Embeddings: learning representations for unsupervised learning

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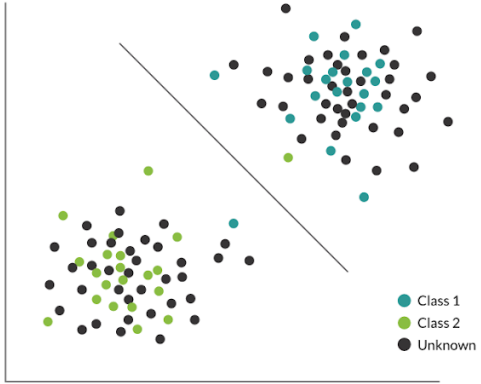
Supervised learning

We observe $\boldsymbol{x}, y$
i.e. classification, regression



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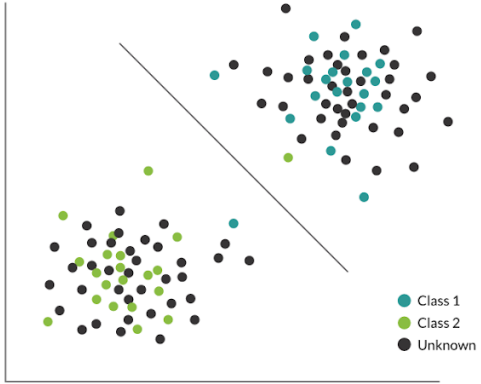
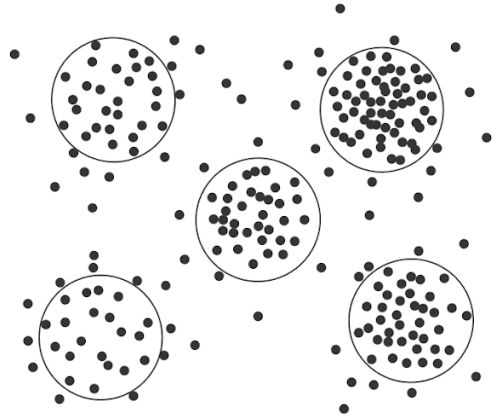


Unsupervised learning

We just observe $\boldsymbol{x}$
i.e. raw text, music, ratings



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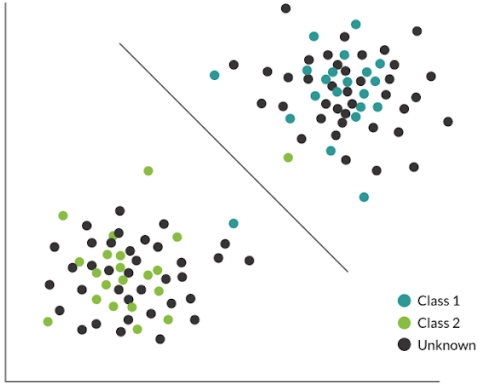

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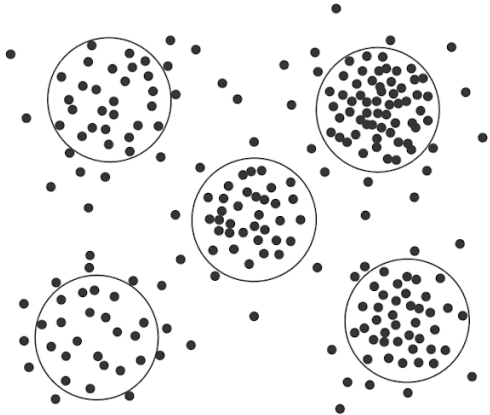


It all deals with learning a representation of the data: embedding entities into $\mathbf{R}^d$

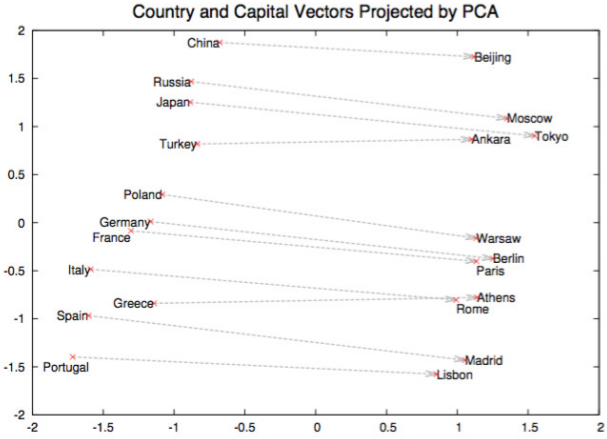
Context

- Dealing with unlabeled data, like raw text
- Dealing with tabular data, which mixes categorical and continuous variables
- Detecting outliers in the dataset
- Or mistakes in labels

Natural language processing

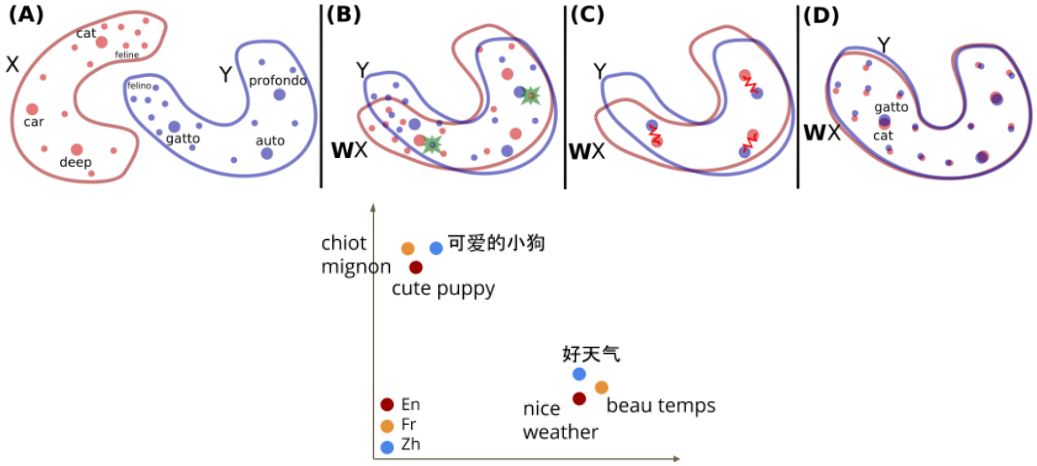
- A document can be represented as a sparse vector $\boldsymbol{x}$ of size 60,000 where $\boldsymbol{x}_i$ is the number of occurrences of the ith word.
- Could we guess meaning from context like humans?

Learned embeddings have interesting properties: word2vec



Tomas Mikolov et al. "Distributed Representations of Words and Phrases and their Compositionality". In: *Advances in Neural Information Processing Systems*. Ed. by C.J. Burges et al. Vol. 26. Curran Associates, Inc., 2013. URL: https://proceedings.neurips.cc/paper/2013/file/9aa42b31882ec039965f3c4923ce901b-Paper.pdf

Multilingual word embeddings (unsupervised)



Guillaume Lample et al. "Word translation without parallel data". In: *International Conference on Learning Representations*. 2018. URL: https://openreview.net/forum?id=H196sainb

Application: Recommender Systems

Problem

- Every user rates few items (1 %)
- How to infer missing ratings?

Example

Sacha	?	5	2	?
Ondine	4	1	?	5
Pierre	3	3	1	4
Joëlle	5	?	2	?

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Encoding the problem

Matrix completion (unsupervised)

Given sparse entries M_{ij} find the other entries M_{ij}

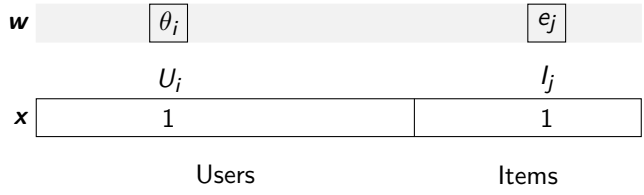
Supervised problem

- $\boldsymbol{X} = \{(i, j)\}$ are the categorical observed indices (ex. user i and item j)
- $\boldsymbol{y} = \{R_{ij}\}$ are the continuous (or categorical) ratings

Learning embeddings

Embedding n entities into $\mathbf{R}^d$ is equivalent to learning a $n \times d$ matrix $\boldsymbol{W}$ s.t. embedding of entity i is W_i.

One-hot encoding $\boldsymbol{e}_j = (0, \ldots, 0, \underbrace{1}_{j}, 0, \ldots, 0)$ so that $\boldsymbol{W}\boldsymbol{e}_j = W_j$



Dimensionality reduction, or best approximation of rank k

Input: $n \times m$ matrix $\boldsymbol{X}$

Minimize: $||\boldsymbol{X} - M||_2^2 = \sum_{i,j}(X_{ij} - M_{ij})^2$ where $rank(M) = k$

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Solution: compute the singular value decomposition (SVD) $\boldsymbol{X} = U\Sigma V^T$ where

- U $(n \times r)$ is orthogonal: $U^T U = I_r$ where $r = rank(\boldsymbol{X})$
- Σ $(r \times r)$ is diagonal: its values $\lambda_1 \geq \ldots \geq \lambda_r > 0$
- V $(m \times r)$ is orthogonal: $V^T V = I_r$

k-SVD is truncated to k biggest singular values. $M = U_k \Sigma_k V_k^T$ is solution. And $W = U_k \Sigma_k$ is a $n \times k$ matrix of embeddings (`pca.transform`).

KNN $\rightarrow$ measure similarity between users (or items)

K-nearest neighbors

- R_u represents the row vector of user u in the rating matrix (users $\times$ items).
- Similarity score between users (cosine):

$$score(u, v) = \frac{R_u \cdot R_v}{||R_u|| \cdot ||R_v||}.$$

- Let's identify the k-nearest neighbors of user u
- And recommend to user u what u's neighbors liked, but u didn't watch

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Hint

If R' the $N \times M$ matrix of rows $\frac{R_u}{||R_u||}$, we can get the $N \times N$ score matrix by computing $R'R'^T$. May not fit in memory.

Matrix factorization $\rightarrow$ reduce dimension to generalize

$$R = \begin{pmatrix} R_1 \\ R_2 \\ \vdots \\ R_n \end{pmatrix} = \boxed{} = \boxed{U} \boxed{P}$$

R: 600 users $\times$ 9k works $\iff$ $\begin{cases} U\text{: 600 users} \times \text{20 profiles} \\ P\text{: 20 profiles} \times \text{9k works} \end{cases}$

$\mathbf{R}_{\text{Bob}}$ is a linear combination of profiles P_1, P_2, etc.

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Interpreting Key Profiles

If P	P_1: adventure	P_2: romance	P_3: plot twist
And U_{Bob}	0.2	-0.5	0.6

$\Rightarrow$ Bob likes a bit adventure, hates romance, loves plot twists.

Matrix factorization $\rightarrow$ reduce dimension to generalize

Train

- R ratings, U user embeddings, V item embeddings.

$$R = UV^T \qquad \hat{r}_{ij} = \boldsymbol{u}_i^T \boldsymbol{v}_j$$

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Test: Will user i' like item j'?

- Just compute $\boldsymbol{u}_{i'}^T \boldsymbol{v}_{j'}$

Objective: regularized squared loss

$$\mathcal{L} = \sum_{i,j} (\underbrace{\boldsymbol{u}_i^T \boldsymbol{v}_j}_{\text{pred}} - \underbrace{r_{ij}}_{\text{real}})^2 + \underbrace{\lambda||\boldsymbol{u}_i||_2^2 + \lambda||\boldsymbol{v}_j||_2^2}_{\text{regularization}}$$

Variants

SVD: $\sum_{\text{all } i,j} (\boldsymbol{u}_i^T \boldsymbol{v}_j - r_{ij})^2$ (missing pairs are imputed to zero)

ALS-WR : $\sum_{i,j \text{ known}} (\boldsymbol{u}_i^T \boldsymbol{v}_j - r_{ij})^2 + \lambda(\sum_i N_i||\boldsymbol{u}_i||^2 + \sum_j M_j||\boldsymbol{v}_j||^2)$

where N_i (resp. M_j): how many times user i rated items (resp. item j was rated)

Computing the gradients

$$\mathcal{L} = \sum_{i,j} (\underbrace{\boldsymbol{u}_i^T \boldsymbol{v}_j}_{\text{pred}} - \underbrace{r_{ij}}_{\text{real}})^2 + \underbrace{\lambda ||\boldsymbol{u}_i||_2^2 + \lambda ||\boldsymbol{v}_j||_2^2}_{\text{regularization}}$$

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$\mathcal{L}$ is (polynomial and) convex in each $\boldsymbol{u}_k$ or $\boldsymbol{v}_\ell$.

