An Exploration of Optimization Algorithms for High Performance Tensor Completion

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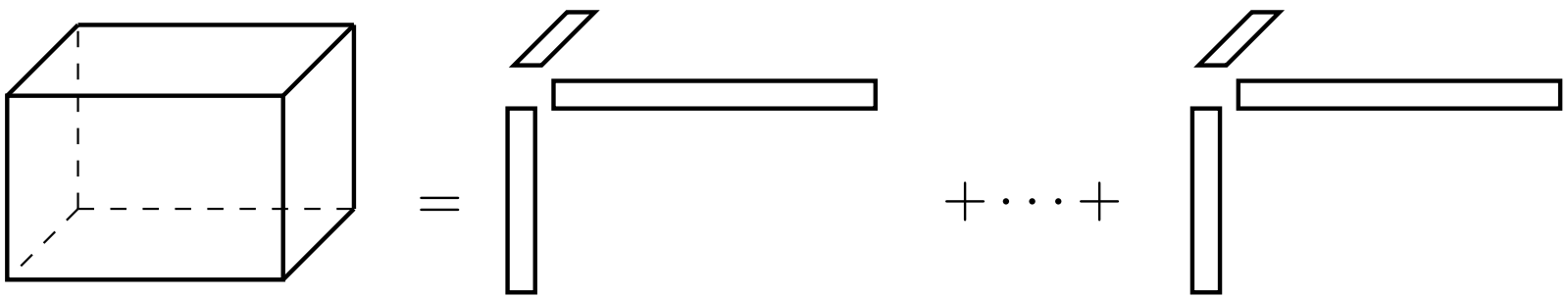
Tensor Introduction

CPD (or: CANDECOMP/PARAFAC)

- Given: tensor $\mathcal{R}^{I \times J \times K}$ and desired rank F
- Compute: low-rank matrices $\mathbf{A}^{I \times F}, \mathbf{B}^{J \times F}, \mathbf{C}^{K \times F}$
- Element-wise: $\mathcal{R}(i,j,k) \approx \sum_{f=1}^{F} \mathbf{A}(i,f)\mathbf{B}(j,f)\mathbf{C}(k,f)$



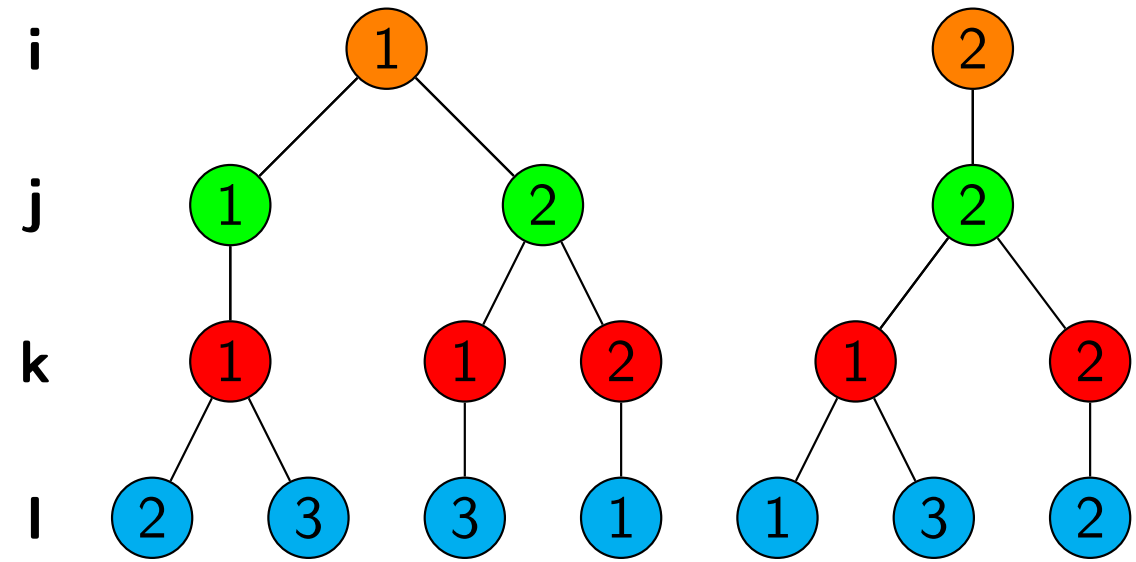
Tensor Storage - Compressed Sparse Fiber (CSF)

(Smith & Karypis '15)

- Values are stored in the leaves (not shown).
- Modes are recursively compressed.
  - Compression naturally exposes opportunities for operation savings.

i	j	k	l
1	1	1	2
1	1	1	3
1	2	1	3
1	2	2	1
2	2	1	1
2	2	1	3
2	2	2	2

→



Tensor Completion: Optimization

Objective

- We only want to model *observed* entries (non-zeros).
  - A least-squares objective would predict zeros!
- The objective is a combination of the predicition ability (the *loss*) and regularization terms (to prevent overfitting).
  - Regularization is controlled by λ, a user-specified parameter.

