Toroidal Grid Optimization via Gradient Descent

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1 Introduction

Gradient descent is an iterative algorithm to optimize (to maximize or minimize) a continuous function. It does so by shifting the value of the paramaters in the direction of its gradient with respect to (w.r.t.) the function. In the context of minimization, it is defined as follows

$$\theta' = \theta - \alpha \frac{d}{d\theta} L(\theta)$$

where θ is the paramater to optimize with the goal of minimizing the value of the function L. α is a scaling factor representing how far the paramater should shift. This equation can be generalized to optimize many paramaters by utilizing partial derivatives instead. Anyhow, it is obvious why a continuous function is required: gradients are only defined with continuous functions.

The primary goal of this essay is to test whether a discrete loss function and its corresponding discrete paramaters can be generalized to a continuous loss function and continuous paramaters, with the purpose of finding optimum discrete variables. What better demonstration than its application on a difficult challenge? So, I chose to address this problem within the context of a programming contest called "Reversing Nearness" held by Al Zimmermann, which traditionally, had been approached with algorithms that do not utilize gradients, such as hill climbing (which modifies each paramater sequentially and keeps changes that optimize the function) and simulated annealing (which is essentially probabilistic hill climbing)[1]. But I wanted to do it with gradients! Because what else would my calculus classes be for.

The objective of Al Zimmermann's programming contest, is to rearrange discrete tokens within a discrete grid, to minimize the the a loss function which depends on the distances between these tokens on a toroidal surface. The intricacies of this problem are explained within the essay.

Hence, my research question: *Is gradient descent a viable approach for toroidal grid optimization?*

There are many techniques used within this essay to accomplish this goal. Among them are

1. Generalization of Euclidean distances to accomodate toroidal surfaces
2. Matric permutations to remove duplicate entries
3. "Superposition" to model discrete tokens being within multiple positions, with their respective "probabilities".[2]
4. Enforcement of probabilities (that they should sum to one), using the Sinkhorn-Knopp algorithm.[1]
5. Use of Jacobian matrices for gradient descent

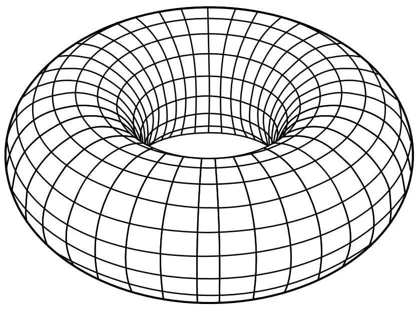
[1]both of which are beyond the scope of this essay

[2]Probabilities here does not refer to the chance of a random event occuring, but rather the "confidence" in which a token is in its position, or the extent in which the position affects the loss function

2 Problem Statement

2.1 Toroidal Grid

According to the problem description on AZsPCs,[2] the initial toroidal grid O is defined as an $N \times N$ grid of unique tokens which "wrap around" (implications are addressed in 2.2.1). These tokens can be arbitrarily defined, as long as they are unique, but for the sake of simplicity (and for reasons explained in 2.2.1), in this essay, a token is of the form by $\boldsymbol{IJ}$, where $\boldsymbol{I}$ and $\boldsymbol{J}$ are alphabetic representations of the indices of the rows and columns respectively, of a token, *within* O[3], eg. AC corresponds to the token in row 1, column 3 of O, DF corresponds to the row 4, column 6 of O, and so on. For $N = 4$, the grid is shown in Figure 1b. The tokens outside of the square grid represent tokens which wrap around the edges, resembling a toroidal surface as shown in Figure 1a.



(a) A Simple Toroid by Yassine Mrabet[3]

	DA	DB	DC	DD	
AD	AA	AB	AC	AD	AA
BD	BA	BB	BC	BD	BA
CD	CA	CB	CC	CD	CA
DD	DA	DB	DC	DD	DA
	DA	DB	DC	DD	

(b) A 4×4 *intial* toroidal grid

Figure 1: Representations of a toroidal grid

2.2 Evaluation Function

The goal of the challenge (and hence this essay) is to create a new grid X — with tokens rearranged arbitrarily from the initial grid O — which minimizes a loss function which is computed with the following procedure:

1. For each unique pair of tokens[4] (eg. (AA, BA) is equivalent to (BA, AA), so (BA, AA) is excluded), calculate the squared distance between them in the new grid,
2. Multiply each of them with the squared distance between the pair of tokens within the original grid
3. The loss is the sum of all of these products

2.2.1 Distance Metric

To evaluate the loss function, a distance metric between two tokens must be established. And to do that, we must define the position of a token in a coordinate system. This is where the methodology we used to define the unique tokens comes in handy; the coordinates of the tokens are simply the indices of the token *within the particular grid* X. To avoid confusion between whether the rows or columns correspond to the x-coordinate or y-coordinate, a token within a grid, with indices (i, j) simply has the coordinate (i, j).[5]

With this definition, we can now define the distance metric. If two two-dimensional coordinates are defined as $s_1 = (x_1, y_1)$ and $s_2 = (x_2, y_2)$, the Euclidean distance d_{euclid} is defined as

$$d_{euclid}(s_1, s_2) = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2} = \sqrt{(\Delta_{euclid}x)^2 + (\Delta_{euclid}y)^2} \tag{1}$$

[3]This is important because after rearranging the tokens, the identity of the token depends on its position within O, and not the rearranged position

[4]Comparisons between a token and itself do not affect the loss, since the distance between them is 0, therefore, their inclusion or exclusion does not affect the computation

[5]Note that this means we are not adhering to Cartesian coordinates, where the index (i, j) would have the coordinate (j, i).

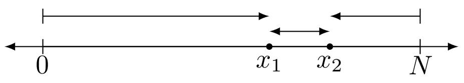


Figure 2: A one-dimensional diagram of toroidal distance, with the two arrows representing two possible distances

and the squared Euclidean distance d^2 evaluates to

$$d^2_{euclid}(s_1, s_2) = (\Delta_{euclid}x)^2 + (\Delta_{euclid}y)^2 \tag{2}$$

simplifying much of the computation.

But to generalize Euclidean distance to the distance on a toroidal surface, we must consider several implications. First of all, Δx or Δy can have 2 possible values. Let us first consider the one-dimensional case. A toroidal surface of length N is illustrated in Figure 2. It can be shown that the corresponding possible values for Δx are as follows:

$$\begin{aligned}\Delta_1(x) &= x_2 - x_1 \\ \Delta_2(x) &= (x_1 - 0) + (N - x_2) = x_1 + N - x_2\end{aligned}$$

To obtain a general equation which works with both $x_1 > x_2$ and $x_1 < x_2$ (as we cannot assume $x_1 < x_2$), we can write

$$\begin{aligned}\Delta_1(x) &= |x_2 - x_1| \\ \Delta_2(x) &= \min(x_1, x_2) + N - \max(x_1, x_2)\end{aligned}$$

where $|a|$ is the absolute value of a, $\min(a, b)$ and $\max(a, b)$ are defined as the minimum and maximum between the values of a and b respectively. They can be defined with piece-wise functions as follows:

$$\min(a,b) = \begin{cases} a & \text{if } a \le b \\ b & \text{if } a > b \end{cases} \qquad \max(a,b) = \begin{cases} a & \text{if } a \ge b \\ b & \text{if } a < b \end{cases}$$

min and max are used to determine the "left-most" and the "right-most" numbers.

Since the distance can only have one value, it is defined as the minimum of the two possible distances:

$$\Delta x = \min(\Delta_1(x), \Delta_2(x))$$

Generalizing it to 2 dimensions, we get

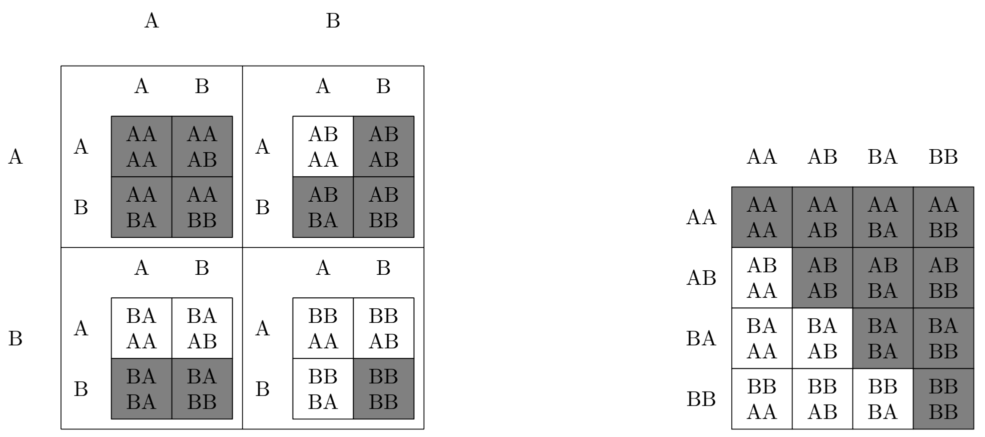
$$\begin{aligned}d(s_1, s_2) &= \sqrt{(\Delta x)^2 + (\Delta y)^2} \\ d^2(s_1, s_2) &= (\Delta x)^2 + (\Delta y)^2\end{aligned}$$

From now on, *distance* refers to d^2.

2.2.2 Token Comparisons

Within this essay, a *comparison* is defined as the distance between two tokens within a toroidal grid X. To be able to perform comparisons for every possible pair of tokens, a grid of comparisons on the grid is required. A viable approach would be to represent the comparison in a 4-dimensional grid (or tensor), where every token in the grid (first 2 dimensions), is compared to every token (next 2 dimensions). An example of the structure of the comparison for a 2×2 grid is shown in Figure 3a. The white boxes denote duplicate comparisons (eg. $\substack{BA \\ AA}$ is identical to $\substack{AA \\ BA}$), because the distance is invariant to the order of the tokens.

But since removing the irregularly shaped duplicate entries is not a trivial task with a 4-dimensional representation — especially if we extend beyond a $N = 2$ grid — we can simplify the problem by reducing the dimensionality of the grid: from an $N \times N \times N \times N$ grid to a $N^2 \times N^2$ grid. The elements within the 4-dimensional matrix are in the form $C_{i,j,k,l}$, and the 2-dimensional grid in the form $C_{ij,kl}$, but both represent the same thing: a the distance between the tokens $\boldsymbol{IJ}$ and $\boldsymbol{KL}$. The two-dimensional representation of Figure 3a is shown in Figure 3b. By doing so, we can easily remove the duplicate entries by multiplying it with an upper triangular matrix, further explained in 2.2.3. Let C_{2d} denote a function mapping from the input toroidal grid X and returning the 2d-comparison grid $C_{2d}(X)$.



(a) 4-dimensional comparison with elements in the form $C(X)_{i,j,k,l}$

(b) 2-dimensional comparison with elements in the form $C(X)_{ij,kl}$

Figure 3: Tensors $C(X)$ representing comparison grids of a 2×2 toroidal grid, where every element represents the distance between X_{ij} and X_{kl}. Shaded cells denote unique comparisons.

2.2.3 Loss Function as Matrix Multiplications

Let $\odot$ denote the element-wise matrix multiplication (eg. $\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \odot \left(\begin{smallmatrix} e & f \\ g & h \end{smallmatrix}\right) = \left(\begin{smallmatrix} a\cdot e & b\cdot f \\ c\cdot g & d\cdot h \end{smallmatrix}\right)$), and O denotes the original grid. The loss function for toroidal grid X is equal to

$$\begin{aligned} L(x) &= \sum_{i}^{N^2} \sum_{j}^{N^2} C(X)_{ij} C(O)_{ij} U_{ij} \\ &= \sum C(X) \odot C(O) \odot U \end{aligned}$$

where $C(X), C(O)$, and U are matrices of the form $N^2 \times N^2$, and U_{ij} is defined with the piece-wise defined function:

$$U_{ij} = \begin{cases} 1, & j \geq i \\ 0, & j < i \end{cases}$$

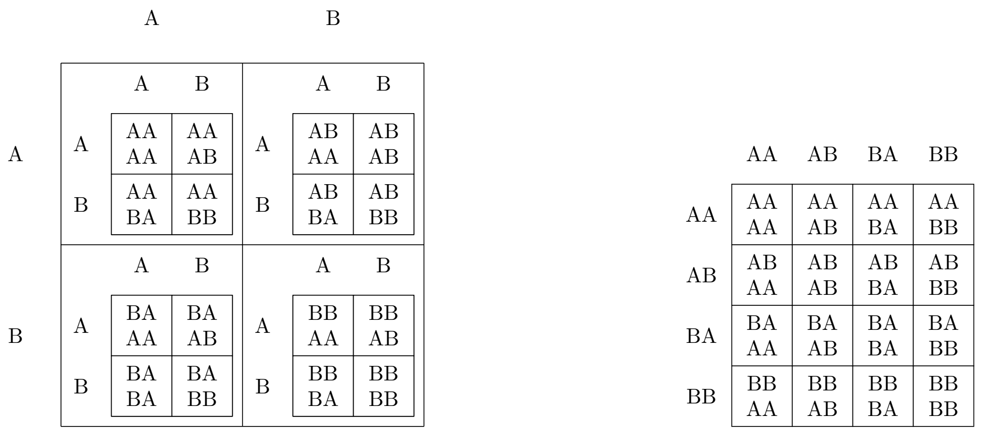
an example the matrix U with shape 4×4 is as follows:

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Multiplying by U has the effect of removing duplicate comparisons, satisfying our requirement of measuring only unique pairs of tokens.

3 Superposition

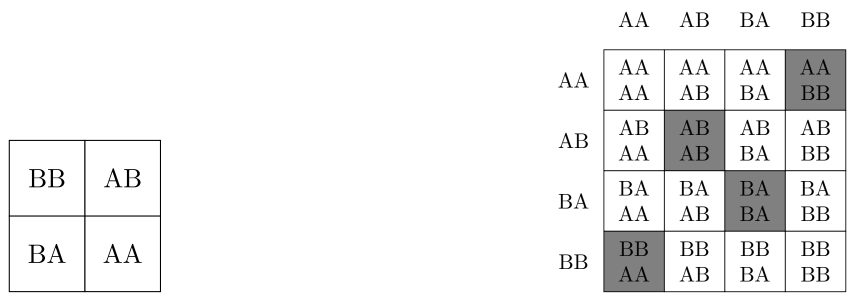
Since the entries into the toroidal grid are discrete (ie. discrete matrix indices correspond to discrete coordinates within the grid), it is not yet possible to optimize the loss function. Therefore, relaxing the constraints to enable “superposition” — here defined as having a token being in multiple positions, with each of its positions having its own “probabilities” — is essential. In this essay, “probability” will not refer to the likeliness of a random event, but rather, the confidence of a token in its posiiton. Let S denote the superposition grid.



(a) A_{ijkl}, a 4-dimensional superposition (b) $A_{ij,kl}$ a 2-dimensional superposition

Figure 4: Tensors S representing superpositions of a 2×2 toroidal grid, where every element S_{ijkl} represents the probability of the token KL being in the of position IJ in the original grid

A simple method of allowing superposition, is by allowing any token to be in any position, which again, can be visualized as a 4-dimensional matrix, and 2-dimensional matrix, as seen in Figure 4, and again, to reduce complexity we choose the 2-dimensional model. But this time, in contrast to Figure 3, the elements of the grid *do not represent comparisons*, but rather, the element $S_{i,j,k,l}$ (in the case of a 4-dimensional superposition) or $S_{ij,kl}$ (in the case of a 2-dimensional superposition), represent the probability of the token $\boldsymbol{KL}$ inhabiting the position of the token $\boldsymbol{IJ}$ *within the original grid* O. Further constraints to enforce the concept of probabilities will be discussed in subsection 4.1. Note that now the rows represents various positions within the grid O, and the columns represents the possible token values. An example is shown in Figure 5.



(a) A_{ijkl}, an example toroidal grid (b) $A_{ij,kl}$ superposition of the grid on the left

Figure 5: Shaded cells represent cells with probability 1, the rest have probability 0

3.0.1 Generalization of the Loss Function

Defining the loss function for this formulation requires us to compare *every* value within *every* position, to *every other* value within *every* position.[6] this is And we must do so, while taking both of their

[6] The wording is important

confidence's into account (ie. the distance metric should be scaled by their confidence). Therefore, the distance should be scaled with

$$S_{ab}S_{cd} \tag{3}$$

The distance between these two probabilities is defined as $C_{a,c}$, because only the indices a and c correspond to positions on the grid (thus being important in calculating distance), whereas b and d correspond to only the token itself.

