

A Configurable Library for Generating and Manipulating Maze Datasets

Michael Igorevich Ivanitskiy¹✉, Aaron Sandoval¹, Alex F. Spies², Rusheb Shah¹, Brandon Knutson¹, Cecilia Diniz Behn¹, and Samy Wu Fung¹

¹ Colorado School of Mines, Department of Applied Mathematics and Statistics ² Imperial College London ✉ Corresponding author

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Summary

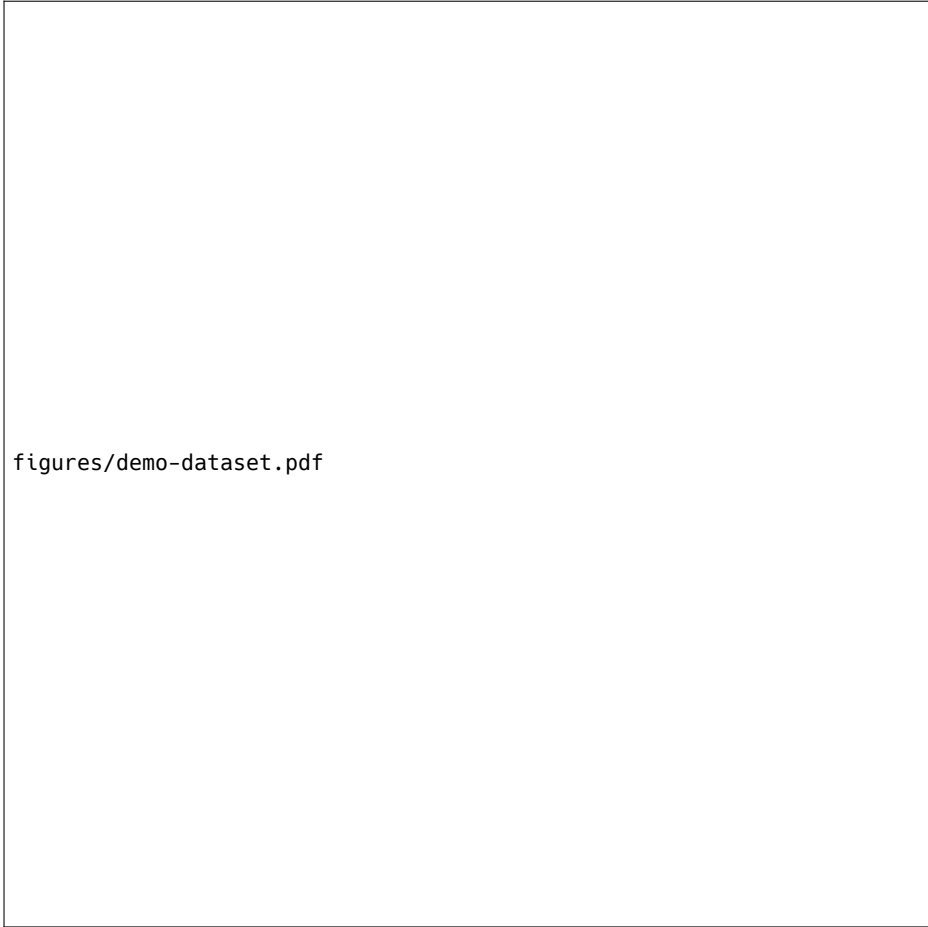
Understanding how machine learning models respond to distributional shifts and different input representations is a key research challenge. Mazes serve as an excellent testbed for this problem due to the degree of control we have over quantifiable distributional shifts. To enable systematic investigations of model behavior on maze tasks, we present `maze-dataset`, a comprehensive library for generating, processing, visualizing, and tokenizing datasets consisting of maze-solving tasks. With this library, researchers can easily create datasets and have extensive control over the generation algorithm used, the parameters fed to the algorithm of choice, and the filters that generated mazes must satisfy. Furthermore, this library supports multiple output formats, including rasterized and a large number of text-based formats, catering to convolutional neural networks and autoregressive transformer models. These formats, along with tools for visualizing and converting between them, ensure versatility and adaptability in research applications.

