SimTensor: A synthetic tensor data generator

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Abstract
SimTensor is a multi-platform, open-source software for generating artificial tensor data (either with CP/PARAFAC or Tucker structure) for reproducible research on tensor factorization algorithms. SimTensor is a stand-alone application based on MATLAB. It provides a wide range of facilities for generating tensor data with various configurations. It comes with a user-friendly graphical user interface, which enables the user to generate tensors with complicated settings in an easy way. It also has this facility to export generated data to universal formats such as CSV and HDF5, which can be imported via a wide range of programming languages (C, C++, Java, R, Fortran, MATLAB, Perl, Python, and many more). The most innovative part of SimTensor is this that can generate temporal tensors with periodic waves, seasonal effects and streaming structure. it can apply constraints such as non-negativity and different kinds of sparsity to the data. SimTensor also provides this facility to simulate different kinds of change-points and inject various types of anomalies. The source code and binary versions of SimTensor is available for download in http://www.simtensor.org.

Keywords: Tensor factorization, CP, Tucker, data generator, synthetic data

1. Introduction
Tensor factorizations have lots of applications in data mining, machine learning, and signal processing as well as chemometrics, and computer vision (Kolda and Bader, 2009; Mørup, 2011; Fanaee-T and Gama, 2016b; Papalexakis et al., 2016). Obviously any improvement in the accuracy of tensor factorization algorithms advances the state-of-the-art in the above-mentioned domains. Developing accurate algorithms for tensor factorization require benchmark data sets with various realistic adjustable configurations. One of the characteristics that is not included in many existing tensor data generators is time-changing behavior of realistic tensors as well as many real issues such as change-points and anomalies. The objective of SimTensor is to provide a standard and comprehensive framework for generating synthetic tensor structured data with focus on the time-changing characteristics of data. The SimTensor is developed based upon of many available codes and techniques in the literature of tensor analysis. So it is benefited a lot from the open-source contributions. Our methodology was to carefully study the available features and considered issues

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in the existing data generators and the presented approaches in the literature for creating test problems. Besides, some ideas such as injecting anomalous tensor is being presented for the first time in SimTensor and is not reported elsewhere. Therefore, SimTensor can be considered as the state-of-the-art tool for generating synthetic tensor data with either CP (Carroll and Chang, 1970; Carroll et al., 1980) or Tucker (Tucker, 1966) structure with focus on time-changing tensors that are very realistic in many applications.

The existing data generators featured in toolboxes such as Tensor Toolbox (Bader et al., 2015) and N-Way Toolbox (Andersson and Bro, 2000) are presented as functions in MATLAB. Hence the access of users of other programming environments is limited since MATLAB is a licensed software. The SimTensor provides a stand-alone solution for wider range of practitioners who develop tensor factorization algorithms in various programming languages and operating systems and want to test their algorithms with several realistic configurations. Therefore, it is expected that SimTensor can contribute to reproducible research on tensor factorization algorithms. It is also open-source, so the community can actively contribute to the project and add their desired features to it according to the requirements that are not considered in the current version.

2. Generating Non-temporal Random Factors

One of the basic step to generate synthetic tensors with CP structure is to create random factor matrices $U^{(n)}$ and then compute sum of multiway-way outer products:

$$x_{ijk} = \sum_{r=1}^{R} u^{(1)}_{ir} u^{(2)}_{jr} u^{(3)}_{kr}.$$  \hspace{1cm} (1)

Where $R$ is the number of components, $I, J, K$ represent the size of tensor in each dimension, and $N$ is order of tensor. If we assume that columns of $U^{(n)}$ are normalized we can introduce the vector $\lambda \in \mathbb{R}^{R}$ and re-write (1) as:

$$x_{ijk} = \sum_{r=1}^{R} \lambda_{r} u^{(1)}_{ir} u^{(2)}_{jr} u^{(3)}_{kr}.$$  \hspace{1cm} (2)

For the Tucker tensor in addition to factor matrices we have to generate a random core tensor $G$ as well. For instance, for a third-order tensor we have:

$$x_{ijk} = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \sum_{r_3=1}^{R_3} g_{r_1 r_2 r_3} u^{(1)}_{ir_1} u^{(2)}_{jr_2} u^{(3)}_{kr_3}.$$  \hspace{1cm} (3)

In order to generate $U^{(n)}$ we can use different approaches. These techniques will be described in the following subsections.

