ML Kit: A Machine Learning Library for Rust

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Application Setting

Rust is a relatively new programming language with a dearth of machine learning infrastructure. We aimed to create a library for Rust programmers to make machine learning convenient, much like NumPy or TensorFlow in Python.

Project Description

Initially, we wanted to create a comprehensive machine learning library for Rust, which would use Rust's safety and speed to implement many algorithms used in data science. We had the original (lofty) goal of being able to run a diffusion model by the end of the semester, or be able to do anything that NumPy/SciKitLearn could do. As we began implementation we recognized that we lacked the time and resources to implement the sheer amount of algorithms we set out to. So, we shifted our focus to what we believe are some of the core algorithms in the field of Machine Learning.

In the end, we created the pure-Rust library `ml_kit`, which implements, from scratch, the following:

- Neural Network based learning, consisting of
  - the basic neural network model with user-defined network shape and activation functions for each layer
  - functionality for handling large datasets for training and testing
  - a stochastic gradient descent trainer, with whatever batch size and epochs a user may want
  - various "gradient update schedules," such as fixed learning rates, time-decay learning rates, AdaGrad, etc.
  - Convolutional Neural Networks (Owen/Ethan talk more on this?)

- Principle Component Analysis, consisting of
  - an implementation of Singular Value Decomposition (SVD),
  - using SVD to obtain a k-dimensional plane of best fit for a set of points in $\mathbb{R}^n$,
  - compressing images (or any data) using SVD by truncating low-variance dimensions

Neural Networks

Principle Component Analysis and SVD

Singular Value Decomposition (SVD) is a factorization of a matrix $A \in \mathbb{R}^{m \times n}$ into

$$A = U \Sigma V^\top$$

where $U \in \mathbb{R}^{m \times m}$ and $V \in \mathbb{R}^{n \times n}$ are orthogonal matrices with columns $\vec{\mathbf{u}}_1, \dots \vec{\mathbf{u}}_m$ and $\vec{\mathbf{v}}_1, \dots, \vec{\mathbf{v}}_n$ respectively, and Σ is a diagonal matrix of the form (assuming $n \leq m$)

$$\Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \\ & & & \end{bmatrix} \in \mathbb{R}^{m \times n}$$

where $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$ are the *singular values* of A. This allows us to write A as the linear combination

$$A = \sum_{i=1}^{n} \sigma_i \vec{\mathbf{u}}_i \vec{\mathbf{v}}_i^\top$$

Note that because the singular values are sorted in decreasing order, we can effectively "save data" in representing A by truncating all but the first $r \leq n$ singular vectors, as the last items in the sum do not contribute as much to the overall product. The immediate application is identifying the most significant axes of correlation in data, allowing dimensionality reduction of datasets by re-writing each item in the basis $\vec{\mathbf{v}}_1, \dots, \vec{\mathbf{v}}_r$. Commonly, the "data" of concern is written into the rows of A.

What we implemented

Our library implements the Golub-Kahan SVD algorithm (described in "Matrix Computations," by Golub and van Loan. [1]) which begins by bi-diagonalizing A, then performing SVD on the bidiagonalization, as the numerical stability and performance are better. Once we were able to compute the SVD of any matrix, we could use SVD as a subroutine in other useful techniques.

The (subjectively) coolest application of SVD we implemented is image compression. By taking an $m \times n$ image and writing it as a 4-tuple of matrices (R, G, B, A) representing the red, green, blue, and alpha channels of the pixels, we can perform SVD on each color channel, store only the SVD representation after truncating insignificant singular vectors, and then de-compress the image later by computing $U\Sigma V^\top$ for each color channel. In practice, one can discard roughly half the singular values and still obtain a recognizeable image. Examples of this and discussion of runtime and compression rates will be left to the evaluation section.

A common goal in statistics is finding the "line of best fit" of a set of points, or in higher dimensions, a k-dimensional plane of best fit. For a cluster of data centered at the origin, the first singular vector, $\vec{\mathbf{v}}_1$, is the line of best fit. This is because SVD is equivalently defined as an optimization proceedure where

$$\vec{\mathbf{v}}_1 = \underset{\|x\|=1}{\operatorname{argmax}} \|Ax\|$$

Since $\vec{\mathbf{v}}_1$ is maximizing the sum of squares of the inner products with all the data points, it is minimizing the sum of squared distances from each data point to the line spanned by $\vec{\mathbf{v}}_1$. More generally, taking the first $\vec{\mathbf{v}}_1, \ldots, \vec{\mathbf{v}}_k$ vectors, we obtain a basis for a k-dimensional "plane of best fit."