Finding $\boldsymbol{u}_k$ that minimizes $\mathcal{L} \Rightarrow$ Finding the zeroes of

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{u}_k} = \sum_{j \text{ rated by } k} 2(\boldsymbol{u}_k{}^T \boldsymbol{v}_j - r_{kj})\boldsymbol{v}_j + 2\lambda \boldsymbol{u}_k = 0$$

can be rewritten $A\boldsymbol{u}_k = B$ so $\boldsymbol{u}_k = A^{-1}B$ (closed form)

Complexity: $O(d^3)$ where d is the (embedding) size of A (but can be parallelized)

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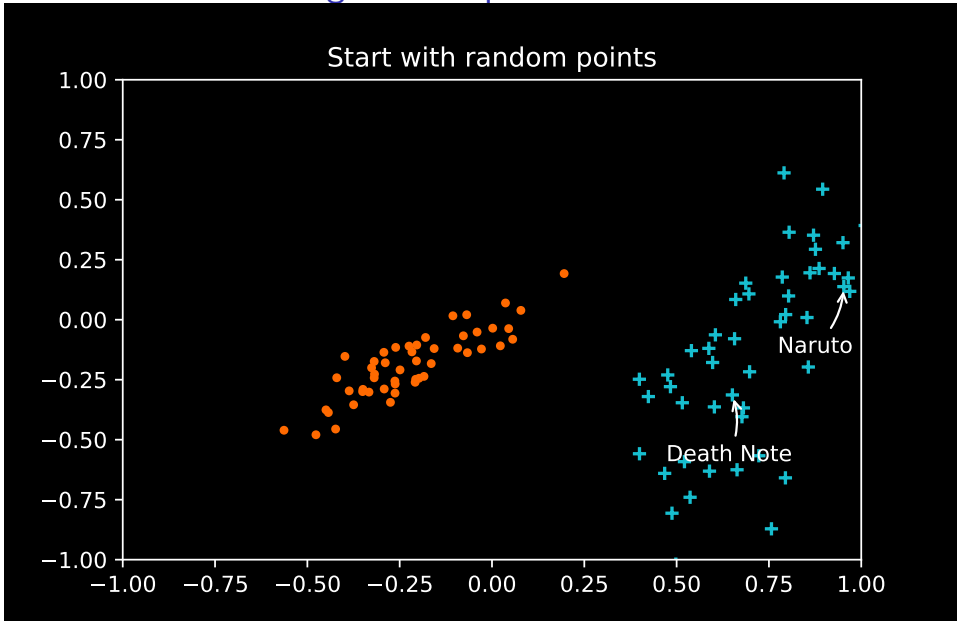
Algorithm ALS: Alternating Least Squares (Zhou, 2008)

- Until convergence (few iterations):
  - Fix U (users) learn V (items) in order to minimize $\mathcal{L}$
  - Fix V find U

Illustration of Alternating Least Squares



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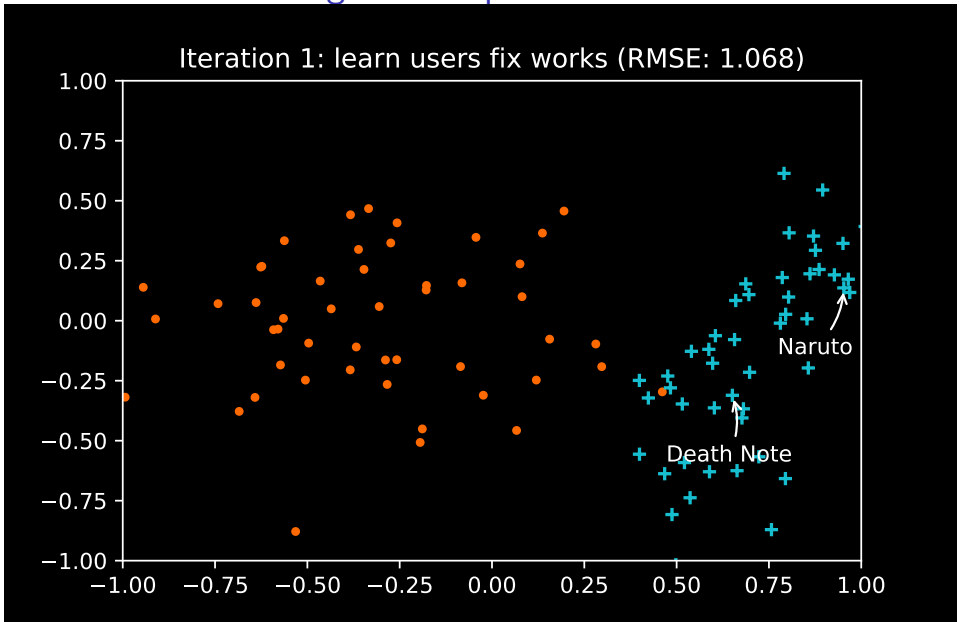

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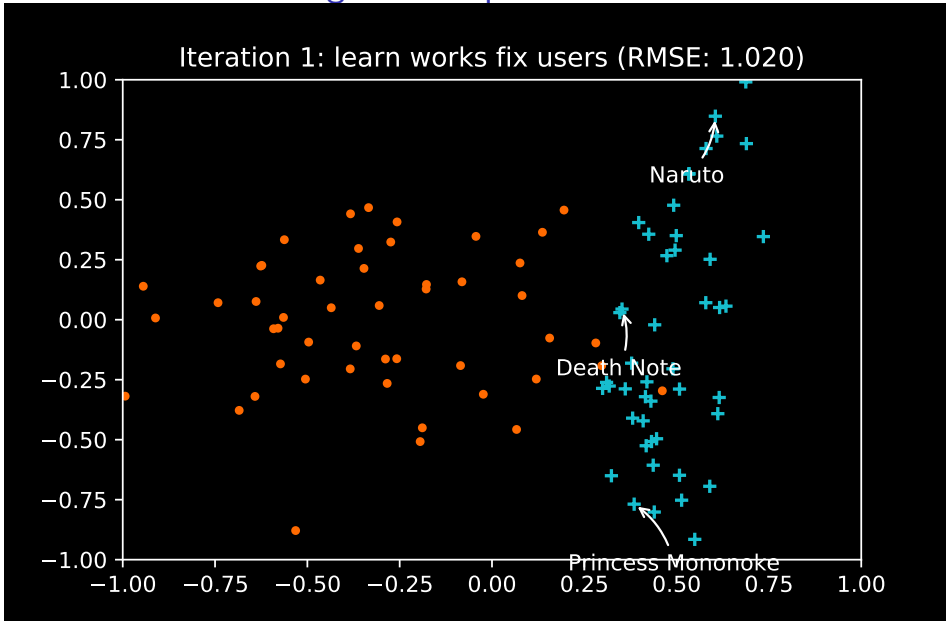

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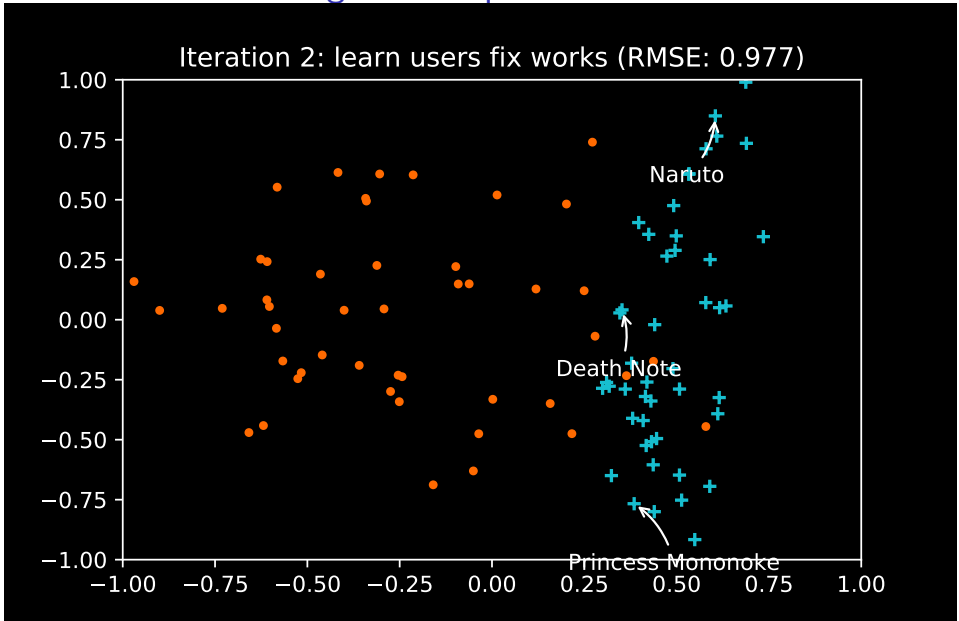

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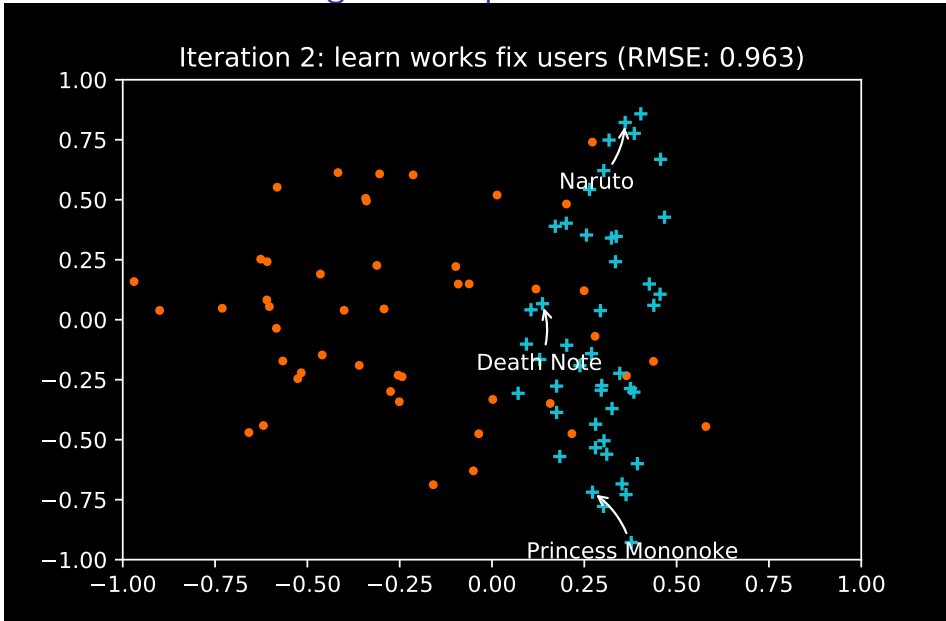

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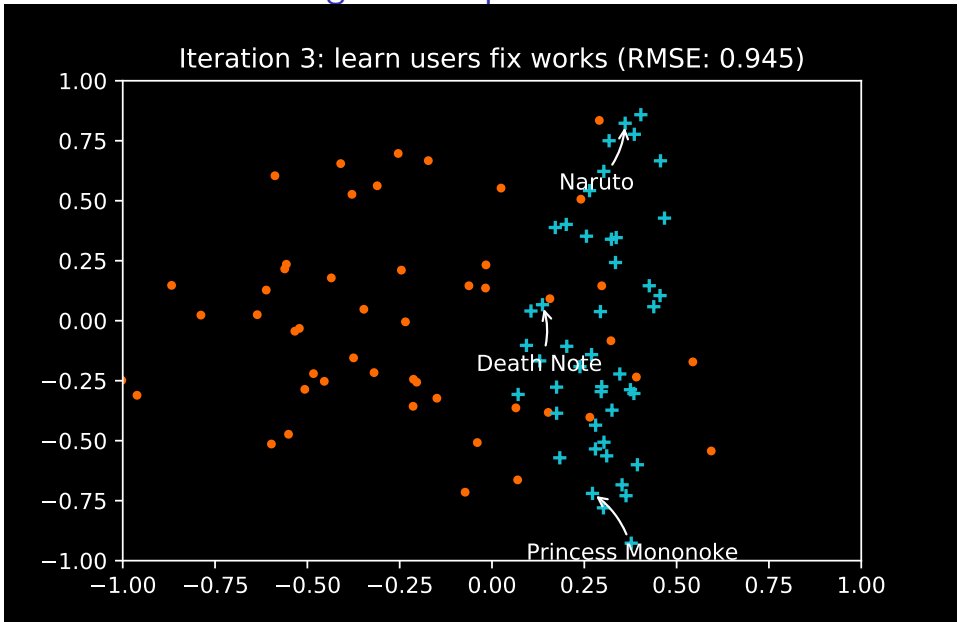

