Exploring Nonnegative Matrix Factorization

Holly Jin
LinkedIn Corp
and
Michael Saunders
Systems Optimization Laboratory, Stanford University

MMDS08

Workshop on Algorithms for Modern Massive Data Sets

Stanford University, June 25–28, 2008

Outline

Introduction

Many applications (signal processing, page rank, imaging) seek *sparse solutions to square or rectangular systems*

$$Ax \approx b \qquad x \text{ sparse}$$

Introduction

Many applications (signal processing, page rank, imaging) seek *sparse solutions to square or rectangular systems*

$$Ax \approx b \qquad x \text{ sparse}$$

Basis Pursuit Denoising (BPDN) seeks sparsity by solving

$$\min \ \tfrac{1}{2}\|Ax - b\|^2 \ + \ \lambda\|x\|_1$$

Introduction

Many applications (signal processing, page rank, imaging) seek *sparse solutions to square or rectangular systems*

$$Ax \approx b \qquad x \text{ sparse}$$

Basis Pursuit Denoising (BPDN) seeks sparsity by solving

$$\min \ \tfrac{1}{2}\|Ax - b\|^2 \ + \ \lambda\|x\|_1$$

Sparse Nonnegative Matrix Factorization (SNMF) involves square or rectangular systems

$$A \ \approx \ WH$$

$$W, H \geq 0 \qquad \text{low rank and sparse}$$

Introduction

Many applications (signal processing, page rank, imaging) seek *sparse solutions to square or rectangular systems*

$$Ax \approx b \qquad x \text{ sparse}$$

Basis Pursuit Denoising (BPDN) seeks sparsity by solving

$$\min \ \tfrac{1}{2}\|Ax - b\|^2 \ + \ \lambda\|x\|_1$$

Sparse Nonnegative Matrix Factorization (SNMF) involves square or rectangular systems

$$A \ \approx \ WH$$

$$W, H \geq 0 \qquad \text{low rank and sparse}$$

Perhaps BPDN can find very sparse approximate W, H

Motivation for Sparse NMF Solver

An example

- Grouping similar items in a grocery store

An example

- Grouping similar items in a grocery store
- Customer check-out receipts:

	Flour	Balloon	Beer	Sugar	Chip
Customer1	0	3	8	0	1
Customer2	0	2	5	1	0
Customer3	5	0	1	10	0
Customer4	0	20	40	2	1
Customer5	10	0	1	10	1

Extract features using SVD

$$U = \begin{pmatrix} -0.1852 & -0.0225 & 0.1457 & 0.9394 & -0.2480 \\ -0.1179 & 0.0282 & -0.1676 & 0.2529 & 0.9451 \\ -0.0338 & 0.6126 & -0.7649 & 0.0793 & -0.1794 \\ -0.9744 & -0.0492 & -0.0030 & -0.2098 & -0.0645 \\ -0.0356 & 0.7881 & 0.6046 & -0.0570 & 0.0945 \end{pmatrix}$$

$$S = \begin{pmatrix} \boxed{45.9457} & 0 & 0 & 0 & 0 \\ 0 & \boxed{17.7720} & 0 & 0 & 0 \\ 0 & 0 & 2.9418 & 0 & 0 \\ 0 & 0 & 0 & 1.1892 & 0 \\ 0 & 0 & 0 & 0 & 0.2783 \end{pmatrix}$$

$$V = \begin{pmatrix} -0.0114 & 0.6158 & 0.7550 & -0.1455 & 0.1719 \\ -0.4414 & -0.0560 & 0.0144 & -0.7337 & -0.5134 \\ -0.8949 & -0.0341 & 0.0164 & 0.3441 & 0.2818 \\ -0.0601 & 0.7842 & -0.6042 & 0.0478 & -0.1191 \\ -0.0260 & 0.0403 & 0.2540 & 0.5656 & -0.7831 \end{pmatrix}$$

