Machine learning for complete intersection Calabi-Yau manifolds

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Abstract

We describe the recent developments in using machine learning techniques to compute Hodge numbers of complete intersection Calabi-Yau (CICY) 3- and 4-folds. The main motivation is to understand how to study data from algebraic geometry and solve problems relevant for string theory with machine learning. We describe the state-of-the art methods which reach near-perfect accuracy for several Hodge numbers, and discuss extrapolating from low to high Hodge numbers, and conversely.

1 Introduction

Calabi-Yau (CY) manifolds are a very active field of research in both mathematics (algebraic geometry) and theoretical physics (string theory). They correspond to Kähler manifolds (complex manifolds with a closed 2-form) whose holonomy group is a subgroup of $\mathrm{SU}(N)$ [1]. These manifolds have a special role in string theory because they are used to describe compactifications: indeed, superstring theory predicts that spacetime must be 10-dimensional, in apparent contradiction with the observed 4-dimensional universe. The solution is to compactify 6 dimensions into a tiny volume at each spacetime point, such that they cannot be observed at the energy scales from the current experiments; consistency of string theory requires the manifold describing these six dimensions to be CY [2, 3]. The shape of the manifold used for the compactification characterizes the low-energy effective action, which should match the existing Standard Model of particle physics. For this reason, classifying CY manifolds by computing their topological and geometrical properties is of the utmost importance in string theory.

String theory is a theory of quantum gravity which also unifies all force and matter fields. Hence, finding the appropriate compactification would allow, in principle, to completely determine the physics of our universe. However, there are some important challenges for pushing this program to its term [4]. First, there is an extremely large number of compactifications, which makes an exhaustive scan impossible. Second, a complete expression for the low-energy effective action is lacking because it requires knowing the CY metric. While existence has been proven by Yau, no metric has been constructed for compact CY until today (though recent progresses with machine learning have been achieved [5–10]). Third, topological properties (which largely constrain the general form of the

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effective theory) can be difficult to compute with standard techniques of algebraic geometry, which lead to complicated algorithms, without closed-form solutions in general. For instance, computing cohomology group dimensions often requiring summing and subtracting huge integers at intermediate steps, to only get relatively small integers at the end.

Progress in string theory goes in hand with understanding better mathematical structures, and machine learning (ML) has been called to the rescue for all three problems [4, 11]. In this paper, we focus on computing Hodge numbers for complete intersection CY (CICY) manifolds [12–19]. This topic is interesting for fundamental mathematics and physics, as argued above, but also for the machine learning community as it showcases a new type of data which has not been properly studied until now. CICYs form a particularly appropriate set with which to begin our investigation since they correspond to the simplest category of CY, they have been completely classified, and their topological properties fully computed. As a consequence, this allows us to design and test new methods in a controlled environment before generalizing to new problems. Moreover, CICYs are often used in string theory model building due to their simple properties.

2 Complete intersection Calabi-Yau manifolds

CY N-folds are N-dimensional complex manifolds with $\mathrm{SU}(N)$ holonomy, or, equivalently, with a vanishing first Chern class [1]. They are characterized by their topological properties, such as the Hodge numbers. These features directly translate into properties of the 4-dimensional effective action, such as the number of chiral multiplets in heterotic compactifications, and the number of hyper and vector multiplets in type II compactifications. Ultimately, they are connected to the number of fermion generations, which could be used to test the effectiveness of the models.

The simplest CYs are constructed as *complete intersections* of hypersurfaces in a product of complex projective spaces $\mathbb{P}^{n_1} \times \cdots \times \mathbb{P}^{n_m}$. They are defined by systems of homogeneous polynomial equations, whose solutions identify CY manifolds. When considering topological properties, it is sufficient to keep track only of the dimensions of the projective spaces and the degree of the equations. In the general case of m projective spaces and k equations, a CICY X is represented by a *configuration matrix*, which will be the input to the network:

$$X = \left[\begin{array}{c|ccc} \mathbb{P}^{n_1} & \alpha_1^1 & \cdots & \alpha_k^1 \\ \vdots & \vdots & \ddots & \vdots \\ \mathbb{P}^{n_m} & \alpha_1^m & \cdots & \alpha_k^m \end{array}\right], \qquad \begin{array}{l} n_i + 1 = \sum_{r=1}^{k} \alpha_r^i, \\ \dim_{\mathbb{C}} X = \sum_{i=1}^{m} n_i - k = N, \end{array} \qquad \alpha_r^i \in \mathbb{N}_+. \tag{1}$$

