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On-the-Fly Rectification for Robust Large-Vocabulary Topic Inference (Supplementary Material)

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Abstract

Our supplementary material aims to help readers better understand the main draft. It answers to a wide range of potential questions from motivation of research to experimental details. It not only consists of the theoretical proofs and empirical supports for our lemmas and findings, but also presents additional result panels that are missing from the main paper due to space limit. We hope our readers find complementary guidance from reading this material.

1. Motivations and Contributions

Q1: What are the major problems of using co-occurrence information?

A1: When data consists of collections of discrete objects, using co-occurrence provides statistical semantics to individual objects (e.g., words, products, items) based on their relations with other objects through the data. As a result, co-occurrence statistics has been widely used for various unsupervised learning, but there are two major drawbacks:

Individual objects naturally exhibit different burstiness. *Frequent objects* that too often co-occurs with many other objects would not provide meaningful semantics. Typical examples in textual data are stop words whose functions are limited to building syntax. *Rare objects* are noisy and unstable because these objects barely appear in the data, making co-occurrences with them prone to poor estimation. But they often provide exclusive markers (like topics) in underlying geometry of the data. Proper tuning of frequency imbalance is the key to successful learning, but it relies mostly on manual elaboration and domain-specific knowledge without any principled approach.

• Co-occurrence provides a great scalability by summarizing millions and billions of examples (e.g., documents, purchases, playlists). However, even the lightest format: co-occurrence matrix between pairs of objects, grows quadratically in the size of vocabulary. Tensor-based models often require co-occurrence between triples of objects, quickly exceeding normal computational budget as the size of vocabulary grows. Improving time and space complexities are crucial for usability of spectral posterior inference for latent variable models.

Q2: Why large vocabulary matters?

A2: Capability to process large vocabulary is the main challenge of the field in the following two reasons:

- Users in representation learning are often required to learn proper data representations for all or majority of their objects. Products in online shopping or items like movies and songs in streaming services form long-tail markets. Thus learning low-dimensional representations only for the frequently appearing objects is not adequate for their profit structures.
- Topic modeling based on co-occurrence often associates each topic with an *anchor word*, which dedicates only to the topic without (or weakly) contributing to the other topics. Using large vocabulary allows users to find better anchor words. In other words, most topic models with large vocabularies are proven to satisfy *separability assumption* (Ding et al., 2015). Our submission shows that topic quality improves both quantitatively and qualitatively as we increase the size of vocabulary.
- Using a large vocabulary improves less subjective interpretation of topics. Our model is capable of finding more specific characteristic words (i.e., relatively rare but associated tightly to each topic), which provide complementary information for interpreting individual topics aligning with their prominent words (i.e., mostly frequent words that are easy to understand).

Q3: Why matrix factorization? What makes rectification interesting?

A3: Matrix/Tensor factorization is a general notion to represent a variety of machine learning problems. Once writing the target inference problem as a factorization form, one

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Preliminary work. Under review by the International Conference on Machine Learning (ICML). Do not distribute.

can identify some necessary geometries with clarity. For
example, low-rankness is often an universal assumption
for unsupervised learning of finding a compact underlying
geometry.

060 • When we have a full generative model of the input data, 061 we can construct co-occurrence as an unbiased moment 062 estimator of the generative process. For instance, if the 063 data exactly follows popular probabilistic processes of 064 topic modeling, the co-occurrence matrix of words must 065 be entry-wise non-negative $(\mathcal{N}\mathcal{N})$, normalized to sum 066 to one (\mathcal{NOR}), and positive semi-definite (\mathcal{PSD}) in ad-067 dition to be low-rank (Lee et al., 2015). However, an 068 empirical co-occurrence cannot jointly satisfy these struc-069 tures due to statistical noises from the finite samples. 070 Rectification provides a principled treatment to fix statis-071 tical unstability by projecting the empirical co-occurrence (constructed from the data) onto a manifold consistent with these necessary geometries, providing an innovative 074 way to improve posterior inference.

075 • It turns out that major spectral algorithms for latent vari-076 able generative models suffer from the similar issue, 077 so called model-data mismatch (Kulesza et al., 2014). 078 Rectification could open a new solution to fix the issue 079 prevalent in spectral inference of mixed-membership latent variable models. In addition, performance of word-081 vector embeddings depends highly on how to correct co-082 occurrences with rare and frequent objects (Levy et al., 083 2015; Pennington et al., 2014). The models themselves do not provide any guidance to fix such co-occurrences, requiring labor-intensive tuning for successful learning 086 of vectorial representations. As their learning tasks can 087 also be written as forms of matrix factorization (Levy 088 & Goldberg, 2014), rectification could be applicable to 089 low-dimensional embedding learning without any ad-hoc 090 treatment. 091

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Q4: It is not easy to understand connections betweenprobabilistic and spectral topic modeling.

