Memory-Efficient Separable Simplex-Structured Matrix Factorization via the Frank-Wolfe Method

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Simplex Structured Matrix Factorization

Simplex Structured Matrix Factorization (SSMF)

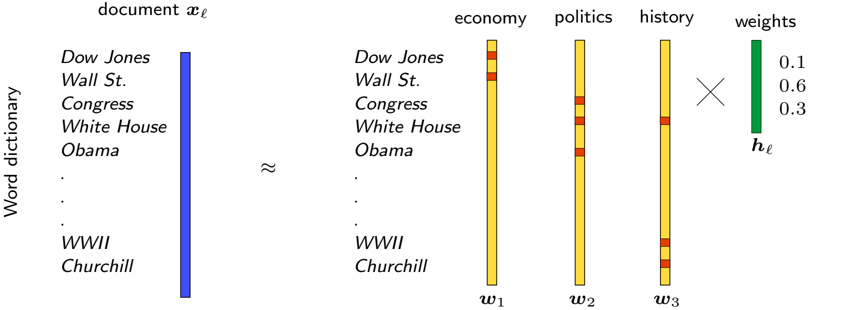
Data matrix $\boldsymbol{X} \in \mathbb{R}^{N \times M}$ is assumed to be generated by $\boldsymbol{W} \in \mathbb{R}^{N \times K}, \boldsymbol{H} \in \mathbb{R}^{K \times M}, K \ll \min(M, N)$ such that

$$\boldsymbol{X} = \boldsymbol{W}\boldsymbol{H} + \boldsymbol{V} \quad \text{subject to } \boldsymbol{H} \geq 0, \mathbf{1}^\top \boldsymbol{H} = \mathbf{1}^\top$$

Given $\boldsymbol{X}$, how do we find the latent factors $\boldsymbol{W}, \boldsymbol{H}$?

- Closely related to nonnegative matrix factorization.
- Has received significant attention across many domains [S. Arora et al. 2012; Sanjeev Arora et al. 2013; T.-H. Chan et al. 2008; X. Fu et al. 2016; Huang et al. 2019; Keshava et al. 2002; Mao et al. 2017b; Panov et al. 2017; Recht et al. 2012]

Application: Topic Modeling



$\boldsymbol{x}_\ell \approx 0.1 \times \boldsymbol{w}_1 + 0.6 \times \boldsymbol{w}_2 + 0.3 \times \boldsymbol{w}_3$

doc. $\approx 0.1 \times$ **economy** $+ 0.6 \times$ **politics** $+ 0.3 \times$ **history**

high prob. word

A demonstration of $\boldsymbol{x}_\ell \approx \boldsymbol{W}\boldsymbol{h}_\ell$

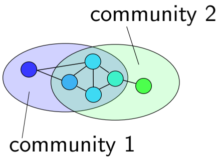
- $\boldsymbol{X}$ is a vocab-document matrix, then $\boldsymbol{X} = \boldsymbol{W}\boldsymbol{H}$ where
  - $\boldsymbol{H} \geq 0, \mathbf{1}^\top \boldsymbol{H} = \mathbf{1}^\top$
  - K is number of topics
- This model has been used in [S. Arora et al. 2012; Sanjeev Arora et al. 2013, 2016; Huang et al. 2016; Recht et al. 2012]

Application: Community Detection

- The mixed membership stochastic blockmodels [Airoldi et al. 2008]

$$P_{i,j} = \boldsymbol{h}_i^\top \boldsymbol{B} \boldsymbol{h}_j$$
$$\boldsymbol{A}(i,j) = \boldsymbol{A}(j,i) \sim \text{Bernoulli}(\boldsymbol{P}(i,j))$$

  where $\boldsymbol{h}_i = [h_{1,i}, \ldots, h_{K,i}]^\top$ represents membership of node i, $\boldsymbol{B}$ represents community-community connection.



Demonstration of a graph with $K = 2$ communities

  - By physical interpretation, $\boldsymbol{H} \geq 0, \mathbf{1}^\top \boldsymbol{H} = \mathbf{1}^\top$.
  - Range space of $\boldsymbol{H}$ can be estimated from K leading eigenvectors of $\boldsymbol{A}$ (denoted as matrix $\boldsymbol{X}$). [Lei et al. 2015; Mao et al. 2017a,b; Panov et al. 2017]

$$\boldsymbol{X} = \boldsymbol{W}\boldsymbol{H} + \boldsymbol{N}$$

Identifiability

- Given a SSMF model with $\boldsymbol{X} = \boldsymbol{W}^\star \boldsymbol{H}^\star$, finding $\boldsymbol{W}^\star, \boldsymbol{H}^\star$ is a difficult problem.

