Machine learning for complete intersection Calabi–Yau manifolds

Harold Erbin

Mit (Usa) & Cea-List (France)

string_data – 16th December 2020

In collaboration with:

- Riccardo Finotello (Università di Torino)

arXiv: 2007.13379, 2007.15706

Massachusetts Institute of Technology

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Outline: 1. Motivations

Motivations

Calabi–Yau 3-folds

Data analysis

Machine learning analysis

Conclusion

String phenomenology

Goal

Find "the" Standard Model from string theory

Method:

- type II / heterotic strings, M-theory, F-theory: $D = 10, 11, 12$
- vacuum choice (flux compactification):
  - typically Calabi–Yau (CY) 3- or 4-fold
  - fluxes and intersecting branes

  $\rightarrow$ reduction to $D = 4$
- check consistency (tadpole, susy...)
- read the $D = 4$ QFT (gauge group, spectrum...)

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No vacuum selection mechanism $\Rightarrow$ string landscape

Landscape mapping

String phenomenology:

- find consistent string models
- find generic/common features
- reproduce the Standard model

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Typical questions:

- understand manifolds
- find parameter distribution
- explore consistent vacua
- find good EFTs for low-energy limit

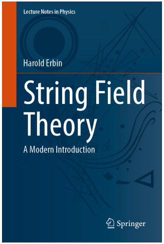
Landscape mapping

String phenomenology:

- find consistent string models
- find generic/common features
- reproduce the Standard model

Typical questions:

- understand manifolds
- find parameter distribution
- explore consistent vacua
- find good EFTs for low-energy limit
- (construct an explicit string field theory)



(to appear in 02/2021)

Number of geometries

Calabi–Yau (CY) manifolds

- CICY (complete intersection in products of projective spaces): 7890 (3-fold), 921,497 (4-fold)
- Kreuzer–Skarke (reflexive polyhedra): 473,800,776 ($d = 4$)

String models and flux vacua

- type IIA/IIB models: 10^{500}
- F-Theory: 10^{755} to 10^{3000} (geometries), $10^{272,000}$ (flux vacua)

[Lerche-Lüst-Schellekens '89; hep-th/0303194, Douglas; hep-th/0307049, Ashok-Douglas; hep-th/0409207, Douglas; 1511.03209, Taylor-Wang; 1706.02299, Halverson-Long-Sun; 1710.11235, Taylor-Wang; 1810.00444, Constantin-He-Lukas]

Challenges

- huge number of possibilities
- difficult math problems (NP-complete, NP-hard, undecidable) [hep-th/0602072, Denef-Douglas; 1009.5386, Cvetič-García-Etxebarria-Halverson; 1809.08279, Halverson-Ruehle; 1911.07835, Halverson-Plesser-Ruehle-Tian]
- methods from algebraic topology: cumbersome, rarely closed-form formulas

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- methods from algebraic topology: cumbersome, rarely closed-form formulas

$\rightarrow$ use machine learning

Selected references: 1404.7359, Abel-Rizos; 1706.02714, He; 1706.03346, Krefl-Song; 1706.07024, Ruehle; 1707.00655, Carifio-Halverson-Krioukov-Nelson; 1804.07296, Wang-Zang; 1806.03121, Bull-He-Jejjala-Mishra; most talks at this conference. . .

Review: Ruehle '20

Plan

Goal

Compute Hodge numbers for CICY 3-folds

1. complete intersection Calabi–Yau (CICY)
2. data analysis for CICY
3. machine learning for CICY

References: [HE-Finotello, 2007.13379, 2007.15706]

Outline: 2. Calabi–Yau 3-folds

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Calabi–Yau 3-folds

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Calabi-Yau

Complete intersection Calabi–Yau (CICY) 3-fold:

- CY: complex manifold with vanishing first Chern class
- complete intersection: non-degenerate hypersurface in products of m projective spaces
- hypersurface = solution to system of k homogeneous polynomial equations

Calabi-Yau

Complete intersection Calabi–Yau (CICY) 3-fold:

- CY: complex manifold with vanishing first Chern class
- complete intersection: non-degenerate hypersurface in products of m projective spaces
- hypersurface = solution to system of k homogeneous polynomial equations
- described by configuration matrix $m \times k$

$$X = \left[\begin{array}{c|ccc} \mathbb{P}^{n_1} & a_1^1 & \cdots & a_k^1 \\ \vdots & \vdots & \ddots & \vdots \\ \mathbb{P}^{n_m} & a_1^m & \cdots & a_k^m \end{array} \right], \qquad a_\alpha^r \in \mathbb{N}$$

$$\dim_{\mathbb{C}} X = \sum_{r=1}^{m} n_r - k = 3, \qquad n_r + 1 = \sum_{\alpha=1}^{k} a_\alpha^r$$

- a_α^r power of coordinates on $\mathbb{P}^{n_r}$ in αth equation

Configuration matrix

Examples

- quintic ($a = 0, \ldots, 4$)

$$\left[\begin{array}{c|c} \mathbb{P}^4_x & 5 \end{array}\right] \implies \sum_a (X^a)^5 = 0$$

- 2 projective spaces, 3 equations ($a, \alpha = 0, \ldots, 3$)

$$\left[\begin{array}{c|ccc} \mathbb{P}^3_x & 3 & 0 & 1 \\ \mathbb{P}^3_y & 0 & 3 & 1 \end{array}\right] \implies \begin{cases} f_{abc}\, X^a X^b X^c = 0 \\ g_{\alpha\beta\gamma}\, Y^\alpha Y^\beta Y^\gamma = 0 \\ h_{a\alpha}\, X^a Y^\alpha = 0 \end{cases}$$

Configuration matrix

Examples

- quintic ($a = 0, \dots, 4$)

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Classification

- invariances $\to$ topologically equivalent manifolds, redundancy
  - permutation of lines and columns
  - identities between subspaces
- but:
  - constraints $\Rightarrow$ bound on matrix size
  - often $\exists$ "favorable" configuration (simplest description)

Topology

Why topology?

- no metric known for compact CY (cannot perform KK reduction explicitly) [but see: Sven's talk, 2012.04656, Anderson-Gerdes-Gray-Krippendorf-Raghuram-Ruehle]
- topological info. $\rightarrow$ properties of 4d low-energy effective action (number of fields, representations, gauge symmetry. . .)

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Topological properties

- Hodge numbers $h^{p,q}$ (number of harmonic (p,q)-forms) here: $h^{1,1}$, $h^{2,1}$
- Euler number $\chi = 2(h^{1,1} - h^{2,1})$
- Chern classes
- triple intersection numbers
- line bundle cohomologies

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Datasets

CICY have been classified

- 7890 configurations (but $\exists$ redundancies)
- number of product spaces: 22
- $h^{1,1} \in [0, 19]$, $h^{2,1} \in [0, 101]$
- 266 combinations $(h^{1,1}, h^{2,1})$
- $a^r_\alpha \in [0, 5]$

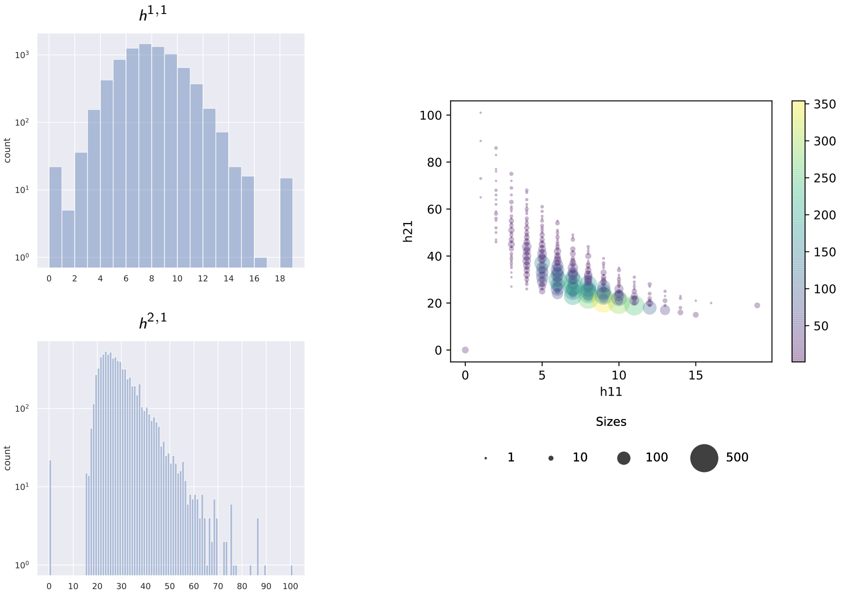
Original data [Candelas-Dale-Lutken-Schimmrigk '88; Green-Hübsch-Lutken '89]:

- maximal matrix size: 12×15
- number of favorable matrices: 4874

Favorable data [1708.07907, Anderson-Gao-Gray-Lee]:

- maximal matrix size: 15×18
- number of favorable matrices: 7820

Data


$h^{1,1}$
count
10^0
10^1
10^2
10^3
0 2 4 6 8 10 12 14 16 18
$h^{2,1}$
count
10^0
10^1
10^2
0 10 20 30 40 50 60 70 80 90 100
h21
0 20 40 60 80 100
h11
0 5 10 15
50 100 150 200 250 300 350
Sizes
1 10 100 500

Goal and methodology

Philosophy

Start with the dataset, derive everything from configuration matrix using data analysis and machine learning only.

Current goal

Input: configuration matrix $\longrightarrow$ Outputs: $h^{1,1}$, $h^{2,1}$

Motivations:

1. CICY: well studied, all topological quantities known
   $\rightarrow$ use as a sandbox
2. improve over [1706.02714, He; 1806.03121, Bull-He-Jejjala-Mishra]
3. $h^{2,1}$ and favorable dataset not studied before

References: [HE-Finotello, 2007.13379, 2007.15706]

Outline: 3. Data analysis

Motivations

Calabi–Yau 3-folds

Data analysis

Machine learning analysis

Conclusion

Feature engineering

Process of creating new features derived from the raw input data.

Some examples:

- number of projective spaces (rows), $m = \texttt{num\_cp}$
- number of equations (columns), k
- number of $\mathbb{C}P^1$
- number of $\mathbb{C}P^2$
- number of $\mathbb{C}P^n$ with $n \neq 1$
- Frobenius norm of the matrix
- list of the projective space dimensions and statistics thereof
- dimensions of ambient space cohomology $\left\{ \prod_{r=1}^{m} \binom{n_r + a_\alpha^r}{n_r} \right\}$
- K-nearest neighbour (KNN) clustering (with $K = 2, \dots, 5$)

Feature selection

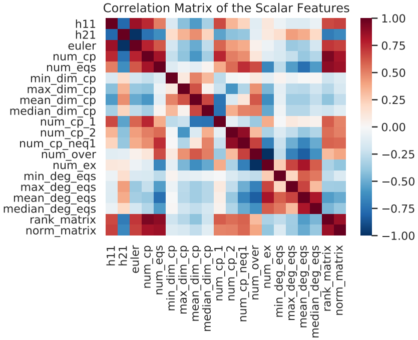
Select the most important features to draw attention of the ML algorithm to salient features in order to ease the learning.

Discovery methods:

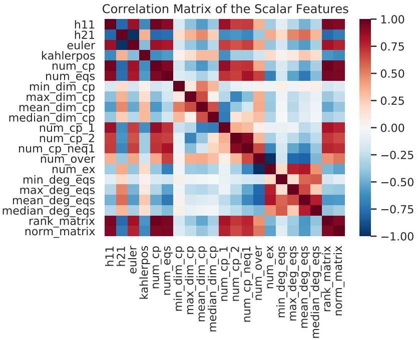
- correlation matrix
- importance from random forests
- scatter plots
- trial and error
- etc.

