Generalizing Linear Autoencoder Recommenders with Decoupled Expected Quadratic Loss

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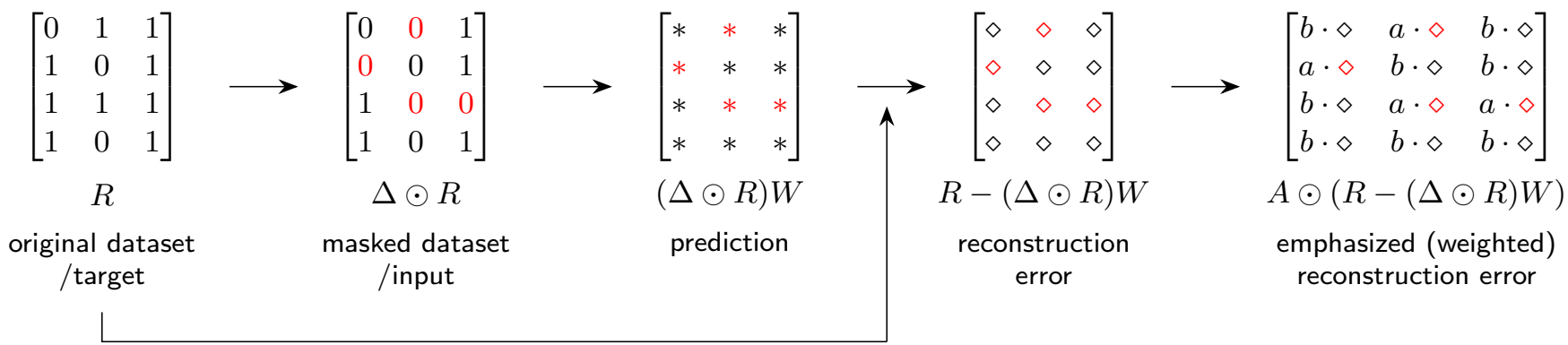
Introduction

In recent years, Linear Autoencoders (LAEs) have demonstrated surprisingly strong performance in recommender systems, even outperforming deep neural network models.

EDLAE [1] is one of the state-of-the-art LAE models, which obtains the optimal model W^* by minimizing the following reconstruction loss:

$$W^* = \arg\min_{W} \lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} \|A^{(k)} \odot (R - (\Delta^{(k)} \odot R)W)\|_F^2 \tag{1}$$

- $R \in \{0,1\}^{m\times n}$: the dataset, with m users and n items.
- $W \in \mathbb{R}^{n\times n}$: the model, a matrix representing item-item relationships.
- $\Delta^{(k)} \in \{0,1\}^{m\times n}$: a random dropout matrix. Δ_{ij} i.i.d. drawn from Bern$(1-p)$.
- $A^{(k)}$: an emphasizing matrix. $A^{(k)}_{ij} = a$ if $\Delta_{ij} = 0$, and $A^{(k)}_{ij} = b$ if $\Delta_{ij} = 1$. Set $a \geq b \geq 0$ to put greater weight on the reconstruction loss of dropped entries.



Introduction

When $b = 0$, EDLAE has a closed-form solution for W^*:

$$W^* = \frac{1}{1-p}\left(I - C \cdot (I \odot C)^{-1}\right), \text{ where } C = \left(R^T R + \frac{p}{1-p} I \odot R^T R\right)^{-1} \tag{2}$$

In this case, the diagonal of W^* is zero.

The main issue is that the closed-form solution of EDLAE is not derived from a statistical perspective, which makes closed-form analysis difficult. Under the original framework, it is hard to answer the following questions:

- Does solutions with $b = 0$ always yield the best test performance?
- When $b > 0$, do closed-form solutions exist? Do they perform better?
- Does emphasizing dropped entries (i.e., choosing $a \geq b \geq 0$) always lead to good performance? What if we instead de-emphasize them by choosing $b > a \geq 0$?
- Why must W^* have a zero-diagonal? Would allowing a non-zero diagonal improve performance?

