MACHINE LEARNING APPROACH TO QUANTUM MECHANICS

> MEDICINE IS A SCIENCE OF UNCERTAINTY AND AN ART OF PROBABILITY.

William Osler

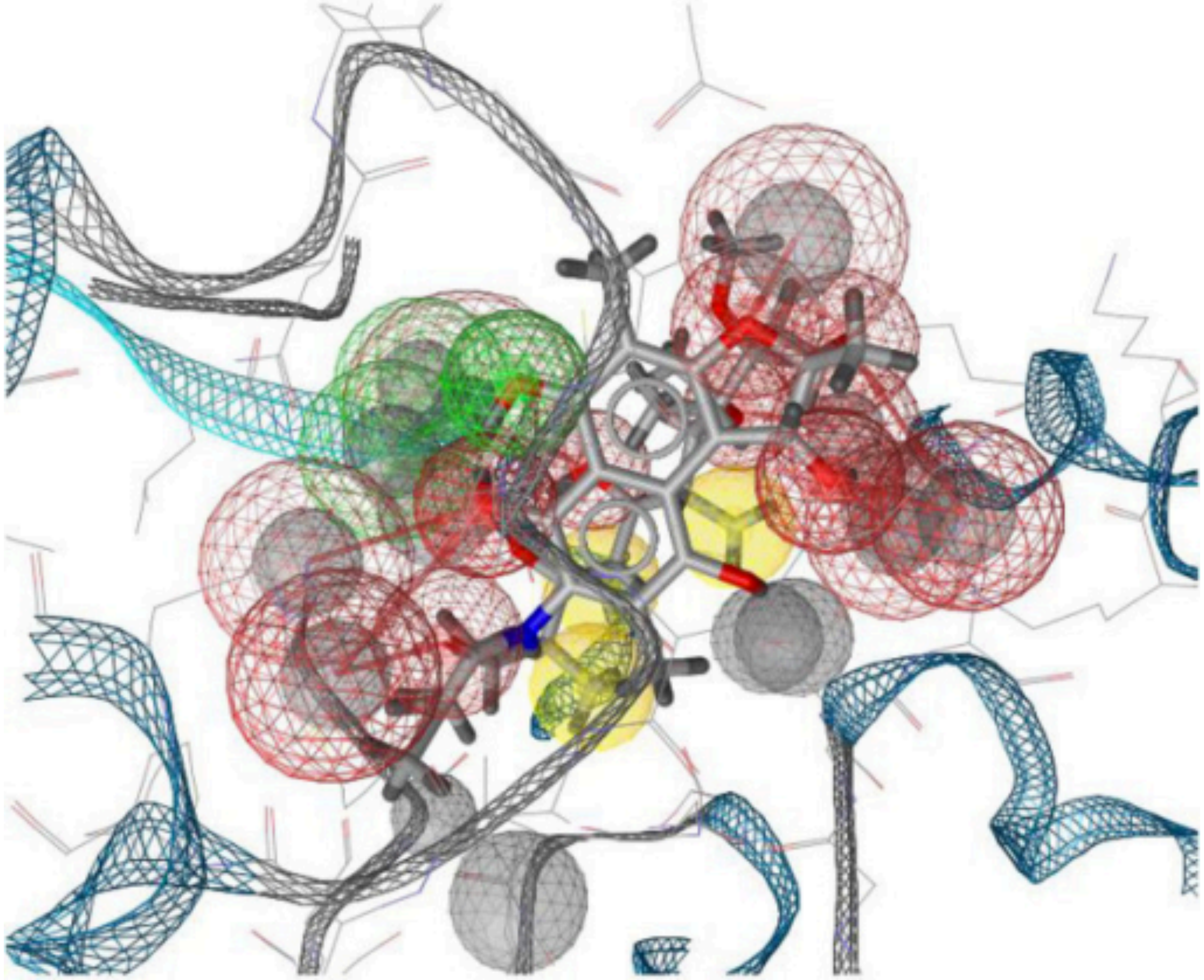
PHARMACEUTICAL R&D COSTS NOW EXCEED $2.87B

