IML2024 Term project Report

Group 190 - Patrik Keinonen, Mikko Kallio, Tuuli Toivanen-Gripentrog

2024-12-18

Introduction

In this project we use a support vector regressor (model) to predict logarithmic saturation vapour pressure of the molecule. We use the idea of producing meaningful features by deriving new features (based on known formulas in chemistry). The SVR model with the augmented dataset is tuned using automatic hyperparameter tuning.

Final Kaggle Score

0.7484 Private (4th place)

0.7571 Public

Feature Engineering

We experimented with a set of different feature engineering methods to discover which changes yielded improvements in model performance.

Feature Correlations

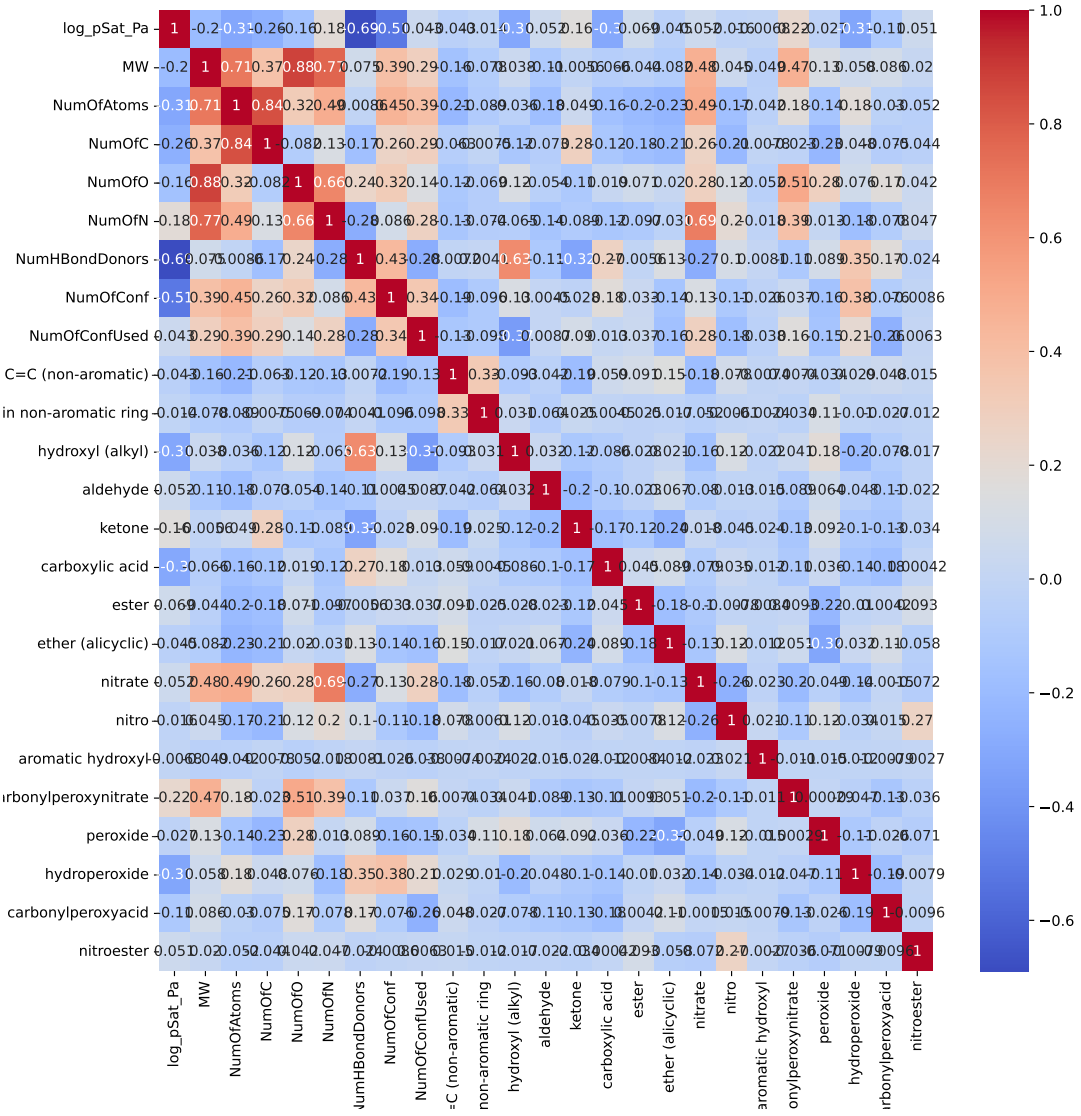
In the early discovery phase of the project, simple data analysis was conducted. We plotted and listed the feature correlations between the target column log_pSat_Pa. Additionally the strongest correlation pairs among the features were identified.

```
## Strongest correlation between the target:
## NumHBondDonors           0.689196
## NumOfConf                0.513653
## hydroperoxide            0.314053
## hydroxyl (alkyl)         0.310452
## NumOfAtoms               0.307337
## carboxylic acid          0.304259
## NumOfC                   0.262769
## carbonylperoxynitrate    0.223739
## MW                       0.199574
## NumOfN                   0.183152
## Name: log_pSat_Pa, dtype: float64
```

```
## ----------------------
```

```
## Strongest correlation pairs:
## NumOfO                 MW               0.880358
## NumOfC                 NumOfAtoms       0.838402
## NumOfN                 MW               0.772575
## NumOfAtoms             MW               0.707009
```

```
## nitrate                    NumOfN             0.687224
## NumOfN                     NumOfO             0.656750
## hydroxyl (alkyl)           NumHBondDonors     0.632023
## carbonylperoxynitrate      NumOfO             0.510409
## nitrate                    NumOfAtoms         0.492108
## NumOfN                     NumOfAtoms         0.491902
## dtype: float64
```