To overcome this limitation, we propose a new framework from the statistical perspective to facilitate closed-form analysis of EDLAE.

Decoupled Expected Quadratic Loss

By the Law of Large Numbers, we can rewrite the EDLAE objective (1) in its expectation form as follows:

$$W^* = \arg\min_W l_{\mathcal{B}}(W), \text{ where } l_{\mathcal{B}}(W) = \mathbb{E}_{\Delta\sim\mathcal{B}}\left[\|A \odot (R - (\Delta \odot R)W)\|_F^2\right]$$
$$= \sum_{i=1}^{n} \mathbb{E}_{\Delta\sim\mathcal{B}}\left[\|A^{(i)}R_{*i} - A^{(i)}(\Delta \odot R)W_{*i})\|_F^2\right], \quad A^{(i)} = \mathrm{diag}(A_{*i}) \tag{3}$$

Let $X = A^{(i)}(\Delta \odot R)$ be the input and $Y_{*i} = A^{(i)}R_{*i}$ be the target, then both X and Y are random variables.

This statistical point of view – considering input and target as random variables and taking expectation of the loss with respect to them – inspires us to propose a general loss function, the Decoupled Expected Quadratic Loss (DEQL):

$$l_{\boldsymbol{\mathcal{D}}}(W) = \sum_{i=1}^{n} h^i_{\mathcal{D}^{(i)}}(W_{*i}), \text{ where } h^i_{\mathcal{D}^{(i)}}(W_{*i}) = \mathbb{E}_{(X,Y)\sim\mathcal{D}^{(i)}}\left[\|Y_{*i} - XW_{*i}\|_F^2\right] \tag{4}$$

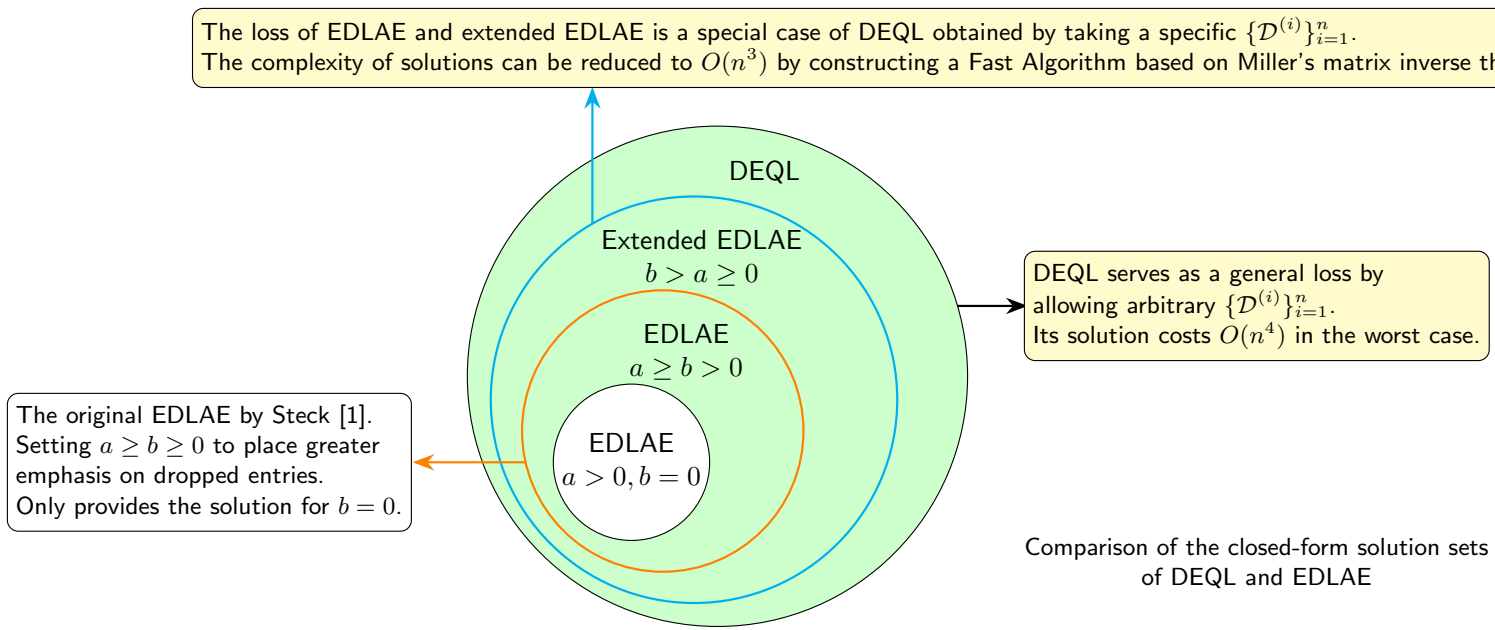
DEQL (4) holds for any collection of distributions $\{\mathcal{D}^{(i)}\}_{i=1}^n$. EDLAE (3) is a special case of (4) obtained by choosing a specific collection.

