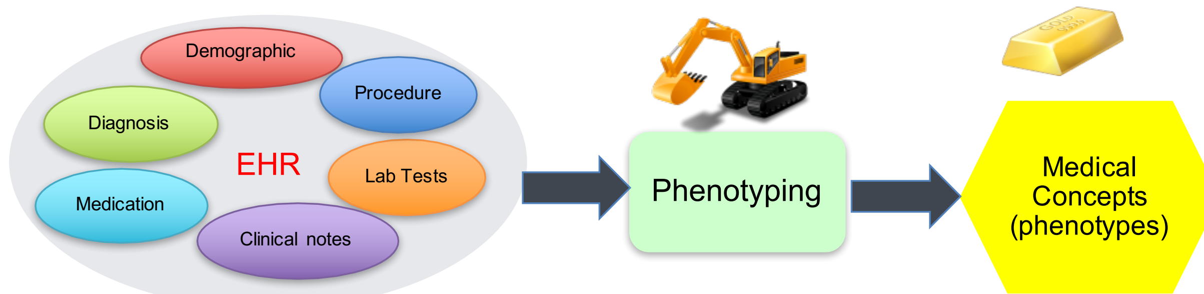
Deep Learning

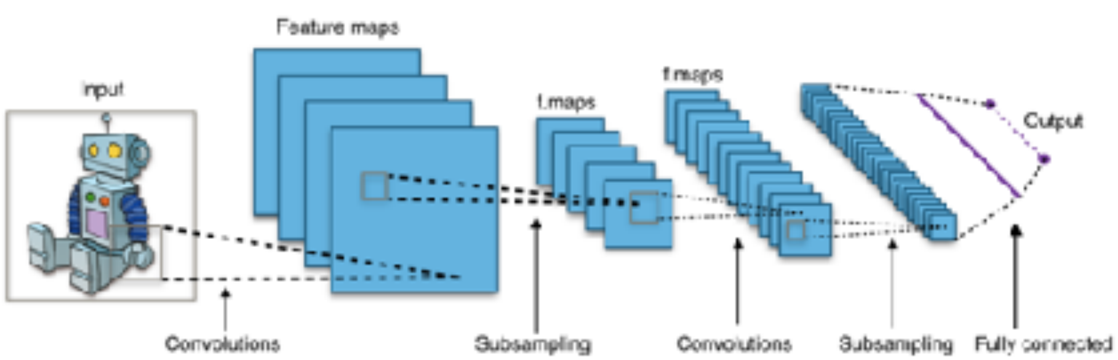
NOT ENOUGH

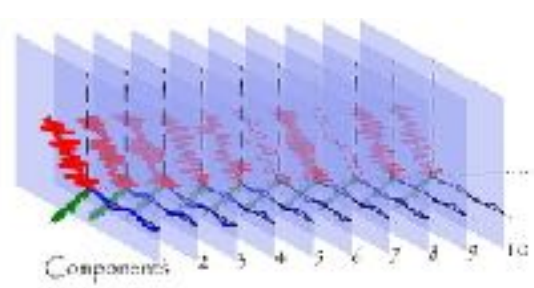
Applications of Tensor Methods

- Data analytics and compression
  - Natural language processing, healthcare analytics, social network analytics, brain signal processing, and deep learning
- Scientific computing
  - Quantum chemistry, computational physics, quantum mechanics



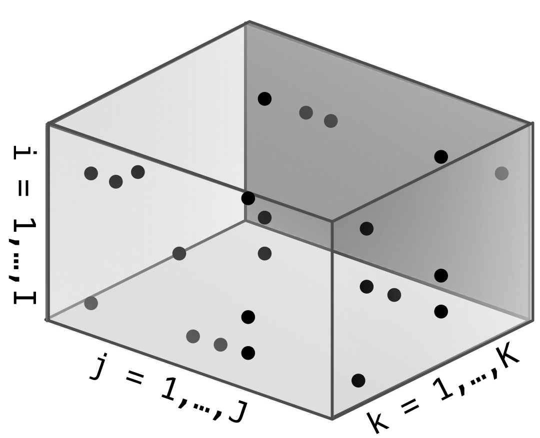






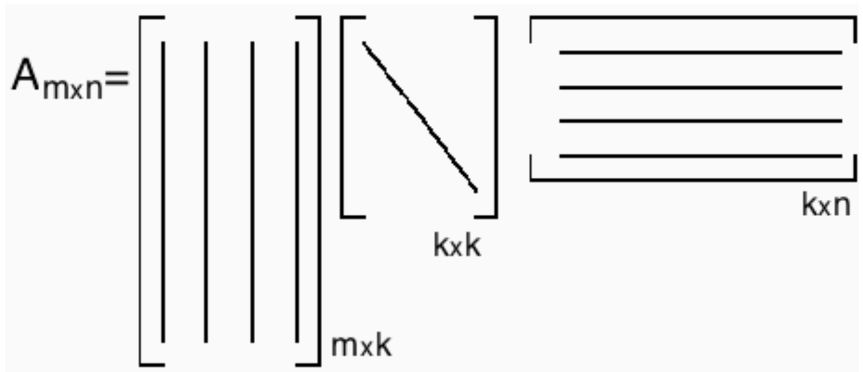
Tensors & Decompositions

- Tensors, multi-way arrays, provide a natural way to represent multidimensional data.
  - Special cases: matrices - 2D tensors, vectors - 1D tensors.
  - Tensor mode or order: tensor dimension.
  - A SPARSE tensor, a tensor consisting mostly of zero entries, widely exists in real applications.



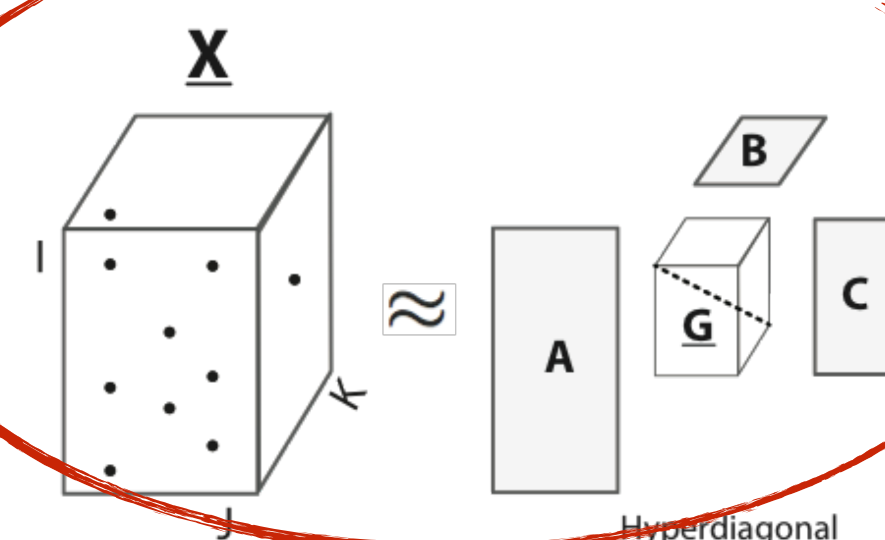
- Tensor decomposition: an extension of matrix factorization to analyze tensor features.

Singular Value Decomposition (SVD)



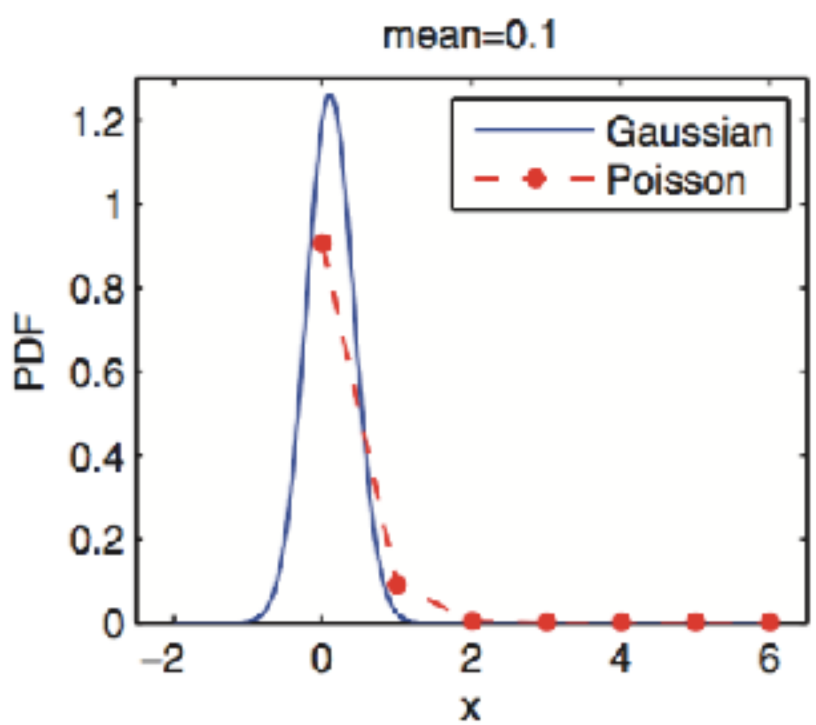
CANDECOMP/PARAFAC

CP Decomposition



CP-ALS and CP-APR

- CP-ALS - alternating least squares
  - For general data
  - Describe input data as Gaussian distribution
  - Fitting function: least squares.
  - Core operation: MTTKRP



- CP-APR – alternating Poisson regression
  - For non-negative data, e.g. count data.
  - Describe input data as Poisson distribution
  - Fitting function:Poisson likelihood fitting algorithm
  - Core operation: element-wise division.

CP-ALS

Bottleneck: MTTKRP

procedure CP-ALS($\mathfrak{X}$,R)
  initialize $\mathbf{A}^{(n)} \in \mathbb{R}^{I_n \times R}$ for $n = 1, \ldots, N$
  repeat
    for $n = 1, \ldots, N$ **do**
      $\mathbf{V} \leftarrow \mathbf{A}^{(1)\mathsf{T}}\mathbf{A}^{(1)} * \cdots * \mathbf{A}^{(n-1)\mathsf{T}}\mathbf{A}^{(n-1)} * \mathbf{A}^{(n+1)\mathsf{T}}\mathbf{A}^{(n+1)} * \cdots * \mathbf{A}^{(N)\mathsf{T}}\mathbf{A}^{(N)}$
      $\mathbf{A}^{(n)} \leftarrow \mathbf{X}_{(n)}(\mathbf{A}^{(N)} \odot \cdots \odot \mathbf{A}^{(n+1)} \odot \mathbf{A}^{(n-1)} \odot \cdots \odot \mathbf{A}^{(1)})\mathbf{V}^{\dagger}$
      normalize columns of $\mathbf{A}^{(n)}$ (storing norms as $\boldsymbol{\lambda}$)
    end for
  until fit ceases to improve or maximum iterations exhausted
  return $\boldsymbol{\lambda}, \mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \ldots, \mathbf{A}^{(N)}$
end procedure

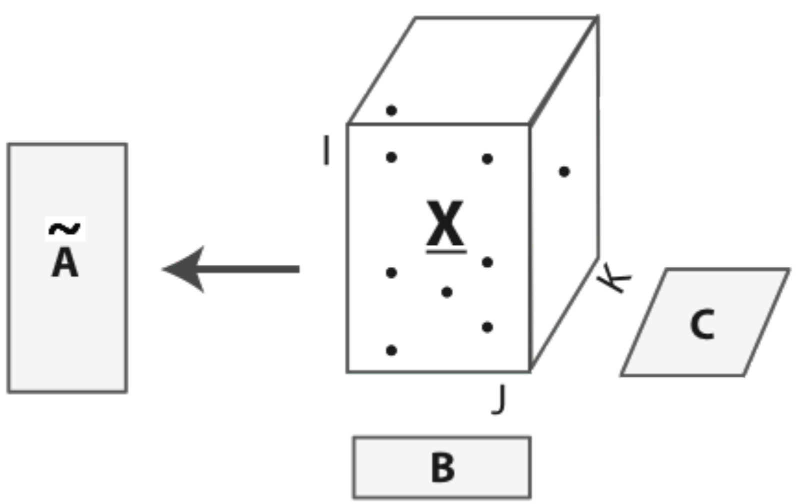
MTTKRP Operation

- Matriced Tensor Times Khatri-Rao Product (MTTKRP)