2.1 Gamma Distribution

In SimTensor, the module gamma generates random factors from $\Gamma(k, \theta)$ where $\Gamma$ is Gamma function, $k$ is positive scalar value called shape parameter, and $\theta$ is nonnegative scalar value called scale parameter. As (Hu et al., 2015) in SimTensor we choose $k$ from $|N(\mu, \sigma^2)|$
where $\mathcal{N}$ is Gaussian distribution, $\mu$ is mean, and $\sigma^2$ is variance. In SimTensor, by default $\mu$ and $\sigma^2$ are set as 0.1 and $\theta$ is set as 0.01.

### 2.2 Multivariate Gaussian Distribution

The module `multi_normal_dist` allows to generate $R$ columns in factor matrix via multivariate Gaussian distribution with different $\mu$ and $\sigma$ parameters (Zhao et al., 2016) for each column. In SimTensor by default $\mu$ and $\sigma$ are set as 0 and 1, for all columns.

### 2.3 Uniformly Distributed Random Numbers

The module `rand` in SimTensor generates random factors with uniformly distributed random numbers on $[0,1]$. This method is widely used for generating random factors, for instance in Tensor toolbox (Bader et al., 2015) and elsewhere.

### 2.4 Standard Normal Distribution

The module `randn` generate factor matrices drawn from the standard normal distribution with $\mu = 0$ and $\sigma = 1$ for all columns. Note that in the current version of SimTensor `randn` is identical to module `multi_normal_dist`. Because by default we set $\mu = 0$ and $\sigma = 1$ in all columns for both methods. However, `multi_normal_dist` opposed to `randn` has this ability to generate columns in factor matrices with different $\mu$ and $\sigma$. The `randn` module is also used in Tensor toolbox (Bader et al., 2015) for creating test problems.

### 2.5 Random Orthogonal Matrices

The module `orthogonal` is borrowed from Tensor toolbox (Bader et al., 2015) and generates a random $n \times n$ orthogonal matrix, a matrix distribution uniform over the manifold of orthogonal matrices with respect to the induced $\mathbb{R}^{n^2}$ Lebesgue measure (Shilon, 2016).

### 2.6 Stochastic

The module `stochastic` as its equivalent in Tensor toolbox (Bader et al., 2015) generates nonnegative factor matrices so that each column sums to one. This method works as follow. First, a factor matrix of $U^n \in \mathbb{R}^{I^n \times R^n}$ is generated via uniformly distributed random numbers on $[0,1]$. Then the sum of each column of $U^n$ is obtained and stored in vector $S$. Final generated matrix is obtained by multiplying $U^n$ to diagonal matrix of $S^{-1}$.

### 2.7 Binary factors

The idea of binary factors is borrowed from work of (Sakurai, 2016) that creates boolean synthetic tensor by generating random binary factors. The method is very simple. First, we generate matrix of $U^n \in \mathbb{R}^{I^n \times R^n}$ filled with zero. Then for each row of matrix we randomly fill one column of matrix with one, such that in each row we will have only one column with one.
2.8 Random Core Tensor/Lambda Generator

SimTensor allows the user to generate random core/tensor (for Tucker) and lambda (for CP). The methods include vector of ones (ones), uniformly distributed random numbers (rand), and standard normal distribution (randn). The user also can customize the generated vector. For Tucker case the generated vector is automatically transformed to the core tensor.