Introduction

Out-of-distribution generalization is a critical challenge in modern machine learning (ML) research. For interpretability and behavioral research in this area, training on algorithmic tasks offers benefits by allowing systematic data generation and task decomposition, as well as simplifying the process of circuit discovery ([Räuker et al., 2023](#)). Although mazes are well suited for these investigations, we have found that existing maze generation packages ([Cobbe et al., 2019](#); [Ehsan, 2022](#); [Harries et al., n.d.](#); [Németh, 2019](#); [Schwarzschild, Borgnia, Gupta, Bansal, et al., 2021](#)) do not support flexible maze generation algorithms that provide fine-grained control of generation parameters and the ability to easily transform between multiple representations of the mazes (Images, Textual, Tokenized) for training and testing models.

This work aims to facilitate deeper research into generalization and interpretability by addressing these limitations. We introduce `maze-dataset`, an accessible Python package ([M. I. Ivanitskiy et al., 2023a](#)). This package offers flexible configuration options for maze dataset generation, allowing users to select from a range of algorithms and adjust corresponding parameters (Section [Generation](#)). Furthermore, this package supports various output formats tailored to different ML architectures (Section [Visual Output Formats](#), Section [Tokenized Output Formats](#)).

TODO: links to docs, not just github



figures/demo-dataset.pdf

Figure 1: Example mazes from various algorithms. Left to right: randomized depth-first search (RDFS), RDFS without forks, constrained RDFS, Wilson's (Wilson, 1996), RDFS with percolation ($p=0.1$), RDFS with percolation ($p=0.4$), random stack RDFS.

Generation and Usage

Our package can be installed from [PyPi](#) via `pip install maze-dataset`, or directly from the [git repository](#) (M. I. Ivanitskiy et al., 2023a).

To create a dataset, we first create a `MazeDatasetConfig` configuration object, which specifies the seed, number, and size of mazes, as well as the generation algorithm and its corresponding parameters. This object is passed to a `MazeDataset` class to create a dataset. Crucially, this `MazeDataset` inherits from a PyTorch (Paszke et al., 2019) Dataset, and can thus be easily incorporated into existing data pre-processing and training pipelines, e.g., through the use of a `Dataloader` class.

```
from maze_dataset import MazeDataset, MazeDatasetConfig, LatticeMazeGenerators
cfg: MazeDatasetConfig = MazeDatasetConfig(
    name="example",
    grid_n=3,
    n_mazes=32,
    maze_ctor=LatticeMazeGenerators.gen_dfs,
)
dataset: MazeDataset = MazeDataset.from_config(cfg)
```

When initializing mazes, further configuration options can be specified through the

`from_config()` factory method as necessary. Options include 1) whether to generate the dataset during runtime or load an existing dataset, 2) if and how to parallelize generation, and 3) where to store the generated dataset. Full documentation of configuration options is available in our repository (M. I. Ivanitskiy et al., 2023a). Available maze generation algorithms are static methods of the `LatticeMazeGenerators` class and include the following:

- `gen_dfs` (**randomized depth-first search**): Parameters can be passed to constrain the number of accessible cells, the number of forks in the maze, and the maximum tree depth. Creates a spanning tree by default or a partially spanning tree if constrained.
- `gen_wilson` (**Wilson’s algorithm**): Generates a random spanning tree via loop-erased random walk (Wilson, 1996).
- `gen_percolation` (**percolation**): Starting with no connections, every possible lattice connection is set to either true or false with some probability p , independently of all other connections. For the kinds of graphs that this process generates, we refer to existing work (Duminil-Copin, 2017; Fisher & Essam, 2004).
- `gen_dfs_percolation` (**randomized depth-first search with percolation**): A connection exists if it exists in a maze generated via `gen_dfs` OR `gen_percolation`. Useful for generating mazes that are not acyclic graphs.

Furthermore, a dataset of mazes can be filtered to satisfy certain properties:

```
dataset_filtered: MazeDataset = dataset.filter_by.path_length(min_length=3)
```

Custom filters can be specified, and several filters are included:

- `path_length(min_length: int)`: shortest length from the origin to target should be at least `min_length`.
- `start_end_distance(min_distance: int)`: Manhattan distance between start and end should be at least `min_distance`, ignoring walls.
- `remove_duplicates(...)`: remove mazes which are similar to others in the dataset, measured via Hamming distance.
- `remove_duplicates_fast()`: remove mazes which are exactly identical to others in the dataset.

