Random Osborne Algorithm for Matrix Balancing

Optimal transport report

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Table of content

Abstract (½ page): What problems is studied? Why is it relevant? What solutions is proposed? Which contributions (theory, numerics, etc)?

1 Introduction (3 pages)

[AP23]

1.1 Presentation of the problem

The matrix balancing problem arises from the recognition that matrices encountered in practical applications may have varying scales across rows and columns. These imbalances can lead to numerical instability and adversely impact the accuracy of numerical computations such as eigenvalues/eigenvectors decomposition [CD00; Che01] or solving linear systems [Che01], . Matrix balancing algorithms aim to address these issues by adjusting the scaling of rows and columns, thereby enhancing the overall numerical properties of the matrix.

Other problems can be reduced to matrix balancing, which gives direct applications. For instance, in optimal transport with problems where decision variables are probability distributions [Alt22]; the approximating Min-Mean-Cycle which can be solved in near-linear runtime in the number of edges [AP22] using results from matrix balancing and in particular, the main result of the studied article.

Notation 1.1 *Let c and r respectively be the column-wise sum and the row-wise sum of matrices ie.*

$$c : \begin{cases} \mathcal{M}_{n,m}(\mathbb{K}) & \to & \mathbb{K} \\ A & \mapsto & A^\top \mathbf{1} \end{cases} \quad \text{and} \quad r : \begin{cases} \mathcal{M}_{n,m}(\mathbb{K}) & \to & \mathbb{K} \\ A & \mapsto & A\mathbf{1}. \end{cases}$$

Definition 1.1 *Let $A \in \mathcal{M}_n(\mathbb{R}_+)$ be a non negative square matrix, $\varepsilon \geq 0$ and $k \in \mathbb{N}^\star$. The matrix A is $(\varepsilon, k$-balanced if*

$$\frac{||c(A) - r(A)||_k}{\sum_{i,j} a_{i,j}} \leq 0. \tag{1}$$

Furthermore, if A is $(0, k)$-balanced, we say that A is balanced.

Definition 1.2 *The ε, k-**approximate matrix balancing problem** is: given a square non-negative matrix $K \in \mathcal{M}_n(\mathbb{R}_+)$, $\varepsilon \geq 0$ and $k \in \mathbb{N}^\star$, find a vector $x \in \mathbb{R}^n$ such that $\mathcal{D}(e^x)K\mathcal{D}(e^x)$ is (ε, k)-balanced.*

1.2 Related work

Iterative algorithms The Osborn algorithm, introduced by Osborn in [Osb60] and later discussed in [PR71], is implemented in Scipy as a default matrix balancing method. Other iterative methods have been introduces. Notably, the Sinkhorn-Knopp algorithm [SK67], a special case of Bregman's balancing method [LS81], iteratively rescales

each row and column until convergence. However, it converges linearly, which is impractical for large and sparse matrices, as discussed by Soules et al. in [Sou91]. Parlett introduced an approach in [PR71] to approximately balance matrices by ensuring the diagonal consists only of powers of 2. The advantage of this method is the elimination of floating-point errors when computing the balanced matrix on base-two computers, making it "good enough" in practice. Some efforts are also made to compare balancing algorithms on real use cases [SZ90].

Issues in Matrix Balancing While matrix balancing is generally effective, there are corner cases where it can worsen the conditioning of matrices. Watkins et al. highlighted some of these cases in [Wat06]. Additionally, James et al. explained, in [JLL14], these issues and proposed modifications to LAPACK to mitigate them.

Theoretical bounds [KK96] establishes an upper bound on the norm of the scaling factors and presents a polynomial-time complexity bound for the computation of scaling factors with a prescribed accuracy.

Characterizations of Non-Negative Balancable Matrices [Osb60] and [Eav+85] offer characterizations of non-negative balancable matrices, contributing to the theoretical understanding of the properties of such matrices. Additionally, [KKS97] provides insights into the complexity aspects of this problem.

Tensor Matrix Balancing Sugiyama et al. extended matrix balancing to tensors in [SNT17], providing a perspective on balancing operations in multi-dimensional spaces. This work contributes to the broader understanding of matrix balancing techniques applied beyond traditional matrices.

1.3 Contributions of the paper

Their main contribution is Theorem 2.2. It exhibits a variant of Osborn's algorithm with near-linear runtime in the input sparsity. It also shows that improving the runtime dependence in ε can be improve from ε^{-2} to ε^{-1} without an additional factor n.