TAXOL: A SUCCESS STORY

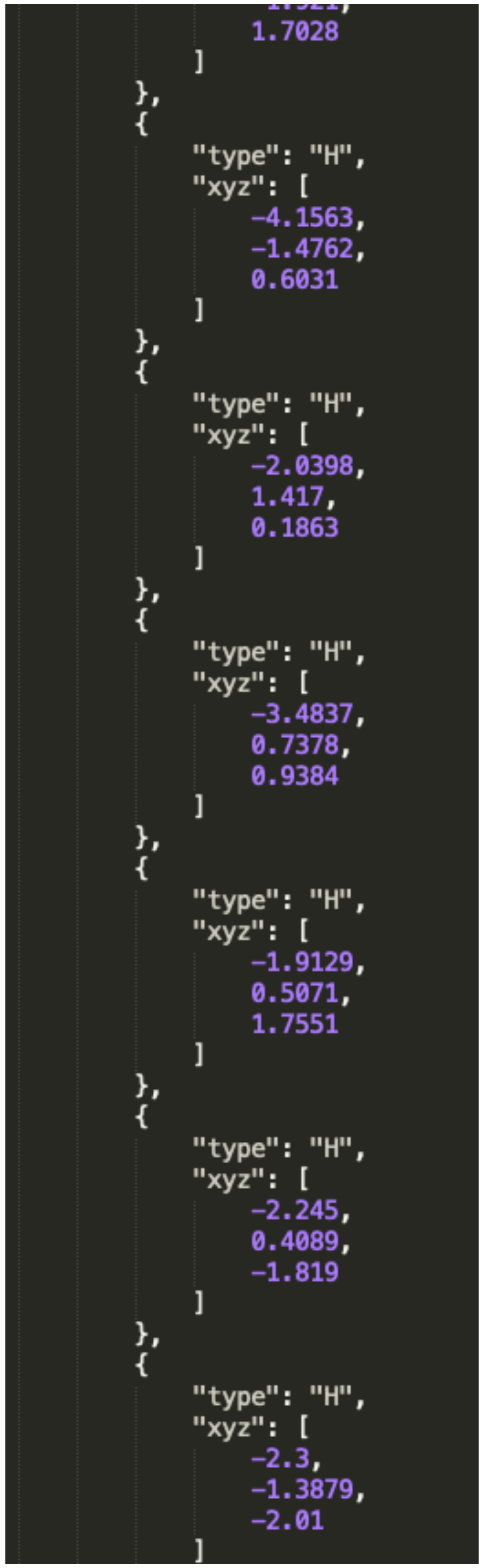
- In the second half of the 20th century, researchers realized the need for systemic treatments for different types of cancer
- A new NCI institution funded such screening programs
- Welcome Taxol
- To date, Taxol is the best-selling cancer drug ever manufactured

OUTLINE

- Describe Data
- Visualizations
- Models
- Parameter Tuning
- Results



DATA



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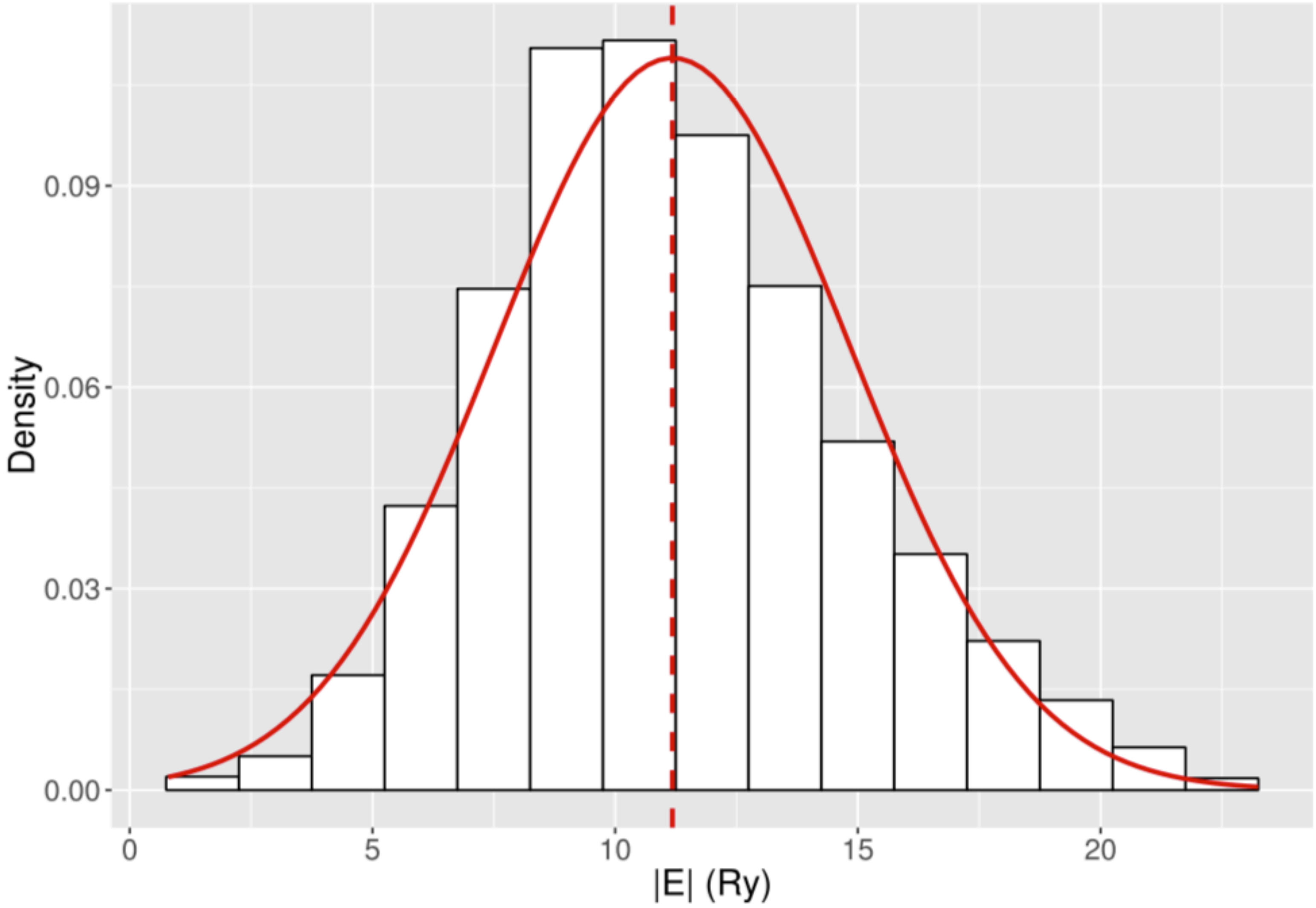


