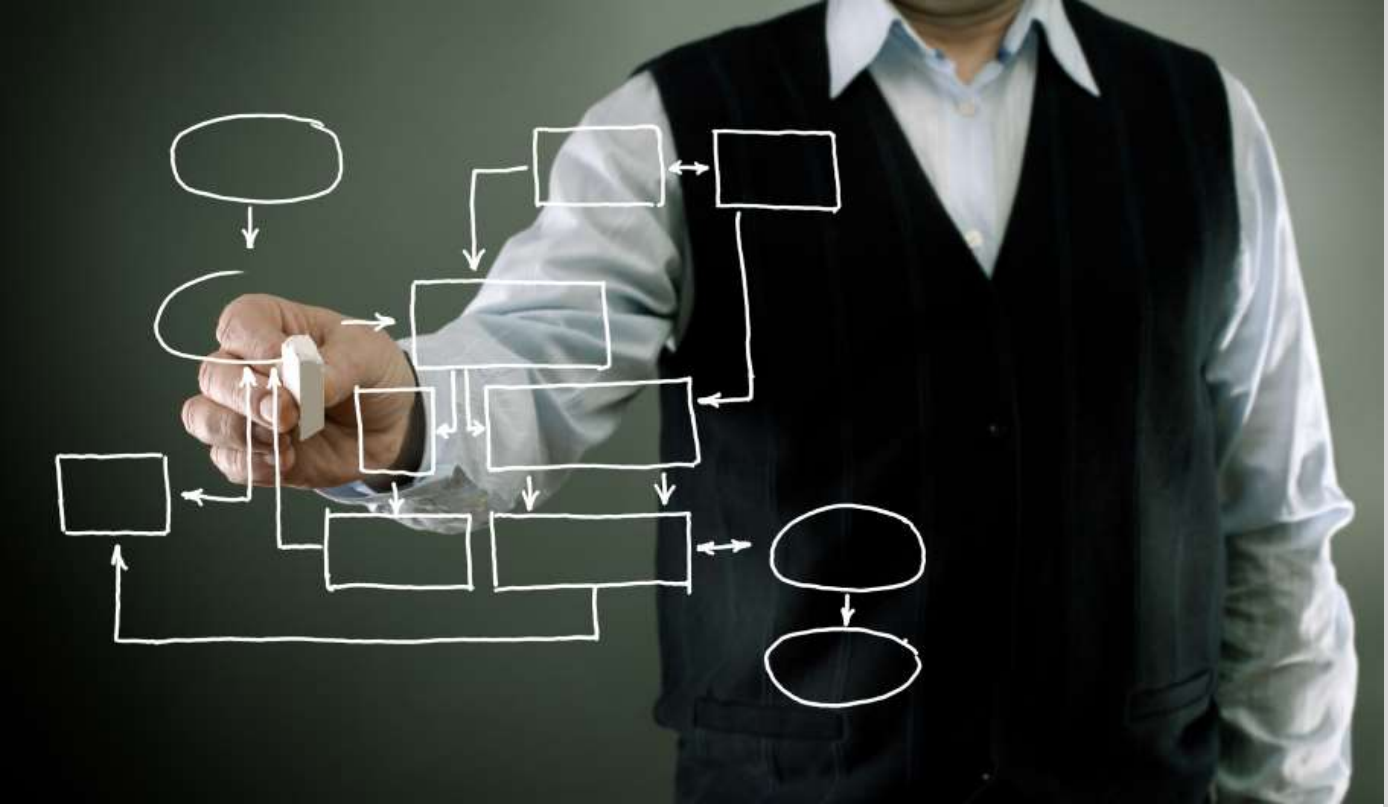

Data Aggregation for Reducing Training Data in Symbolic Regression

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SymReg
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EuroCAST 2019

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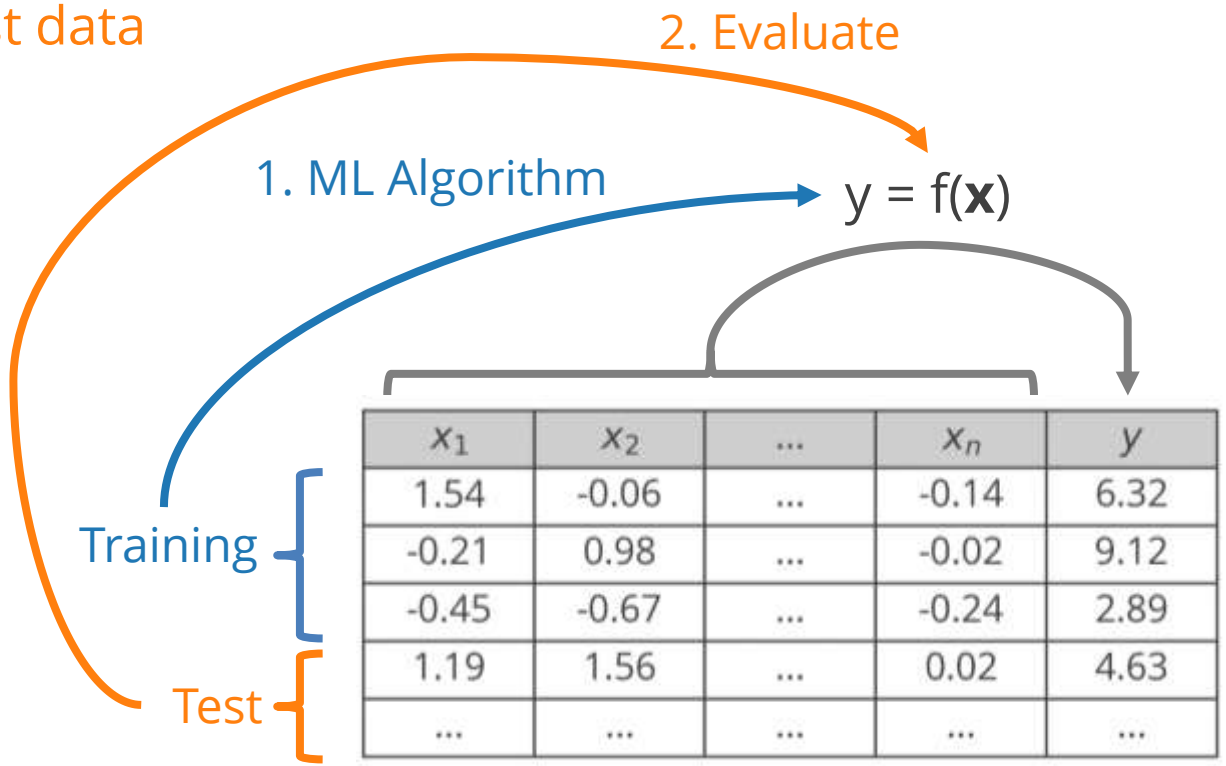
Supervised Machine Learning

1. Find model with minimal error on training data
2. Check that model works with unseen test data

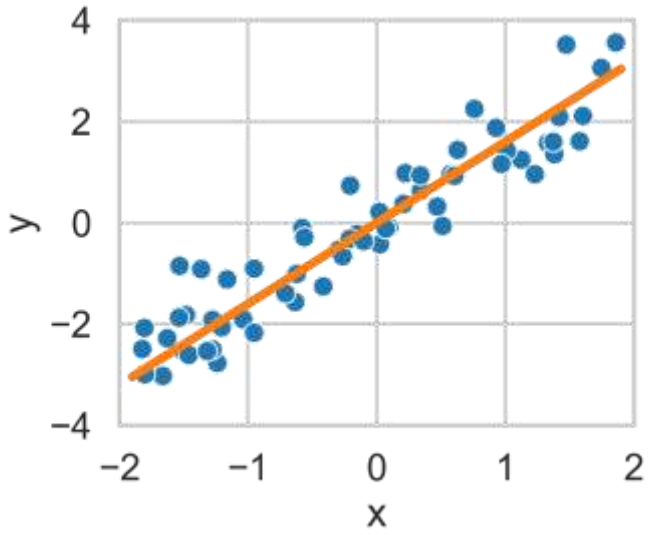


x_1	x_2	...	x_n	y
1.54	-0.06	...	-0.14	6.32
-0.21	0.98	...	-0.02	9.12
-0.45	-0.67	...	-0.24	2.89
1.19	1.56	...	0.02	4.63
...	...	...	...	...