Tensor Matricization   Khatri-Rao Product

$$\tilde{\mathbf{A}} \leftarrow \mathbf{X}_{(1)} \, (\mathbf{C} \odot \mathbf{B})$$

Updated Factor Matrix   Factor Matrix



MTTKRP Operation

- Matriced Tensor Times Khatri-Rao Product (MTTKRP)

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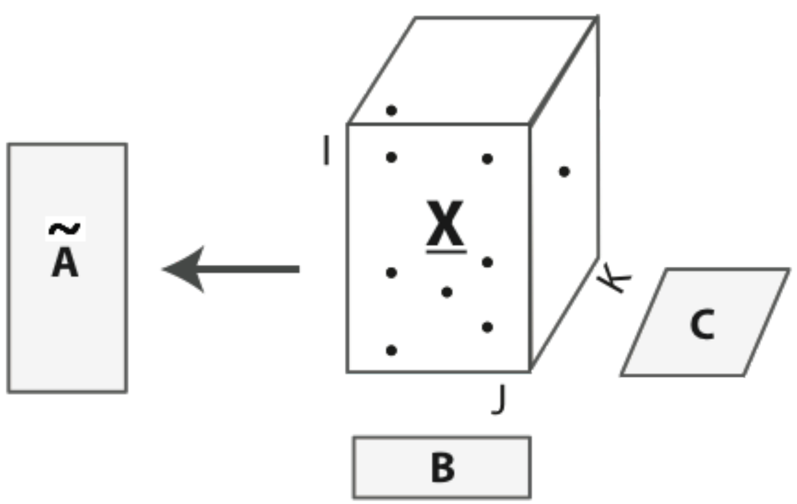
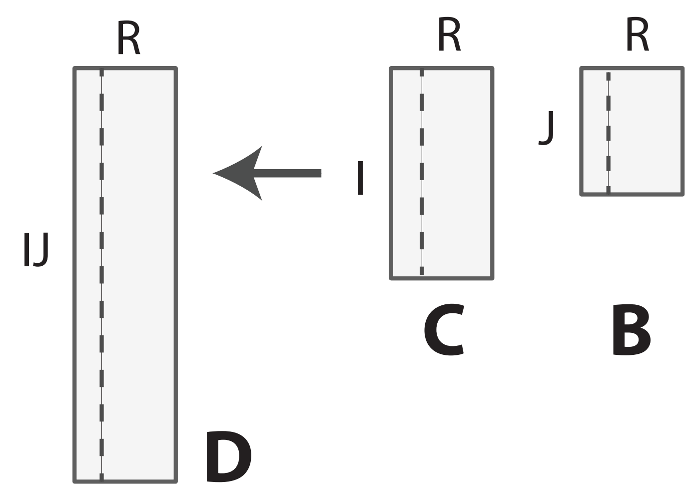
Factor Matrix



- Khatri-Rao Product

$$\mathbf{D} \leftarrow \mathbf{C} \odot \mathbf{B}$$

Matrix



CP-APR

for $k = 1, 2, \dots, k_{\max}$ **do**
  isConverged $\leftarrow$ true
  for $n = 1, \dots, N$ **do**

$$\mathbf{S}(i,r) \leftarrow \begin{cases} \kappa, & \text{if } k > 1, \mathbf{A}^{(n)}(i,r) < \kappa_{\text{tol}}, \text{ and } \mathbf{\Phi}^{(n)}(i,r) > 1, \\ 0, & \text{otherwise} \end{cases}$$

$$\mathbf{B} \leftarrow (\mathbf{A}^{(n)} + \mathbf{S})\mathbf{\Lambda}$$

$$\mathbf{\Pi} \leftarrow \left(\mathbf{A}^{(N)} \odot \cdots \odot \mathbf{A}^{(n+1)} \odot \mathbf{A}^{(n-1)} \odot \cdots \odot \mathbf{A}^{(1)}\right)^{\mathsf{T}}$$

    for $\ell = 1, 2, \dots, \ell_{\max}$ **do** ▷ subproblem loop

$$\mathbf{\Phi}^{(n)} \leftarrow \left(\mathbf{X}_{(n)} \oslash \left(\max(\mathbf{B\Pi}, \epsilon)\right)\right) \mathbf{\Pi}^{\mathsf{T}}$$

      if $|\min(\mathbf{B}, \mathbf{E} - \mathbf{\Phi}^{(n)})| < \tau$ **then**
        break
      end if
      isConverged $\leftarrow$ false
      $\mathbf{B} \leftarrow \mathbf{B} * \mathbf{\Phi}^{(n)}$
    end for
    $\boldsymbol{\lambda} \leftarrow \mathbf{e}^{\mathsf{T}}\mathbf{B}$
    $\mathbf{A}^{(n)} \leftarrow \mathbf{B\Lambda}^{-1}$
  end for
  if isConverged = true **then**
    break
  end if
end for

Bottleneck:
element-wise product

Bottleneck of CP-APR

- Consider CP-APR MU

$$\mathbf{\Phi}^{(n)} \leftarrow \left(\mathbf{X}_{(n)} \oslash \left(\max(\mathbf{B}\mathbf{\Pi}, \epsilon)\right)\right) \mathbf{\Pi}^{\mathsf{T}}$$

$$\mathbf{\Pi} \leftarrow \left(\mathbf{A}^{(N)} \odot \cdots \odot \mathbf{A}^{(n+1)} \odot \mathbf{A}^{(n-1)} \odot \cdots \odot \mathbf{A}^{(1)}\right)^{\mathsf{T}}$$

Stored in sparse format, size nnz * R

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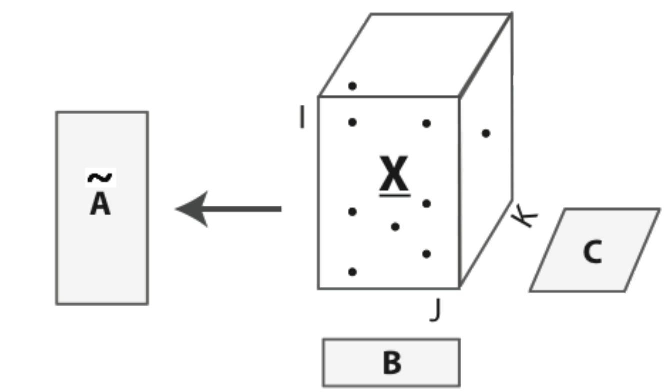
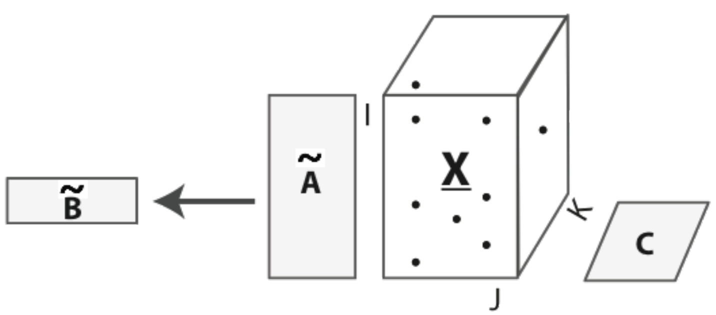
Mode Orientation

Tensor decomposition

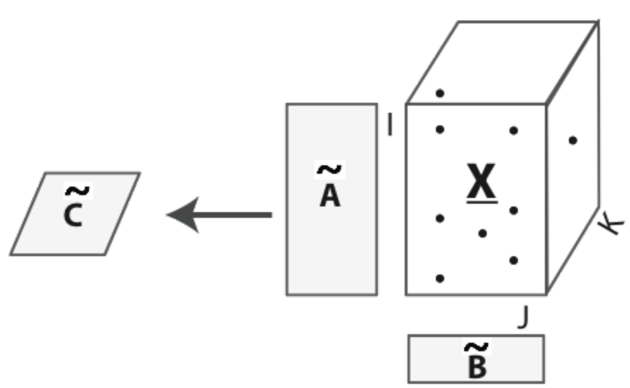
<u>Kernel in Mode-1</u>



<u>Kernel in Mode-2</u>



<u>Kernel in Mode-3</u>



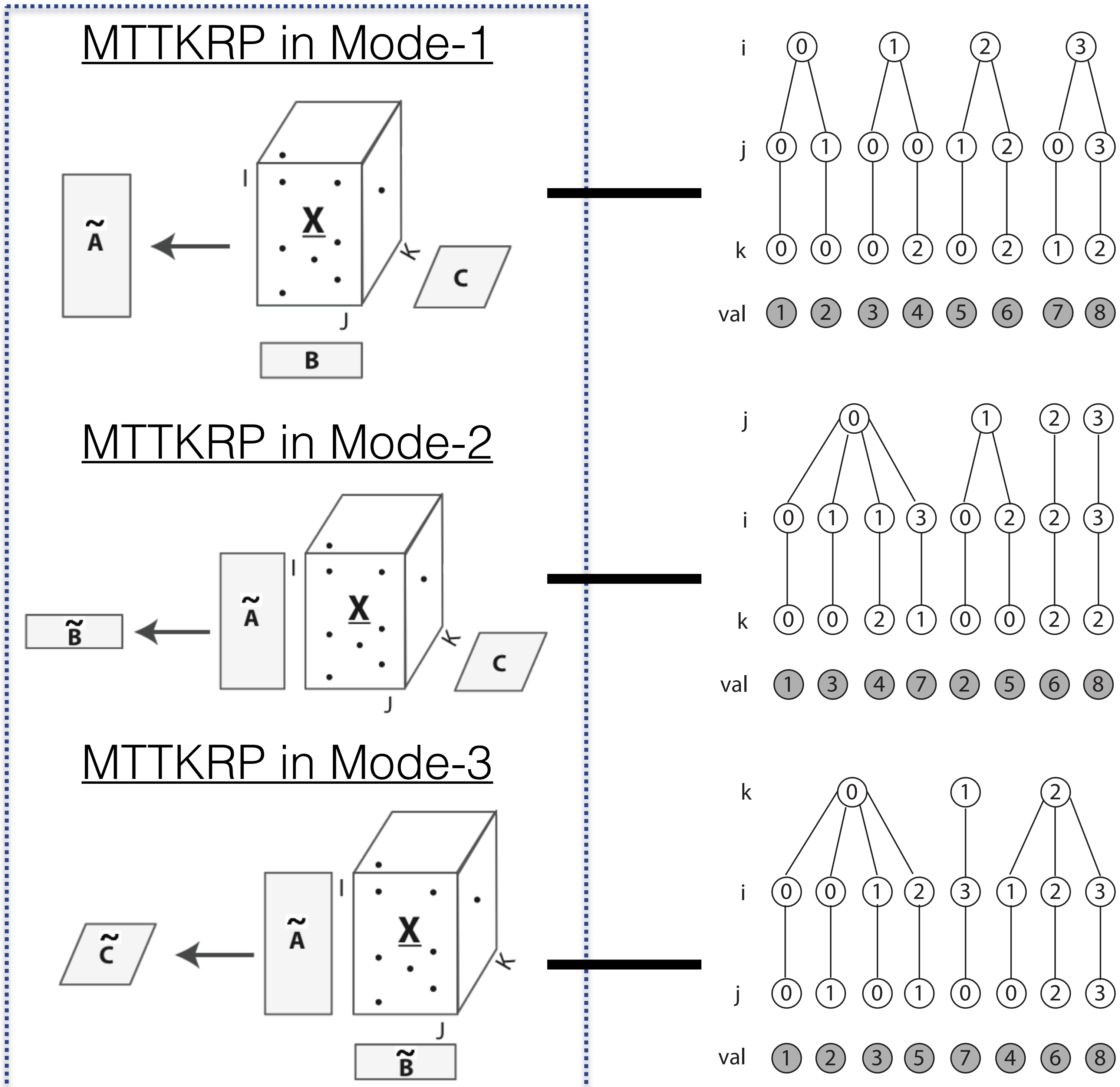
	Mode Oriented	Neutral Mode Orientation
	Mode-1 oriented (CSF)	Coordinate (COO)
Kernel in Mode-1	**Efficient**	**Inefficient**
Kernel in Mode-2	**?**	**?**
Kernel in Mode-3	**?**	**?**

Mode Oriented Formats

- Three CSF/F-COO representations are required/preferred for the three MTTKRPs.