Decoupled Expected Quadratic Loss

Advantages of DEQL:

- It enables a simpler and better-understood closed-form analysis.
- It extends the solution space, allowing us to obtain solutions for $b > 0$ and overcoming the $b = 0$ limitation of EDLAE.
- Solutions with $b > 0$ can achieve better test performance than those with $b = 0$.
- It supports choosing arbitrary distributions $\{\mathcal{D}^{(i)}\}_{i=1}^{n}$, which could facilitate designing objectives that outperform EDLAE.

Overall Framework:



Comparison of the closed-form solution sets of DEQL and EDLAE

Closed-Form Solutions of DEQL: $b > 0$ Case

When $b > 0$, the optimal solution of DEQL W^* is solved column-wisely by

$$W^*_{*i} = \mathbb{E}_{(X,Y)\sim\mathcal{D}^{(i)}}\left[X^T X\right]^{-1} \mathbb{E}_{(X,Y)\sim\mathcal{D}^{(i)}}\left[X^T Y_{*i}\right] \text{ for } i = 1, 2, ..., n$$

Applying to EDLAE case, we plug in $X = A^{(i)}(\Delta \odot R)$ and $Y_{*i} = A^{(i)} R_{*i}$ and get

$$W^*_{*i} = {H^{(i)}}^{-1} v^{(i)} \text{ for } i = 1, 2, ..., n, \text{ where} \tag{5}$$
$$H^{(i)} = \mathbb{E}_{\Delta\sim\mathcal{B}}\left[(\Delta \odot R)^T {A^{(i)}}^2 (\Delta \odot R)\right],\ v^{(i)} = \mathbb{E}_{\Delta\sim\mathcal{B}}\left[(\Delta \odot R)^T {A^{(i)}}^2 R_{*i}\right]$$

where $H^{(i)}$ and $v^{(i)}$ can be expressed in a more explicit form

Lemma 1

$H^{(i)} = G^{(i)} \odot R^T R$ and $v^{(i)} = u^{(i)} \odot R^T R_{*i}$, where

$$G^{(i)}_{kl} = \begin{cases} (1-p)b^2 & \text{if } k = l = i \\ (1-p)^2 b^2 & \text{if } k \neq l = i \text{ or } l \neq k = i \\ (1-p)pa^2 + (1-p)^2 b^2 & \text{if } k = l \neq i \\ (1-p)^2 pa^2 + (1-p)^3 b^2 & \text{if } i \neq k \neq l \neq i \end{cases}, \quad u^{(i)}_k = \begin{cases} (1-p)b^2 & \text{if } k = i \\ (1-p)pa^2 + (1-p)^2 b^2 & \text{if } k \neq i \end{cases}$$

for $k, l \in \{1, 2, ..., n\}$.

A Fast Algorithm for Computing $b > 0$ Solutions

The major challenge in computing $b > 0$ solutions by $W^*_{*i} = {H^{(i)}}^{-1} v^{(i)}$ for all i is computational inefficiency.