Theorem 1.1 *Let $K \in \mathcal{M}_n(\mathbb{R}_+)$ be a balanceable non negative square matrix and $\varepsilon \geq 0$. Random Osborn solves $(\varepsilon, 1)$-approximate matrix balancing problem in T operations where there exists $c > 0, \delta > 0$ such that*

$$\mathbb{E}(T) = \mathcal{O}\left(\frac{m}{\varepsilon} \min\left\{\frac{1}{\varepsilon}; d\right\} \log \kappa\right) \quad \textit{and} \quad \mathbb{P}\left(T \leq c\frac{m}{\varepsilon} \min\left\{\frac{1}{\varepsilon}; d\right\} \log \kappa \log \frac{1}{\delta}\right) \geq 1 - \delta$$

where m is the number of nonzero entries in K, d is the diameter of the graph associated to K and $\kappa = \sum_{i,j} K_{i,j} / \min_{i,j} K_{i,j}$.

1.4 Our contributions

numerics? limits? optimization ?

2 Main body (10 pages)

2.1 Notations

2.2 Presentation of the method

```
osborn(K, ε):
    x = 0 ∈ ℝ^n
    while not(is_balanced(𝔻(e^x)K𝔻(e^{-x}), ε)):
        Choose k ∈ [n] # This is where variants differ
        x += (log(c_k(𝔻(e^x)K𝔻(e^{-x}))) - log(r_k(𝔻(e^x)K𝔻(e^{-x}))))/2
    return x
```

There are *many* way to choose the next coordinate to update and hence many variants of the algorithm. The article focuses on four of them:

- **Cyclic Osborn** Cycle through the coordinates. (*eg.* 1, 2, 3, 1, 2, 3, 1, ...).
- **Random-Reshuffle Cyclic Osborn** Cycle through the coordinates using a new random permutation for each cycle. (*eg.* 2, 1, 3, 1, 2, 3, 1, 3, 2, ...).
- **Greedy Osborn** Choose k where the imbalance is maximal *eg.*

$$k = \text{argmax}_k \left| \sqrt{r_k(\mathbb{D}(e^x)K\mathbb{D}(e^{-x}))} - \sqrt{c_k(\mathbb{D}(e^x)K\mathbb{D}(e^{-x}))} \right|.$$

- **Random Osborn** Uniformly sample k independently between each call.

2.2.1 Implementation

The implementations were carried out in Python, providing us with a transparent and customizable framework for thorough experimentation. The source code for our implementations is available on GitHub. The implementation uses sparse representation for matrices and aimed to provide an implementation using data structures as close as possible as those used to compute the theoretical results. However, we were not able to find a detailed presentation of those and had to do our best to match the article. We did not give any focus on bit complexity. The authors recommanded a log-domain implementation to enable a logarithmic bit-complexity for some variants. However, we decided not to follow through in order to increase speed because we did not worry about bit-complexity.

At each update of x, we update the balanced matrix by multiplying the corresponding row and column. With the sparse representation, this operation is proportional to m. It is even $\mathcal{O}(m/n)$ on average! To compute the optimization function, the sum of elements in DAD^{-1} is computed in $\mathcal{O}(m)$ thanks to the sparse representation and $||c(A) - r(A)||_1$ is also computed in $\mathcal{O}(m)$. Indeed, we use $||c(A) - r(A)||_1 = \sum_j \left|\sum_i (DAD^{-1} - (DAD^{-1})^\top)_{i,j}\right|$. **Those techniques are not presented in the article and we had to come up with on our own.**

2.3 Matrix balancing as a convex optimization problem

A key part of the proofs of convergence given on the paper and other works rely mainly on a seeing the matrix balancing problem as an optimization problem. Let $\Phi : x \mapsto \log \sum_{i,j} e^{x_i - x_j} K_{i,j}$. The gradient of this function is

$$\nabla \Phi(x) = \frac{r\left(\mathcal{D}(e^x) K \mathcal{D}(e^x)\right) - c\left(\mathcal{D}(e^x) K \mathcal{D}(e^x)\right)}{\sum_{i,j} \left(\mathcal{D}(e^x) K \mathcal{D}(e^x)\right)_{i,j}}.$$

We can clearly notice a connection with Equation (1) and see that x is a solution to the ε, k-matrix balancing problem if and only if $||\nabla \Phi(x)||_k \leq \varepsilon$. The function Φ is convex and approximately solving the convex optimization problem $\min_x \Phi(x)$ solves the matrix balancing problem.

Alexandre d'Aspremont says in his MVA course on convex optimization that writing a problem as a convex optimization problem is almost solving it, which shows how important this statement is.