Regression Algorithms

Linear Regression

- Find linear relations in data



Symbolic Regression

- Find mathematical formulas of any structure
- Search with genetic programming with strict offspring selection[1]
- Optimize constants with gradient descent

Random Forest Regression

- Build many decision trees with differently sampled training data

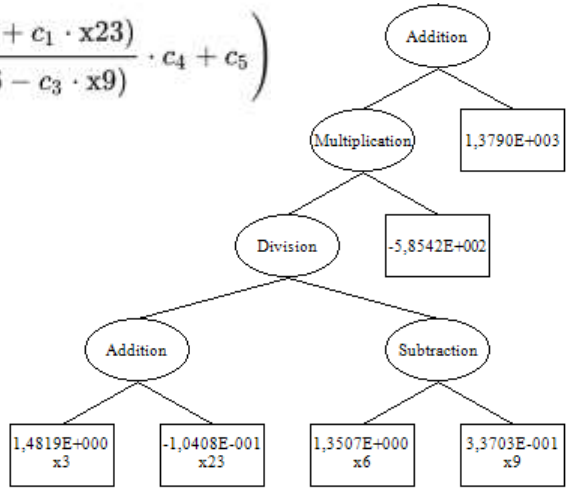
1) Affenzeller, M., Wagner, S., Winkler, S., & Beham, A. (2009). *Genetic Algorithms and Genetic Programming: Modern Concepts and Practical Applications*. Chapman and Hall/CRC.

Regression Algorithms

- Linear Regression
  - Find linear relations in data

- **Symbolic Regression**
  - Find mathematical formulas of any structure
  - Search with genetic programming with strict offspring selection[1]
  - Optimize constants with gradient descent

$$e = \left(\frac{(c_0 \cdot \mathrm{x3} + c_1 \cdot \mathrm{x23})}{(c_2 \cdot \mathrm{x6} - c_3 \cdot \mathrm{x9})} \cdot c_4 + c_5 \right)$$



- Random Forest Regression
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Regression Algorithms

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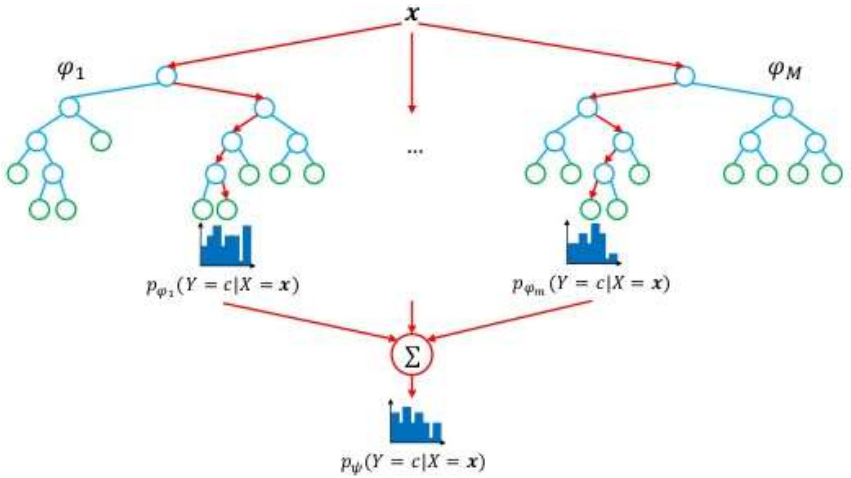
Image: Ilan Reinstein, KDnuggets™, www.kdnuggets.com/2017/10/random-forests-explained.html

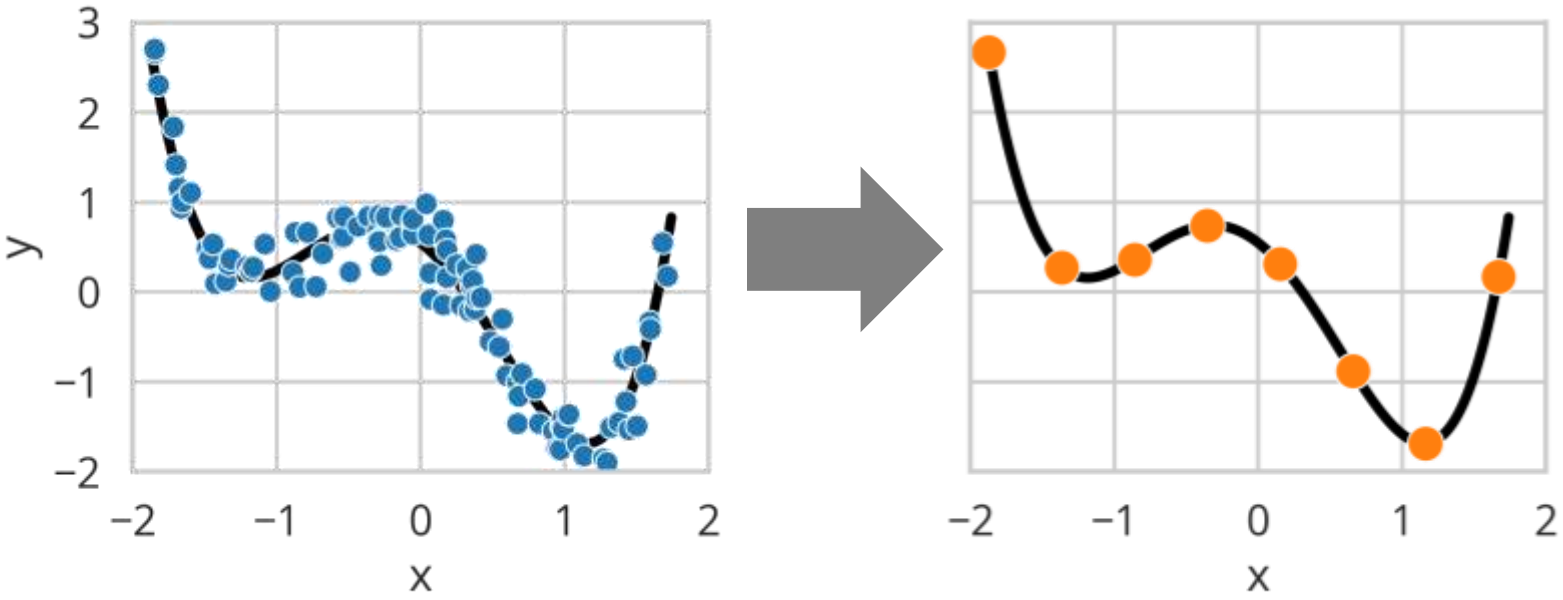


1) Affenzeller, M., Wagner, S., Winkler, S., & Beham, A. (2009). *Genetic Algorithms and Genetic Programming: Modern Concepts and Practical Applications*. Chapman and Hall/CRC.

Make Big Data small again!

GP with Big Data is impractical → Problem: Evaluation

Can we reduce training data with without loss in accuracy?