$$
\begin{aligned}
&\text{find} && \boldsymbol{W}, \boldsymbol{H} && \text{(1a)}\\
&\text{subject to} && \boldsymbol{X} = \boldsymbol{W}\boldsymbol{H} && \text{(1b)}\\
& && \boldsymbol{H} \geq 0, \mathbf{1}^\top \boldsymbol{H} = \mathbf{1}^\top && \text{(1c)}
\end{aligned}
$$

- The solution is not unique. There exists non-singular $\boldsymbol{Q}$ such that

$$
\boldsymbol{X} = \boldsymbol{W}^\star \boldsymbol{H}^\star = (\underbrace{\boldsymbol{W}^\star \boldsymbol{Q}^{-1}}_{\boldsymbol{W}'})(\underbrace{\boldsymbol{Q}\boldsymbol{H}^\star}_{\boldsymbol{H}'}), \text{ and } \boldsymbol{H}' \geq 0, \mathbf{1}^\top \boldsymbol{H}' = \mathbf{1}^\top
$$

Definition (Identifiability [Xiao Fu et al. 2019])

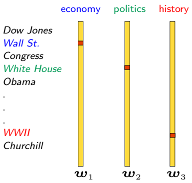
A SSMF model where $\boldsymbol{X} = \boldsymbol{W}^\star \boldsymbol{H}^\star$ is called identifiable respect to criterion (1) if for all $\boldsymbol{W}, \boldsymbol{H}$ satisfying criterion (1), it holds that $\boldsymbol{W} = \boldsymbol{W}^\star \boldsymbol{\Pi}, \boldsymbol{H} = \boldsymbol{\Pi}^\top \boldsymbol{H}^\star$, where $\boldsymbol{\Pi}$ is a permutation matrix.

Separability Condition

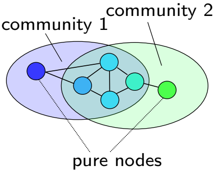
Separability condition [Donoho et al. 2003]

There exists set $\mathcal{K}$ so that $\boldsymbol{H}^\star(:,\mathcal{K}) = \boldsymbol{I}$.

- Have been adapted in many works [Sanjeev Arora et al. 2016; Tsung-Han Chan et al. 2011; Gillis et al. 2014a; Nascimento et al. 2005]
- Finding $\mathcal{K}$ is the key to estimate ground truth $\boldsymbol{W}^\star, \boldsymbol{H}^\star$.
  - In noiseless case, $\boldsymbol{X}(:,\mathcal{K}) = \boldsymbol{W}^\star \boldsymbol{H}^\star(:,\mathcal{K}) = \boldsymbol{W}^\star$.
- Physical interpretation
  - Anchor word [S. Arora et al. 2012] in topic modeling
  - Pure node [Mao et al. 2017b] in community detection



Demonstration of anchor word



Demonstration of pure node

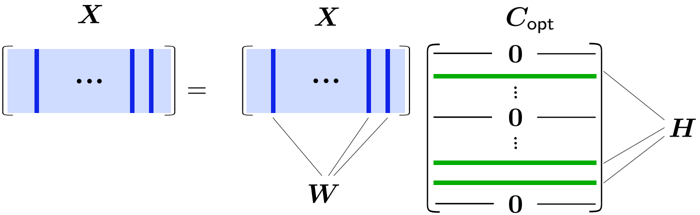
  - Expert annotator in crowd-sourcing [Ibrahim et al. 2019]
  - Pure pixels in hyperspectral unmixing [Ma et al. 2014]

A Self-Dictionary Perspective

- Consider the self-dictionary and sparse regression formulation,
  [Elhamifar et al. 2012; Esser et al. 2012; Iordache et al. 2014; Recht et al. 2012]

$$\begin{aligned} \underset{\boldsymbol{C}}{\text{minimize}} \quad & \|\boldsymbol{C}\|_{\text{row-0}} \\ \text{subject to} \quad & \boldsymbol{X} = \boldsymbol{X}\boldsymbol{C} \\ & \boldsymbol{C} \geq 0, \mathbf{1}^\top \boldsymbol{C} = \mathbf{1}^\top \end{aligned}$$

- $\boldsymbol{C}_{\text{opt}}(\mathcal{K},:) = \boldsymbol{H}, \boldsymbol{C}_{\text{opt}}(\mathcal{K}^c,:) = \mathbf{0}$ is an optimal solution point.
  - $\|\boldsymbol{C}_{\text{opt}}\|_{\text{row-0}} = K$.
  - For a full rank $\boldsymbol{W}$, one needs at least K non-zero rows of $\boldsymbol{C}$ to construct $\boldsymbol{X}$.



