Fast Newton-type Methods for Nonnegative Matrix and Tensor Approximation

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Outline

Nonnegative matrix approximation (NNMA) problem:

- $A = [a_1, \ldots, a_N], \quad a_i \in \mathbb{R}_+^M$, is input nonnegative matrix
- **Goal :** Approximate A by conic combinations of *nonnegative representative vectors* $b_1, \ldots, b_K$ such that

$$a_i \approx \sum_{j=1}^{K} b_j c_{ji}, \quad c_{ji} \geq 0, \quad b_j \geq 0,$$

$$\text{i.e.} \quad A \approx BC, \quad B, C \geq 0.$$

The quality of the approximation $A \approx BC$ is

- Measured using an appropriate distortion function
- For example, the Frobenius norm distortion or the Kullback-Leibler divergence

In this presentation, we focus on the Frobenius norm distortion, which leads to the *least squares NNMA* problem:

$$\underset{B,C \geq 0}{\text{minimize}} \quad \mathscr{F}(B;C) = \frac{1}{2}\|A - BC\|_{\mathrm{F}}^2,$$

- NNMA objective function is not simultaneously convex in B & C
- But is individually convex in B & in C
- Most NNMA algorithms are iterative and perform an alternating optimization

Basic Framework for NNMA algorithms

1. Initialize B^0 and/or C^0; set $t \leftarrow 0$.
2. Fix B^t and solve the problem w.r.t C, Obtain C^{t+1}.
3. Fix C^{t+1} and solve the problem w.r.t B, Obtain B^{t+1}.
4. Let $t \leftarrow t+1$, & repeat Steps 2 and 3 until convergence criteria are satisfied.

Nonnegative Tensor Approximation

Problem Setting

- For brevity, consider 3-mode tensors only
- Least squares objective function

$$\mathscr{A}, \mathscr{T} \in \mathbb{R}_+^{\ell \times m \times n}$$

$$\|\mathscr{A} - \mathscr{T}\|_F^2 = \sum_{i=1}^{l} \sum_{j=1}^{m} \sum_{k=1}^{n} \left([\mathscr{A}]_{ijk} - [\mathscr{T}]_{ijk}\right)^2.$$

- Given a nonnegative tensor $\mathscr{A} \in \mathbb{R}^{\ell \times m \times n}$, find a nonnegative approximation $\mathscr{T} \in \mathbb{R}^{\ell \times m \times n}$ which consists of nonnegative *components*
- Tensor decomposition :
  "PARAFAC" or "Tucker"

Nonnegative PARAFAC Decomposition

- PARAFAC or Outer Product Decomposition:

$$
\begin{aligned}
\text{minimize} \quad & \|\mathscr{A} - \mathscr{T}\|_F^2 \\
\text{subject to} \quad & \mathscr{T} = \sum_{i=1}^{k} p^i \otimes q^i \otimes r^i, \\
\text{where} \quad & \mathscr{A},\ \mathscr{T} \in \mathbb{R}^{\ell \times m \times n}, \\
& P = [p^i] \in \mathbb{R}^{\ell \times k},\ Q = [q^i] \in \mathbb{R}^{m \times k},\ R = [r^i] \in \mathbb{R}^{n \times k}, \\
& P,\ Q,\ R \geq 0.
\end{aligned}
$$

Nonnegative Tucker Decomposition

- Tucker decomposition of tensors,

$$
\begin{array}{rl}
\text{minimize} & \|\mathscr{A} - \mathscr{T}\|_{\mathrm{F}}^2 \\
\text{subject to} & \mathscr{T} = \big(P, Q, R\big) \cdot \mathscr{Z}, \\
\text{where} & \mathscr{A},\ \mathscr{T} \in \mathbb{R}^{\ell\times m\times n},\ \mathscr{Z} \in \mathbb{R}^{p\times q\times r}, \\
 & P \in \mathbb{R}^{\ell\times p},\ Q \in \mathbb{R}^{m\times q},\ R \in \mathbb{R}^{n\times r}, \\
 & \mathscr{Z},\ P,\ Q,\ R \geq 0.
\end{array}
$$

