ABSTRACT

Matrix factorization, one of the most popular methods in machine learning, has recently benefited from introducing non-linearity in prediction tasks using tropical semiring. The non-linearity enables a better fit to extreme values and distributions, thus discovering high-variance patterns that differ from those found by standard linear algebra. However, the optimization process of various tropical matrix factorization methods is slow. In our work, we propose a new method FastSTMF based on Sparse Tropical Matrix Factorization (STMF), which introduces a novel strategy for updating factor matrices that results in efficient computational performance. We evaluated the efficiency of FastSTMF on synthetic and real gene expression data from the TCGA database, and the results show that FastSTMF outperforms STMF in both accuracy and running time. Compared to NMF, we show that FastSTMF performs better on some datasets and is not prone to overfitting as NMF. This work sets the basis for developing other matrix factorization techniques based on many other semirings using a new proposed optimization process.

Keywords data embedding, tropical matrix factorization, sparse data, matrix completion, tropical semiring, optimization strategy

1 Introduction

One of the most popular and widely used machine learning and data mining methods is matrix factorization. Matrix factorization methods achieve good results in various applications such as clustering, imputation of missing data, recommender systems, image processing, and bioinformatics, e.g., see [Xu et al.(2003)] [Omanović et al.(2021)] [Koren et al.(2009)] [Haefele et al.(2014)] [Brunet et al.(2004)]. The main idea of matrix factorization is to approximate the input data matrix as a product of lower-dimensional matrices, called factor matrices. Factor matrices enable a more straightforward interpretation of the rows and columns of the input matrix. The multiplication of factor matrices is mainly defined by applying standard linear algebra [Lee and Seung(1999)]. However, some recent approaches take advantage of the tropical semiring for matrix multiplication [De Schutter and De Moor(1997)] [Karaev and Miettinen(2016)] [Omanović et al.(2021)].

Semirings are widely used to solve graph optimization problems [Gondran and Minoux(2008)]. Different semirings can describe related problems depending on the definitions of addition and multiplication. Finding the shortest path in a graph can be characterized using the (min, +) semiring, the longest path using the (max, +) semiring (known as tropical semiring), while finding the minimum spanning tree using the (max, min) semiring. In [Belle and
with tropical entries. For each matrix which includes the model and solver, SP allows us to combine and integrate a wide range of specifications freely. One of the most well-studied matrix factorization methods is NMF [Lee and Seung(1999)], where input and factor matrices are limited to non-negative values. The factor model is additive, which simplifies the interpretation of the results.

Recent research results showed that to understand and interpret the deep neural network models, we need to understand the relevant tropical geometry [Zhang et al.(2018)]. Because the matrix factorization model is a kind of a simple neural network, the first step in bringing a new paradigm in the machine learning field would be to introduce semirings in matrix factorization methods, which could be later applied to understand deep models. Standard linear algebra enables quick model optimization; nevertheless, the drawback represents the linear relations found by the model. At the same time, tropical semiring produces nonlinear models, which can explain complex relations, but the optimization is costly compared to methods using standard linear algebra [Omanović et al.(2021)], [Karaev and Miettinen(2016)].

The main challenge is designing a matrix factorization method based on tropical semiring while achieving fast model optimization.

In our work, we propose an efficient sparse data matrix factorization method for the prediction of missing values, called FastSTMF, which is available on https://github.com/Ejmric/FastSTMF. The new method is based on Sparse Tropical Matrix Factorization (STMF, [Omanović et al.(2021)]), which ensures a better fit to extreme values and distributions, thus discovering high-variance patterns. At the same time, FastSTMF eliminates the main drawback of a slow computational performance of its ancestor STMF. The proposed method achieves better results by introducing a novel strategy to update the factor matrices. We evaluate its performance on synthetic and real datasets and show that FastSTMF outperforms STMF by achieving better results with less computation. We include the widely used NMF method in the evaluation process, and we do not include the Cancer method, since it cannot perform matrix completion, i.e., predict missing values. In conclusion, we give a thorough discussion and present plans for future work.

2 Related work

The most well-studied matrix factorization method is NMF [Lee and Seung(1999)], where input and factor matrices are limited to non-negative values. The factor model is additive, which simplifies the interpretation of the results. There are many different variants of NMF designed for a diverse set of applications [Zhang et al.(2010)], [Mnih and Salakhutdinov(2008)], [Stražar et al.(2016)], [Žitnik and Zupan(2015)]. These methods use standard linear algebra, where addition (+) and multiplication (×) are standard operations.

Standard linear algebra is limited to discovering patterns that arise from linear combinations of features. The usage of other semiring operations is expected to identify additional nonlinear patterns. Such a substitution of operations has already been successfully implemented in [Karaev and Miettinen(2016)], [Karaev and Miettinen(2016)], [Karaev et al.(2018)], [Omanović et al.(2021)], [Omanović et al.(2020)]

To perform data analysis and discover interesting patterns. In our work, we use tropical semiring $\mathbb{R}_{\text{max}} = \mathbb{R} \cup \{-\infty\}$ as in [Omanović et al.(2021)], where we replace the standard addition (+ in $\mathbb{R}$) with the maximum operator (max) and the standard multiplication (× in $\mathbb{R}$) with addition (+). Since data are usually summarized in a matrix, we will generalize the tropical operations to $\mathbb{R}_{\text{max}}^{m \times n}$, the set of $m \times n$ matrices with tropical entries. For each matrix $R \in \mathbb{R}_{\text{max}}^{m \times n}$, we denote by $R_{ij}$ its entry in the $i$-th row and the $j$-th column. Tropical operations give rise to matrix addition $A \oplus B$, where the entries of the sum of matrices $A, B \in \mathbb{R}_{\text{max}}^{m \times n}$ are defined as

$$ (A \oplus B)_{ij} := \max\{A_{ij}, B_{ij}\}, $$

$i = 1, \ldots, m, j = 1, \ldots, n$, and to the matrix multiplication $A \otimes B$ of matrices $A \in \mathbb{R}_{\text{max}}^{m \times p}, B \in \mathbb{R}_{\text{max}}^{p \times n}$, and its entries are defined as

$$ (A \otimes B)_{ij} := \max_{1 \leq k \leq p} \{A_{ik} + B_{kj}\}, $$

$i = 1, \ldots, m, j = 1, \ldots, n$.

