New Algorithms for Nonnegative Matrix Factorization and Beyond

Ankur Moitra

Institute for Advanced Study and Princeton University

Challenge: develop tools for automatic comprehension of data



Challenge: develop tools for automatic comprehension of data



- Discover hidden topics
- Annotate documents according to these topics
- Organize and summarize the collection

Challenge: develop tools for automatic comprehension of data

- Discover hidden topics
- Annotate documents according to these topics
- Organize and summarize the collection

Challenge: develop tools for automatic comprehension of data

Parceling Out a Nest Egg, Without Emptying It

By PAUL SULLIVAN

What clients often forget are fixed costs — homes, cars, insurance — that must come down but take time to reduce, she said. Beyond that is her clients' skittish approach to risk; putting all of their money in cash may make them feel safe, she said, but it probably will not support the lifestyle they want for decades.

A generational disconnect is at work here: most people plan to retire at 65, the retirement age established for <u>Social Security</u> in 1935, when the average <u>life expectancy</u> was 61. Today the average is over 80 for men and women with a college degree.

So the \$5.12 million gift exemption — created in a compromise between President Obama and Congress in 2010 — presents the well-off with a decision laden with short- and long-term consequences. How much should they give heirs now — and thus avoid giving the government in <u>estate taxes</u> later — while maintaining their lifestyle over a probably longer but still unpredictable remaining life span?

- Discover hidden topics
- Annotate documents according to these topics
- Organize and summarize the collection

Challenge: develop tools for automatic comprehension of data

- Discover hidden topics
- Annotate documents according to these topics
- Organize and summarize the collection

Challenge: develop tools for automatic comprehension of data



- Discover hidden topics
- Annotate documents according to these topics
- Organize and summarize the collection

Challenge: develop tools for automatic comprehension of data

- Discover hidden topics
- Annotate documents according to these topics
- Organize and summarize the collection

Challenge: develop tools for automatic comprehension of data



- Discover hidden topics
- Annotate documents according to these topics
- Organize and summarize the collection

Parceling Out a Nest Egg, Without Emptying It

What clients often forget are fixed costs — homes, cars, insurance — that must come down but take time to reduce, she said. Beyond that is her clients' skittish approach to risk; putting all of their money in cash may make them feel safe, she said, but it probably will not support the lifestyle they want for decades.

A generational disconnect is at work here: most people plan to retire at 65, the retirement age established for <u>Social Security</u> in 1935, when the average <u>life expectancy</u> was 61. Today the average is over 80 for men and women with a college degree.

So the \$5.12 million gift exemption — created in a compromise between President Obama and Congress in 2010 — presents the well-off with a decision laden with short- and long-term consequences. How much should they give heirs now — and thus avoid giving the government in <u>estate taxes</u> later — while maintaining their lifestyle over a probably longer but still unpredictable remaining life span?

Parceling Out a Nest Egg, Without Emptying It

What clients often forget are fixed costs — homes, cars, insurance — that must come down but take time to reduce, she said. Beyond that is her clients' skittish approach to risk; putting all of their money in cash may make them feel safe, she said, but it probably will not support the lifestyle they want for decades.

A generational disconnect is at work here: most people plan to retire at 65, the retirement age established for <u>Social Security</u> in 1935, when the average <u>life expectancy</u> was 61. Today the average is over 80 for men and women with a college degree.

So the \$5.12 million gift exemption — created in a compromise between President Obama and Congress in 2010 — presents the well-off with a decision laden with short- and long-term consequences. How much should they give heirs now — and thus avoid giving the government in <u>estate taxes</u> later — while maintaining their lifestyle over a probably longer but still unpredictable remaining life span?

Politics: (President Obama, 0.10), (congress, 0.08), (government, 0.07), ...

Parceling Out a Nest Egg, Without Emptying It

What clients often forget are fixed costs — homes, cars, insurance — that must come down but take time to reduce, she said. Beyond that is her clients' skittish approach to risk; putting all of their money in cash may make them feel safe, she said, but it probably will not support the lifestyle they want for decades.

A generational disconnect is at work here: most people plan to retire at 65, the retirement age established for <u>Social Security</u> in 1935, when the average <u>life expectancy</u> was 61. Today the average is over 80 for men and women with a college degree.

