Randomized Short-Recurrence Iterative Methods for Approximate Low-Rank Factorizations

Workshop on
Computational and Mathematical Methods in Data Sciences
Technical University of Chemnitz

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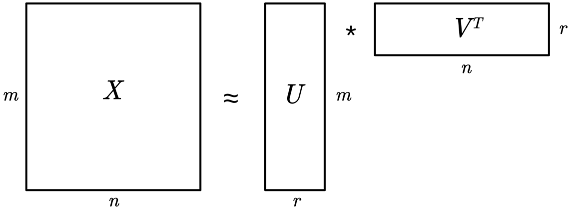
Outline I

Outline II

Introduction

Low-rank matrix approximation — the "What?"

- Given a matrix $X \in \mathbb{R}^{m\times n}$, we seek some factor matrices $U \in \mathbb{R}^{m\times r}$ and $V \in \mathbb{R}^{n\times r}$, with $r \leq \min(m,n)$, s.t. $X - UV^T$ is small in some sense:



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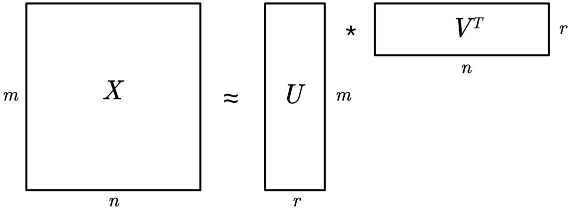

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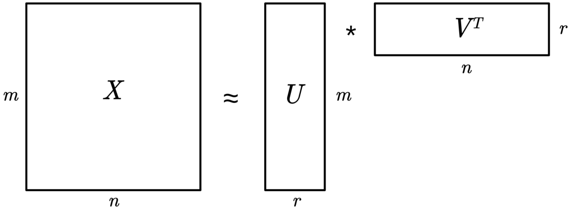

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- In this talk, we aim at minimizing the Frobenius residual norm:

$$\boxed{\text{Find } (U, V) \in \mathbb{R}^{m \times r} \times \mathbb{R}^{n \times r} \text{ s.t. } f(U, V) := \|X - UV^T\|_F^2 \text{ is minimized}}$$

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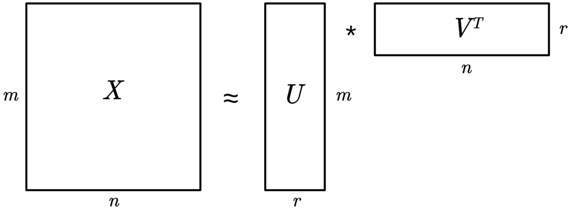

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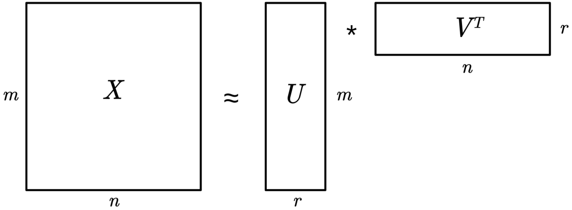

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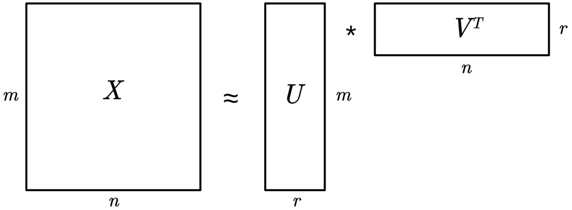

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- f is invariant under orthogonal transformation, i.e., $f(UQ, VQ) = f(U, V)$.
- regularization terms can be added to f to promote sparsity, orthogonality, balanced norms, or else, in the factors; making the problem convex, ...

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- Applications in multiple fields:
  - Pre-training of LLMs, recommendation systems, regularization of DNNs, pattern (e.g., face or signal) recognition, preconditioning of challenging numerical problems, approximating dynamical systems, ...

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- In those cases, gradient descent algorithms and other first-order iterative methods are often the best alternative.
- In this work, we propose enhanced gradient descent algorithms for the computation of approximate low-rank matrix factorizations.