Correlation matrix

Original



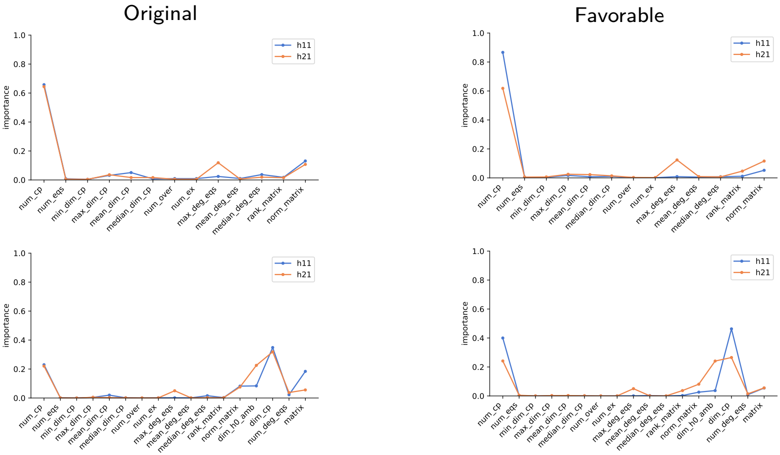
Favorable



Feature importance from random forests

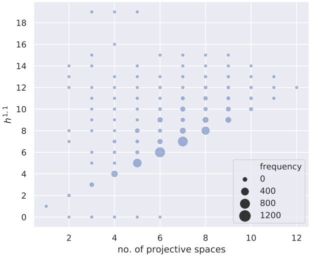
Random forest

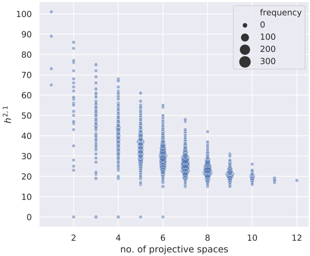
Large number of decision trees trained on different subsets. The most relevant features appear at the top of the trees.



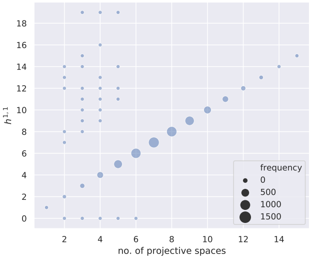
Scatter plots

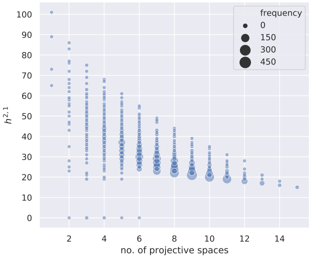
Original





Favorable





Outline: 4. Machine learning analysis

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Calabi–Yau 3-folds

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Strategy

Questions:

- classification or regression?
- feature engineering?
- data diminution: remove outliers (39 matrices, 0.49%)?
- data augmentation: generate more inputs using invariances?
- single- or multi-tasking?

Strategy

Questions:

- classification or regression?
  - classification: assume knowledge of boundaries
    (in practice, performs less well) [thanks to Robin Schneider]
  - regression: better for generalization
    different scales $\rightarrow$ normalize data $\approx$ use continuous variable
    (in practice, not needed)
- feature engineering?
  $\rightarrow$ helps only for non-neural network algorithms
- data diminution: remove outliers (39 matrices, 0.49%)?
  $\rightarrow$ remove outliers from training set
- data augmentation: generate more inputs using invariances?
  $\rightarrow$ adding row/column permutations decreases performance
- single- or multi-tasking?
  $\rightarrow$ multi-tasking slightly decreases performance

Setup

Algorithms:

- linear regression
- linear-kernel SVM
- Gaussian-kernel SVM
- random forests
- gradient boosted trees
- neural networks

Evaluation:

- train/validation/test splits: 80/10/10 and 30/10/60
- optimization using MSE
- final evaluation with accuracy after rounding