Note that $H^{(i)} = G^{(i)} \odot R^T R$, and each $G^{(i)}$ differs only in the ith row and column:

$$G^{(1)} = \begin{bmatrix} \times & * & * & * & * \\ * & + & \circ & \circ & \circ \\ * & \circ & + & \circ & \circ \\ * & \circ & \circ & + & \circ \\ * & \circ & \circ & \circ & + \end{bmatrix} \quad G^{(2)} = \begin{bmatrix} + & * & \circ & \circ & \circ \\ * & \times & * & * & * \\ \circ & * & + & \circ & \circ \\ \circ & * & \circ & + & \circ \\ \circ & * & \circ & \circ & + \end{bmatrix} \quad \cdots \quad G^{(n)} = \begin{bmatrix} + & \circ & \circ & \circ & * \\ \circ & + & \circ & \circ & * \\ \circ & \circ & + & \circ & * \\ \circ & \circ & \circ & + & * \\ * & * & * & * & \times \end{bmatrix}$$

$$\times : (1-p)b^2, \quad * : (1-p)^2 b^2, \quad + : (1-p)pa^2 + (1-p)^2 b^2, \quad \circ : (1-p)^2 pa^2 + (1-p)^3 b^2$$

Each column W^*_{*i} requires computing the inversion ${H^{(i)}}^{-1}$, which takes $O(n^3)$. Since W^* has n columns, the total computation cost is $O(n^4)$! This complexity is impractical for real world datasets with large n.

Question: Can we design a more efficient algorithm for computing W^* when $b > 0$?

The answer is YES. We will show an algorithm that reduces the complexity to $O(n^3)$.

A Fast Algorithm for Computing $b > 0$ Solutions

Note that we can decompose $G^{(1)}, G^{(2)}, ..., G^{(n)}$ as follows:

$$G^{(1)}\begin{bmatrix} \times & * & * & * & * \\ * & + & \circ & \circ & \circ \\ * & \circ & + & \circ & \circ \\ * & \circ & \circ & + & \circ \\ * & \circ & \circ & \circ & + \end{bmatrix} = \begin{bmatrix} + & \circ & \circ & \circ & \circ \\ \circ & + & \circ & \circ & \circ \\ \circ & \circ & + & \circ & \circ \\ \circ & \circ & \circ & + & \circ \\ \circ & \circ & \circ & \circ & + \end{bmatrix} + \begin{bmatrix} \triangle & & & & \\ \diamond & & & & \\ \diamond & & & & \\ \diamond & & & & \\ \diamond & & & & \end{bmatrix} + \begin{bmatrix} & \diamond & \diamond & \diamond & \diamond \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix}$$

$$G^{(2)}\begin{bmatrix} + & * & \circ & \circ & \circ \\ * & \times & * & * & * \\ \circ & * & + & \circ & \circ \\ \circ & * & \circ & + & \circ \\ \circ & * & \circ & \circ & + \end{bmatrix} = \begin{bmatrix} + & \circ & \circ & \circ & \circ \\ \circ & + & \circ & \circ & \circ \\ \circ & \circ & + & \circ & \circ \\ \circ & \circ & \circ & + & \circ \\ \circ & \circ & \circ & \circ & + \end{bmatrix} + \begin{bmatrix} & \diamond & & & \\ & \triangle & & & \\ & \diamond & & & \\ & \diamond & & & \\ & \diamond & & & \end{bmatrix} + \begin{bmatrix} \diamond & & \diamond & \diamond & \diamond \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix}$$

