Wasserstein-Fisher-Rao Document Distance

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Abstract

As a fundamental problem of natural language processing, it is important to measure the distance between different documents. Among the existing methods, the Word Mover’s Distance (WMD) has shown remarkable success in document semantic matching for its clear physical insight as a parameter-free model. However, WMD is essentially based on the classical Wasserstein metric, thus it often fails to robustly represent the semantic similarity between texts of different lengths. In this paper, we apply the newly developed Wasserstein-Fisher-Rao (WFR) metric from unbalanced optimal transport theory to measure the distance between different documents. The proposed WFR document distance maintains the great interpretability and simplicity as WMD. We demonstrate that the WFR document distance has significant advantages when comparing the texts of different lengths. In addition, an accelerated Sinkhorn based algorithm with GPU implementation has been developed for the fast computation of WFR distances. The KNN classification results on eight datasets have shown its clear improvement over WMD.

1 Introduction

Measuring the similarity between documents plays an important role in natural language processing. Recently, Word Mover’s Distance (WMD) [19], as a metric in probability space, has clear interpretation, solid theoretical foundation and demonstrated great success in many applications, e.g. metric learning [16], document retrieval [31], question answering [6] and machine translation [33]. More concretely, in the word embedding space, WMD employs the Wasserstein metric on the space of normalized bag of words (nBOW) distribution of documents, i.e. given two documents $D_s = \{x_1^s, ..., x_m^s\}$ and $D_t = \{x_1^t, ..., x_n^t\}$ with nBOW distributions $f^s$ and $f^t$, the WMD of $D_s$ and $D_t$ is

$$\text{WMD}(D_s, D_t) = \min_{R \in \mathbb{R}^{m \times n}} \left\{ \sum_{ij} C_{ij} R_{ij} \left| \sum_j R_{ij} = f_i^s, \sum_i R_{ij} = f_j^t \right. \right\}$$

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Figure 1: Illustration of transport plans by WMD (Example 1) and WFR Document Distance (Example 2). “(key, 0.2, 0.15)” denotes the mass of the word “key” is 0.2 in WMD while 0.15 in WFR.

Table 1: Transport plan by Example 1 (a) and Example 2 (b)

(a) WMD transport plan

| word   | awful  | indiv. cost | mass | amount | total |
|--------|--------|-------------|------|--------|-------|
| A      | happy  | 1.43        | 1    | 1.43   | 1.43  |
|        | sad    | 1.20        | 0.20 | 0.40   | 0.60  |
|        | lost   | 1.49        | 0.20 | 0.30   | 0.60  |
| C      | key    | 1.50        | 0.20 | 0.30   | 0.60  |
|        | evening| 1.56        | 0.20 | 0.30   | 0.60  |
|        | restaurant | 1.75   | 0.20 | 0.35   |       |

(b) WFR transport plan

| word   | awful  | indiv. cost | mass | amount | total |
|--------|--------|-------------|------|--------|-------|
| A      | happy  | 2.04        | 1    | 2.04   | 2.04  |
|        | sad    | 1.45        | 0.47 | 0.68   |       |
|        | lost   | 2.21        | 0.16 | 0.35   |       |
| C      | key    | 2.25        | 0.15 | 0.34   | 1.96  |
|        | evening| 2.42        | 0.12 | 0.30   |       |
|        | restaurant | 3.07   | 0.09 | 0.30   |       |

where $C_{ij} = ||x^t_i - x^s_j||$ is the transport cost and $x^t$ is the word vector. With the help of optimal transport, WMD naturally bridges the document distance and the word similarity in the embedding space. Moreover, it is worth to note that optimal transport metric (Wasserstein metric) has shown many new insights in generative adversarial networks [3], domain adaptation [28], representation learning [25], and etc.

Classical optimal transport models require that every piece of mass in the source distribution is transported to an equal-weight piece of mass in the target distribution. However, this requirement is too restrictive for varying-length document classification, especially when there are words semantically far away from the motifs of the documents. The following example illustrates that the semantic outliers correspond to distant points and can mislead the output of WMD.

Example 1 Consider the three sentences in Figure 1. Indeed, sentence A has positive semantics while B and C are negative. Therefore, well-defined document distance should reveal $D_{AB} > D_{BC}$. 
After removing stop words[^1], the cost to transport from B to A or C is listed in Table 1(a). During the transport from B to C, the mass at “awful” in B is equally allocated to the five words in C. Since four out of the five words are semantically far from “awful”, the average individual cost is pulled up, which makes \( \text{WMD}(A, B) < \text{WMD}(B, C) \).