CP Decomposition

More storage



CSF-1

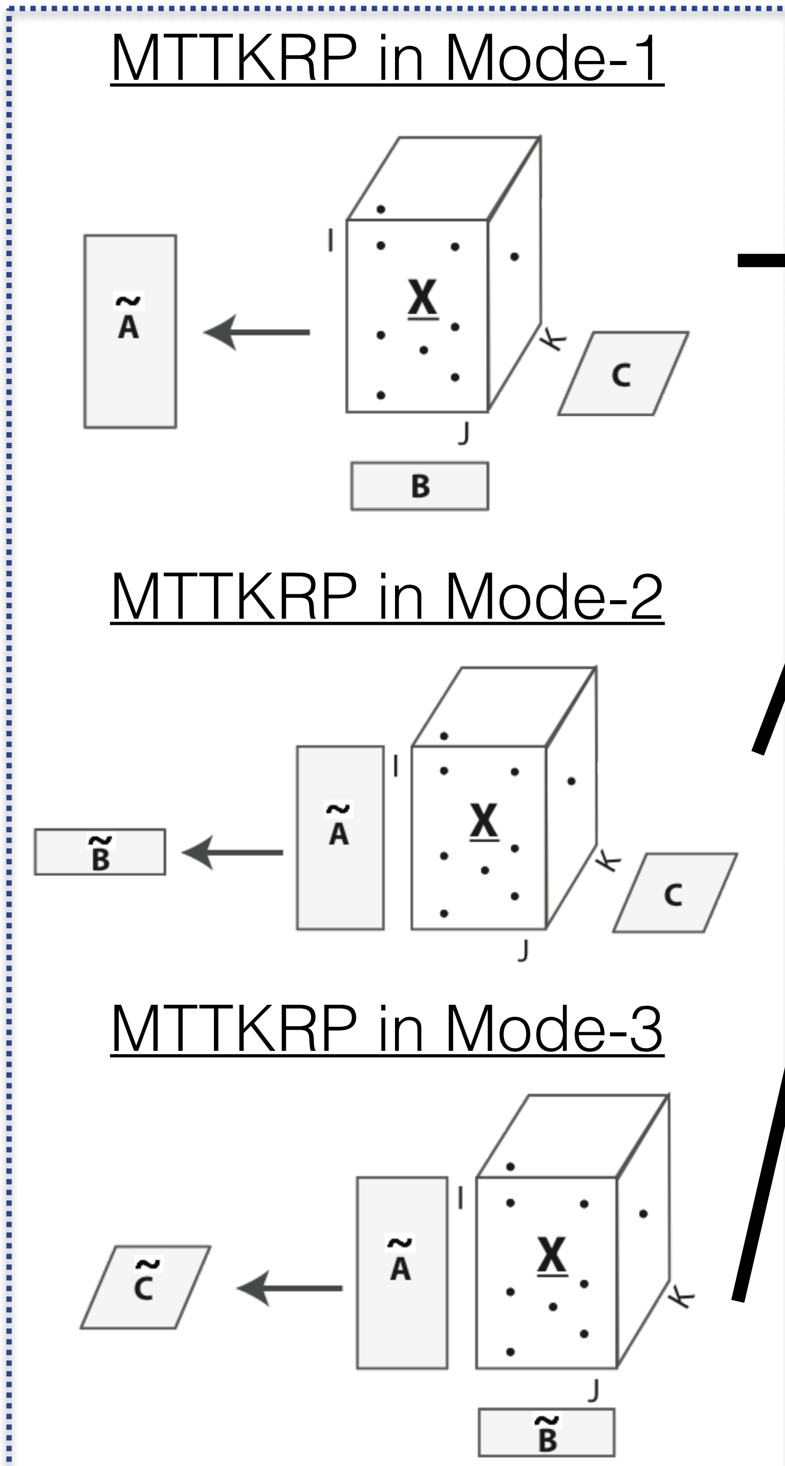
CSF-2

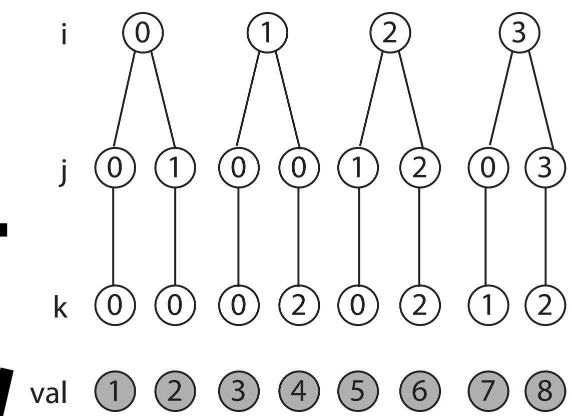
CSF-3

Mode Oriented Formats

- Three CSF/F-COO representations are required/preferred for the three MTTKRPs.

CP Decomposition



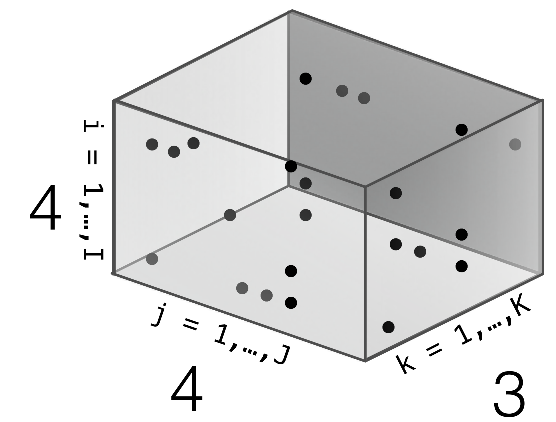


CSF-1

Performance payoff

Current Sparse Tensor Formats

- **COO**: coordinate formats [Bader et al., 2006]
- **CSF**: Compressed Sparse Fibers, extension of CSR. [Smith et al. 2015]
- **F-COO**: Flagged COO format [Liu et al., 2017]



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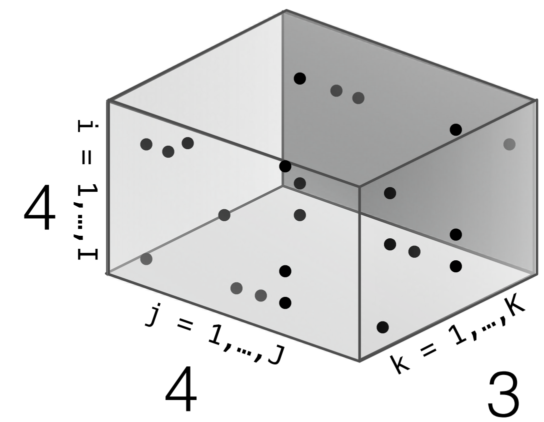
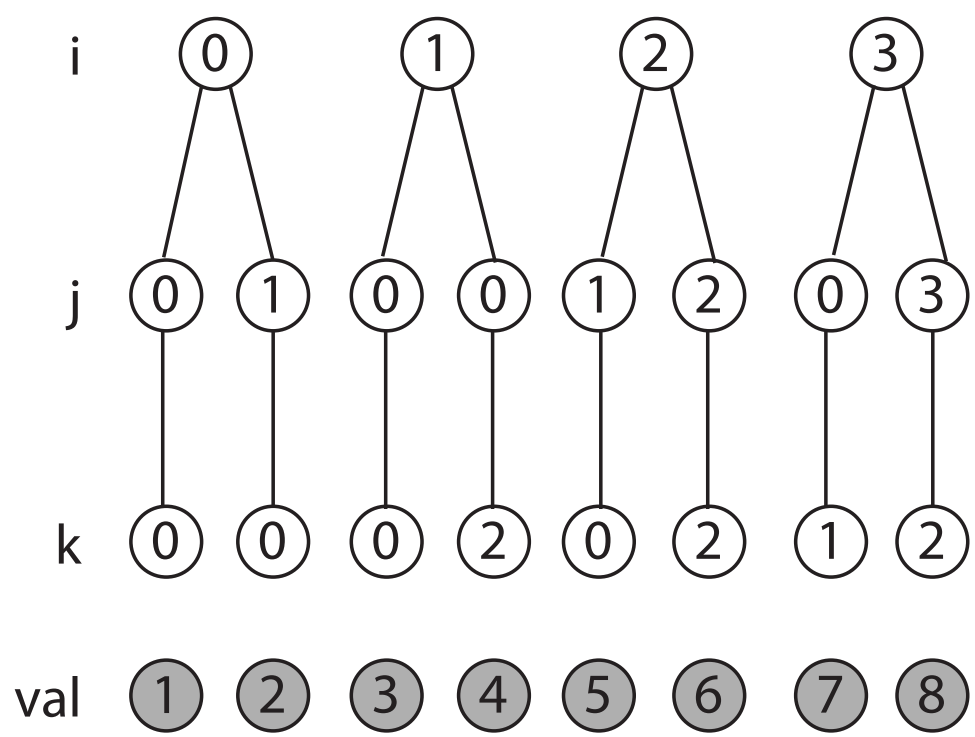


i	j	k	val
0	0	0	1
0	1	0	2
1	0	0	3
1	0	2	4
2	1	0	5
2	2	2	6
3	0	1	7
3	3	2	8

(a) COO



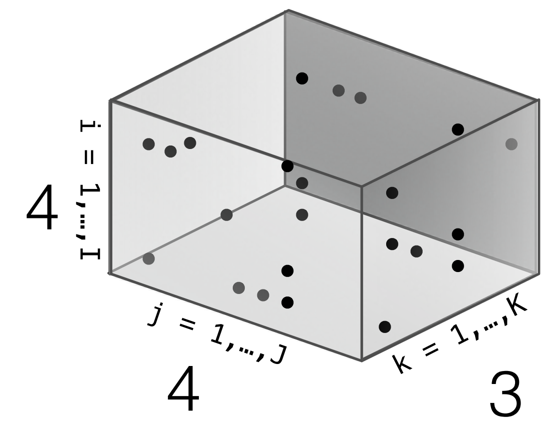
(b) CSF

	bf	j	k	val
sf[0]=1	1	0	0	1
	0	1	0	2
	1	0	0	3
	0	0	2	4
sf[1]=1	1	1	0	5
	0	2	2	6
	1	0	1	7
	0	3	2	8