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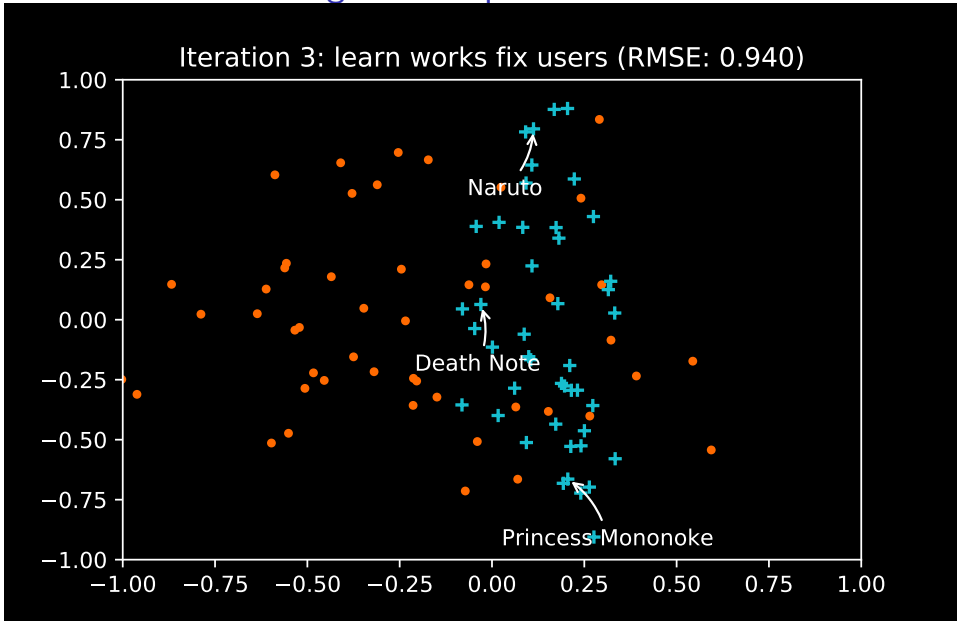

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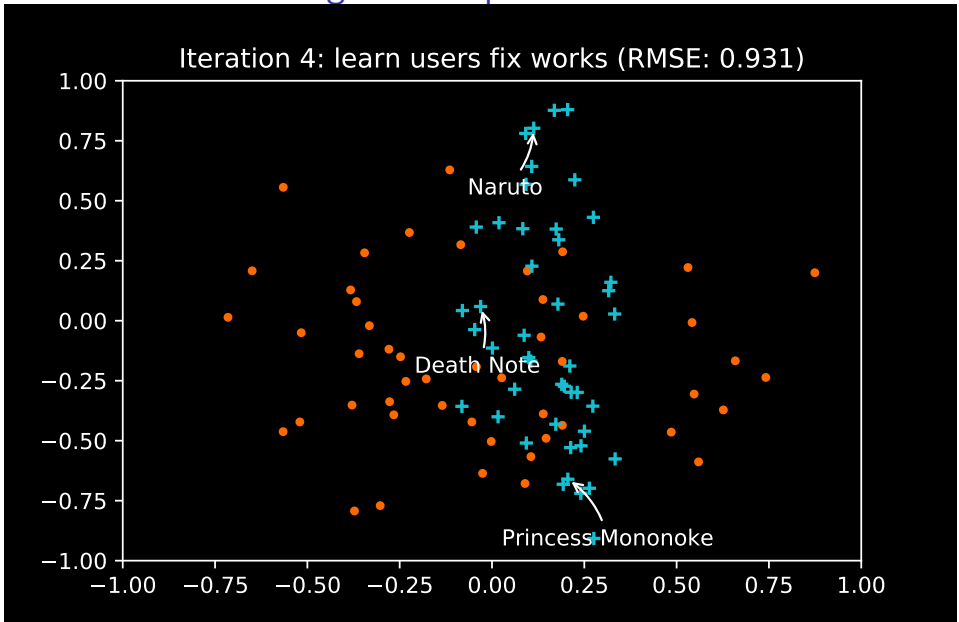

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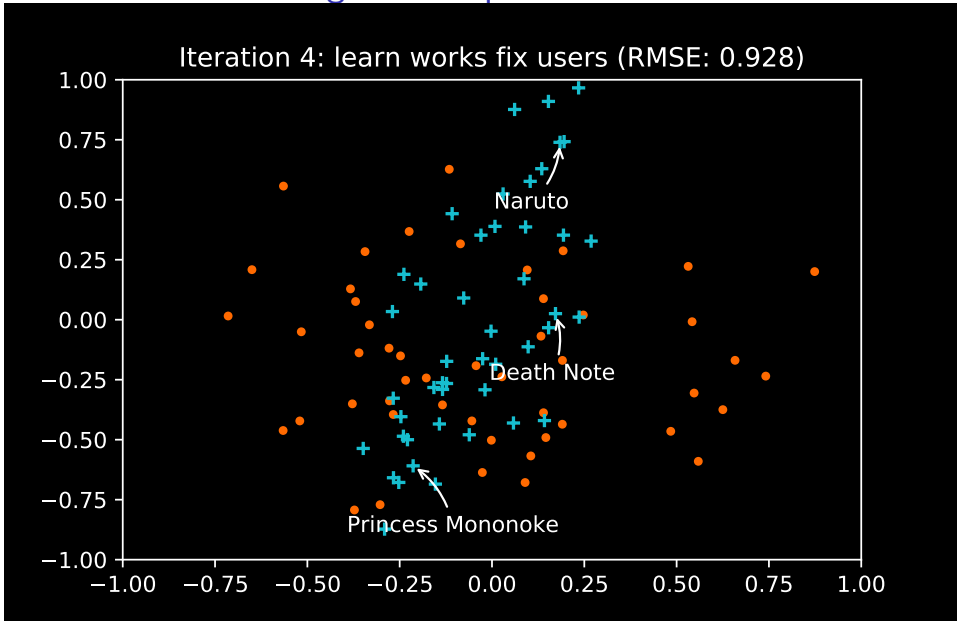

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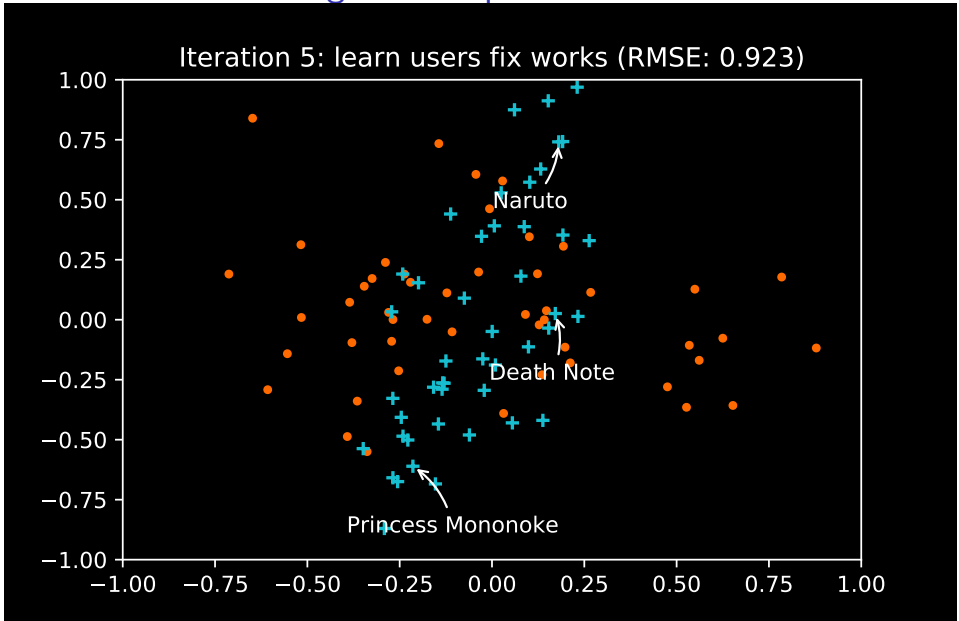

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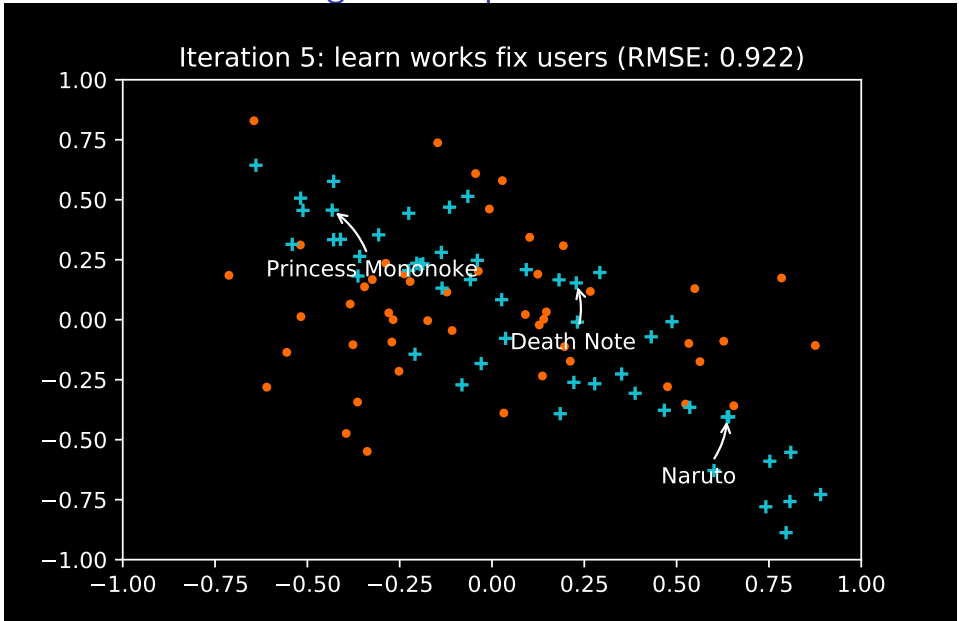

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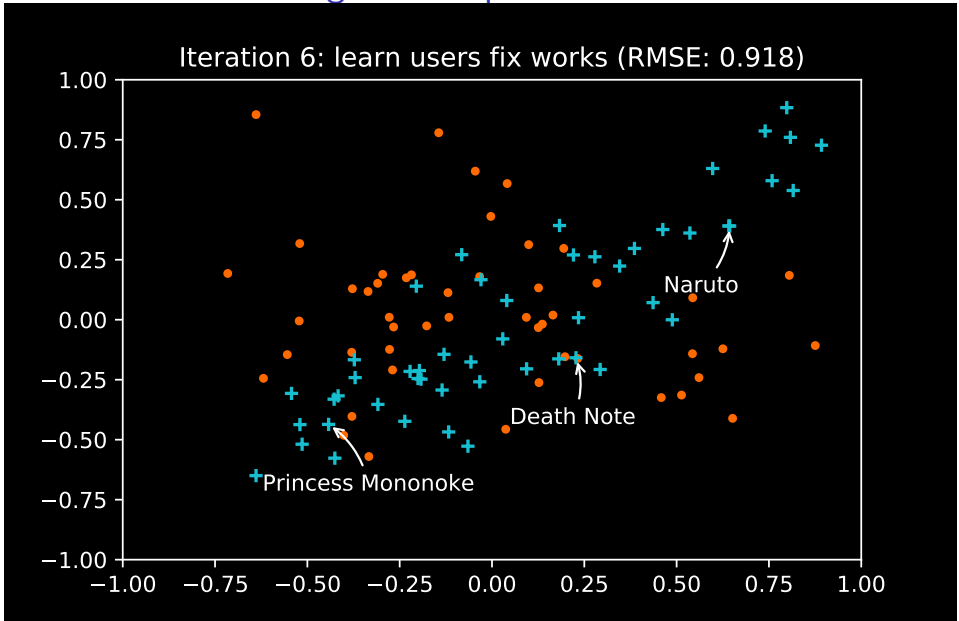