We conducted feature selection experiments by selecting only the most correlated variables and excluding others. Additionally, we tried dropping some of the features which were highly correlated with another feature. These experiments did not improve the models performance. Hence, we moved on to some more advanced feature engineering techniques.

Data Cleaning

By replacing infinite values and missing data with zero, we ensured the dataset is well-suited for downstream modeling, and prevented issues with invalid numerical values.

Creation of Derived Features

We quickly realized lacking domain knowledge in chemistry and physiscs, the competence required analysing molecular data. The principal idea was to compose *meaningful features*, something we were inspired by the discussion at *Bayesian Data Analysis* course in the context of GLM (generalized linear models). After studying the university guidelines provided in the course page, we interpreted the rules so that we were able to use an external AI consultant. Hence, providing a listing of the features with descriptions to ChatGPT, we asked which formulas in chemistry use the given covariates as parameters. We received a listing of formulas which we then implemented in the feature engineering phase.

- AtomFraction: Proportion of carbon, oxygen, and nitrogen atoms in the molecule relative to the total atom count.
- Polarity: Ratio of hydrogen bond donors to molecular weight.
- HBondDensity: Ratio of hydrogen bond donors to the total number of atoms.
- GroupDensity_CarboxylicAcid: Concentration of carboxylic acid groups per unit molecular weight
- Unsaturation: Sum of non-aromatic double bonds and C=C-C=O bonds in non-aromatic rings.
  `df['Unsaturation'] = df['C=C (non-aromatic)'] + df['C=C-C=O in non-aromatic ring']`
- ConfigurationalComplexity: Ratio of the number of stable conformers to molecular weight.
  `df['ConfigurationalComplexity'] = df['NumOfConf'] / df['MW']`
- HydrogenBondPotential: Total potential for hydrogen bonding based on hydrogen bond donors and nitrogen/oxygen atoms.
  `df['HydrogenBondPotential'] = df['NumHBondDonors'] + (df['NumOfO'] + df['NumOfN'])`
- PolarGroupCount: Count of polar functional groups.
  `polar_groups = ['hydroxyl (alkyl)', 'aldehyde', 'ketone', 'carboxylic acid', 'ester', 'nitro']`
- AromaticGroupFraction: Proportion of aromatic hydroxyl groups relative to all polar groups.
  `df['AromaticGroupFraction'] = df['aromatic hydroxyl'] / (df[polar_groups + ['aromatic hydroxyl']].sum(axis=1) + 1e-9)`
- MolecularSize: Combined measure of molecular weight and atom count.
- Hydrophobicity: Ratio of carbon atoms to the total atom count.
- DegreeOfUnsaturation: Measure of molecular unsaturation based on carbon and atom counts.
- ShapeCompactness: Ratio of atom count to the number of conformers used in calculations.
- SymmetryIndex: Ratio of symmetric to asymmetric functional groups.
- VolatilityIndex: Proxy for molecular volatility based on carbon-to-polar group ratio and molecular weight.
- PolarityIndex: A combined measure of molecular polarity.
- OxygenToCarbonRatio: Relative proportion of oxygen to carbon atoms.