Gradient descent algorithms

- Gradient descent algorithms are defined upon setting search directions of a block coordinate descent along the gradients of the objective function:

$$\nabla_U f(U,V) = -2RV \quad \text{and} \quad \nabla_V f(U,V) = -2R^T U \quad \text{where} \quad R := X - UV.$$

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Given a pair of initial approximate low-rank factors $U_0 \in \mathbb{R}^{m\times r}$ and $V_0 \in \mathbb{R}^{n\times r}$, 2-block gradient descent (2BGD) iterates are defined as follows:

Algorithm 2 2BGD(X, U_0, V_0)

$R_0 := X - U_0 V_0^T$
for $t = 0, 1, \dots$ **do**
    $P_t := -R_t V_t$
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    $U_{t+1} := U_t + \eta_t P_t$ $\triangleright$ $\eta_t \in (0, \infty)$ is learning rate
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6: $\quad V_{t+1} := V_t + \eta_t Q_t$
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Properly decreasing learning rates guarantee convergence to stationary points of f, but we want to try and achieve faster convergence.

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Definition (A2BSCD methods)

- Given $X \in \mathbb{R}^{m\times n}$, $U_0 \in \mathbb{R}^{m\times r}$, $V_0 \in \mathbb{R}^{n\times r}$ and $r \leq \min(m,n)$, a sequence of A2BSCD with search directions $P_t \in \mathbb{R}^{m\times r}$ and $Q_t \in \mathbb{R}^{n\times r}$ is defined by:

$$\begin{cases} U_{t+1} \in U_t + \mathrm{span}\{P_t\} \;\text{ s.t. }\; \nabla_U f(U,V_t)|_{U_{t+1}} \propto \tilde{R}_t V_t \perp \mathrm{span}\{P_t\} \\ V_{t+1} \in V_t + \mathrm{span}\{Q_t\} \;\text{ s.t. }\; \nabla_V f(U_{t+1},V)|_{V_{t+1}} \propto R_{t+1}^T U_{t+1} \perp \mathrm{span}\{Q_t\} \end{cases}$$

where $\tilde{R}_t := X - U_{t+1}V_t^T$ and $R_{t+1} := X - U_{t+1}V_{t+1}^T$.
- Proper descent algorithms are s.t. $f(U_{t+1},V_{t+1}) \leq f(U_{t+1},V_t) \leq f(U_t,V_t)$.

Optimality of A2BSCD iterates

- Particular A2BSCD methods are instantiated by the definition of update formulae for the search directions $(P_t, Q_t) \in \mathbb{R}^{m\times r} \times \mathbb{R}^{n\times r}$ for the iterates U_{t+1} and V_{t+1}, respectively, for $t = 0, 1, \ldots$

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Theorem (Optimality of A2BSCD iterates)

Irrespective of the choice of search directions $(P_t, Q_t) \in \mathbb{R}^{m\times r} \times \mathbb{R}^{n\times r}$:

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$$U_{t+1} = \arg \min_{U \in U_t + \textit{span}\{P_t\}} f(U, V_t) \;\; \textit{and} \;\; V_{t+1} = \arg \min_{V \in V_t + \textit{span}\{Q_t\}} f(U_{t+1}, V).$$

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- *all non-trivial A2BSCD methods are proper block descent algorithms, i.e., s.t. $f(U_{t+1}, V_{t+1}) \leq f(U_t, V_t)$, and converge to stationary points of f.*

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Proof.

Based on the theorem of orthogonal projections. $\square$

Alternating 2-block subspace gradient descent

- A natural instance of A2BSCD method is obtained by setting the search directions P_t and Q_t along gradient directions of f:

Definition (A2BSGD method and iterates)

- Given $X \in \mathbb{R}^{m\times n}$, $U_0 \in \mathbb{R}^{m\times r}$, $V_0 \in \mathbb{R}^{n\times r}$ and $r \leq \min(m,n)$, a sequence of alternating 2-block subspace gradient descent (A2BSGD) iterates is defined by setting the search directions of the A2BSCD algorithm to:

$$P_t := R_t V_t \propto \nabla_U f(U, V_t)|_{U_t} \quad \text{and} \quad Q_t := \tilde{R}_t^T U_{t+1} \propto \nabla_V f(U_{t+1}, V)|_{V_t}\,.$$

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- The main iterates of the A2BSGD method are given by:

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for $t = 0, 1, \ldots,$ in which the optimal step sizes $\alpha_t, \gamma_t \in \mathbb{R}$ are:

$$\alpha_t := \frac{\|P_t\|_F^2}{(P_t V_t^T V_t, P_t)_F} \quad \text{and} \quad \gamma_t := \frac{\|Q_t\|_F^2}{(Q_t U_{t+1}^T U_{t+1}, Q_t)_F}.$$

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Theorem (Alternating local optimality)