$$\underset{\mathbf{A},\mathbf{B},\mathbf{C}}{\text{minimize}} \quad \underbrace{\mathcal{L}(\mathcal{R},\mathbf{A},\mathbf{B},\mathbf{C})}_{\text{Loss}} + \underbrace{\lambda\left(||\mathbf{A}||_F^2 + ||\mathbf{B}||_F^2 + ||\mathbf{C}||_F^2\right)}_{\text{Regularization}}$$

$$\mathcal{L}(\mathcal{R},\mathbf{A},\mathbf{B},\mathbf{C}) = \frac{1}{2}\sum_{\text{nnz}(\mathcal{R})}\left(\mathcal{R}(i,j,k) - \sum_{f=1}^{F}\mathbf{A}(i,f)\mathbf{B}(j,f)\mathbf{C}(k,f)\right)^2$$

Challenges

Optimization Algorithms

- Optimization algorithms for *matrix* completion are relatively mature
  - How do they adapt to tensors?
- We must consider multiple properties when comparing algorithms:
  1. Number of operations
  2. Convergence rate
  3. Computational intensity
  4. Parallelism

Tensor Properties

- Most matrix optimization algorithms parallelize over the many rows and columns (e.g., users and items).
- Many domains have a mix of short and long modes.
  - Context-aware recommender systems will have orders of magnitude fewer contexts than users or items.

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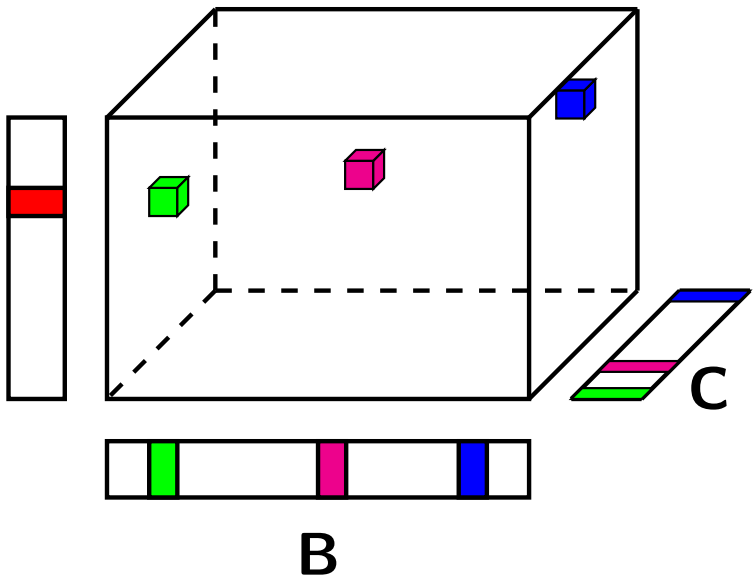
Alternating Least Squares (ALS)

Problem Formation

- Hold $\mathbf{B}$ and $\mathbf{C}$ constant, solving for $\mathbf{A}$ convex.
- Each row of $\mathbf{A}$ is a linear least squares problem.
- $\mathbf{H}_i$ is an $|\mathcal{R}(i,:,:)| \times F$ matrix:
  - $\mathcal{R}(i,j,k) \rightarrow \mathbf{B}(j,:) * \mathbf{C}(k,:)$. (element-wise multiplication)
- $\mathbf{A}(i,:) \leftarrow \left(\mathbf{H}_i^T \mathbf{H}_i + \lambda \mathbf{I}\right)^{-1} \mathbf{H}_i^T \text{vec}(\mathcal{R}(i,:,:))$
- $\mathcal{O}(F^2)$ work per non-zero.



Alternating Least Squares (ALS)

Shao '12, Karlsson '15

- Normal equations $\mathbf{N}_i = \mathbf{H}_i^T \mathbf{H}_i$ are formed one non-zero at a time.
- $\mathbf{H}_i^T \text{vec}(\mathcal{R}(i,:,:))$ is similarly accumulated into a vector q_i.

Algorithm 1 ALS: updating $\mathbf{A}(i,:)$

1: $\mathbf{N}_i \leftarrow \mathbf{0}^{F \times F}$
2: $q_i \leftarrow \mathbf{0}^{F \times 1}$
3: **for** $(i,j,k) \in \mathcal{R}(i,:,:)$ **do**
4: $\quad x \leftarrow \mathbf{B}(j,:) * \mathbf{C}(k,:)$
5: $\quad \mathbf{N}_i \leftarrow \mathbf{N}_i + x^T x$
6: $\quad q_i \leftarrow q_i + \mathcal{R}(i,j,k) x^T$
7: **end for**
8: $\mathbf{A}(i,:) \leftarrow (\mathbf{N}_i + \lambda \mathbf{I})^{-1} q_i$

ALS - Parallelism

Shared-Memory (Shao '12)

- Least squares problems are solved in batches of size $B = \mathcal{O}(100)$.
- Each core independently accumulates the B sets of $\mathbf{N}_i$ and q_i.
- Corresponding $\mathbf{N}_i$ and q_i are aggregated.
- Finally, the B inversions and updates are performed in parallel.