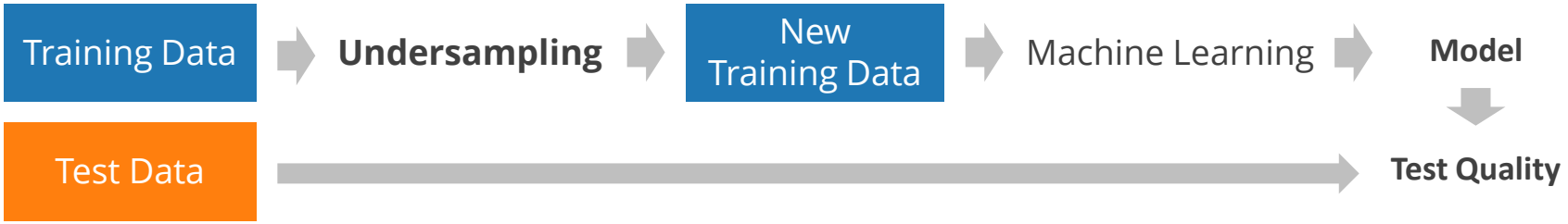


Idea

Kugler et al.[1] suggest data clustering

→ Cancel out noise

→ Remove inconsistencies



Used undersampling methods:

- Random sampling
- K-means clustering
- Data binning

1) Kugler, C., Hochrein, T., Dietl, K., Heidemeyer, P., Bastian, M.: *Softsensoren in der Kunststoffverarbeitung: Qualitätssicherung für die Compoundierung und Extrusion*. SKZ - Forschung und Entwicklung. Shaker Verlag GmbH (2015)

K-Means Clustering

Finds *K* centroids, so that the total (Euclidean) distance of all points to their closest centroid becomes minimal.

- → Stochastic
- → Scaling of variables
- → Mini-Batch K-Means[1]

  Much faster with similar accuracy[1]

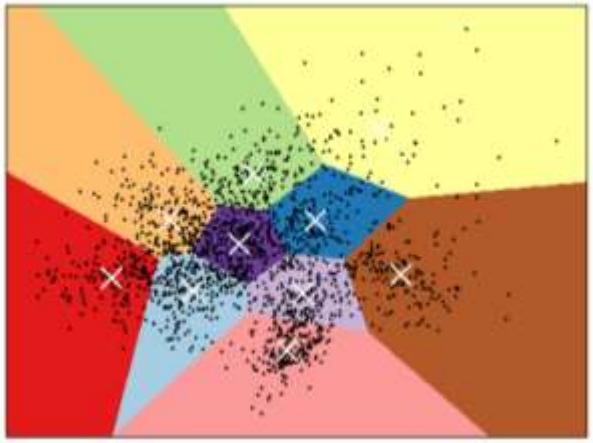


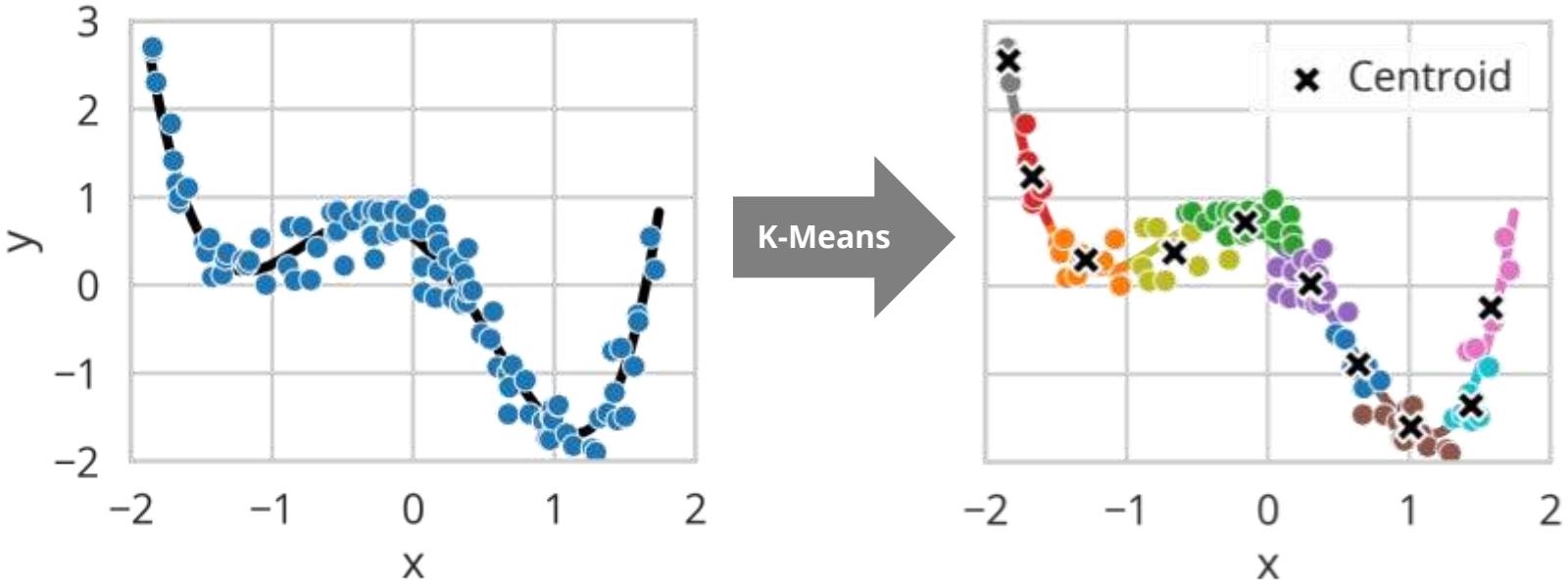
Image: Scikit-learn: *Machine Learning in Python*, Pedregosa et al., JMLR 12 pp. 2825-2830, 2011

1) Sculley, D. (2010, April). *Web-Scale K-Means Clustering*. In Proceedings of the 19th international conference on World wide web (pp. 1177-1178). ACM.

K-Means Clustering

Result of K-Means are *K* centroids

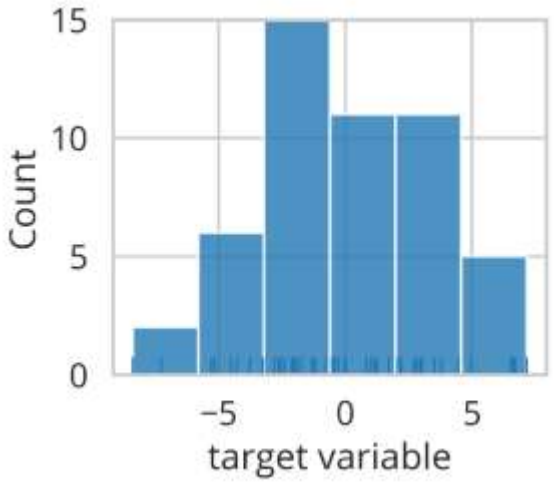
→ Use these centroids as training data!



Data Binning

1. Group the data along the target variable into bins of fixed width (similar to a histogram).
2. Use the average of each variable per bin as representative.
3. Use these representatives as training data.