(c) F-COO

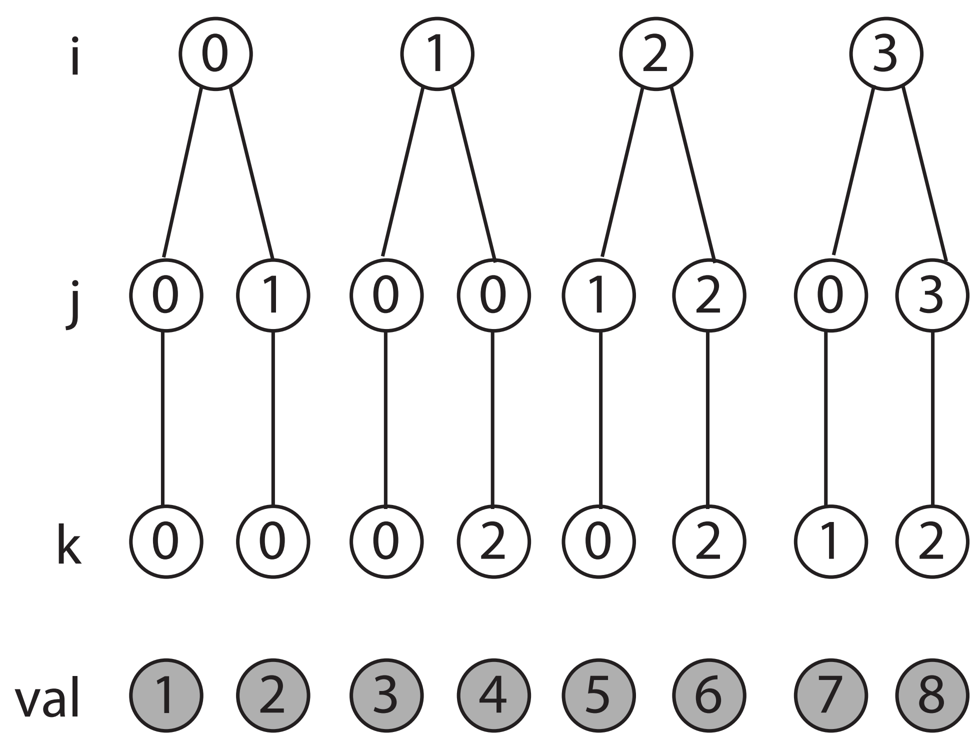
Current Sparse Tensor Formats

- **COO**: coordinate formats [Bader et al., 2006]
- **CSF**: Compressed Sparse Fibers, extension of CSR. [Smith et al. 2015]
- **F-COO**: Flagged COO format [Liu et al., 2017]



i	j	k	val
0	0	0	1
0	1	0	2
1	0	0	3
1	0	2	4
2	1	0	5
2	2	2	6
3	0	1	7
3	3	2	8

(a) COO



(b) CSF

	bf	j	k	val
sf[0]=1	1	0	0	1
	0	1	0	2
	1	0	0	3
	0	0	2	4
sf[1]=1	1	1	0	5
	0	2	2	6
	1	0	1	7
	0	3	2	8

(c) F-COO

neutral
mode orientation

mode oriented,
prefer different representations for different modes.

HiCOO Format

- Store a sparse tensor in units of small sparse blocks, saving storage
  - Shorten the bit-length of element indices
  - Compress the number of block indices
  - an improvement of the Compressed Sparse Blocks (CSB) format

32-bit

i	j	k	val
0	0	0	1
0	1	0	2
1	0	0	3
1	0	2	4
2	1	0	5
2	2	2	6
3	0	1	7
3	3	2	8

(a) COO

32-bit **8-bit**

	bptr	bi	bj	bk	ei	ej	ek	val
B0	0	0	0	0	0	0	0	1
					0	1	0	2
					1	0	0	3
B1	3	0	0	1	1	0	0	4
B2	4	1	0	0	0	1	0	5
					1	0	1	7
B3	6	1	1	1	0	0	0	6
					1	1	0	8

(b) HiCOO

$i = bi * B + ei$

<u>For the tensor</u>: Reduce its storage and memory footprints

<u>For matrices</u>: Better data locality

Construct HiCOO Representation

- Morton-order sorting for the input COO tensor.
- Partition to blocks and determine each block location.
- Construct HiCOO representation by compressing index length.

bits: β_{int}

i	j	k	val
0	0	0	1
0	1	0	2
1	0	0	3
1	0	2	4
2	1	0	5
2	2	2	6
3	0	1	7
3	3	2	8

COO

Z-Order Sorting →

β_{int}

i	j	k	val
0	0	0	1
0	1	0	2
1	0	0	3
1	0	2	4
2	1	0	5
3	0	1	7
2	2	2	6
3	3	2	8

Partition →

β_{long} β_{int}

bptr	i	j	k	val
0	0	0	0	1
	0	1	0	2
	1	0	0	3
3	1	0	2	4
4	2	1	0	5
	3	0	1	7
6	2	2	2	6
	3	3	2	8

Compress →

β_{long} β_{int} β_{byte}

	bptr	bi	bj	bk	ei	ej	ek	val
B0	0	0	0	0	0	0	0	1
					0	1	0	2
					1	0	0	3
B1	3	0	0	1	1	0	0	4
B2	4	1	0	0	0	1	0	5
					1	0	1	7
B3	6	1	1	1	0	0	0	6
					1	1	0	8

HiCOO

$i = bi*B+ei;\ \ j = bj*B+ej;\ \ k = bk*B+ek$

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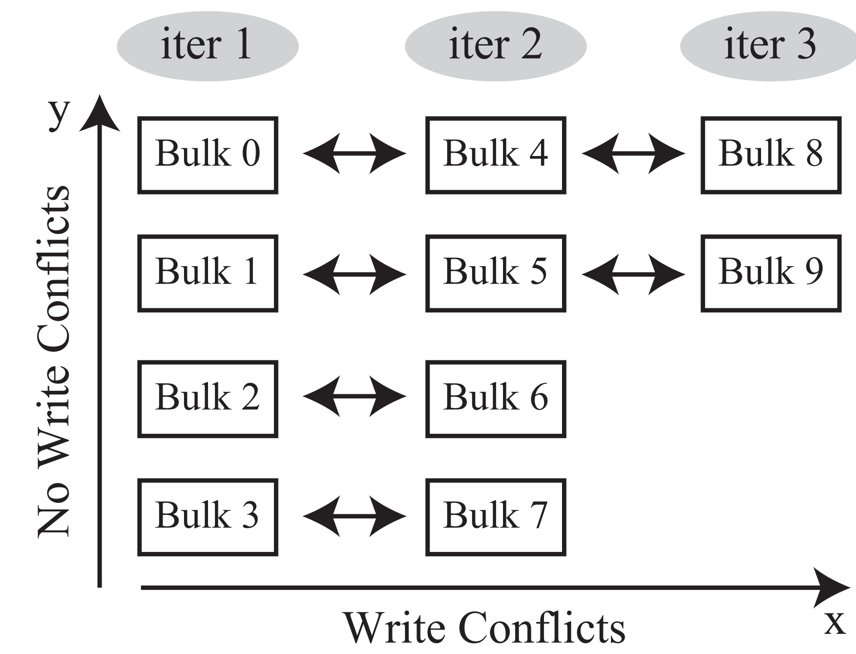
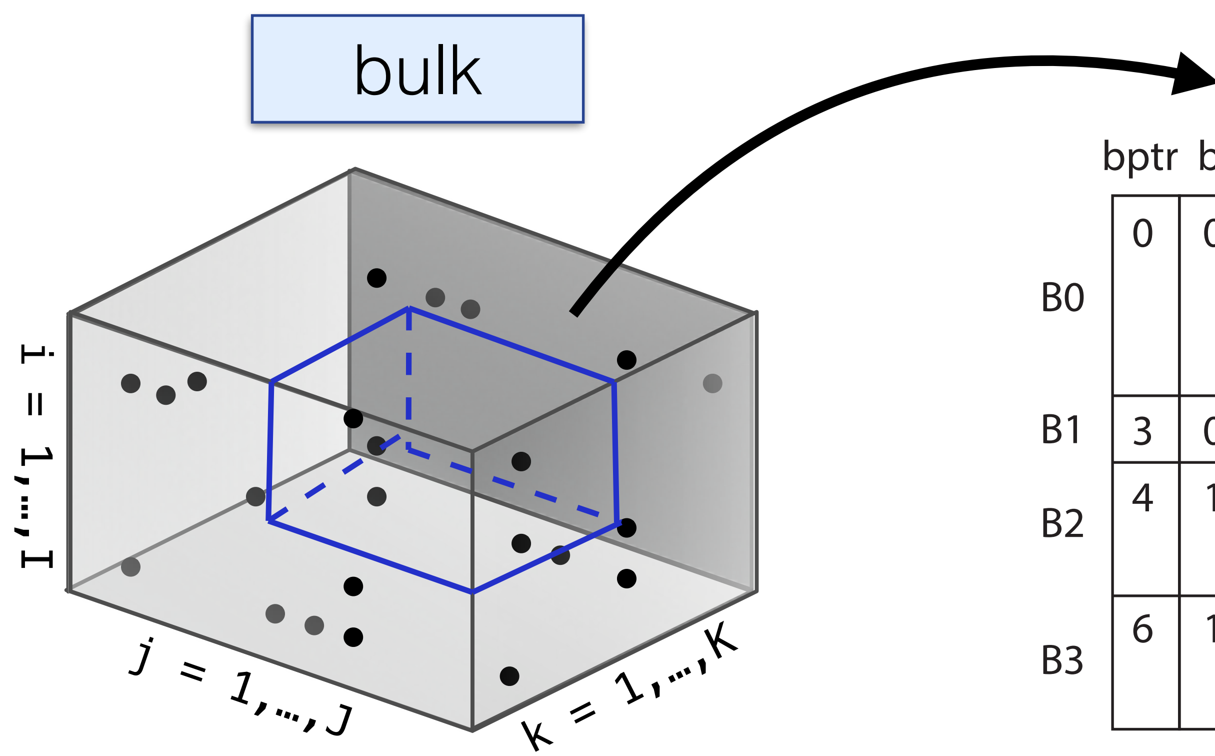
Two-level Blocking for Efficient Thread Parallelism

- Use two-level blocking strategy
  - Large bulks (logical) + small blocks (physical)
  - To avoid using locks, we add a bit extra storage for scheduling information.





	bptr	bi	bj	bk	ei	ej	ek	val
B0	0	0	0	0	0	0	0	1
					0	1	0	2
					1	0	0	3
B1	3	0	0	1	1	0	0	4
B2	4	1	0	0	0	1	0	5
					1	0	1	7
B3	6	1	1	1	0	0	0	6
					1	1	0	8

HiCOO

Platform and Dataset

- **Platform**: Intel Xeon CPU E7-4850 platform consisting 56 physical cores with gcc 5.4.1 and parallelized by OpenMP.
- **Dataset**: FROSTT [Smith et al. 2017] and HaTen2 [Jeon et al. 2015]

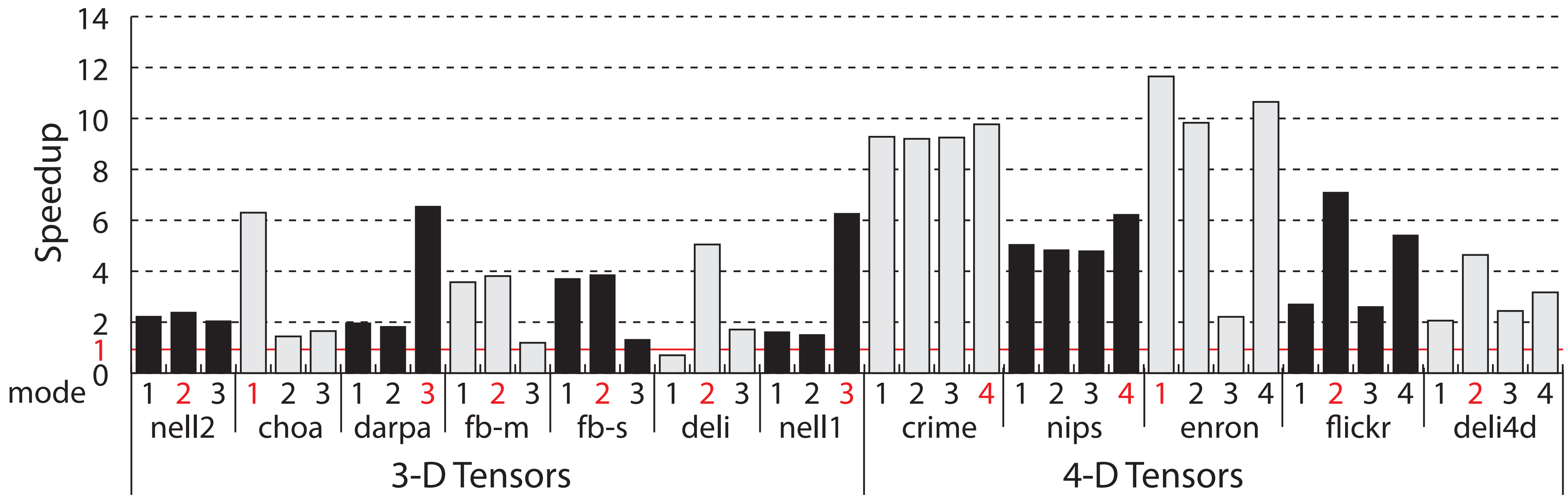
DESCRIPTION OF SPARSE TENSORS.