Truncated SVD

- Choose $k = 2$ principal features according to matrix S:

$$Uk = \begin{pmatrix} -0.1852 & 0.0225 \\ -0.1179 & -0.0282 \\ -0.0338 & -0.6126 \\ -0.9744 & 0.0492 \\ -0.0356 & -0.7881 \end{pmatrix}$$

$$Sk = \begin{pmatrix} 45.9457 & 0 \\ 0 & 17.7720 \end{pmatrix}$$

$$Vk = \begin{pmatrix} -0.0114 & -0.6158 \\ -0.4414 & 0.0560 \\ -0.8949 & 0.0341 \\ -0.0601 & -0.7842 \\ -0.0260 & -0.0403 \end{pmatrix}$$

Truncated SVD

- Choose $k = 2$ principal features according to matrix S:

$$Uk = \begin{pmatrix} -0.1852 & 0.0225 \\ -0.1179 & -0.0282 \\ -0.0338 & -0.6126 \\ -0.9744 & 0.0492 \\ -0.0356 & -0.7881 \end{pmatrix}$$

$$Sk = \begin{pmatrix} 45.9457 & 0 \\ 0 & 17.7720 \end{pmatrix}$$

$$Vk = \begin{pmatrix} -0.0114 & -0.6158 \\ -0.4414 & 0.0560 \\ -0.8949 & 0.0341 \\ -0.0601 & -0.7842 \\ -0.0260 & -0.0403 \end{pmatrix}$$

- Error $\|A - USV^T\| = $ 1.5e-14
  vs $\|A - U_k S_k V_k^T\| = 2.9$ (minimized Frobenius norm)

Clustering and ranking

- Row and column clustering and rankings:

$$Rr = \begin{pmatrix} (1,1) & 2 \\ (2,1) & 3 \\ (4,1) & 1 \\ (3,2) & 2 \\ (5,2) & 1 \end{pmatrix} \qquad Rc = \begin{pmatrix} (2,1) & 2 \\ (3,1) & 1 \\ (1,2) & 2 \\ (4,2) & 1 \\ (5,2) & 3 \end{pmatrix}$$

Clustering and ranking

- Row and column clustering and rankings:

$$Rr = \begin{pmatrix} (1,1) & 2 \\ (2,1) & 3 \\ (4,1) & 1 \\ (3,2) & 2 \\ (5,2) & 1 \end{pmatrix} \quad Rc = \begin{pmatrix} (2,1) & 2 \\ (3,1) & 1 \\ (1,2) & 2 \\ (4,2) & 1 \\ (5,2) & 3 \end{pmatrix}$$

- Order of k preserves the ranking of cluster importance

Clustering and ranking

- Row and column clustering and rankings:

$$Rr = \begin{pmatrix} (1,1) & 2 \\ (2,1) & 3 \\ (4,1) & 1 \\ (3,2) & 2 \\ (5,2) & 1 \end{pmatrix} \qquad Rc = \begin{pmatrix} (2,1) & 2 \\ (3,1) & 1 \\ (1,2) & 2 \\ (4,2) & 1 \\ (5,2) & 3 \end{pmatrix}$$

- Order of k preserves the ranking of cluster importance
- Cluster example meanings:

	Flour	Balloon	Beer	Sugar	Chip
Customer 1	0	3	8	0	1
Customer 2	0	2	5	1	0
Customer 3	5	0	1	10	0
Customer 4	0	20	40	2	1
Customer 5	10	0	1	10	1

Clustering and ranking

- Row and column clustering and rankings:

$$Rr = \begin{pmatrix} (1,1) & 2 \\ (2,1) & 3 \\ (4,1) & 1 \\ (3,2) & 2 \\ (5,2) & 1 \end{pmatrix} \quad Rc = \begin{pmatrix} (2,1) & 2 \\ (3,1) & 1 \\ (1,2) & 2 \\ (4,2) & 1 \\ (5,2) & 3 \end{pmatrix}$$

- Order of k preserves the ranking of cluster importance
- Cluster example meanings:

	Flour	Balloon	Beer	Sugar	Chip
Customer 1	0	3	8	0	1
Customer 2	0	2	5	1	0
Customer 3	5	0	1	10	0
Customer 4	0	20	40	2	1
Customer 5	10	0	1	10	1

- Features extraction:

	Partying	Baking
Customers	1, 2, 4	3, 5
Products	Balloon, Beer	Flour, Sugar, Chip

NMF

- $A = WH, \quad A \approx W_k H_k$

NMF

- $A = WH, \quad A \approx W_k H_k$
- Factorization not unique: (via Chih-Jen Lin's NMF solver)

$$W_k = \begin{pmatrix} 0 & 1.2850 \\ 0.4711 & 0.8065 \\ 8.4380 & 0.0365 \\ 0.0217 & 6.7563 \\ 10.8476 & 0 \end{pmatrix}$$

$$H_k = \begin{pmatrix} 0.7968 & 0 & 0.0928 & 1.0214 & 0.0567 \\ 0 & 2.9321 & 5.9337 & 0.2885 & 0.1667 \end{pmatrix}$$

NMF

- $A = WH, \quad A \approx W_k H_k$
- Factorization not unique: (via Chih-Jen Lin's NMF solver)

$$W_k = \begin{pmatrix} 0 & 1.2850 \\ 0.4711 & 0.8065 \\ 8.4380 & 0.0365 \\ 0.0217 & 6.7563 \\ 10.8476 & 0 \end{pmatrix}$$

$$H_k = \begin{pmatrix} 0.7968 & 0 & 0.0928 & 1.0214 & 0.0567 \\ 0 & 2.9321 & 5.9337 & 0.2885 & 0.1667 \end{pmatrix}$$

- Clustering and Ranking:

$$Rr = \begin{pmatrix} (1,2) & 2 \\ (2,2) & 3 \\ (4,2) & 1 \\ (3,1) & 2 \\ (5,1) & 1 \end{pmatrix} \qquad Rc = \begin{pmatrix} (2,2) & 2 \\ (3,2) & 1 \\ (5,2) & 3 \\ (1,1) & 2 \\ (4,1) & 1 \end{pmatrix}$$

NMF

- $A = WH, \quad A \approx W_k H_k$
- Factorization not unique: (via Chih-Jen Lin's NMF solver)

$$W_k = \begin{pmatrix} 0 & 1.2850 \\ 0.4711 & 0.8065 \\ 8.4380 & 0.0365 \\ 0.0217 & 6.7563 \\ 10.8476 & 0 \end{pmatrix}$$

$$H_k = \begin{pmatrix} 0.7968 & 0 & 0.0928 & 1.0214 & 0.0567 \\ 0 & 2.9321 & 5.9337 & 0.2885 & 0.1667 \end{pmatrix}$$

- Clustering and Ranking:

$$Rr = \begin{pmatrix} (1,2) & 2 \\ (2,2) & 3 \\ (4,2) & 1 \\ (3,1) & 2 \\ (5,1) & 1 \end{pmatrix} \qquad Rc = \begin{pmatrix} (2,2) & 2 \\ (3,2) & 1 \\ (5,2) & 3 \\ (1,1) & 2 \\ (4,1) & 1 \end{pmatrix}$$

- Order of k does not preserve the ranking of cluster importance

Sparse Nonnegative Factorization

Sparse NMF

$$A \approx WH, \quad W, H \geq 0, \quad \text{low rank and sparse}$$

Kim and Park (2007)

$$\boxed{\min_{W,H\geq 0} \frac{1}{2}\|A - WH\|_F^2 + \eta\|W\|_F^2 + \beta \sum \|h_j\|_1^2}$$

Sparse NMF

$$A \approx WH, \quad W, H \geq 0, \quad \text{low rank and sparse}$$

Kim and Park (2007)

$$\boxed{\min_{W,H\geq 0} \tfrac{1}{2}\|A - WH\|_F^2 + \eta\|W\|_F^2 + \beta \sum \|h_j\|_1^2}$$

Alternating nonnegative least squares (NLS) on

$$\boxed{\min_{W\geq 0} \left\| \begin{pmatrix} H^T \\ \sqrt{\eta} I \end{pmatrix} W^T - \begin{pmatrix} A^T \\ 0 \end{pmatrix} \right\|_F^2, \qquad \min_{H\geq 0} \left\| \begin{pmatrix} W \\ \sqrt{\beta} e^T \end{pmatrix} H - \begin{pmatrix} A \\ 0 \end{pmatrix} \right\|_F^2}$$

Sparse H

Sparse NMF via BPDN

$$\boxed{\min_{W,H\geq 0} \ \frac{1}{2}\|A - WH\|_F^2 + \beta \sum \|w_i\|_1 + \eta \sum \|h_j\|_1}$$