Example 1 shows that WMD tends to overestimate the semantic dissimilarity when the longer document contains additional details that not involved in the shorter one. In this length-varying case, WMD may not be an effective metric for comparing documents with rich semantic details. Especially, this situation becomes extremely severe in some advanced tasks such as text summarizing [17], title generation [32] and length-varying matching [14].

Supervised Word Mover’s Distance (S-WMD) [16] tried to partly alleviate this overestimation issue by introducing global modification. S-WMD introduced the histogram importance vector to re-weight the nBOW distribution. The re-weight parameters in S-WMD do not rely on any specific texts but the training corpus. However, as shown in Example 1, a reasonable re-weight mechanism should reduce the additional detail, which should be determined text-specifically.

To address issues above, we introduce a robust document distance based on the Wasserstein-Fisher-Rao (WFR) metric, a natural extension of Wasserstein metric newly developed from the theory of unbalanced optimal transport [30, 21, 8, 9]. Unlike traditional Wasserstein metric, WFR metric allows transport from a piece of mass to another piece with different mass by adding a penalty term accounting for the unbalanced mass. WFR document distance allows the unbalanced transport among semantic words, which naturally re-weights the transport plan based on the squared distances in word embedding space. This unique property of WFR alleviates the overestimation effects caused by WMD in a text-specific way. The following Example 2 illustrates how WFR document distance remains effective in the case where WMD fails.

Example 2  The unbalanced transport plan from B to A or C and its cost that derives WFR document distance are listed in Table 1(b). As we can see, the points closer to “awful”, such as “sad”, are more preferable in the transport plan from B to C. This effect naturally re-weights the five words in C and the distance of “awful” to them, making the total cost to transport from B to C lower than B to A.

The main contributions of this paper are three folds.

- The Wasserstein-Fisher-Rao metric is applied for measuring document distance. Theoretically, this new WFR document distance is highly interpretable and differentiable as WMD and has only one hyper-parameter which is not sensitive.
- A GPU implementation is introduced for the WFR document distance, which improves the computation efficiency nearly by an order of magnitude. Furthermore, an effective prune strategy is designed for fast top-k smallest WFR document distance query.
- We conduct extensive experiments in the tasks of varying-length matching and document classification. WFR document distance is proved to be far more robust than WMD when applied to varying-length documents. Moreover, the results of the eight document classification tasks comprehensively show the advantage of the WFR document distance.

2 Related Work

In this section, we briefly review the literature from the following three perspectives.

(a) Representation of documents. There have been many ways for documents representation. Latent Semantic Indexing [11] and Latent Dirichlet Allocation [5] are based on inferred latent variables generated by the graphical model. However, most of those models are lack of the semantic information in word embedding space [24]. Stack denoising auto encoders [13], Doc2Vec [20] and skip-thoughts [18] are neural network based similarities. Despite their numerical success, those models are difficult to explain, and the performance always relies on the training samples.

Recently, WMD [19] is proposed as an implicit document representation. By considering each document as a set of words in the word embedding space, it defines the minimal transportation

[^1]: stop words are not colored in the text and removed in the figure by referring to this stop words list [https://www.textfixer.com/tutorials/common-english-words.txt](https://www.textfixer.com/tutorials/common-english-words.txt)
cost as the distance between two documents. This metric is interpretable with the consideration of semantic movements. Many other metric learning models are inspired by the metric property of WMD. S-WMD \cite{16} employed the derivative of WMD to optimize the parameterized transformation in word embedding space and histogram importance vector. Word Mover’s Embedding \cite{31} designed a kernel method on WMD metric space. However, those methods are still more or less suffer from the overestimation issue. They do not have the document-specific re-weight mechanism as WFR Document Distance.

(b) (Un)balanced optimal transport. Optimal transport (OT) has been one of the hottest topics of applied mathematics in the past few years. It is also closely related to some subjects in pure mathematics such as geometric analysis \cite{23,22} and non-linear partial differential equations \cite{12,15}. As the most fundamental and important object of OT, Wasserstein metric can be applied to measure the similarity of two probability distributions. The objective functions defined by this metric are usually convex, insensitive to noise, and can be effectively computed. Thus, Wasserstein metric has been deeply exploited by many researchers and has been successfully applied to machine learning \cite{5}, image processing \cite{27} and computer graphics \cite{29}.