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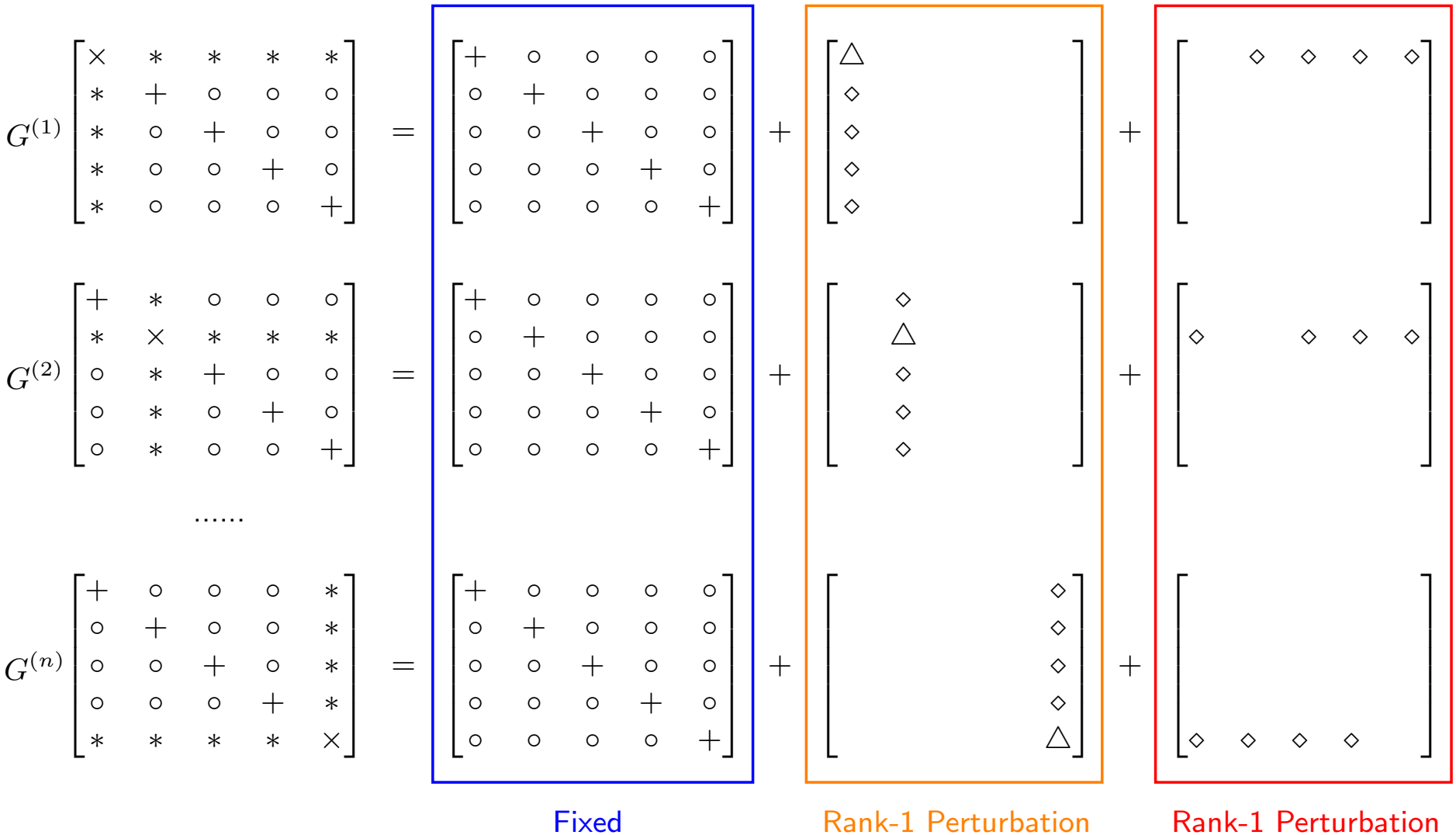
$$G^{(n)}\begin{bmatrix} + & \circ & \circ & \circ & * \\ \circ & + & \circ & \circ & * \\ \circ & \circ & + & \circ & * \\ \circ & \circ & \circ & + & * \\ * & * & * & * & \times \end{bmatrix} = \begin{bmatrix} + & \circ & \circ & \circ & \circ \\ \circ & + & \circ & \circ & \circ \\ \circ & \circ & + & \circ & \circ \\ \circ & \circ & \circ & + & \circ \\ \circ & \circ & \circ & \circ & + \end{bmatrix} + \begin{bmatrix} & & & \diamond & \\ & & & \diamond & \\ & & & \diamond & \\ & & & \diamond & \\ & & & \triangle & \end{bmatrix} + \begin{bmatrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ \diamond & \diamond & \diamond & \diamond & \end{bmatrix}$$