Sparse NMF via BPDN

$$\boxed{\min_{W,H\geq 0} \ \tfrac{1}{2}\|A - WH\|_F^2 + \beta \sum \|w_i\|_1 + \eta \sum \|h_j\|_1}$$

Alternating BPDN on

$$\min_{W\geq 0} \ \tfrac{1}{2}\|H^T W^T - A^T\|^2 + \eta \sum \|w_i\|_1$$

$$\min_{H\geq 0} \ \tfrac{1}{2}\|WH - A\|^2 + \beta \sum \|h_j\|_1$$

Sparse W and H

L1^2 or L1?

- Kim and Park (2007):

$$\min_{x \geq 0} \frac{1}{2}\|Ax - b\|^2 + \lambda \|x\|_1^2$$

$x \to 0$ only as $\lambda \to \infty$

(Nevertheless, Kim and Park report sparse solutions with moderate λ)

L1^2 or L1?

- Kim and Park (2007):

$$\min_{x\geq 0} \frac{1}{2}\|Ax-b\|^2 + \lambda\|x\|_1^2$$

$x \to 0$ only as $\lambda \to \infty$
(Nevertheless, Kim and Park report sparse solutions with moderate λ)

- BPDN:

$$\min_{x\geq 0} \frac{1}{2}\|Ax-b\|^2 + \lambda\|x\|_1$$

$x = 0$ for $\lambda \geq \|A^Tb\|_\infty$
x very sparse for $\lambda = 0.9\|A^Tb\|_\infty$ say

Easy to control the sparsity of x

SNMF via BPDN implementation

$$\boxed{\min_{U,D,V\geq 0} \tfrac{1}{2}\|A - UDV^T\|_F^2 + \sum \beta_i \|Du_i\|_1 + \sum \eta_j \|Dv_j\|_1}$$

Alternating BPDN on

$$\min_{v_j\geq 0} \tfrac{1}{2}\|Uv_j - a_{.j}\|^2 + \eta_j\|v_j\|_1, \qquad \text{normalize } V \rightarrow VD$$

$$\min_{u_i\geq 0} \tfrac{1}{2}\|Vu_i - a_{i.}\|^2 + \beta_i\|u_i\|_1, \qquad \text{normalize } U \rightarrow UD$$

SNMF via BPDN implementation

$$\boxed{\min_{U,D,V\geq 0} \ \tfrac{1}{2}\|A - UDV^T\|_F^2 + \sum \beta_i \|Du_i\|_1 + \sum \eta_j \|Dv_j\|_1}$$

Alternating BPDN on

$$\min_{v_j\geq 0} \ \tfrac{1}{2}\|Uv_j - a_{.j}\|^2 + \eta_j\|v_j\|_1, \qquad \text{normalize } V \to VD$$

$$\min_{u_i\geq 0} \ \tfrac{1}{2}\|Vu_i - a_{i.}\|^2 + \beta_i\|u_i\|_1, \qquad \text{normalize } U \to UD$$

- $\eta_j \leq \sigma\|U^T a_{.j}\|_\infty$ $\quad$ σ = "sparsity" input parameter
  $\beta_i \leq \sigma\|V^T a_{i.}\|_\infty$ $\quad$ = 0.9 or 0.8 say

SNMF via BPDN implementation

$$\boxed{\min_{U,D,V\geq 0} \tfrac{1}{2}\|A - UDV^T\|_F^2 + \sum \beta_i \|Du_i\|_1 + \sum \eta_j \|Dv_j\|_1}$$

Alternating BPDN on

$$\min_{v_j \geq 0} \tfrac{1}{2}\|Uv_j - a_{.j}\|^2 + \eta_j \|v_j\|_1, \qquad \text{normalize } V \to VD$$

$$\min_{u_i \geq 0} \tfrac{1}{2}\|Vu_i - a_{i.}\|^2 + \beta_i \|u_i\|_1, \qquad \text{normalize } U \to UD$$

- $\eta_j \leq \sigma \|U^T a_{.j}\|_\infty$ $\qquad \sigma =$ "sparsity" input parameter
  $\beta_i \leq \sigma \|V^T a_{i.}\|_\infty$ $\qquad = 0.9$ or 0.8 say
- At some point, *freeze* D $\qquad$ (Also η_j β_i stop changing)