The Hodge numbers $h^{(p,q)}$ are topological invariants which count the dimensions of the Dolbeault cohomology groups, whose elements are complex (p, q)-forms.

We will investigate the CICY 3- and 4-folds. The numbers, matrix size, and statistics (written as $\langle\cdot\rangle = \text{average}_{\text{min}}^{\text{max}}$) of their Hodge numbers are:

- $N = 3$: 7890 CICYs with 15×18 matrices, $\langle h^{(1,1)}\rangle = 7.4_1^{19}$, $\langle h^{(2,1)}\rangle = 29_{15}^{101}$ [20, 21].
- $N = 4$: 921 497 CICYs with 16×20 matrices, $\langle h^{(1,1)}\rangle = 10_1^{24}$, $\langle h^{(2,1)}\rangle = 0.8_0^{33}$, $\langle h^{(3,1)}\rangle = 40_{20}^{426}$, $\langle h^{(2,2)}\rangle = 240_{204}^{1752}$ [22, 23].

3 Methodology

In this section, we present briefly the CICYMiner architecture and explain its main characteristics.

The paper [17] performed a complete data analysis for the 3-folds dataset, including feature engineering and selection. It was found that no derived feature helped in computing the Hodge numbers, and that neural networks outperform any other tested algorithm. As a consequence, we will focus on the latter, and review the architecture with the highest performance.

CICYMiner [18] is built from a series of Inception modules [16, 17], starting with a common trunk which splits in branches, such that it computes the different Hodge numbers at the same time given a configuration matrix $m \times k$. Inception modules are inspired by GoogleNet [24] and perform

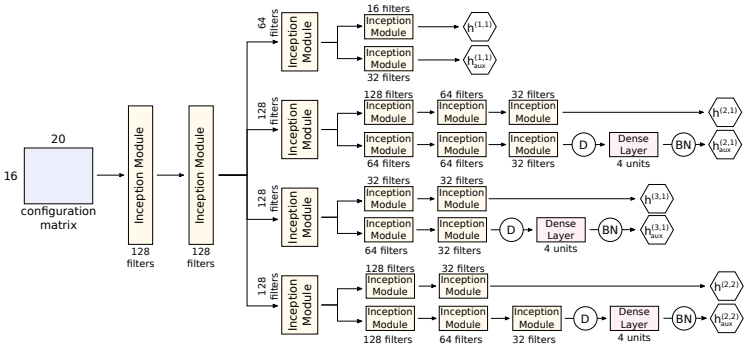


Figure 1: CICYMiner architecture, with dropout (D) with rate 0.2, and batch normalization (BN). The auxiliary branches replicate the output predictions and help to stabilize the learning process.

two parallel convolutions with $1d$ kernels $m \times 1$ and $1 \times k$, followed by concatenation and batch normalization. This structure is important 1) to put on an equal footing all the equations and projective spaces defining the configuration matrix (thanks to weight sharing), while also 2) taking into account the symmetries of the system. The ablation study performed in [16] displayed strikingly how both these ingredients are necessary to reach the highest accuracy. A neural network made of 3 Inception modules [16, 17] also achieved a near-perfect accuracy for the 3-folds $h^{(1,1)}$ while requiring much fewer parameters compared to earlier results [12, 13]. The architecture, inspired from [25], is shown in Figure 1 for the 4-folds; the network contains approximately 10^7 parameters. The same architecture can be used for the 3-folds which is achieved by removing the legs for $h^{(2,2)}$ and $h^{(3,1)}$ (3.3×10^6 parameters). Hyperparameter optimization is performed on the 4-folds dataset using a grid search over a reasonable portion of the hyperparameter space defined using insights from other architectures which used Bayesian or BOHB optimizations.