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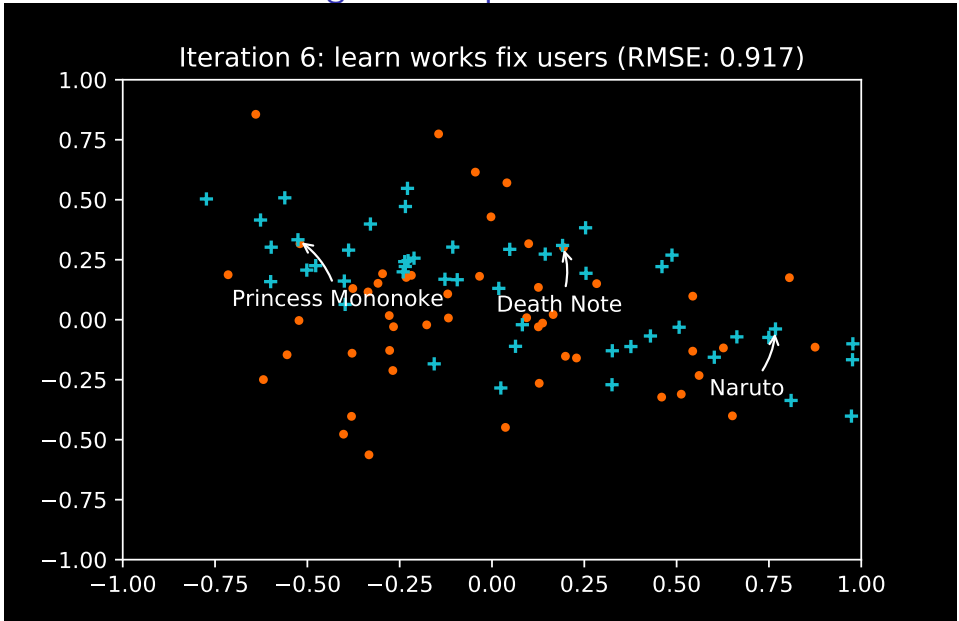

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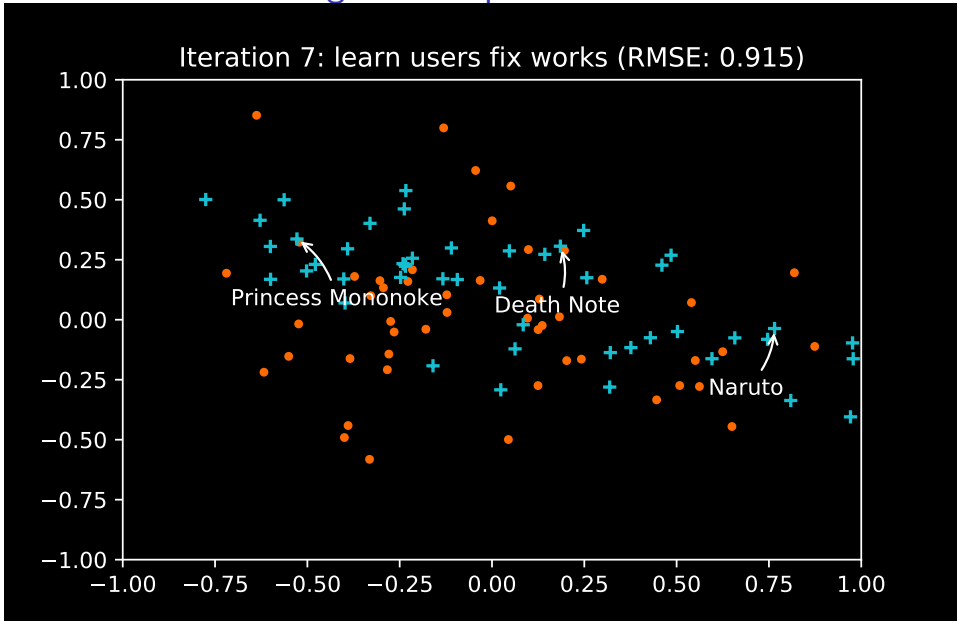

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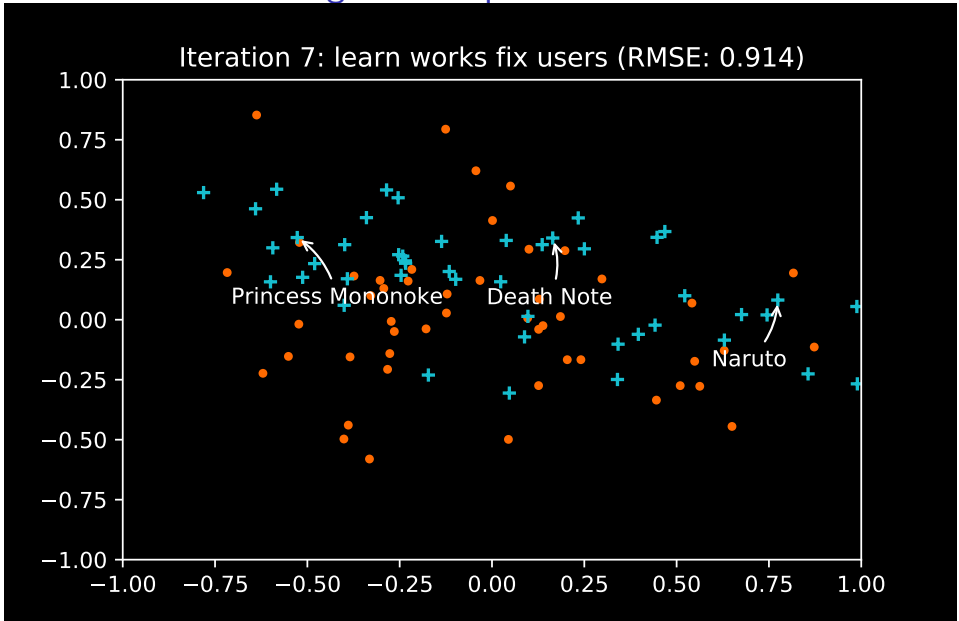

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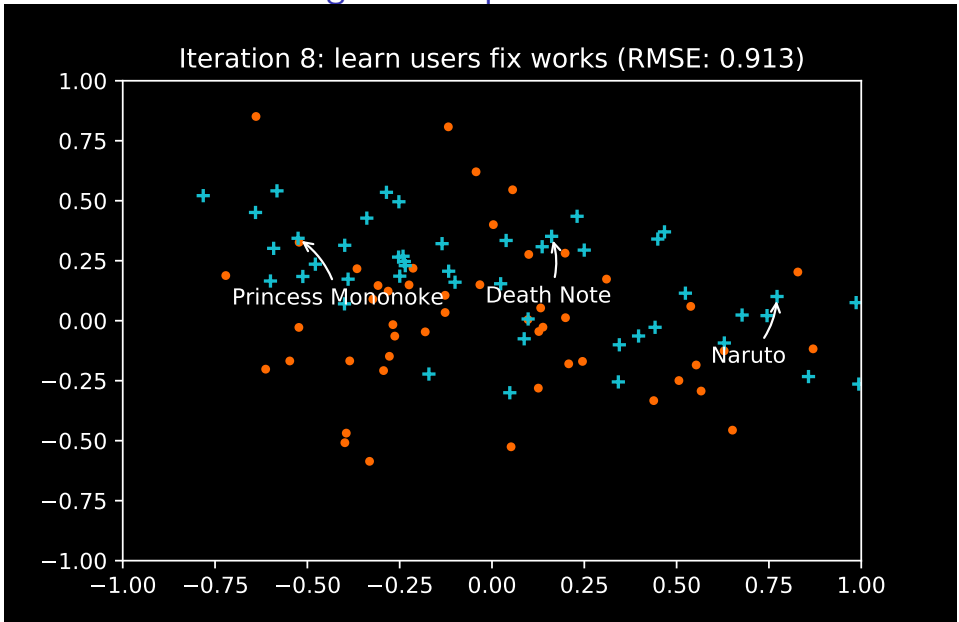

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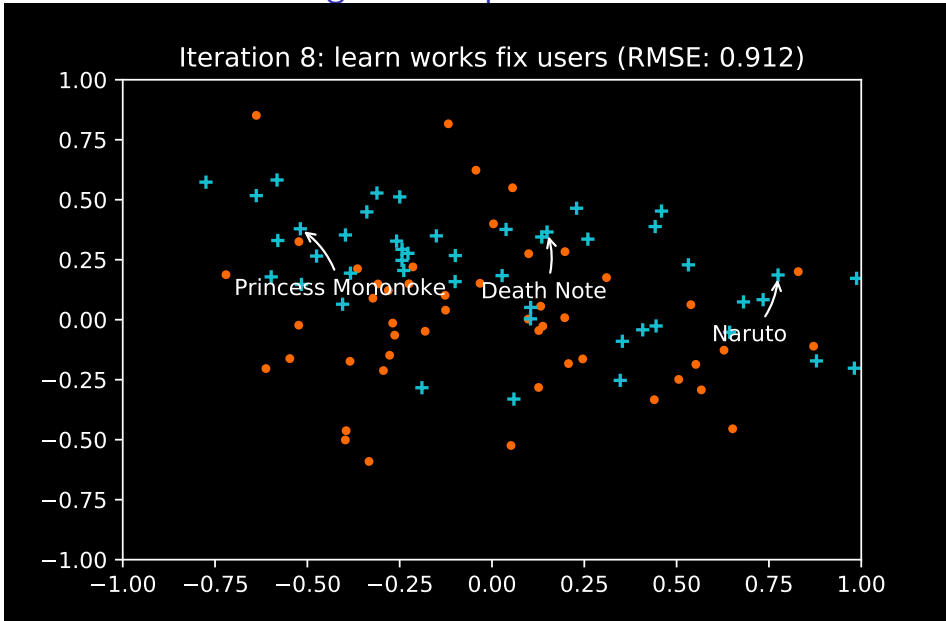

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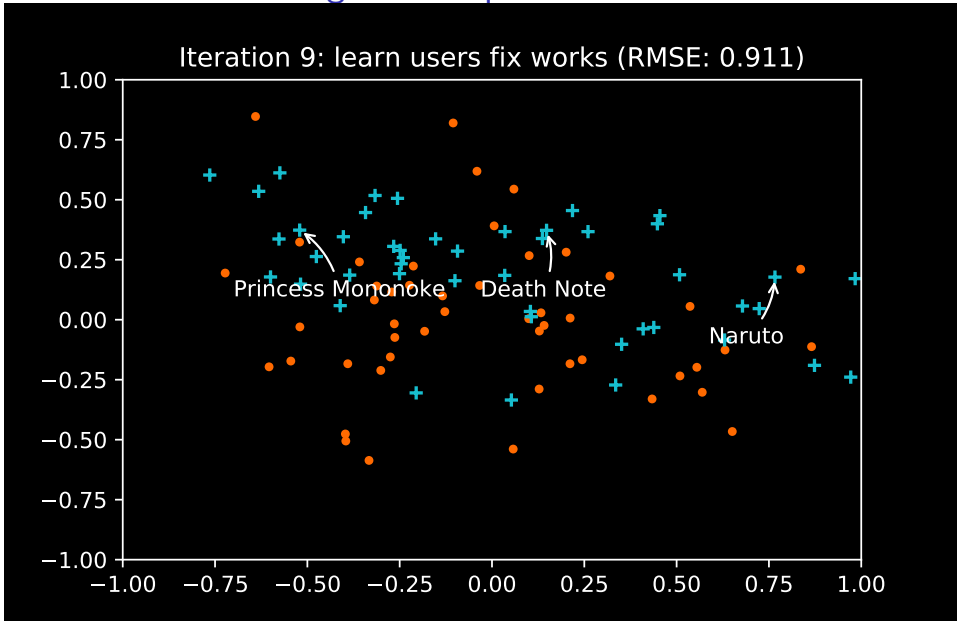

