

SWIFT: Scalable Wasserstein Factorization for Sparse Nonnegative Tensors

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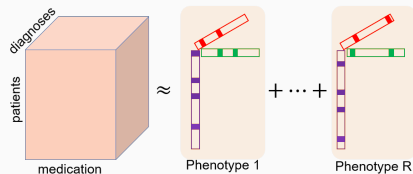
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Background: CP Tensor Factorization

CP factorization¹ approximates a tensor \mathcal{X} as the sum of R rank-one tensors:



An example of CP factorization with input of a patient-diagnosis-medication tensor.

$$\mathcal{X} \approx \hat{\mathcal{X}} = \llbracket \mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \dots, \mathbf{A}^{(N)} \rrbracket = \sum_{r=1}^R \mathbf{a}_r^{(1)} \circ \mathbf{a}_r^{(2)} \circ \dots \circ \mathbf{a}_r^{(N)},$$

- $\mathbf{A}^{(n)}$: Factor matrix for the n -th mode.
 - $\mathbf{a}_r^{(n)}$: the r -th column of $\mathbf{A}^{(n)}$
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- It is widely-used in various applications, e.g. healthcare data analytics.
 - It is highly interpretable: each rank-one tensor can be treated as a latent factor.

¹ Tamara G Kolda and Brett W Bader. "Tensor decompositions and applications". In: *SIAM Review* (2009).

Existing tensor factorization models assume certain distributions of input, for example:

- **Gaussian distribution:** $\min_{\hat{\mathcal{X}}} \|\mathcal{X} - \hat{\mathcal{X}}\|_F^2 \quad \leftarrow \text{MSE loss}^2$
- **Poisson distribution:** $\min_{\hat{\mathcal{X}}} \hat{\mathcal{X}} - \mathcal{X} * \log(\hat{\mathcal{X}}) \quad \leftarrow \text{KL divergence}^3$
- **Bernoulli distribution:** $\min_{\hat{\mathcal{X}}} \log(1 + e^{\hat{\mathcal{X}}}) - \mathcal{X} * \hat{\mathcal{X}} \quad \leftarrow \text{logit loss}^4$

Do we always know the distribution of a given input tensor?

- Real-world data often have very complex distributions.
- We usually do not know the underlying distribution of the input tensor.

²J Carroll and J Chang. "Analysis of individual differences in multidimensional scaling via an N-way generalization of "Eckart-Young" decomposition". In: *Psychometrika* (1970).

³E Chi and T Kolda. "On tensors, sparsity, and nonnegative factorizations". In: *SIAM Journal on Matrix Analysis and Applications* (2012).

⁴D Hong, T Kolda, and J Duersch. "Generalized canonical polyadic tensor decomposition". In: *SIAM Review* (2020).

Instead of assuming a specific distribution, the **Wasserstein distance** can be an alternative.

- *a.k.a.* Earth Mover Distance (EMD);
- is a potentially better measure of the difference between two distributions;
- does not assume any particular distributions of input data; and
- can leverage correlation relationship within each mode by defining the cost matrix.

Preliminaries: Wasserstein Distance and Optimal Transport

Definition (Wasserstein distance between vectors)

Wasserstein distance between probability vectors \mathbf{a} and \mathbf{b} is defined as

$$W(\mathbf{a}, \mathbf{b}) = \langle \mathbf{C}, \mathbf{T} \rangle \quad (1)$$

- \mathbf{C} is the cost matrix, where c_{ij} is the cost of moving a_i to b_j .
- $\mathbf{T} \in U(\mathbf{a}, \mathbf{b})$ is an Optimal Transport (OT) solution between \mathbf{a} and \mathbf{b} .
- $U(\mathbf{a}, \mathbf{b}) = \{\mathbf{T} \in \mathbb{R}_+^{n \times m} \mid \mathbf{T}\mathbf{1}_m = \mathbf{a}, \mathbf{T}^T \mathbf{1}_n = \mathbf{b}\}$ is the feasible set of the OT problem.

Solving this OT problem is very expensive⁵: it has a complexity of $O(n^3)$.