BPDN solvers

BPDN solvers

$$\min \lambda\|x\|_1 + \tfrac{1}{2}\|Ax - b\|^2$$

OMP	Davis, Mallat et al 1997	Greedy
BPDN-interior	Chen, Donoho & S, 1998, 2001	Interior, CG
PDSCO, PDCO	Saunders 1997, 2002	Interior, LSQR
BCR	Sardy, Bruce & Tseng 2000	Orthogonal blocks
Homotopy	Osborne et al 2000	Active-set, all λ
LARS	Efron, Hastie, Tibshirani 2004	Active-set, all λ
STOMP	Donoho, Tsaig, et al 2006	Double greedy
l1_ls	Kim, Koh, Lustig, Boyd et al 2007	Primal barrier, PCG
GPSR	Figueiredo, Nowak & Wright 2007	Gradient Projection
SPGL1	van den Berg & Friedlander 2007	Spectral GP, all λ
BPdual	Friedlander & Saunders 2007	Active-set on dual
LPdual	Friedlander & Saunders 2007	Active-set on dual, $x \geq 0$
lsNMF, lsNTF	Friedlander & Hatz 2007	Sparse NMF *and* NTF (BCLS subproblem solver)

LPdual solver

Active-set method for *dual* of regularized LP:

$$\min_{x,\,y}\ e^T x + \tfrac{1}{2}\lambda\|y\|^2 \quad \text{st} \quad Ax + \lambda y = b, \quad x \geq 0$$

$$\boxed{\min_y\ -b^T y + \tfrac{1}{2}\lambda\|y\|^2 \quad \text{st} \quad A^T y \leq e}$$

LPdual solver

Active-set method for *dual* of regularized LP:

$$\min_{x,\,y}\ e^T x + \tfrac{1}{2}\lambda\|y\|^2 \quad \text{st} \quad Ax + \lambda y = b, \quad x \geq 0$$

$$\boxed{\min_y\ -b^T y + \tfrac{1}{2}\lambda\|y\|^2 \quad \text{st} \quad A^T y \leq e}$$

$B \equiv$ columns of A for active constraints ($B^T y = e$)
Initially $y = 0$, B empty
Selects columns of B in mostly *greedy* manner

LPdual solver

Active-set method for *dual* of regularized LP:

$$\min_{x,\,y}\; e^T x + \tfrac{1}{2}\lambda\|y\|^2 \quad \text{st} \quad Ax + \lambda y = b, \quad x \geq 0$$

$$\boxed{\min_y\; -b^T y + \tfrac{1}{2}\lambda\|y\|^2 \quad \text{st} \quad A^T y \leq e}$$

$B \equiv$ columns of A for active constraints ($B^T y = e$)
Initially $y = 0$, B empty
Selects columns of B in mostly *greedy* manner

Main work per iteration:

Solve $\min \|Bx - g\|$
Form $dy = (g - Bx)/\lambda$
Form $dz = A^T dy$
Add or delete a column of B

SNMF Results

Sparse NMF example

- Sparse solution: $k = 2$

$$U_k = \begin{pmatrix} 0.1859 & \\ 0.1170 & \\ & 0.6146 \\ 0.9756 & \\ & 0.7889 \end{pmatrix} \qquad V_k = \begin{pmatrix} & 0.6153 \\ 0.4428 & \\ 0.8963 & \\ & 0.7877 \\ 0.0253 & 0.0303 \end{pmatrix}$$

$$D_k = \begin{pmatrix} 27.51 & \\ & 10.69 \end{pmatrix}$$

Sparse NMF example

- Sparse solution: $k = 2$

$$U_k = \begin{pmatrix} 0.1859 & \\ 0.1170 & \\ & 0.6146 \\ 0.9756 & \\ & 0.7889 \end{pmatrix} \qquad V_k = \begin{pmatrix} & 0.6153 \\ 0.4428 & \\ 0.8963 & \\ & 0.7877 \\ 0.0253 & 0.0303 \end{pmatrix}$$

$$D_k = \begin{pmatrix} 27.51 & \\ & 10.69 \end{pmatrix}$$

- Clustering and Ranking:

$$Rr = \begin{pmatrix} (1,1) & 2 \\ (2,1) & 3 \\ (4,1) & 1 \\ (3,2) & 2 \\ (5,2) & 1 \end{pmatrix} \qquad Rc = \begin{pmatrix} (2,1) & 2 \\ (3,1) & 1 \\ (1,2) & 2 \\ (4,2) & 1 \\ (5,2) & 3 \end{pmatrix}$$