We implement a proceedure which takes a data matrix $D \in \mathbb{R}^{n \times m}$ whose columns are each $\mathbb{R}^n$ data points, and returns $\vec{\mu} \in \mathbb{R}^n$ and $V \in \mathbb{R}^{n \times k}$ such that the plane defined by

$$\left\{ \vec{\mu} + \sum_{i=1}^{k} \alpha_i \vec{\mathbf{v}}_i \mid \alpha_i \in \mathbb{R} \right\}$$

is the plane of best fit for the data. Examples of this will be left to the evaluations section.

Relationship to Other Work

Linear algebra is the foundatin to machine learning, so we needed to use a good linear algebra library. Sylvan had previously spent winter break working on `matrix_kit`,

1. Gene H. Golub and Charles F. van Loan, *Matrix Computations*, Fourth (JHU Press, 2013), ISBN: 1421407949 9781421407944, http://www.cs.cornell.edu/cv/GVL4/golubandvanloan.htm.

which is a pure-Rust linear algebra package that implemented incredibly basic matrix-vector operations. We continued developing this library in parallel with `ml_kit` over the semester as we recognized more features that were needed from the linear algebra library. So, the sum of our work for the course can be thought of as the entirety of `ml_kit`, as well as significant improvement to the functionality of `matrix_kit`.

The `matrix_kit` library can be found on GitHub at https://github.com/SylvanM/matrix_kit.

Evaluation

Gradient Descent

Principle Component Analysis

In this section, we discuss the performance of our SVD-based algorithms in terms of their speed and correctness.

Singular Value Decomposition

Correctness

In numerical methods such as SVD, the accumulation of floating point error prevents us from measuring exact correctness. Instead, we define some small ε, and consider two matrices $A \approx_\varepsilon B$ to be "basically equal" if for all i, j, $|a_{ij} - b_{ij}| < \varepsilon$. When testing on large matrices, we chose $\varepsilon = 1 \times 10^{-5}$ to be our goal, though in practice on smaller matrices ($m, n \leq 50$) we attain correctness up to $\varepsilon = 1 \times 10^{-9}$.

To test correctness of our SVD implementation, we start with a randomly generated matrix $A \in \mathbb{R}^{m \times n}$ where each entry is sampled from the normal distribution $\mathcal{N}(0, 1)$, and compute its SVD into U, V, and Σ. We then check that U and V are orthogonal by testing $U^\top U \approx_\varepsilon I_m$ and $V^\top V \approx_\varepsilon I_n$. We then check that $A \approx_\varepsilon U \Sigma V^\top$.

Sometimes, our SVD implemention does not converge on a particular matrix, and so we abort the execution. The main loop of the Golub-Kahan algorithm should in theory take $\mathcal{O}(n)$ steps, so we introduced a check that if the main loop runs more than $30n$ times, we declare the instance a failure, and return empty 0×0 matrices.

With m and n sampled randomly in the range 2 through 20, we ran the above testing proceedure 10,000 times and found no correctness failures, though we observe a divergence rate of about 2.49%. That is, on small matrices, our algorithm failed to converge on 249 out of the 10,000 random matrices.

The issue of convergence seems to become better with larger matrices. When we sample m and n randomly from the range 2 through 200, we found that out of 300 trials, only 1 instance failed to converge, a rate of .33%.

For matrices with $200 \leq m, n \leq 300$, we found no matrices with failed to converge out of 30 trials.

Runtime Performance

Our SVD implementation is absurdly slow. It became impractical to test at a large scale for matrices with more than $500 \times 500 = 250,000$ entries. This is unfortunate, as most real-world applications would require much larger matrices. When we first tried image compression, we used a 4K image taken by an iPhone, and running SVD on each color channel took so long that even when let to run for 12 hours overnight, it didn't terminate. It is hard to know if this is because it genuinely just took so long, or if it fell into the small fraction of cases that caused divergence. Because of the decaying rate of divergence for larger dimensions, we believe it is the former. We also tried running SVD on matrices of comparable size (with m and n in the low thousands) and were unable to get it to terminate after several hours.