We preprocess the input data by simply rescaling the entries of the configuration matrices in the training set in the $[0, 1]$ range, but we don't rescale the labels. The computation is performed as a regression:[1] outputs are forced to be positive by adding a ReLU after each output layer, and predictions are rounded to the closest integer before computing the accuracy of the network. We train with the Huber loss with hyperparameter $\delta = 1.5$, and loss weights of 0.05, 0.3, 0.25 and 0.35 for $h^{(1,1)}$, $h^{(2,1)}$, $h^{(3,1)}$ and $h^{(2,2)}$, respectively, in the 4-folds case (determined using hyperparameter optimization as described above). In order to maintain a similar ratio, we use 0.17 and 0.83 for $h^{(1,1)}$ and $h^{(2,1)}$ for the CICY 3-folds. Performance of the network is assessed by computing the accuracy (agreement between the predicted and real integer values). Training has been performed on a single NVIDIA V100 GPU over a fixed amount of 300 epochs for CICY 4-folds, while we use 1500 epochs in the 3-folds case, due to limited cluster time. We use the Adam optimizer with an initial learning rate of 10^{-3} and a mini-batch size of 64 configuration matrices. The learning rate is reduced by a factor 0.3 after 75 epochs without improvement in the validation loss.

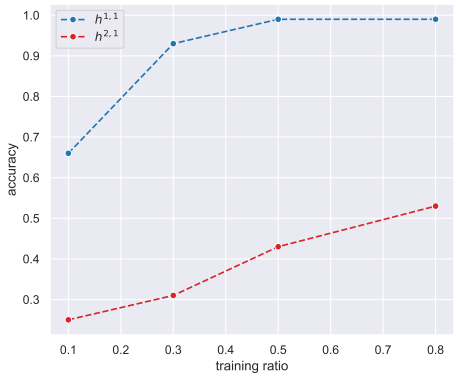
The code is available at: `https://github.com/thesfinox/ml-cicy-4folds`, `https://github.com/melsophos/cicy`.

4 Results

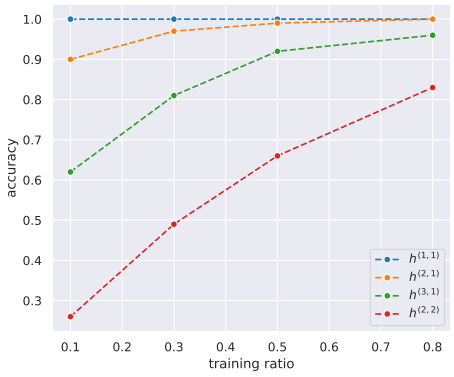
We provide three applications of the CICYMiner network: 1) Hodge numbers predictions, extrapolation after training only with 2) low and 3) high Hodge numbers. Except for the 4-folds predictions in 1), the results are new.

Predicting Hodge numbers We are interested in predicting the Hodge numbers, using the configuration matrix as input of the neural network. We will train with $x\%$ of the data selected by stratifying on $h^{(2,1)}$ in order to preserve the distribution of the samples, and varying x how the accuracy improves with the size of the training set. The validation set is chosen totally at random,

[1] Approaching the problem as a classification task does not make sense because it would assume an a priori knowledge of the value ranges, which is not desirable.



(a) 3-folds.



(b) 4-folds.

Figure 2: Accuracy for CICYMiner as a function of percentage of training data.