- Basic Idea: build a matrix approximation problem
- For example, for matrix factor P,
  - Fix Q and R
  - Form $Z \in \mathbb{R}^{k \times mn}$ where i-th row corresponds to vectorized $q^i \otimes r^i$
  - Form $A \in \mathbb{R}^{\ell \times mn}$ where i-th row corresponds to vectorized $\mathscr{A}(i,:,:)$
  - Now the problem is

$$\underset{P \geq 0}{\text{minimize}} \quad \|A - PZ\|_{\mathrm{F}}^2.$$

Nonnegative Tucker Decomposition

Algorithm - Update Matrix Factors by Reducing to NNMA

- Basic Idea: build a matrix approximation problem
- For example, for matrix factor P,
  - Fix $\mathscr{Z}$, Q and R
  - Form $Z \in \mathbb{R}^{p \times mn}$ by flattening the tensor $\big(Q, R\big) \cdot \mathscr{Z}$ along mode-1
  - Computing $\mathscr{T} = \big(P, Q, R\big) \cdot \mathscr{Z}$ is equivalent to PZ
  - Flatten the tensor $\mathscr{A}$ similarly, obtain a matrix $A \in \mathbb{R}^{\ell \times mn}$
  - Now the problem is

$$\underset{P,Z \geq 0}{\text{minimize}} \quad \|A - PZ\|_{\mathrm{F}}^2.$$

- The Frobenius norm is the sum of Euclidean norms over columns
- Optimization over B (or C) boils down to a series of *nonnegative least squares (NNLS)* problems
- For example, fix B and find a solution x — i-th column of C reduces a NNLS problem:

$$\begin{array}{ll} \underset{x}{\text{minimize}} & f(x) = \frac{1}{2}\|Bx - a_i\|_2^2, \\ \text{subject to} & x \geq 0. \end{array}$$

Existing NNMA Algorithms

Exact Methods

Basic Framework for *Exact* Methods

1. Initialize B^0 and/or C^0; set $t \leftarrow 0$.
2. Fix B^t and find C^{t+1} such that

$$C^{t+1} = \operatorname*{argmin}_C \mathscr{F}(B^t, C),$$

3. Fix C^{t+1} and find B^{t+1} such that

$$B^{t+1} = \operatorname*{argmin}_B \mathscr{F}(B, C^{t+1}),$$

4. Let $t \leftarrow t+1$, & repeat Steps 2 and 3 until convergence criteria are satisfied.

Exact Methods

- Based on NNLS algorithms:
  - Active set procedure [Lawson & Hanson, 1974]
  - FNNLS [Bro & Jong, 1997]
  - Interior-point gradient method
- Projected gradient method [Lin, 2005].

Existing NNMA Algorithms

Inexact Methods

Basic Framework for *Inexact* Methods

1. Initialize B^0 and/or C^0; set $t \leftarrow 0$.
2. Fix B^t and find C^{t+1} such that

$$\mathscr{F}(B^t, C^{t+1}) \leq \mathscr{F}(B^t, C^t),$$

3. Fix C^{t+1} and find B^{t+1} such that

$$\mathscr{F}(B^{t+1}, C^{t+1}) \leq \mathscr{F}(B^t, C^{t+1}),$$

4. Let $t \leftarrow t+1$, & repeat Steps 2 and 3 until convergence criteria are satisfied.

Inexact Methods

- Multiplicative method [Lee & Seung, 1999]
- Alternating Least Squares (ALS) algorithm
- “Projected Quasi-Newton” method [Zdunek & Cichocki, 2006]

- Active Set based methods

> NOT suitable for large-scale problems

- Gradient Descent based methods

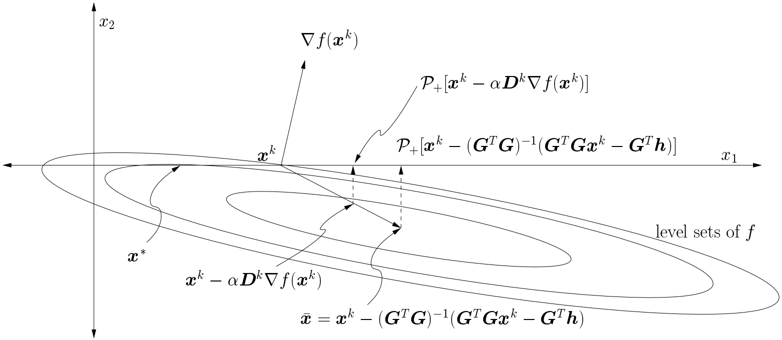
> May suffer from slow convergence — known as zigzagging