Alike with the situation in subsubsection 2.2.2, we must prevent duplicate comparisons between values (not position), for example: each of $[\frac{AA}{AA}, \frac{AB}{AA}, \frac{BA}{AA}, \frac{BB}{AA}]$ should be compared to $[\frac{AA}{AB}, \frac{AB}{AB}, \frac{BA}{AB}, \frac{BB}{AB}]$, but not vice versa, because the values (not the positions) will have been compared already. Again, to do so, we must construct an upper triangular matrix U, of the shape $N^2 \times N^2$.

Therefore, the loss function can be written as

$$L(X) = \sum_{a}^{N^2}\sum_{b}^{N^2}\sum_{c}^{N^2}\sum_{d}^{N^2} S_{a,b}S_{c,d}C_{a,c}C_{b,d}U_{a,c} \tag{4}$$

$\sum_a^{N^2}$	Represents an iteration over Source Positions
$\sum_b^{N^2}$	Represents an iteration over Source Values
$\sum_c^{N^2}$	Represents an iteration over Target Positions
$\sum_d^{N^2}$	Represents an iteration over Target Values
$S_{a,b}$	Represents the Probability of the Source Position and Value
$S_{c,d}$	Represents the Probability of the Target Position and Value
$C_{a,c}$	Represents the Distance between Source and Target Position
$C_{b,d}$	Represents the Distance between the Source and Target Values in the original grid
$U_{a,c}$	Upper triangular matrix to remove redundant value comparisons

4 Optimization

4.1 Constraints

To be able to properly model probability, the sum of the probabilities of each token in all of its positions must be equal to one. Similarly, the sum of the probabilities of each position, in all of its values must be equal to one. Therefore, the sums of each of the rows and each of the columns must be equal to one, this is called a Doubly Stochastic Matrix. To be able to enforce this constraint, the Sinkhorn-Knopp algorithm was developed.

4.1.1 Sinkhorn-Knopp Algorithm

Given K an $n \times n$ non-negative matrix, by repetitively normalizing the rows and columns, a doubly stochastic matrix can be obtained. A single iteration can be seen through the following equation

$$K' = \left(\sum_{i}^{N} K_{ij} \right)^{-1} K \left(\sum_{j}^{N} K_{ij} \right)^{-1} \tag{5}$$

4.1.2 Non-negative Matrices

Since Sinkhorn-Knopp requires a non-negative matrix, and because negative probabilities make no sense, at every iteration of Sinkhorn-Knopp and Gradient Descent, the values have to be maintained above 0.

$$K'_{ij} = \max(K_{ij}, 0) \tag{6}$$

4.2 Gradient Descent

Gradient Descent is an algorithm to iteratively optimize a convex function, with knowledge of the derivative of the function with respect to all of the function parameters θ. In the case of optimizing a loss function, steps must be taken in the direction opposite to the gradient, therefore, the equation is as follows

$$\theta' = \theta - \alpha \frac{\delta}{\delta\theta} L(\theta) \tag{7}$$

where α is a parameter determining how big of a change there is between iterations of gradient descent.

4.2.1 Derivative of Loss Function coming Soon

5 Evaluation

5.1 Graphs of Loss over Time

5.2 Comparison to State of the Art Lower Bounds

5.3 Limitations of Computational Complexity

5.4 Limitations of How to Discretive Superpositions

5.5 Summary

References

[1] Richard Sinkhorn and Paul Knopp. “Concerning nonnegative matrices and doubly stochastic matrices”. In: *Pacific Journal of Mathematics* 21.2 (1967), pp. 343–348.

[2] Al Zimmermann. *Reversing Nearness.* URL: `http://azspcs.com/Contest/Nearness` (visited on 02/25/2020).

[3] Yassine Mrabet. *A simple Torus.* 2007. URL: `https://upload.wikimedia.org/wikipedia/commons/c/c6/Simple_Torus.svg` (visited on 02/25/2020). License: Creative Commons BY-SA.