→ Deterministic
→ Imposes n:1 mapping of features to target variable
→ Should cancel out inconsistencies in process states



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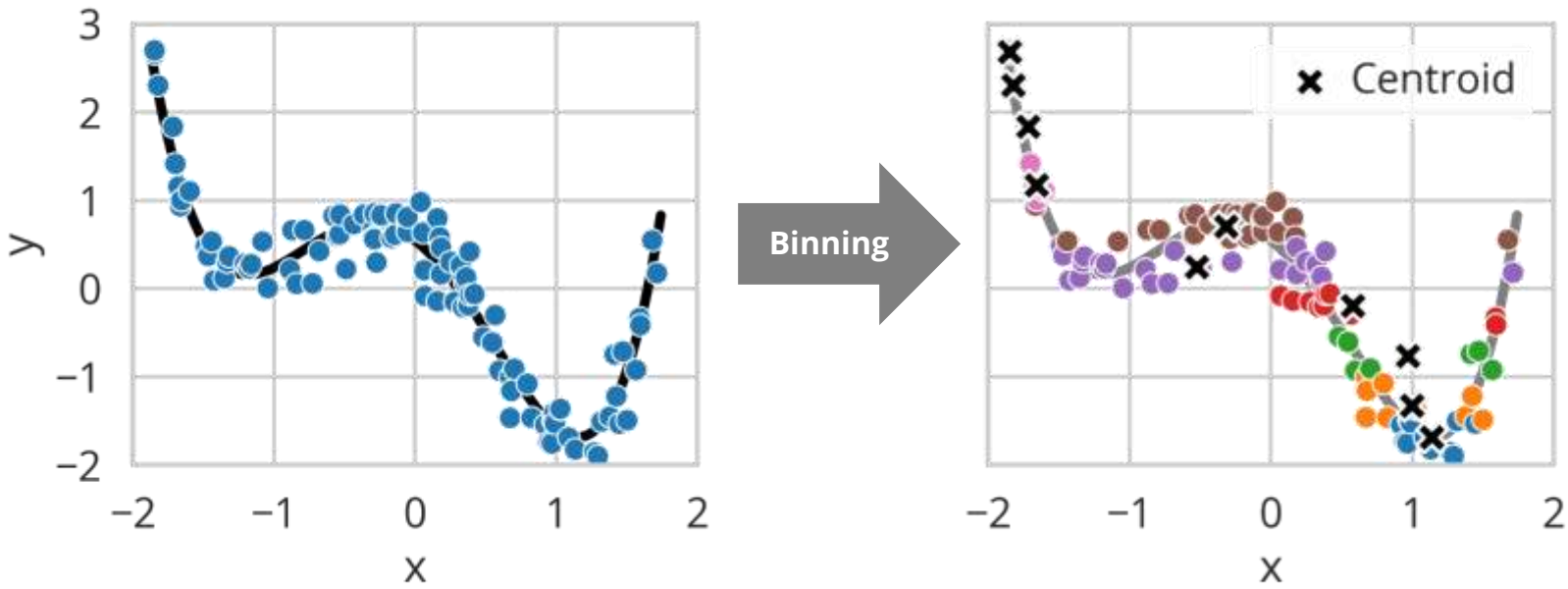
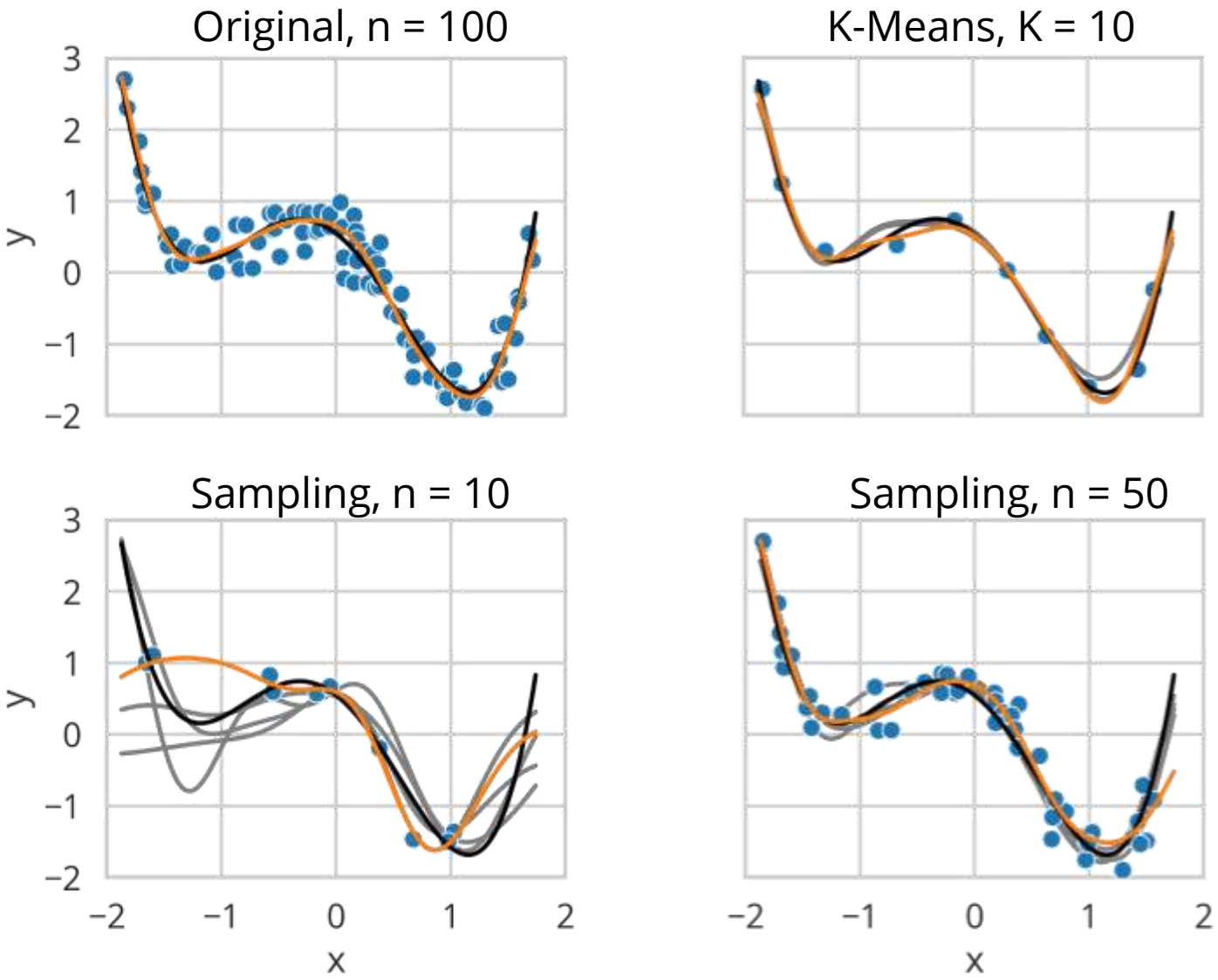
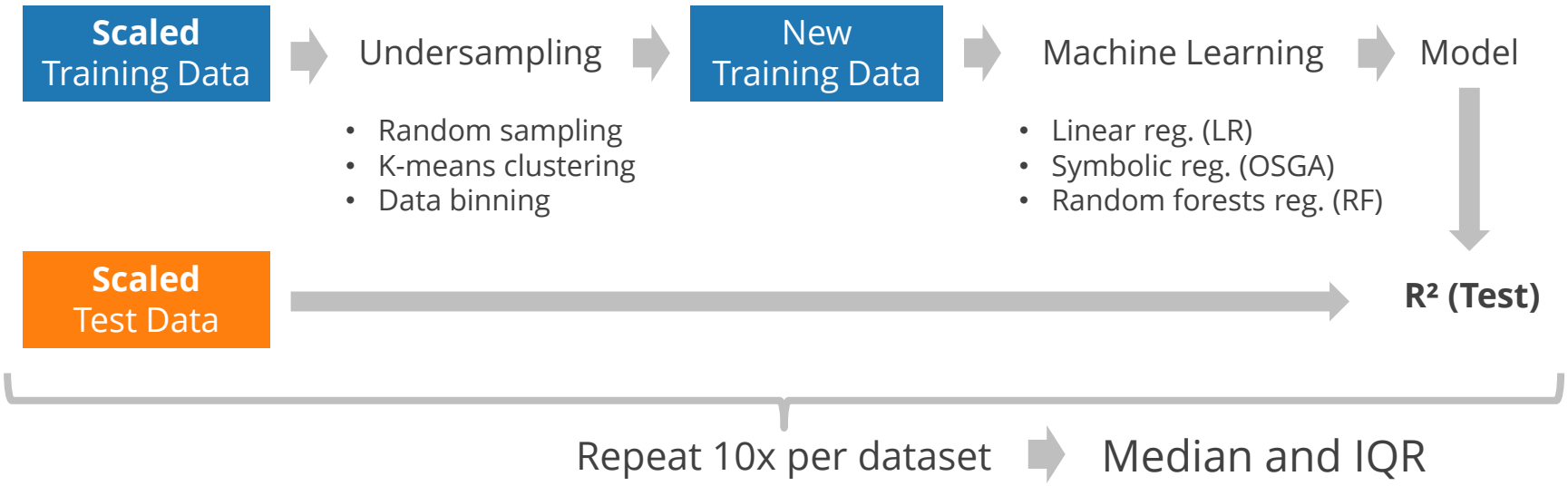