Given $X \in \mathbb{R}^{m\times n}$, $U_0 \in \mathbb{R}^{m\times r}$, $V_0 \in \mathbb{R}^{n\times r}$, *and* $r \leq \min(m,n)$, *with search directions satisfying Eq.* (1), $P_{-1} := 0_{m\times r}$ *and* $Q_{-1} := 0_{n\times r}$, *we have:*

$$\begin{cases} \displaystyle\min_{U\in U_t+\textit{span}\{P_{t-1},R_tV_t\}} f(U,V_t) \leq \min_{U\in U_t+\textit{span}\{R_tV_t\}} f(U,V_t) \\ \displaystyle\min_{V\in V_t+\textit{span}\{Q_{t-1},\tilde{R}_t^TU_{t+1}\}} f(U_{t+1},V) \leq \min_{V\in V_t+\textit{span}\{\tilde{R}_t^TU_{t+1}\}} f(U_{t+1},V) \end{cases}$$

for $t = 0, 1, \dots$.

Andrew Knyazev (2001). Toward the optimal preconditioned eigensolver: Locally optimal block preconditioned conjugate gradient method. SIAM journal on scientific computing, 23(2):517–541.

Alternating 2-block subspace locally optimal gradient descent

Definition (A2BSLOGD method and iterates)

- Given $X \in \mathbb{R}^{m\times n}$, $U_0 \in \mathbb{R}^{m\times r}$, $V_0 \in \mathbb{R}^{n\times r}$ and $r \leq \min(m,n)$, a sequence of A2BSLOGD iterates is defined by:

$$\begin{cases} U_{t+1} & := \arg \min\limits_{U \in U_t + \mathrm{span}\{R_t V_t, P_{t-1}\}} \|X - UV_t^T\|_F \\ V_{t+1} & := \arg \min\limits_{V \in V_t + \mathrm{span}\{\tilde{R}_t^T U_{t+1}, Q_{t-1}\}} \|X - U_{t+1}V^T\|_F \end{cases} \quad \text{for} \quad t = 0, 1, \ldots$$

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$$\|R_t V_t\|_F^2,\ (R_t V_t V_t^T V_t, R_t V_t)_F,$$
$$(P_{t-1} V_t^T V_t, P_{t-1})_F,\ (R_t V_t V_t^T V_t, P_{t-1})_F,\ (R_t V_t, P_{t-1})_F$$

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and the corresponding search direction is updated by:

$$P_t := R_t V_t + (\beta_t / \alpha_t) P_{t-1} \;\; \text{for} \;\; t = 0, 1, \ldots$$

Alternating 2-block subspace locally optimal gradient descent

Definition (A2BSLOGD method and iterates, cont'd)

- The main right iterates of the A2BSLOGD method are given by:

$$V_{t+1} := V_t + \gamma_t \tilde{R}_t^T U_{t+1} + \omega_t Q_{t-1} \quad \text{for} \quad t = 0, 1, \ldots$$

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where the optimal step sizes γ_t and ω_t depend on:

$$\|\tilde{R}_t^T U_{t+1}\|_F^2,\ (\tilde{R}_t^T U_{t+1} U_{t+1}^T U_{t+1}, \tilde{R}_t^T U_{t+1})_F$$

$$(Q_{t-1} U_{t+1}^T U_{t+1}, Q_{t-1})_F,\ (\tilde{R}_t^T U_{t+1} U_{t+1}^T U_{t+1}, Q_{t-1})_F,\ (\tilde{R}_t^T U_{t+1}, Q_{t-1})_F$$

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and the corresponding search direction is updated by:

$$Q_t := \tilde{R}_t^T U_{t+1} + (\omega_t / \gamma_t) Q_{t-1} \quad \text{for} \quad t = 0, 1, \dots$$

Simultaneous 2-block subspace coordinate descent methods

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Definition (S2BSCD methods)

- Given $X \in \mathbb{R}^{m\times n}$, $U_0 \in \mathbb{R}^{m\times r}$, $V_0 \in \mathbb{R}^{n\times r}$ and $r \leq \min(m, n)$, a sequence of simultaneous 2-block subspace coordinate descent iterates is defined by:

$$\begin{cases} U_{t+1} \in U_t + \text{span}\{P_t\} \\ V_{t+1} \in V_t + \text{span}\{Q_t\} \end{cases} \quad \text{s.t.} \quad \begin{cases} R_{t+1} V_t \perp \text{span}\{P_t\} \\ R_{t+1}^T U_t \perp \text{span}\{Q_t\} \end{cases}$$

where $P_t \in \mathbb{R}^{m\times r}$ and $Q_t \in \mathbb{R}^{n\times r}$ are given search directions.
- Proper descent algorithms are s.t. $f(U_{t+1}, V_{t+1}) \leq f(U_t, V_t)$.