A key condition of Wasserstein metric is that the total mass of the measures to be compared should be identical. This requirement prevents further application of Wasserstein metric as it cannot capture the features with mass difference, growth or decay. To overcome the shortage, WFR metric is proposed \cite{30,21,8,9} and applied to the situations where the similarity of objects (distributions) cannot be characterized by transport alone. Thus, it is not surprising that WFR has shown great performance in many applications, e.g. image processing \cite{9} and tumor growth modeling \cite{7}.

(c) Fast calculation of (un)balanced optimal transport. Sinkhorn algorithm \cite{10} solves the entropy regularized optimal transport problems. By reducing the entropy regularization term, the solution of each Sinkhorn iteration approximates to that of the original OT problem. A greedy coordinate descent version of Sinkhorn iteration \cite{2} called Greenkhorn is proposed to improve the convergence property. Recently, Sinkhorn algorithm is applied to solve the unbalanced optimal transport problem \cite{9} with modification on log-domain stabilization. In the case of document classification, an approximated solution of WFR is sufficient to serve as a good metric for documents. We accelerate the Sinkhorn algorithm by GPUs to obtain a large amount of WFR simultaneously. Furthermore, as the dual problem of each sinkhorn iteration is computationally cheap and provides the lower bound of WFR Document Distance distance, we can further accelerate the KNN by introducing a prune strategy.

3 Methods

3.1 Introduction of WFR metric

Like traditional Wasserstein metric, WFR metric can be interpreted as the square root of the minimum cost of a transport problem. The most intuitive approach to formulate this optimization is by introducing the Benamou-Brenier formulation of optimal transport theory:

Definition 1 (WFR metric) Given two measure $\mu$ and $\nu$ over some metric space $\langle X, \| \cdot \| \rangle$ and $\eta > 0$. Then the WFR distance is defined by the following optimization problem:

$$\text{WFR}_\eta(\mu, \nu) = \left( \inf_{\rho, v, \alpha} \int_0^1 \int_{\Omega} \left( \frac{1}{2} \| v(t, x) \|^2 + \frac{\eta^2}{2} \alpha(t, x)^2 \right) dx dt \right)^{\frac{1}{2}}$$

The infimum is taken over all the triplets $(\rho, v, \alpha)$ satisfying the following continuity equation:

$$\begin{align*}
\partial_t \rho + \nabla \cdot (\rho v) &= \rho \alpha, \\
\rho(0, \cdot) &= \mu, \quad \rho(1, \cdot) = \nu.
\end{align*}$$

The “source term” $\rho \alpha$ in the continuity equation and the corresponding penalty term $\eta^2 \alpha(t, x)^2 / 2$ in the objective function in the formulation of WFR metric are the main difference between WFR and classical Wasserstein metric. They quantify the failure of conservation law (mass balance) in the transport plan. The parameter $\eta$ controls the interpolation of the transport cost and the penalty term, which also determines the maximum distance that transport could occur. One can refer to \cite{8} for more details.
3.1.1 Discrete WFR metric

Discrete measure \( \mu \) over \( \mathbb{R}^n \) could be considered as \( \mu = \sum_i \mu_i \delta_{x_i} \), where \( \delta_x \) is the Dirac function on \( x \in \mathbb{R}^n \). When \( \sum_i \mu_i = 1 \), \( \mu \) is probabilistic distribution. In the following context, we begin with the explicit formula of the transport between two Diracs and the proof is from Section 4 in [8].

Lemma 1 Given two Diracs of mass \( h_0 \) and \( h_1 \) and location \( x_0 \) and \( x_1 \), the WFR metric between them is

\[
WFR_\eta(h_0 \delta_{x_0}, h_1 \delta_{x_1}) = 
\sqrt{2\eta \left[ h_0 + h_1 - 2\sqrt{h_0 h_1} \cos \left( \frac{|x_1 - x_0|}{2\eta} \right) \right]^2},
\]

where

\( \cos_+ (x) = \begin{cases} 
\cos (x), & x \in [-\pi/2, \pi/2]; \\
0, & x \notin [-\pi/2, \pi/2]. 
\end{cases} \)