A4: Our submission tries not to use probability notations.
It helps increasing consistency but decreases readability.
Among many explanations to describe foundations in probabilistic and spectral topic models, we find Section 2 in (Lee et al., 2020) is particularly insightful. Here we retype it for your convenience.

We begin this section with a formal introduction to spectral topic modeling. Consider a dataset of M documents consisting of tokens drawn from a vocabulary of N words. Topic models assume that K topics are used to generate this dataset, where each topic is a distribution over the words; we summarize the latent topics by the column-stochastic matrix $\boldsymbol{B} \in \mathbb{R}^{N \times K}$ where each column $\boldsymbol{b}_k \in \Delta^{N-1}$ represents the distribution of the topic k. For each document m, choose a topic composition $\boldsymbol{w}_m \in \Delta^{K-1}$ first from a certain prior \mathfrak{f} ; we collect these hidden compositions into another column-stochastic matrix $\boldsymbol{W} \in \mathbb{R}^{K \times M}$. These models assume that each of the n_m tokens in the document m is then generated independently from the categorical distribution given by the word-probability vector $\boldsymbol{B}\boldsymbol{w}_m \in \mathbb{R}^N$.

Different models adopt different f such as $f = \text{Dir}(\alpha)$ for Latent Dirichlet Allocation (LDA) (Blei et al., 2003); $f = \mathcal{LN}(\mu, \Sigma)$ or $f = \mathcal{PN}(\mu, \Sigma)$ for Logistic/Probit-Normal Correlated Topic Models (CTMs) (Blei & Lafferty, 2007; Yu & Fokoue, 2014). Let $H \in \mathbb{R}^{N \times M}$ be the word-document matrix where the *m*-th column vector h_m counts the occurrences of each word in the document *m*, and let \widetilde{H} be the column-normalized version of H that specifies the relative frequencies of each word rather than the raw counts. Then topic modeling aims to learn *latent topics* Band *hidden compositions* W given the *observed collections of words* H. Equivalently, we seek a non-negative matrix factorization $\widetilde{H} \approx BW$ but with a prior to make individual topic compositions { w_m } coherent within a corpus.

Joint Stochastic Matrix Factorization (JSMF) The matrix \widetilde{H} of word frequencies is sparse, noisy, and often inconveniently large. Let us consider instead the word cooccurrence matrix $C \in \mathbb{R}^{N \times N}$, where C_{ij} indicates the joint probability of observing a pair of words (i, j). Then topic modeling corresponds to a second-order non-negative matrix factorization: $C \approx BAB^{\mathsf{T}}$ where the column-stochastic matrix $B \in \mathbb{R}^{N \times K}$ represents the topics as before and the joint-stochastic matrix $A \in \mathbb{R}^{K \times K}$ represents the *topic correlations*. If the true compositions W^* that generate the data are known, we can define the true correlations by $A^* := \frac{1}{M}W^*W^{*\mathsf{T}}$ where A_{kl}^* is the joint probability for a pair of latent topics (k, l). By forming C as an unbiased estimator of the underlying generative process, we can identify B and A close to the true topics and their correlations.¹

It is helpful to compare the matrix-based view of JSMF to the generative view of standard topic models. For each document m, the generative view begins with the topic composition w_m , focusing on how to produce streams of tokens. We keep choosing a topic z from w_m and then a word x from b_z for each of the n_m positions. The correlations between words that $w_m \sim f$ induces are not explicitly modeled. In contrast, the matrix-based view starts with *individual topic correlations* A_m for each document m. Then for each of the possible $n_m(n_m - 1)$ position pairs, a pair of topics (z_1, z_2) is selected first from A_m , then a pair of words (x_1, x_2) is

¹As the number of documents M grows, A converges to the true A^* and the prior $\mathbb{E}_{w \sim f}[ww^T]$ (Arora et al., 2012).

110 chosen according to the topics (b_{z_1}, b_{z_2}) , respectively. The 111 word co-occurrence matrix explicitly captures the resulting 112 correlations induced by the *prior topic correlations* A. This 113 pair generation view has the following two important im-114 plications: Recall that sharing the prior f for $\{w_m\} \sim f$ is 115 the crux of modern topic modeling (Asuncion et al., 2009), 116 and our flexible matrix prior A takes the role of f for JSMF.