Distributed-Memory (Karlsson '15)

- Non-zeros can be distributed in any fashion.
- All $\mathbf{N}_i$ and q_i aggregated (`MPI_Allreduce`).
  - $\mathcal{O}(IF^2)$ data communicated per process.
- Processes evenly divide the inversions and then exchange updates (`MPI_Allgather`).

Contributions - Shared Memory

Tensor Representations

- Storing multiple representations of $\mathcal{R}$ allows us to parallelize over rows of $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$.
  - No parallel reductions or synchronization required.
  - Each core only requires $\mathcal{O}(F^2)$ intermediate storage.
- If mode is short, use method of (Shao '12) with a single batch of size equal to the dimension of that mode.

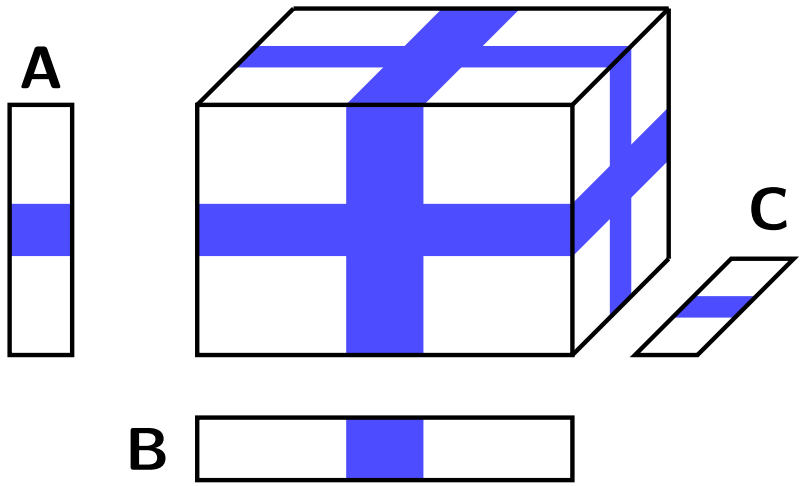
BLAS-3 Formulation

- Element-wise computation is an outer product formulation.
  - F^2 work with F^2 data per non-zero.
- Instead, we store $(\mathbf{B}(j,:) * \mathbf{C}(k,:))$ into rows of a thread-local buffer $\mathbf{Z}$.
  - When $\mathbf{Z}$ is full, do a rank-k update: $\mathbf{N}_i \leftarrow \mathbf{N}_i + \mathbf{Z}^T\mathbf{Z}$.

Contributions - Distributed Memory

Coarse-Grained Decomposition (following Shin & Kang '14)

- Avoid communicating normal equations by using separate 1D decompositions of **A**, **B**, and **C**.
- Each process owns all necessary non-zeros and only needs to exchange the updated factor rows.
- If mode is short, use method of (Karlsson '15) with `MPI_Allreduce`.



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Stochastic Gradient Descent (SGD)

Problem Formulation

- Randomly select entry $\mathcal{R}(i,j,k)$ and update rows of $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$.
  - $\mathcal{O}(F)$ work per non-zero.
- η is the step size; typically $\mathcal{O}(10^{-3})$.

$$\delta \leftarrow \mathcal{R}(i,j,k) - \sum_{f=1}^{F} \mathbf{A}(i,f)\mathbf{B}(j,f)\mathbf{C}(k,f)$$

$$\mathbf{A}(i,:) \leftarrow \mathbf{A}(i,:) + \eta\left[\delta\left(\mathbf{B}(j,:) * \mathbf{C}(k,:)\right) - \lambda\mathbf{A}(i,:)\right],$$

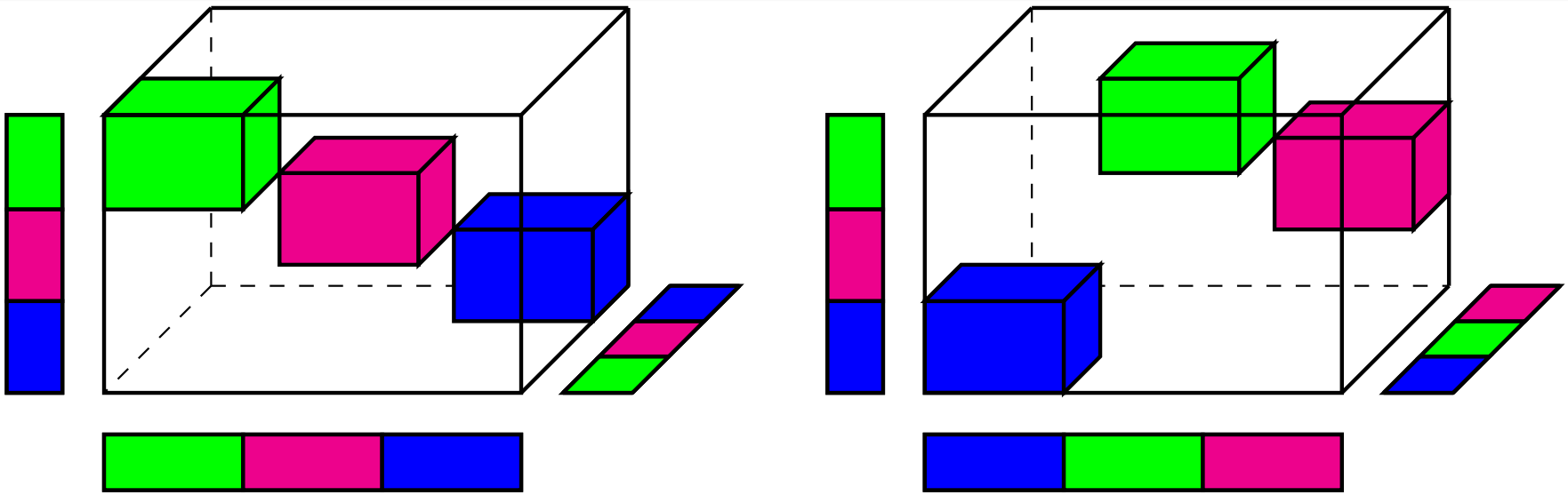
$$\mathbf{B}(j,:) \leftarrow \mathbf{B}(j,:) + \eta\left[\delta\left(\mathbf{A}(i,:) * \mathbf{C}(k,:)\right) - \lambda\mathbf{B}(j,:)\right],$$