- Newton-type methods

> Naïve combination with projection does NOT guarantee convergence

Previous Attempts at Newton-type Methods for NNMA

Difficulties



- Naïve Combination of projection step and non-diagonal gradient scaling does not guarantee convergence
- An iteration may actually lead to an increase of objective

The active set :

- If active variables at the final solution are known in advance,
  - Original problem reduces to an **equality-constrained** problem
  - Equivalently one can solve an **unconstrained** sub-problem over inactive variables

Projection :

- The projection step identifies active variables at each iteration

Gradient :

- The gradient information gives a guideline to determine which variables *will not* be optimized at the next iteration

- Combine Projection with non-diagonal gradient scaling
- At each iteration, partition variables into two disjoint set, Fixed and Free variables
- Optimize the objective function over Free variables
- Convergence to a stationary point of $\mathscr{F}$ is guaranteed
- Any positive definite gradient scaling scheme is allowed, i.e., the inverse of full Hessian, an approximated Hessian by BFGS, conjugate gradient, etc

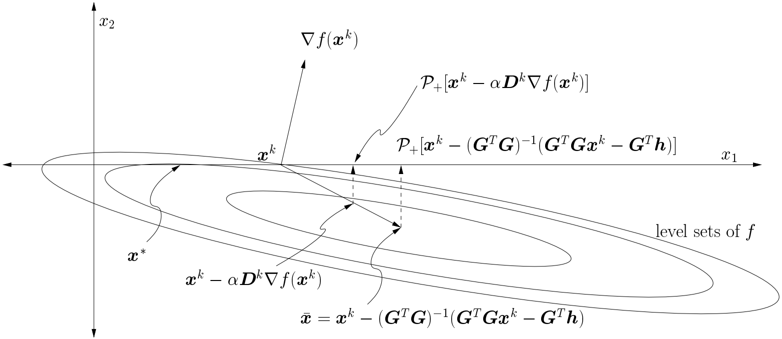
Divide variables into *Free* variables and *Fixed* variables.

- *Fixed* Set: Indices listing entries of x^k that are held *fixed*
- Definition: a set of indices

$$I^k = \left\{ i \middle| x_i^k = 0, \, [\nabla f(x^k)]_i > 0 \right\}.$$

- A **subset** of active variables at iteration k
- Contains active variables that satisfy the KKT conditions

Newton-type Methods



Fast Newton-type Nonnegative Matrix Approximation

FNMA^{E} & FNMA^{I}– an *exact* and *Inexact* Method

A subprocedure to update C in FNMA^{E}

1. Compute the gradient matrix $\nabla_C \mathscr{F}(B; C^{old})$.
2. Compute fixed set I_+ for C^{old}.
3. Compute the step length vector α.
4. Update C^{old} as

$$U \leftarrow \mathscr{Z}_+\left[\nabla_C \mathscr{F}(B; C^{\text{old}})\right]; \quad \textit{//Remove gradient info. from fixed vars}$$

$$U \leftarrow \mathscr{Z}_+\left[DU\right]; \quad \textit{//Fix fixed vars}$$

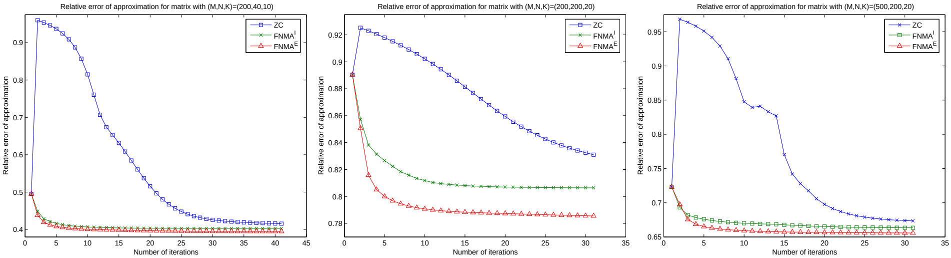
$$C^{\text{new}} \leftarrow \mathscr{P}_+\left[C^{\text{old}} - U \cdot \text{diag}(\alpha)\right] \quad \textit{//Enforce feasibility}$$