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Q5: Why don't you compare against existing methods like Variational Inference, Gibbs Sampling or tensorbased spectral topic models? Why only comparing to AP for rectification?

122 A5: We mainly compare against RAW (=AP+AW) as our 123 main contribution is to scale the anchor-based algorithms to 124 larger vocabularies. Earlier work (Lee et al., 2015) shows 125 that RAW learns quality topics comparable to those from 126 Collapsed Gibbs Sampling. Previous work (Lee et al., 2019) 127 already shows that RAW performs both quantitatively and 128 qualitatively better than Online Variational Inference and 129 the tensor-based spectral method with CP-decomposition. 130 It also tests Douglas-Rachford rectification (DR) instead of 131 AP for RAW, but there was no difference in performance. 132 Therefore our submission compares the performance only 133 to RAW. 134

Q6: Likelihood-based methods do not suffer from the model-data mismatch issue. What are the benefits of using spectral methods instead of using standard probabilistic inference?

A6: Whereas likelihood-based methods keeps iterating
through the input data (e.g., documents or playlists) until convergence, spectral methods no longer revisit the input data once it is summarized into a co-occurrence statistics. Note that we often operate on millions or billions
of documents, whereas the size of vocabulary is order-ofmagnitudes smaller. In addition, spectral methods are

- Consistent. Predictions are consistent in the limit of infinite data.
- Transparent. The overall inference consists of clearly separated three steps: co-occurrence construction, rectification, and factorization.
- Interpretable. Each topic associates with a unique identifier called anchor words. Our Table 1 show that the *Characteristic Words (CWs)* from each anchor word can contribute to a specific understanding of each topic.
- Provable. Though this is not the main point of our paper, one can show finite sample convergence bounds.

Q7: For large vocabularies, the original Anchor Word algorithm already uses random projections of co-occurrence given Johnson-Lindenstrauss lemma. What

makes your work different?

A7: The original Anchor Word algorithm (AW) (Arora et al., 2013) uses two types of random projections. Both transform the empirical co-occurrence into low-dimensional spaces. However,

- As studied in (Lee & Mimno, 2014), the projected cooccurrence matrix has many non-negligible negative entries, which break the next step of inferring topics *B* (or concretely topic-word matrix *B*) as this step is based mainly on Bayes Rule. As an additional result, the learned topic correlations *A* consist of many negative entries, being far from a legal joint distribution.
- Even if the random projections are used only for fast finding of anchor words, the result set of anchors *S* cannot be better than the anchor words found in the original space. Our Figure 1 clearly demonstrates that the anchor words found from the raw co-occurrence without any rectification are far from covering the convex hull of co-occurrence space.

The key implication is that *rectification* is an essential step for high-quality topic and correlation inference as well as high-quality anchor finding. But the previously available rectifications like AP and DR cannot scale to increasing vocabularies. Our contribution: ENN and PALM are to simultaneously achieve compression and rectification of co-occurrence statistics. Our another contribution LAW indeed scales similarly to AW with random projection, but it infers topics and topic correlations more naturally from the outputs of ENN and PALM. In particular, it avoids forming any rectified C, which would incur a cost of $\mathcal{O}(N^2)$. In our LR-JSMF pipeline, we can completely bypass this $\mathcal{O}(N^2)$ constraint by constructing a low-rank approximation of the full co-occurrence directly from the raw data.

3. Algorithms and Pipeline

Q8: The paper has a number of different but related algorithms. Which algorithm is used in which step? What algorithms are from prior work and what are new in this work?

A8: Our framework consists of three main steps: 1) cooccurrence construction; 2) rectification; and 3) factorization. See our flowchart in Figure 1 together with the following explanations.

• For rectification, Algorithm 2 (RAW) consists of Alternating Projection rectification (AP) from the prior work (Lee et al., 2015). For simultaneous rectification and compression, we propose the *Epsilon Non-negative rectification* (*ENN*) in Algorithm 3 and the *Proximal Alternating Linearized Minimization rectification* (*PALM*) in Algorithm

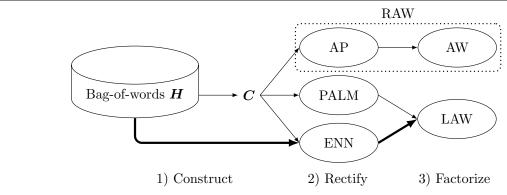


Figure 1. Flowchart of the framework. The bold arrows represent our proposed pipeline, LR-JSMF.