Tensors	Order	Dimensions	#Nonzeros	Density
nell2	3	$12K \times 9K \times 29K$	77M	2.4×10^{-5}
choa	3	$712K \times 10K \times 767$	27M	5.0×10^{-6}
darpa	3	$22K \times 22K \times 24M$	28M	2.4×10^{-9}
fb-m	3	$23M \times 23M \times 166$	100M	1.1×10^{-9}
fb-s	3	$39M \times 39M \times 532$	140M	1.7×10^{-10}
deli	3	$533K \times 17M \times 2.5M$	140M	6.1×10^{-12}
nell1	3	$3M \times 2M \times 25M$	144M	9.1×10^{-13}
crime	4	$6K \times 24 \times 77 \times 32$	5M	1.5×10^{-2}
nips	4	$2K \times 3K \times 14K \times 17$	3M	1.8×10^{-6}
enron	4	$6K \times 6K \times 244K \times 1K$	54M	5.5×10^{-9}
flickr	4	$320K \times 28M \times 2M \times 731$	113M	1.1×10^{-14}
deli4d	4	$533K \times 17M \times 2M \times 1K$	140M	4.3×10^{-15}

J. Li, J. Sun, R. Vuduc. “HiCOO: Hierarchical Storage of Sparse Tensors”. 2018

Multicore MTTKRP

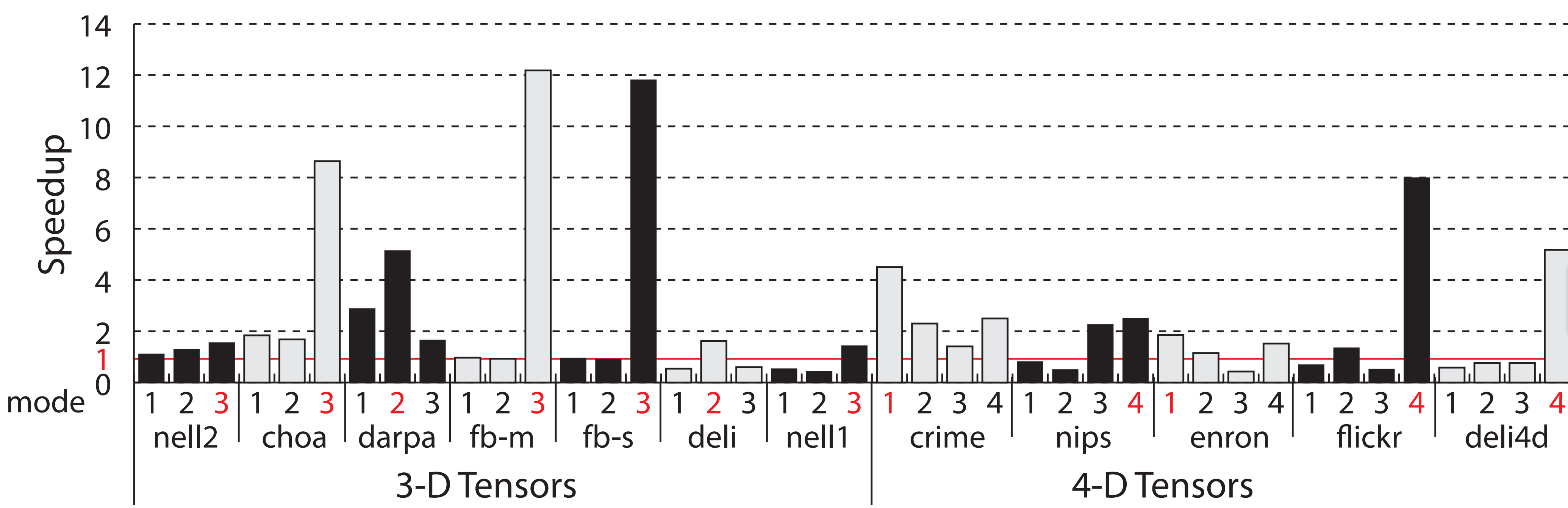
- ParTI! library: Speedups of HiCOO over COO



0.8x

- SPLATT library: Speedups of HiCOO over CSF

Storage size:

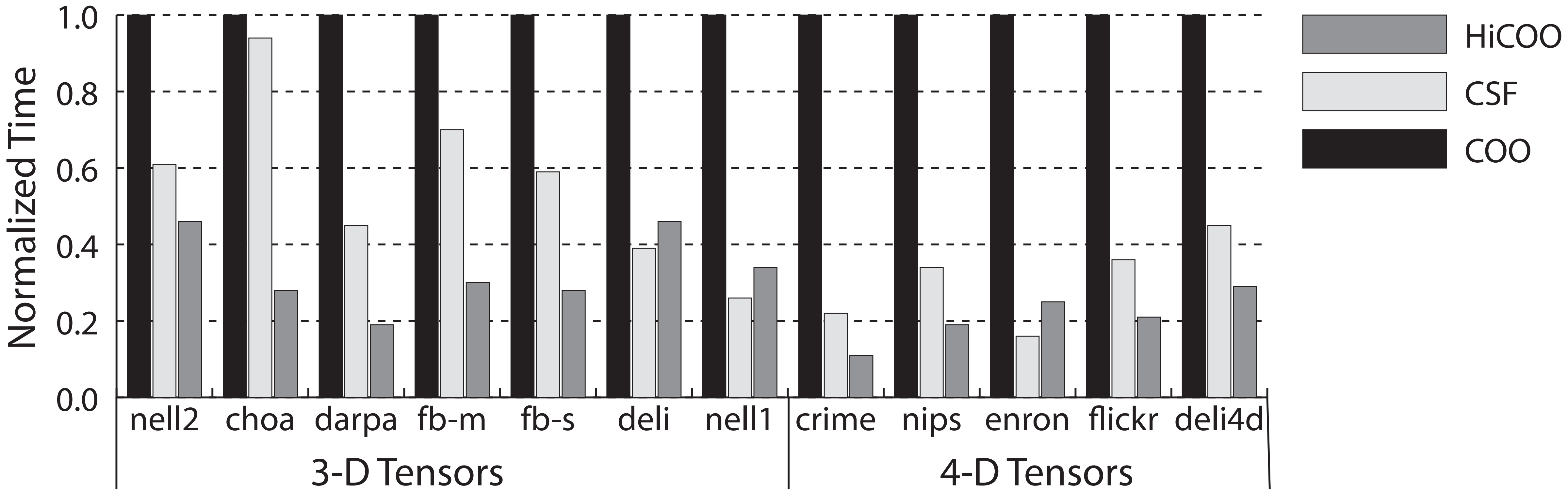


0.3x

comparable

Multicore CP-ALS

- HiCOO outperforms COO by up to 9.4× and CSF up to 3.4×.



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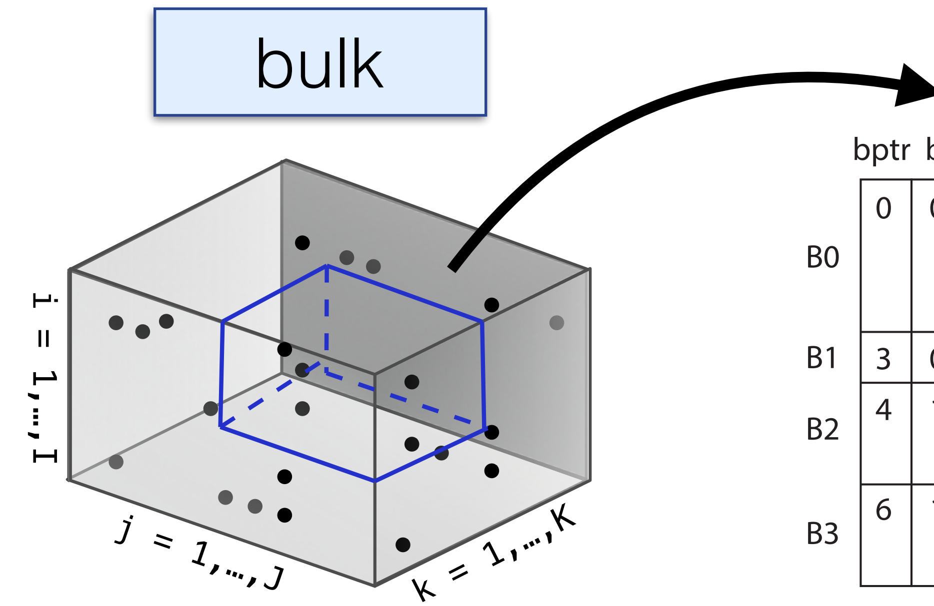
Data Distribution



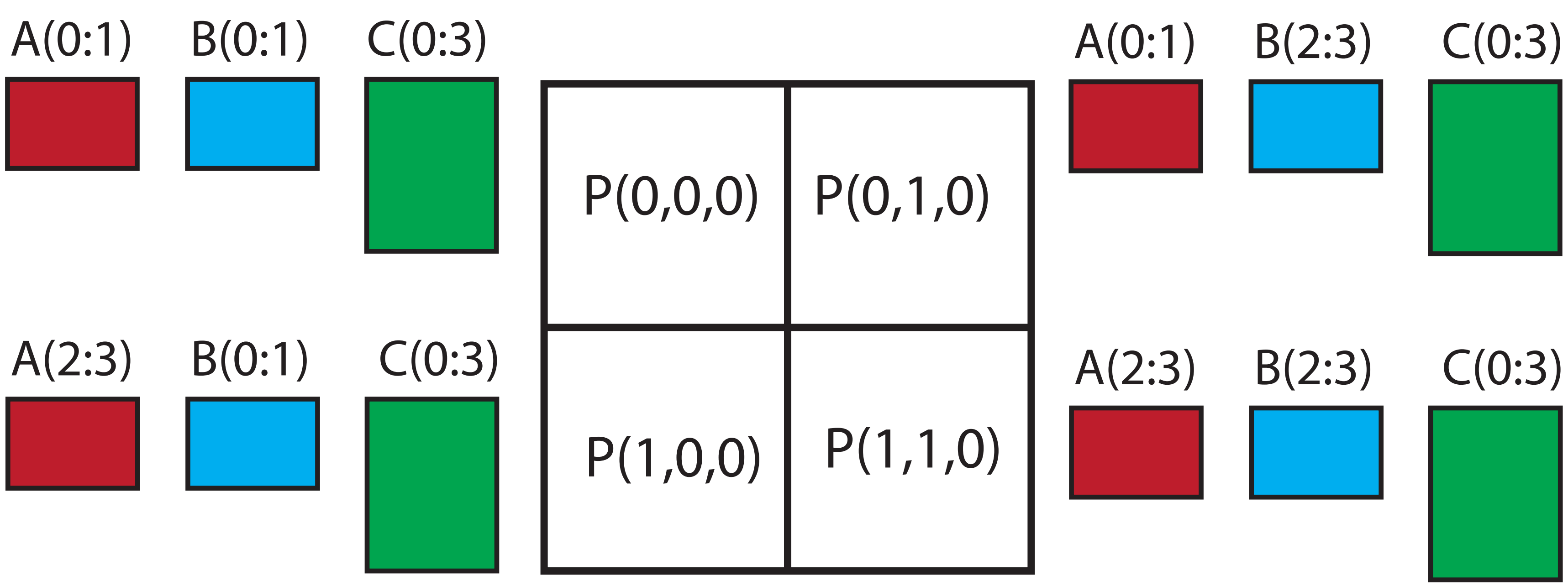
	bptr	bi	bj	bk	ei	ej	ek	val
B0	0	0	0	0	0	0	0	1
					0	1	0	2
					1	0	0	3
B1	3	0	0	1	1	0	0	4
B2	4	1	0	0	0	1	0	5
					1	0	1	7
B3	6	1	1	1	0	0	0	6
					1	1	0	8

HiCOO

- Tensor:
  - Two-level blocking
  - Bulk level: node partitioning to ensure nonzero balance
  - Block level: ensure fast local computation
- Factor matrices
  - Each processor owns the portion of factor matrices its local tensor needs.
  - Some duplication exists.