Row-sparsity matrix $\boldsymbol{C}_{\text{opt}}$

Greedy Approach

$$\begin{aligned} \underset{\boldsymbol{C}}{\text{minimize}} \quad & \|\boldsymbol{C}\|_{\text{row-0}} \\ \text{subject to} \quad & \boldsymbol{X} = \boldsymbol{X}\boldsymbol{C} \\ & \boldsymbol{C} \geq 0, \mathbf{1}^\top \boldsymbol{C} = \mathbf{1}^\top \end{aligned}$$

- The greedy approach identifies the set $\mathcal{K}$ by adding one index at a time [Xiao Fu et al. 2015b].
- Successive projection algorithm (SPA) [Araújo et al. 2001] is a representative.
- Extracting $\mathcal{K}$ is guaranteed even in noisy case [Gillis et al. 2014a].
- All greedy-based methods have a Gram-Schmidt structure which is prone to error propagation under noisy conditions.

Convex Relaxation Approach

- Relax the problem to a convex optimization problem [Ammanouil et al. 2014; Elhamifar et al. 2012; Gillis 2013; Gillis et al. 2018, 2014b; Recht et al. 2012]
- An example of this approach is [Esser et al. 2012; Xiao Fu et al. 2015a; Gillis et al. 2018]

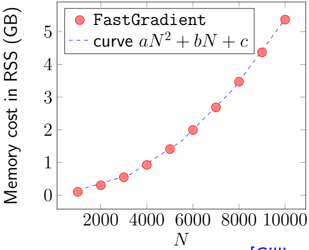
$$\begin{aligned} \underset{\boldsymbol{C}}{\text{minimize}} \quad & \frac{1}{2}\|\boldsymbol{X} - \boldsymbol{X}\boldsymbol{C}\|_{\mathrm{F}}^2 + \lambda R(\boldsymbol{C}) \\ \text{subject to} \quad & \boldsymbol{C} \geq 0, \mathbf{1}^\top \boldsymbol{C} = \mathbf{1}^\top \end{aligned}$$

  where $R(\boldsymbol{C})$ is some regularization term to promote row-sparsity.
- $\mathcal{K}$ is identified in noisy conditions.
- Often more robust than greedy approach.

Potential Memory Issue

The variable $\boldsymbol{C}$ has size $N \times N$.

A dense matrix $\boldsymbol{C}$ with $N = 100000$ requires 74.5GB.



Memory consumption of FastGradient [Gillis et al. 2018]

Proposal: Frank-Wolfe

In order to gain noise robustness and memory efficiency while obtaining identifiability,

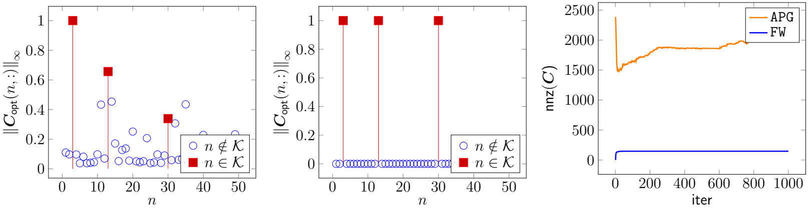
- We follow the convex relaxation approach.
- We propose to use Frank-Wolfe as the optimization method to guarantee $O(KN)$ memory consumption.

Warm-up with the Noiseless Case

$$
\begin{aligned}
\underset{\boldsymbol{C}}{\text{minimize}} \quad & \frac{1}{2}\|\boldsymbol{X} - \boldsymbol{X}\boldsymbol{C}\|_{\mathrm{F}}^2 && \text{(2a)}\\
\text{subject to} \quad & \boldsymbol{C} \geq 0, \mathbf{1}^\top \boldsymbol{C} = \mathbf{1}^\top && \text{(2b)}
\end{aligned}
$$

Problem (2) can have several solutions

- A desired solution $\boldsymbol{C}^\star(\mathcal{K}, :) = \boldsymbol{H}, \boldsymbol{C}^\star(\mathcal{K}^c, :) = \mathbf{0}$
- A trivial solution $\boldsymbol{I}_N$



APG - Objective value: $3.99e{-5}$ FW - Objective value: $2.86e{-5}$ Number of nonzeros (nnz) of $\boldsymbol{C}$

Accelerated proximal gradient (APG) vs Frank-Wolfe (FW). Unlike APG, FW outputs exact $\boldsymbol{C}^\star$ and keeps $\boldsymbol{C}$ sparse during its procedure. $M = 10, N = 50, K = 3$

Frank-Wolfe (FW) method [Frank et al. 1956]

- Assume $f(\boldsymbol{x})$ is convex and $\mathcal{D}$ is a compact convex constraint

$$
\begin{aligned}
\underset{\boldsymbol{x}}{\text{minimize}} \quad & f(\boldsymbol{x}) \\
\text{subject to} \quad & \boldsymbol{x} \in \mathcal{D}
\end{aligned}
$$