IDENTIFY AND DESIGN

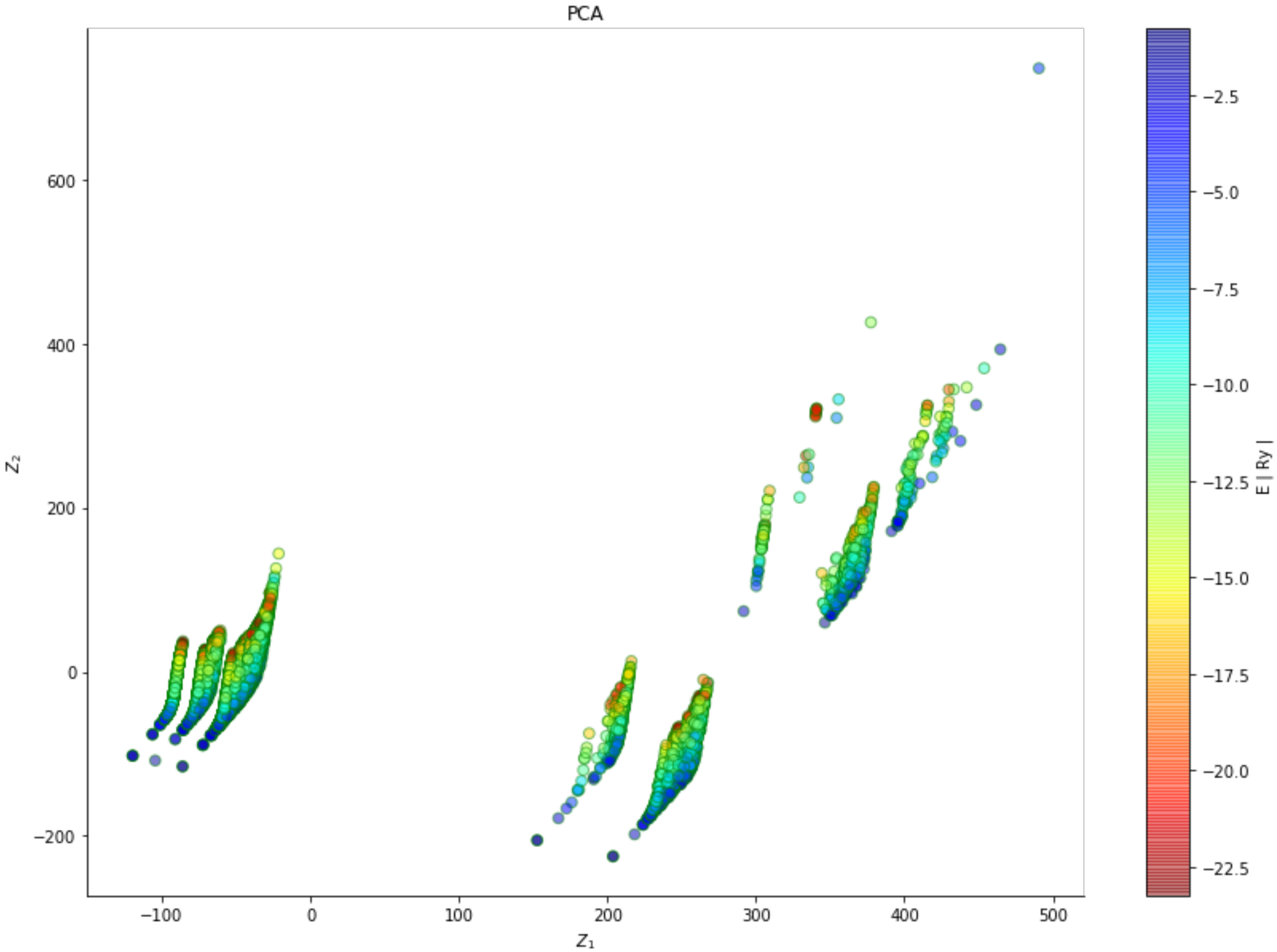
- Chemical & electrical properties
- Quantum mechanics
- Coulomb Matrix
- Computationally expensive

$$C_{IJ} = \begin{cases} 0.5\, Z_I^{2.4} & I = J \\ \frac{Z_I Z_J}{|\mathbf{R}_I - \mathbf{R}_J|} & I \neq J \end{cases}$$