All implemented maze generation algorithms are stochastic by nature. For reproducibility, the seed parameter of `MazeDatasetConfig` may be set. In practice, we do not find that exact duplicates of mazes are generated with any meaningful frequency, even when generating large datasets.

Visual Output Formats

Internally, mazes are `SolvedMaze` objects, which have path information, and a connection list optimized for storing sub-graphs of a lattice. These objects can be converted to and from several formats.

<code>as_ascii()</code>	<code>as_pixels()</code>	<code>MazePlot()</code>
Simple text format for displaying mazes, useful for debugging in a terminal environment.	numpy array of dtype=uint8 and shape (height, width, 3). The last dimension is RGB color.	feature-rich plotting utility with support for multiple paths, heatmaps over positions, and more.

Figure 2: Various output formats. Top row (left to right): ASCII diagram, rasterized pixel grid, and advanced display.

Visual Outputs for Training and Evaluation

In previous work, maze tasks have been used with Recurrent Convolutional Neural Network (RCNN) derived architectures (Schwarzschild, Borgnia, Gupta, Huang, et al., 2021). To facilitate the use of our package in this context, we replicate the format of (Schwarzschild, Borgnia, Gupta, Bansal, et al., 2021) and provide the RasterizedMazeDataset class which returns rasterized pairs of (input, target) mazes as shown in Figure below.

Figure 3: Input is the rasterized maze without the path marked (left), and provide as a target the maze with all but the correct path removed. Configuration options exist to adjust whether endpoints are included and if empty cells should be filled in.

Tokenized Output Formats

To train autoregressive text models such as transformers, we convert mazes to token sequences in two steps. First, the maze is stringified using `as_tokens()`. The `MazeTokenizerModular` class provides a powerful interface for configuring maze stringification behavior. Second, the sequence of strings is tokenized into integers using `encode()`. Tokenization uses a fixed vocabulary for simplicity. Mazes up to 50x50 are supported using unique tokens, and up to 128x128 when using coordinate tuple tokens.

Stringification Options and MazeTokenizerModular

There are many algorithms by which one might tokenize a 2D maze into a 1D format usable by autoregressive text models. Training multiple models on the encodings output from each of these algorithms may produce very different internal representations, learned solution algorithms, and levels of performance. To explore how different maze tokenization algorithms affect these models, the `MazeTokenizerModular` class contains a rich set of options to customize how mazes are stringified. This class contains 19 discrete parameters, resulting in 5.9 million unique tokenizers. But wait, there's more! There are 6 additional parameters available in the library which are untested but further expand the the number of tokenizers by a factor of 44/3 to 86 million.

All output sequences consist of four token regions representing different features of the maze. These regions are distinguished by color in Figure below.

- Adjacency list: A text representation of the lattice graph
- Origin: Starting coordinate
- Target: Ending coordinate
- Path: Maze solution sequence from the start to the end

Figure 4: Example text output format with token regions highlighted.

Each MazeTokenizerModular is constructed from a set of several _TokenizerElement objects, each of which specifies how different token regions or other elements of the stringification are produced.

figures/TokenizerElement_structure.pdf

Figure 5: Nested internal structure of _TokenizerElement objects inside a typical MazeTokenizerModular object.

Optional delimiter tokens may be added in many places in the output. Delimiter options are all configured using the parameters named pre, intra, and post in various _TokenizerElement classes. Each option controls a unique delimiter token. Here we describe each _TokenizerElement and the behaviors they support. We also discuss some of the model behaviors and properties that may be investigated using these options.

Coordinates

The _CoordTokenizer object controls how coordinates in the lattice are represented in across all token regions. Options include:

- **Unique tokens:** Each coordinate is represented as a single unique token "(i,j)"
- **Coordinate tuple tokens:** Each coordinate is represented as a sequence of 2 tokens, respectively encoding the row and column positions: ["i", ",", "j"]

Adjacency List

The _AdjListTokenizer object controls this token region. All tokenizations represent the maze connectivity as a sequence of connections or walls between pairs of adjacent coordinates in the lattice.