3. Generating Temporal Random Factors

SimTensor enables the user to create temporal factors with different strategies such as periodic waves, seasonal effects, and streaming.

3.1 Periodic waves

In SimTensor is possible to simulate periodic waves such as Cosine, Sine, as well as Square and Sawtooth waves. The user is able to determine the number of waves and frequency of waves in each setting. The idea is inspired by (Lemm et al., 2011) for generating artificial data for testing algorithms for factroization of shift-invariant multilinear data which is a real case in neuroimaging data.

3.2 Seasonal effects

Seasonal effects are very realistic for those data sets that are generated by humans. In such data sets there is a repeating pattern during specific time interval such as days, weeks, seasons, and so forth. For instance, in disease surveillance data (Fanaee-T and Gama, 2015a) disease outbreaks such as Influenza are more frequent in winters. In computer networks different traffic usage pattern can be detected. For instance, it is observed that traffic peak occurs around mid-day and during the night (Tune and Roughan, 2013). In transportation systems the peak of traffic is on the morning when people go to work and evening when they back home (Tan et al., 2013). There are lots of examples of such temporal seasonality. In SimTensor is possible to simulate different seasonal effects with various temporal granularities. Sometimes also in some other applications such as animal migration we may find some specific seasonality patterns which can be different from human-centered systems. In SimTensor the user is able to define some customized seasonal effects like this as well. The user also is able to define a particular growth rate. In this case, the data items in each cycle will be multiplied by a weight.

As in many realistic scenarios (e.g. in transportation systems) also we may experience multiple seasonality patterns in data. It is extremely easy to simulate such scenarios in SimTensor with defining multiple factors with different seasonal grounds.

3.3 Streaming tensor

In the approach that is exploited in (Nion and Sidiropoulos, 2009) for generating time-varying factor matrices it is assumed that data arrives in a streaming fashion and it is expected that data in \( t+1 \) is a sample of data of \( t \) with some little changes. This change is controlled by a parameter that is called variation control parameter and can be defined by
the user. This can be used for evaluation of any incremental or streaming tensor analysis algorithm (Sun et al., 2008; Zhou et al., 2016; Fanaee-T and Gama, 2015b).

4. Simulating Change Points

Shifts and drifts are realistic characteristics in many applications. It is important to assess the performance of tensor factorization algorithms in dealing with such changes. In SimTensor it is possible to create artificial change points in the factor matrices related to the temporal dimension. Depending on the defined period by the user different types of changes can be simulated, including temporary changes, structural shifts, and singular outliers. For instance, if temporal mode has size of 100, the user can simulate a shift by defining the change point with start point of 51 and end point of 100. Example of short-term changes (or events) can be start point of 20 and end point of 25. And finally if user is interested to simulate singular changes (or temporal outliers) she can define start/end point at the same time instant.

5. Simulating Anomalies

Those patterns in data that do not conform to expected behavior are called anomalies (Chandola et al., 2009; Fanaee-T and Gama, 2016b). In different contexts anomalies may have diverse interpretations. In medical domain, for instance it can be translated to disease outbreak. In industrial settings it might be a fault. Or in transportation systems it might be translated as a events (Fanaee-T and Gama, 2016a). However, anomalies are different from outliers, in the sense that anomalies occur in a systematic way. In fact anomalies are generated by anomalous process while outliers can be only small errors in information systems or data gathering (Fanaee-T et al., 2014). In SimTensor we for the first time propose a new method for simulating anomalies. The idea is that we first create a smaller random tensor with CP structure and then inject it inside the bigger generated tensor. Actually we replace a small portion of the original tensor with the new generated tensor. This will be a challenge for tensor factorization algorithms to discover this small injected tensor. It is assumed that those approaches that can detect the smaller tensor should perform well for detecting anomalies from tensor-structured data.

6. Simulating Noise

Noise is the inherent part of many data sets. Three methods are available in SimTensor for simulating noises. The user is able to apply noise directly to the factor matrices; apply an additive white Gaussian noise with controllable noise level on the final generated tensor (more common) via the method of (Viswanathan, 2015); or apply sparse white noise on the final tensor.