5. $C^{\text{old}} \leftarrow C^{\text{new}}$
6. Update D if necessary

FNMA^{I}: To speed up computation,

- Step-size α is parameterized
- Inverse Hessian is used for non-diagonal gradient scaling

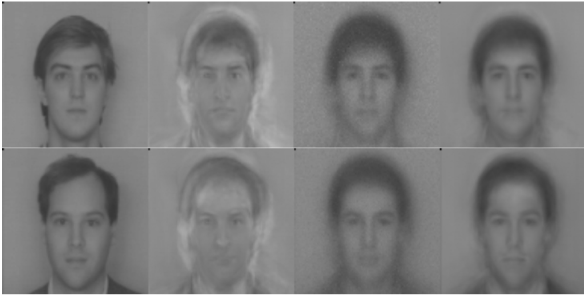
Experiments
Comparisons against ZC



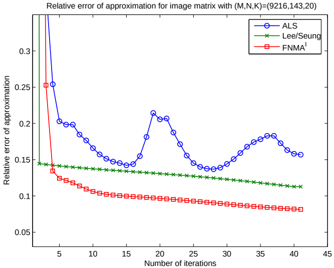
(a) Dense (b) Sparse (c) Sparse

- Relative approximation error against iteration count for ZC, FNMA^{I} & FNMA^{E}
- Relative errors achieved by both FNMA^{I} and FNMA^{E} are lower than ZC.
- Note that ZC does not decrease the errors monotonically

Experiments
Application to Image Processing



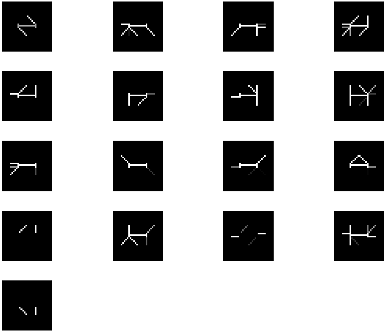
Original ALS LS FNMA^{I}



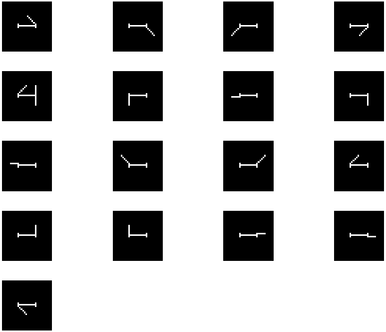
- Image reconstruction as obtained by the ALS, LS, and FNMA^{I} procedures
- Reconstruction was computed from a rank-20 approximation
- ALS leads to a non-monotonic change in the objective function value