The tropical matrix factorization problem is defined as follows: given an input data matrix $R \in \mathbb{R}_{\text{max}}^{m \times n}$ and factorization rank $r$, find coefficient factor $U \in \mathbb{R}_{\text{max}}^{m \times r}$ and basis factor $V \in \mathbb{R}_{\text{max}}^{r \times n}$ such that

$$ R \cong U \otimes V. $$

The STMF method uses tropical semiring on sparse data and can better fit extreme values and distributions compared to NMF [Omanović et al.(2021)]. The two key parts of STMF are algorithms to update the coefficient factor $U$ (algorithm...
ULF) and the basis factor $V$ (algorithm URF). Each of them uses the operation $(\min, +)$, defined as
\[(A \otimes^* B)_{ij} := \min_{A_{ik}, B_{kj} \text{are given}} \{A_{ik} + B_{kj}\}\]
for matrices $A \in \mathbb{R}_{\max}^{m \times p}$ and $B \in \mathbb{R}_{\max}^{p \times n}$, $i = 1, \ldots, m$, $j = 1, \ldots, n$, which imitates multiplication with the inverse matrix, since invertible tropical matrices are rarely found. The fact that the STMF method computes ULF/URF for each element of the input matrix results in low computational performance.

Here is where we found the motivation for FastSTMF: the average running time of STMF is slow compared to NMF’s, see [Omanović et al. (2021), Table 3]. Note that given a factorization rank $r$, STMF attempts updating the factor matrices $r$ times for each element $R_{ij}$ until approximation error is decreased and therefore performs poorly in terms of running time. Our work presents several novel strategies for updating factor matrices more efficiently. We explored different approaches and the method that gave the best results, we named it FastSTMF (Algorithm 3).

3 Methods

The update procedure of factor matrices $U \in \mathbb{R}_{\max}^{m \times r}$ and $V \in \mathbb{R}_{\max}^{r \times n}$ to approximate a given input data matrix $R \in \mathbb{R}_{\max}^{m \times n}$ is the crucial part of each matrix factorization algorithm. The speed of convergence depends on how effectively we make changes in the factor matrices $U$ and $V$. STMF updates the factor matrices $r$ times for each element $R_{ij}$ until the approximation error decreases. It starts in the upper left corner of the matrix $R$, therefore focusing the optimization more on the entries in the upper rows and leftmost columns and slowly progresses to the lower part of the matrix. Namely, for every pair of indices $(i, j)$ algorithm ULF (URF, respectively) in STMF contains a loop that searches for the optimal column index $k$ of the coefficient factor $U$ (row index $k$ of the basis factor $V$, respectively) to update.

3.1 Our contribution

We propose new update rules (defined as the ByRow strategy in Section 3.2.1) in which we identify for each row $i$ of $R$ only one column $j$ and the optimal $k$ to update in each iteration of $R$. We provide the triple $(i, j, k)$ as an input parameter in algorithms F-ULF (see Algorithm 1) and F-URF (see Algorithm 2) to change in one update step only the entries of the $k$-th column of $U$, denoted by $U_{ik}$, and the $k$-th row of $V$, denoted by $V_{kj}$. This results in an update of all entries in the current approximation of the matrix $R$, based on the change of only one row of coefficient factor $U$ and only one column of basis factor $V$.

**Algorithm 1** Fast update of $U, V$ based on the element from the $i$-th row of the coefficient factor $U$ (F-ULF)

**Input:** data matrix $R \in \mathbb{R}_{\max}^{m \times n}$, coefficient factor $U \in \mathbb{R}_{\max}^{m \times r}$, basis factor $V \in \mathbb{R}_{\max}^{r \times n}$, position $(i, j, k)$

**Output:** $U, V, f, U_{ik}', V_{kj}'$

$U_{ik}' \leftarrow U_{ik} - R_{ij}$
$V_{kj}' \leftarrow V_{kj} - R_{ij}$

**Algorithm 2** Fast update of $U, V$ based on the element from the $j$-th column of the basis factor $V$ (F-URF)

**Input:** data matrix $R \in \mathbb{R}_{\max}^{m \times n}$, coefficient factor $U \in \mathbb{R}_{\max}^{m \times r}$, basis factor $V \in \mathbb{R}_{\max}^{r \times n}$, position $(i, j, k)$

**Output:** $U, V, f, U_{ik}', V_{kj}'$

$U_{ik}' \leftarrow U_{ik} - R_{ij}$
$V_{kj}' \leftarrow V_{kj} - R_{ij}$

The difference between ULF/URF and F-ULF/F-URF is in the efficiency of matrix operations and in their implementations. ULF and URF in STMF contain a loop that searches for the optimal $k$. In contrast, FastSTMF identifies $k$ in advance.
and provides it as an input parameter in F-ULF and F-URF, see Algorithms 1 and 2. ULF/URF both use whole matrices \( U, V \) in all matrix operations to get new updated \( U, V \). However, we obtain the same updated \( U, V \) in the proposed F-ULF/F-URF by changing only the appropriate rows/columns from \( U, V \), since only specific values change in the factor matrices. In this way, we speed up the process of computing new factor matrices by getting the same result faster (see Supplementary Figure S10).

### 3.2 Update strategies

Instead of having multiple attempts to update each element in factor matrices as in STMF, we propose three novel update strategies: by row (ByRow), by element (ByElement) and by entire matrix (ByMatrix). Modified update strategies result in more iterations through all matrix elements in the same amount of time compared to STMF. For each strategy, we define its own error, defined with \( err \), which guides the selection of factor matrices’ indices to update.

#### 3.2.1 The ByRow strategy

In the central part of our work, we investigate the different selection approaches for choosing the best indices \( j \) and \( k \) to update for a fixed row \( i \). In the ByRow strategy, we iterate through all rows of the matrix \( R \). For each row \( i \) of \( R \), we update the factor matrices only once for each iteration over \( R \\

- **In the sequential selection (SEQ),** we choose for each \( i \) the smallest \( j \) and \( k \) that decrease the approximation error \( \| \|_b \) the most, defined as the sum of the absolute values of matrix entries (for definitions, see Subsection 3.6). After updating the row \( i \), we continue to select \((j, k)\) for the next row \( i + 1 \).