So the \$5.12 million gift exemption — created in a compromise between President Obama and Congress in 2010 — presents the well-off with a decision laden with short- and longterm consequences. How much should they give heirs now — and thus avoid giving the government in estate taxes later — while maintaining their lifestyle over a probably longer but still unpredictable remaining life span?

Politics: (President Obama, 0.10), (congress, 0.08), (government, 0.07), ...

Parceling Out a Nest Egg, Without Emptying It

What clients often forget are fixed costs — homes, cars, insurance — that must come down but take time to reduce, she said. Beyond that is her clients' skittish approach to risk; putting all of their money in cash may make them feel safe, she said, but it probably will not support the lifestyle they want for decades.

A generational disconnect is at work here: most people plan to retire at 65, the retirement age established for <u>Social Security</u> in 1935, when the average <u>life expectancy</u> was 61. Today the average is over 80 for men and women with a college degree.

So the \$5.12 million gift exemption — created in a compromise between President Obama and Congress in 2010 — presents the well-off with a decision laden with short- and longterm consequences. How much should they give heirs now — and thus avoid giving the government in estate taxes later — while maintaining their lifestyle over a probably longer but still unpredictable remaining life span?

• Each **document** is a distribution on **topics**

Politics: (President Obama, 0.10), (congress, 0.08), (government, 0.07), ...

Parceling Out a Nest Egg, Without Emptying It

What clients often forget are fixed costs — homes, cars, insurance — that must come down but take time to reduce, she said. Beyond that is her clients' skittish approach to risk; putting all of their money in cash may make them feel safe, she said, but it probably will not support the lifestyle they want for decades.

A generational disconnect is at work here: most people plan to retire at 65, the retirement age established for <u>Social Security</u> in 1935, when the average <u>life expectancy</u> was 61. Today the average is over 80 for men and women with a college degree.

So the \$5.12 million gift exemption — created in a compromise between President Obama and Congress in 2010 — presents the well-off with a decision laden with short- and longterm consequences. How much should they give heirs now — and thus avoid giving the government in estate taxes later — while maintaining their lifestyle over a probably longer but still unpredictable remaining life span?

- Each **document** is a distribution on **topics**
- Each **topic** is a distribution on words



Are there efficient algorithms to find the topics?

Are there efficient algorithms to find the topics?

Challenge: We cannot **rigorously** analyze algorithms used in practice! (When do they work? run quickly?)

Are there efficient algorithms to find the topics?

Challenge: We cannot **rigorously** analyze algorithms used in practice! (When do they work? run quickly?)

Part I: An Optimization Perspective

- Nonnegative Matrix Factorization
- Separability and Anchor Words
- Algorithms for Separable Instances

Are there efficient algorithms to find the topics?

Challenge: We cannot **rigorously** analyze algorithms used in practice! (When do they work? run quickly?)

Part I: An Optimization Perspective

- Nonnegative Matrix Factorization
- Separability and Anchor Words
- Algorithms for Separable Instances
- Part II: A Bayesian Perspective
 - Topic Models (e.g. LDA, CTM, PAM, ...)
 - Algorithms for Inferring the Topics
 - Experimental Results

documents (n)







relative frequency of word i in document j

documents (n)











E.g. "personal finance", (0.15, money), (0.10, retire), (0.03, risk), ...



E.g. "personal finance", (0.15, money), (0.10, retire), (0.03, risk), ...



E.g. "personal finance", (0.15, money), (0.10, retire), (0.03, risk), ...



nonnegative

E.g. "personal finance", (0.15, money), (0.10, retire), (0.03, risk), ...



nonnegative

Machine Learning and Statistics:

- Introduced by [Lee, Seung, '99]
- Goal: extract latent relationships in the data

• Applications to text classification, information retrieval, collaborative filtering, etc [Hofmann '99], [Kumar et al '98], [Xu et al '03], [Kleinberg, Sandler '04],...

Machine Learning and Statistics:

- Introduced by [Lee, Seung, '99]
- Goal: extract latent relationships in the data

• Applications to text classification, information retrieval, collaborative filtering, etc [Hofmann '99], [Kumar et al '98], [Xu et al '03], [Kleinberg, Sandler '04],...