⁵Gabriel Peyré, Marco Cuturi, et al. "Computational optimal transport". In: *Foundations and Trends® in Machine Learning* (2019).

Preliminaries: Wasserstein Distance and Optimal Transport

An efficient alternative:

Definition (Entropy regularized OT problem⁶)

The entropy regularized OT problem is defined as:

$$W_V(\mathbf{a}, \mathbf{b}) = \underset{\mathbf{T} \in U(\mathbf{a}, \mathbf{b})}{\text{minimize}} \quad \langle \mathbf{C}, \mathbf{T} \rangle - \frac{1}{\rho} E(\mathbf{T}), \quad (2)$$

where $E(\mathbf{T}) = -\sum_{i,j=1}^{M,N} t_{ij} \log(t_{ij})$ is the entropy of \mathbf{T} .

- It is strictly convex with a unique solution.
- It can be tackled with \mathbf{u} and \mathbf{v} such that $\text{diag}(\mathbf{u}) \exp(-\rho \mathbf{C}) \text{diag}(\mathbf{v}) \in U(\mathbf{a}, \mathbf{b})$.
- Optimal \mathbf{u} and \mathbf{v} can be computed via the Sinkhorn's algorithm⁷.

⁶ Marco Cuturi. "Sinkhorn distances: Lightspeed computation of optimal transport". In: *Advances in Neural Information Processing Systems*. 2013.

⁷ Richard Sinkhorn and Paul Knopp. "Concerning nonnegative matrices and doubly stochastic matrices". In: *Pacific Journal of Mathematics* (1967)

However, applying Wasserstein distance to tensor factorization is challenging:

1. **Wasserstein distance is not well-defined for tensors:** It is well-defined for vectors, yet vectorizing tensor yields extremely large vectors, making it infeasible to solve.
2. **Wasserstein distance is difficult to scale:** It requires to solve the OT problems many times in each iteration, which is extremely time consuming.
3. **Real-world input are often large, sparse and non-negative:** Efficient algorithms are possible only when the sparsity structure are fully utilized.

Our Contributions

Contribution 1: Defining Wasserstein Tensor Distance

- SWIFT is the first work that defines Wasserstein distance for tensors.
- It does not assume any particular distribution.
- Therefore, it can handle non-negative inputs, including binaries, counts, and real-values.

Contribution 2: Formulating Wasserstein Tensor Factorization

- We propose SWIFT model to minimize the Wasserstein distance between the input and its CP reconstructions.

Contribution 3: Efficiently Solving Wasserstein Tensor Factorization

- SWIFT effectively explores the sparsity structure of the input and reduces the number of times required to compute OT.
- It reduces the computational time by efficient rearrangement of its sub-problems.
- As a result, it achieves 921x speed up over a naive implementation.

Defining Wasserstein Tensor Distance

We first define the Wasserstein distance for matrices by **summing that over their columns**:

Definition (Wasserstein Matrix Distance)

Given a cost matrix $\mathbf{C} \in \mathbb{R}_+^{M \times M}$, the Wasserstein distance between two matrices $\mathbf{A} = [\mathbf{a}_1, \dots, \mathbf{a}_P] \in \mathbb{R}_+^{M \times P}$ and $\mathbf{B} = [\mathbf{b}_1, \dots, \mathbf{b}_P] \in \mathbb{R}_+^{M \times P}$ is denoted by $W_M(\mathbf{A}, \mathbf{B})$, and given by:

$$W_M(\mathbf{A}, \mathbf{B}) = \sum_{p=1}^P W_V(\mathbf{a}_p, \mathbf{b}_p) = \underset{\bar{\mathbf{T}} \in U(\mathbf{A}, \mathbf{B})}{\text{minimize}} \langle \bar{\mathbf{C}}, \bar{\mathbf{T}} \rangle - \frac{1}{\rho} E(\bar{\mathbf{T}}), \quad (3)$$

where $\bar{\mathbf{C}} = [\underbrace{\mathbf{C}, \dots, \mathbf{C}}_{P \text{ times}}]$, $\bar{\mathbf{T}} = [\mathbf{T}_1, \dots, \mathbf{T}_P]$, and the feasible set $U(\mathbf{A}, \mathbf{B})$ is given by:

$$U(\mathbf{A}, \mathbf{B}) = \left\{ \bar{\mathbf{T}} \in \mathbb{R}_+^{M \times MP} \mid \mathbf{T}_p \mathbf{1}_M = \mathbf{a}_p, \mathbf{T}_p^T \mathbf{1}_M = \mathbf{b}_p \quad \forall p \right\} = \left\{ \bar{\mathbf{T}} \in \mathbb{R}_+^{M \times MP} \mid \Delta(\bar{\mathbf{T}}) = \mathbf{A}, \Psi(\bar{\mathbf{T}}) = \mathbf{B} \right\}, \quad (4)$$

where $\Delta(\bar{\mathbf{T}}) = [\mathbf{T}_1 \mathbf{1}_M, \dots, \mathbf{T}_P \mathbf{1}_M] = \bar{\mathbf{T}}(\mathbf{I}_P \otimes \mathbf{1}_M)$, $\Psi(\bar{\mathbf{T}}) = [\mathbf{T}_1^T \mathbf{1}_M, \dots, \mathbf{T}_P^T \mathbf{1}_M]$ and $\mathbf{1}_M$ is a vector of all ones with the size of M .

Defining Wasserstein Tensor Distance

Then we can define the Wasserstein distance for tensors by **summing that over the matricization along each mode of the tensor**:

Definition (Wasserstein Tensor Distance)

The Wasserstein distance between N -th order tensor $\mathcal{X} \in \mathbb{R}_+^{I_1 \times \dots \times I_N}$ and its reconstruction $\hat{\mathcal{X}} \in \mathbb{R}_+^{I_1 \times \dots \times I_N}$ is denoted by $W_T(\hat{\mathcal{X}}, \mathcal{X})$:

$$W_T(\hat{\mathcal{X}}, \mathcal{X}) = \sum_{n=1}^N W_M(\hat{\mathbf{X}}_{(n)}, \mathbf{X}_{(n)}) \equiv \sum_{n=1}^N \left\{ \underset{\bar{\mathbf{T}}_n \in U(\hat{\mathbf{X}}_{(n)}, \mathbf{X}_{(n)})}{\text{minimize}} \quad \langle \bar{\mathbf{C}}_n, \bar{\mathbf{T}}_n \rangle - \frac{1}{\rho} E(\bar{\mathbf{T}}_n) \right\}, \quad (5)$$

where $\mathbf{X}_{(n)} \in \mathbb{R}_+^{I_n \times I_{(-n)}}$ is the n -th mode matricization of \mathcal{X} , $\bar{\mathbf{C}}_n = [\mathbf{C}_n, \mathbf{C}_n, \dots, \mathbf{C}_n] \in \mathbb{R}_+^{I_n \times I_n I_{(-n)}}$, and $\bar{\mathbf{T}}_n = [\mathbf{T}_{n1}, \dots, \mathbf{T}_{nj}, \dots, \mathbf{T}_{nI_{(-n)}}] \in \mathbb{R}_+^{I_n \times I_n I_{(-n)}}$. $\mathbf{T}_{nj} \in \mathbb{R}_+^{I_n \times I_n}$ is the transport matrix between the columns $\hat{\mathbf{X}}_{(n)}(:, j) \in \mathbb{R}_+^{I_n}$ and $\mathbf{X}_{(n)}(:, j) \in \mathbb{R}_+^{I_n}$.

The Wasserstein distance $W_T(\mathcal{X}, \mathcal{Y})$ defined above is a valid distance and satisfies the metric axioms of positivity, symmetry, and triangle inequality.