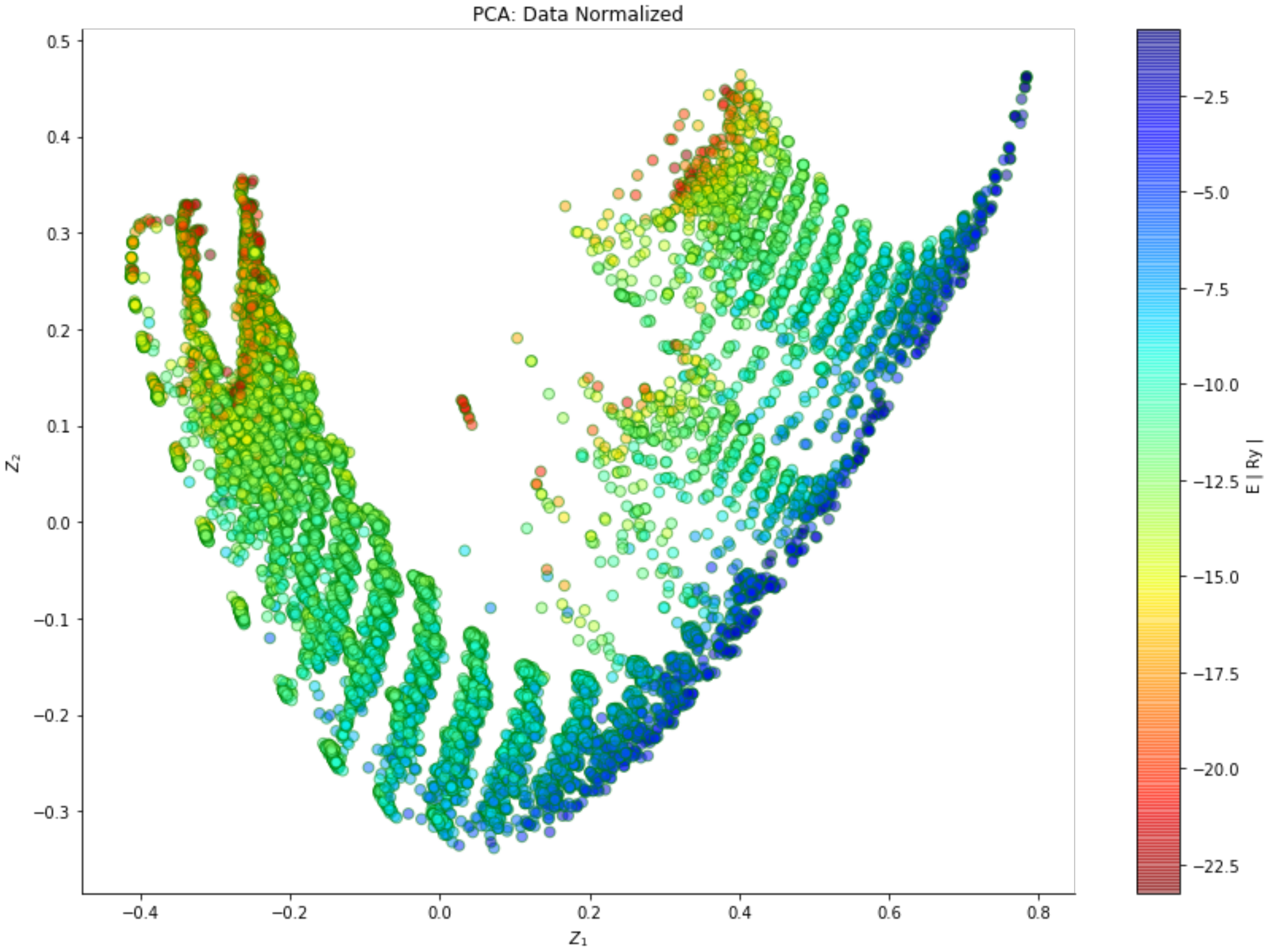
PREVIOUS WORK

- Electronic state simulations via Density Functional Theory
- B. Himmetoglu (2016) Tree based machine learning framework for predicting ground state energies of molecules
  - Data available on Kaggle / GitHub
  - Objective: Predict Enthalpy of Atomization Energy