In general, the transport of two distributions composed of multiple Diracs can be interpreted as the linear combination of point-to-point transports. Mathematically speaking, consider two distributions,

\[
\mu = \sum_{i=1}^I \mu_i \delta_{x_i}, \quad \nu = \sum_{j=1}^J \nu_j \delta_{y_j}, \quad \mu_i \geq 0, \quad \nu_j \geq 0,
\]

we can split the mass \( \mu_i, \nu_j \) into different pieces \( \alpha_{ij} \geq 0, \beta_{ji} \geq 0 \) as

\[
\sum_{j=1}^J \alpha_{ij} = \mu_i, \quad i = 1, \ldots, I,
\]

\[
\sum_{i=1}^I \beta_{ji} = \nu_j, \quad j = 1, \ldots, J, \quad (1)
\]

and assign each pair of \( (\alpha_{ij}, \beta_{ji}) \) to the transport between \( x_i \) and \( y_j \). The WFR distance between \( \mu \) and \( \nu \) is

\[
WFR^2_\eta(\mu, \nu) = \min_{\alpha_{ij}, \beta_{ji}} \sum_{i,j} WFR^2_\eta(\alpha_{ij} \delta_{x_i}, \beta_{ji} \delta_{y_j})
\]

\( \text{s.t.} \ \alpha_{ij} \text{ and } \beta_{ji} \text{ satisfy (1)} \) \hspace{1cm} (2)

It is noted that the problem of (2) is equivalent to the minimization problem in Definition 1. However, it is difficult to find a numerical method to implement (2). By taking dual form and changing variables alternatively, we derive Theorem 1 which is more numerically friendly.

Theorem 1 Wasserstein-Fisher-Rao metric \( WFR_\eta(\mu, \nu) \) for two discrete measure \( \mu, \nu \) is the optimum of the primal problem:

\[
WFR_\eta(\mu, \nu) = \inf_{R_{ij} \geq 0} J_\eta(R; \mu, \nu).
\]

(3)

\( R_{ij} \) is the transport plan and the objective function \( J_\eta \) is

\[
J_\eta(R; \mu, \nu) = 
\sum_{i,j} C_{ij} R_{ij} + K\mathcal{L} \left( \sum_j R_{ij} ||\mu|| \right) + K\mathcal{L} \left( \sum_i R_{ij} ||\nu|| \right)
\]

where \( C_{ij} = -2\log(\cos_+ (|x_i - y_j|/2\eta)) \) is the cost matrix and \( K\mathcal{L} \) denotes the KL divergence. The corresponding dual problem is

\[
\sup_{\phi_i, \psi_j} D_\eta(\phi, \psi; \mu, \nu)
\]

\( \text{s.t.} \ \phi_i + \psi_j \leq C_{ij} \text{ for any } i, j. \) \hspace{1cm} (4)

where the dual objection function is

\[
D_\eta(\phi, \psi; \mu, \nu) = \sum_i (1 - e^{-\phi_i}) \mu_i + \sum_j (1 - e^{-\psi_j}) \nu_j.
\]

(5)
3.1.2 Sinkhorn iteration for WFR metric

Sinkhorn iteration aims at solving the family of “entropy regularized” optimal transport problems. We use the calligraphy letter to distinguish the regularized problem form the original one. The entropy regularized optimal transport problem is the minimization of

$$\inf_{R_{ij} > 0} J_{\eta, \epsilon}(R) := J_\eta(R) + \epsilon \sum_{ij} R_{ij} \log(R_{ij}),$$

which is strictly convex. Up to a multiplier $2\eta^2$, we have

$$J_{\eta, \epsilon}(R) = KL\left( \sum_j R_{ij} \| \mu \right) + KL\left( \sum_i R_{ij} \| \nu \right) + \epsilon KL(R_{ij} \| \exp(-C/\epsilon))$$

By convex optimization theory \cite{26}, the dual problem of (6) is

$$\sup_{\phi, \psi} D_{\eta, \epsilon}(\phi, \psi),$$

where $K_\epsilon = e^{-C/\epsilon}$, $(\phi \oplus \psi)_{ij} = \phi_i + \psi_j$ and

$$D_{\eta, \epsilon}(\phi, \psi) = \langle 1 - e^{-\phi}, \mu \rangle + (1 - e^{-\psi}, \nu) + \epsilon(1 - e^\phi, K_\epsilon).$$

The WFR Sinkhorn iteration $S_\epsilon$ solves problem (7) for fixed $\epsilon$. We use Bregman iteration \cite{4} to update the $\phi$ and $\psi$ alternatively, i.e.