- FW's standard procedure: at iteration t,

$$
\begin{aligned}
&\boldsymbol{s}^t \leftarrow \arg\min_{\boldsymbol{s} \in \mathcal{D}} \ \nabla f(\boldsymbol{x}^t)^\top \boldsymbol{s} \\
&\boldsymbol{x}^{t+1} \leftarrow \boldsymbol{x}^t + \alpha^t(\boldsymbol{s}^t - \boldsymbol{x}^t), \quad \alpha^t = 2/(2+t)
\end{aligned} \tag{3}
$$

- For our problem,

When $\mathcal{D} = \left\{\boldsymbol{x} \in \mathbb{R}^n \mid \boldsymbol{x} \geq 0, \mathbf{1}^\top \boldsymbol{x} = 1\right\}$, solving (3) only cost $O(n)$, i.e.,

$$
\boldsymbol{s} = \boldsymbol{e}_{n^\star}, \ n^\star = \arg\min_n [\nabla f(\boldsymbol{x}^t)]_n
$$

FW in the Noiseless Case

- The original problem can be solved for each column $\boldsymbol{c}$ independently.

$$\begin{aligned} \underset{\boldsymbol{c}\in\mathbb{R}^N}{\text{minimize}} \quad & \frac{1}{2}\|\boldsymbol{x}-\boldsymbol{X}\boldsymbol{c}\|_{\mathrm{F}}^2 := f(\boldsymbol{c}) \\ \text{subject to} \quad & \boldsymbol{c}\geq 0, \mathbf{1}^\top\boldsymbol{c}=1 \end{aligned}$$

- Updating procedure:

$$\begin{aligned} &\boldsymbol{s}^t \leftarrow \boldsymbol{e}_{n^\star}, \quad n^\star = \arg\min_n \, [\nabla f(\boldsymbol{x}^t)] \\ &\boldsymbol{c}^{t+1} \leftarrow \boldsymbol{c}^t + \alpha^t(\boldsymbol{s}^t - \boldsymbol{c}^t), \quad \alpha^t = 2/(2+t) \end{aligned}$$

- If FW picks $n^\star \in \mathcal{K}$ in all iterations, then with $\boldsymbol{c}^0 = \mathbf{0}$,

$$\mathsf{supp}(\boldsymbol{c}^t) \subseteq \mathcal{K}$$

holds in all iterations t until FW terminates.

FW in the Noiseless Case

FW always picks $n^\star \in \mathcal{K}$.

- Gradient

$$\nabla f(\mathbf{c}) = [\boldsymbol{h}_1^\top \boldsymbol{q}, \dots, \boldsymbol{h}_N^\top \boldsymbol{q}]^\top, \quad \boldsymbol{q} = \boldsymbol{W}^\top \boldsymbol{W}(\boldsymbol{H}\boldsymbol{c} - \boldsymbol{h})$$

- For $n^\star = \arg\min_n \boldsymbol{h}_n^\top \boldsymbol{q}$, either
  - $\boldsymbol{h}_{n^\star} = \boldsymbol{e}_{k^\star}$, where $k^\star = \arg\min_{k \in [K]} q_k$. By definition, $n^\star \in \mathcal{K}$.
  - $\boldsymbol{q} = \boldsymbol{0} \Rightarrow$ desired solution $\boldsymbol{c}^\star$ is found because,

$$\boldsymbol{q} = \boldsymbol{0} \Leftrightarrow \boldsymbol{H}\boldsymbol{c} = \boldsymbol{h} \xLeftrightarrow{\text{assume } \mathcal{K} = [K]} \begin{bmatrix} \boldsymbol{I} & \boldsymbol{H}' \end{bmatrix} \boldsymbol{c} = \boldsymbol{h} \Leftrightarrow \boldsymbol{c} = \begin{bmatrix} \boldsymbol{h} \\ \boldsymbol{0} \end{bmatrix} = \boldsymbol{c}^\star$$

To sum up, in the noiseless case, with $\boldsymbol{c}^0 = \boldsymbol{0}$,

- $\text{supp}(\boldsymbol{c}^t) \subseteq \mathcal{K}$ for all t.
- FW terminates when $\boldsymbol{c}^t = \boldsymbol{c}^\star = \begin{bmatrix} \boldsymbol{h} \\ \boldsymbol{0} \end{bmatrix}$.

Therefore, FW outputs $\boldsymbol{C}_{\text{opt}} = \boldsymbol{C}^\star$ using only $O(KN)$ memory.