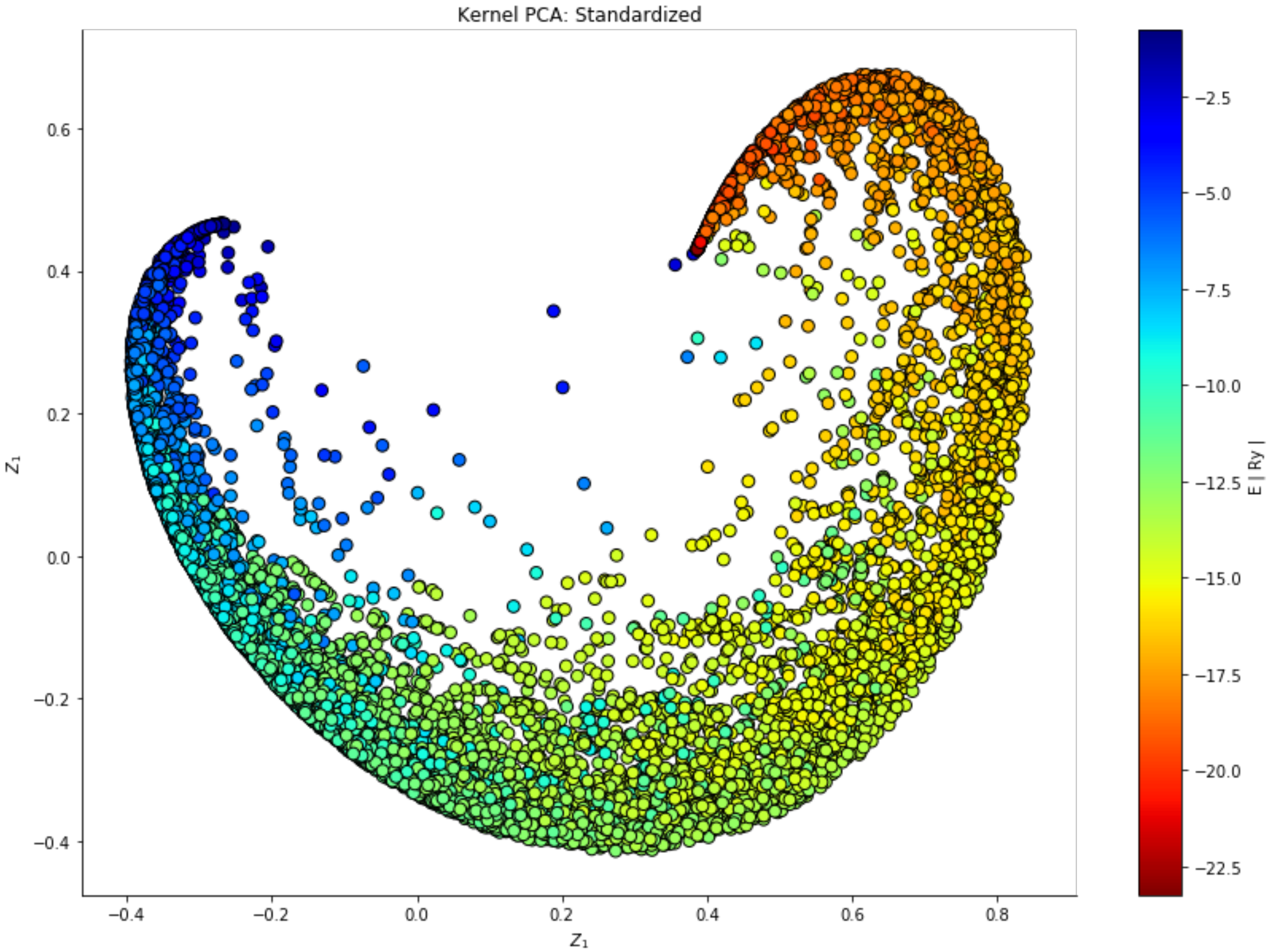
VISUALIZATION: PCA



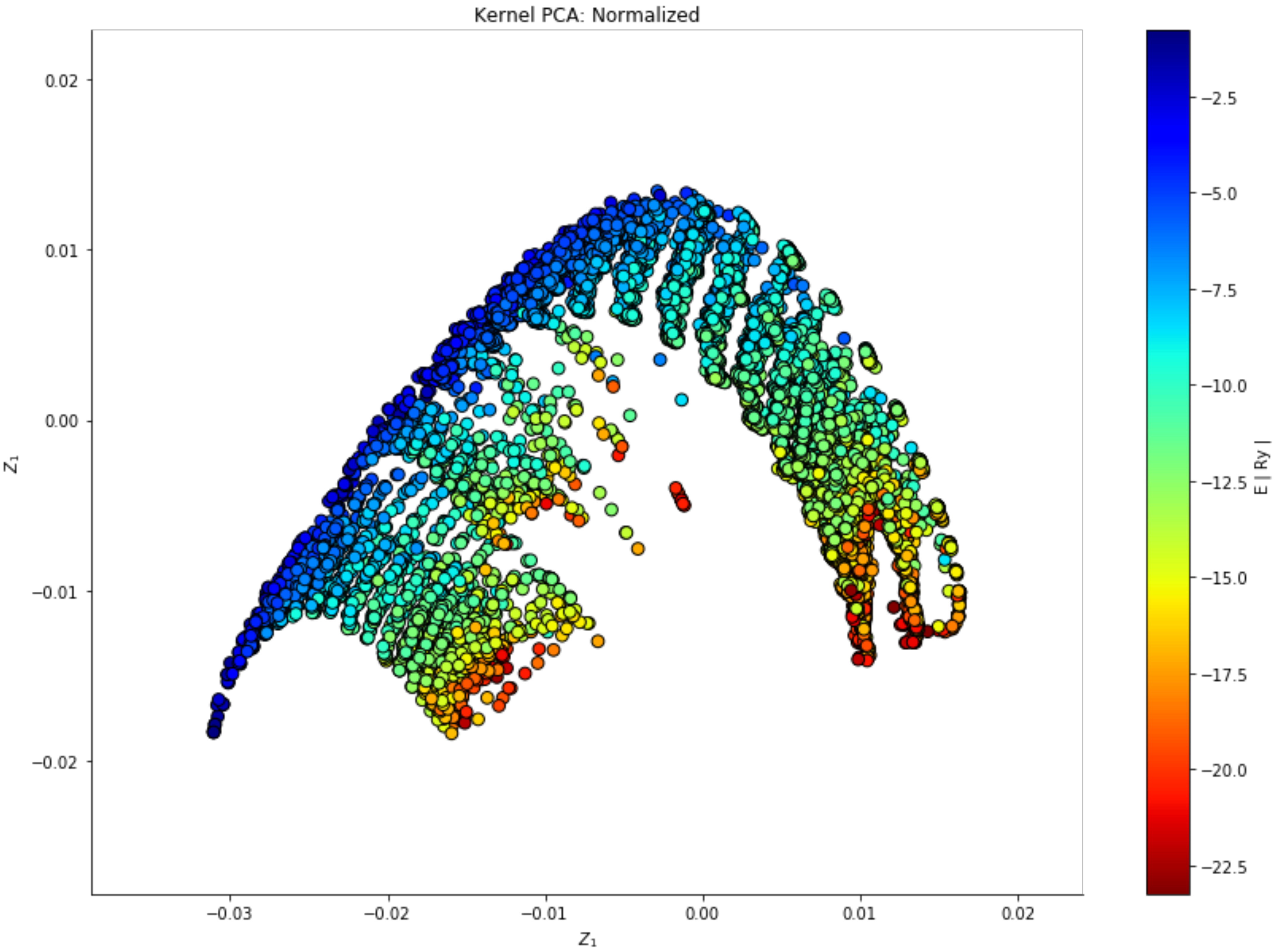
VISUALIZATION: PCA (NORMALIZED)