Defining Wasserstein Tensor Distance

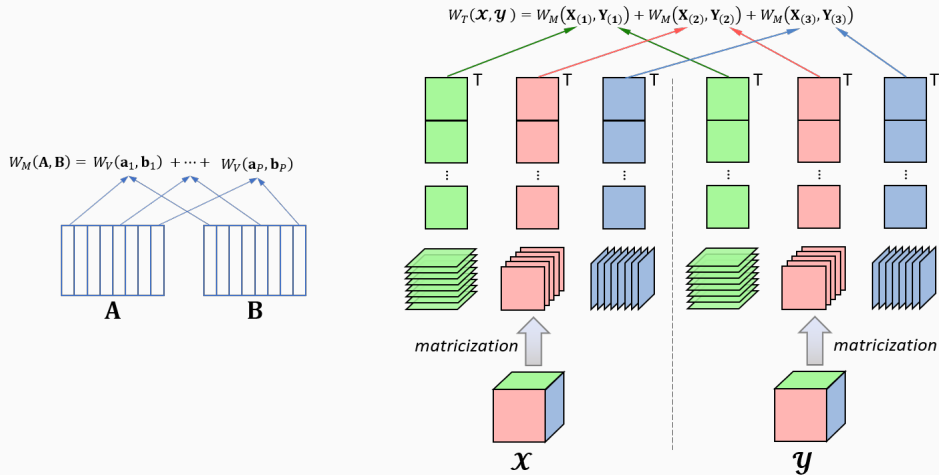


Illustration of the Wasserstein distances. Left: Wasserstein matrix distance; right: Wasserstein tensor distance.

Wasserstein Tensor Factorization

SWIFT minimizes the Wasserstein tensor distance between input and its CP reconstruction:

Optimization problem

$$\begin{aligned} & \underset{\{\mathbf{A}_n \geq 0, \bar{\mathbf{T}}_n\}_{n=1}^N}{\text{minimize}} && \sum_{n=1}^N \left(\langle \bar{\mathbf{C}}_n, \bar{\mathbf{T}}_n \rangle - \frac{1}{\rho} E(\bar{\mathbf{T}}_n) \right) \\ & \text{subject to} && \hat{\mathcal{X}} = \llbracket \mathbf{A}_1, \dots, \mathbf{A}_N \rrbracket \\ & && \bar{\mathbf{T}}_n \in U(\hat{\mathbf{X}}_{(n)}, \mathbf{X}_{(n)}), \quad n = 1, \dots, N \end{aligned}$$

Constraint Relaxation using the generalized KL-divergence

$$\underset{\{\mathbf{A}_n \geq 0, \bar{\mathbf{T}}_n\}_{n=1}^N}{\text{minimize}} \quad \sum_{n=1}^N \left(\underbrace{\langle \bar{\mathbf{C}}_n, \bar{\mathbf{T}}_n \rangle - \frac{1}{\rho} E(\bar{\mathbf{T}}_n)}_{\text{Part } P_1} + \lambda \left(\underbrace{KL(\Delta(\bar{\mathbf{T}}_n) \| \mathbf{A}_n (\mathbf{A}_{\odot}^{(-n)})^T)}_{\text{Part } P_2} + \underbrace{KL(\Psi(\bar{\mathbf{T}}_n) \| \mathbf{X}_{(n)})}_{\text{Part } P_3} \right) \right) \quad (6)$$

We alternate between \mathbf{A}_n and $\bar{\mathbf{T}}_n$ to solve Eq. (6).

Efficient Algorithms: 1. Solving for OT Problems ($\bar{\mathbf{T}}_n$)

Note that: $\bar{\mathbf{T}}_n = [\mathbf{T}_{n1}, \dots, \mathbf{T}_{nj}, \dots, \mathbf{T}_{nl_{(-n)}}] \in \mathbb{R}_+^{I_n \times I_{(-n)}}$.

The number of optimal transport problems to solve is: $l_{(-n)} = l_1 \times \dots \times l_{n-1} \times l_{n+1} \times \dots \times l_N$.