7. Constraints on factor matrices

SimTensor enables the user to add non-negativity constraint in two ways, either on factor matrices or on the final tensor. The user can also apply different constraints such as correlation between columns in the factor matrices on the factor matrices or angle between
| Component                  | Module                | Target tensor factorization algorithm | Target Data                                            |
|---------------------------|-----------------------|---------------------------------------|--------------------------------------------------------|
| Non-temporal factor generator | rand, randn, multinormal,list | Traditional approaches, for example CP-ALS (Carroll and Chang, 1970; Carroll et al., 1980) or Tucker-ALS (Tucker, 1966)  | High quality multi-linear data                          |
| Orthogonal                | HOSVD (De Lathauwer et al., 2000b), HOOI (De Lathauwer et al., 2000a) or similar |                          | High quality multi-linear data                          |
| Stochastic                | Non-negative algorithms like (Carroll et al., 1989; Kim and Choi, 2007) |                          | Visual data (e.g. image or video) and count data (e.g. recommender systems) |
| Binary                    | Boolean algorithms such as (Miettinen, 2011) |                          | Social network data                                    |
| Temporal factor generator | Periodic waves        | Shift-invariant TD algorithms like ShiftCP (Morup et al., 2008) | Neuroimaging data (e.g. EEG)                          |
| Seasonal effects          | All Algorithms        |                          | Human generated data sets (e.g. Internet traffic, mobility data, etc.) |
| Streaming                 | Online Algorithms like PARAFAC-SDT (Nion and Sidiropoulos, 2000), OnlineCP (Zhou et al., 2016) or similar |                          | Streaming data                                          |
| Change-points             | Incremental algorithms such as DTA, STA, or WTA (Sun et al., 2008) |                          | Temporal tensors                                       |
| Effects                   | Anomalies             | All algorithms (with focus on the evaluation of model’s discriminability) | Data sets with structural anomalies                    |
|                          | Noise                 | All algorithms (with focus on the evaluation of model’s power) | All Data sets                                           |
|                          | Non-negativity constraints | Non-negative algorithms like (Carroll et al., 1989; Kim and Choi, 2007) | Visual data (e.g. image or video) and count data (e.g. recommender systems) |
|                          | Sparsity constraints  | Sparse-friendly algorithms such as (Kolda and Sun, 2008) | Incomplete data sets                                    |
|                          | Sparse Count Tensors  | Sparse Bayesian algorithms such as (Hu et al., 2015) | Large-scale sparse count data in recommender systems and social networks |

Table 1: A guide to choose the the component and module in SimTensor for evaluation of a specific tensor factorization algorithm or testing an algorithm in a particular application.

columns of the factor matrices. Note that this can be applied to non-temporal modes. It is also possible to normalize the final tensor or perform a sign fix operation on the final tensor.

8. Generating Sparse tensors

Three mechanisms are included for generating sparse tensors. The first one is to apply sparsity constraint on the factor matrices by randomly removing non-zero elements from the dense created factor matrices. The second strategy is to generate CP or Tucker tensor with the dense factor matrices and then remove some random non-zero elements. The third methodology is to create sparse count tensors based on the idea of (Hu et al., 2015). In this method we firstly generate random factors with Gamma random numbers. Then we create CP tensor with the generated random factors and finally feed this tensor as input parameters for generating tensor with Poisson distribution. This kind of synthetic data can be used for evaluation of Bayesian tensor factorization algorithms (Hu et al., 2015).
9. How to use SimTensor?

Depending on the evaluation objective SimTensor can generate synthetic data for various family of tensor factorization algorithms. It also can create data sets with different realistic characteristics that exists in many applications. In Table 1 a guide is presented to choose the right module and component for generating synthetic tensor when any specific type of algorithms or data sets is desired.

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