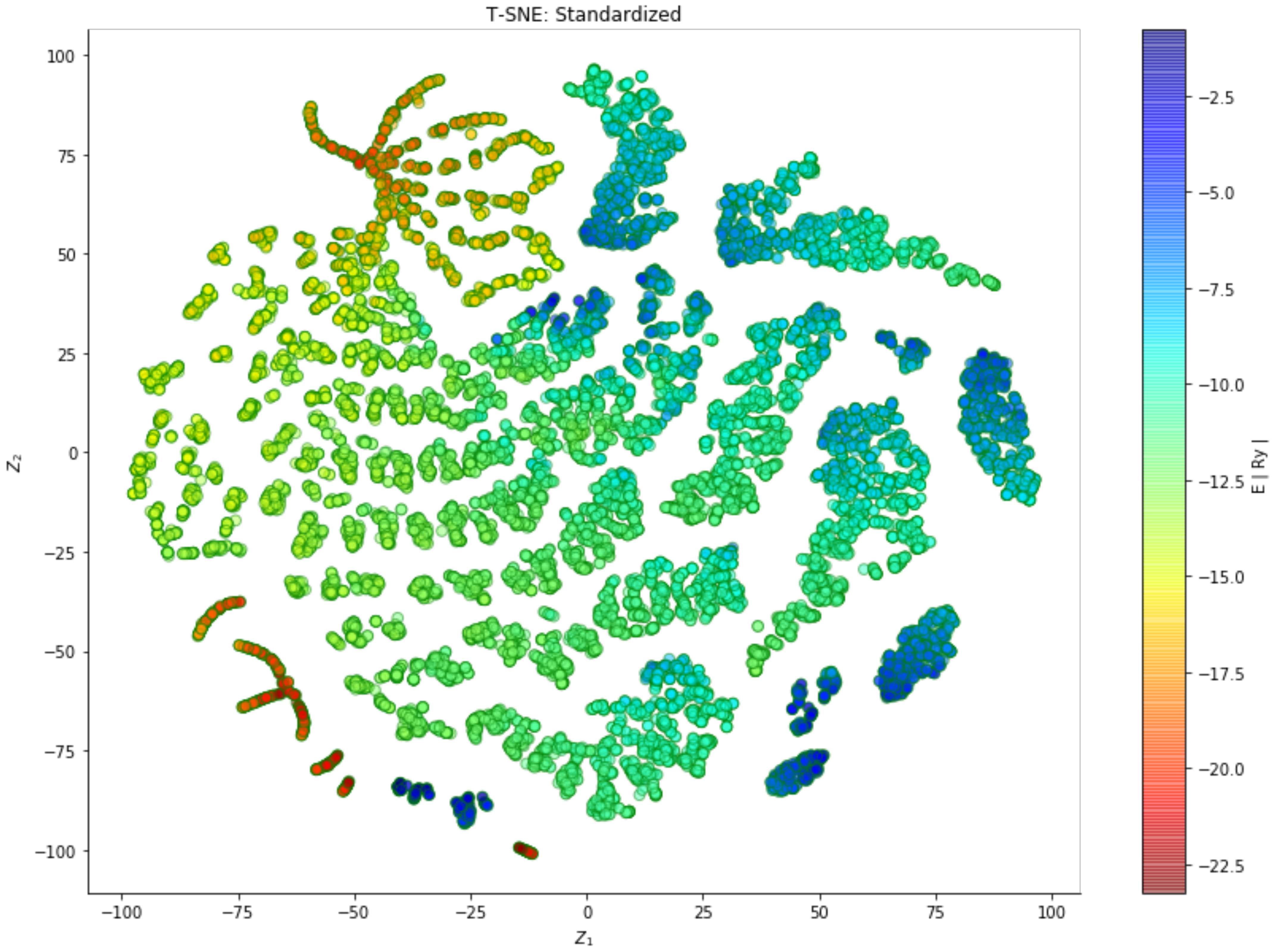
VISUALIZATION: KERNEL PCA (STANDARDIZED)



VISUALIZATION: KERNEL PCA (NORMALIZED)



VISUALIZATION: T-SNE (STANDARDIZED)