4. Note that AP outputs $N \times N$ rectified co-occurrence C^* , whereas our ENN and PALM output $N \times K$ rectified compression of co-occurrence Y.

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- 182 • For inference given full co-occurrence C, we use the 183 original Anchor Word algorithm (AW) in Algorithm 1 184 from the prior work (Arora et al., 2013). For inference 185 given the rectified and compressed co-occurrence Y, we 186 propose the Low-rank Anchor Word algorithm (LAW). 187 AP+AW, together known as the Rectified Anchor Word 188 algorithm (RAW), is from the previous work (Lee et al., 189 2015). 190
- From co-occurrence construction to factorization, our 192 *Low-Rank Joint Stochastic Matrix Factorization (LR-JSMF)* constructs only a low-rank approximation of the 195 input data H, bypassing the construction of any full co-196 occurrence C. Then it enjoys total computational cost 197 linear in N by initializing ENN by the low-rank approxi-198 mation of the input data.

Q9: ENN could lead to a co-occurrence matrix with neg-ative values. Is it fine?

A9: ENN only leads to *tiny* negative values in the decompressed version $C^* = YY^{\mathsf{T}}$. Our experimental results show that ENN+LAW has no visible difference from AP+AW 204 qualitatively in the learned topics as well as quantitatively in a number of metrics. Indeed, strictly enforcing non-206 negativity constraint of the decompressed C^* in PALM deteriorates the quality of topics although they still perform 208 much better than the original Anchor Word algorithm (AW) 209 without any rectification. Note also that many other previ-210 ous already claim provable guarantees under even bigger 211 violations in non-negativity (Arora et al., 2012; 2013; 2016). 212 Different from these papers, our ENN can also control the 213 214 degree of violation ϵ .

215 Q10: What is the intuition behind using column-pivoted QR on $\overline{C}^{\mathsf{T}}$ to find the anchor words?

A10: Previous work (Lee et al., 2015) shows that separability enables us to represent all non-anchor rows in \overline{C} as a convex combination of the anchor rows (i.e. $\overline{C}_{i*} = \sum_k \breve{B}_{ki} \overline{C}_{s_k*}$). To infer topics (concretely topicword matrix \breve{B}), therefore, we need to find K number of rows in \overline{C} that form a large enough convex hull to enclose all the other rows, the co-occurrence space in Figure 1. *Column-pivoted QR* is a greedy approach to this problem: in each step, we pick a pivot that is farthest away from the points picked so far, orthogonally project all the remaining points, and repeat this Gram-Schmidt process until we pick K points. We particularly use the algorithm in (Lee et al., 2019) for finding the set of anchor words S.

Q11: The Low-rank Anchor Word algorithm (LAW) shown in Algorithm 5 involves computing the QR decomposition of Y = QR. What is the additional cost incurred by this step?

A11: Computing the QR decomposition of $\boldsymbol{Y} \in \mathbb{R}^{N \times K}$ takes $\mathcal{O}(NK^2)$ time without affecting to our computational complexity linear in N.

4. Dataset and Experimental Results

Q12: How exactly is the raw data pre-processed before constructing co-occurrence matrix *C*?

A12: Given the bag-of-words, we first filter out all stop words such as $\{a, the, of, ...\}$. Then we measure the tf-idf scoring of all words and keep the top N words, where N is the user-specified vocabulary size. Unlike the usual tf-idf scoring, we integer floor all inverse document frequency scores. This consequently removes words that occur in more than 50% of the documents. Lastly, we discard all documents that contain less than 3 unique words or are less than 5 tokens long. Note that this produces exactly identical dataset on which the previous work measures the performance of RAW (=AP+AW) (Lee et al., 2015; 2019; 2020).

Q13: For most datasets used, the number of documents M exceeds the vocabulary size N. In such cases, does $\mathcal{O}(NMK)$ runtime of the proposed LR-JSMF pipeline exceed $\mathcal{O}(N^2K)$?

A13: Since the word-document matrix H is much sparser 221 than the word co-occurrence C, using H to construct com-222 pressed co-occurrence statistics V and D turns out to be 223 much more efficient than explicitly constructing C even in 224 cases where M > N. To be specific, a tighter bound on the 225 cost of initializing ENN directly from H gives $\mathcal{O}(LMK)$ 226 time and $\mathcal{O}(NK)$ space, where L is the average number 227 of unique words in each document. For the previous Recti-228 fied Anchor Word algorithm (RAW), the tighter bounds of 229 constructing C are $\mathcal{O}(L^2M)$ time and $\mathcal{O}(N^2)$ space.