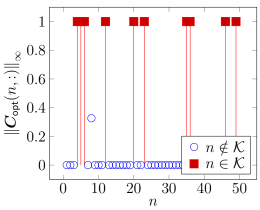
FW in the Noisy Case

- In the noisy case, i.e., $\boldsymbol{X} = \boldsymbol{W}\boldsymbol{H} + \boldsymbol{V}, \boldsymbol{V} \neq \boldsymbol{0}$, the gradient is

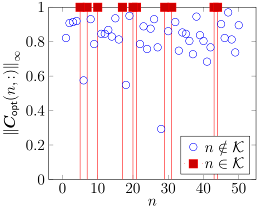
$$\nabla f(\boldsymbol{c}) = [\boldsymbol{h}_1^\top \boldsymbol{q}, \ldots, \boldsymbol{h}_n^\top \boldsymbol{q}] + \boldsymbol{n}, \quad (\boldsymbol{n} \text{ depends on the noise } \boldsymbol{V})$$

  then the picked index $n^\star$ could be outside of $\mathcal{K}$.

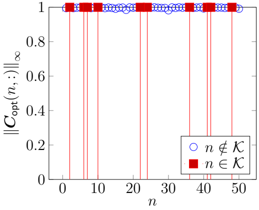
- FW is no longer guaranteed to output $\boldsymbol{C}^\star$.



SNR= 35dB



SNR= 25dB



SNR= 15dB

$\boldsymbol{C}_{\text{opt}}$ obtained by FW; $M = 40, N = 50, K = 10$.

Enhancement in the Noisy Case

- Different regularizations have been used to promote row-sparsity [Elhamifar et al. 2012; Esser et al. 2012; Xiao Fu et al. 2015a; Gillis et al. 2018, 2014b; Recht et al. 2012]. For example, [Esser et al. 2012; Xiao Fu et al. 2015a] use

$$\|\boldsymbol{C}\|_{\infty,1} := \sum_{i=1}^{N} \|\boldsymbol{C}(i,:)\|_{\infty}$$

- FW works best with smooth functions

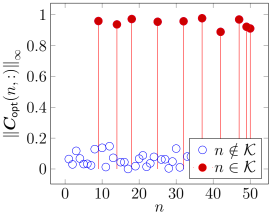
$$\Phi_\mu(\boldsymbol{C}) = \sum_{i=1}^{N} \varphi_\mu(\boldsymbol{C}(i,:)), \quad \varphi_\mu(\boldsymbol{C}(i,:)) = \mu \log\left(\frac{1}{N}\sum_{j=1}^{N} \exp\left(\frac{c_{i,j}}{\mu}\right)\right)$$

- We propose `MERIT`, a FW-based algorithm for solving:

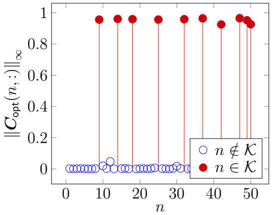
$$\begin{aligned} \underset{\boldsymbol{C}}{\text{minimize}} \quad & \frac{1}{2}\|\boldsymbol{X} - \boldsymbol{X}\boldsymbol{C}\|_{\mathrm{F}}^2 + \lambda \Phi_\mu(\boldsymbol{C}) \\ \text{subject to} \quad & \boldsymbol{C} \geq 0, \mathbf{1}^\top \boldsymbol{C} = \mathbf{1}^\top \end{aligned}$$

Identifiability

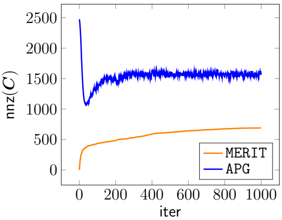
- With regularization, we can guarantee the extraction of $\mathcal{K}$ exactly in the noisy case under some reasonable assumptions [Nguyen et al. 2021].
- This result is obtained using a similar idea to [Xiao Fu et al. 2015a].
- Any convex optimization method can be used to obtain $\mathcal{K}$ via solution $\boldsymbol{C}_{\text{opt}}$.



`MERIT` - Objective value: $3.58e{-}01$



`APG` - Objective value: $4.41e{-}01$



Number of nonzeros (nnz) of $\boldsymbol{C}$

$$M = 40, K = 10, N = 50, \texttt{SNR} = 30\text{dB}, \mu = 1e{-}6, \lambda = 0.1.$$

Memory

- The objective function

$$h(\boldsymbol{C}) = \underbrace{\frac{1}{2}\left\|\boldsymbol{X} - \boldsymbol{X}\boldsymbol{C}\right\|_{\mathrm{F}}^{2}}_{f(\boldsymbol{C})} + \lambda \Phi_{\mu}(\boldsymbol{C}) = f(\boldsymbol{C}) + \lambda \Phi_{\mu}(\boldsymbol{C})$$