Sparse NMF example

- Sparse solution: $k = 2$

$$U_k = \begin{pmatrix} 0.1859 & \\ 0.1170 & \\ & 0.6146 \\ 0.9756 & \\ & 0.7889 \end{pmatrix} \quad V_k = \begin{pmatrix} & 0.6153 \\ 0.4428 & \\ 0.8963 & \\ & 0.7877 \\ 0.0253 & 0.0303 \end{pmatrix}$$

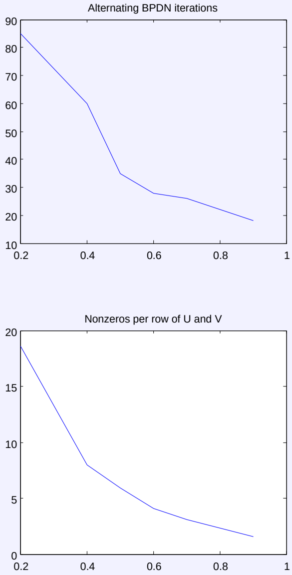
$$D_k = \begin{pmatrix} 27.51 & \\ & 10.69 \end{pmatrix}$$

- Clustering and Ranking:

$$Rr = \begin{pmatrix} (1,1) & 2 \\ (2,1) & 3 \\ (4,1) & 1 \\ (3,2) & 2 \\ (5,2) & 1 \end{pmatrix} \quad Rc = \begin{pmatrix} (2,1) & 2 \\ (3,1) & 1 \\ (1,2) & 2 \\ (4,2) & 1 \\ (5,2) & 3 \end{pmatrix}$$

- Order of k does preserve the ranking of cluster importance

$m = n = 450, \quad k = 200, \quad$ increasing sparsity



Real Application Examples

Keyword clusterings

- About 8000 stem terms

Keyword clusterings

- About 8000 stem terms
- Create term similarity matrix A

Keyword clusterings

- About 8000 stem terms
- Create term similarity matrix A
- Sample clusters:

googladword	c++
adword	cc++
googl	java
googlanalyt	c++java
yahoo	c++program
searchmarket	c++unix
omnitur	pascal
msn	c++develop
webtrend	c++programm
adbrit	javaprogram

User input standardization

- Field-of-study user input, about 400k unique entries
- Cluster user inputs automatically
- Sample clusters:
  - Abbreviations, variation of the same word or typos

    hr, human resources, hrm

    film production, film, theatre, acting, theater
  - New words

    physical therapy, kinesiology
  - Similar disciplines

    materials science and engineering, materials science, materials engineering
  - Foreign language

    business economics, bedrijfseconomie

    bedrijfskundige informatica, business informatics, informatica
  - Noise elimination, or crowded cluster

    business administration, business, mba, project management, master in business administration, business administration, master of business administration, technology, business admin, general education

Thanks

- Michael Friedlander (BP solvers)

Thanks

- Michael Friedlander (BP solvers)
- Sou-Cheng Choi
  Lek-Heng Lim

Thanks

- Michael Friedlander (BP solvers)
- Sou-Cheng Choi
  Lek-Heng Lim
- Jay Kreps
  Jonathan Goldman
  Huitao Luo

Thanks

- Michael Friedlander (BP solvers)
- Sou-Cheng Choi
  Lek-Heng Lim
- Jay Kreps
  Jonathan Goldman
  Huitao Luo
- Understanding Complex Datasets
  Data Mining with Matrix Decompositions
  (useful book by David Skillicorn)

Thanks

- Michael Friedlander (BP solvers)
- Sou-Cheng Choi
  Lek-Heng Lim
- Jay Kreps
  Jonathan Goldman
  Huitao Luo
- Understanding Complex Datasets
  Data Mining with Matrix Decompositions
  (useful book by David Skillicorn)
- Michael Saunders