This is almost certainly due to the fact that at this stage of development we did *not* fully optimize our Golub-Kahan implementation. The first step, which relies on bi-diagonalizing the matrix, uses a sequence of Householder reflections, which if implemented efficiently can take linear time as they only affect two rows of a matrix. Further optimization would include only applying the reflection to a sub-matrix of A, and not the entire matrix. Instead, we applied the householder reflection matrix to the entire matrix A, taking $\mathcal{O}(n^3)$ time for each step. This easily balloons the runtime, since this is done inside an inner loop. At first, we tried implementing the fully optimized Golub-Kahan algorithm, but were unable to get it to work correctly. So, we focused on just trying to get a *correct* implementation instead of premature optimization. The natural next steps after this project would be to get this running faster!

Image Compression

As discussed above, we were unable to run our image compression on large images, so we started with low-resolution images. We ran our image compression algorithm on two images, one of some sheep,[2], and one of a cat.

When a matrix A is decomposed into U, Σ, V, and all but the first k singular values are ditched, we are left with three matrices of sizes $m \times k$, k and $n \times k$ (we need

2. The sheep are in the teaching barn by the Vet School. I highly recommend that you go visit and pet them! It's free and you can just walk right up to them!

only store the diagonal of Σ). So, the number of floating point values we must store as a fraction of the amount we would need to fully represent A is what we call the "compression ratio," computed as

$$r = \frac{r + rm + rn}{mn}$$

For small matrices and large values of r, this doesn't save much. However, this scales incredibly well for large matrices, as we can pick modestly small values of r and end up with impressive compression ratios while still being able to recognize the original image. A small caveat here is that typically a single pixel's channel for one color only uses one byte to represent it, whereas we are using 64-bit floating points, so one could argue that we need to include a factor of 8 in our compression ratio. However, our compression would work just as well if each color channel was represented as a floating point value between 0 and 1 (since this is what we convert the image to anyway when we begin compression), so we think it is fair to compare the sizes when thinking of the original channel as being a decimal between 0 and 1 as opposed to an integer between 0 and 255.

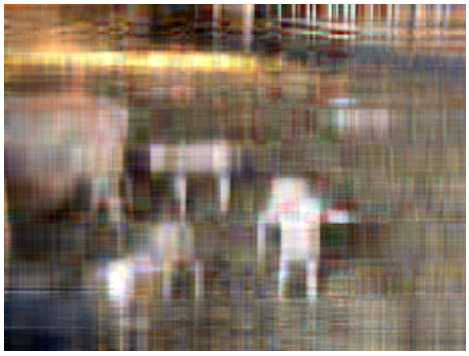
Sheep

We used a 240×320 pixel image of some sheep laying in a barn, and truncated the singular values up to the first $k \in \{100, 50, 10\}$. Running SVD to decompose the image took **1m 15s**.

Original

$k = 100$, 73.0% compression

$k = 50$, 36.5% compression



$k = 10$, 7.3% compression

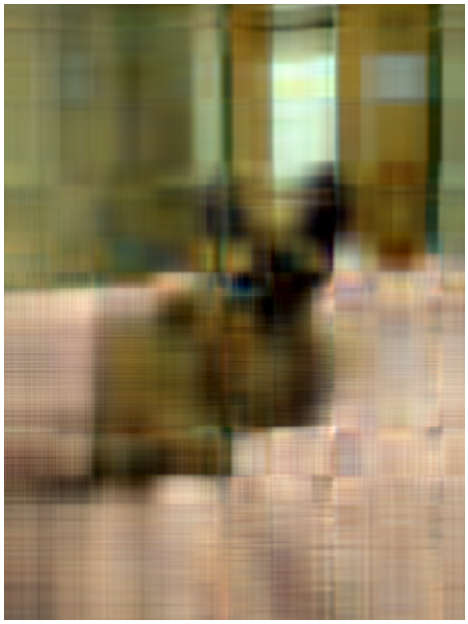
Panini (the cat)

On a 640×480 image of Panini, SVD took **20m 50s** to finish. Here are the results using the first $k \in \{150, 50, 7\}$ singular values.

Original

$k = 150$, 54.7% compression

$k = 50$, 18.2% compression



$k = 7$, 2.6% compression

Planes of Best Fit

References

Golub, Gene H., and Charles F. van Loan. *Matrix Computations*. Fourth. JHU Press, 2013. ISBN: 1421407949 9781421407944. http://www.cs.cornell.edu/cv/GVL4/golubandvanloan.htm.