Data Distribution Cont.

- X: 4*4*4 sparse tensor
- Processors are split to 2*2*2 grids.
- Use sub-communicator to update factor matrices.



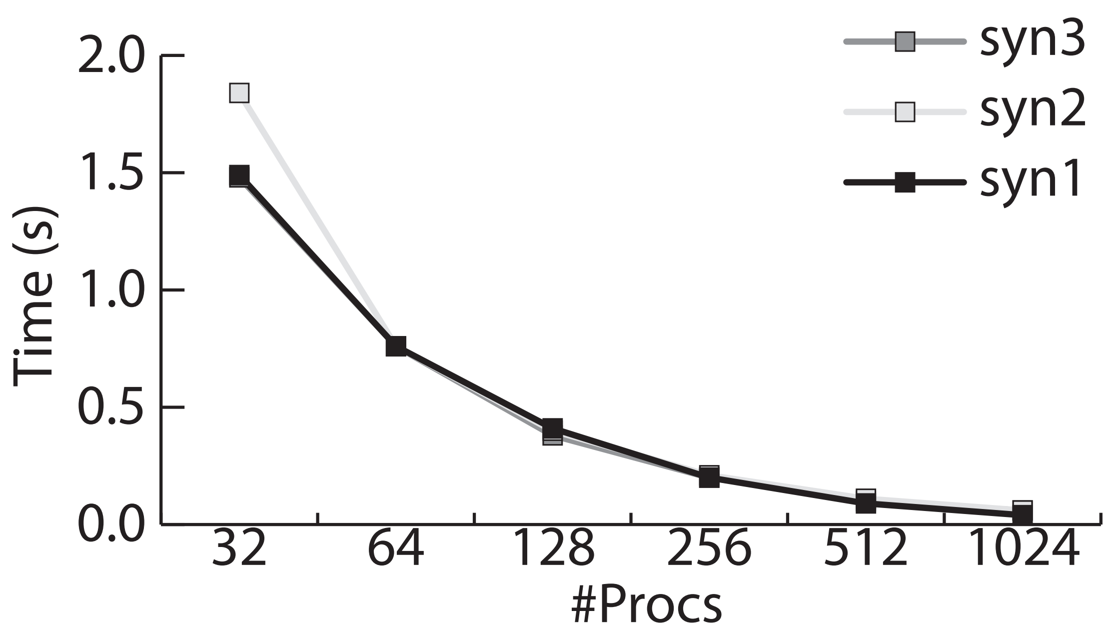
Platform and Dataset

- **Platform**: Cori supercomputer in NERSC, which is Cray XC40. Each node is Intel Xeon CPU E5-2698 v3 ("Haswell") consisting 32 physical cores. We use Intel MPI 2018 version.
  - We test 32 to 1024 processors with 32 processors per node.
- **Dataset**: Synthetic tensors from Poisson distribution.

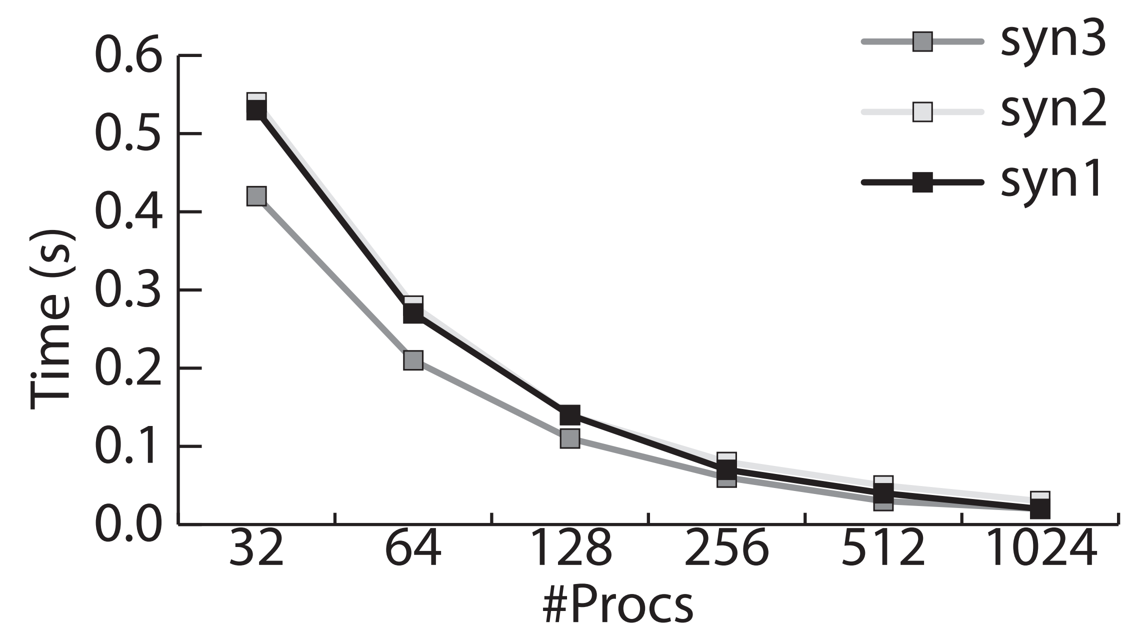
Tensors	Order	Dimensions	#Nonzeros	Density
syn1	3	$10K \times 10K \times 10K$	100M	1.0×10^{-4}
syn2	3	$50K \times 50K \times 50K$	125M	1.0×10^{-6}
syn3	3	$40K \times 40K \times 40K$	128M	2.0×10^{-6}