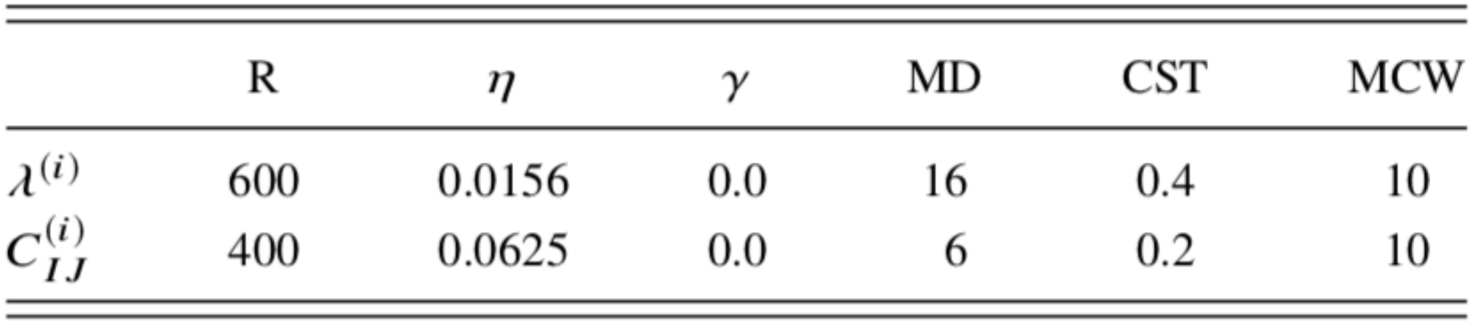


MODELS

- Linear Regression
- Boosted Regression Models
- Ensemble Models

PARAMETER TUNING

- Literature - optimal?
- Grid Search
- Manual Tuning
  - Trial and error/intuition



	R	η	γ	MD	CST	MCW
$\lambda^{(i)}$	600	0.0156	0.0	16	0.4	10
$C_{IJ}^{(i)}$	400	0.0625	0.0	6	0.2	10