Theoretical Computer Science:

• Introduced by [Yannakakis '90] in context of extended formulations; also related to the log-rank conjecture

Machine Learning and Statistics:

- Introduced by [Lee, Seung, '99]
- Goal: extract latent relationships in the data

• Applications to text classification, information retrieval, collaborative filtering, etc [Hofmann '99], [Kumar et al '98], [Xu et al '03], [Kleinberg, Sandler '04],...

Theoretical Computer Science:

• Introduced by [Yannakakis '90] in context of extended formulations; also related to the log-rank conjecture

Physical Modeling:

- Introduced by [Lawton, Sylvestre '71]
- Applications in chemometrics, environmetrics, economics

ALGORITHMS FOR NMF?

ALGORITHMS FOR NMF?

Local Search: given A, compute W, compute A....
Local Search: given A, compute W, compute A....

• known to fail on worst-case inputs (stuck in local optima)

Local Search: given A, compute W, compute A....

- known to fail on worst-case inputs (stuck in local optima)
- highly sensitive to cost-function, update procedure, regularization

Local Search: given A, compute W, compute A....

- known to fail on worst-case inputs (stuck in local optima)
- highly sensitive to cost-function, update procedure, regularization

Can we give an efficient algorithm that works on all inputs?

Theorem [Vavasis '09]: It is NP-hard to compute NMF

Theorem [Vavasis '09]: It is NP-hard to compute NMF

Theorem [Cohen, Rothblum '93]: Can solve NMF in time (nm)^{O(nr+mr)}

Theorem [Vavasis '09]: It is NP-hard to compute NMF

Theorem [Cohen, Rothblum '93]: Can solve NMF in time (nm)^{O(nr+mr)}

What is the complexity of NMF as a function of **r**?

Theorem [Vavasis '09]: It is NP-hard to compute NMF

Theorem [Cohen, Rothblum '93]: Can solve NMF in time (nm)^{O(nr+mr)}

What is the complexity of NMF as a function of r?

Theorem [Arora, Ge, Kannan, Moitra, STOC'12]: Can solve NMF in time (nm) $O(r^2)$ yet any algorithm that runs in time (nm) $O(r^2)$ would yield a $2^{O(n)}$ algorithm for 3-SAT.

Theorem [Vavasis '09]: It is NP-hard to compute NMF

Theorem [Cohen, Rothblum '93]: Can solve NMF in time (nm)^{O(nr+mr)}

What is the complexity of NMF as a function of **r**?

Theorem [Arora, Ge, Kannan, Moitra, STOC'12]: Can solve NMF in time (nm) $O(r^2)$ yet any algorithm that runs in time (nm) $O(r^2)$ would yield a $2^{O(n)}$ algorithm for 3-SAT.



system of polynomial inequalities

Theorem [Vavasis '09]: It is NP-hard to compute NMF

Theorem [Cohen, Rothblum '93]: Can solve NMF in time (nm)^{O(nr+mr)}

What is the complexity of NMF as a function of **r**?

Theorem [Arora, Ge, Kannan, Moitra, STOC'12]: Can solve NMF in time (nm) $O(r^2)$ yet any algorithm that runs in time (nm) $O(r^2)$ would yield a $2^{O(n)}$ algorithm for 3-SAT.



Can we reduce the number of variables from nr+mr to $O(r^2)$?

Local Search: given A, compute W, compute A....

- known to fail on worst-case inputs (stuck in local optima)
- highly sensitive to cost-function, update procedure, regularization

Can we give an efficient algorithm that works on all inputs?

Local Search: given A, compute W, compute A....

- known to fail on worst-case inputs (stuck in local optima)
- highly sensitive to cost-function, update procedure, regularization

Can we give an efficient algorithm that works on all inputs?

Yes, if and only if **r** is constant

Local Search: given A, compute W, compute A....

- known to fail on worst-case inputs (stuck in local optima)
- highly sensitive to cost-function, update procedure, regularization

Can we give an efficient algorithm that works on all inputs?

Yes, if and only if **r** is constant

Are the instances we actually want to solve somehow easier?

Local Search: given A, compute W, compute A....

- known to fail on worst-case inputs (stuck in local optima)
- highly sensitive to cost-function, update procedure, regularization

Can we give an efficient algorithm that works on all inputs?