$\times : (1-p)b^2$, $* : (1-p)^2b^2$, $+ : (1-p)pa^2 + (1-p)^2b^2$, $\circ : (1-p)^2pa^2 + (1-p)^3b^2$

$\triangle : -(1-p)p(a^2-b^2)$, $\diamond : -(1-p)^2p(a^2-b^2)$

A Fast Algorithm for Computing $b > 0$ Solutions



This special decomposition structure inspires us to use a more specialized matrix inversion algorithm to reduce the computational complexity.

A Fast Algorithm for Computing $b > 0$ Solutions

Miller's Matrix Inverse Theorem [2]: Let G and $G+Q$ be non-singular matrices. Suppose Q is of rank r and can be decomposed as $Q = E_1 + E_2 + ... + E_r$, where each E_k is of rank 1, and $P_{k+1} = G + E_1 + E_2 + ... + E_k$ is non-singular for $k = 1, 2, ..., r$. Let $P_1 = G$, then

$$P_{k+1}^{-1} = P_k^{-1} - \frac{1}{1 + \text{tr}\left(P_k^{-1} E_k\right)} P_k^{-1} E_k P_k^{-1}$$

The computation of ${H^{(1)}}^{-1}, {H^{(2)}}^{-1}, ..., {H^{(n)}}^{-1}$ is a special case of Miller's theorem with $r = 2$. Based on this, we design the following fast algorithm for computing $W_{*i}^* = {H^{(i)}}^{-1} v^{(i)}$ for all i, with a total cost $O(n^3)$.

Fast Algorithm: First, precompute these matrices

$$R^T R, \quad H_0^{-1} = \left(G_0 \odot R^T R\right)^{-1}, \quad [H_0^{-1} v^{(1)}, H_0^{-1} v^{(2)}, ..., H_0^{-1} v^{(n)}] = H_0^{-1}(U \odot R^T R),$$

$$[H_0^{-1} e_1^{(1)}, H_0^{-1} e_1^{(2)}, ..., H_0^{-1} e_1^{(n)}] = H_0^{-1}(G_1 \odot R^T R), \quad [e_2^{(1)}, e_2^{(2)}, ..., e_2^{(n)}] = G_2 \odot R^T R$$

Then for $i = 1, 2, ..., n$, compute each $W_{*i}^* = {H^{(i)}}^{-1} v^{(i)}$ as follows:

$$r = H_0^{-1} v^{(i)}, \quad w = H_0^{-1} e_1^{(i)}, \quad s = r - \frac{1}{1 + w_i} r_i w, \quad t = (H_0^{-1})_{*i} - \frac{(H_0^{-1})_{ii}}{1 + w_i} w,$$

$$ {H^{(i)}}^{-1} v^{(i)} = s - \frac{1}{1 + {e_2^{(i)}}^T t} ({e_2^{(i)}}^T s) t$$

Closed-Form Solutions of DEQL: $b = 0$ Case

When $b = 0$, the optimal solution of DEQL is given by

$$W^*_{*i,-i} = (H^{(i)}_{-i})^{-1} v^{(i)}_{-i} \quad \text{and} \quad W^*_{ii} \in \mathbb{R} \quad \text{for } i = 1, 2, ..., n \tag{6}$$

- $H^{(i)}_{-i}$ is obtained by removing the ith row and column of $H^{(i)}$.
- $v^{(i)}_{-i}$ is obtained by removing the ith row of $v^{(i)}$.

This implies that, the optimal solutions for $b = 0$ have infinite many; they share the same off-diagonal and allow arbitrary diagonal.