Intuition


Original, n = 100
K-Means, K = 10
Sampling, n = 10
Sampling, n = 50
y
x
3
2
1
0
−1
−2
−2
−1
0
1
2

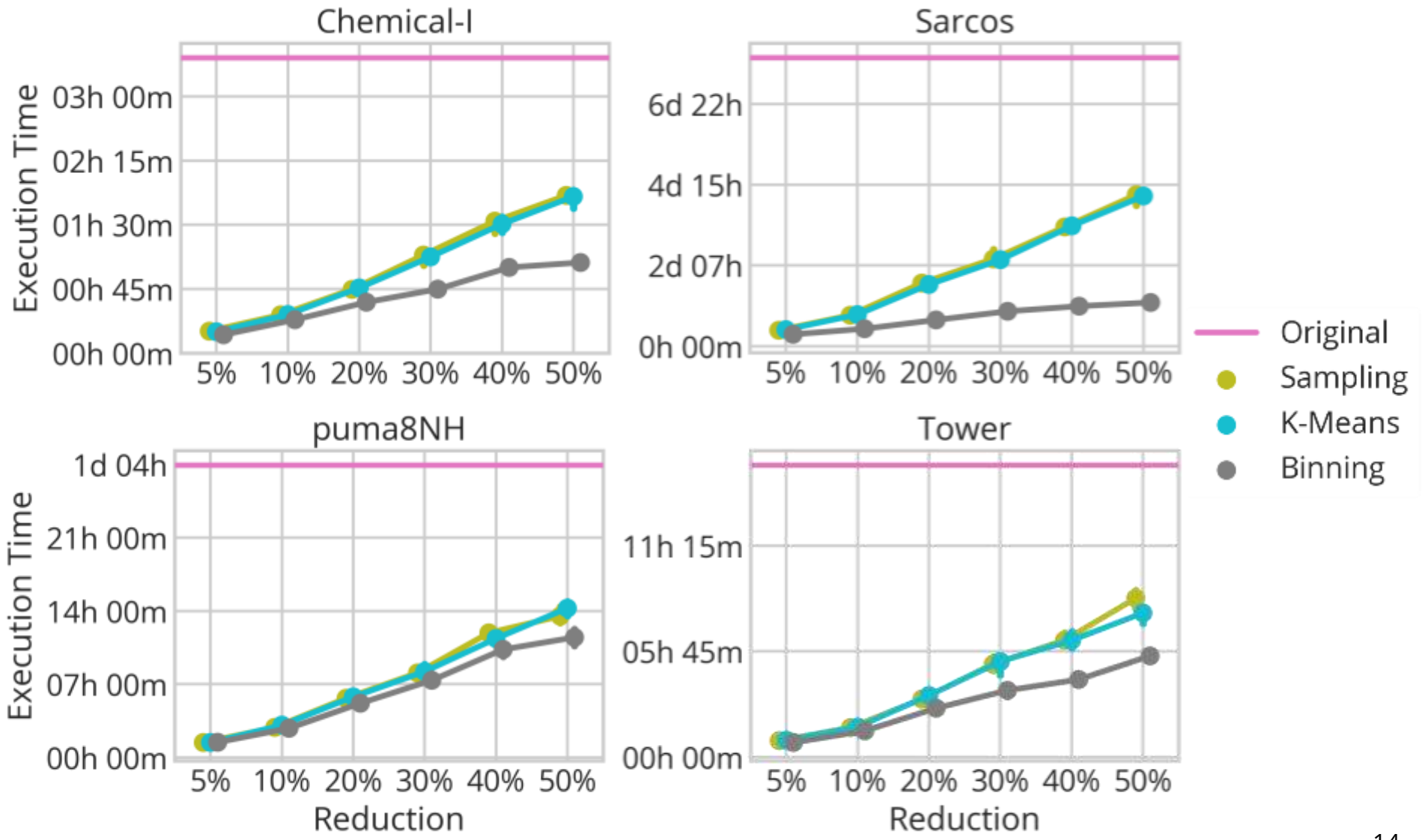
Experiment Setup



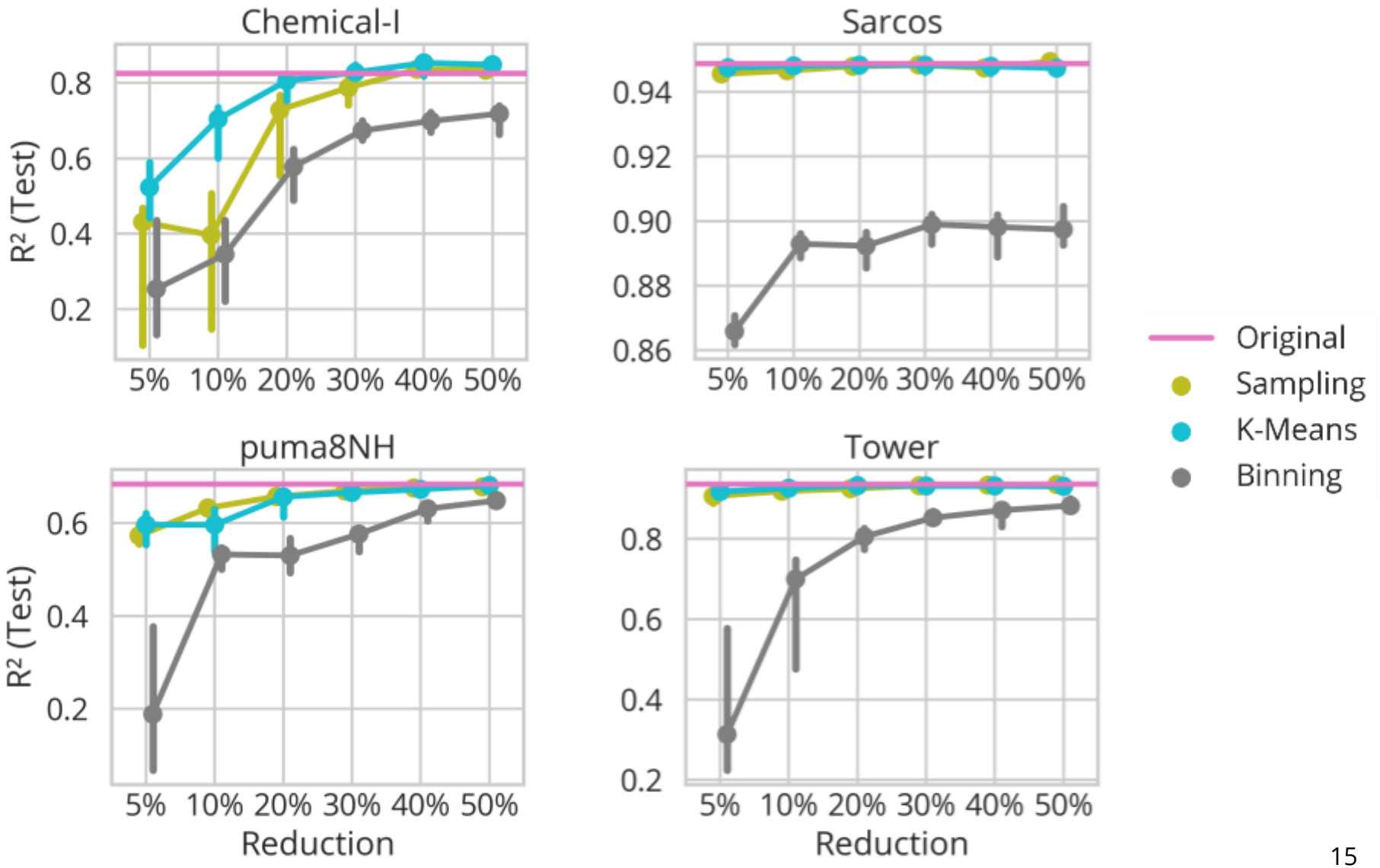
Used datasets:

	training rows	features
Chemical-I	711	57
Sarcos	~44 500	21
puma8NH	6144	8
Tower	3136	25

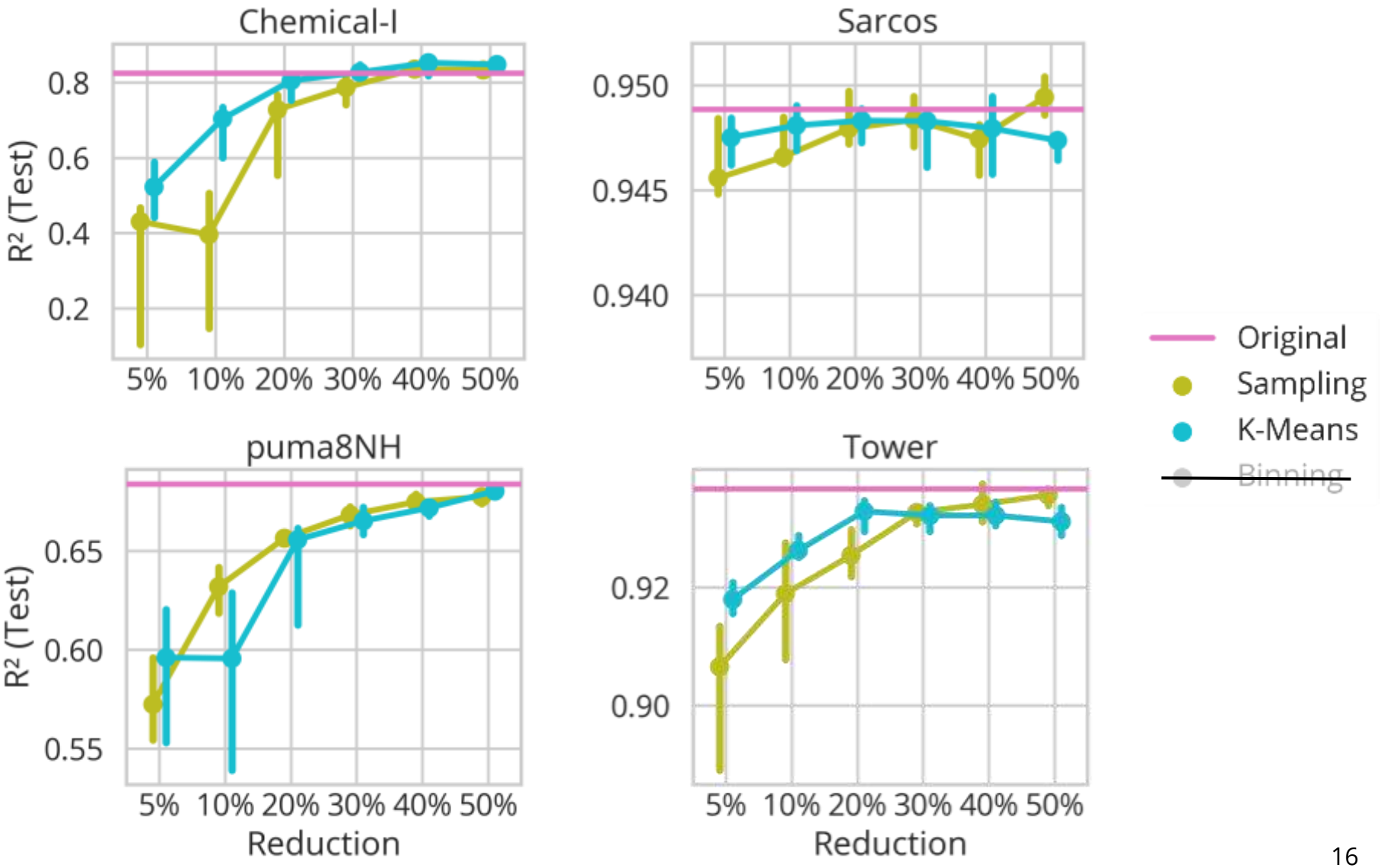
OSGA Speedup



Loss in Quality with OSGA

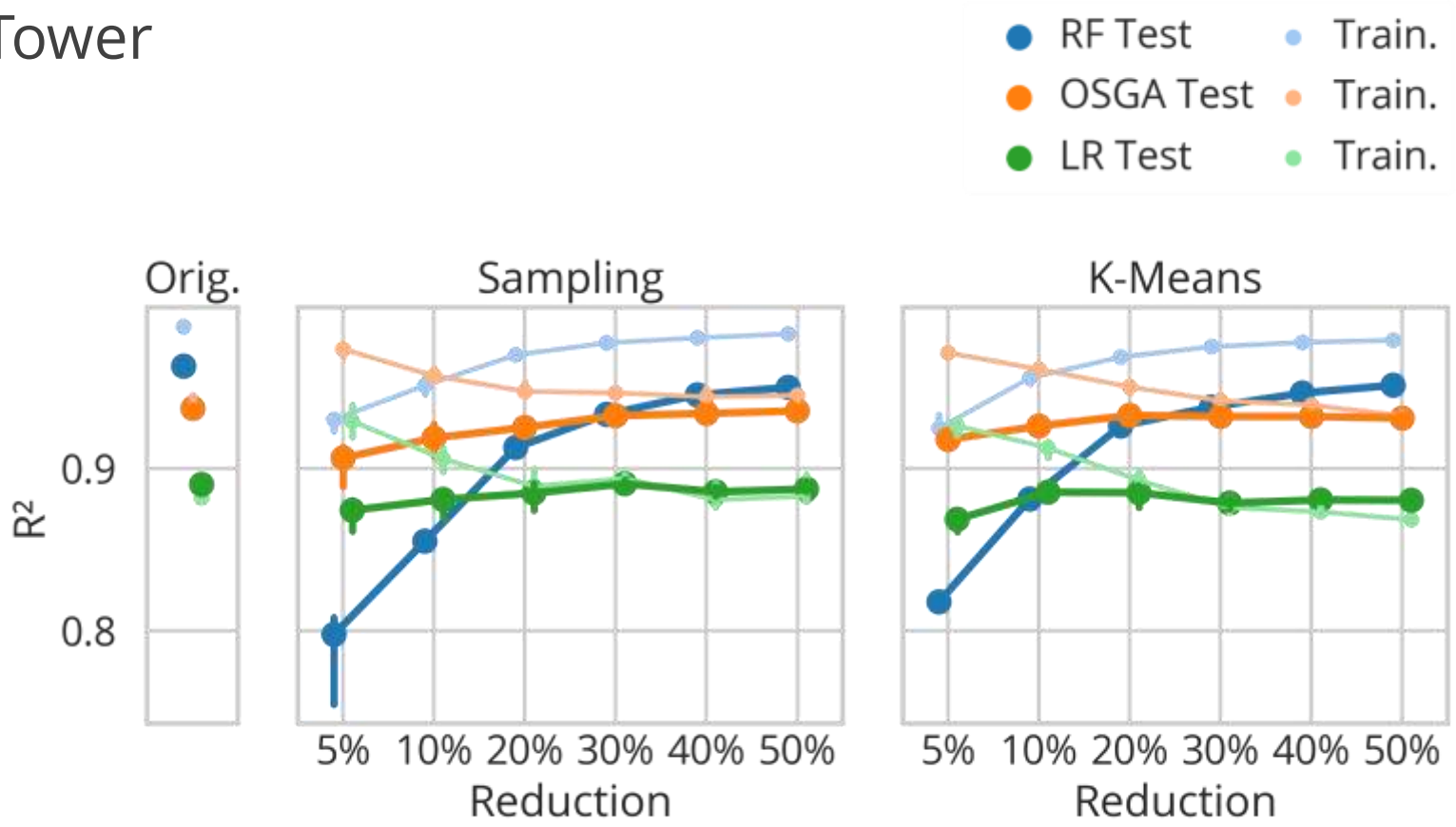


Loss in Quality with OSGA



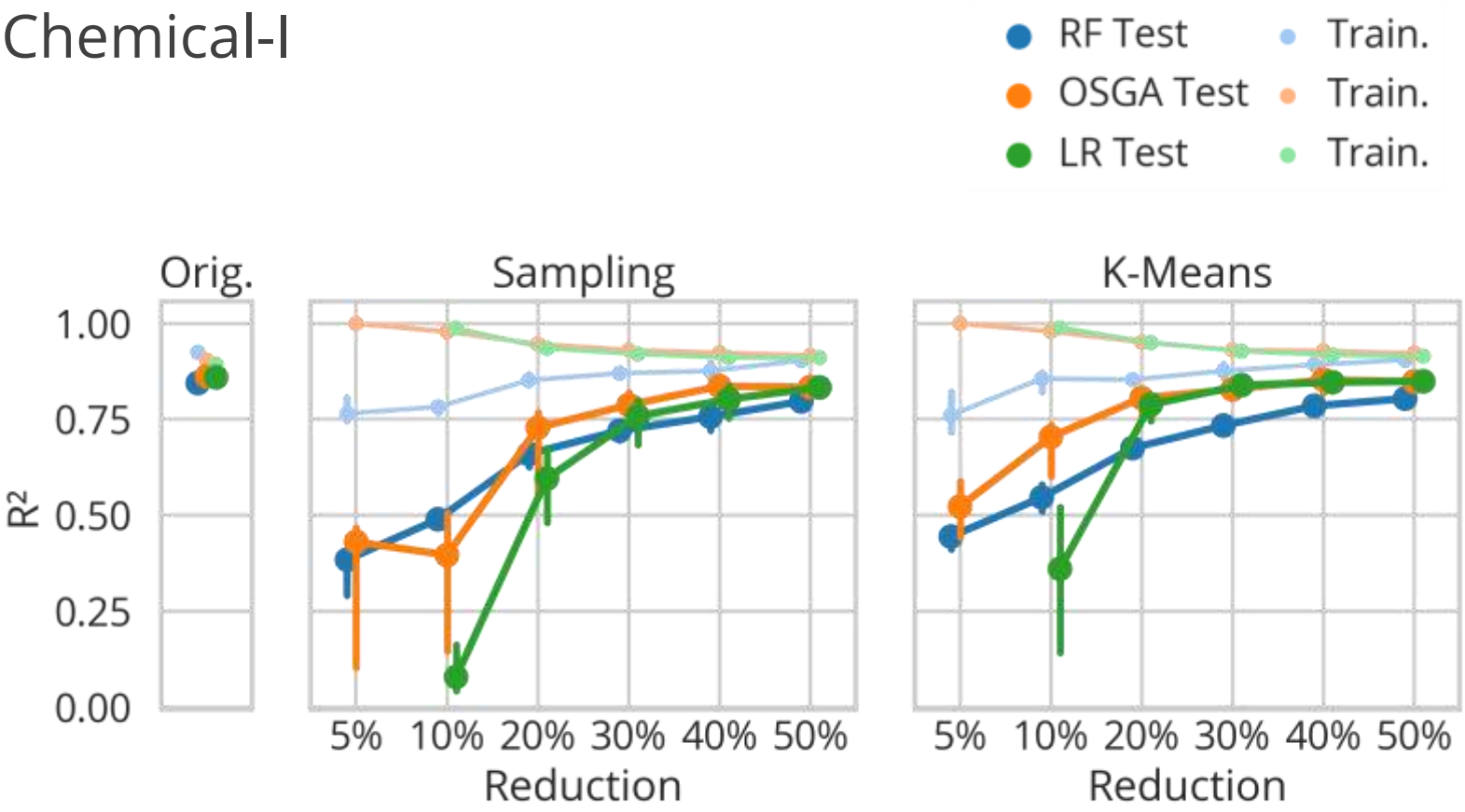
Algorithm Comparison

Tower



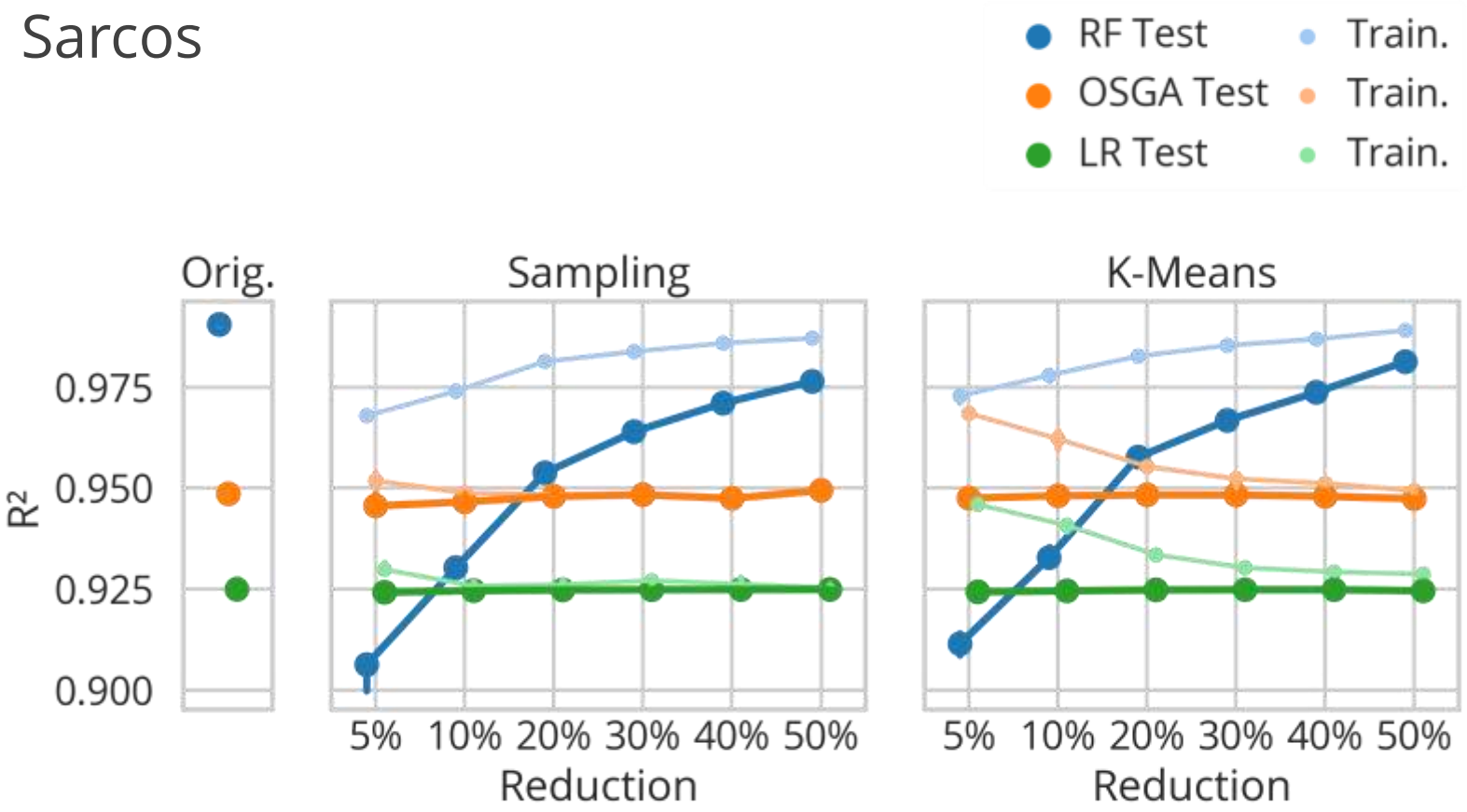
Algorithm Comparison

Chemical-I



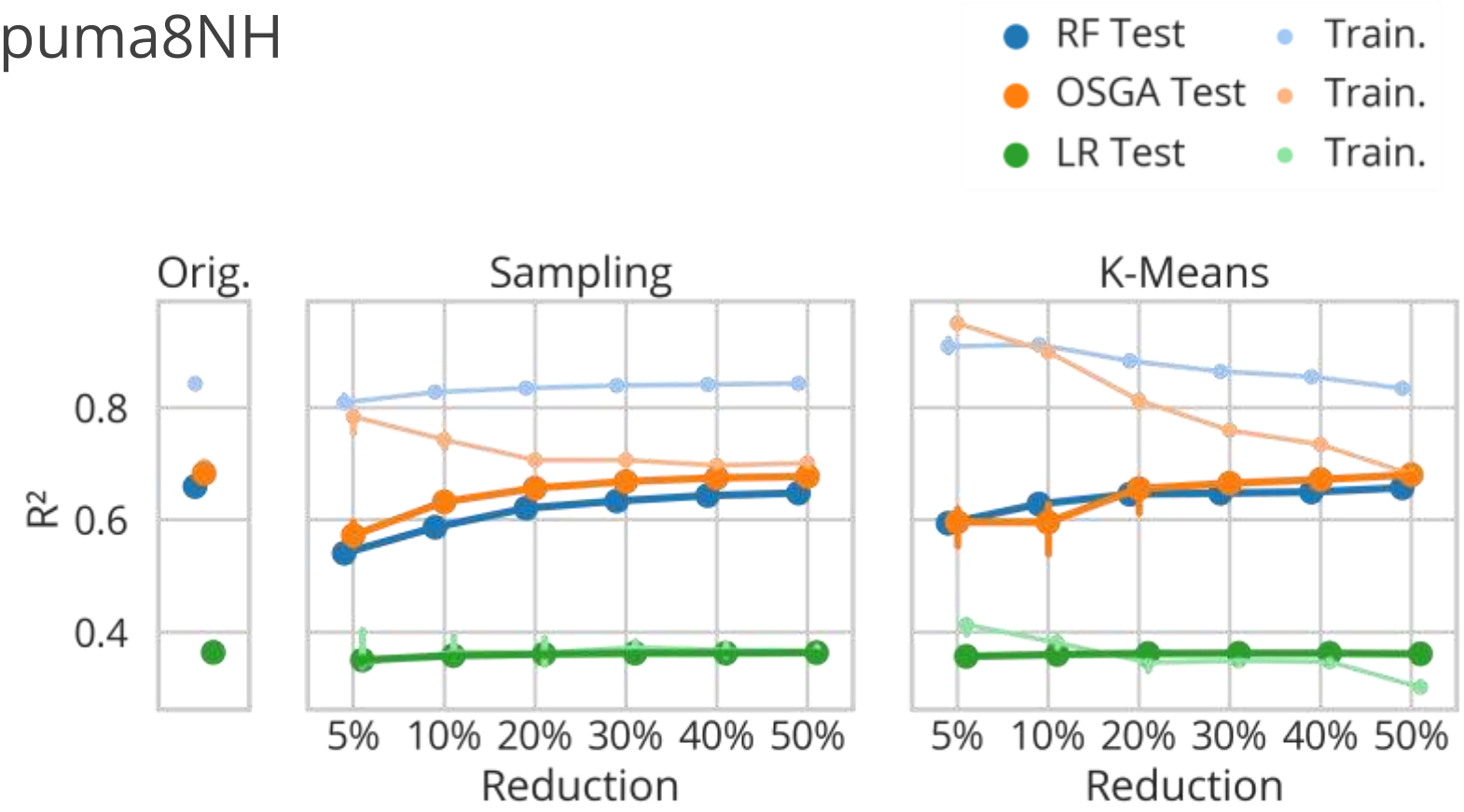
Algorithm Comparison

Sarcos



Algorithm Comparison