$$\phi^{(l+1)} = \arg\max_\phi (1 - e^{-\phi}, \mu) + \epsilon(1 - e^\phi, K_\epsilon),$$

$$\psi^{(l+1)} = \arg\max_\psi (1 - e^{-\psi}, \nu) + \epsilon(1 - e^\psi, K_\epsilon).$$

Those two subproblems could be solved in Proposition 1

**Proposition 1** Let $u = e^{\phi/\epsilon}$ and $v = e^{\psi/\epsilon}$, the analytical solution of subproblems in Equation (8) is

$$u_i^{(l+1)} = \left( \mu_i / \sum_j e^{-C_{ij}/\epsilon} v_j^{(l)} \right)^{1/(1+\epsilon)},$$

$$v_j^{(l+1)} = \left( \nu_j / \sum_i e^{-C_{ij}/\epsilon} u_i^{(l+1)} \right)^{1/(1+\epsilon)},$$

where $i = 1, \ldots, I$ and $j = 1, \ldots, J$. Equation (9) is the iteration step solves $S_\epsilon$

The details of the Sinkhorn method for WFR distance is given in Algorithm 1. It is noted that in \cite{2}, the term $e^{-C_{ij}/\epsilon}$ or $u_i, v_j$ might get extremely small or large which could cause the numerical instability in the implementation. In Algorithm 1, we take $\exp((\phi_i + \psi_j - C_{ij})/\epsilon)$ as a whole for improving the numerical stability. To solve the original problem (3), we sequentially perform WFR Sinkhorn iteration $\{S_{\epsilon_n}\}$ on descending $\{\epsilon_n\}$ where $\epsilon_n \to 0$, and adopt the optimal $\phi, \psi$ for $S_{\epsilon_n}$ as the initial value for $S_{\epsilon_{n+1}}$. The precision of WFR metric is controlled by the gap between the primal and dual problem. Besides, the WFR Sinkhorn iteration could be accelerated by packing batch of $\mu, \nu$ and precomputed cost matrix $C$ to GPU simultaneously.

3.1.3 Derivatives of WFR metric

Suppose the optimizers of the primal problem (5) and the dual problem (4) are $R^*$ and $(\phi^*, \psi^*)$ respectively. The derivative of WFR with respect to the discrete measure could be derived from envelop theorem \cite{1}. By symmetry, the derivative of the first discrete measure $\mu = \sum_{i=1}^I \mu_i \delta x_i$ is

$$\frac{\partial \text{WFR}_\eta(\mu, \nu)}{\partial \mu_i} = 1 - e^{-\phi_i^*},$$

$$\frac{\partial \text{WFR}_\eta(\mu, \nu)}{\partial x_i} = \sum_j R_{ij}^* \frac{\partial C_{ij}}{\partial x_i}.$$
To apply WFR document distance, one document should be formulated as one discrete measure \( \mu \) for entropy regularization, and number of iteration \( n \), dual potential \( \phi \) and \( \psi \).

\[ \text{Algorithm 2 WFRDocDist}(\mu, \nu, C, \epsilon, n, \phi, \psi) \]

**Input:** discrete measure \( \mu \) and \( \nu \), cost matrix \( C \), \( \epsilon \) for entropy regularization, and number of iteration \( n \), dual potential \( \phi \) and \( \psi \).

**Output:** Optimal transport plan \( R \) and potential \( \phi \), \( \psi \).

- if \( \phi \) is None or \( \psi \) is None then
  - \((b, \phi, \psi) \leftarrow (1_J, 0_J, 0_J)\)
- else
  - \((b, \phi, \psi) \leftarrow (1_J, \phi, \psi)\)
- end if

for \( k = 1 \) to \( n \) do
  - \( a_i \leftarrow (\mu_i / \exp(\phi_i \sum_j R_{ij} b_j))^{1/(1+\epsilon)}\)
  - \( b_j \leftarrow (\nu_j / \exp(\psi_j \sum_i R_{ij} a_i))^{1/(1+\epsilon)}\)
  - if \( \|a\| \) or \( \|b\| \) is too large, or \( k \) equals to \( n \) then
    - \( \phi \leftarrow \phi + \epsilon \log(a), \quad \psi \leftarrow \psi + \epsilon \log(b)\)
    - \( R_{ij} \leftarrow \exp((\phi_i + \psi_j - C_{ij}) / \epsilon)\)
  - end if
- end for

Return \((R, \phi, \psi)\).