- FW's updating procedure on this problem can be executed column by column sequentially

$$\boldsymbol{s}_{\ell}^{t} \leftarrow \boldsymbol{e}_{n^\star}, \quad n^\star = \arg\min_{n}\, [\nabla h(\boldsymbol{c}_{\ell})]_{n}$$
$$\boldsymbol{c}_{\ell}^{t+1} \leftarrow \boldsymbol{c}_{\ell}^{t} + \alpha(\boldsymbol{s}_{\ell}^{t} - \boldsymbol{c}_{\ell}^{t}), \quad \alpha^{t} = 2/(2+t)$$

- Gradient is given by

$$\nabla h(\boldsymbol{c}_{\ell}) = \nabla f(\boldsymbol{c}_{\ell}) + \lambda [\nabla \Phi_{\mu}(\boldsymbol{C})]_{:,\ell}$$

- Question: If at iteration t, supp$(\boldsymbol{c}_{\ell}^{t}) \subseteq \mathcal{K}$, can FW pick

$$n^\star \in \mathcal{K},$$

where $n^\star := \arg\min_{n}\, [\nabla h(\boldsymbol{c}_{\ell})]_{n}$ in iteration $t+1$?

Effect of Noise

- Gradient of $f(\boldsymbol{c}_\ell) = 1/2 \, \|\boldsymbol{X} - \boldsymbol{X}\boldsymbol{C}\|_{\mathrm{F}}^2$

$$\nabla f(\boldsymbol{c}_\ell) = [\boldsymbol{h}_1^\top \boldsymbol{q}_\ell, \ldots, \boldsymbol{h}_N^\top \boldsymbol{q}_\ell]^\top + \boldsymbol{n}_\ell$$

- A demonstration of effect of noise that causes

$$n^\star := \arg\min_n \, [\nabla f(\boldsymbol{c}_\ell)]_n \notin \mathcal{K}.$$

$$\nabla f(\boldsymbol{c}_\ell) = \begin{array}{r} n^\star \dashrightarrow \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{bmatrix} 0.5 \\ 1.5 \\ 1.5 \\ 2.0 \\ \vdots \\ 1.5 \end{bmatrix} \begin{array}{l} \left.\begin{matrix} \\ \\ \\ \end{matrix}\right\} \mathcal{K} \\ \\ \\ \\ \\ \end{array} + \begin{bmatrix} 0.5 \\ 1.5 \\ -0.5 \\ 1.0 \\ \vdots \\ -1.0 \end{bmatrix} = \begin{bmatrix} 1.0 \\ 3.0 \\ 1.0 \\ 3.0 \\ \vdots \\ 0.5 \end{bmatrix} \begin{array}{l} \left.\begin{matrix} \\ \\ \\ \end{matrix}\right\} \mathcal{K} \\ \\ \\ \\ \dashleftarrow n^\star \end{array}$$

Regularization

- Gradient of the regularization

$$\boldsymbol{y}_\ell = [\nabla \Phi_\mu(\boldsymbol{C})]_{:,\ell}, \quad y_{n,\ell} = \frac{\exp(c_{n,\ell}/\mu)}{\sum_{i=1}^{N} \exp(c_{n,i}/\mu)}$$

- Assume that at iteration t, $\operatorname{supp}(\boldsymbol{c}_\ell^t) \subseteq \mathcal{K}$ for all ℓ.
  - For $n \notin \mathcal{K}$, $y_{n,\ell} = 1/N$.
  - If $\exists n_0 \in \mathcal{K}$ such that $c_{n_0,\ell}$ is not the largest element in row n_0 (*), then $y_{n_0,\ell} < \exp((c_{n_0,\ell} - c_{n_0,\star})/\mu)$, $\quad c_{n_0,\star} = \max_i c_{n_0,i}$.
  - (*) can be enforced with some initialization.
- An example of $\boldsymbol{C}$ and $\boldsymbol{y}_\ell$,

$$\boldsymbol{C} = \begin{array}{cc} & \begin{array}{ccc} \ell & & m \end{array} \\ \begin{array}{c} \mathcal{K}\left\{ \begin{array}{c} \\ \\ \\ \end{array} \right. \\ \\ \\ \end{array} & \begin{bmatrix} 0.3 & \dots & 0.1 \\ 0.2 & \dots & 0.6 \\ 0.5 & \dots & 0.3 \\ & & \\ \mathbf{0} & \vdots & \mathbf{0} \end{bmatrix} \begin{array}{c} \\ \leftarrow n_0 \\ \\ \\ \\ \end{array} \end{array} \quad \Longrightarrow \quad \boldsymbol{y}_\ell = \begin{bmatrix} 0.5 \\ 0.001 \\ 0.9 \\ 1/N \\ \vdots \\ 1/N \end{bmatrix} \begin{array}{c} \\ \leftarrow n_0 \\ \\ \\ \\ \\ \end{array}$$

Effect of Regularization

Regularization can ensure $n^\star \in \mathcal{K}$ under some reasonable assumptions.

