Data Augmentation for Mathematical Objects

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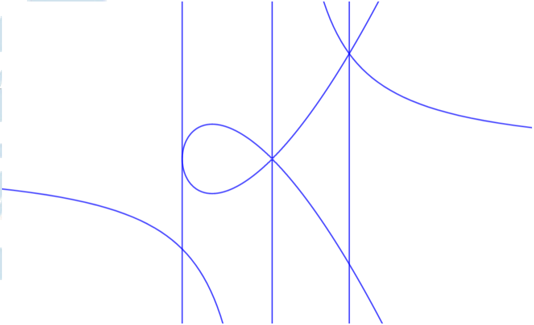
[2] Supported by UKRI EPSRC Grant EP/T015748/1, "*Pushing Back the Doubly-Exponential Wall of Cylindrical Algebraic Decomposition*" (DEWCAD).

Outline

Introduction to CAD

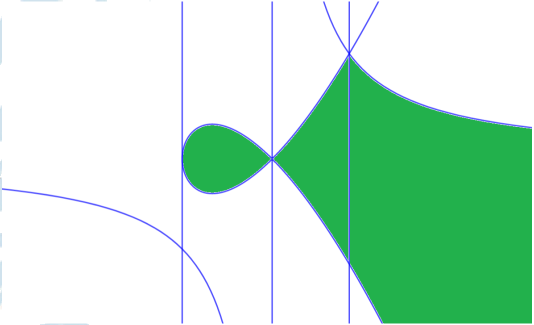
Given a set of polynomials

$$S = \{xy - 1, y^2 - x^3 - x^2\}$$



Introduction to CAD

We may want to know where $xy - 1 < 0$ and $y^2 - x^3 - x^2 < 0$.



The only implemented general-purpose algorithm that guarantees to answer such questions is CAD, firstly proposed in [Collins(1975)].

Pros and cons

- Useful in biology [Röst and Sadeghimanesh(2021)], robotics, proving mathematical inequalities [Gerhold and Kauers(2006)], ...
- Davenport proved in [Davenport and Heintz(1988)] that CAD has doubly exponential complexity with respect to the number of variables.
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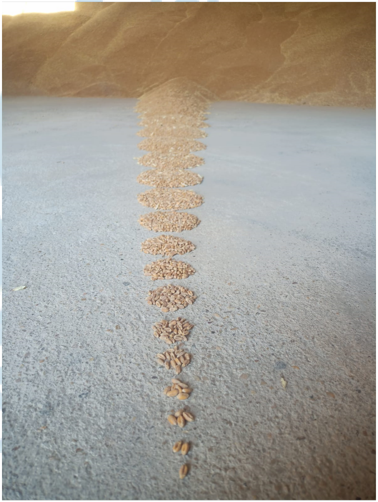
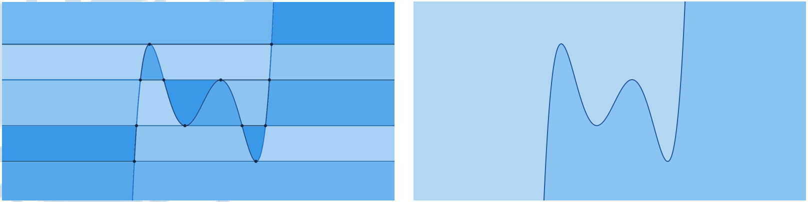
A little story



Variable ordering

Brown and Davenport [Brown and Davenport(2007)]:
Depending on variable ordering, **constant** or **doubly exponential** complexity.



Variable ordering

Choosing the right variable ordering:

- Humans have proposed heuristics for this task: e.g. `sotd` [Dolzmann et al.(2004)Dolzmann, Seidl, and Sturm]; `brown` [Brown(2004)] and `mods` [?]
- Machine Learning models have been trained for this purpose e.g. [?] and [Chen et al.(2020)Chen, Zhu, and Chi]

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.

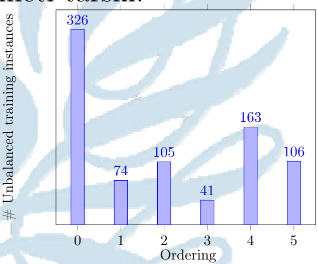
Training models

In [England and Florescu(2019)] multiple models were trained.