Yes, if and only if **r** is constant

Are the instances we actually want to solve somehow easier?

Focus of this talk: a natural condition so that a **simple** algorithm **provably** works, **quickly**

topics (r)



words (m)

topics (r)



words (m)

topics (r) personal finance



words (m)

topics (r) personal finance



topics (r)



topics (r) baseball



topics (r) baseball



bunt

topics (r)



topics (r) movie reviews



topics (r) movie reviews



If an **anchor word** occurs then the document is at least partially about the topic

oscar-winning

topics (r) movie reviews



If an **anchor word** occurs then the document is at least partially about the topic

oscar-winning

topics (r) movie reviews



If an **anchor word** occurs then the document is at least partially about the topic

A is **p-separable** if each topic has an anchor word that occurs with probability ≥ p

Topic Models: documents are **stochastically** generated as a convex combination of topics

Topic Models: documents are **stochastically** generated as a convex combination of topics

Theorem [Arora, Ge, Moitra, FOCS'12]: There is a polynomial time algorithm that learns the parameters of **any** topic model provided that the topic matrix **A** is p-separable.

Topic Models: documents are **stochastically** generated as a convex combination of topics

Theorem [Arora, Ge, Moitra, FOCS'12]: There is a polynomial time algorithm that learns the parameters of **any** topic model provided that the topic matrix **A** is p-separable.

In fact our algorithm is **highly practical**, and runs **orders of magnitude faster** with nearly-identical performance as the current best (Gibbs Sampling)

Topic Models: documents are **stochastically** generated as a convex combination of topics

Theorem [Arora, Ge, Moitra, FOCS'12]: There is a polynomial time algorithm that learns the parameters of **any** topic model provided that the topic matrix **A** is p-separable.

In fact our algorithm is **highly practical**, and runs **orders of magnitude faster** with nearly-identical performance as the current best (Gibbs Sampling)

See also [Anandkumar et al '12], [Rabani et al '12] that give algorithms based on the method of moments

How do anchor words help?

ANCHOR WORDS \cong VERTICES




Observation: If **A** is separable, the rows of **W** appear as rows of **M**, we just need to find the anchor words!

Observation: If **A** is separable, the rows of **W** appear as rows of **M**, we just need to find the anchor words!

How can we find the anchor words?

















Observation: If **A** is separable, the rows of **W** appear as rows of **M**, we just need to find the anchor words!

How can we find the anchor words?

How can we find the anchor words?

How can we find the anchor words?

The NMF Algorithm:
7

How can we find the anchor words?

The NMF Algorithm:	
 find the anchor words (linear programming) 	
	7

How can we find the anchor words?

The NMF Algorithm:	
 find the anchor words (linear programming) 	
 paste these vectors in as rows in W 	

How can we find the anchor words?

The NMF Algorithm:	
 find the anchor words (linear programming) 	
 paste these vectors in as rows in W 	
 find the nonnegative A so that AW ≈ M 	
(convex programming)	-7

OUTLINE

Are there efficient algorithms to find the topics?

Challenge: We cannot **rigorously** analyze algorithms used in practice! (When do they work? run quickly?)

Part I: An Optimization Perspective

- Nonnegative Matrix Factorization
- Separability and Anchor Words
- Algorithms for Separable Instances
- Part II: A Bayesian Perspective
 - Topic Models (e.g. LDA, CTM, PAM, ...)
 - Algorithms for Inferring the Topics
 - Experimental Results





document #1: (1.0, personal finance)



document #1: (1.0, personal finance)

fixed stochastic











Latent Dirichlet Allocation (Blei, Ng, Jordan)





Correlated Topic Model (Blei, Lafferty)













document #2: (0.5, baseball); (0.5, movie review)

These models differ only in how W is generated

ALGORITHMS FOR TOPIC MODELS?

ALGORITHMS FOR TOPIC MODELS?

What if documents are **short**; can we still find **A**?

ALGORITHMS FOR TOPIC MODELS?

What if documents are **short**; can we still find **A**?

The crucial observation is, we can work with the **Gram matrix** (defined next...)










 $W W^{\mathsf{T}}$













Anchor words are extreme rows of the Gram matrix!

What if documents are **short**; can we still find **A**?