- _EdgeSubset: Specifies the subset of lattice edges to be tokenized
 - **All edges:** Every edge in the lattice
 - **Connections:** Only edges which contain a connection
 - **Walls:** Only edges which contain a wall
- _EdgePermuter: Specifies how to sequence the two coordinates in each lattice edge
 - **Random**
 - **Sorted:** The smaller coordinate always comes first
 - **Both permutations:** Each edge is represented twice, once with each permutation. This option attempts to represent connections in a more directionally symmetric manner. Including only one permutation of each edge may affect models' internal

representations of edges, treating a path traversing the edge differently depending on if the coordinate sequence in the path matches the sequence in the adjacency list.

- `shuffle_d0`: Whether to shuffle the edges randomly or sort them in the output by their first coordinate
- `connection_token_ordinal`: Location in the sequence of the token representing whether the edge is a connection or a wall

Path

The `_PathTokenizer` object controls this token region. Paths are all represented as a sequence of steps moving from the start to the end position.

- `_StepSize`: Specifies the size of each step
 - **Singles**: Every coordinate traversed between start and end is directly represented
 - **Forks**: Only coordinates at forking points in the maze are represented. The paths between forking points are implicit. Using this option might train models more directly to represent forking points differently from coordinates where the maze connectivity implies an obvious next step in the path.
- `_StepTokenizer`: Specifies how an individual step is represented
 - **Coordinate**: The coordinates of each step are directly tokenized using a `_CoordTokenizer`
 - **Cardinal direction**: A single token corresponding to the cardinal direction taken at the starting position of that step. E.g., NORTH, SOUTH. If using a `_StepSize` other than **Singles**, this direction may not correspond to the final direction traveled to arrive at the end position of the step.
 - **Relative direction**: A single token corresponding to the first-person perspective relative direction taken at the starting position of that step. E.g., RIGHT, LEFT.
 - **Distance**: A single token corresponding to the number of coordinate positions traversed in that step. E.g., using a `_StepSize` of **Singles**, the **Distance** token would be the same for each step, corresponding to a distance of 1 coordinate. This option is only of interest in combination with a `_StepSize` other than **Singles**.

A `_PathTokenizer` contains a sequence of one or more unique `_StepTokenizer` objects. Different step representations may be mixed and permuted, allowing for investigation of model representations of multiple aspects of a maze solution at once.

Tokenized Outputs for Training and Evaluation

During deployment we provide only the prompt up to the `<PATH_START>` token.

Examples of usage of this dataset to train autoregressive transformers can be found in our maze-transformer library (M. I. Ivanitskiy et al., 2023b). Other tokenization and vocabulary schemes are also included, such as representing each coordinate as a pair of i, j index tokens.

Extensibility

The tokenizer architecture is purposefully designed such that adding and testing a wide variety of new tokenization algorithms is fast and minimizes disturbances to functioning code. This is enabled by the modular architecture and the automatic inclusion of any new tokenizers in integration tests. To create a new tokenizer, developers forking the library may simply create their own `_TokenizerElement` subclass and implement the abstract methods. If the behavior change is sufficiently small, simply adding a parameter to an existing `_TokenizerElement` subclass and updating its implementation will suffice. For small additions, simply adding new cases to existing unit tests will suffice.