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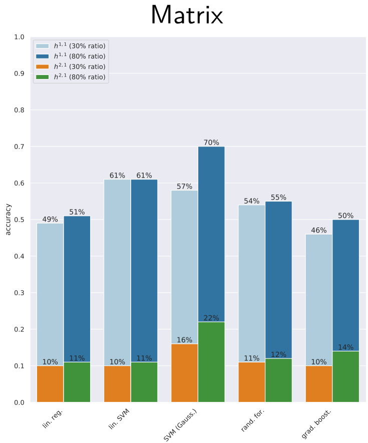
Preliminary observations:

- all algo. give 99 % for $h^{1,1}$ in favorable dataset with engineered features (without engineering: 90-95 % for standard algo.)
- $h^{2,1}$ equivalently hard in both sets

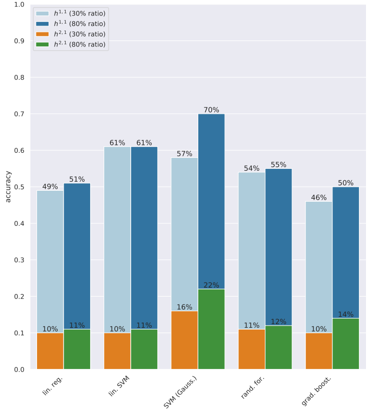
→ focus on original dataset

Results: simple algorithms

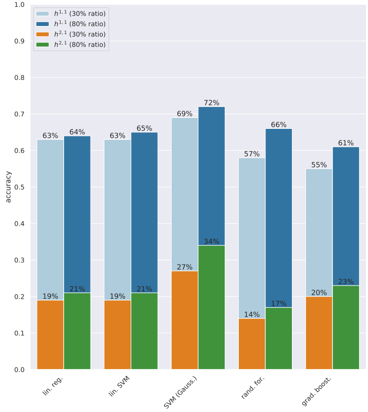


Results: simple algorithms

Matrix



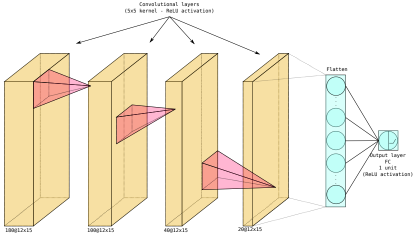
Matrix + engineered features



Convolutional neural network

Architecture and training:

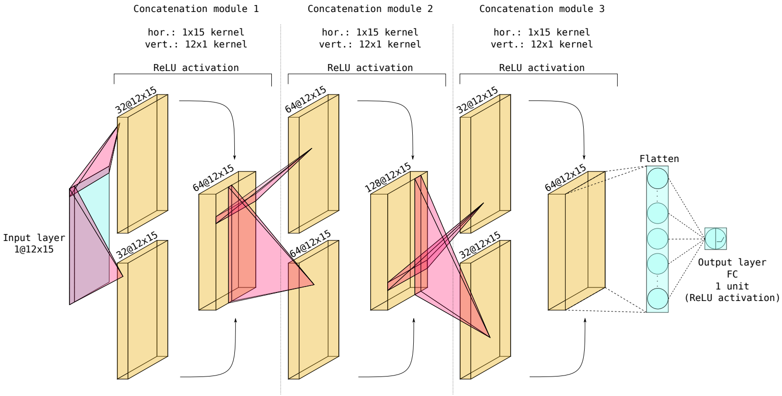
- 4 convolutional layers, kernel 5×5:
  - $h^{1,1}$: 180, 100, 40, 20 units
  - $h^{2,1}$: 250, 150, 100, 50 units
- after each layer: batch normalization, ReLU activation
- at the end: dropout $p = 0.2$, ReLU (enforces positive output)
- early stopping & learning rate decay primordial to increase accuracy beyond 90 %
- number of parameters:
  - $h^{1,1}$: 5.8×10^5
  - $h^{2,1}$: 2.1×10^6