Name	**Accuracy**
`brown`	0.553
`gmods`	0.563
KNN	0.555
DT	0.573
SVC	0.549
MLP	0.569

A glance at the dataset

Extracted from QFNRA problems of the SMT-LIB; mainly meti-tarski.



Changing a label

If the optimal ordering for $\{x_1x_2^3 + x_2^2x_3^2, x_2x_3^3 - 1\}$ is 0.

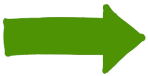
The six possible variable orderings

Ordering Name	**Ordering**
Ordering 0	$x_1 \succ x_2 \succ x_3$
Ordering 1	$x_1 \succ x_3 \succ x_2$
Ordering 2	$x_2 \succ x_1 \succ x_3$
Ordering 3	$x_2 \succ x_3 \succ x_1$
Ordering 4	$x_3 \succ x_1 \succ x_2$
Ordering 5	$x_3 \succ x_2 \succ x_1$

By simply swapping the names of x_1 and x_2 we get an instance with optimal ordering 2: $\{x_2x_1^3 + x_1^2x_3^2, x_1x_3^3 - 1\}$.

Analogy with arrows for computer vision

Normally, we cannot change the labels on demand but our problem is symmetric.



Arrow pointing right

Arrow pointing up

Analogy with arrows for computer vision

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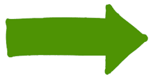
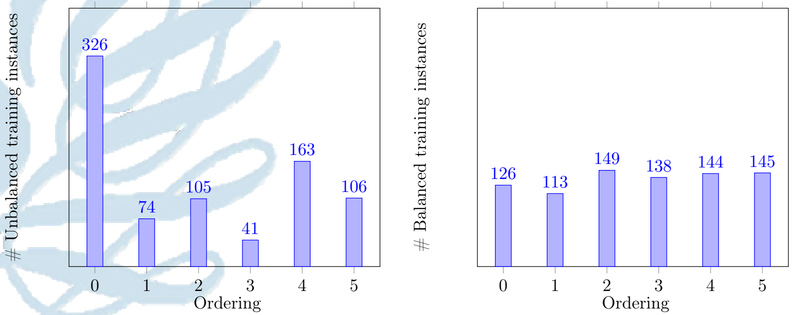


Arrow pointing right

Arrow pointing down

Balancing the dataset

By randomly permuting variables in an instances we can balance our datasets.



Problems caused by unbalancedness

Models trained on unbalanced data do not perform well on balanced data.

Testing dataset	Unbalanced	Balanced
KNN-Unbalanced	0.51	0.21
DT-Unbalanced	0.53	0.31
SVC-Unbalanced	0.48	0.23
RF-Unbalanced	**0.58**	**0.35**
MLP-Unbalanced	0.51	0.32

Accuracy of models trained on the unbalanced dataset, when tested on the different testing datasets.

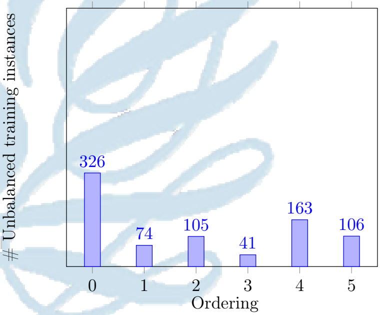
Balancing solves this issue

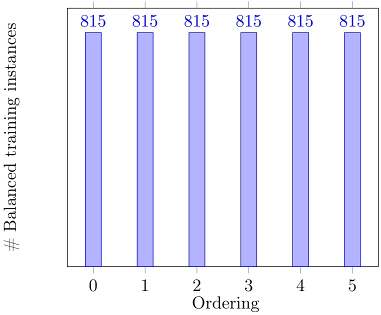
Testing dataset	Unbalanced	Balanced
KNN-Balanced	0.41	0.36
DT-Balanced	0.43	0.45
SVC-Balanced	0.25	0.3
RF-Balanced	**0.49**	**0.52**
MLP-Balanced	0.45	0.43

Accuracy of models trained on the balanced dataset, when tested on the different testing datasets.

