# Automating the Detection of Anomalies and Trends from Text <br> NGDM'07 Workshop <br> Baltimore, MD 

Michael W. Berry

Department of Electrical Engineering \& Computer Science
University of Tennessee

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## NNMF Origins

- NNMF (Nonnegative Matrix Factorization) can be used to approximate high-dimensional data having nonnegative components.
- Lee and Seung (1999) demonstrated its use as a sum-by-parts representation of image data in order to both identify and classify image features.
■ Xu et al. (2003) demonstrated how NNMF-based indexing could outperform SVD-based Latent Semantic Indexing (LSI) for some information retrieval tasks.


## NNMF for Image Processing



Sparse NNMF verses Dense SVD Bases; Lee and Seung (1999)
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## NNMF Analogue for Text Mining (Medlars)



Interpretable NNMF feature vectors; Langville et al. (2006)

## Derivation

- Given an $m \times n$ term-by-document (sparse) matrix $X$.

■ Compute two reduced-dim. matrices $W, H$ so that $X \simeq W H$; $W$ is $m \times r$ and $H$ is $r \times n$, with $r \ll n$.

- Optimization problem:

$$
\min _{W, H}\|X-W H\|_{F}^{2}
$$

subject to $W_{i j} \geq 0$ and $H_{i j} \geq 0, \forall i, j$.
■ General approach: construct initial estimates for $W$ and $H$ and then improve them via alternating iterations.

## Minimization Challenges and Formulations [Berry et al., 2007]

- Local Minima: Non-convexity of functional $f(W, H)=\frac{1}{2}\|X-W H\|_{F}^{2}$ in both $W$ and $H$.
- Non-unique Solutions: $W D D^{-1} \mathrm{H}$ is nonnegative for any nonnegative (and invertible) $D$.
■ Many NNMF Formulations:
- Lee and Seung (2001) - information theoretic formulation based on Kullback-Leibler divergence of $X$ from WH.
- Guillamet, Bressan, and Vitria (2001) - diagonal weight matrix $Q$ used ( $X Q \approx W H Q$ ) to compensate for feature redundancy (columns of $W$ ).
- Wang, Jiar, Hu, and Turk (2004) - constraint-based formulation using Fisher linear discriminant analysis to improve extraction of spatially localized features.
- Other Cost Function Formulations - Hamza and Brady (2006), Dhillon and Sra (2005), Cichocki, Zdunek, and Amari (2006)


## Multiplicative Method (MM)

- Multiplicative update rules for $W$ and $H$ (Lee and Seung, 1999):

1 Initialize $W$ and $H$ with nonnegative values, and scale the columns of $W$ to unit norm.
2 Iterate for each $c, j$, and $i$ until convergence or after $k$ iterations:

$$
\begin{aligned}
& 1 H_{c j} \leftarrow H_{c j} \frac{\left(W^{\top} X\right)_{c j}}{\left(W^{\top} W H\right)_{c j}+\epsilon} \\
& 2 W_{i c} \leftarrow W_{i c} \frac{\left(X H^{\top}\right)_{i c}}{\left(W H H^{\top}\right)_{i c}+\epsilon}
\end{aligned}
$$

3 Scale the columns of $W$ to unit norm.

- Setting $\epsilon=10^{-9}$ will suffice to avoid division by zero [Shahnaz et al., 2006].


## Multiplicative Method (MM) contd.

Multiplicative Update MATLAB ${ }^{\circledR}$ Code for NnMF

```
W = rand(m,k); % W initially random
H}=\operatorname{rand}(\textrm{k},\textrm{n});\quad%\mathbf{H}\mathrm{ initially random
for i = 1:maxiter
    H = H .* (W'W}\mathbf{\top}\mathbf{A})./(\mp@subsup{\mathbf{W}}{}{\top}\mathbf{W}\mathbf{H}+\epsilon)
    W = W .* (AH'`})./(\mathbf{WHH}\mp@subsup{}{}{\mathbf{T}}+\epsilon)
end
```