MODELS: RESULTS

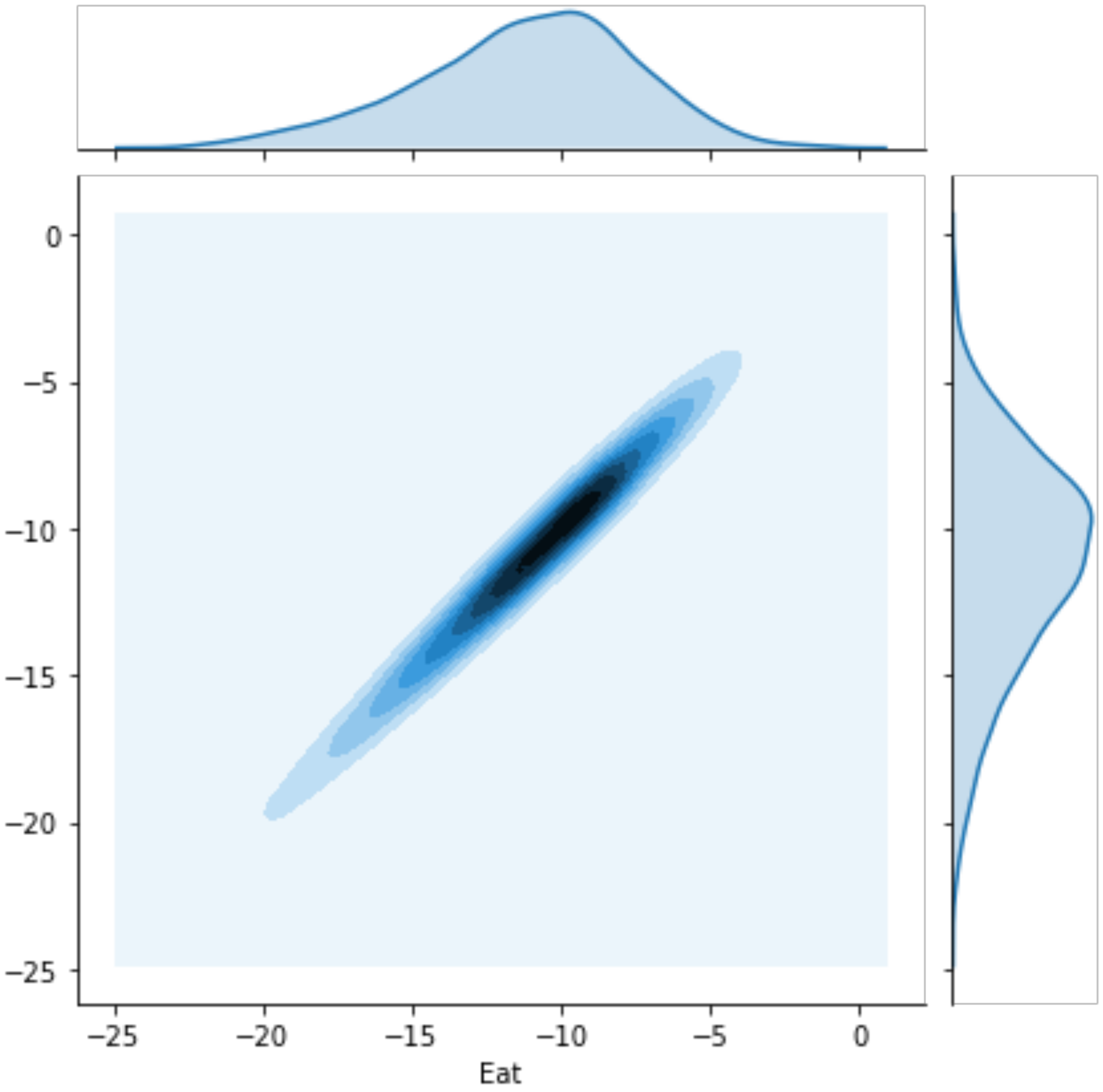
PREVIOUS MODEL

- RMSE: 36.63

MODEL TYPE	RMSE[Ry]	TEST SCORE	RMSE [kcal/mol]
LightGBM	0.00505493	0.99963	**1.588**
XGBoost	0.00522919	0.99957	**1.636**
Gradient Boosting	0.09485	0.9993	**29.682**
Extra Tree	0.12229	0.9989	**38.268**
Bagging	0.148732	0.9983	**46.543**
Random Forest	0.284132	0.994	**88.914**
K-Nearest Neighbors (k=3)	0.547451	0.9776	**171.314**
Linear Regression (PCA)	0.809693	0.9509	**253.378**
Elastic Net	0.882564	0.9417	**276.182**
Passive Aggressive	1.022587	0.922	**319.999**
Support Vector Machine Regression	1.698415	0.7848	**531.487**
Linear Regression (Kernel PCA)	3.3874	0.1439	**1060.023**
Linear Regression	116.05917	-1004.0646	**36318.519**

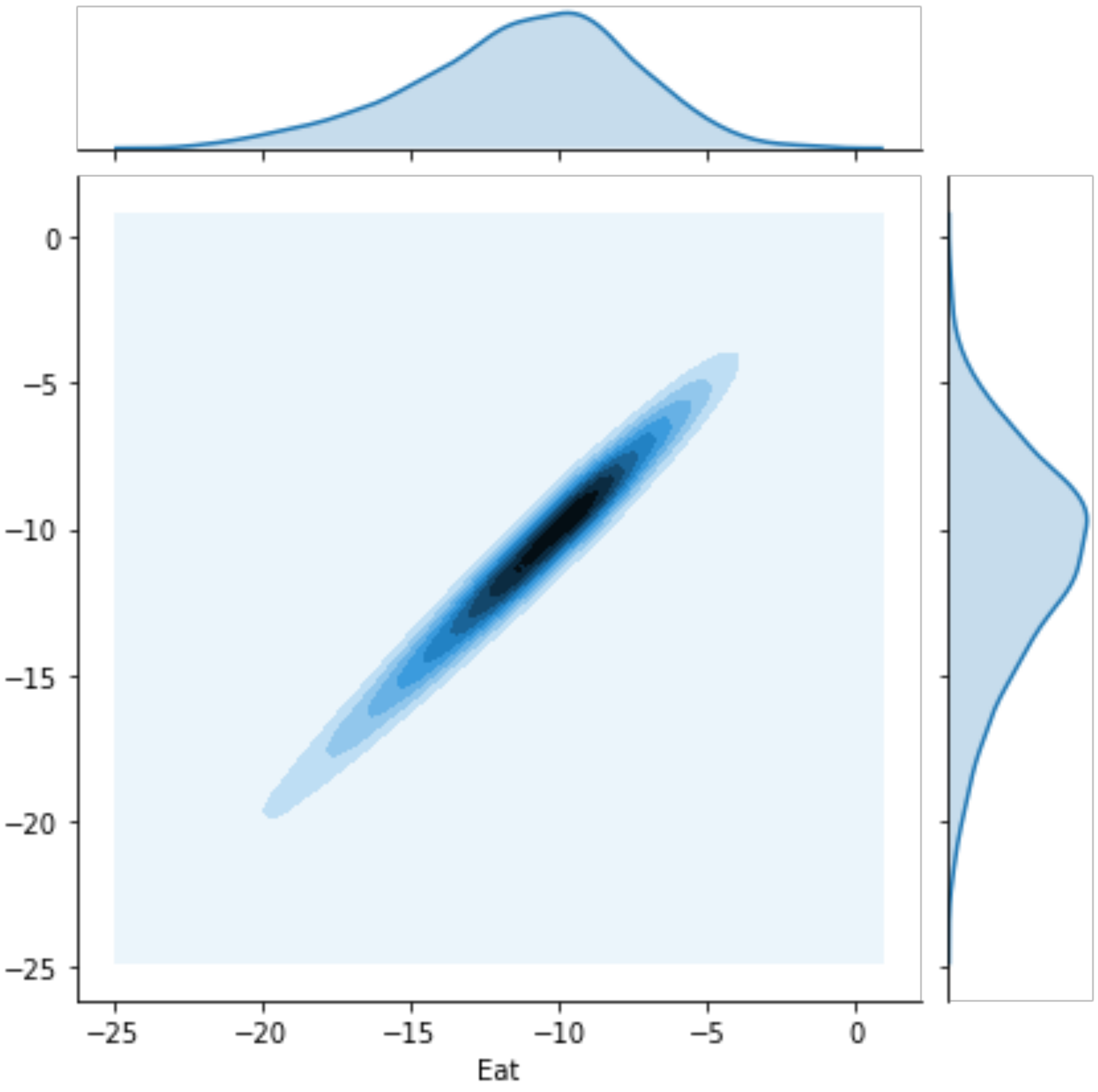
PARAMETERS

- booster = gbdt
- learning_rate = 0.09
- reg_alpha = 0.115
- reg_lambda = 0.58
- max_depth=8
- num_leaves=17
- subsample = 0.6
- gamma = 0.001
- eval_metric = rmse



PARAMETERS

- booster = gbdt
- learning_rate = 0.09
- num_leaves = 100
- reg_alpha, reg_lambda = 0
- min_child_samples = 7
- min_child_weight = 1
- base_score = 0.5
- eval_metric = l2



- WHY ARE XGBOOST/LIGHTGBM SO FAST?
- SHORTCOMINGS

Q&A