$$\mathbf{C}(k,:) \leftarrow \mathbf{C}(k,:) + \eta\left[\delta\left(\mathbf{A}(i,:) * \mathbf{B}(j,:)\right) - \lambda\mathbf{C}(k,:)\right].$$

SGD - Stratification

Beutel '14

- *Strata* identify independent blocks of non-zeros.
- Each stratum is processed in parallel.



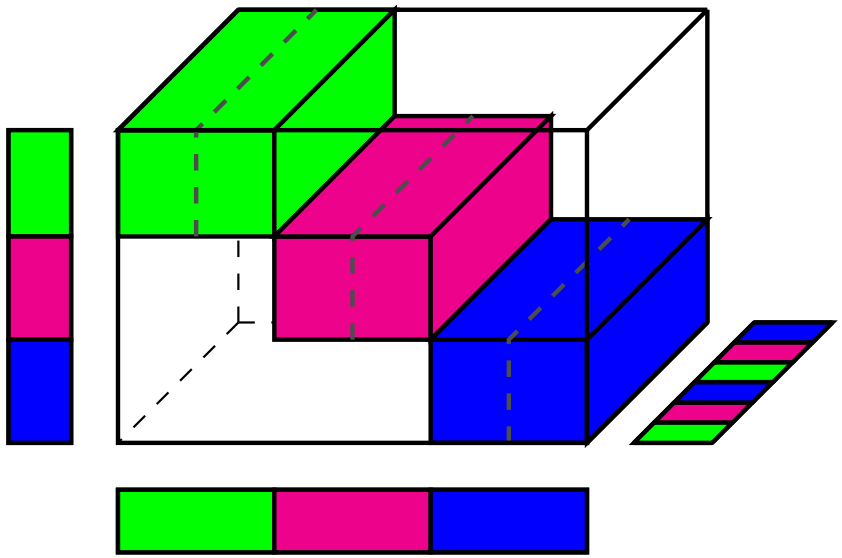
Limitation of Stratification

- There is only as much parallelism as the smallest dimension.
- Sparsely populated strata are communication bound.

Contributions - SGD

Problem Relaxation: Cheat!

- Shared-memory: go Hogwild! and allow race conditions.
- Distributed-memory: limit the number of strata to reduce communication and handle short modes.
- Assign multiple processes to the same stratum (called a *team*).
- Each performs updates on its own versions of the factors.
- At the end, the updates are exchanged among the team.



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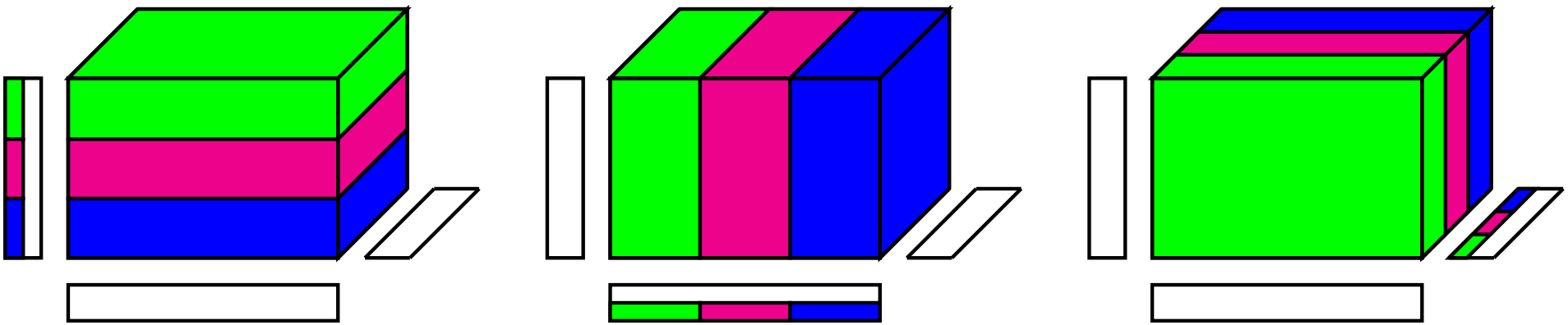
Coordinate Descent (CCD++)

- Rank-1 factors are updated in sequence.
- $\mathcal{O}(F)$ work per non-zero (same as SGD).