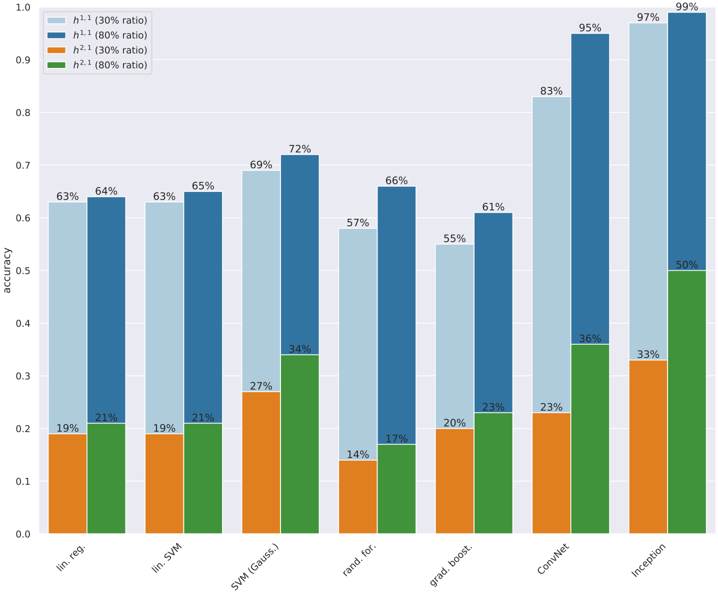
Inception neural network (1)

- designed by Google for computer vision
  $\rightarrow$ breakthrough in image classification
  [Szegedy et al., 1409.4842, 1512.00567, 1602.07261]
- sequence of inception modules
  $\rightarrow$ parallel convolutions with kernels of $\neq$ sizes
- learns different combinations of features at different scales
- 3 inception modules, kernels $(12 \times 1, 1 \times 15)$:
  - $h^{1,1}$: 32, 64, 32 units
  - $h^{2,1}$: 128, 128, 64 units
- numbers of parameters:
  - $h^{1,1}$: 2.3×10^5, $7\times$ less than [1806.03121, Bull-He-Jejjala-Mishra]
  - $h^{2,1}$: 1.1×10^6

Inception neural network (2)

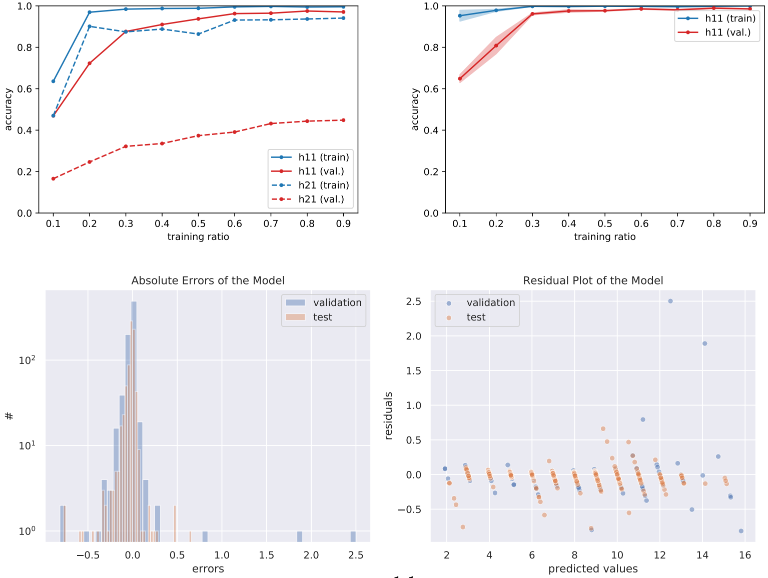


Results



$h^{1,1}$ (30% ratio)
$h^{1,1}$ (80% ratio)
$h^{2,1}$ (30% ratio)
$h^{2,1}$ (80% ratio)
accuracy
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
63% 64% 19% 21%
63% 65% 19% 21%
69% 72% 27% 34%
57% 66% 14% 17%
55% 61% 20% 23%
83% 95% 23% 36%
97% 99% 33% 50%
lin. reg.
lin. SVM
SVM (Gauss.)
rand. for.
grad. boost.
ConvNet
Inception

Learning curve and errors



$h^{1,1}$

Why do convolutional / Inception networks work?