puma8NH



Conclusion

- Results of k-means and random sampling comparable
  - Implications on…
    - hyperparameter optimization?
    - statistical tests?
    - etc.?
- Binning not usable
  - Unusable loss in accuracy in all cases

- Little loss of accuracy with >30% undersampling rate
- Speedup linear to undersampling rate

Discussion

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Algorithm Settings

Offspring Selection Genetic Programming

Max. Tree Size	Depth: 30 Length:50
Grammar	+ - × ÷ exp log square sqrt cbrt sin cos tan
Population Size	300
Mutation Rate	20 %
Selector	GenderSpecific (Random & Proportional)

Random Forest

R	30 %
M	50 %
Number of Trees	50

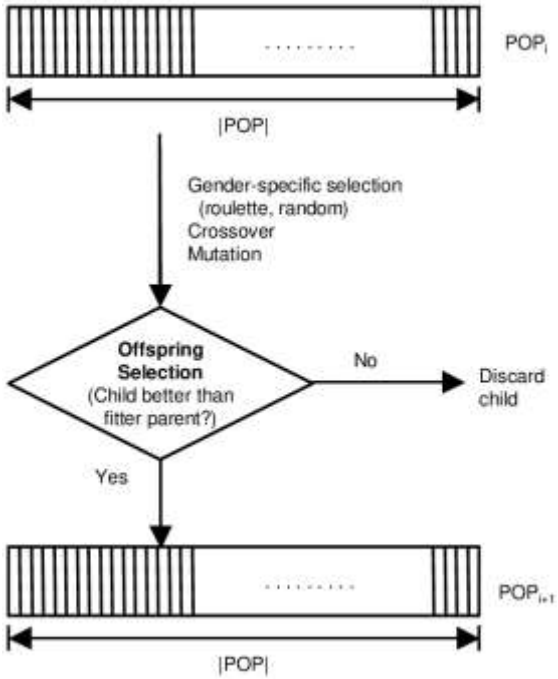

Image: Affenzeller, M., Wagner, S., & Winkler, S. (2007, July). *Aspects of adaptation in natural and artificial evolution*. In Proceedings of the 9th annual conference companion on Genetic and evolutionary computation (pp. 2595-2602). ACM