Distributed MTTKRP Performance

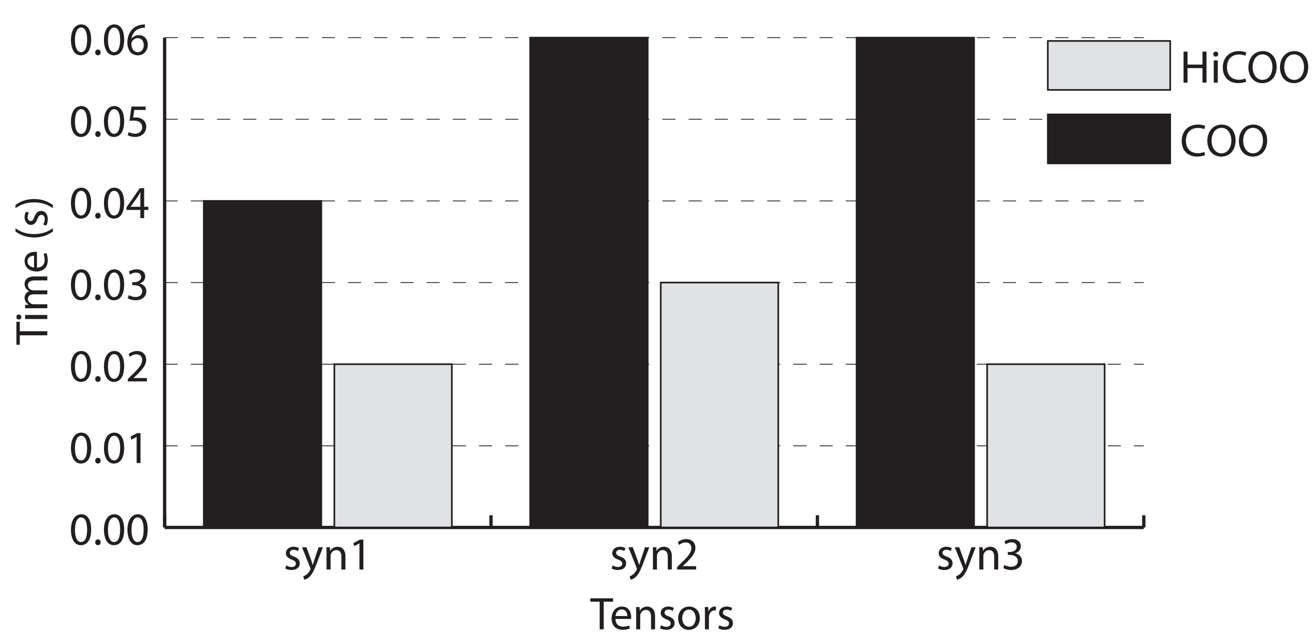
COO



HiCOO

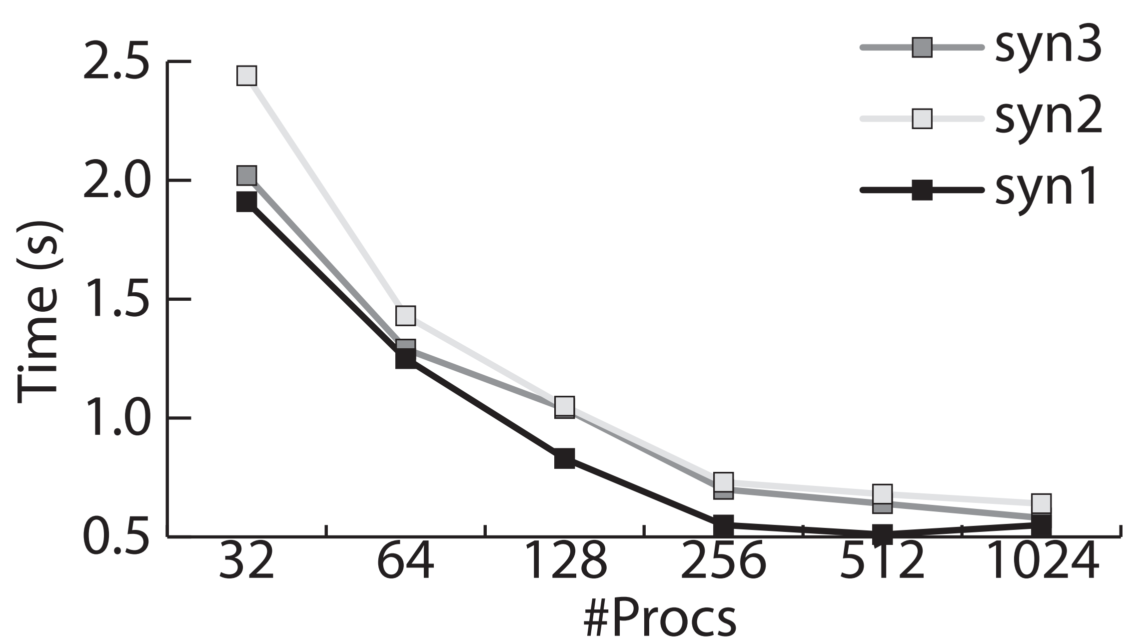


MTTKRP time using 1024 procs



Distributed CP-ALS Performance

COO



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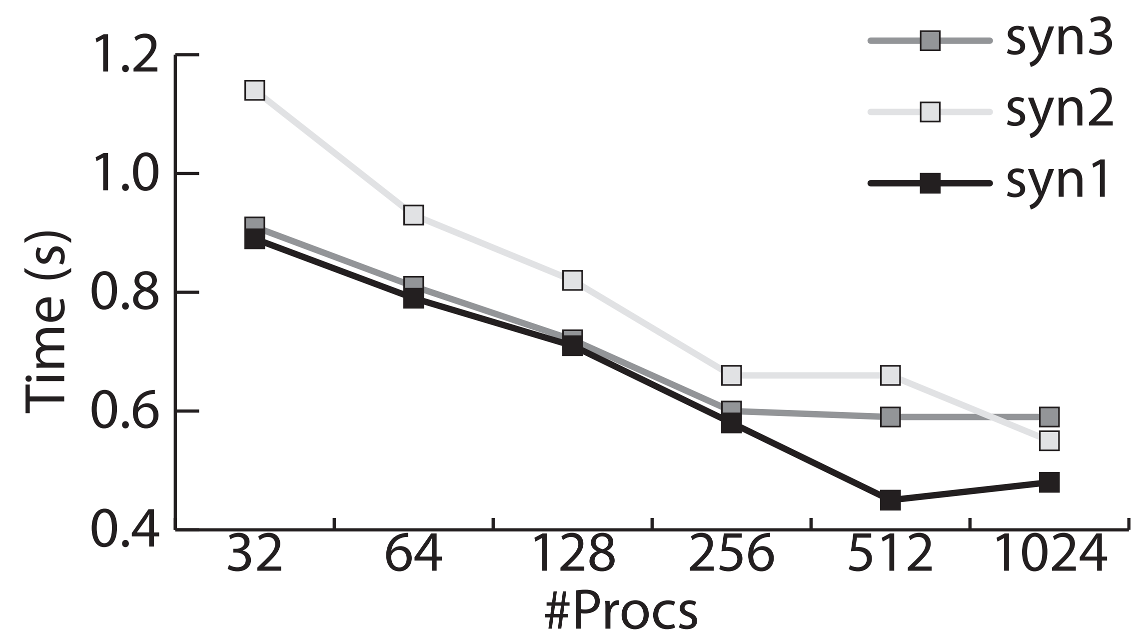
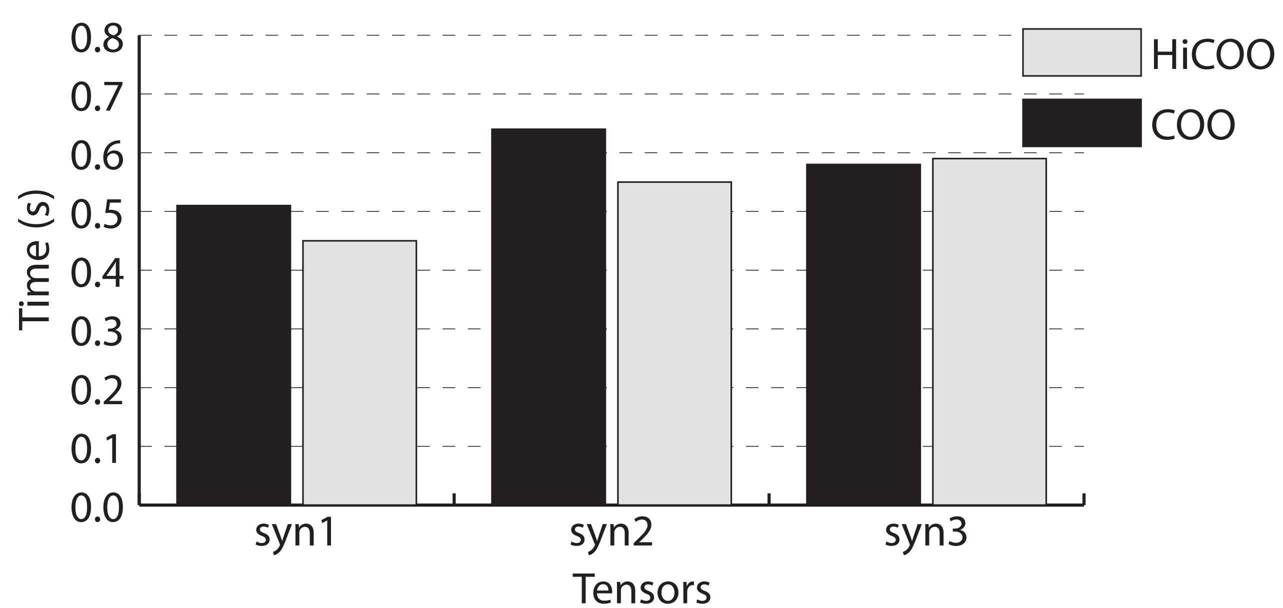
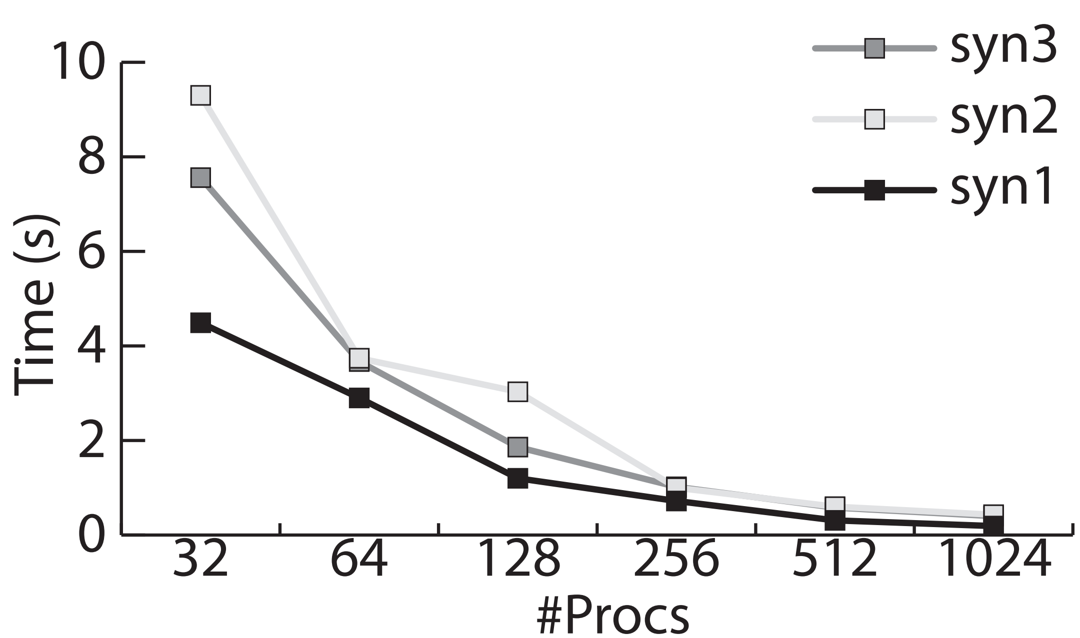