Q14: Why are the different metrics shown in Figures 2 and 3?

A14: We only present 7 metrics for each experiment 233 for readability in the limited space. The panels that 234 were missing are shown in Figure 2 of this supple-235 mentary. In addition to evaluation metrics discussed 236 in the main paper, here we present two more metrics 237 to maximize comparability with other work: Sparsity 238 $(\frac{1}{K}\sum_{k}\frac{\sqrt{N}-(\|\mathbf{b}_{k}\|_{1}/\|\mathbf{b}_{k}\|_{2})}{\sqrt{N}-1})$ measures how concentrated the 239 topics are on specific words, and the traditional Coherence 240 $(\frac{1}{K}\sum_{k}\sum_{x_1\neq x_2}^{x_1,x_2\in Top_k}\log\frac{D_2(x_1,x_2)+\epsilon}{D_1(x_2)})$ measures how often 241 the top Prominent Words of each topic co-occur within 242 243 training documents. $D_1(\cdot)$ and $D_2(\cdot, \cdot)$ denote document 244 frequencies and co-document frequencies within the corpus, 245 respectively.

246 247 248 Q15: For metrics involving C, were they measured with the original C or the rectified C?

A15: All metrics presented are measured against the orig-249 inal C. Particularly for the large-vocabulary experiments 250 in Figure 3, we use approximated versions of RelativeRe-251 covery and RelativeApproximation instead since vocabulary 252 sizes over 15k prohibit explicit use of full co-occurrence C253 on standard hardware. We verified that the approximated 254 versions agree with the exact versions in their trends when 255 measuring on the datasets with small vocabularies. 256

Q16: Why the patterns over increasing x-axis values arenot always consistent?

259 A16: Say we generate a dataset from a probabilistic topic model with two topics. As topic modeling is also a cluster-261 ing, learning two or four clusters from the dataset is much easier than learning three clusters or five clusters. Therefore 263 our metric values or runtimes are not necessarily mono-264 tone when increasing the number of topics. Similarly, the 265 difficulty of learning some number of topics varies when 266 changing the size of vocabularies, thereby creating some amount of inconsistency. 267

268 269 270 Q17: Why some of the metrics are changed to relative versions?

A17: We change three intrinsic metrics: Recovery error, Approximation error, and Diagonal Dominancy into their relative versions from the original ones in (Lee et al., 2015;

2017; 2019). This is because we here compare different sizes of vocabularies as well as different numbers of topics.

Q18: According to the source code, the proposed algorithms seem to use fixed number of iterations rather than running until convergence. Is it fair?

A18: It is primarily because the previous work (Lee et al., 2015) that we directly compare against uses the fixed number of iterations for its rectification step by AP. However, we significantly test both fixed number of iterations and fixed thresholds for convergence. Then we set the proper number of iterations for our ENN and PALM empirically, so that the learned topics are in convergence. However, such convergence in topics is not easy to be translated into the uniform convergence criteria for different rectifications. Although we cannot guarantee these number of iterations are optimal for every possible textual and non-textual datasets, our experimental designs are fair on these four datasets.

Q19: How did you choose the parameters in your algorithm?

A19: Most of them are selected empirically through careful experimentation. We are able to find these which perform well across all datasets we have tested on. Some other parameters in our numerical methods are by the recommendation of the original paper.

Q20: What was the hardware setup for the experiments presented in Section 5?

A20: All experiments were performed on a highperformance computing cluster running on RedHat 6.6 OS. The non-monotonic increase in runtimes are due to preemptive load-balancing of the cluster's job scheduler. To reduce fluctuation, we took the average over 10 runs for all runtime measurements shown in the main paper.

Q21: Will be source code be released upon publication? A21: Yes. We will include a Github link to our libraries in the final draft. The anonymized source codes are submitted with the datasets used in the experiments.