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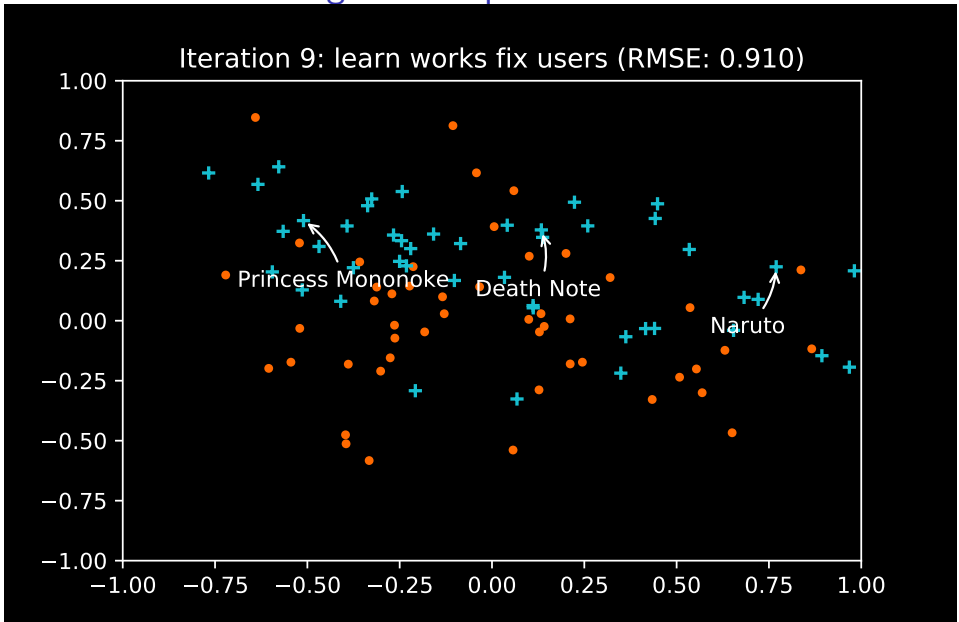

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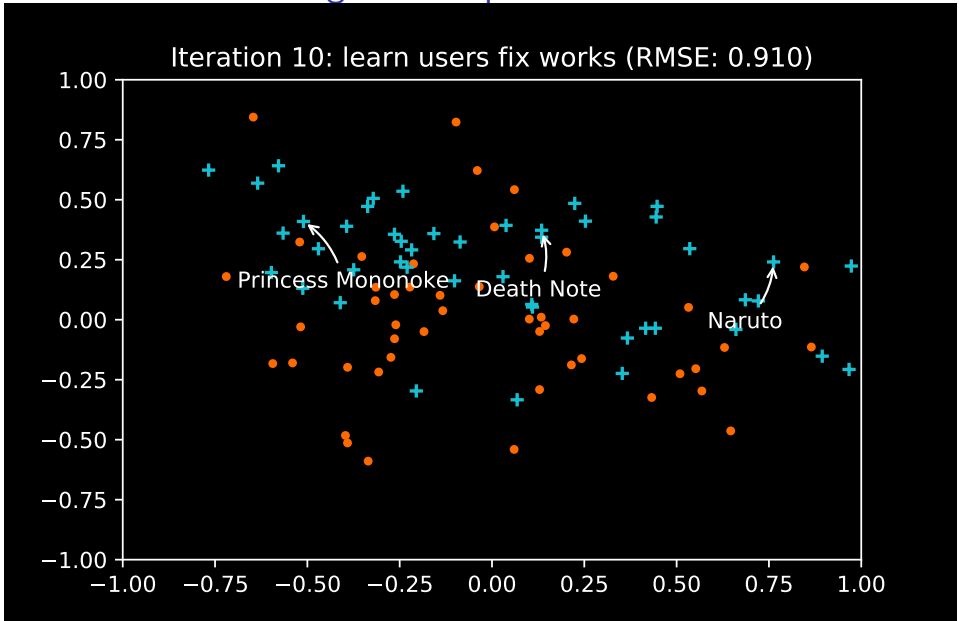

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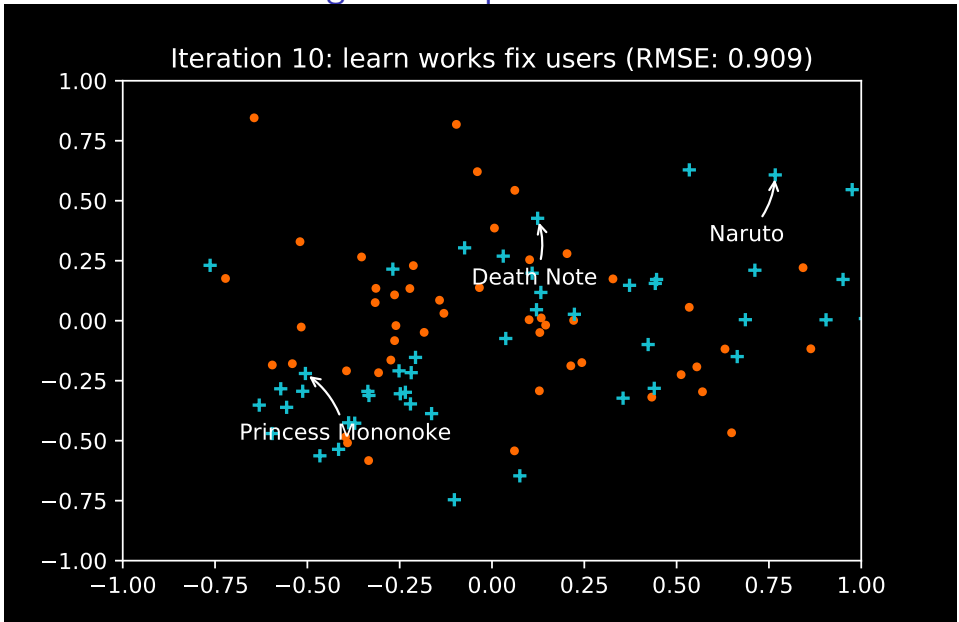

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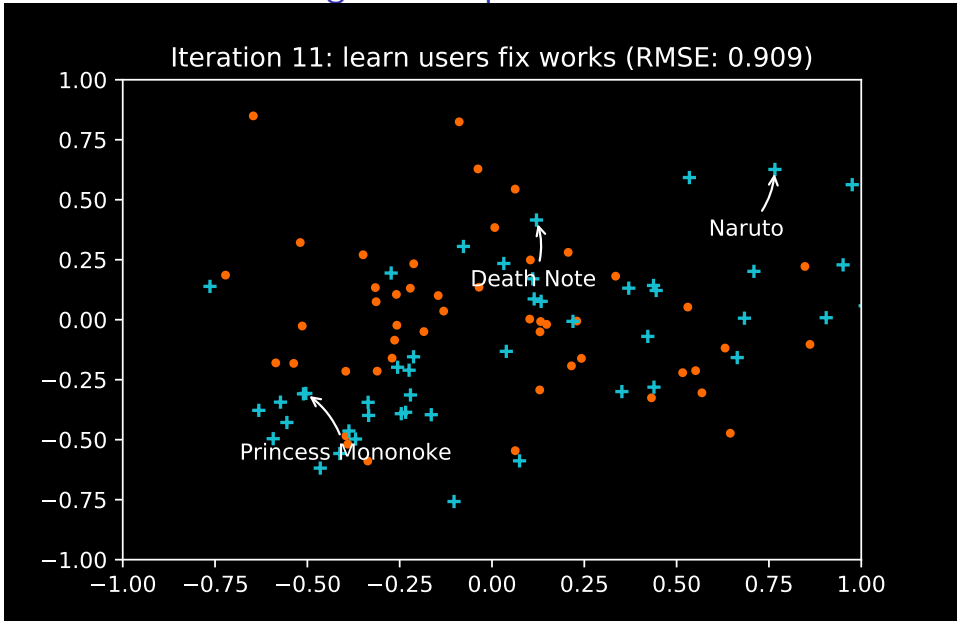

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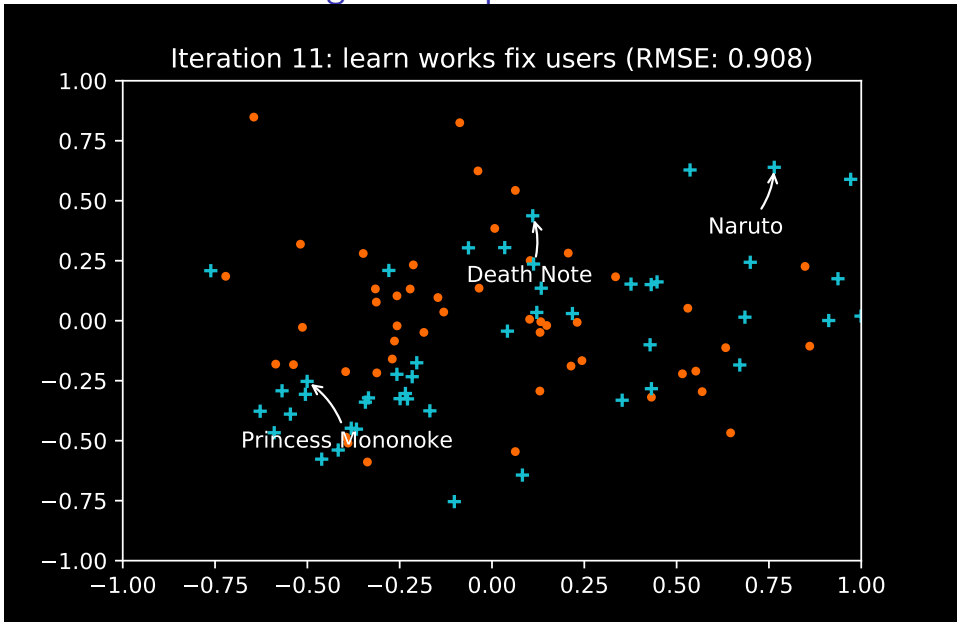

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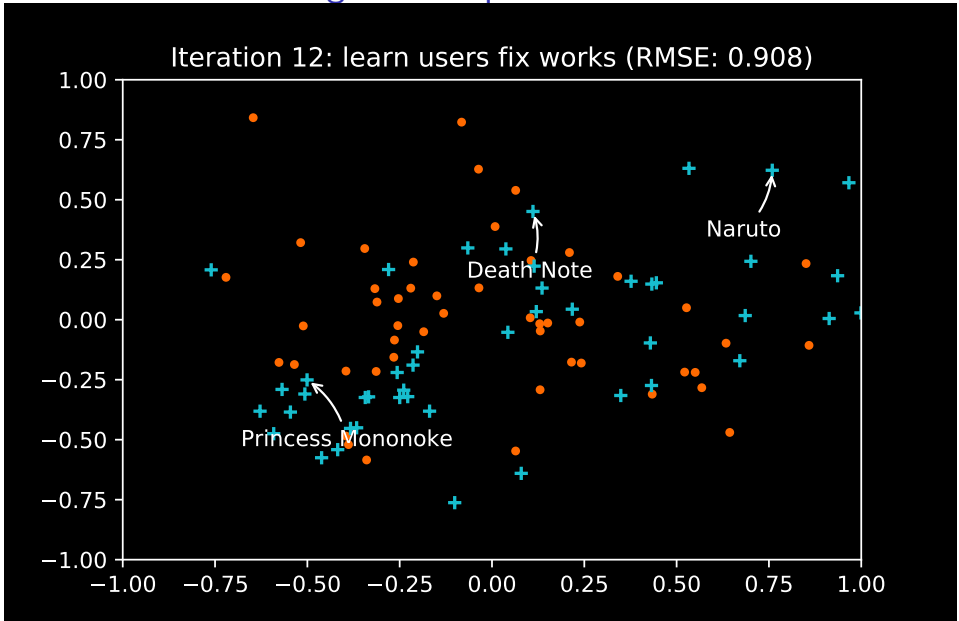