- **The tropical distance selection (TD) aims for** \((U \otimes V)_{ij} = \max_{1 \leq k \leq r} \{U_{ik} + V_{kj}\}\) to be as close to \( R_{ij} \) in the shortest time. Therefore, when \( R_{ij} \) is given, the TD selection chooses for each \( i \) the index \( j \) with the highest tropical distance

\[
\text{td}(R, U, V, i, j) = \left| R_{ij} - \max_{1 \leq k \leq r} (U_{ik} + V_{kj}) \right|
\]

and still decreases the approximation error \( \| \|_b \). For each pair \((i, j)\), the tropical distance \( \text{td}(R, U, V, i, j) \) measures the error at position \((i, j)\) between \( R \) and the current iteration \( U \otimes V \) in tropical semiring. Intuitively, we can interpret the function \( f \) as the indicator of the most suitable location in the factor matrices to update. For each pair \((i, j)\), we denote the value of index \( k \) selected in \( \text{td} \) as

\[
f(i, j) = \arg\max_{1 \leq t \leq r} (U_{it} + V_{tj}).
\]

The TD selection chooses \( k = f(i, j) \) and when multiple \( \ell \) indices give the same maximum value, the smaller \( \ell \) is chosen as \( k \). We expect the tropical distance selection criteria to find the tropical patterns in the matrix and correct the largest entry-wise error.

- **We investigate two subvariants of TD, denoted TD_A and TD_B.** Instead of comparing the error only locally at position \((i, j)\) in TD, these subvariants will act more globally and will scan a whole row and column to find the best index \( k \). We define the tropical distance for row \( i \) as

\[
\text{td}_{row}(R, U, V, i) = \sum_{t=1}^{n} \text{td}(R, U, V, i, t)
\]

and for column \( j \) as

\[
\text{td}_{col}(R, U, V, j) = \sum_{t=1}^{m} \text{td}(R, U, V, t, j).
\]

Both variants select the index \( j \) to be the one that results in the maximum value of

\[
\text{err}(R, U, V, i, j) = \text{td}_{col}(R, U, V, j).
\]

Since the row \( i \) is predetermined and the value of \( \text{td}_{row}(R, U, V, i) \) is fixed, we are only interested in selecting the column index \( j \) with the highest \( \text{err} \). The variant TD_A selects \( k \) as the index that occurs the most times in \( \text{td}_{row}(R, U, V, i) \) and \( \text{td}_{col}(R, U, V, j) \) together. Formally,

\[
k = \arg\max_{\ell} \left( \text{count}_\ell \left( \{ f(i, t) : t = 1, \ldots, n \} \cup \{ f(t, j) : t = 1, \ldots, m \} \right) \right),
\]

where the function \( \text{count}_\ell \) returns the number of occurrences of \( \ell \) in the multiset \( \{ \cdot \} \).
For variant TD_B, we first define $j_0 = \arg\max_{1 \leq t \leq n} (err(R, U, V, i, t))$ and $i_0 = \arg\max_{1 \leq t \leq n} (err(R, U, V, t, j))$ as indices, where the maximal $err$ is achieved in the $i$-th row and the $j$-th column. We choose $k$ as
\[
  k = \begin{cases} 
    f(i, j_0), & (U \otimes V)_{ij_0} \geq (U \otimes V)_{i_0j}, \\
    f(i_0, j), & \text{otherwise.}
  \end{cases}
\]

### 3.2.2 The ByElement strategy

The ByElement strategy updates the factor matrices, when $R_{ij}$ is given, only once by choosing the index $k = k_{ij}$ using TD selection. For a fixed $(i, j)$, we compute $td(R, U, V, i, j)$, which represents the $err$:
\[
  err(R, U, V, i, j) = td(R, U, V, i, j).
\]

In case $err$ equals 0, we have a perfect approximation of $(i, j)$ and we skip updating that element.

### 3.2.3 The ByMatrix strategy

On the contrary, the ByMatrix strategy selects only one $i$ and $j$ over the entire data matrix $R$ in each iteration through all given elements of the matrix. Namely, we define the error of every pair $(i, j)$ as
\[
  err(R, U, V, i, j) = td_{row}(R, U, V, i) + td_{col}(R, U, V, j) - td(R, U, V, i, j).
\]

Since $(i, j)$ appears in $td_{row}(R, U, V, i)$ and in $td_{col}(R, U, V, j)$, we subtract $td(R, U, V, i, j)$ in $err$ to avoid double counting. We sort all $err$ in decreasing order and select a pair of indices $(i, j)$ with the highest $err$, while the index $k$ is chosen using TD selection for $(i, j)$. Since ByMatrix strategy compares the errors of all matrix elements before the update, it is extremely slow. Our aim is to create a fast tropical method, thus we randomly apply F-ULF or F-URF to the chosen triple $(i, j, k)$ instead of testing them both. We halve the running time at the expense of skipping potential good indices to update.

### 3.3 Comparison of strategies

In each of these three strategies, we choose the indices $(i, j, k)$ with the highest value $err$ that decreases the approximation error and $k$ as described above. The reason for a more time-efficient updating of the factor matrices is the introduction of $td$-based heuristics in a given running time. If the selected indices $(i, j, k)$ do not decrease the approximation error, we use the indices computed from the next highest $err$.

For some of the proposed methods, we first choose to perform permuting of rows (PermR) or columns (PermC) in the data matrix. All permutations sort rows or columns in increasing order by their minimum values, consistent with the proven efficient criteria used in STMF (see Omanović et al. (2021), Fig. 3). In the ByMatrix strategy, the permutation of rows or columns is unnecessary, since the values of $err$ are always computed for all entries of the matrix, and the permuting procedure would not influence the algorithm’s results.

In total, we will compare and evaluate twelve methods with various combinations of update strategies and data permutations on synthetic data. Among ten ByRow strategies, we chose the one that performed best, see Subsection 4.1.1. We selected the preferred data matrix shape for ByElement, ByRow and ByMatrix, see Subsection 4.1.2. We summarize three final methods that gave the best results in Table 1 and give their pseudocodes in Algorithm 3 and in the Supplement, Section B.

| STMF | update strategy | permutation by columns | permutation by rows | candidate selection | preferred shape |
|------|-----------------|------------------------|---------------------|---------------------|----------------|
| STMF_ByElement_PermC_TD_W | 5 times per element | incr. by minimum | X | X | wide |
| STMF_ByRow_RandPerm_TD_A_W (FastSTMF) | once per element | incr. by minimum | random | TD | wide |
| STMF_ByMatrix_NoPerm_TD_W | once per row | X | X | TD | wide |
| | once per matrix | X | X | TD | wide |

Table 1: Comparison of proposed methods with the STMF method given the update strategy, performed data matrix permutations, performed candidate selection and preferred data matrix shape (see Section B).