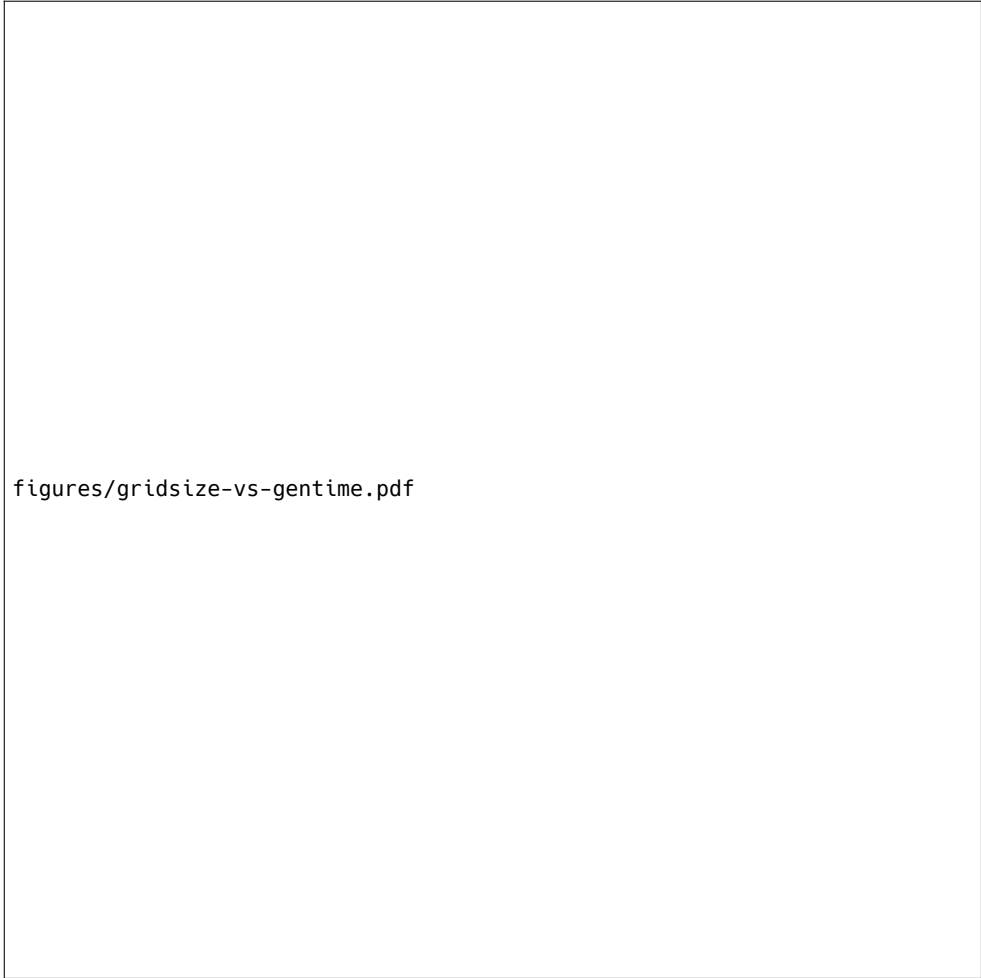
The breadth of tokenizers is also easily scaled in the opposite direction. Due to the exponential

scaling of parameter combinations, adding a small number of new features can significantly slow certain procedures which rely on constructing all possible tokenizers, such as integration tests. If any existing subclass contains features which aren't needed, a developer tool decorator is provided which can be applied to the unneeded `_TokenizerElement` subclasses to prune those features and compact the available space of tokenizers.

Benchmarks of Generation Speed

We provide approximate benchmarks for relative generation time across various algorithms, parameter choices, maze sizes, and dataset sizes.

Method & Parameters	Average time per maze (ms)				
Generation algorithm	Generation parameters	all sizes	small ($g \leq 10$)	medium ($10 < g \leq 32$)	large ($g > 32$)
gen_dfs	accessible_cells=20	2.4	2.4	2.6	2.4
gen_dfs	do_forks=False	3.0	2.4	3.7	3.8
gen_dfs	max_tree_depth=455	2.2	2.2	4.9	11.6
gen_dfs	—	31.1	2.8	28.0	136.5
gen_dfs_percolation	p=0.1	53.9	3.6	42.5	252.9
gen_dfs_percolation	p=0.4	58.8	3.7	44.7	280.2
gen_percolation	—	59.1	3.3	43.6	285.2
gen_wilson	—	767.9	10.1	212.9	4530.4
median (all runs)		10.8	6.0	44.4	367.7
mean (all runs)		490.0	11.7	187.2	2769.6



figures/gridsizes-vs-gentime.pdf

Figure 6: Plots of maze generation time. Generation time scales exponentially with maze size for all algorithms (left). Generation time does not depend on the number of mazes being generated, and there is minimal overhead to initializing the generation process for a small dataset (right). Wilson's algorithm is notably less efficient than others and has high variance. Note that for both plots, values are averaged across all parameter sets for that algorithm, and parallelization is disabled.