Simultaneous 2-block subspace gradient descent

- A natural instance of S2BSCD method is obtained by setting the search directions P_t and Q_t along gradient directions of f:

Definition (S2BSGD method and iterates)

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$$P_t := R_t V_t \propto \nabla_U f(U, V_t)|_{U_t} \quad \text{and} \quad Q_t := R_t^T U_t \propto \nabla_V f(U_t, V)|_{V_t} .$$

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- The main iterates of the S2BSGD method are given by:

$$U_{t+1} := U_t + \alpha_t P_t \quad \text{and} \quad V_{t+1} := V_t + \gamma_t Q_t$$

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for $t = 0, 1, \ldots$, in which the optimal step sizes $\alpha_t, \gamma_t \in \mathbb{R}$ depend on:

$$\|P_t\|_F^2, (P_t V_t^T V_t, P_t)_F, (U_t Q_t^T V_t, P_t)_F, (P_t Q_t^T V_t, P_t)_F,$$
$$\|Q_t\|_F^2, (V_t P_t^T U_t, Q_t)_F, (Q_t U_t^T U_t, Q_t)_F, (Q_t P_t^T U_t, Q_t)_F.$$

Simultaneous 2-block subspace locally optimal gradient descent

Definition (S2BSLOGD method and iterates)

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- The main left iterates are given by:

$$\begin{cases} U_{t+1} := U_t + \alpha_tR_tV_t + \beta_tP_{t-1} \\ V_{t+1} := V_t + \gamma_t\tilde{R}_t^TU_{t+1} + \omega_tQ_{t-1} \end{cases} \quad \text{for} \;\; t = 0, 1, \ldots$$

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  and the corresponding search directions are updated by:

$$\begin{cases} P_t := R_tV_t + (\beta_t/\alpha_t)P_{t-1} \\ Q_t := \tilde{R}_t^TU_{t+1} + (\omega_t/\gamma_t)Q_{t-1} \end{cases} \quad \text{for} \;\; t = 0, 1, \ldots$$

Simultaneous 2-block subspace locally optimal gradient descent

Definition (S2BSLOGD method and iterates, cont'd)

- The optimal step sizes γ_t, β_t, γ_t and ω_t depend on:

$$\|R_tV_t\|_F^2, (R_tV_t, P_{t-1})_F, (R_tV_tV_t^TV_t, R_tV_t)_F, (R_tV_tV_t^TV_t, P_{t-1})_F,$$
$$(P_{t-1}V_t^TV_t, R_tV_t)_F, (P_{t-1}V_t^TV_t, P_{t-1})_F, (U_tU_t^TR_tV_t, R_tV_t)_F,$$
$$(U_tU_t^TR_tV_t, P_{t-1})_F, (U_tQ_{t-1}^TV_t, R_tV_t)_F, (U_tQ_{t-1}^TV_t, P_{t-1})_F,$$
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Randomization

Random subspace embeddings

- The main building block of randomization is subspace embedding:

Definition ((ε, δ, d)-oblivious embedding)

A random linear map $x \in \mathbb{R}^n \mapsto \Theta x \in \mathbb{R}^k$ is an (ε, δ, d)-oblivious subspace embedding (OSE) of dimension $k < n$ with some $\delta \in (0, 1)$ if, for any d-dimensional subspace $\mathcal{S} \subset \mathbb{R}^n$, we have:

$$\text{Pr}\left\{(1-\varepsilon)\|x\|_2 \leq \|\Theta x\|_2 \leq (1+\varepsilon)\|x\|_2\right\} \geq 1-\delta \;\; \forall \;\; x \in \mathcal{S}.$$

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Random subspace embeddings can be used to reduce problem dimension, FLOP counts and data movement.

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- The practicality of randomization lies in finding subspace embeddings s.t.:
  - The embedding dimension k is sufficiently smaller than n, and
  - Sketching, i.e., the linear map $x \mapsto \Theta x$, can be applied efficiently.

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- The practicality of randomization lies in finding subspace embeddings s.t.:
  - The embedding dimension k is sufficiently smaller than n, and
  - Sketching, i.e., the linear map $x \mapsto \Theta x$, can be applied efficiently.
- Common sketching strategies include:
  - CountSketch, scaled random Gaussian matrices, sub-sampled fast transforms, random sign matrices.

Randomization of simultaneous 2-block coordinate descent

- All the block subspace coordinate descent algorithms presented thus far may be recast to make use of randomization in order to reduce FLOP counts and data movement while minimally impacting convergence.