Augmenting the dataset

Including all possible permutations we can augmentate the dataset.



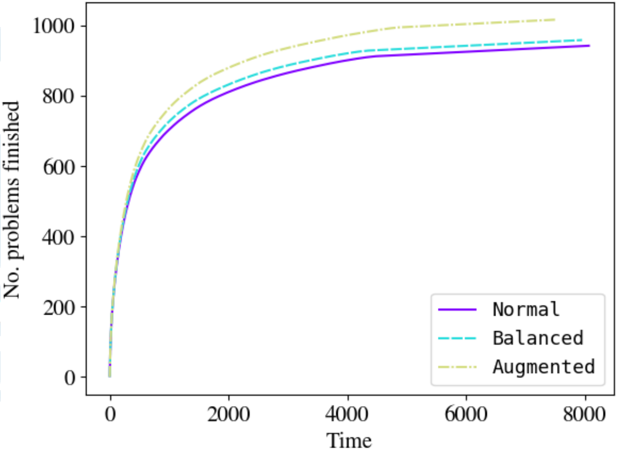


Augmenting boosts the results

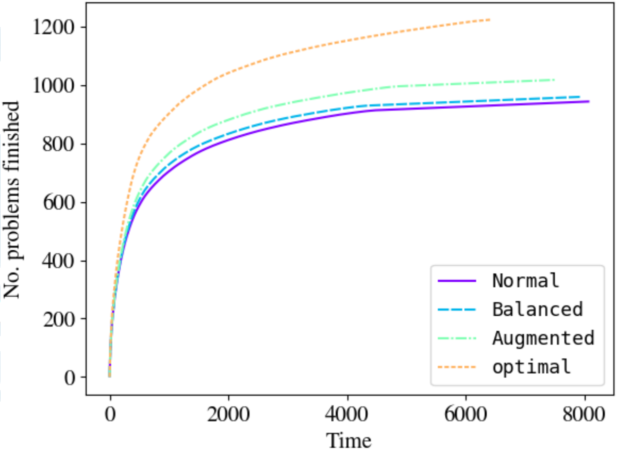
Testing dataset	Unbalanced	Balanced
KNN-Augmented	0.54	0.55
DT-Augmented	0.54	0.55
SVC-Augmented	0.46	0.48
RF-Augmented	**0.62**	**0.63**
MLP-Augmented	0.48	0.5

Accuracy of models trained on the augmented dataset, when tested on the different testing datasets.

Survival plot SVC



Survival plot SVC



Comparing accuracies

Training dataset	Normal	Balanced	Augmented
KNN	0.3	0.42	**0.55**
DT	0.35	0.43	**0.54**
MLP	0.35	0.45	**0.47**
SVC	0.23	0.29	**0.48**
RF	0.46	0.53	**0.61**

Accuracy of models on the balanced testing dataset, having been trained on the different training datasets.

Comparing timings

Training dataset	Normal	Balanced	Augmented
KNN	21 603	20 927	18 850
DT	20 352	17 299	17 404
SVC	25 004	23 913	19 980
RF	19 909	17 391	16 301
MLP	21 977	20 210	18 509

Accuracy of models on the balanced testing dataset, having been trained on the different training datasets.

Comparison with [Hester et al.(2023)Hester, Hitaj, Passmore, Owre, Shankar

- Very similar results.
- I removed loads of repeated examples (around 8000 vs around 1000).
- I used some more features.
- I still have to check if those two make any difference.

Future work

- Extra augmentation methods.
- Using regression instead of classification.
- Using reinforcement learning (pick one variable at a time).
- Encode sets of polynomials as graph and using Graph NN.

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Comparing with regression

Classification	
Name	**Time**
KNN	18 850
DT	17 404
SVC	19 980
RF	16 301
MLP	18 509

Regression	
Name	**Time**
DTR	17 206
SVR	26 100
RFR	11 391
KNNR	15 362
MLPR	25 219

Timings for different paradigms

Lesson to take from this talk

Representations of mathematical objects often have symmetries and those can be exploited to augmentate the number of representations that we have of a given object.
Very rarely we can give a mathematical object to a machine learning model (variable length), and augmentation is a tool to give as many views of the same object as possible.

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Apendix