- matrix not invariant under rotation/translation, but conv. layers encodes only translation equivariance (pooling and data augmentation induces invariance under rotation and invariance) [Goodfellow-Bengio-Courville '16]
- $1d$ parallel kernels of maximal sizes: look at all $\mathbb{C}P^n$/equations for each equation/$\mathbb{C}P^n$ at the same time
- weight sharing (convolution): same operations for each $\mathbb{C}P^n$ and equation since they all enter symmetrically (expected for a math formula)

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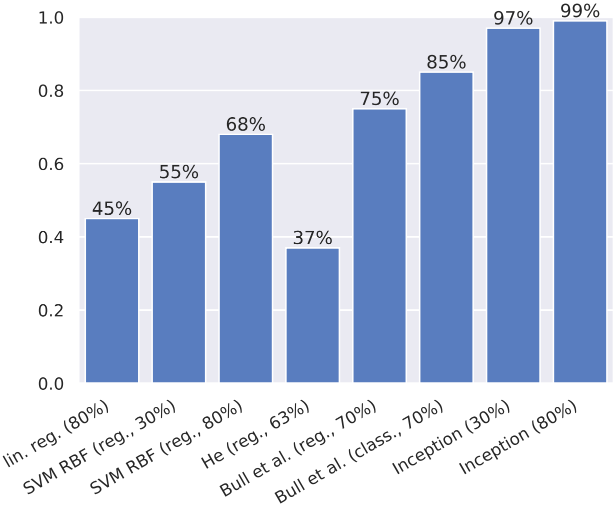
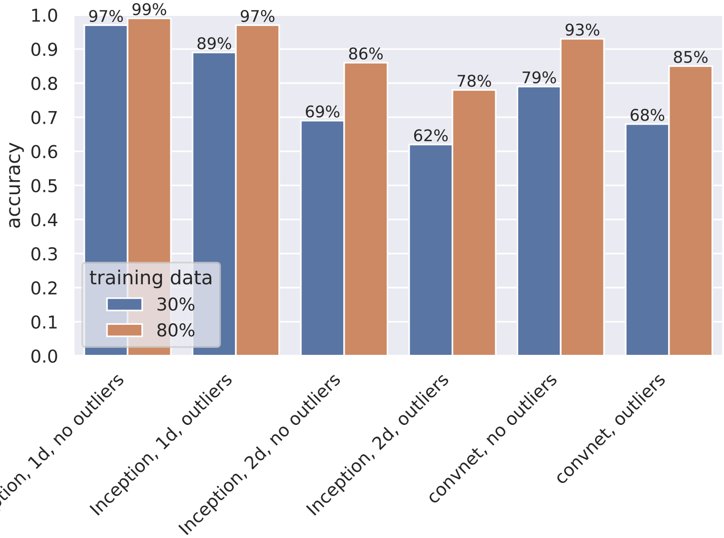
Next: focus on $h^{1,1}$

Comparing architectures



He: 1706.02714; Bull et al.: 1806.03121; percentage: training data

Ablation study



Outline: 5. Conclusion

Motivations

Calabi–Yau 3-folds

Data analysis

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Conclusion

Results:

- rigorous data analysis for the computation of Hodge numbers for CICY 3-folds
- almost perfect accuracy for predicting $h^{1,1}$
- accuracy of 50 % for $h^{2,1}$

Outlook:

- improve accuracy for $h^{2,1}$
    1. use engineered data as auxiliary inputs to the Inception network
    2. use another data representation (e.g. graph [Hübsch '92; 2003.13679, Krippendorf-Syvaeri], learned from variational autoencoder. . .)
- dissect neural network data to understand what it learns
- extension to CICY 4-folds