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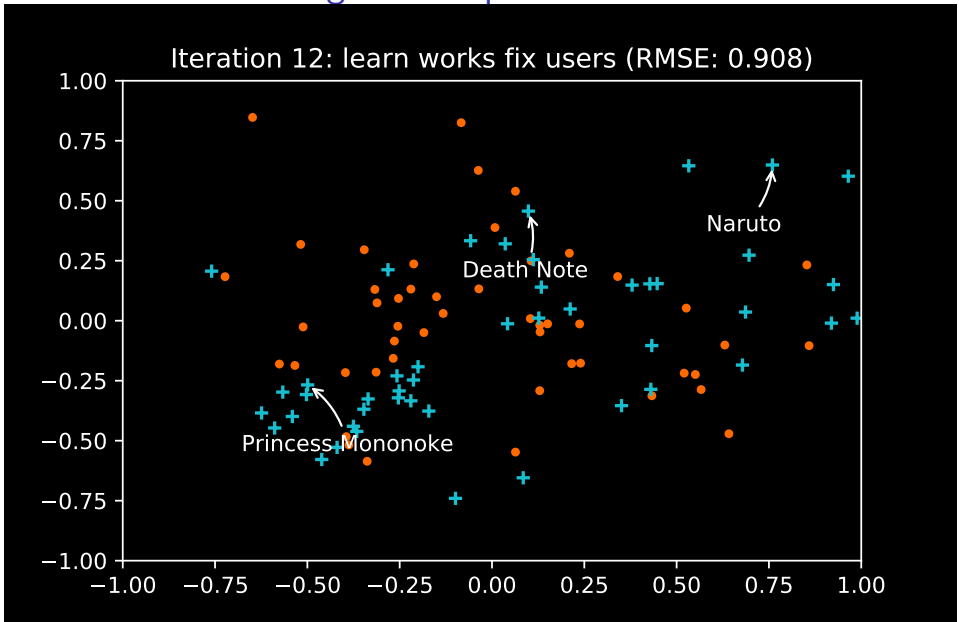

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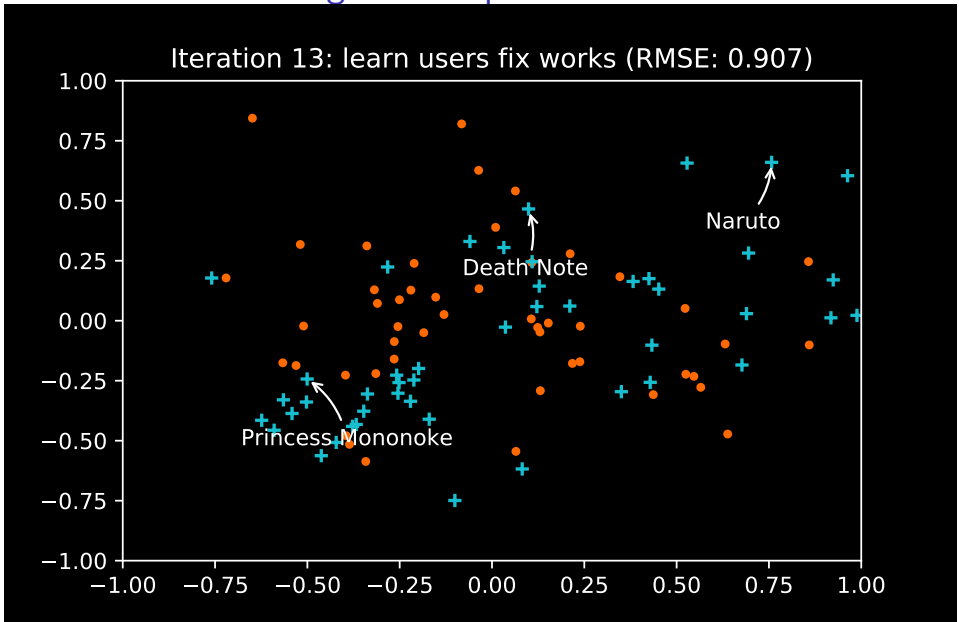

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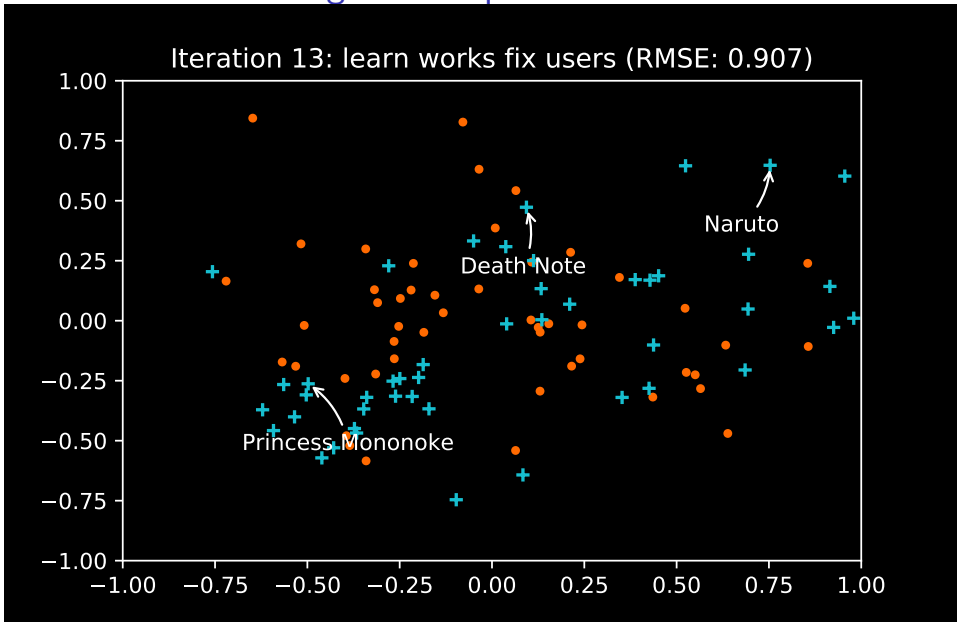

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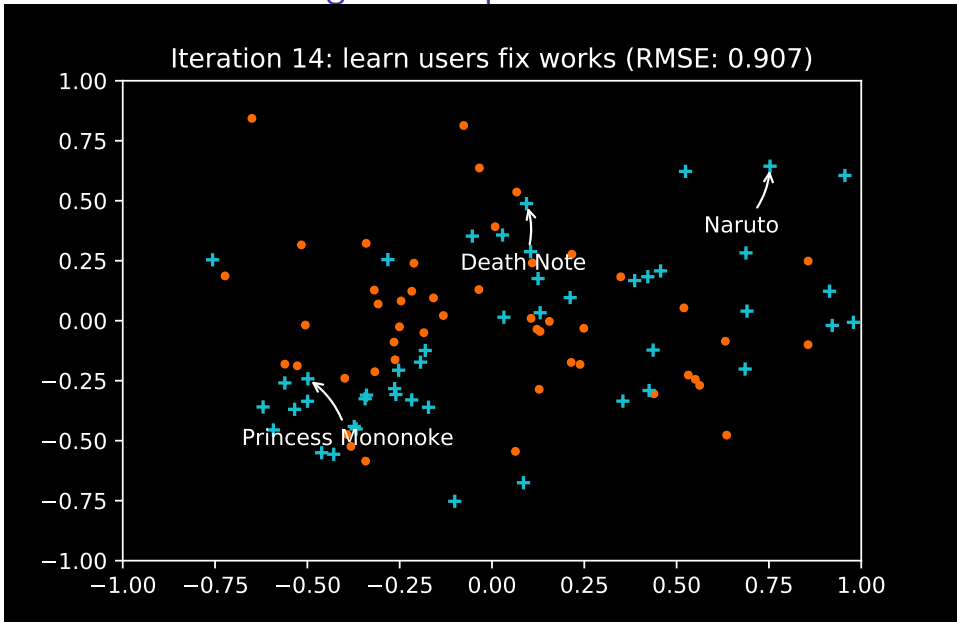

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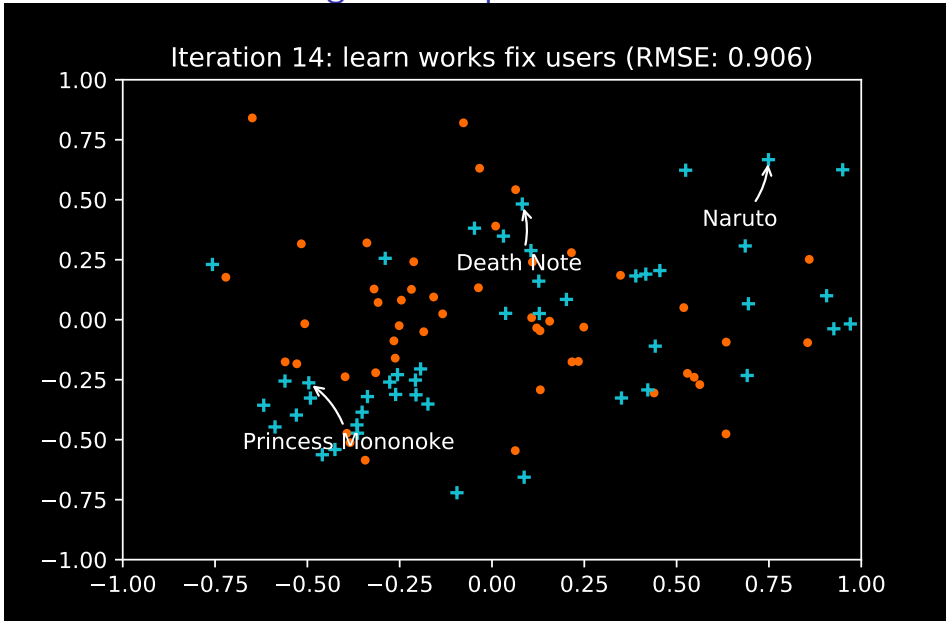

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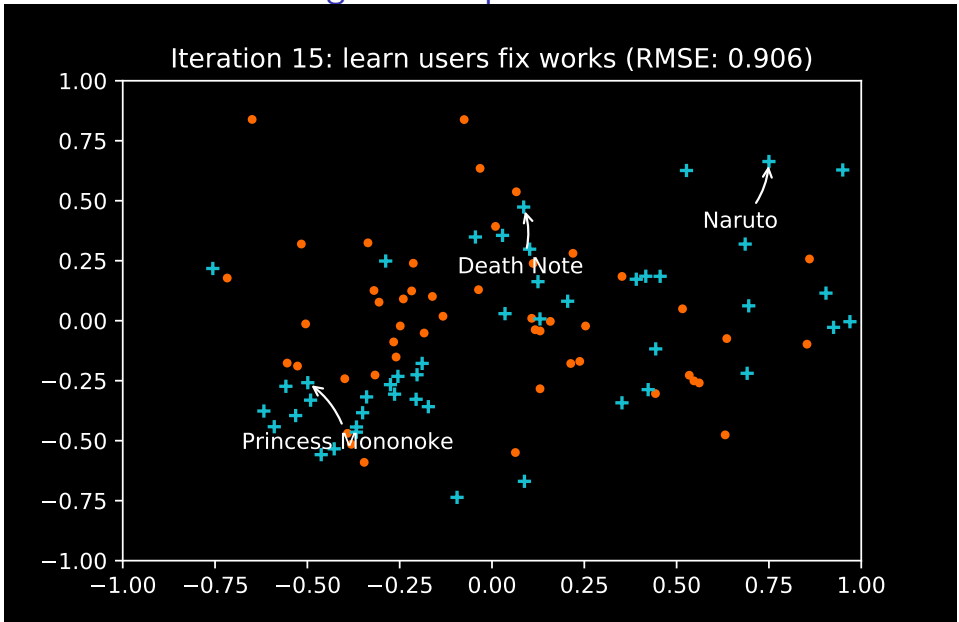