## Lee and Seung MM Convergence

■ Convergence: when the MM algorithm converges to a limit point in the interior of the feasible region, the point is a stationary point. The stationary point may or may not be a local minimum. If the limit point lies on the boundary of the feasible region, one cannot determine its stationarity [Berry et al., 2007].
■ Several modifications have been proposed: Gonzalez and Zhang (2005) accelerated convergence somewhat but stationarity issue remains; Lin (2005) modified the algorithm to guarantee convergence to a stationary point; Dhillon and Sra (2005) derived update rules that incorporate weights for the importance of certain features of the approximation.

## Hoyer's Method

- From neural network applications, Hoyer (2002) enforced statistical sparsity for the weight matrix $H$ in order to enhance the parts-based data representations in the matrix $W$.
- Mu et al. (2003) suggested a regularization approach to achieve statistical sparsity in the matrix $H$ : point count regularization; penalize the number of nonzeros in $H$ rather than $\sum_{i j} H_{i j}$.
- Goal of increased sparsity (or smoothness) - better representation of parts or features spanned by the corpus $(X)$ [Berry and Browne, 2005].


## GD-CLS - Hybrid Approach

■ First use MM to compute an approximation to $W$ for each iteration - a gradient descent (GD) optimization step.

- Then, compute the weight matrix $H$ using a constrained least squares (CLS) model to penalize non-smoothness (i.e., non-sparsity) in $H$ - common Tikohonov regularization technique used in image processing (Prasad et al., 2003).
- Convergence to a non-stationary point evidenced (proof still needed).


## GD-CLS Algorithm

1 Initialize $W$ and $H$ with nonnegative values, and scale the columns of $W$ to unit norm.
2 Iterate until convergence or after $k$ iterations:
$\boxed{1} W_{i c} \leftarrow W_{i c} \frac{\left(X H^{T}\right)_{i c}}{\left(W H H^{T}\right)_{i c}+\epsilon}$, for $c$ and $i$
2 Rescale the columns of $W$ to unit norm.
3 Solve the constrained least squares problem:

$$
\min _{H_{j}}\left\{\left\|X_{j}-W H_{j}\right\|_{2}^{2}+\lambda\left\|H_{j}\right\|_{2}^{2}\right\}
$$

where the subscript $j$ denotes the $j^{\text {th }}$ column, for $j=1, \ldots, m$.

- Any negative values in $H_{j}$ are set to zero. The parameter $\lambda$ is a regularization value that is used to balance the reduction of the metric $\left\|X_{j}-W H_{j}\right\|_{2}^{2}$ with enforcement of smoothness and sparsity in $H$.


## Two Penalty Term Formulation

- Introduce smoothing on $W_{k}$ (feature vectors) in addition to $H^{k}$ :

$$
\min _{W, H}\left\{\|X-W H\|_{F}^{2}+\alpha\|W\|_{F}^{2}+\beta\|H\|_{F}^{2}\right\}
$$

where $\|\cdot\|_{F}$ is the Frobenius norm.
■ Constrained NNMF (CNMF) iteration:

$$
\begin{aligned}
& H_{c j} \leftarrow H_{c j} \frac{\left(W^{T} X\right)_{c j}-\beta H_{c j}}{\left(W^{T} W H\right)_{c j}+\epsilon} \\
& W_{i c} \leftarrow W_{i c} \frac{\left(X H^{T}\right)_{i c}-\alpha W_{i c}}{\left(W H H^{T}\right)_{i c}+\epsilon}
\end{aligned}
$$

## Improving Feature Interpretability

## Gauging Parameters for Constrained Optimization

How sparse (or smooth) should factors $(W, H)$ be to produce as many interpretable features as possible?

To what extent do different norms $\left(I_{1}, l_{2}, l_{\infty}\right)$ improve/degradate feature quality or span? At what cost?

Can a nonnegative feature space be built from objects in both images and text? Are there opportunities for multimodal document similarity?