The crucial observation is, we can work with the **Gram matrix** (defined next...)

What if documents are **short**; can we still find **A**?

The crucial observation is, we can work with the Gram matrix (defined next...)

Given enough documents, we can still find the anchor words!

What if documents are **short**; can we still find **A**?

The crucial observation is, we can work with the **Gram matrix** (defined next...)

Given enough documents, we can still find the anchor words!

How can we use the anchor words to find the rest of **A**?

What if documents are **short**; can we still find **A**?

The crucial observation is, we can work with the **Gram matrix** (defined next...)

Given enough documents, we can still find the anchor words!

How can we use the anchor words to find the rest of **A**?

The **posterior distribution** Pr[topic|word] is supported on just one topic, for an anchor word

What if documents are **short**; can we still find **A**?

The crucial observation is, we can work with the Gram matrix (defined next...)

Given enough documents, we can still find the anchor words!

How can we use the anchor words to find the rest of **A**?

The **posterior distribution** Pr[topic|word] is supported on just one topic, for an anchor word

We can use the anchor words to find Pr[topic|word] for all the other words...

points are now (normalized) rows of $\widehat{M} \widehat{M}^{\mathsf{T}}$







points are now (normalized) rows of $\widehat{M} \widehat{M}^{\mathsf{T}}$





points are now (normalized) rows of $\widehat{M} \widehat{M}^{\mathsf{T}}$ Α

word #3: (0.5, anchor #2); (0.5, anchor #3)

points are now (normalized) rows of $\widehat{M} \widehat{M}^{\mathsf{T}}$ Α

word #3: (0.5, anchor #2); (0.5, anchor #3) Pr[topic|word #3]: (0.5, topic #2); (0.5, topic #3)



what we have:



word #3: (0.5, anchor #2); (0.5, anchor #3) Pr[topic|word #3]: (0.5, topic #2); (0.5, topic #3)



Pr[topic|word #3]: (0.5, topic #2); (0.5, topic #3)



Pr[topic|word #3]: (0.5, topic #2); (0.5, topic #3)

Pr[word|topic] = $\frac{Pr[topic|word] Pr[word]}{\sum_{word'} Pr[topic|word'] Pr[word']}$

Pr[word|topic] = $\frac{\Pr[topic|word] \Pr[word]}{\sum_{word'}} \Pr[topic|word'] \Pr[word']$

The Topic Model Algorithm:
V

Pr[word|topic] = $\frac{Pr[topic|word] Pr[word]}{\sum_{word'} Pr[topic|word'] Pr[word']}$

The Topic Model Algorithm:	
 form the Gram matrix and find the anchor words 	
	\square

Pr[word|topic] = $\frac{\Pr[topic|word] \Pr[word]}{\sum_{word'}} \Pr[topic|word'] \Pr[word']$

The Topic Model Algorithm:

 form the Gram matrix and find the anchor words
 write each word as a convex combination of the anchor words to find Pr[topic|word]

Pr[word|topic] = $\frac{\Pr[topic|word] \Pr[word]}{\sum_{word'}} \Pr[topic|word'] \Pr[word']$

The Topic Model Algorithm:

• form the Gram matrix and find the anchor words

• write each word as a convex combination of the anchor words to find **Pr[topic|word]**

• compute **A** from the formula above

Pr[word|topic] = $\frac{\Pr[topic|word] \Pr[word]}{\sum_{word'}} \Pr[topic|word'] \Pr[word']$

The Topic Model Algorithm:

• form the Gram matrix and find the anchor words

• write each word as a convex combination of the anchor words to find **Pr[topic|word]**

• compute **A** from the formula above

This **provably** works for **any** topic model (LDA, CTM, PAM, etc ...) provided **A** is separable and **R** is non-singular

Our first attempt used matrix inversion, which is noisy and unstable and can produce small **negative** values

Our first attempt used matrix inversion, which is noisy and unstable and can produce small **negative** values

METHODOLOGY:

We ran our algorithm on real and synthetic data:

 synthetic data: train an LDA model on 1100 NIPS abstracts, use this model to run experiments

Our first attempt used matrix inversion, which is noisy and unstable and can produce small **negative** values

METHODOLOGY:

We ran our algorithm on real and synthetic data:

 synthetic data: train an LDA model on 1100 NIPS abstracts, use this model to run experiments

Our algorithm is **fifty times faster** and performs nearly the same on all metrics we tried (I_1, log-likelihood, coherence,...) when compared to MALLET






EXPERIMENTAL RESULTS

[Arora, Ge, Halpern, Mimno, Moitra, Sontag, Wu, Zhu, ICML'13]:



The previous algorithm was **inspired by experiments!**

Our first attempt used matrix inversion, which is noisy and unstable and can produce small **negative** values

METHODOLOGY:

We ran our algorithm on real and synthetic data:

 synthetic data: train an LDA model on 1100 NIPS abstracts, use this model to run experiments

Our algorithm is **fifty times faster** and performs nearly the same on all metrics we tried (I_1, log-likelihood, coherence,...) when compared to MALLET

The previous algorithm was **inspired by experiments!**

Our first attempt used matrix inversion, which is noisy and unstable and can produce small **negative** values

METHODOLOGY:

We ran our algorithm on real and synthetic data:

 synthetic data: train an LDA model on 1100 NIPS abstracts, use this model to run experiments

Our algorithm is **fifty times faster** and performs nearly the same on all metrics we tried (I_1, log-likelihood, coherence,...) when compared to MALLET

• real data: UCI collection of 300,000 NYT articles, 10 minutes!

Is Learning Computationally Easy?



computational geometry



computational geometry















Pearson (1896) and the Naples crabs:



Pearson (1896) and the Naples crabs:

• Can we infer the parameters of a mixture of Gaussians from random samples?



Pearson (1896) and the Naples crabs:

- Can we infer the parameters of a mixture of Gaussians from random samples?
- Introduced the method of moments, but no provable guarantees



Pearson (1896) and the Naples crabs:

- Can we infer the parameters of a mixture of Gaussians from random samples?
- Introduced the method of moments, but no provable guarantees



Theorem [Kalai, Moitra, Valiant STOC'10, FOCS'10]: there is a polynomial time alg. to learn the parameters of a mixture of a constant number of Gaussians (even in high-dimensions)

Pearson (1896) and the Naples crabs:

- Can we infer the parameters of a mixture of Gaussians from random samples?
- Introduced the method of moments, but no provable guarantees



Theorem [Kalai, Moitra, Valiant STOC'10, FOCS'10]: there is a polynomial time alg. to learn the parameters of a mixture of a constant number of Gaussians (even in high-dimensions)



This settles a long line of work starting with [Dasgupta, '99] that assumed negligible overlap.

Pearson (1896) and the Naples crabs:

- Can we infer the parameters of a mixture of Gaussians from random samples?
- Introduced the **method of moments**, but no provable guarantees



Theorem [Kalai, Moitra, Valiant STOC'10, FOCS'10]: there is a polynomial time alg. to learn the parameters of a mixture of a constant number of Gaussians (even in high-dimensions)



This settles a long line of work starting with [Dasgupta, '99] that assumed negligible overlap. See also [Belkin, Sinha '10]













Approximation Algorithms, Metric Embeddings



Approximation Algorithms, Metric Embeddings





Information Theory, Communication Complexity

Approximation Algorithms, Metric Embeddings





Information Theory, Communication Complexity

Combinatorics, Smooth Analysis



• Often optimization problems abstracted from learning are intractable!

• Often optimization problems abstracted from learning are intractable!

• Are there new models that better capture the instances we actually want to solve in practice?

• Often optimization problems abstracted from learning are intractable!

• Are there new models that better capture the instances we actually want to solve in practice?

• These new models can lead to interesting **theory** questions and highly practical and **new** algorithms

• Often optimization problems abstracted from learning are intractable!

• Are there new models that better capture the instances we actually want to solve in practice?

• These new models can lead to interesting **theory** questions and highly practical and **new** algorithms

• There are **many** exciting questions left to explore at the intersection of algorithms and learning

Any Questions?

Summary:

• Often optimization problems abstracted from learning are intractable!

• Are there new models that better capture the instances we actually want to solve in practice?

• These new models can lead to interesting **theory** questions and highly practical and **new** algorithms

• There are **many** exciting questions left to explore at the intersection of algorithms and learning