Instead, we use the property of the OT solution $\mathbf{T}_{nj}^* \mathbf{1} = \text{diag}(\mathbf{u}_j) \mathbf{K}_n \mathbf{v}_j = \mathbf{u}_j * (\mathbf{K}_n \mathbf{v}_j)$; therefore:

Proposition 2

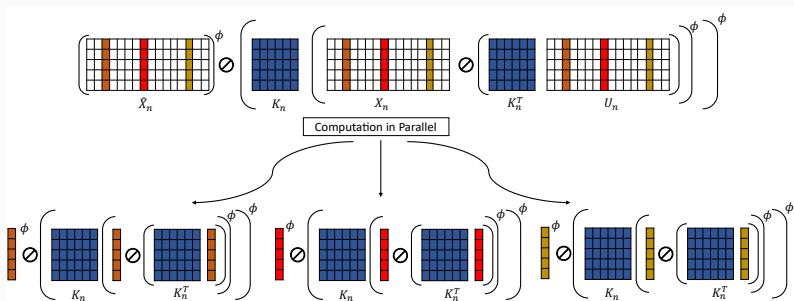
$$\Delta(\bar{\mathbf{T}}_n) = [\mathbf{T}_{n1} \mathbf{1}, \dots, \mathbf{T}_{nj} \mathbf{1}, \dots, \mathbf{T}_{nl_{(-n)}} \mathbf{1}] = \mathbf{U}_n * (\mathbf{K}_n \mathbf{V}_n) \quad (7)$$

minimizes (6), where $\mathbf{K}_n = e^{(-\rho \mathbf{C}_n - 1)} \in \mathbb{R}_+^{I_n \times I_n}$, $\mathbf{U}_n = (\hat{\mathbf{X}}_{(n)})^\Phi \oslash (\mathbf{K}_n (\mathbf{X}_{(n)} \oslash (\mathbf{K}_n^T \mathbf{U}_n))^\Phi)^\Phi$, $\mathbf{V}_n = (\mathbf{X}_{(n)} \oslash (\mathbf{K}_n^T \mathbf{U}_n))^\Phi$, $\Phi = \frac{\lambda \rho}{\lambda \rho + 1}$, and \oslash indicates element-wise division.

Efficient Algorithms: 1. Solving for OT Problems (\bar{T}_n)

Exploring the sparsity structure for efficiently computing $\Delta(\bar{T}_n)$

- Many columns of the $\mathbf{X}_{(n)}$ are all zeros; thus they can be ignored when computing \mathbf{V}_n .
- Besides, each column of \mathbf{V}_n can be computed in parallel.



SWIFT explores sparsity structure in input data $\mathbf{X}_{(n)}$ and drops zero values columns.

Efficient Algorithms: 2. Updating CP factors (\mathbf{A}_n)

Sub-problem for the CP factor matrices \mathbf{A}_n

$$\underset{\mathbf{A}_n \geq 0}{\text{minimize}} \quad \sum_{i=1}^N KL\left(\Delta(\bar{\mathbf{T}}_i) \parallel \mathbf{A}_i(\mathbf{A}_{\odot}^{(-i)})^T\right) \quad (8)$$

Challenge: \mathbf{A}_n is also involved in the Khatri-Rao product $\mathbf{A}_{\odot}^{(-i)}$.

To tackle this, we define an rearranging operator Π , such that

Efficient rearranging operation

$$\Pi(\mathbf{A}_i(\mathbf{A}_{\odot}^{(-i)})^T, n) = \mathbf{A}_n(\mathbf{A}_{\odot}^{(-n)})^T \in \mathbb{R}_+^{I_n \times I_{(-n)}} \quad \forall i \neq n. \quad (9)$$

In this way, the Khatri-Rao product term no longer contain the factor matrix \mathbf{A}_n .

Efficient Algorithms: 2. Updating CP factors (\mathbf{A}_n)

With this operator, the sub-problem is equivalent to:

Rearranged sub-problem for \mathbf{A}_n

$$\underset{\mathbf{A}_n \geq 0}{\text{minimize}} \quad KL \left(\begin{bmatrix} \Pi(\Delta(\bar{\mathbf{T}}_1), n) \\ \vdots \\ \Pi(\Delta(\bar{\mathbf{T}}_i), n) \\ \vdots \\ \Pi(\Delta(\bar{\mathbf{T}}_N), n) \end{bmatrix} \parallel \begin{bmatrix} \mathbf{A}_n(\mathbf{A}_{\odot}^{(-n)})^T \\ \vdots \\ \mathbf{A}_n(\mathbf{A}_{\odot}^{(-n)})^T \\ \vdots \\ \mathbf{A}_n(\mathbf{A}_{\odot}^{(-n)})^T \end{bmatrix} \right) \quad (10)$$

With the rearranged objective function, the factor matrix \mathbf{A}_n can be efficiently updated via multiplicative update rules⁸.