## Anomaly Detection (ASRS)

- Classify events described by documents from the Airline Safety Reporting System (ASRS) into 22 anomaly categories; contest from SDM07 Text Mining Workshop.
- General Text Parsing (GTP) Software Environment in C++ [Giles et al., 2003] used to parse both ASRS training set and a combined ASRS training and test set:

| Dataset | Terms | ASRS Documents |
| ---: | ---: | ---: |
| Training | 15,722 | 21,519 |
| Training+Test | 17,994 | $28,596(7,077)$ |

- Global and document frequency of required to be at least 2; stoplist of 493 common words used; char length of any term $\in[2,200]$.
- Download Information:

GTP: http://www.cs.utk.edu/~1si
ASRS: http://www.cs.utk.edu/tmw07

## Initialization Schematic

H


H

(Filtered)

## Anomaly to Feature Mapping and Scoring Schematic



## Training/Testing Performance (ROC Curves)

- Best/Worst ROC curves (False Positive Rate versus True Positive Rate)

| Anomaly |  | Type (Description) |  |
| :---: | :--- | :---: | :---: |

## Anomaly Summarization Prototype - Sentence Ranking



Sentence rank $=\mathrm{f}($ global term weights $)-$ B. Lamb三

## Improving Summarization and Steering

## What versus why:

Extraction of textual concepts still requires human interpretation (in the absence of ontologies or domain-specific classifications).

How can previous knowledge or experience be captured for feature matching (or pruning)?

To what extent can feature vectors be annotated for future use or as the text collection is updated? What is the cost for updating the NNMF (or similar) model?

## Unresolved Modeling Issues

## Parameters and dimensionality:

Further work needed in determining effects of alternative term weighting schemes (for $X$ ) and choices of control parameters (e.g., $\alpha, \beta$ for CNMF).

How does document (or object) clustering change with different ranks (or features)?

How should feature vectors from competing models (Bayesian, neural nets, etc.) be compared in both interpretability and computational cost?

## Email Collection

■ By-product of the FERC investigation of Enron (originally contained 15 million email messages).

- This study used the improved corpus known as the Enron Email set, which was edited by Dr. William Cohen at CMU.
- This set had over 500,000 email messages. The majority were sent in the 1999 to 2001 timeframe.


## Enron Historical 1999-2001

■ Ongoing, problematic, development of the Dabhol Power Company (DPC) in the Indian state of Maharashtra.

- Deregulation of the Calif. energy industry, which led to rolling electricity blackouts in the summer of 2000 (and subsequent investigations).
■ Revelation of Enron's deceptive business and accounting practices that led to an abrupt collapse of the energy colossus in October, 2001; Enron filed for bankruptcy in December, 2001.


## Multidimensional Data Analysis via PARAFAC



Temporal Assessment via PARAFAC


## Mathematical Notation

- Kronecker product

$$
A \otimes B=\left(\begin{array}{ccc}
A_{11} B & \cdots & A_{1 n} B \\
\vdots & \ddots & \vdots \\
A_{m 1} B & \cdots & A_{m n} B
\end{array}\right)
$$

- Khatri-Rao product (columnwise Kronecker)

$$
A \odot B=\left(\begin{array}{lll}
A_{1} \otimes B_{1} & \cdots & A_{n} \otimes B_{n}
\end{array}\right)
$$

- Outer product

$$
A_{1} \circ B_{1}=\left(\begin{array}{ccc}
A_{11} B_{11} & \cdots & A_{11} B_{m 1} \\
\vdots & \ddots & \vdots \\
A_{m 1} B_{11} & \cdots & A_{m 1} B_{m 1}
\end{array}\right)
$$

## PARAFAC Representations

- PARAllel FACtors (Harshman, 1970)
- Also known as CANDECOMP (Carroll \& Chang, 1970)
- Typically solved by Alternating Least Squares (ALS)