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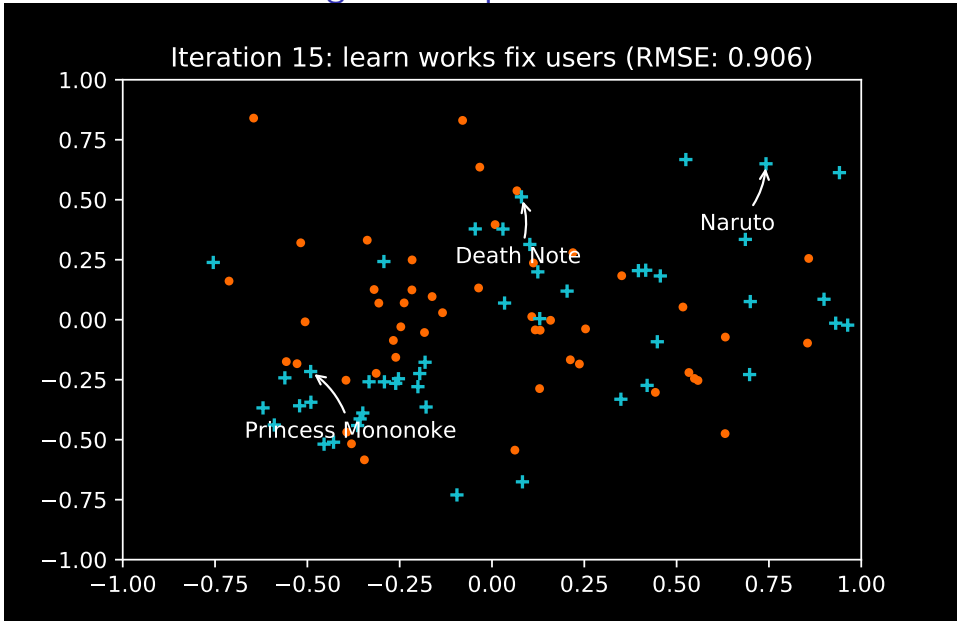


Illustration of Alternating Least Squares

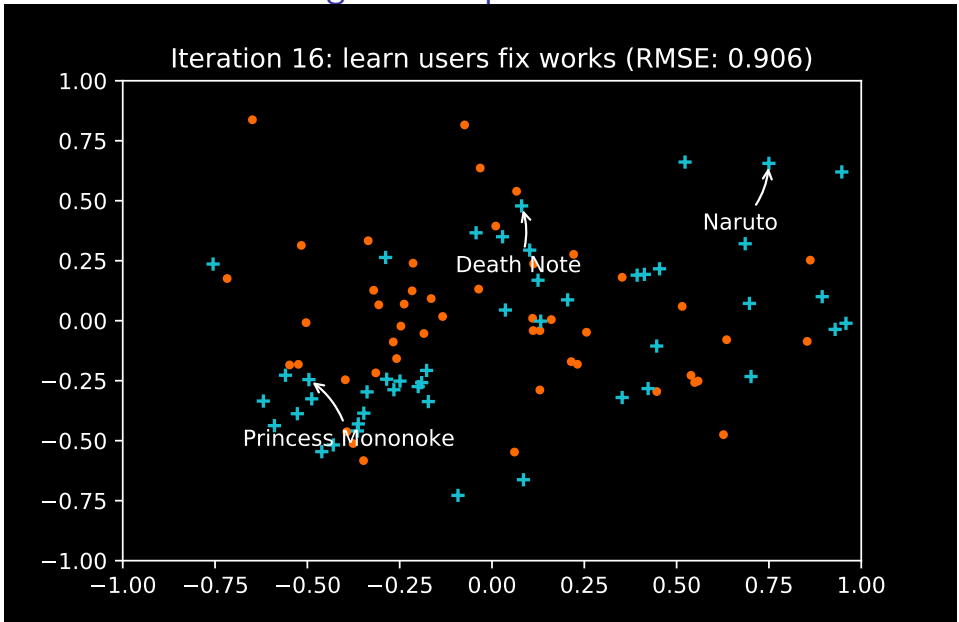
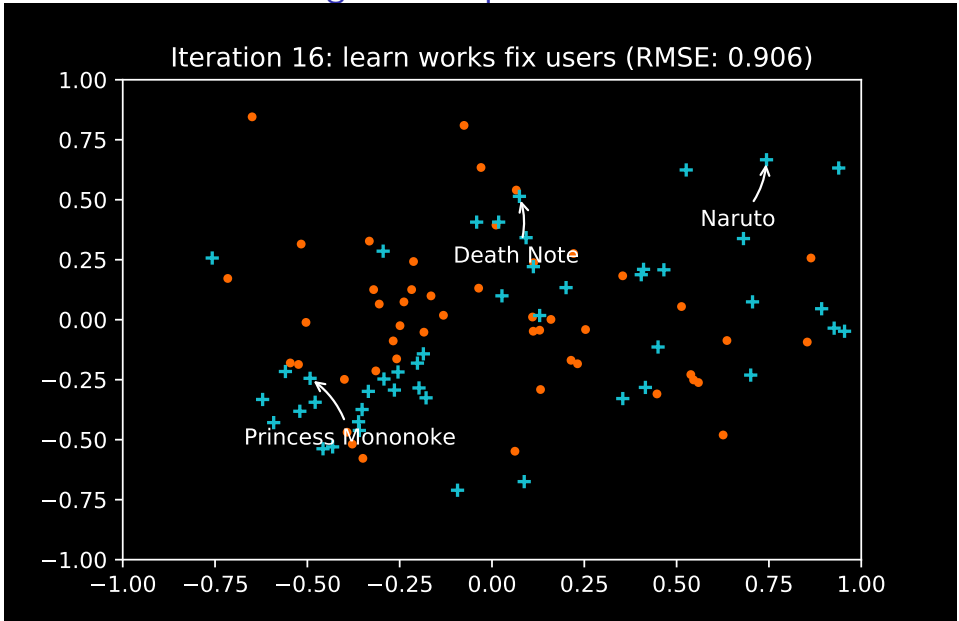


Illustration of Alternating Least Squares



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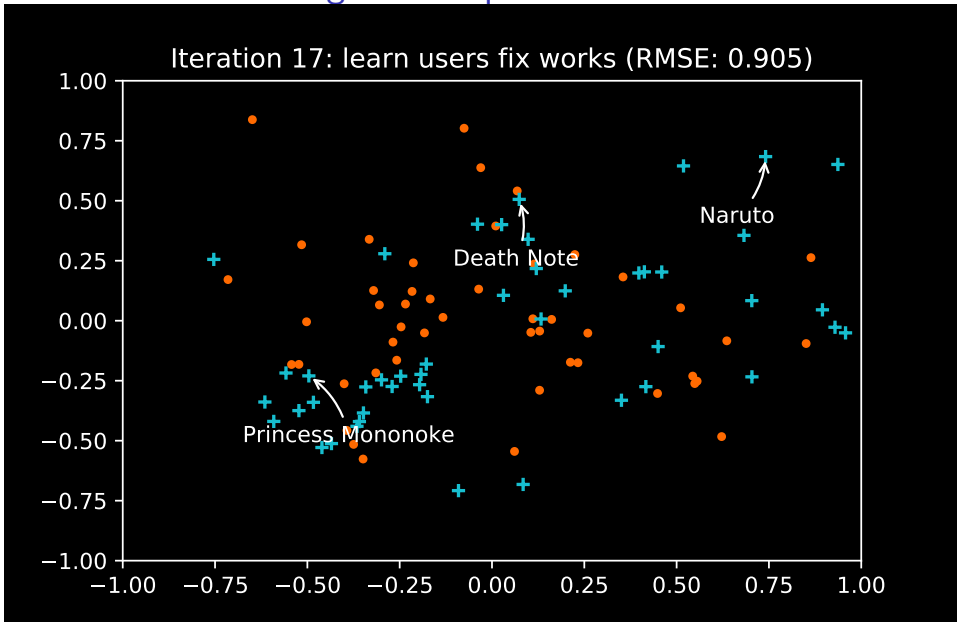
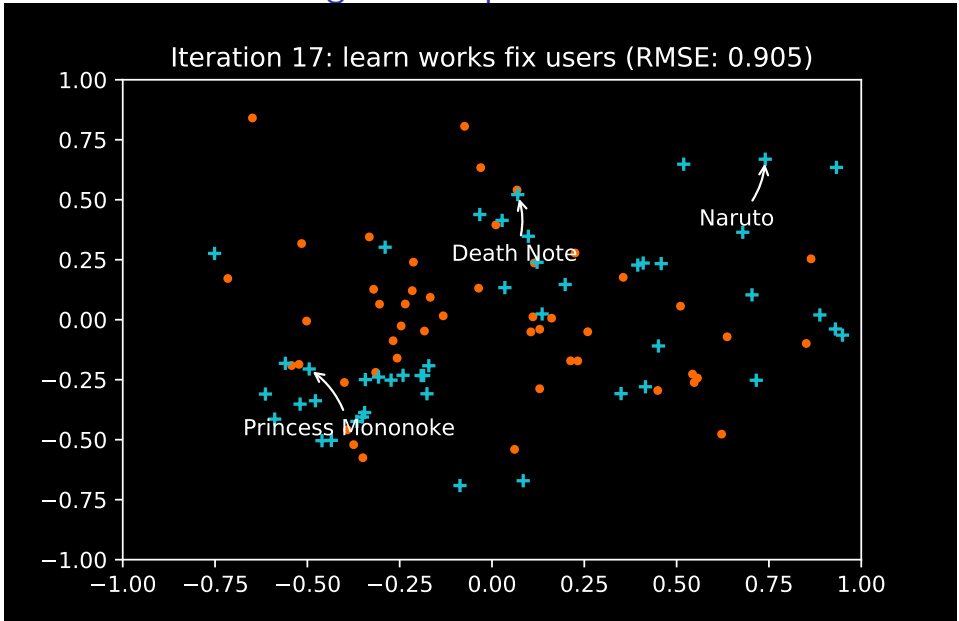


Illustration of Alternating Least Squares



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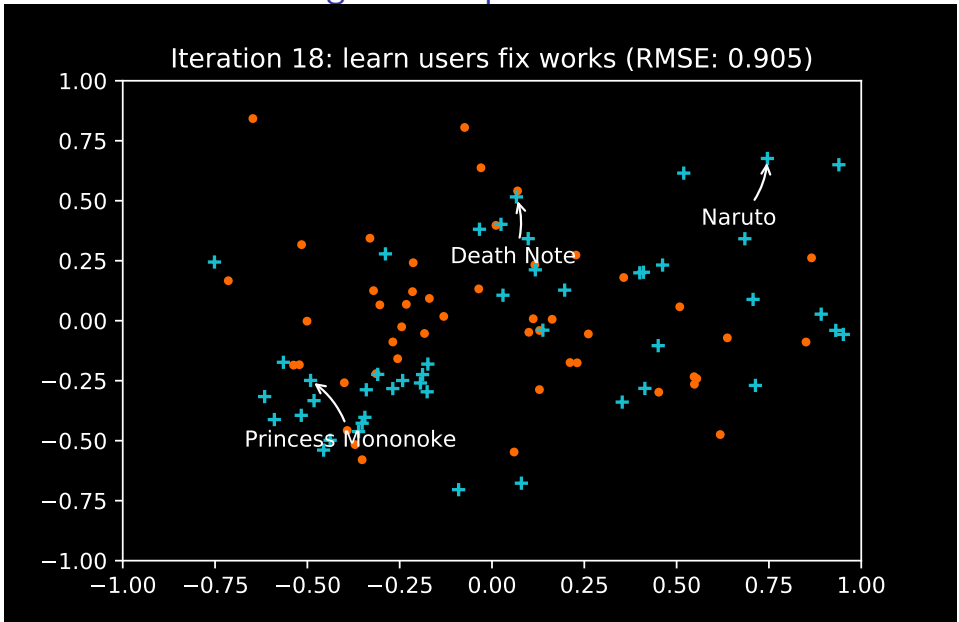