Furthermore, we show that the EDLAE solution corresponds to one of these by choosing a zero diagonal:

Theorem 2

The EDLAE solution (2) is equivalent to the DEQL solution of the $b = 0$ case (6) with $W^*_{ii} = 0$ for all i.

Since any model in the solution space – whether with a zero diagonal or not – equally minimizes the EDLAE objective, a zero-diagonal solution does not necessarily yield better test performance than a non-zero-diagonal one.

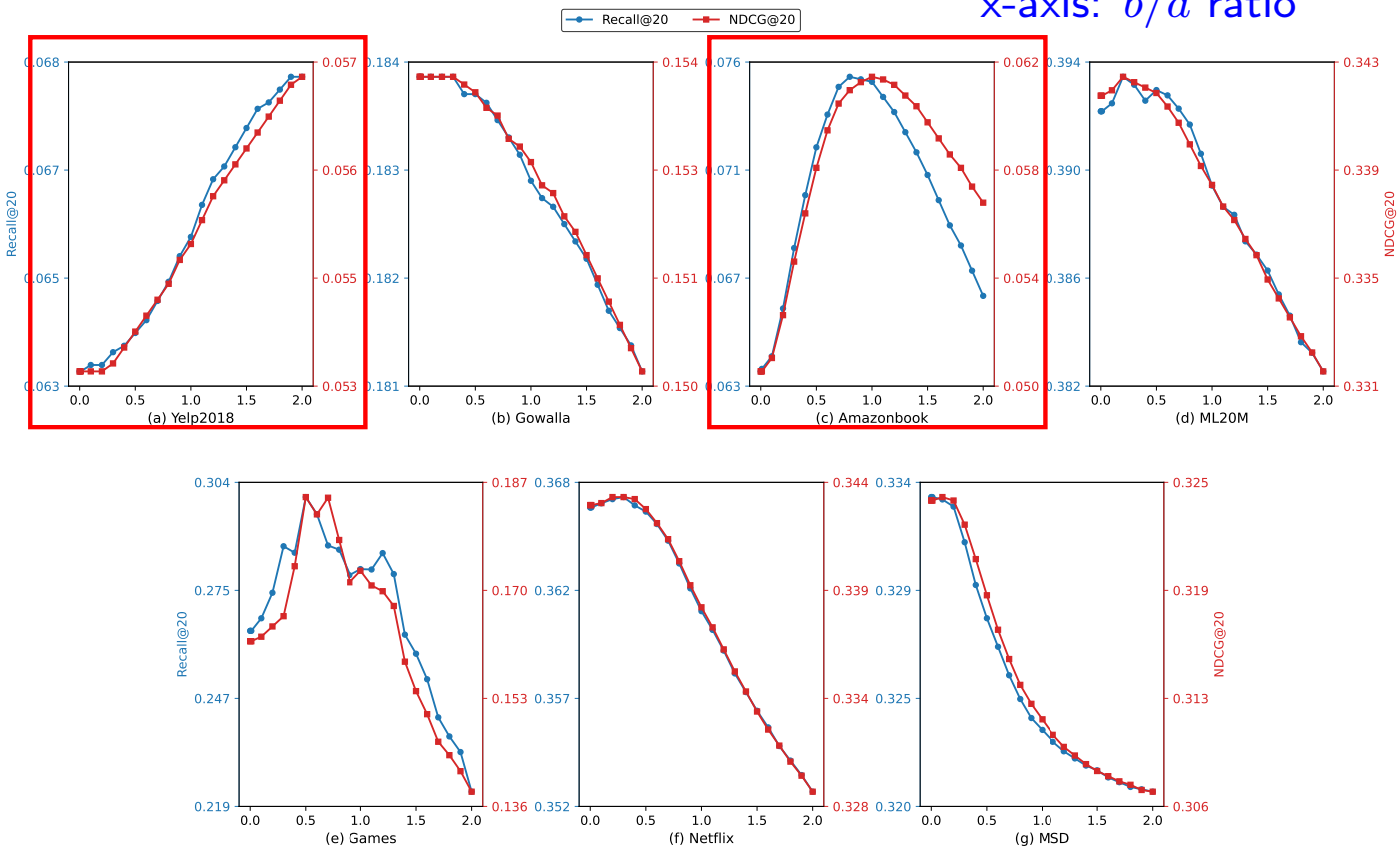
Experiment: Comparison with SOTA LAE Recommenders