5. Topic Variations when Increasing or Decreasing Vocabularies

Figure 3 shows qualitatively that users can learn more distinguishable topics by using larger vocabularies. It is especially because the algorithms make use of rarer words for more specific contexts. Moving from left to right columns, we can observe that the set of *Prominent Words (PWs)* becomes more specific. For instance, the topic corresponding to the third row are slightly vague when the sizes of vocabulries are smaller than N=5000, whereas we gain access to highly topic-specific words such as *hjb* (Hamilton-Jacobi-Bellman equation) or *pid* (Proportional Integral Derivative) when N = 5000, signifying the pertinence to dynamical and control systems of the topic. When using smaller vocabularies,

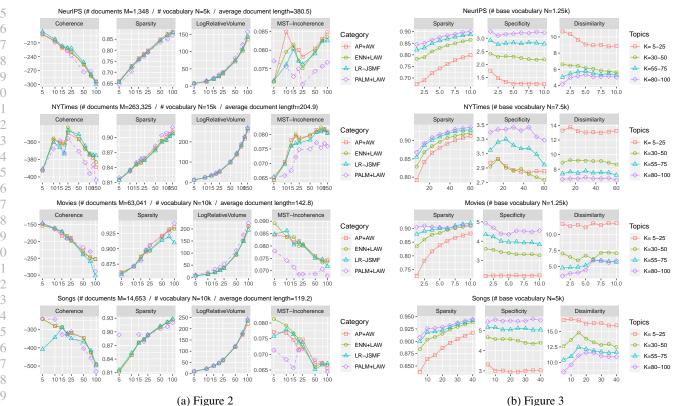


Figure 2. Additional panels for Figures 2 and 3 of the main paper. The x-axes show the number of topics K in Figure 2, and the vocabulary size N in Figure 3. In y-axes, higher is better for all metrics except for MST-Incoherence. We cannot measure Coherence for the increasing-vocabulary experiment in Figure 3 due to the large memory cost of storing co-document counts for every pair of words.

we also observe that words normally considered as less interesting terms can often contribute highly to topics. For example, the topic corresponding to the bottom row shows red shade when N = 1250, indicating that general terms such as *equivalent* or *cambridge* are strongly connected to the machine learning literature.

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396			V	ocabulary Size			
397	1250	2500	3750	5000 (base)	6250	7500	8750
398	refractory	interspike	bursting	neuron	signalling	ipsp	tst
399	interconnection	marder	stomatogastric	circuit	meilijson	stg	am
400	seen	abbott	konishi	synaptic	quiescent	substances	hyperpolarized
401	detail	acad	axonal	cell	ryckebusch	inactivation	memorized
402	transmission	pyloric	modulatory	layer	leech	depolarized	transposed
403	considered	bird	ionic	signal	silent	shapiro	tsividis
404	san	male	kanji	recognition	radical	sicl	subword
405	additional	henderson	phonemic	layer	npm	joe	phoneroes
406	amount	jackel	subsystem	hidden	demi	chinese	otherfilter
407	considered	recog	dtw	word	shikano	hanazawa	sdnn
408	developed	dictionary	strokes	speech	letterform	lexicon	perplexity
409	significant	ocr	gender	net	tebelskis	preprocessed	males
410	cambridge	discounted	tutor	control	hjb	jacobi	ovi
411	pendulum	bradtke	lqr	action	rein	forcement	pid
	requires	discount	disturbances	dynamic	biped	viscosity	idm
412	con	eligibility	disturbance	optimal	trol	sel	umass
413	bellman	indirect	hamilton	reinforcement	handicapped	bizzi	missile
414	plan	amherst	smdp	controller	gullapalli	swinging	queueing
415	directional	transparent	luminance	cell	unoriented	aftereffect	moc
416	seen	adelson	ruderman	field	heeger	blast	ori
417	dark	geniculate	andersen	visual	thalamus	mae	taube
418	neuroscience	amacrine	bergen	motion	directionally	knierim	muller
419	soc	deg	selectively	direction	hayashi	mexican	swindale
420	supported	mcnaughton	lond	image	werblin	specimen	skagg
421	equivalent	fix	solvable	gaussian	birmingham	boxplot	pbr
422	computing	satisfying	distribu	noise	kolmogorov	dependences	owi
423	cambridge	royal	barber	approximation	gmm	cb2	danish
424	considered	opper	parametrized	hidden	winther	$\operatorname{trigonometric}$	ylz
425	simply	leibler	const	bound	imation	colt	diabetes
425	detail	treatment	eter	matrix	statist	minimizer	devroye
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Figure 3. Losses or gains in Prominent Words (PWs) depending on the vocabulary size. Each row represents a topic from the NeurIPS dataset, with the top 6 PWs shown in the middle column. The red and green cells denote PWs that are lost or gained by shifting the vocabulary size from the default size N = 5000, respectively. The color intensities indicate the each word's contribution towards the corresponding topic.