## Alternative PARAFAC formulations

$$
\begin{aligned}
& X_{i j k} \approx \sum_{i=1}^{r} A_{i r} B_{j r} C_{k r} \\
& \mathcal{X} \approx \sum_{i=1}^{r} A_{i} \circ B_{i} \circ C_{i}, \text { where } \mathcal{X} \text { is a 3-way array (tensor). } \\
& X_{k} \approx A \operatorname{diag}\left(C_{k:}\right) B^{T}, \text { where } X_{k} \text { is a tensor slice. } \\
& X^{I \times J K} \approx A(C \odot B)^{T}, \text { where } X \text { is matricized. }
\end{aligned}
$$

## PARAFAC (Visual) Representations



Outer product form


Tensor slice form


Matrix form

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## Nonnegative PARAFAC Algorithm

- Adapted from (Mørup, 2005) and based on NNMF by (Lee and Seung, 2001)

$$
\begin{aligned}
\left\|X^{I \times J K}-A(C \odot B)^{T}\right\|_{F} & =\left\|X^{J \times I K}-B(C \odot A)^{T}\right\|_{F} \\
& =\left\|X^{K \times I J}-C(B \odot A)^{T}\right\|_{F}
\end{aligned}
$$

■ Minimize over $A, B, C$ using multiplicative update rule:

$$
\begin{aligned}
A_{i \rho} \leftarrow A_{i \rho} \frac{\left(X^{I \times J K} Z\right)_{i \rho}}{\left(A Z^{T} Z\right)_{i \rho}+\epsilon}, & Z=(C \odot B) \\
B_{j \rho} \leftarrow B_{j \rho} \frac{\left(X^{J \times I K} Z\right)_{j \rho}}{\left(B Z^{T} Z\right)_{j \rho}+\epsilon}, & Z=(C \odot A) \\
C_{k \rho} \leftarrow C_{k \rho} \frac{\left(X^{K \times I J} Z\right)_{k \rho}}{\left(C Z^{T} Z\right)_{k \rho}+\epsilon}, & Z=(B \odot A)
\end{aligned}
$$

## Tensor-Generated Group Discussions

■ NNTF Group Discussions in 2001

- 197 authors; 8 distinguishable discussions

■ "Kaminski/Education" topic previously unseen


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## Gantt Charts from PARAFAC Models

NNTF/PARAFAC


PARAFAC


## Day-level Analysis for PARAFAC (Three Groups)

■ Rank-25 tensor for 357 out of 365 days of 2001:
$A(69,157 \times 25), B(197 \times 25), C(357 \times 25)$

- Groups 3,4,5:



## Day-level Analysis for NN-PARAFAC (Three Groups)

■ Rank-25 tensor (best minimizer) for 357 out of 365 days of 2001: $A(69,157 \times 25), B(197 \times 25), C(357 \times 25)$

- Groups $1,7,8$ :



## Day-level Analysis for NN-PARAFAC (Two Groups)

- Groups 20 (California Energy) and 9 (Football) (from C factor of best minimizer) in day-level analysis of 2001:



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## Four-way Tensor Results (Sept. 2007)

- Apply NN-PARAFAC to term-author-recipient-day array $(39,573 \times 197 \times 197 \times 357)$; construct a rank- 25 tensor (best minimizer among 10 runs).
- Goal: track more focused discussions between individuals/ small groups; for example, betting pool (football).



## Four-way Tensor Results (Sept. 2007)

■ Four-way tensor may track subconversation already found by three-way tensor; for example, RTO (Regional Transmission Organization) discussions.


## NNTF Optimal Rank?

■ No known algorithm for computing the rank of a $k$-way array for $k \geq 3$ [Kruskal, 1989].

- The maximum rank is not a closed set for a given random tensor.
■ The maximum rank of a $m \times n \times k$ tensor is unknown; one weak inequality is given by

$$
\max \{m, n, k\} \leq \operatorname{rank} \leq \min \{m \times n, m \times k, n \times k\}
$$

■ For our rank-25 NNTF, the size of the relative residual norm suggests we are still far from the maximum rank of the 3-way and 4-way arrays.

## Further Reading

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