- Gradient

$$\nabla h(\boldsymbol{c}_\ell) = \nabla f(\boldsymbol{c}_\ell) + \lambda \boldsymbol{y}_\ell,$$

- We have

$$\begin{cases} y_{n,\ell} = 1/N & \text{if } n \notin \mathcal{K} \\ y_{n_0,\ell} \approx 0 & \text{for some } n_0 \in \mathcal{K} \end{cases}$$

$$\Rightarrow n^\star := \arg\min_n \, [\nabla h(\boldsymbol{c}_\ell)]_n = n_0 \quad \text{for some } \lambda$$

- An example of $\boldsymbol{C}$ and $\nabla h(\boldsymbol{c}_\ell)$,

$$\Longrightarrow \nabla h(\boldsymbol{c}_\ell) = \begin{array}{r} \mathcal{K}\left\{\begin{array}{l} \\ \\ \\ \end{array}\right. \\ \\ \\ \\ \\ \end{array}\begin{bmatrix} 1.0 \\ 3.0 \\ 1.0 \\ 3.0 \\ \vdots \\ 0.5 \end{bmatrix} + \lambda \begin{bmatrix} 0.5 \\ 0.001 \\ 0.9 \\ 1/N \\ \vdots \\ 1/N \end{bmatrix}$$

the smallest element

MERIT in the Noisy Case

To sum up, in the noisy case, under some reasonable assumptions, the proposed method MERIT can

- Extract $\mathcal{K}$ exactly.
- If $\boldsymbol{C}^t$ satisfies supp$(\boldsymbol{c}_\ell^t) \subseteq \mathcal{K}$ for all ℓ, then supp$(\boldsymbol{c}_\ell^{t+1}) \subseteq \mathcal{K}$ for all ℓ, and hence MERIT can guarantee a memory consumption of $O(KN)$.

You should have an informal theorem here!

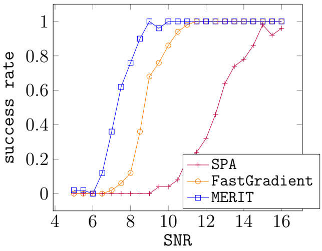
Synthetic Data

Data generation

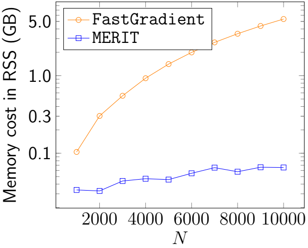
- $\boldsymbol{W} \sim \mathcal{U}(0, 1)$
- $\boldsymbol{H} \sim \text{Dir}(\mathbf{1}), \boldsymbol{H}(:, 1:K) = \boldsymbol{I}$
- $\boldsymbol{V} \sim \mathcal{N}(0, \sigma)$
- After shuffling $\boldsymbol{H}$, $\boldsymbol{X} = \boldsymbol{W}\boldsymbol{H} + \boldsymbol{V}$
- Noise level is measured in $\texttt{SNR} = 10 \log_{10}(\sum_{\ell=1}^{N} \|\boldsymbol{W}\boldsymbol{h}_\ell\|_2^2)/(MN\sigma^2)$dB

Metric

- $\texttt{success rate} = P(\mathcal{K} = \widehat{\mathcal{K}})$
- Estimate `success rate` by 50 trials



(a) `success rate` under different SNRs; $N = 200$, $M = 50$, $K = 40$.



(b) Memory consumption under different N's; SNR $= 10$dB, $M = 50$, $K = 40$.