We use the Random Acol initialization strategy for the matrix $U$ as used in STMF (Omanović et al. (2021)). Random Acol is the element-wise average strategy of randomly selected columns from the input data matrix $R$. The convergence of the proposed algorithm FastSTMF, defined in Algorithm 3, is checked similarly to that of STMF (Omanović et al. (2021)). The update rules of FastSTMF step-by-step reduce the approximation error, since the factor matrices $U$ and $V$ are only
We create two groups of synthetic datasets when different number of features are given. We merge similar genes into 100 features, representing our features for the BIC data. All the real data is in the form of data matrices, and merge into 1000 features for the large synthetic datasets.

Algorithm 3: FastSTMF (STMF_byRow_RandPerm_TD_A_W)

**Input:** data matrix $R \in \mathbb{R}^{m \times n}$, factorization rank $r$

**Output:** factorization $U \in \mathbb{R}^{m \times r}$, $V \in \mathbb{R}^{r \times n}$

1. if $R$ not wide then transpose $R$
2. $perm \leftarrow$ random permutation of indices $1 \ldots m$
3. $R \leftarrow R[perm, :]$
4. initialize $U$ and compute $V$
5. while not converged do
   1. for each row $i$ of $R$
      1. $row\_indices \leftarrow \{f(i, t) : t = 1, \ldots, n\}$
      2. $errors, columns\_indices \leftarrow [], []$
      3. for each column $j$ of $R$
         1. $e \leftarrow td\_col(R, U, V, j)$
         2. append $e$ to $errors$
         3. $col\_indices \leftarrow \{f(t, j) : t = 1, \ldots, m\}$
         4. append $col\_indices$ to $columns\_indices$
      4. for each $j$ in argsort($errors$) in decreasing order
         1. $k \leftarrow \text{argmax}_{t} (\text{count}_t(row\_indices \cup columns\_indices[j]))$
         2. $(U, V, f, U_{t}', V_{k}') \leftarrow F\_ULF(R, U, V, i, j, k)$
         3. if $f$ decreases then break
         4. else $(U, V, f, U_{t}', V_{k}') \leftarrow F\_ULF(R, U, V, i, j, k)$
         5. if $f$ decreases then break
         6. else $(U, V, f, U_{t}', V_{k}') \leftarrow F\_ULF(R, U, V, i, j, k)$
      5. if $R$ transposed then $(U, V) \leftarrow (V^T, U[perm^{-1}, :)^T])$
      6. else $(U, V) \leftarrow (U[perm^{-1}, :], V)$
6. return $U, V$

3.4 Synthetic data

We create two groups of synthetic datasets $R_{\lambda}$ with matrices of rank three: smaller, of size $200 \times 200$, and larger, of size $10000 \times 300$. In each group, the dataset $R_{\lambda}$ is computed using the following formula:

$$R_{\lambda} = \lambda(A \otimes B) + (1 - \lambda)(A \cdot B),$$

where $A$ and $B$ are two random non-negative matrices sampled from a uniform distribution over $[0, 1)$, and $A \otimes B$ is the tropical product and $A \cdot B$ is the standard product of generated matrices. Thus, when $\lambda = 0$ the dataset $R_{\lambda}$ has a completely linear structure and $\lambda = 1$ represents a completely tropical structure of $R_{\lambda}$. Note that since the entries of $A$ and $B$ are uniformly distributed in $[0, 1)$, the average entry of $A \otimes B$ will be in general larger than the average entry of $A \cdot B$. Since we are interested in tropical factorization, we also consider $\lambda = 0.5$ to generate data matrix $R$ with a more tropical than linear structure, called mixture. We generate 50 small synthetic datasets and 100 large synthetic datasets. We split the large synthetic data in 50 matrices representing the training set and 50 representing the validation set.

3.5 Real data

In our work, we use the following preprocessing gene expression datasets from the Cancer Genome Atlas (TCGA) database [Rappoport and Shamir (2018)]: Acute Myeloid Leukemia (AML), Breast Invasive Carcinoma (BIC), Colon Adenocarcinoma (COLON), Glioblastoma Multiforme (GBM), Liver Hepatocellular Carcinoma (LIHC), Lung Squamous Cell Carcinoma (LUSC), Ovarian Serous Cystadenocarcinoma (OV), Skim Cutaneous Melanoma (SKCM) and Sarcoma (SARC).

Similarly as in the evaluation of STMF, we use feature agglomeration [Murtagh and Legendre (2014)] to merge similar genes and to minimize the influence of non-informative genes. In addition, we compare the performance of methods when different number of features are given. We merge similar genes into 100 features, representing our small real data matrices, and merge into 1000 features for the large real data matrices. We use the 50 known PAM genes [Parker et al. (2009)] representing our features for the BIC data. All the real data is in the form of patients x meta-genes.
3.6 Evaluation metrics

*b-norm* is defined as a sum of the absolute values of matrix entries \(|W|_b = \sum_{i,j} |W_{ij}|\), and it can be applied as an objective function in matrix factorization methods. As in [Omanović et al.(2021)], we use the *b-norm* to minimize the approximation error of FastSTMF.

**Normalized error (NE).** For each of the tested method, we measure *normalized error* \(\text{NE}_t\) compared to baseline STMF’s error at timestamp \(t\) as:

\[
\text{NE}_t = \frac{e_t - \gamma t_{\text{max}}}{\gamma t_{\text{max}} - \gamma t_{\text{max}}},
\]

where \(\gamma_t\) is the approximation error of STMF at the timestamp \(t\) and \(e_t\) is the error of a specific method at the timestamp \(t\) computed using the *b-norm*. We choose \(t_{\text{init}}\) as the time after initialization in STMF. \(\text{NE}_t\) allows us to compare different methods on multiple datasets and observe how fast the error drops below 0, which is \(\gamma t_{\text{max}}\) for STMF. Negative NE values imply that the specific method achieves better results in less time compared to STMF.