Table 1: Accuracy when training with an upper bound on $h^{(1,1)}$ or lower bound on $h^{(2,2)}$ (4-folds). As a reminder, extremal values for both Hodge numbers are $h^{(1,1)} \leq 24, h^{(2,2)} \geq 204$.

	ratio	$h^{(1,1)}$	$h^{(2,1)}$	$h^{(3,1)}$	$h^{(2,2)}$
$h^{(1,1)} \leq 5$	$2\,\%$	0.06	0.70	0.07	0.02
$h^{(1,1)} \leq 8$	$26\,\%$	0.53	0.83	0.27	0.11
$h^{(1,1)} \leq 10$	$59\,\%$	0.93	0.95	0.62	0.40
$h^{(2,2)} > 225$	$50\,\%$	1.00	0.88	0.39	0.04
$h^{(2,2)} > 250$	$27\,\%$	0.98	0.80	0.09	0.03
$h^{(2,2)} > 300$	$8\,\%$	0.95	0.72	0.05	0.03
$h^{(2,2)} > 400$	$1.6\,\%$	0.76	0.70	0.03	0.0

using $10\,\%$ of the samples. The remaining samples are included in the test set. The results for the 3- and 4-folds are given in Figures 2a and 2b.

For the 4-folds and $h^{(1,1)}$ of the 3-folds, the CICYMiner network is capable of learning accurately the discreteness of the Hodge numbers: for most of them, the regression metrics show values which indicate confidently integer numbers (MAE $\ll 0.50$ and MSE $\ll 0.25$). Note that the network is still underfitting the training set: longer training or different choices of the learning rate may be needed to investigate this aspect.

Extrapolation from low Hodge numbers We focus on the CICY 4-folds dataset. Following [14], we test the ability to predict the entire range of Hodge numbers when training only with samples whose $h^{(1,1)}$ is below a fixed value. Then, we test how well the network performs in predicting Hodge numbers outside the training range. The motivation is that, for other datasets, CYs with low $h^{(1,1)}$ are easier to understand, such that one can be interested in training for those instances and extrapolate the predictions. We reuse the same hyperparameters as before, but train CICYMiner on the reduced training set. Results are summarized in Table 1, where the ratio of the data refers to the size of the training set. As we can see, the performance increases quickly for the first two Hodge numbers, but remain lower than in the previous study for the last two.

Extrapolation from high Hodge numbers The same experiment can be run by imposing a lower bound on $h^{(2,2)}$ (largest number of outliers and largest interval of variation). As previously, no hyperparameter optimization is run in this case. Results are shown in Table 1. As in the previous case, good results on $h^{(1,1)}$ and $h^{(2,1)}$ can be recovered starting from approximately $50\,\%$ of the training samples, but $h^{(2,2)}$ performance stays low in any case. In this and previous cases, it is not clear why the network behaves this way.

5 Conclusion

This paper described the state-of-the-art in predicting CICY Hodge numbers with neural networks. This shows that machine learning techniques, and especially deep learning, are completely adapted to manipulate data in algebraic geometry. While the other topological quantities of the CICY are relatively easy to compute, it would still be interesting to explore if neural networks can predict them accurately. These different studies open the stage for attacking more difficult problems in algebraic geometry, such as studying CY built from the Kreuzer-Skarke polytopes [26, 27].

Computing accurately $h^{(2,1)}$ for the 3-folds is still an open problem. While the CICYMiner architecture performs slightly better than the pure Inception model from [16, 17], the drawback is a much slower training time and many more parameters. Moreover, while results are more precise for the 4-folds, it would be desirable to increase the accuracy of $h^{(2,2)}$. Work in progress explores if the graph representation of the data [1, 28, 29] can help.

Finally, the last step is extracting analytical formulas in order to interpret the neural network and improve our knowledge. The simplest approach is to perform symbolic regression on the neural network following [30, 31]. It can be expected that the result contains piecewise functions, given the structure of the analytic expressions found for line bundle cohomologies [32–36].

Broader impacts

Historically, codes used to compute properties of CY for string theory have not been made open source, which made the barrier to enter the field high. One goal of developing ML algorithms and make them open source is to help people get involved in the field.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] See Section 5.
   (c) Did you discuss any potential negative societal impacts of your work? [N/A]
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [N/A]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [N/A]
   (b) Did you include complete proofs of all theoretical results? [N/A]
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes]
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Sections 3 and 4.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [No] Because of computational cost.
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