Performance of `MERIT` compared to baselines

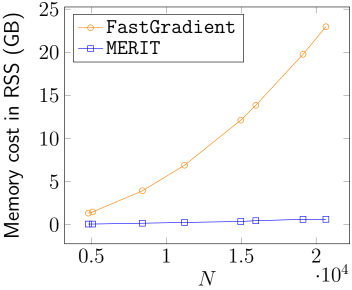
Real Data: Topic Modeling

Accuracy

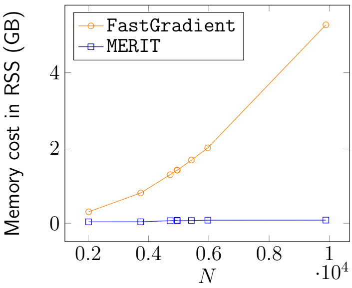
	Method $\backslash K$	3	4	5	6	7	8	9	10
TDT2	SPA	0.87	0.83	0.81	0.81	0.78	0.76	0.75	0.72
	FastAnchor	0.77	0.72	0.67	0.63	0.66	0.63	0.65	0.65
	XRAY	0.87	0.82	0.80	0.81	0.78	0.75	0.75	0.71
	LDA	0.78	0.77	0.74	0.75	0.73	0.72	0.68	0.70
	FastGradient	0.70	0.71	0.65	0.64	0.61	0.56	0.58	0.57
	MERIT	**0.88**	**0.88**	**0.85**	**0.86**	**0.84**	**0.82**	**0.80**	**0.77**
Reuters-21578	SPA	0.64	0.57	0.54	0.51	0.49	0.44	0.42	0.40
	FastAnchor	0.60	0.57	0.52	0.52	0.46	0.42	0.38	0.37
	XRAY	0.63	0.57	0.54	0.51	0.49	0.45	0.42	0.40
	LDA	0.63	0.57	0.53	0.51	0.46	0.44	0.41	0.42
	FastGradient	0.62	0.57	**0.56**	0.51	0.50	**0.48**	**0.44**	**0.46**
	MERIT	**0.66**	**0.62**	0.53	**0.53**	**0.51**	**0.48**	0.43	0.45

Bold, and blue indicate the best and second best scores, resp.

Real Data: Topic Modeling



TDT2



Reuters-21578

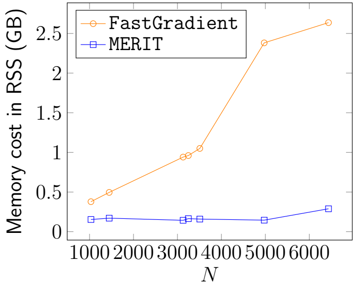
Memory consumption of `FastGradient` and `MERIT`

Real Data: Community detection

- Metric: Spearman's rank correlation (SRC). SRC $\in [-1, 1]$, higher value is better.
- Data: co-authorship networks, a community ground truth is defined by
  - DBLP: group of conferences
  - MAG: "field of study" tag

Dataset	GeoNMF	SPOC	FastGradient	MERIT
DBLP1	0.2974	0.2996	**0.3145**	0.2937
DBLP2	0.2948	0.2126	0.3237	**0.3257**
DBLP3	0.2629	**0.2972**	0.1933	0.2763
DBLP4	0.2661	0.3479	0.1601	**0.3559**
DBLP5	0.1977	0.1720	0.0912	**0.1983**
MAG1	**0.1349**	0.1173	0.0441	0.1149
MAG2	0.1451	0.1531	**0.2426**	0.2414

SRC Performance on DBLP and MAG. **Bold** and blue indicate the best and second best scores.



Memory consumption of FastGradient and MERIT

Conclusion

- FW is proposed as a memory efficient method for solving separable simplex-structured matrix factorization via convex relaxation.
- When noise is absent, using FW can bring identification with memory $O(KN)$
- For the noisy case, we have proposed using a smooth regularization to guarantee identifiability.
- For the noisy case, we have also shown that running FW only cost $O(KN)$ under some reasonable assumptions.

The talk is based on [Tri Nguyen et al. "Memory-efficient convex optimization for self-dictionary separable nonnegative matrix factorization: A frank-wolfe approach". In: *arXiv preprint arXiv:2109.11135* [2021], IEEE TSP, revised. (2nd round revision).]

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Condition (*)

Claim:

$\exists n_0 \in \mathcal{K}$ such that $\boldsymbol{C}(n_0, :)$ is not a constant
$\Rightarrow \exists n_0 \in \mathcal{K}$ such that $c_{n_0,\ell}$ is not the largest element in row n_0 (*).

- Assume that for all $n \in \mathcal{K}$, $c_{n,\ell}$ is the largest element in row n.
- Then for row n_0 such that $\boldsymbol{C}(n_0, :)$ is not a constant,

$$\exists m, \quad c_{n_0,\ell} > c_{n_0,m}$$

- That leads to

$$1 = \mathbf{1}^\top \boldsymbol{c}_\ell > \mathbf{1}^\top \boldsymbol{c}_m = 1$$

- The contradiction concludes our claim.

An example of $\boldsymbol{C}$,

$$\boldsymbol{C} = \begin{array}{c} \mathcal{K}\left\{ \begin{array}{c} \\ \\ \\ \end{array} \right. \\ \\ \end{array} \begin{array}{ccc} \overbrace{}^{\ell} & & \overbrace{}^{m} \\ \end{array} \left[\begin{array}{ccc} \cdot & \cdots & \cdot \\ 0.6 & \cdots & 0.5 \\ \cdot & \cdots & \cdot \\ \mathbf{0} & \vdots & \mathbf{0} \end{array} \right]$$