**3.2 WFR Document Distance**

**3.2.1 Approximate WFR document distance**

To apply WFR document distance, one document should be formulated as one discrete measure \( \mu = \sum_{k=1}^{K} \mu_k \delta_{x_k} \). Following the bag of words representation, a document \( D \) is considered as a multi-set with \( K \) elements \( D = \{w_1, \ldots, w_K\} \) and the number of occurrence of each word \( C_D = \{c_1, \ldots, c_K\} \). Each word \( w_i \) belongs to the vocabulary \( \mathcal{V} \). The nBOW distribution is defined by normalizing the number of occurrences: \( \mu_k = c_k / \sum_j c_j \) for \( k = 1, \ldots, K \). Given a word embedding \( \mathcal{X} : \mathcal{V} \rightarrow \mathbb{R}^n \), each word \( w_k \) in Document \( D \) is mapped to a point in \( \mathbb{R}^n \), i.e. \( x_k = \mathcal{X}(w_k) \) for \( k = 1, \ldots, K \). Formally, we define the WFR document distance as follows.

**Definition 2 (WFR document distance)** Given a pair of documents \( D_1 \) and \( D_2 \) and a constant \( \eta > 0 \). Let \( \mu = \sum_{i=1}^{m_1} \mu_i \delta_{y_i} \) and \( \nu = \sum_{j=1}^{m_2} \nu_j \delta_{y_j} \) be the nBOW probability distribution of \( D_1 \) and \( D_2 \) respectively. The WFR document distance of \( D_1 \) and \( D_2 \) is defined as

\[ \text{Dist}(D_1, D_2) = \text{WFR}_q(\mu, \nu). \]

The numerical method for calculating the WFR document distance is present in Algorithm 2. In our experiment, we use \( M = 5 \) WFR Sinkhorn iterations with parameter \( \{(\epsilon_m, n_m) = \{(e^{-m/2}, 32m)\}\} \) for the \( m \)-th iteration. Experiments show that the mean relative error of the approximate solution is no more than 0.001 by evaluation the duality gap which achieves the desired accuracy.
Algorithm 3 Top-k smallest WFR document distance query

```
Input: Test document $D_0$ and training document set $\{(D_m, y_n)_{n=1}^N\}$, number of iteration $M$, parameter $\{(\epsilon_m, n_m)\}_{m=1}^M$ for each WFR Sinkhorn iteration, $\eta$ for WFR document distance and $K$ for KNN.
Output: k indices of top-k smallest WFR document distance samples
for each $D_m$ in training set do
    $C_{ij}^{(n)} \leftarrow -2 \log \left( \frac{\cos[(x_j - y_i^{(n)})^2]}{2\eta} \right)$
    $(u^{(n)}, v^{(n)}) \leftarrow (\text{None, None})$
end for
FilteredIndex $\leftarrow [1, \ldots, N]$
for $m$ from 1 to $M$ do
    CandidateIndex $\leftarrow$ FilteredIndex
    FilteredIndex $\leftarrow [\ ]$
    threshold $\leftarrow 0$
    for $k$ from 1 to $K$ do
        $t \leftarrow \text{WFRDocDist}(\mu_{D_m}, \nu_{D_m}, M, \{(\epsilon_m, n_m)\}, \eta)$
        if $t \geq$ threshold then
            threshold $\leftarrow t$
        end if
    end for
    for each $i \in$ CandidateIndex do
        $(R^{(i)}, u^{(i)}, v^{(i)}) \leftarrow \text{WFRSinkhorn}(\mu_{D_m}, \nu_{D_m}, C^{(i)}, \epsilon_m, n_m, u^{(i)}, v^{(i)})$
        if $D_0(u^{(i)}, v^{(i)}; \mu_{D_m}, \nu_{D_0}) <$ threshold then
            append $i$ to FilteredIndex
        end if
    end for
    Sort FilteredIndex by $J_\eta(R^{(i)}; \mu_{D_m}, \nu_{D_0})$ in ascending order.
end for
Return the first-$K$ elements of FilteredIndex.
```

3.2.2 Prune strategy for top-k smallest WFR document distance query

Top-k smallest WFR document distance query is significant in applications like document retrieval. [19] proposed a prune strategy for fast WMD-KNN classification based on the lower bound of WMD. In the case of WFR document distance, it is natural to adopt the evaluated value of the dual objective function [3] as a lower bound. With the descending of the entropy regularization’s coefficient $\epsilon$, the dual lower bound gets more and more tight.