Illustration of Alternating Least Squares

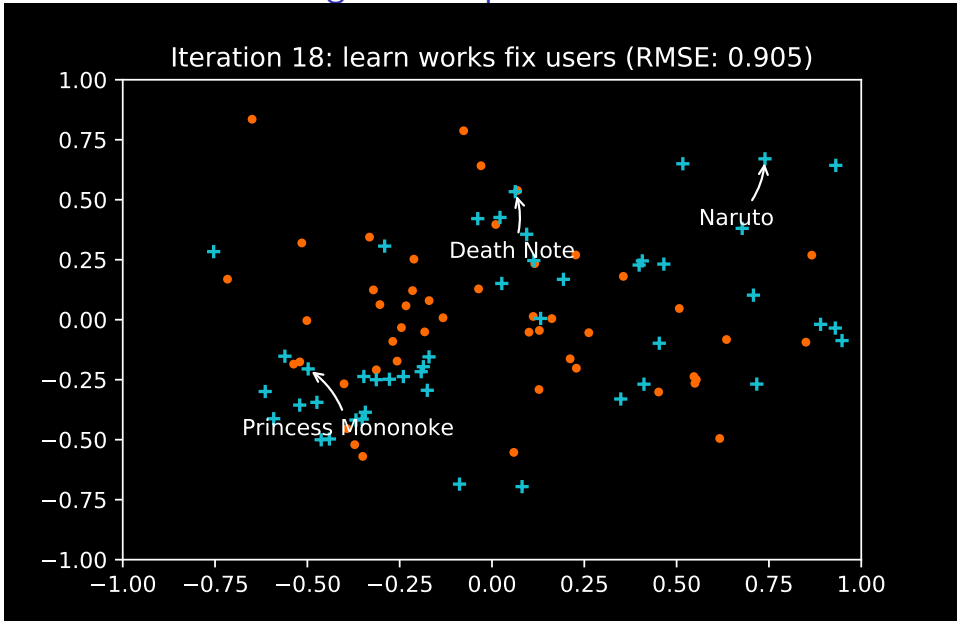


Illustration of Alternating Least Squares

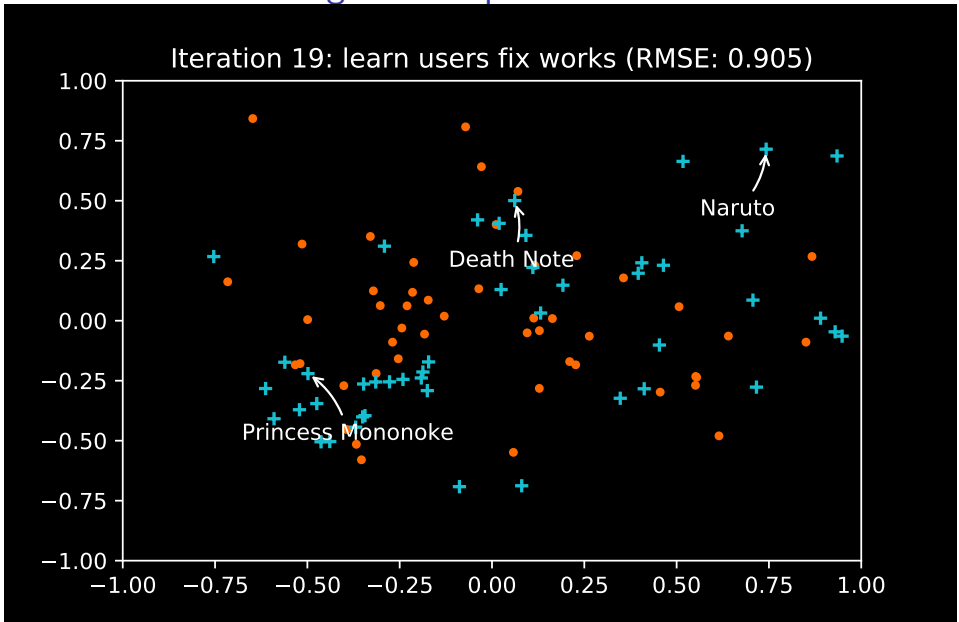
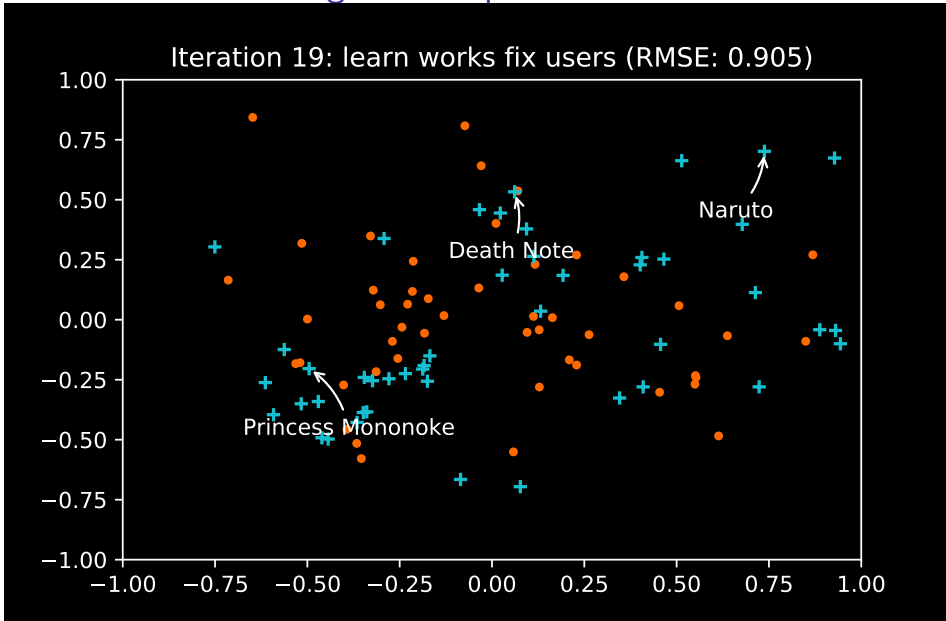
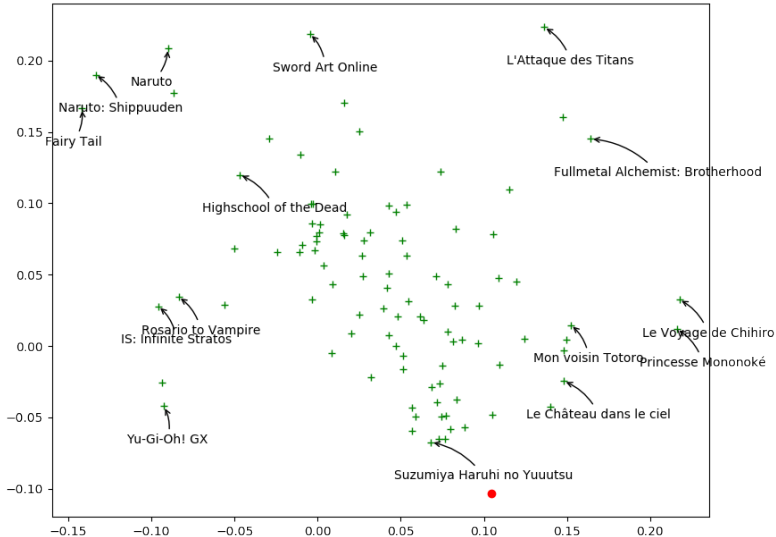


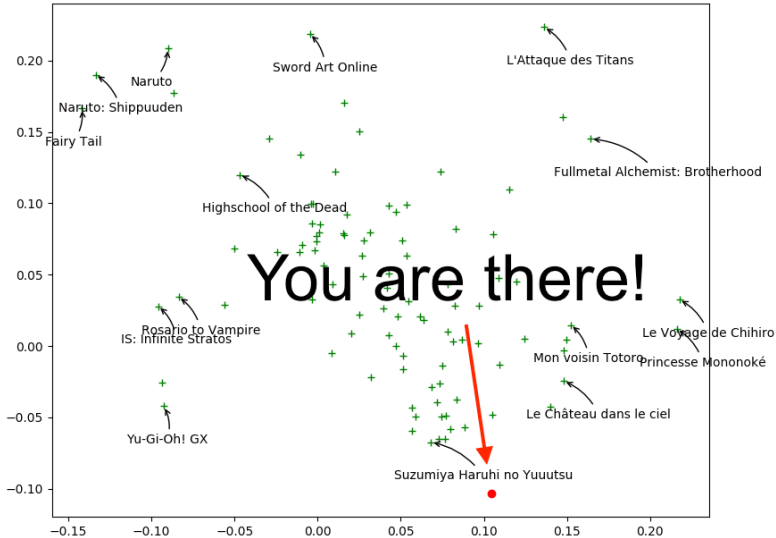
Illustration of Alternating Least Squares



Close $\boldsymbol{v}_j$ mean similar movies



u_i will like movies in its direction



word2vec: the Skip-Gram model

We want, given a word $w \sim P(W)$, to predict its context (i.e. the words around it).

Oh, it's a classification problem! With 60,000 classes.

$$P(c|w) = \text{softmax}(\boldsymbol{u}_w^T \boldsymbol{v}_c) \propto \exp(\boldsymbol{u}_w^T \boldsymbol{v}_c)$$

Cross-entropy would look like:

$$\mathcal{L} = \log \sigma(\boldsymbol{u}_w^T \boldsymbol{v}_c) + \sum_{\substack{i=1 \\ c_i \neq c}}^{60000} \log(1 - \sigma(\boldsymbol{u}_w^T \boldsymbol{v}_{c_i}))$$

So instead let's just sample k words from vocabulary proportionally to their occurrence:

$$\mathcal{L} = \sum_{w,c} \log \sigma(\boldsymbol{u}_w^T \boldsymbol{v}_c) + \sum_{\substack{i=1 \\ c_i \sim P(W)}}^{k} \log(1 - \sigma(\boldsymbol{u}_w^T \boldsymbol{v}_{c_i}))$$

Neural Word Embedding as Implicit Matrix Factorization

Noise contrastive estimation

$$\mathcal{L} = \sum_{w,c} \log \sigma(\boldsymbol{u}_w^T \boldsymbol{v}_c) + \sum_{\substack{i=1 \\ c_i \sim P(W)}}^{k} \log(1 - \sigma(\boldsymbol{u}_w^T \boldsymbol{v}_{c_i}))$$

Negative sampling (similar objective)

$$\mathcal{L} = \sum_{w,c} \log \sigma(\boldsymbol{u}_w^T \boldsymbol{v}_c) + \sum_{\substack{i=1 \\ c_i \sim P(W)}}^{k} \log \sigma(-\boldsymbol{u}_w^T \boldsymbol{v}_{c_i}))$$

This objective is equivalent to factorizing the pointwise mutual information matrix:

$$\log \frac{\#(w,c)N}{\#w\#c} - \log k = \boldsymbol{u}_w^T \boldsymbol{v}_c \text{ where } N \text{ is the number of pairs.}$$

Omer Levy and Yoav Goldberg. "Neural Word Embedding as Implicit Matrix Factorization". In: *Advances in Neural Information Processing Systems*. Ed. by Z. Ghahramani et al. Vol. 27. Curran Associates, Inc., 2014. URL: https://proceedings.neurips.cc/paper/2014/file/feab05aa91085b7a8012516bc3533958-Paper.pdf

Practical datasets

A toy dataset of matrix completion

You are given some entries of $M = UV$ where the shapes are $(10, 3) \cdot (3, 5)$
The goal is to recover the other entries

Movielens

100,000 ratings (1–5 stars) of 600 users on 9,000 movies.
https://files.grouplens.org/datasets/movielens/ml-latest-small.zip

The Adventures of Sherlock Holmes

By Arthur Conan Doyle
https://github.com/theeluwin/pytorch-sgns

[1] Guillaume Lample et al. "Word translation without parallel data". In: *International Conference on Learning Representations*. 2018. URL: https://openreview.net/forum?id=H196sainb.

[2] Omer Levy and Yoav Goldberg. "Neural Word Embedding as Implicit Matrix Factorization". In: *Advances in Neural Information Processing Systems*. Ed. by Z. Ghahramani et al. Vol. 27. Curran Associates, Inc., 2014. URL: https://proceedings.neurips.cc/paper/2014/file/feab05aa91085b7a8012516bc3533958-Paper.pdf.

[3] Tomas Mikolov et al. "Distributed Representations of Words and Phrases and their Compositionality". In: *Advances in Neural Information Processing Systems*. Ed. by C.J. Burges et al. Vol. 26. Curran Associates, Inc., 2013. URL: https://proceedings.neurips.cc/paper/2013/file/9aa42b31882ec039965f3c4923ce901b-Paper.pdf.