**Distance correlation (DC)** is a well-known measure for detecting a wide range of relationships, including nonlinear [Szekely and Rizzo(2009)]. The DC coefficient is defined on the interval [0, 1] and equals 0 when the variables are independent. The coefficient tells us the strength of association between the original and approximated matrix. In our previous study [Omanovic et al.(2021)], we used DC to evaluate the predictive performance of different matrix factorization methods.

**Root-mean-square error (RMSE)** measure is used to assess the approximation error of the training data, denoted RMSE-A, and to rate the prediction error on the real test data, denoted RMSE-P. The value of RMSE is always non-negative, and 0 indicates a perfect fit to data. It is a commonly used metric to evaluate matrix factorization methods [Bokde et al.(2015)].

**Critical difference (CD)** graph defined by Demšar [Demšar(2006)] is used to compare the performance of multiple algorithms on multiple datasets. CD is computed using a statistical test for the average performance ranks of methods over different datasets for the significance level \(\alpha = 0.05\). We rank the methods by the time needed to achieve STMF’s final \(\text{NE}_{t_{\text{max}}}\) and by their final \(\text{NE}_{t_{\text{max}}}\). Observing the CD graph, the group of methods not connected to another group indicates that there is a significant difference between the two groups. It is a rigorous method for evaluating algorithms since it only observes rankings in performance without considering how much one method is numerically better than others.

**Bootstrap** is a resampling technique used to compute confidence intervals of statistics such as mean, standard deviation, or other. It is performed by sampling a dataset with replacement without assumptions about distributions or variances [Hesterberg(2011)]. In our work, we use bootstrap to estimate the confidence interval of the mean statistic.

3.7 Evaluation

We compare all our proposed methods with STMF on synthetic datasets, while on real datasets we compare the proposed FastSTMF with NMF and STMF. Since we cannot directly compare the tested methods and STMF by the number of iterations, we measure their errors \(\text{NE}_t\) at regular wall clock time points \(t\) during execution. We limit the execution to the wall clock running time \(t_{\text{max}}\). We then observe the running time needed to achieve STMF’s final \(\text{NE}_{t_{\text{max}}}\) and use the running time to rank the methods. We also rank the methods by their final \(\text{NE}_{t_{\text{max}}}\) error at running time \(t_{\text{max}}\). For large synthetic datasets and large real datasets, we set the maximum running time to \(t_{\text{max}} = 600s\). For small synthetic datasets, we set the time to \(t_{\text{max}} = 100s\). For small real datasets, we set the time to \(t_{\text{max}} = 300s\), since all methods converge faster on smaller data. We evaluate the proposed methods on a server with 48 cores on two 2.3 GHz Intel CPUs and 492 GB RAM. For a fair comparison and to prevent the methods from interrupting each other, we run experiments in parallel and ensure that the CPUs never reach full load.

We perform ten runs with different initializations of factor matrices on each dataset and select the median NE. Experiments on synthetic data used factorization rank three, but the experiments on real data were performed for the selected optimal factorization rank, already chosen in [Omanovic et al.(2021), see Table 3]. We randomly and uniformly mask 20% of data as missing for all datasets, which we use as a test set for the prediction task.

4 Results

We use synthetic data to improve all proposed algorithms and to choose which method to name FastSTMF. We then performed experiments on small and large real data matrices to compare the performance of the models obtained by STMF, FastSTMF, and NMF. We do not compare with the Cancer method, as it cannot predict missing values.
4.1 Synthetic data

First, we demonstrate the benefits of using tropical distance versus sequential selection of indices on small synthetic matrices. Second, we use large synthetic training data to determine the data matrix shape (wide or tall matrix) where each proposed method achieves the smallest error (we refer to it as the method’s preferred shape) of the input data matrix. We then include the appropriate transposition of the input data at the beginning of each method and evaluate the performance on the synthetic validation data.

4.1.1 Comparing selections in the ByRow strategy

We compare selections TD, TD_A, TD_B and SEQ as described in Subsection 3.2.1. The performance between tropical distance selection, sequential selection and NMF differs depending on different $\lambda$ values (see Figure 1). As expected, when $\lambda = 0$, NMF achieves best approximation since the data has linear structure, while for tropical structure ($\lambda = 1$), TD methods achieve almost perfect approximation. In the case of mixed linear-tropical structure ($\lambda = 0.5$), TD_A and TD_B selections have best results. NMF uses the Frobenius norm in the optimization process, which is monotone decreasing. The reason why the NMF’s error slightly increases in Figure 1 is because we are using the $b$-norm in NE computation, which allows us to compare all methods fairly (see Supplementary Figure S11).

![Figure 1](image1.png)

Figure 1: Comparison of the median NE and the first and third quantiles between sequential selection (SEQ) of indices, tropical distance (TD) selections, and NMF for different ByRow strategies on one small synthetic dataset for: (a) $\lambda = 0$, linear structure, (b) $\lambda = 0.5$, mixture and (c) $\lambda = 1$, tropical structure. The black horizontal dashed line represents STMF’s final $NE_{t_{\text{max}}}$, while the grey horizontal dashed line represents perfect approximation, i.e., approximation error being equal to 0.

The results of NE for all 50 datasets are summarized in a graph showing the ranking of methods (Figure 2). For each second of running time, we rank the methods by their current NE and compute the average ranking and the 95% confidence interval.

![Figure 2](image2.png)

Figure 2: Average rankings with 95% confidence interval from bootstrap on 50 datasets for: (a) $\lambda = 0$, linear structure, (b) $\lambda = 0.5$, mixture, and (c) $\lambda = 1$, tropical structure.

We rank the methods by the time needed to achieve STMF’s final $NE_{t_{\text{max}}}$ and by their final $NE_{t_{\text{max}}}$. If value $\lambda$ is known in advance, we can choose the specific selection method as the best choice, as shown in Supplementary Figures S12, S13, and S14. We show in Figure 3(c) the average ranking for all $\lambda$ values that may be used when there is no prior knowledge about $\lambda$. Figure 3(c) shows the average ranking when both criteria STMF’s final $NE_{t_{\text{max}}}$ and final $NE_{t_{\text{max}}}$ are
taken into account. Methods that use the TD_A selection achieve the best results according to all three criteria. Based on this, we focus on the TD_A methods in the ByRow strategies.