In the top-k smallest WFR document distance query setting, the query document $D_0$ is formulized as $\mu_{D_0} = \sum_{i=1}^J \mu_i \delta_{x_i}$, and the document samples are $\{(D_n, y_n)\}_{n=1}^N$ where each $D_n$ as $\nu_{D_n} = \sum_{j=1}^J \nu_j^{(n)} \delta_{y_j^{(n)}}$, $n = 1, \ldots, N$. Considering the task with hyper-parameter $k$, after each WFR Sinkhorn iteration, we sort the document samples by the value of primal objective [3] and take the maximum of WFR document distance among the first $k$ smallest value as the threshold. Furthermore, we evaluate the dual lower bound, document samples with lower bound that larger than the threshold will be dropped. By this way, we only need to perform few WFR Sinkhorn iterations for most of the samples, which saves a lot of time.

Algorithm 3 demonstrates the details of top-k smallest WFR document distance query with prune strategy. For WFR document distance described in Definition 2, the number of WFR Sinkhorn iterations $M$ and parameters $\{(\epsilon_m, n_m)\}$ for each WFR Sinkhorn iteration is fixed. Given document size $L$, the time complexity of the Sinkhorn iteration is $O(L^2)$ for a fixed parameter. Given the size of training samples $N$, the time complexity of Algorithm 3 is bounded by $O(NL^2)$. It is noticed that this asymptotic bound cannot be further improved since the time complexity of the distance/cost matrices calculation between the evaluated sample and $N$ labeled samples are $O(NL^2)$.
Table 2: The datasets used for evaluation and their description.

| DATASET     | # TRAIN | # TEST | AVG NDW | STD NDW |
|-------------|---------|--------|---------|---------|
| BBCSPORTS   | 517     | 220    | 117.0   | 55.0    |
| TWITTER     | 2175    | 933    | 9.9     | 5.1     |
| RECIPE      | 3059    | 1311   | 48.4    | 29.8    |
| OHSUMED     | 3999    | 5153   | 59.2    | 22.3    |
| CLASSIC     | 4965    | 2128   | 48.8    | 27.7    |
| REUTERS     | 5485    | 2189   | 37.1    | 36.6    |
| AMAZON      | 5600    | 2400   | 45.1    | 22.8    |
| 20NEWS      | 11293   | 7528   | 69.7    | 70.1    |

Table 3: KNN Classification Error Rate for WMD and WFR

| DATASET     | BBCSPORT | TWITTER | RECIPE | OHSUMED |
|-------------|-----------|---------|--------|---------|
| WMD         | 4.6 ± 0.7 | 28.7 ± 0.6 | 42.6 ± 0.3 | 44.5    |
| S-WMD       | 2.1 ± 0.5 | 27.5 ± 0.5 | 39.2 ± 0.3 | 34.3    |
| WFR         | 0.8 ± 0.3 | 26.4 ± 0.2 | 38.9 ± 0.1 | 41.82   |

| DATASET     | CLASSIC   | REUTERS  | AMAZON  | 20NEWS  |
|-------------|-----------|---------|---------|---------|
| WMD         | 2.8 ± 0.1 | 3.5     | 7.4 ± 0.3 | 28.3    |
| S-WMD       | 3.2 ± 0.2 | 3.2     | 5.8 ± 0.1 | 26.8    |
| WFR         | 2.6 ± 0.2 | 3.2     | 4.8 ± 0.2 | 22.3    |

4 Experiment and Discussion

In this section, we demonstrate the supreme of WFR Document Distance over WMD and other WMD-based metrics in two tasks. The first task directly illustrates the robustness of WFR over WMD when matching length-varying documents. The second task examines the effectiveness of WFR Document Distance on a vast number of documents by KNN classification. The WMD is computed by the author’s Matlab-mex code.

(a) Dataset description We evaluate the effectiveness of WFR Document Distance on eight document classification datasets: BBCSPORTS: BBC sports article at 2004-2005; TWITTER: sentiment classification corpus of tweets; RECIPE: recipe procedures from different origin; OHSUMED: medical abstracts from cardiovascular disease groups; CLASSIC: academical paper by different publishers; REUTERS and 20NEWS: news articles by topics. The preprocessing procedures and the choice of word embeddings are the same as that described by [19, 16]. We use directly the preprocessed version of datasets from the authors. Table 2 presents the key information of the datasets, including the number of train/test samples and the average and the standard deviation of the number of distinct words (NDW).