2.4 Theoretical guarantees

Lemma 2.1 *A matrix $K \in \mathcal{M}_n(\mathbb{R}_+^\star)$ is balanceable if and only if its associated graph is strongly connected [Osb60].*

Theorem 2.1 *Let $K \in \mathcal{M}_n(\mathbb{R}_+)$ be a balanceable non negative square matrix and $\varepsilon \geq 0$. Greedy Osborn solves $(\varepsilon, 1)$-approximate matrix balancing problem in*

$$\mathcal{O}\left(\frac{n^2}{\varepsilon} \min\left\{\frac{1}{\varepsilon}; d\right\} \log \kappa\right)$$

where d is the diameter of the graph associated to K and $\kappa = \sum_{i,j} K_{i,j} / \min_{i,j} K_{i,j}$.

Theorem 2.2 *Let $K \in \mathcal{M}_n(\mathbb{R}_+)$ be a balanceable non negative square matrix and $\varepsilon \geq 0$. Random Osborn solves $(\varepsilon, 1)$-approximate matrix balancing problem in T operations where there exists $c > 0, \delta > 0$ such that*

$$\mathbb{E}(T) = \mathcal{O}\left(\frac{m}{\varepsilon} \min\left\{\frac{1}{\varepsilon}; d\right\} \log \kappa\right) \quad \text{and} \quad \mathbb{P}\left(T \leq c \frac{m}{\varepsilon} \min\left\{\frac{1}{\varepsilon}; d\right\} \log \kappa \log \frac{1}{\delta}\right) \geq 1 - \delta$$

where m is the number of nonzero entries in K, d is the diameter of the graph associated to K and $\kappa = \sum_{i,j} K_{i,j} / \min_{i,j} K_{i,j}$.

Theorem 2.3 *Let $K \in \mathcal{M}_n(\mathbb{R}_+)$ be a balanceable non negative square matrix and $\varepsilon \geq 0$. Random cyclic Osborn solves $(\varepsilon, 1)$-approximate matrix balancing problem in T operations where there exists $c > 0, \delta > 0$ such that*

$$\mathbb{E}(T) = \mathcal{O}\left(\frac{mn}{\varepsilon} \min\left\{\frac{1}{\varepsilon}; d\right\} \log \kappa\right) \quad \text{and} \quad \mathbb{P}\left(T \leq c \frac{mn}{\varepsilon} \min\left\{\frac{1}{\varepsilon}; d\right\} \log \kappa \log \frac{1}{\delta}\right) \geq 1 - \delta$$

where m is the number of nonzero entries in K, d is the diameter of the graph associated to K and $\kappa = \sum_{i,j} K_{i,j} / \min_{i,j} K_{i,j}$.

2.5 Numerics

Computing numeric experiments was not easy. Getting the actual number of arithmetic operations is a complex endeavour, especially with a high-level language such as Python. We decided do use the running time to estimate how the number of arithmetic operations will evolve as a function of given parameters. This is not a precise measurement. However, all algorithms presented are are basically the same and this measure should be a fair assessment of convergence speed.

2.5.1 Data generation

In order to conduct numerical experiments, it is useful to be able to generate matrices with given parameters such as value of κ and sparsity. For that, we start by generating a (n, n) random matrix with m non-zero values using `scipy.sparse.random`. Then we assign values to those non-zero entries according to a EXPONENTIAL distribution of scale 1. We then want to modify those values to get the expected value for κ. To do so, we add a value x to all non-zeros entries. If the generated matrix was K, to find x, we solve

$$\kappa = \frac{\sum_{i,j} K_{i,j} + m \times x}{K_{\min} + x}.$$

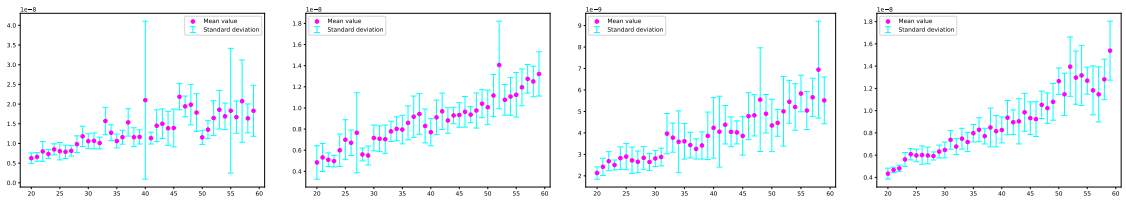
We then find that the value to add is

$$x = \frac{\kappa \times K_{\min} - \sum_{i,j} K_{i,j}}{m - \kappa}.$$

Sometimes, x is negative and K end up not being non-negative and we just start again from the start. Finally, we want the matrix to be balanceable. Hence, we start again until its associated graph is strongly connected (Lemma 2.1).