![Figure 3: CD graph of averaged rankings for all three values of \( \lambda \in \{0, 0.5, 1\} \) on 50 datasets. Ranking of methods using different criteria: (a) time needed to achieve STMF’s final \( NE_{t_{\text{max}}} \), (b) final \( NE_{t_{\text{max}}} \) of its method and (c) averaged rankings of both (a) and (b).]

The TD_A selection contains two methods: STMF_ByRow_PermR_TD_A and STMF_ByRow_NoPerm_TD_A, which work best on the mixed linear-tropical structure (\( \lambda = 0.5 \)). The NoPerm version of the method achieves better rankings than PermR for all three values of \( \lambda \) (see Figure 2). Thus, we continue our synthetic experiments with the \( \lambda = 0.5 \) and the NoPerm version.

Since experiments are performed on randomly generated synthetic datasets where the order of rows bear no meaning, we notice that the NoPerm is a special case of RandPerm. On the contrary, in real datasets, rows can have meaning and their initial permutation (NoPerm) can contain a structure that could lead to a biased approximation. An example of such a real-world dataset would be the gene expression data matrix, where cells are sorted by their class (e.g., healthy cells first and then cancer cells). In limited running time, it could happen that the ByRow strategy would fit only a single class and not the entire matrix. We decide to address this issue by performing a random permutation of the rows RandPerm before fitting the data. The motivation comes from other machine learning resampling procedures, such as cross-validation, where data are shuffled randomly at the beginning, or in stochastic gradient optimization where data can be shuffled after each epoch to reduce overfitting and variance [Bottou(2012)]. Based on this, we decide to use STMF_ByRow_RandPerm_TD_A as the best representative of the ByRow strategy in the rest of the paper.

### 4.1.2 Determining the preferred shape on training data

In our experiments, the 50 generated synthetic 10000 \( \times \) 300 matrices are tall, since the number of rows is greater than the number of columns. Moreover, we transpose each of the matrices to obtain a 300 \( \times \) 10000 wide matrix. Since \((U \otimes V)^T = V^T \otimes U^T\), transposing each matrix into a tall dataset is an equivalent but faster way of constructing a wide dataset compared to generating a new wide synthetic dataset. For each method, we test tall and wide synthetic matrices to verify on which matrix shape a method returns a smaller approximation error. The value \( \omega \) reports the proportion of tests when a smaller error is achieved on the wide matrix compared to the tall matrix. The algorithm would not have a preferred matrix shape when \( \omega = 0.5 \). Tall matrices perform better than wide matrices when \( \omega = 0 \), while \( \omega = 1 \) indicates that the wide matrix shape is better than the tall matrix shape. In our case, the strategies ByElement, ByMatrix and ByRow achieve \( \omega = 0.92 \), \( \omega = 0.92 \) and \( \omega = 1.0 \), respectively. We repeat the procedure for 100 synthetic datasets, 50 tall and 50 wide (for results on one dataset, see Figure 4). For each method, we compute the distribution of the differences between the final errors on tall and wide matrices. We used the mean value of the distribution (red vertical line) in Figure 5 to decide for each method whether it performs better on tall or wide matrices. All the methods tested perform better on wide matrices. Note that ByRow strategy on wider matrices is closer to ByMatrix strategy, but on taller matrices closer to ByElement strategy. Hence we see the reason for ByRow strategy preferring wide matrices in choosing precision of the ByMatrix strategy over the fast but less accurate choice of indices in the ByElement strategy. The another potential reason for the preference for wide over tall matrices in all three proposed strategies is the Random Arcol initialization of matrix \( U \). Note that Random Arcol uses random columns of the data matrix \( R \) to initialize matrix \( U \), and it better transfers the variance from the data when selecting columns in the wide matrix than in the tall matrix, resulting in better initialization. In the case of a limited running time on large data matrices, the initialization step is crucial, making the wide matrix the preferred shape for all proposed strategies.
Figure 4: Comparison of median NE among different methods on one example of large synthetic rank three training data matrix presented in a tall matrix of size $10000 \times 300$ and a wide matrix of size $300 \times 10000$.

Figure 5: Distribution of differences between final errors on tall and wide matrices, where negative values mean that error on tall matrices is smaller than on wide, while positive values indicate that error on wide matrices is smaller than on tall. The mean value (red line) denotes the mean of the distribution of differences.

4.1.3 Selecting the FastSTMF method on validation data

Given the results on synthetic training data, we include a step for checking the matrix shape at the beginning. Each of the methods first inspects the shape of the matrix and, if necessary, transposes the matrix to a wider shape.

We rank the methods by the time needed to achieve STMF’s final $NE_{t_{\text{max}}}$, see Figure 5. If the method never achieves the final STMF’s $NE_{t_{\text{max}}}$, it gets the lowest ranking, and if the two methods achieve error at the same time, they share the ranking position.
Figure 6: Median NE between methods on one large synthetic test rank three matrix of size $10000 \times 300$. Note that STMF does not use matrix transposition, so it has a larger error at the beginning compared to other methods.

When we compare the three proposed methods with STMF on synthetic validation data, we conclude that there are two groups of methods that differ significantly, see CD graph in Figure 7. The first group consists of our three proposed methods, and there is no significant difference between them. The second group contains only the original STMF method. The average ranking on 50 datasets is the highest for the STMF_ByRow_RandPermR_TD_A_W method (see Algorithm 3), which we propose as FastSTMF (Table 2).

Figure 7: Critical difference (CD) graph of average performance ranks from Table 2 for different methods tested on 50 large validation datasets, for $\alpha = 0.05$.