(b) Baseline Besides WMD, we consider an additional supervised baseline named Supervised Word Mover’s Distance (S-WMD). Compared to WMD, this method employed a histogram importance vector \( w \) of vocabulary to re-weight the nBOW distribution \( \tilde{f}_i = \frac{w_i f_i}{\sum_j w_j f_j} \), and a linear transformation \( A : x_i \mapsto Ax_i \) to modify the distances in the word embedding space. The parameters are trained by gradient descent of the loss defined by Neighborhood Components Analysis (NCA). Other traditional document representation or similarity baselines are proved to be significantly weaker than WMD and SWMD [19, 16]. So they are not included.

(c) Setup Throughout the experiments, we optimize over the neighborhood size \( k \in \{1, \ldots, 19\} \) in KNN and the only hyper-parameter \( \eta \in \{1, 1/2, 1/3, 1/4\} \) by 5-fold cross-validation. We obtain the original code from the authors and re-conduct the evaluation process. For datasets without predefined train/test splits (bbcsport, twitter, recipe, classic, amazon), we report mean and standard deviation of the performance over five random 70/30 train/test splits.

(d) Discussion In Table 3 we output the results from three different document distances and eight datasets. Firstly, we compare the performance between WFR with WMD. As presented, WFR Document Distance has less KNN classification error rate at all datasets. Furthermore, for the  

https://github.com/gaohuang/S-WMD
datasets with large standard deviation of NDW (exceeds 40, see Table 2), i.e. dataset BBCSPORTS, AMAZON and 20NEWS, WFR outperforms the document distance with a clear margin. For those datasets with less standard deviations of NDW, the reduction of the KNN classification error is not that significant.

Secondly, we compare the performance between WFR with S-WMD. WFR successfully outperforms S-WMD in six out of eight datasets even though S-WMD has more supervised parameters. The successful of WFR over S-WMD since a more effective way to re-weight the transport plan is automatically captured by WFR, rather than text-independent global re-weighting in S-WMD. We notice that S-WMD only outperforms WFR and WMD at OHSUMED dataset. The medical term for cardiovascular disease in the OHSUMED dataset may not have proper word vector. The text-independent deficiency of the word embedding might be relieved by supervised transformation by S-WMD.

(e) Prune Efficiency and GPU acceleration The prune strategy for top-k smallest WFR document distance query and GPU parallelism is important to constrain the computation cost of KNN in an affordable range. Table 4 demonstrates the effect of prune strategy and GPU parallelism.

The columns in Table 4 named by Prune shows the average percent of samples left after m-th round of prune. For BBCSPORTS dataset, since the training set has only 517 samples, 3.87% of the training set contains 20 samples, which is the minimal number required for KNN classifier when K = 20. For other larger datasets, we noticed that after 2 rounds, more than 98% of the training samples are pruned. For all datasets, one could examine that after 3 rounds, the number of left samples is about 20, which is suitable for the following KNN classification. With this prune strategy, most of the computing cost is at the 1st Sinkhorn iteration, which is of time complexity $O(NL^2)$. In other words, one could improve the final precision for top-k smallest WFR document distance with merely little cost.

Figure 2 shows the averaging time of one KNN classification on eight datasets. The value is scaled by the minimal time cost (TWITTER dataset by GPU). The column in Table 4 named by GPU Acc.
Ratio denotes the acceleration ratio. For example, 3.9 for bbcsports means that one CPU (Core i7-7700HQ) computation costs 3.9 times as one GPU (GTX-1080Ti). For TWITTER, this dataset is too small so that all the data could be placed into the visual memory of GPU at single batch, which allows extremely high parallelism. Discard the highest and lowest value of the acceleration ratio, we observe that the GPU parallelism provides about 8.9 times acceleration.

5 Conclusion

In this paper, the Wasserstein-Fisher-Rao metric is applied as one unsupervised document distance (WFR document distance) which is demonstrated to be theoretically solid, easy to interpret and proved to be much more robust than WMD. WFR and its derivatives could be calculated efficiently by WFR Sinkhorn iterations with GPU acceleration. Similar to its ancestors, WFR document distance benefits from the semantic similarity of word embedding space while employs automatically re-weighted transport plan overcome the overestimation issue appearing in varying-length situations. Numerical expriments confirm the effectiveness and efficiency of the new proposed metric.

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