⁸Daniel D Lee and H Sebastian Seung. "Algorithms for non-negative matrix factorization". In: *Advances in Neural Information Processing Systems*. 2001.

Experiments: Datasets and Evaluation Metrics

BBC News⁹

- a third-order counting tensor with size of 400 articles by 100 words by 100 words
- downstream task: article category classification; evaluated by *accuracy*.

Sutter

- a dataset collected from a large real-world health provider network
- a third-order binary tensor with size of 1000 patients by 100 diagnoses by 100 medications
- downstream task: heart failure onset; evaluated by *PR-AUC*.

We use the pair-wise cosine distance to compute the cost matrices for each mode of the two datasets.

⁹Derek Greene and Pádraig Cunningham. "Practical Solutions to the Problem of Diagonal Dominance in Kernel Document Clustering". In: *International Conference on Machine learning*. 2006.

Experiments: Baselines

We compare against the following tensor factorization models with different loss functions:

Model	Loss Type	Underlying Distribution Assumption	Reference
CP-ALS	MSE Loss	Gaussian	(Bader & Kolda 2007)
CP-NMU	MSE Loss	Gaussian	(Bader & Kolda 2007)
Supervised CP	MSE Loss	Gaussian	(Kim et al. 2017)
Similarity based CP	MSE Loss	Gaussian	(Kim et al. 2017)
CP-Continuous	Gamma Loss	Gamma	(Hong et al. 2020)
CP-Binary	Log Loss	Bernoulli	(Hong et al. 2020)
CP-APR	KL Loss	Poisson	(Chi & Kolda 2012)

Experimental Results: Classification Performance

		R=5	R=10	R=20	R=30	R=40
BBC News Dataset	CP-ALS	.521 ± .033	.571 ± .072	.675 ± .063	.671 ± .028	.671 ± .040
	CP-NMU	.484 ± .039	.493 ± .048	.581 ± .064	.600 ± .050	.650 ± .031
	Supervised CP	.506 ± .051	.625 ± .073	.631 ± .050	.665 ± .024	.662 ± .012
	Similarity Based CP	.518 ± .032	.648 ± .043	.638 ± .021	.662 ± .034	.673 ± .043
	CP-Continuous	.403 ± .051	.481 ± .056	.528 ± .022	.559 ± .024	.543 ± .043
	CP-Binary	.746 ± .058	.743 ± .027	.737 ± .008	.756 ± .062	.743 ± .044
	CP-APR	.675 ± .059	.768 ± .033	.753 ± .035	.743 ± .033	.746 ± .043
	SWIFT	.759 ± .013	.781 ± .013	.803 ± .010	.815 ± .005	.818 ± .022
Sutter Data	CP-ALS	.327 ± .072	.333 ± .064	.311 ± .068	.306 ± .065	.332 ± .098
	CP-NMU	.300 ± .054	.294 ± .064	.325 ± .085	.344 ± .068	.302 ± .071
	Supervised CP	.301 ± .044	.305 ± .036	.309 ± .054	.291 ± .037	.293 ± .051
	Similarity Based CP	.304 ± .042	.315 ± .041	.319 ± .063	.296 ± .041	.303 ± .032
	CP-Continuous	.252 ± .059	.237 ± .043	.263 ± .065	.244 ± .053	.256 ± .077
	CP-Binary	.301 ± .061	.325 ± .079	.328 ± .080	.267 ± .074	.296 ± .063
	CP-APR	.305 ± .075	.301 ± .068	.290 ± .052	.313 ± .082	.304 ± .086
	SWIFT	.364 ± .063	.350 ± .031	.350 ± .040	.369 ± .066	.374 ± .044

SWIFT outperforms all models consistently by a large margin.