Implementation

We refer to our GitHub repository ([M. I. Ivanitskiy et al., 2023a](#)) for documentation and up-to-date implementation details.

This package utilizes a simple, efficient representation of mazes. Using an adjacency list to represent mazes would lead to a poor lookup time of whether any given connection exists, whilst using a dense adjacency matrix would waste memory by failing to exploit the structure (e.g., only 4 of the diagonals would be filled in). Instead, we describe mazes with the following simple representation: for a d -dimensional lattice with r rows and c columns, we initialize a boolean array $A = \{0, 1\}^{d \times r \times c}$, which we refer to in the code as a `connection_list`. The value at $A[0, i, j]$ determines whether a downward connection exists from node $[i, j]$ to $[i + 1, j]$. Likewise, the value at $A[1, i, j]$ determines whether a rightwards connection to $[i, j + 1]$ exists. Thus, we avoid duplication of data about the existence of connections, at the cost of requiring additional care with indexing when looking for a connection upwards or to the left. Note that this setup allows for a periodic lattice.

To produce solutions to mazes, two points are selected uniformly at random without replacement

from the connected component of the maze, and the A^* algorithm (Hart et al., 1968) is applied to find the shortest path between them.

Parallelization is implemented via the multiprocessing module in the Python standard library, and parallel generation can be controlled via keyword arguments to the `MazeDataset.from_config()` function.

Relation to Existing Works

As mentioned in the introduction, a multitude of public and open-source software packages exist for generating mazes (Ehsan, 2022; Németh, 2019; Schwarzschild, Borgnia, Gupta, Bansal, et al., 2021). However, our package provides more flexibility and efficiency in the following ways:

- For rigorous investigations of the response of a model to various distributional shifts, preserving metadata about the generation algorithm with the dataset itself is essential. To this end, our package efficiently stores the dataset along with its metadata in a single human-readable file (M. Ivanitskiy, n.d.). This metadata is loaded when the dataset is retrieved from disk and reduces the complexity of discerning the parameters under which a dataset was created.
- Prior works provide maze datasets in only a rasterized format, which is not suitable for training autoregressive text-based transformer models. As discussed in Section [Visual Output Formats](#) and Section [Tokenized Output Formats](#), our package provides these different formats natively.
- Our package provides a selection of maze generation algorithms, which all write to a single unified format. All output formats are reversible, and operate to and from this unified format.

As mentioned in Section [Training](#), we also include the `RasterizedMazeDataset` class in our codebase, which can exactly mimic the outputs provided in `easy-to-hard-data` (Schwarzschild, Borgnia, Gupta, Bansal, et al., 2021). Our `as_ascii()` method provides a format similar to that used in (Singla, 2023). The text format provided by `as_tokens()` is similar to that of (Liu & Wu, 2023), but provides a custom tokenization scheme.

Limitations of maze-dataset

For simplicity, the package primarily supports mazes that are sub-graphs of a 2-dimensional rectangular lattice. Some support for higher-dimensional lattices is present, but not all output formats are adapted for higher dimensional mazes. [Implementation Implementation](#)

Conclusion

The `maze-dataset` library (M. I. Ivanitskiy et al., 2023a) introduced in this paper provides a flexible and extensible toolkit for generating, processing, and analyzing maze datasets. By supporting various procedural generation algorithms and conversion utilities, it enables the creation of mazes with customizable properties to suit diverse research needs. Planned improvements to the `maze-dataset` include adding more generation algorithms (such as Prim's algorithm (Dijkstra, 1959; Jarník, 1930; Prim, 1957) and Kruskal's algorithm (Kruskal, 1956), among others (Gabrovšek, 2019)), adding the ability to augment a maze with an adjacency list to add "shortcuts" to the maze, and resolving certain limitations detailed in Section [Limitations](#). Future work will make extensive use of this library to study interpretability and out-of-distribution generalization in autoregressive transformers (M. I. Ivanitskiy et al., 2023b), recurrent convolutional neural networks (Schwarzschild, Borgnia, Gupta, Huang, et al., 2021), and implicit networks (Fung et al., 2022; McKenzie et al., 2023).

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