CCD++ - Parallelism

Distributed-Memory (Karlsson '15, Shin '15)

- Each entry of $\mathbf{A}(:, f)$ is computed in parallel.
  - Distributing non-zeros requires α_i and β_i to be aggregated.
  - Communication volume is $\mathcal{O}(IF)$ per process.
- All δ_{ijk} can be maintained in a residual tensor.
  - All updates are totally parallel - no communication needed.

$$\delta_{ijk} \leftarrow \boldsymbol{\mathcal{R}}(i,j,k) - \sum_{f=1}^{F} \mathbf{A}(i,f)\mathbf{B}(j,f)\mathbf{C}(k,f)$$

$$\alpha_i \leftarrow \sum_{\boldsymbol{\mathcal{R}}(i,:,:)} \delta_{ijk} \left(\mathbf{B}(j,f)\mathbf{C}(k,f)\right)$$

$$\beta_i \leftarrow \sum_{\boldsymbol{\mathcal{R}}(i,:,:)} \left(\mathbf{B}(j,f)\mathbf{C}(k,f)\right)^2$$

$$\mathbf{A}(i,f) \leftarrow \frac{\alpha_i}{\lambda + \beta_i}$$

Contributions - Shared Memory

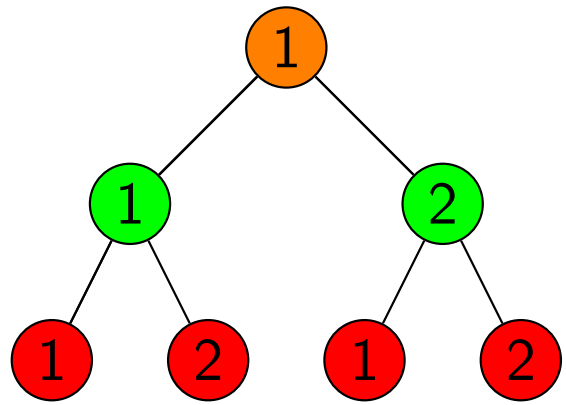
CSF Formulation

- Column-wise methods require F passes over the sparse tensor.
  - CCD++ requires a high memory bandwidth.
- CSF shrinks the memory footprint of the tensor and structures memory accesses.
  - Fewer operations and a reduced memory bandwidth.
- One example is during residual computation:

$$\mathbf{v} \leftarrow \mathbf{A}(i,:) * \mathbf{B}(j,:),$$

$$\delta_{ijk} \leftarrow \boldsymbol{\mathcal{R}}(i,j,k) - \sum_{f=1}^{F} \mathbf{v}(f)\mathbf{C}(k,f),$$

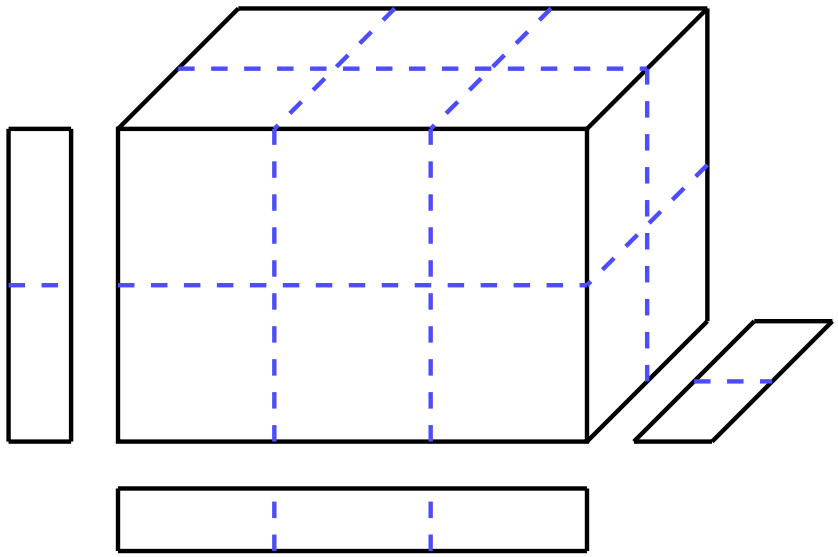
$$\delta_{ijk'} \leftarrow \boldsymbol{\mathcal{R}}(i,j,k') - \sum_{f=1}^{F} \mathbf{v}(f)\mathbf{C}(k',f).$$



Contributions - Distributed Memory

Medium-Grained Decomposition (Smith & Karypis '16)

- Distributing non-zeros over a grid limits communication to the grid layer.
- For short modes, we use a grid dimension of one and fully replicate the factor.
  - Non-zeros are still distributed and processed in parallel.