Randomization of simultaneous 2-block coordinate descent

- All the block subspace coordinate descent algorithms presented thus far may be recast to make use of randomization in order to reduce FLOP counts and data movement while minimally impacting convergence.
- For example, we have:

Definition (RS2BSCD methods)

Given a matrix $X \in \mathbb{R}^{m \times n}$ with approximate factors $U_0 \in \mathbb{R}^{m \times r}$, $V_0 \in \mathbb{R}^{n \times r}$ of rank $r \leq \min(m, n)$, and two random subspace embeddings:

$$x \in \mathbb{R}^m \mapsto \Theta_1 x \in \mathbb{R}^k \quad \text{and} \quad y \in \mathbb{R}^n \mapsto \Theta_2 y \in \mathbb{R}^\ell,$$

a sequence of randomized simultaneous 2-block subspace coordinate descent (RS2BSCD) iterates is defined by:

$$\begin{cases} U_{t+1} \in U_t + \mathrm{span}\{P_t\} \\ V_{t+1} \in V_t + \mathrm{span}\{Q_t\} \end{cases} \quad \text{s.t.} \quad \begin{cases} \Theta_1(R_{t+1}V_t) \perp \mathrm{span}\{\Theta_1 P_t\} \\ \Theta_2(R_{t+1}^T U_t) \perp \mathrm{span}\{\Theta_2 Q_t\} \end{cases}$$

where $P_t \in \mathbb{R}^{m \times r}$ and $Q_t \in \mathbb{R}^{n \times r}$ are given search directions.

Summary of methods

Summary of FLOPs per iteration

- Methods for general matrices:

Method	FLOPs per iteration (dense X)
2BGD	$(6r+3)mn + 2r\cdot(m+n)$
A2BSGD	$(8r+4)mn + (4r^2+6r)(m+n)$
RA2BSGD	$(8r+4)mn + (2r^2+2r)(m+n) + (2r^2+4r)(k+\ell)$
A2BSLOGD	$(8r+4)mn + (6r^2+16r)(m+n)$
RA2BSLOGD	$(8r+4)mn + (2r^2+6r)(m+n) + (4r^2+10r)(k+\ell)$
S2BSGD	$(6r+3)mn + (10r^2+10r)(m+n)$
RS2BSGD	$(6r+3)mn + (4r^2+2r)(m+n) + (6r^2+8r)(k+\ell)$
S2BSLOGD	$(6r+3)mn + (22r^2+42r)(m+n)$
RS2BSLOGD	$(6r+3)mn + (6r^2+6r)(m+n) + (16r^2+36r)(k+\ell)$

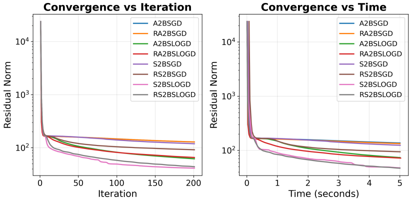
- Methods for symmetric positive semi-definite matrices:

Method	FLOPs per iteration (dense X)
1BGD	$(4r+3)n^2 + 2r\cdot n$
S1BSGD	$(4r+3)n^2 + (10r^2+9r)n$
RS1BSGD	$(4r+3)n^2 + (4r^2+2r)n + (6r^2+7r)k$
S1BSLOGD	$(4r+3)n^2 + (22r^2+33r)n$
RS1BSLOGD	$(4r+3)n^2 + (6r^2+6r)n + (16r^2+27r)k$

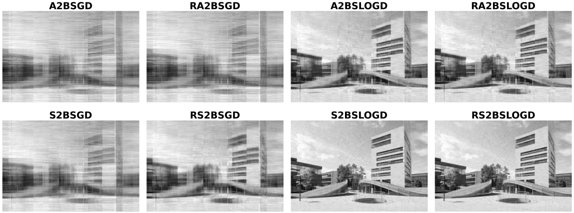
Numerical experiments

Toy example

- Rank-100 approximation of a 800-by-1,200 grayscale image:



- Low-rank approximations achieved in 5 seconds:



- We observe that:
  - Simultaneous schemes converge faster than alternating ones,
  - Local optimality accelerates convergence,
  - Randomization minimally impacts convergence.

Closing remarks

Conclusion

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  - Find this presentation at:

    venkovic.github.io/research

Related ongoing and future work

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    - Parallelization.
  - Low-rank approximation:
    - Application to matrix recovery (completion and sensing problems).
    - Non-negative matrix factorizations.
    - Tensor factorizations.