2.5.2 Complexity as a function of n

In order to experimentally show the convergence speed of theorems presented in Section 2.4, we fixed the parameters m and ε and let n in $[\![20, 60]\!]$. Each matrix is generated using an exponential distribution according to the scheme[3] presented in Section 2.5.1. The Figure 1 shows the results.



(a) Random. (b) Random cyclic. (c) Greedy. (d) Cyclic.

Figure 1: Plot of $\text{avg}(\text{time}/(m \min(d, 1/\varepsilon) \log(\kappa)/\varepsilon))$ as a function of n, using various variations with $\varepsilon = 10^{-4}$ and $m = 175$. Matrices are generated according to the framework presented in Section 2.5.1. Forall $n \in [\![20, 60]\!]$, we generate 10 matrices of size n and sparsity m.

We can assess the convergence depicted in Figure 1 by comparing it to the outcomes presented in Section 2.4. As outlined in Theorem 2.3, our anticipation was a linear

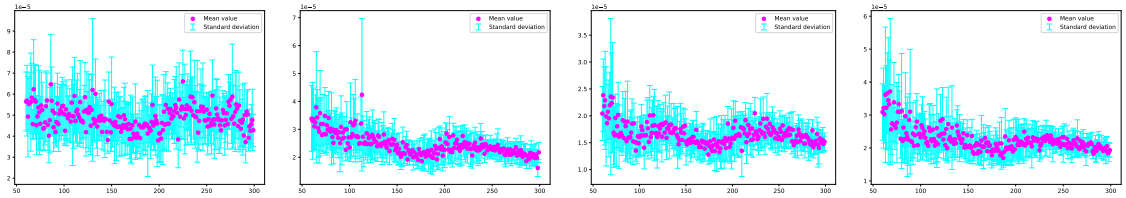
3 Note that here κ is not fixed.

progression concerning n in Figure 1b and Figure 1d. Remarkably, this linear trend is observed, even though it was originally expected only in terms of expectation. Referring to Theorem 2.1, an evolution in $\mathcal{O}(n^2/m)$ is expected in Figure 1c, and this prediction aligns with the observed outcomes. These numerical results are indeed promising.

The final validation involves examining Theorem 2.2, suggesting that Figure 1a should remain constant. Contrary to this expectation, the figure does not exhibit constancy. However, the growth rate is noticeably lower compared to the other variants, and there appears to be a tendency for the curve to plateau as n increases which is encouraging.

2.5.3 Complexity as a function of m

In order to experimentally show the convergence speed of theorems presented in Section 2.4, we fixed the parameters n and ε and let m in $[\![60, 300]\!]$. Each matrix is generated using an exponential distribution according to the scheme[4] presented in Section 2.5.1. The Figure 2 displays the results.

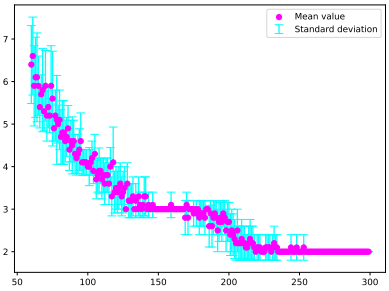


(a) Random. (b) Random cyclic. (c) Greedy. (d) Cyclic.

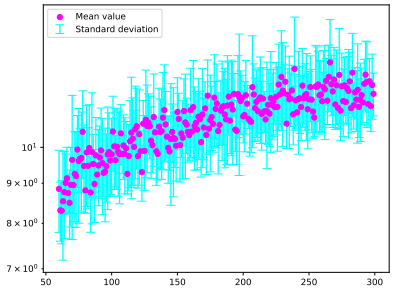
Figure 2: Plot of $\text{avg}(\text{time}/(\min(d, 1/\varepsilon)\log(\kappa)/\varepsilon))$ as a function of m, using various variations with $\varepsilon = 10^{-2}$ and $n = 60$. Matrices are generated according to the framework presented in Section 2.5.1. Forall $m \in [\![60, 300]\!]$, we generate 10 matrices of size n and sparsity m.

Interpreting the plots in Figure 2 using the theorems outlined in Section 2.4 poses challenges due to intrinsic connections between certain variables, such as d and m in the results. The expectation, based on Theorem 2.1, is that the plot using the greedy OSBORN method should remain flat, indicating no dependence on m. However, contrary to this theoretical expectation, the observed plot does not exhibit this characteristic. A more nuanced understanding is provided by Figure 3, where the relationship between Figure 2c and Figure 3a suggests non-monotonic behavior.