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Experimental Setup

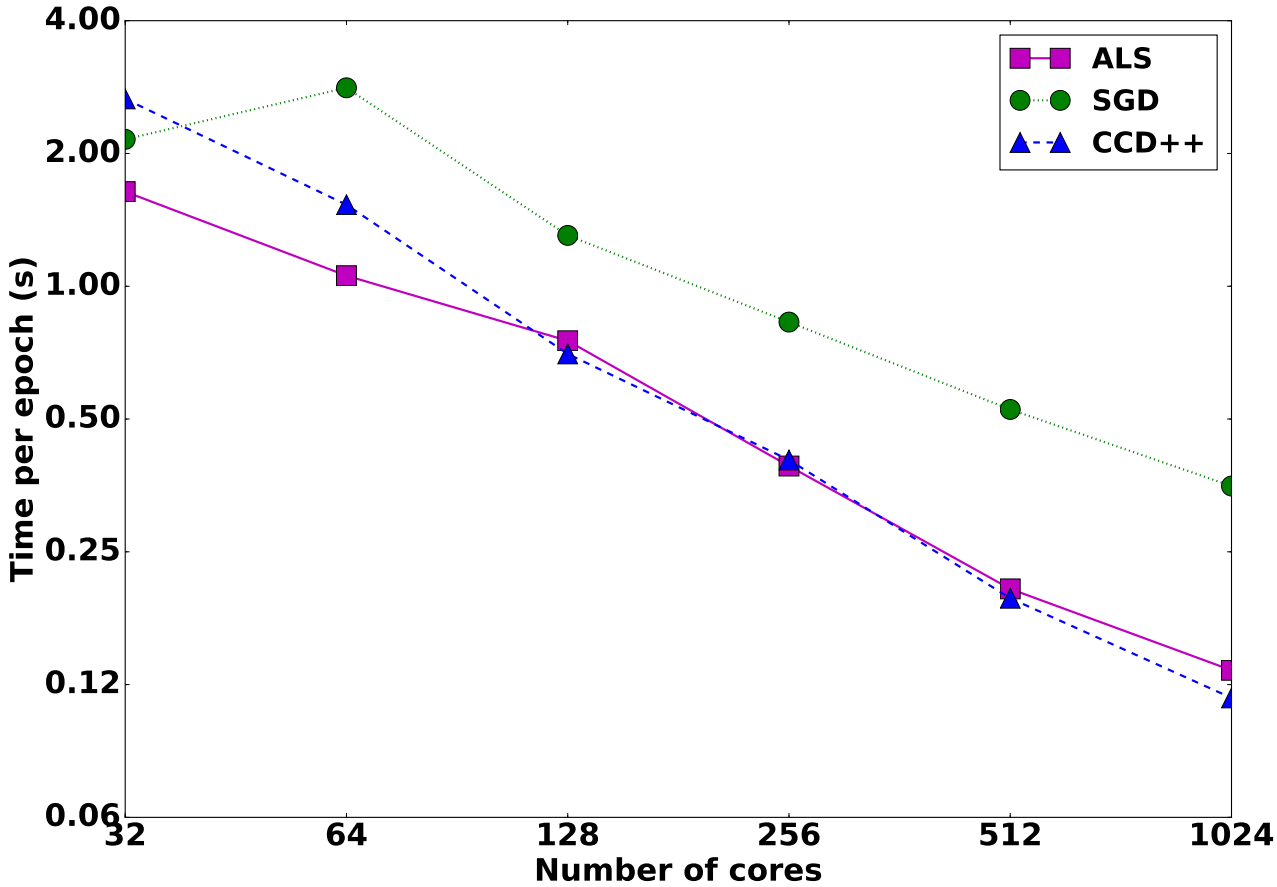
Tensor Dataset

- We use Yahoo! Music ratings from the 2011 KDD Cup.
- 1M users $\times$ 625K songs $\times$ 133 months with 210M ratings.
- More datasets in paper (SC'16)