Experimental Results: Classification Performance

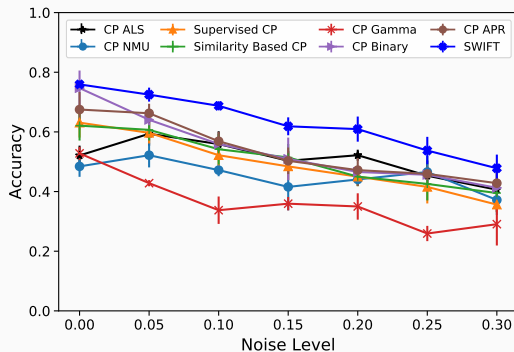
Comparison against widely-adopted classifiers:

	Accuracy on BBC	PR-AUC on Sutter
Lasso Logistic Regression	.728 \pm .013	.308 \pm .033
Random Forest	.628 \pm .049	.318 \pm .083
Multi-Layer Perceptron	.690 \pm .052	.305 \pm .054
K-Nearest Neighbor	.596 \pm .067	.259 \pm .067
SWIFT (R=5)	.759 \pm .013	.364 \pm .063
SWIFT (R=40)	.818 \pm .020	.374 \pm .044

SWIFT with rank of 5 already outperforms all other classifiers compared.

Experimental Results: Classification Performance on Noisy Data

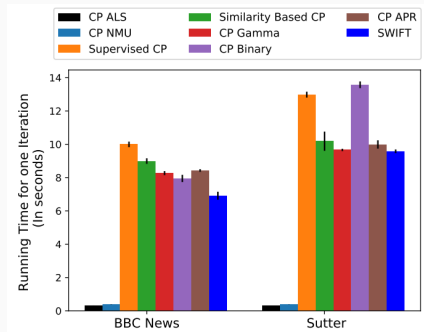
We inject random noise to the BBC News data and run all models using the noisy data:



SWIFT outperforms all baselines, especially for medium and high noise levels.

Experimental Results: Scalability of SWIFT

We set $R = 40$, switch off all parallelization of SWIFT for fair comparison and measure the running time of all models.



SWIFT is as scalable as other CP factorization models.

Experimental Results: Interpretability of SWIFT

We interpret the factor matrices learned for Sutter datasets. Following are three examples:

Atrial Fibrillation (Weight= 21.93)

Dx-Essential hypertension [98.]
Dx-Disorders of lipid metabolism [53.]
Dx-Cardiac dysrhythmias [106.]
Rx-Calcium Channel Blockers
Rx-Alpha-Beta Blockers
Rx-Angiotensin II Receptor Antagonists

Cardiometabolic Disease (Weight= 19.58)

Dx-Diabetes mellitus without complication [49.]
Dx-Essential hypertension [98.]
Dx-Disorders of lipid metabolism [53.]
Rx-Diagnostic Tests
Rx-Biguanides
Rx-Diabetic Supplies

Mental Disorder (Weight= -16.22)

Dx-Anxiety disorders [651]
Dx-Menopausal disorders [173.]
Dx-Depressive disorders [6572]
Rx-Benzodiazepines
Rx-Selective Serotonin Reuptake Inhibitors (SSRIs)
Rx-Serotonin Modulators

- Each group (phenotype) contains clinically relevant diagnoses and medications.
- The weight indicates the lasso logistic regression coefficient for heart failure (HF) prediction.
- First two groups are clinically relevant to HF, but the third is not.
- The clinical meaningfulness is endorsed by a medical expert.

SWIFT yields interpretable factor matrices.

Conclusion

- We define the Wasserstein distance between two tensors and propose SWIFT, a Wasserstein tensor factorization model.
- We derive an efficient learning algorithm by exploring the sparsity structure and introducing efficient rearrangement operator.
- Empirical evaluations demonstrate that SWIFT consistently outperforms baselines in downstream prediction tasks, even in the presence of heavy noise.
- SWIFT is also shown scalable and interpretable.

Thank you!

All questions and comments are greatly appreciated!