4 Note that here κ is not fixed.



(a) Evolution of d.



(b) Evolution of $\log \kappa$.

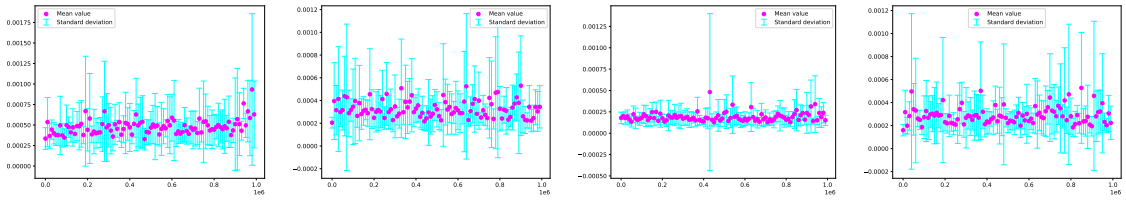
Figure 3: Plots of $\text{avg}(d)$ and $\text{avg}(\log \kappa)$ as a function of m, using $n = 60$ and the framework presented in Section 2.5.1. Forall $m \in [\![60, 300]\!]$, we generate 10 matrices of size n and sparsity m.

Specifically, as Figure 3a decreases, Figure 2c increases, and vice versa, elucidating the non-monotonous trend observed. Additionally, insights from Figure 3b contribute to an understanding of why the scaled time is decreasing overall for the greedy variant. Similar principles apply to the interpretation of the other plots. Notably, the random variant appears to be less affected by overall trends, suggesting a higher dependency on m.

Unfortunately, the observed plots do not align with our expectations. They fail to exhibit a clear linear dependency for the three variants, contrary to the anticipated linear relationship.

2.5.4 Complexity as a function of κ

Finally, same experiments were ran to showcase the linear dependency in $\log \kappa$ in theorems outlined in Section 2.4. The result, provided in Figure 4 clearly fails to showcase any dependency in κ.



(a) Random. (b) Random cyclic. (c) Greedy. (d) Cyclic.

Figure 4: Plot of $\text{avg}(\text{time}/(\min(d, 1/\varepsilon)/\varepsilon))$ as a function of κ, using various variations with $\varepsilon = 10^{-2}$, $n = 10$ and $m = 30$. Matrices are generated according to the framework presented in Section 2.5.1. Forall $\kappa \in [\![40, 10^6]\!]$, we generate 10 matrices of size n and sparsity m.

2.5.5 Convergence plot

2.5.6 Per iteration runtime

Only if I have time

2.6 Applications

2.6.1 Displacement Interpolation

[Pey11]
Discrete barycenters 9.4 ?

2.7 Optimal mass distribution using Osborn

Given a mass distribution and a cost matrix we can compute optimal mass distribution to the second set

2.8 Osborn in Optimal Transport and connection to Sinkhorn's algorithm

A connection with Sinkhorn's Algorithm must be drawn. Those two algorithms compute a scaling of a matrix. The main difference is Osborn returns a scaling of the form DAD^{-1} whereas Sinkhorn returns a scaling of the form XAY with X and Y diagonals.

Sinkhorn is an optimal transport algorithm, as we have seen in the course. It computes a solution to

$$\min_{P \in U(a,b)} \langle P, C \rangle + \varepsilon \mathrm{KL}(P | \mathbb{1}_{n \times m})$$

using notations from the course. Unlike with Osborn's algorithm, we do not need to work with square matrices.

Osborn's algorithm does not compute an optimal transport. We tried to modify it to be able to use it to compute optimal transport solutions. However, we failed to do so. It still has some advantages : its scaling has a form that preserves eigenspaces.

2.8.1 Osborn's algorithm as a preprocess step for Sinkhorn's algorithm

[Pey11]
Approximate solution using Osborn (Can easily compute optimal solution using (1.1))
Osborn before SInkhorn ?
Osborn as a measure ? Read about Sinkhorn as a measure ?

3 Conclusion and perspective

Summary of the result obtained: pros and cons (limitation, problems, error in the articles, etc) Possible improvement/extension

4 Connexion with the course

MANDATORY SECTION:. What are the notions/results/algorithms presented in the course that are used or related to the one presented in this paper?
Osborn gives solutions valable in the context of Kantorovich discrete relaxation : Osborn$(K) \in_a U(a, a)$ (does not need to be a permutation).
Sinkhorn

Unblanced OT ?

Todo list

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