Model	Amazon-Books		Yelp2018		Gowalla	
	R@20	N@20	R@20	N@20	R@20	N@20
Deep learning based models						
PinSage	0.0282	0.0219	0.0471	0.0393	0.1380	0.1196
LightGCN	0.0411	0.0315	0.0649	0.0530	0.1830	0.1554
DGCF	0.0422	0.0324	0.0654	0.0534	0.1842	0.1561
SGL-ED	0.0478	0.0379	0.0675	0.0555	–	–
SimpleX	0.0583	0.0468	0.0701	0.0575	0.1872	0.1557
SSM (MF)	0.0473	0.0367	0.0509	0.0404	0.1231	0.0878
SSM (GNN)	0.0590	0.0459	**0.0737**	**0.0609**	**0.1869**	**0.1571**
LAE-based models						
DLAE	**0.0751**	0.0610	0.0678	0.0570	0.1839	0.1533
EASE	0.0710	0.0566	0.0657	0.0552	0.1765	0.1467
EDLAE	0.0711	0.0566	0.0673	0.0565	0.1844	0.1539
ELSA	0.0719	0.0594	0.0629	0.0541	0.1755	0.1490
DEQL(plain)	0.0695	0.0537	0.0647	0.0543	0.1749	0.1453
DEQL(L2+zero-diag)	0.0711	0.0567	0.0672	0.0565	0.1844	0.1539
DEQL(L2)	**0.0751**	**0.0613**	0.0685	0.0576	0.1845	0.1540

DEQL(L2): DEQL with L_2 regularization, DEQL(L2+zero-diag): DEQL with L_2 regularization and zero diagonal constraint.

- The original EDLAE solution ($b = 0$) is not optimal. DEQL solutions with $b > 0$ achieves higher test performance.
- L_2 regularization is essential for improving performance.
- The zero-diagonal constraint does not necessarily lead to better performance.

Experiment: Sensitivity Analysis of b



- The overall results show that models with $b > 0$ can achieve better performance than those with $b = 0$, highlighting the effectiveness of DEQL.
- The results on datasets Amazonbook and Yelp2018 are counter-intuitive: the peak model performance occurs at $b > a$ (emphasize the remained entries rather than dropped ones), which is contrary to the EDLAE assumption $a \geq b$. One possible reason is that on these datasets, item interactions are extremely sparse; choosing $a > b$ forces the model to learn unreliable cross-item correlations, which degrades performance.

Conclusion

DEQL facilitates closed-form solution analysis and reveals new theoretical insights:

- When $b = 0$, the closed-form minimizer is not unique – solutions share identical off-diagonal entries while allowing arbitrary diagonal.
- When $b > 0$, a unique closed-form solution always exists, including the previously unexplored region $b > a$.

Experiments show that

- Solutions with $b > 0$ consistently outperform the original EDLAE solutions with $b = 0$, as well as other recent LAE-based and deep learning-based recommender models.
- The previously assumed constraint $a \geq b$ does not universally guarantee optimal performance.

One future direction is to use DEQL (4) to design alternative objectives by choosing distributions $\{\mathcal{D}^{(i)}\}_{i=1}^{n}$ that more closely align with the MSE testing criterion than EDLAE (3), which may enhance recommendation performance.

References

[1] Harald Steck. Autoencoders that don't overfit towards the identity. NeurIPS, 2020.

[2] Kenneth S Miller. On the inverse of the sum of matrices. Mathematics magazine, 54(2):67–72, 1981.

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Thank you for attention!