Experiments

Application to Image Processing - Swimmer dataset - rank 13



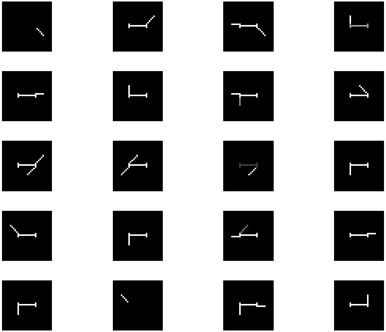
Lee & Seung's rank 17



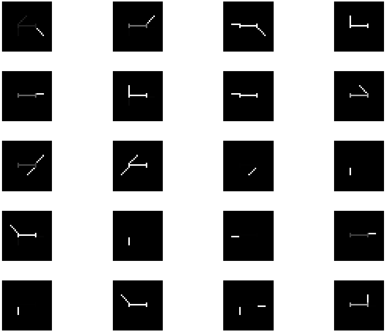
FNMA^{E} rank 17

Experiments

Application to Image Processing - Swimmer dataset - rank 20



Lee & Seung's rank 20

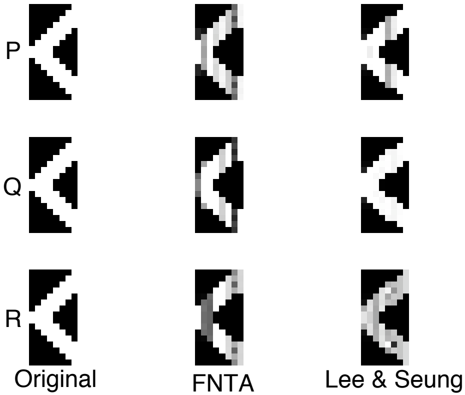


FNMA^E rank 20

	Lee & Seung's	FNMA^E	
Rank 13	140.53	47.06	Elapsed CPU Time
	4.49×10^7	2.01×10^7	Objective Function Value
Rank 17	182.24	62.29	Elapsed CPU Time
	2.41×10^7	$\mathbf{6.85 \times 10^{-4}}$	Objective Value
Rank 20	156.18	41.93	Elapsed CPU Time
	5.61×10^5	4.71×10^3	Objective Function Value

Experiments

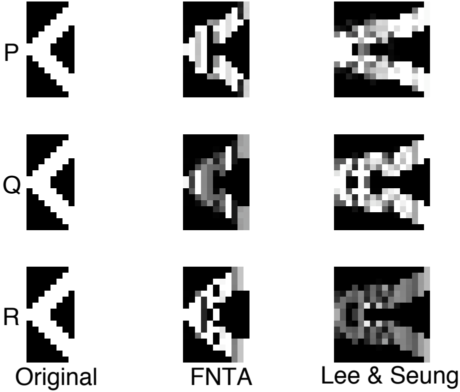
Comparison against Lee & Seung-type Algorithms - PARAFAC/ $k = 8$



- Nonnegative PARAFAC decomposition with $k = 8$
- Original $P, Q, R \in \mathbb{R}^{16\times 8}$ and rank 8
- Final rank is 8 for both FNTA and Lee & Seung
- FNTA gives smaller reconstruction error

Experiments

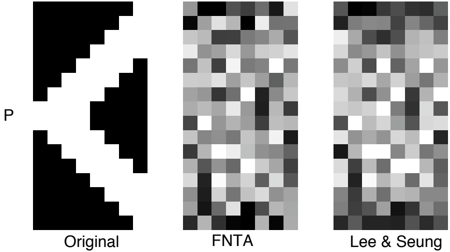
Comparison against Lee & Seung-type Algorithms - PARAFAC/ $k = 16$



- Nonnegative PARAFAC decomposition with $k = 16$
- Original $P, Q, R \in \mathbb{R}^{16 \times 8}$ and rank 8
- Final ranks are 11 for FNTA and 16 for Lee & Seung
- FNTA produces sparser and low-rank solution

Experiments

Comparison against Lee & Seung-type Algorithms - Tucker



- Nonnegative Tucker decomposition with $[p\ q\ r] = [8\ 8\ 8]$
- Original P, Q, R as before
- Original core tensor has 1 for all entries
- FNTA gives smaller reconstruction error
- Both methods fit the original tensor very well (error < 1e-4)
- Unlike PARAFAC, Both are unable to discover factors

Simultaneous Update of Factors

- Instead of alternating optimization between B and C,
- Update B and C jointly
- For example, after computing $\bar{B}$ and $\bar{C}$ s.t.

$$\bar{B} = \operatorname*{argmin}_{B \geq 0} \|A - BC_k\|_F^2, \quad \bar{C} = \operatorname*{argmin}_{C \geq 0} \|A - B_k C\|_F^2.$$

- Solve two-dimensional bound-constrained optimization,

$$\min_{0 \leq (\beta, \gamma) \leq 1} \|A - \big(B_k + \beta(\bar{B} - B_k)\big)\big(C_k + \gamma(\bar{C} - C_k)\big)\|_F^2.$$

Summary

- Nonnegative matrix and tensor approximation problems
- Non-diagonal gradient scaling can give faster convergence
- Algorithmic framework based on partitioning of variables
  - an *exact* & probably convergent method (more accurate)
  - an *inexact* method analogous to ALS (faster)
  - extensions to NNTA
- In progress...
  - More general distortion functions, e.g., Bregman divergences
  - Publicly available software toolbox
- A MATLAB Implementation of FNMA^E is now available at www.cs.utexas.edu/users/dmkim/Source/software/nnma/index.html

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