Table 2: The average ranking of time needed to achieve STMF’s final $\text{NE}_{t_{\text{max}}}$ for proposed methods on 50 large synthetic validation datasets.

| Method                                      | Average Ranking |
|---------------------------------------------|-----------------|
| STMF                                        | 3.54            |
| STMF_ByElement_Permc_TD_W                  | 1.32            |
| STMF_ByRow_RandPermR_TD_A_W (FastSTMF)      | 1.26            |
| STMF_ByMatrix_NoPerm_TD_W                  | 1.54            |

4.2 Real data

In Table, we present the results on the predicted performance, measured with DC, RMSE-P, and RMSE-A, for small datasets. We have already shown [Omanović et al. (2021)] that on six out of nine datasets, STMF outperforms NMF according to DC. Most DC values are improved by FastSTMF and therefore FastSTMF outperforms STMF and NMF on most datasets. Moreover, FastSTMF also achieves a smaller RMSE-A compared to STMF, but NMF still achieves the smallest RMSE-A in most cases. However, in most cases, RMSE-P is the highest for NMF, indicating its tendency to overfit. STMF and FastSTMF do not have this issue, which we can see from the fact that the differences in RMSE-A and RMSE-P are minor.
Table 3: Median DC, median RMSE-P and median RMSE-A of final (at $t_{\text{max}}$) approximation matrix on gene expression data on small datasets. Result of the best method in the comparison between STMF and FastSTMF is shown in bold. Best result among all three methods (STMF, FastSTMF, NMF) are indicated by asterisk.

Table 4: Median DC, median RMSE-P and median RMSE-A of final (at $t_{\text{max}}$) approximation matrix on gene expression data on large datasets. Result of best method in the comparison between STMF and FastSTMF shown in bold. Best result among all three methods (STMF, FastSTMF, NMF) indicated by asterisk.

Table 5 includes DC, RMSE-P, and RMSE-A for large datasets. We can see that according to DC, FastSTMF outperforms STMF on most datasets, however their RMSE results are similar. In all cases except GBM, where the winner is FastSTMF, the best results among the three methods are achieved by NMF. This behavior is very different from the one computed on small datasets. We believe that the reason behind this is that NMF tends towards the mean value of the data matrix entries, while FastSTMF and STMF can better fit to extreme values and distributions. Hence, the errors of the non-extremal entries are large, which in high-dimensional data matrices produces a larger RMSE of FastSTMF and STMF compared to NMF.

Figure 9 shows the results on the small and large SARC data where we can see that FastSTMF achieves a smaller final NE$_{t_{\text{max}}}$ compared to STMF and NMF. Moreover, FastSTMF reaches smaller NE than STMF's in dozens of seconds and NMF's final NE in sixty seconds. As we expected, NMF converges quickly, but it does not improve over time. For all other small datasets, similar figures are available in Supplement, Section A.1.

Figure 10 shows the results on the small and large SARC data where we can see that FastSTMF achieves a smaller final NE$_{t_{\text{max}}}$ faster than STMF. Moreover, FastSTMF reaches smaller NE than STMF's final NE$_{t_{\text{max}}}$ in dozens of seconds, see Figure 10(a). NMF converges quickly and achieves the smallest NE compared to other methods since it also achieves the smallest RMSE-A in Tables 3 and 4. For all other large datasets, the figures are available in Supplement, Section A.2.
5 Conclusion

Matrix factorization methods are one of the most widely used techniques in machine learning with various applications. The redefinition of basic operations, which mainly used standard linear algebra, enables to develop nonlinear models. However, all recent tropical semiring matrix factorization models have the main drawback in the slow optimization process, and in our work, we improve the speed of previous methods, while also achieving better results.

In this paper, we evaluate three strategies ByElement, ByRow and ByMatrix resulting in twelve methods tested on three types of structure in synthetic data: linear structure ($\lambda = 0$), tropical structure ($\lambda = 1$) and their mixture ($\lambda = 0.5$). ByRow strategy achieves better results than ByElement and ByMatrix since its update is focused on only one entry in each row. ByMatrix strategy is extremely slow compared to other two strategies, since it firstly compares the errors of all matrix elements before the update. On the other extreme, ByElement iterates quickly, but it often chooses wrong elements to update since it chooses locally and does not consider the impact of the update on the approximation of the rest of the matrix. ByRow strategy solves these problems by partitioning the matrix into rows and finding the best column and factor candidates that have the largest impact not only on the row, but also on the corresponding column. In this way, the ByRow strategy achieves the best results by being faster than the ByMatrix strategy and more accurate than the ByElement strategy. For them we tested different $td$-based heuristics that have different efficiencies for different choices of $\lambda$, so for a specific data pattern one might compare and select the most appropriate heuristic. We proved that $TD_A$ selection, which is more global than $TD$ selection, gives the best results when there is no prior knowledge about $\lambda$.

We propose an algorithm based on tropical semiring called FastSTMF, which has proven to be an efficient matrix factorization method for the prediction of missing values (matrix completion task). FastSTMF is based on STMF, but it introduces a new way of updating factor matrices, which results in higher performance, i.e., achieving better results in a shorter time. The results on synthetic data show that FastSTMF outperforms STMF in achieving a smaller approximation error in less time, while on real small data FastSTMF outperforms STMF and NMF in achieving a higher distance correlation and a smaller prediction and approximation error. The results on real large data confirm the superior performance of FastSTMF over STMF in terms of distance correlation, but it is shown that NMF outperforms both methods if we have high-dimensional data.

A limitation of our FastSTMF method is its inability to achieve comparable results on high-dimensional data to methods that use standard linear algebra. In our future work, we should explore how to reduce the dimensionality of the data to select more suitable features for tropical optimization. Another drawback in the algorithm’s speed is in the update procedure compared to methods that use standard linear algebra. NMF uses gradient descent and updates all factor matrices’ values simultaneously. Since the gradient descent cannot be used in tropical semiring, we change the entries of only one column of the coefficient factor and only one row of the basis factor in one update step (F-ULF or F-URF). With this, we guarantee the convergence of FastSTMF, but addressing the simultaneous update of more rows and columns of factor matrices in tropical semiring deserves further detailed research. Note that RMSE favors the normally distributed data and models that tend toward the mean approximation, such as NMF. On the other hand, FastSTMF prefers extreme values and hence RMSE penalizes the large errors of the non-extremal entries. We should explore which metrics could better compare different methods independently of preferred data distribution. Our ideas articulate a wide range of research questions of dependence of proposed methods on different probability distributions for generating synthetic datasets (e.g., beta, Poisson), and also the question whether substituting the $b$-norm in our objective function with the $\ell_\infty$-norm [Maragos et al.(2021)] would give better results.
This paper presents a novel and faster way to guide the optimization process in matrix factorization methods based on tropical semiring. We show how to identify the best method based on the patterns that appear in the data. We believe that the proposed FastSTMF and its variants are essential to develop other techniques based on general semirings, which could help to find different structures not explainable by standard linear algebra.