Computing Environment

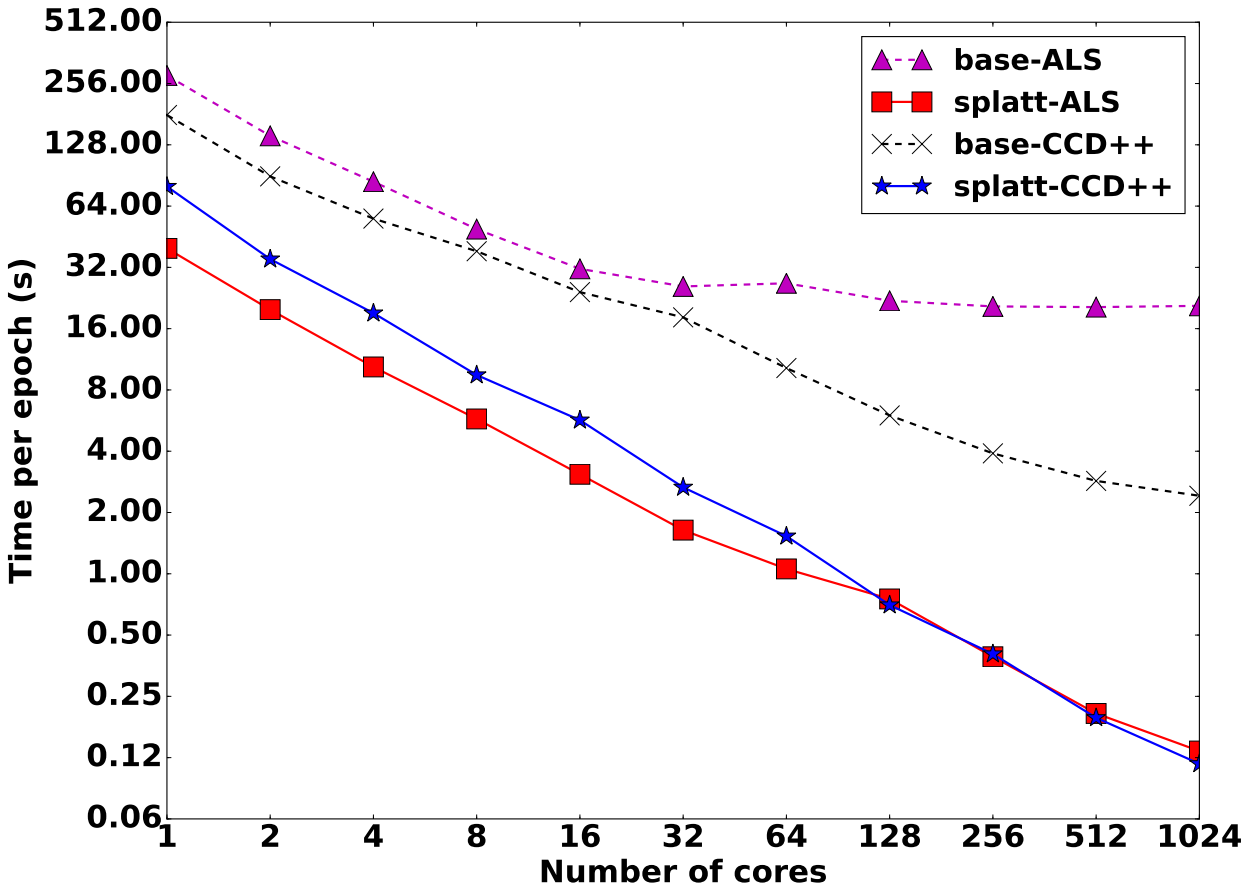
- All experiments performed on the Cori supercomputer at NERSC.
- Nodes have two sixteen-core Intel processors (Haswell).
- Implemented as part of open source library SPLATT.
  - Written in C with hybrid MPI+OpenMP parallelism.