CP-ALS time using 1024 procs

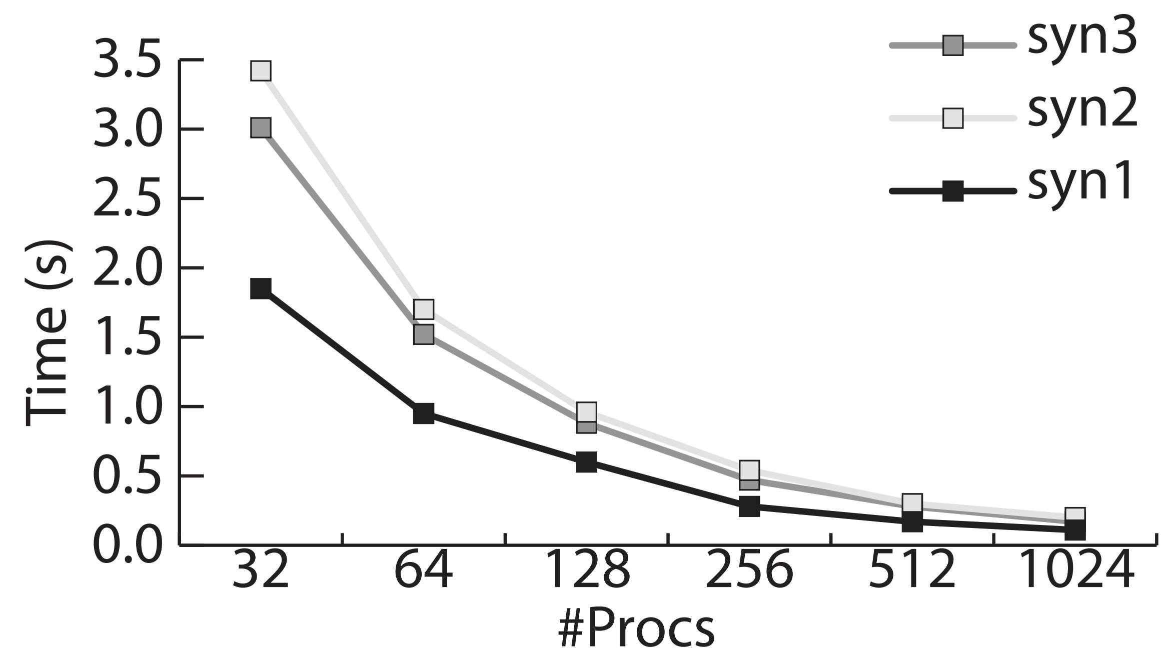


Distributed CompPhi Performance

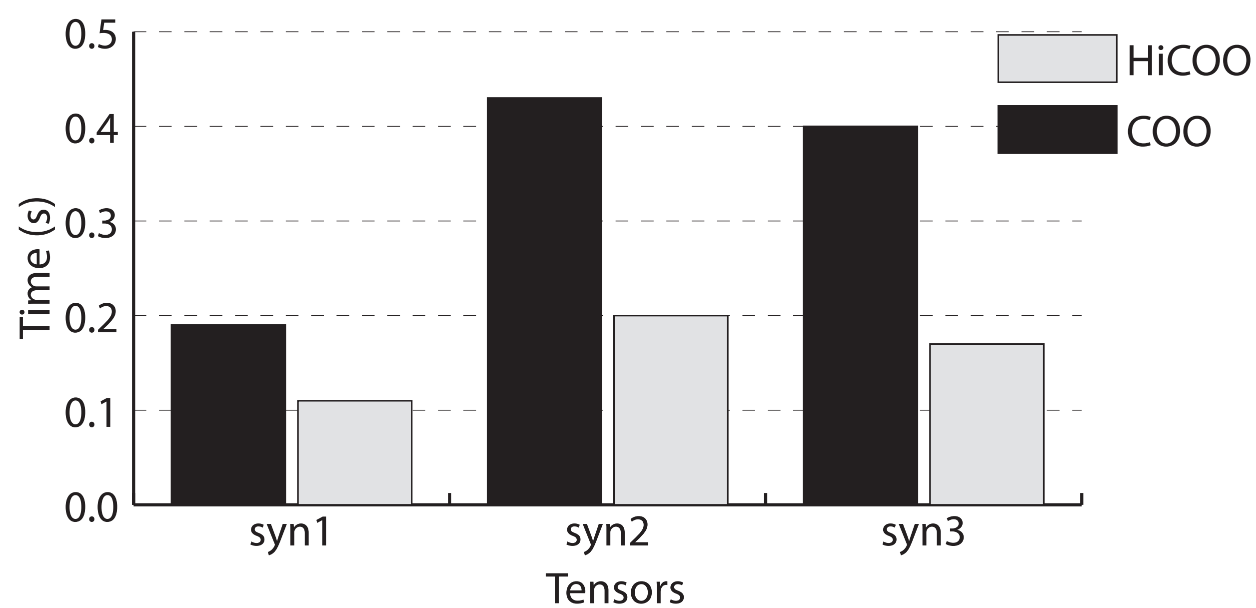
COO



HiCOO

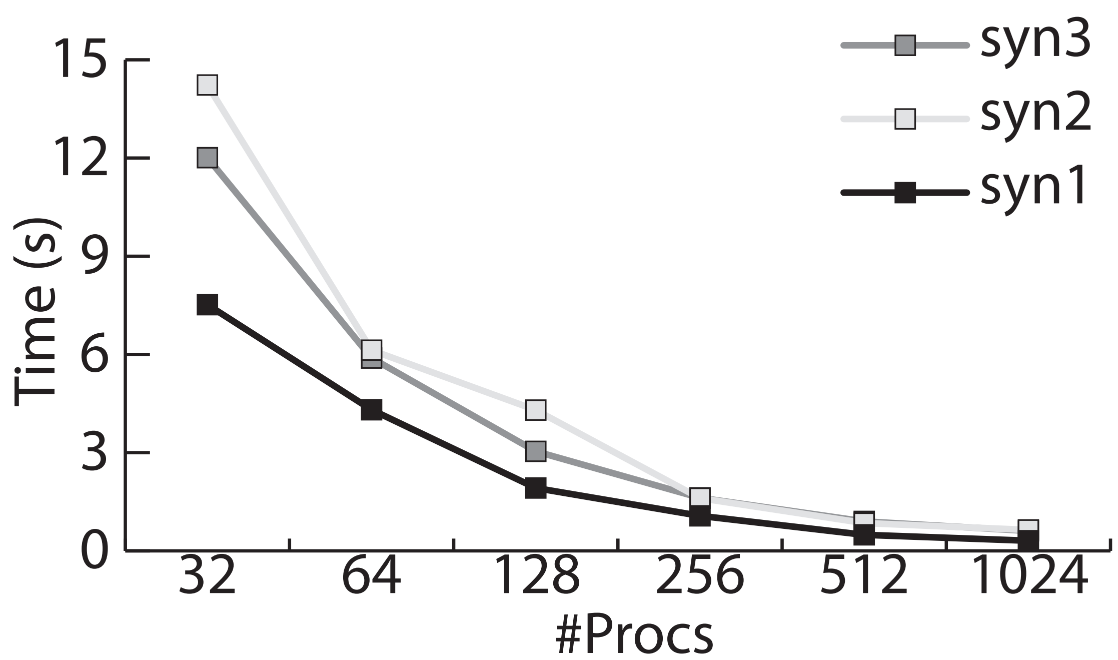


CompPhi time using 1024 procs

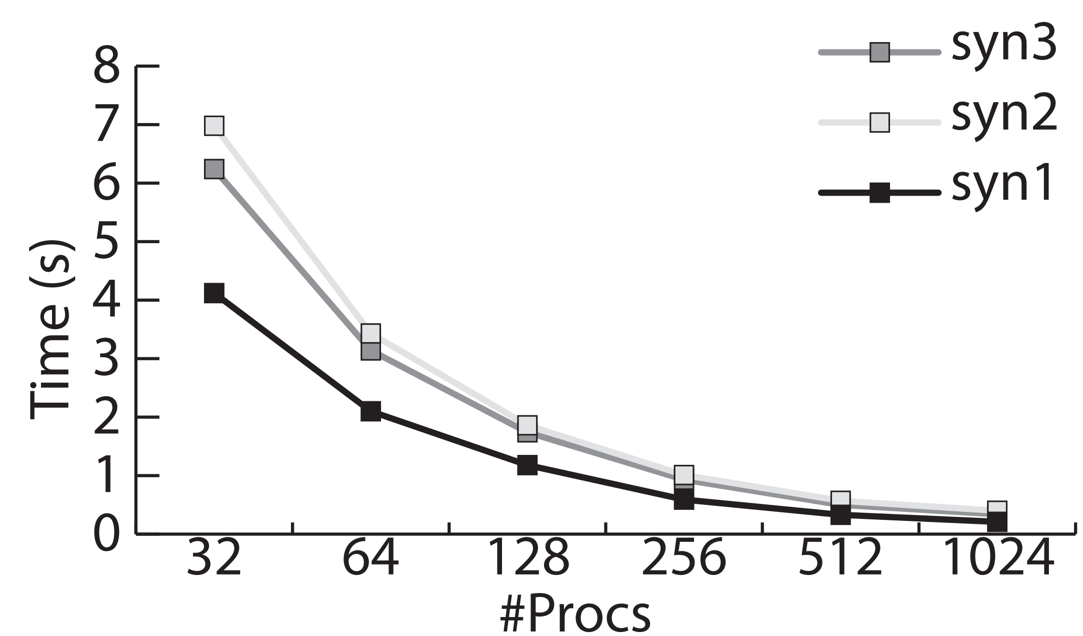


Distributed CP-APR Performance

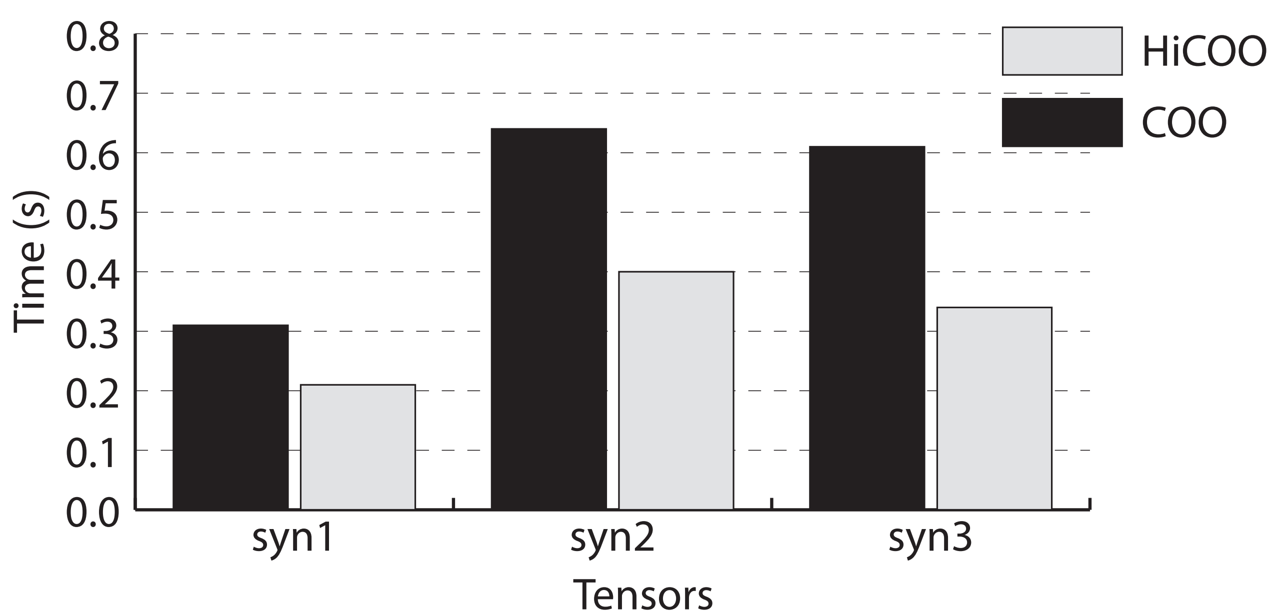
COO



HiCOO



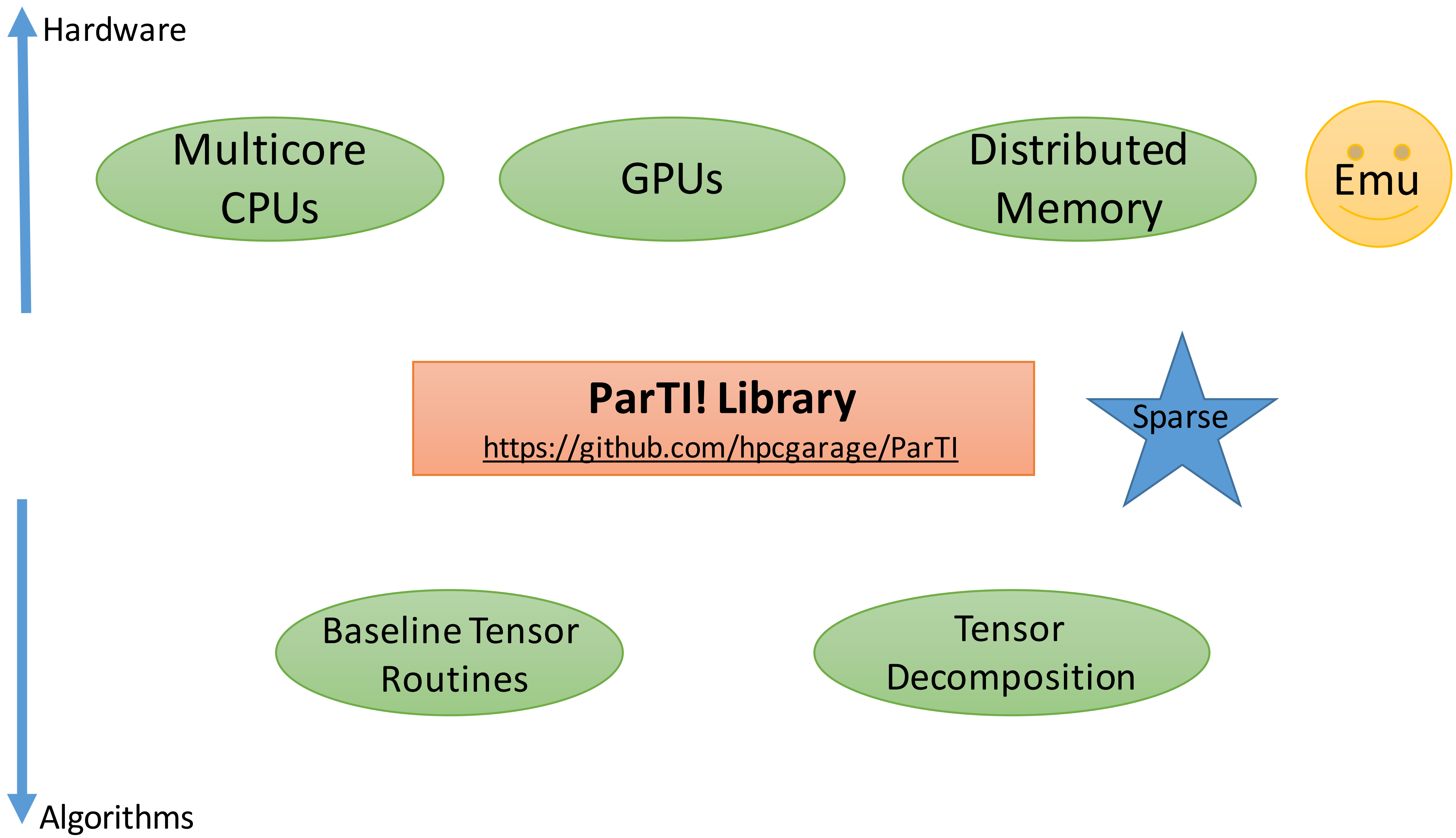
CP-APR time using 1024 procs



Conclusion and Future Work

- Conclusion
  - **HiCOO WORKS!**
- Future work
  - Combine multicore and distributed parallelism together to build hybrid MPI+OpenMP HiCOO CPDs.
  - Also include our GPU implementations.
  - Consider CP-APR algorithms to Newton-based optimization methods.

ParTI! Project



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Emu TECHNOLOGY

Related Work

- S. Smith et al. “A Medium-Grained Algorithm for Distributed Sparse Tensor Factorization”, IPDPS’16
- O. Kaya et al. “Scalable Sparse Tensor Decompositions in Distributed Memory Systems”, SC’15
- E. Solomonik et al. “Sparse Tensor Algebra as a Parallel Programming Model”, TR, 2015
- S. Rajbhandari et al. “A communication-optimal framework for contracting distributed tensors”, SC'14
- W. Austin et al. “Parallel Tensor Compression for Large-Scale Scientific Data”, IPDPS’16
- J. Choi et al. “DFacTo: Distributed Factorization of Tensors”, NIPS’14