**Author’s contributions**

AO, TC and PO designed the study. AO wrote the software application and performed experiments. AO and TC analyzed and interpreted the results on real data. AO wrote the initial draft of the paper and all authors edited and approved the final manuscript.

**Declaration of Competing Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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**Availability of data and materials**

This paper uses the real TCGA data available on [http://acgt.cs.tau.ac.il/multi_omic_benchmark/download.html](http://acgt.cs.tau.ac.il/multi_omic_benchmark/download.html). PAM50 data can be found on [https://github.com/CSB-IG/pa3bc/tree/master/bioclassifier_R/](https://github.com/CSB-IG/pa3bc/tree/master/bioclassifier_R/). BIC subtypes are collected from [https://www.cbioportal.org/](https://www.cbioportal.org/) STMF code, PAM50 data and BIC subtypes are available on [https://github.com/Ejmric/FastSTMF](https://github.com/Ejmric/FastSTMF).

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Supplementary material

A  Performance comparison

Supplementary Figure S 10: Difference between ULF and F-ULF.

Supplementary Figure S 11: Comparison between Frobenius and $b$-norm norm in NMF.

Supplementary Figure S 12: CD graphs for $\lambda = 0$. Average rankings of methods and critical difference (CD) at 0.05 significance level calculated on 50 datasets.

(a) Ranking on time needed to achieve STMF’s final $\text{NE}_{t_{\text{max}}}$.

(b) Ranking on final $\text{NE}_{t_{\text{max}}}$.

Supplementary Figure S 13: CD graphs for $\lambda = 0.5$. Average rankings of methods and critical difference (CD) at 0.05 significance level calculated on 50 datasets.

(a) Ranking on time needed to achieve STMF’s final $\text{NE}_{t_{\text{max}}}$.

(b) Ranking on final $\text{NE}_{t_{\text{max}}}$.
(a) Ranking on time needed to achieve STMF's final $NE_{t_{\text{max}}}$.

(b) Ranking on final $NE_{t_{\text{max}}}$.

Supplementary Figure S 14: CD graphs for $\lambda = 1$. Average rankings of methods and critical difference (CD) at 0.05 significance level calculated on 50 datasets.
A.1 Small datasets, normalized errors of Fast-STMF, STMF and NMF

Supplementary Figure S 15: AML small

Supplementary Figure S 15: COLON small

Supplementary Figure S 16: GBM small

Supplementary Figure S 16: LIHC small

Supplementary Figure S 17: LUSC small

Supplementary Figure S 17: BIC small

Supplementary Figure S 18: SARC small

Supplementary Figure S 18: SKCM small
A.2 Large datasets, normalized errors of Fast-STMF, STMF and NMF

Supplementary Figure S 19: AML large

Supplementary Figure S 19: COLON large

Supplementary Figure S 20: GBM large

Supplementary Figure S 20: LIHC large

Supplementary Figure S 21: LUSC large

Supplementary Figure S 21: OV large

Supplementary Figure S 22: SARC large

Supplementary Figure S 22: SKCM large
B Pseudocodes

### STMF_ByElement_PermC_TD_W

**Input:** data matrix \( R \in \mathbb{R}^{m \times n} \), factorization rank \( r \)

**Output:** factorization \( U \in \mathbb{R}^{m \times r} \), \( V \in \mathbb{R}^{r \times n} \)

if \( R \) not wide then transpose \( R \)

\( perm \leftarrow \) permutation that orders columns in \( R \) by the minimum value in the increasing order

\( R \leftarrow R[:, perm] \)

initialize \( U \) and compute \( V \)

while not converged do

  for each element \((i, j)\) of \( R \)

  \( k \leftarrow f(i, j) \)

  \((U, V, f, U'_k, V'_k) \leftarrow F-ULF(R, U, V, i, j, k)\)

  if \( f \) decreases then break

  else \((U_k, V_k) \leftarrow (U'_k, V'_k)\)

  \((U, V, f, U'_k, V'_k) \leftarrow F-URF(R, U, V, i, j, k)\)

  if \( f \) decreases then break

  else \((U_k, V_k) \leftarrow (U'_k, V'_k)\)

if \( R \) transposed then \((U, V) \leftarrow (V[:, perm^{-1}]^T, U^T)\)

else \((U, V) \leftarrow (U, V[:, perm^{-1}])\)

return \( U, V \)

---

### STMF_ByMatrix_NoPerm_TD_W

**Input:** data matrix \( R \in \mathbb{R}^{m \times n} \), factorization rank \( r \)

**Output:** factorization \( U \in \mathbb{R}^{m \times r} \), \( V \in \mathbb{R}^{r \times n} \)

if \( R \) not wide then transpose \( R \)

initialize \( U \) and compute \( V \)

while not converged do

  rows \( \leftarrow \{\text{td}_\text{row}(R, U, V, i): i = 1, \ldots, m\}\}

  cols \( \leftarrow \{\text{td}_\text{col}(R, U, V, j): j = 1, \ldots, n\}\}

  errors, errors_indices \( \leftarrow [\], [\] \)

  for each element \((i, j)\) of \( R \)

  \( e \leftarrow \text{rows}[i] + \text{cols}[j] - \text{td}(R, U, V, i, j) \)

  append \( e \) to \( \text{errors} \)

  append \((i, j, f(i, j))\) to \( \text{errors_indices} \)

  for each \( d \) in \( \text{argsort(\text{errors})} \) in decreasing order

  \((i, j, k) \leftarrow \text{errors_indices}[d]\)

  if \( \text{random()} < 0.5 \) then \((U, V, f, U'_k, V'_k) \leftarrow F-ULF(R, U, V, i, j, k)\)

  else \((U, V, f, U'_k, V'_k) \leftarrow F-URF(R, U, V, i, j, k)\)

  if \( f \) decreases then break

  else \((U_k, V_k) \leftarrow (U'_k, V'_k)\)

if \( R \) transposed then \((U, V) \leftarrow (V^T, U^T)\)

else \((U, V) \leftarrow (U, V)\)

return \( U, V \)