Strong Scaling - Rank 10



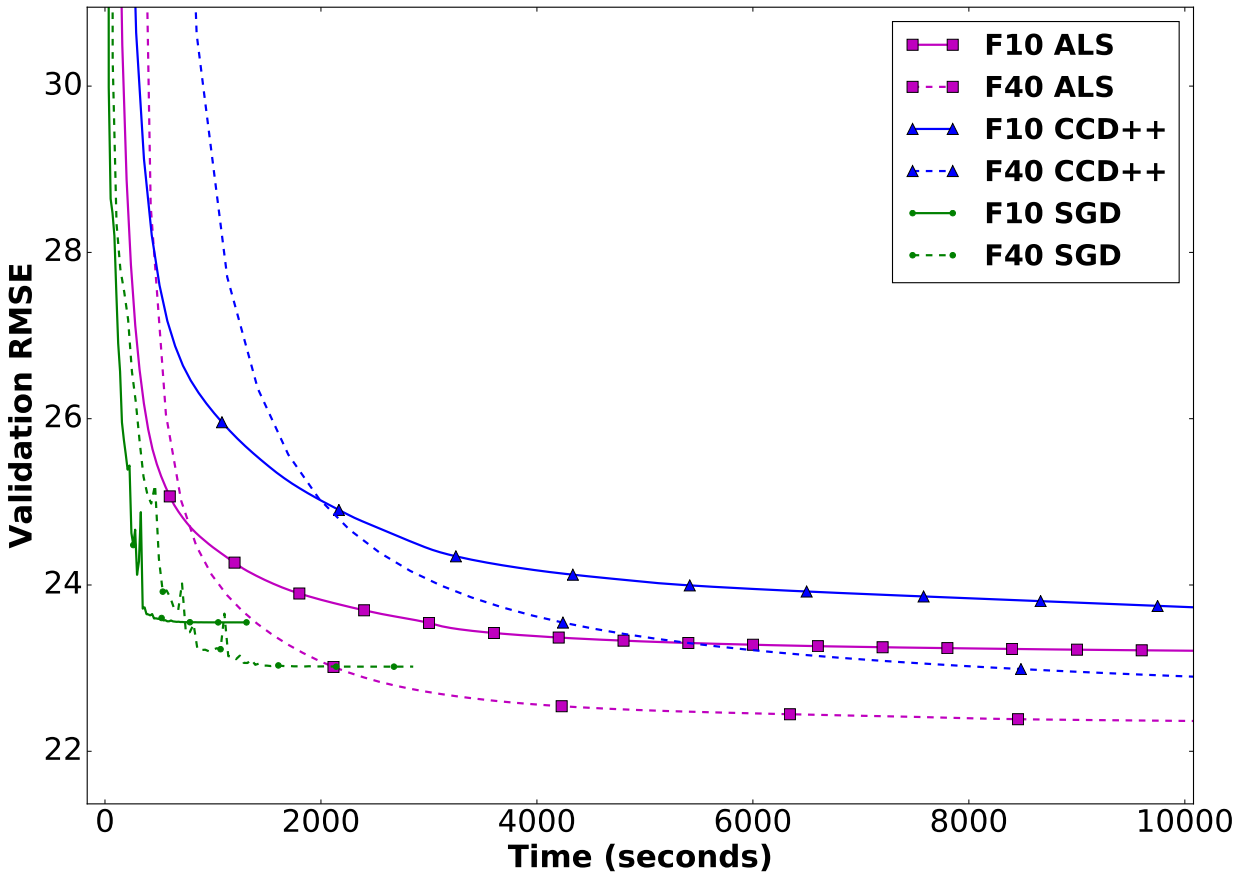
Benchmarking - Rank 10

- base-ALS and base-CCD++ from Karlsson '15 (C++ and MPI).



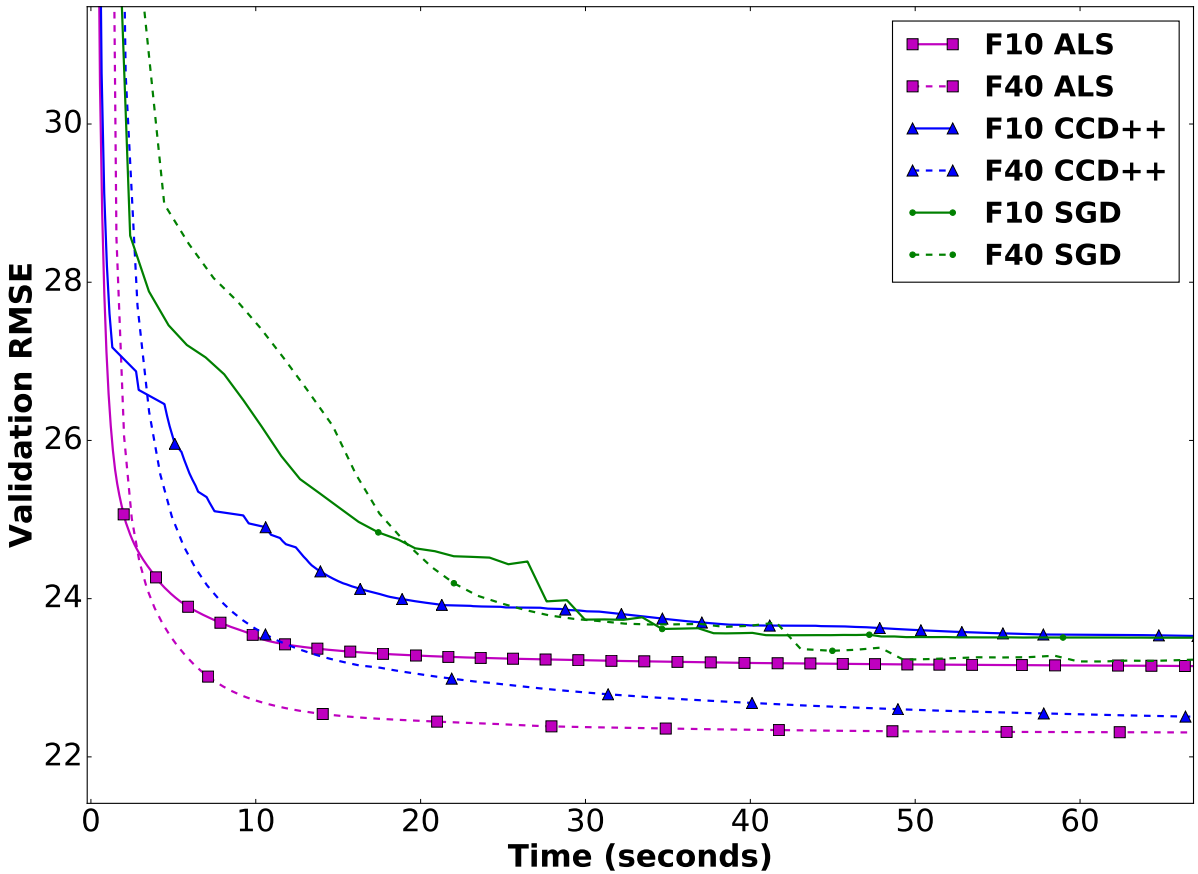
Convergence @ 1 core

- Convergence is detected if the RMSE was not improved after 20 epochs.



Convergence @ 1024 cores

- Convergence is detected if the RMSE was not improved after 20 epochs.



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Conclusions

Optimization Algorithms

- We scale ALS, SGD, and CCD++ to (past?) 1024 cores.
- SGD is best for small-scale systems.
- ALS is more expensive but shows fastest convergence at scale.
- CCD++ strong scales best.
  - Maybe overtake ALS convergence at larger scale?

Release

- Paper to appear in SC'16
- Pre-print and source code to come next month:
  - `http://cs.umn.edu/~splatt/`