Interaction Features

To capture non-linear relationships, several interaction terms were introduced. We experimented with Sklearn `PolynomialFeatures(degree=2, intercation_only=True)`. This resulted in a convoluted dataset.

Principal component analysis was also employed to reduce the complexity of the model.
However, we defaulted into a more crude, manual process by defining the interactions by hand using semi-brute-force strategy. Hence, we tried different interactions:

```
df['AtomFraction * Hydrophobicity'] = df['AtomFraction'] * df['Hydrophobicity']
df['HydrogenBondPotential * NumOfC'] = df['HydrogenBondPotential'] * df['NumOfC']
df['Hydrophobicity * NumOfC'] = df['Hydrophobicity'] * df['NumOfC']
df['PolarityIndex_FlexibilityRatio'] = df['PolarityIndex'] * df['FlexibilityRatio']
df['VolatilityIndex_DegreeOfUnsaturation'] = df['VolatilityIndex'] * df['DegreeOfUnsaturation']
df['ShapeCompactness_FlexibilityRatio'] = df['ShapeCompactness'] * df['FlexibilityRatio']
df['PolarityIndex * NumOfC'] = df['PolarityIndex'] * df['NumOfC']
df['DegreeOfUnsaturation * NumOfC'] = df['DegreeOfUnsaturation'] * df['NumOfC']
df['NumOfC * NumOfO'] = df['NumOfC'] * df['NumOfO']
```

in order to model potential synergistic effects between molecular properties.

Feature Transformations

As part of the preprocessing pipeline, we systematically explored various mathematical transformations of the input features to improve the model's performance. Transforming features can help normalize distributions, reduce the influence of outliers, and capture nonlinear patterns.

We developed a function to iterate through features and apply transformations based on a predefined set of transformation functions. Using a brute-force approach, we systematically evaluated each transformation for all features by assessing their impact on model performance.

Transformation Functions Explored

- Logarithmic (log): Compresses large values and expands small ones, effective for reducing skewness.
- Square root (sqrt): Reduces the magnitude of large values while preserving smaller ones.
- Square (square): Amplifies differences in values, highlighting larger magnitudes.
- Cubic (cube): A stronger version of the square transformation to capture higher-order relationships.
- Exponential (exp): Expands small differences in values, useful for features with compressed scales.
- Reciprocal (1/x): Inverts the scale, useful for features with large values that need downweighting.
- Box-Cox: A parameterized transformation that aims to stabilize variance and make data approximately normal (applied only for strictly positive features). [1]
- Yeo-Johnson: Similar to Box-Cox but works with both positive and negative values. [2]

Results From Feature Engineering

The model performance increased by introducing derived, interaction and transformed features. Hence, we continued to explore which combination of the above-mentioned new features yields best results.

Experiments With Different Models

In the discovery phase of the project, several models from different families were evaluated:

- Dummy regressor
- Linear Regression
- Random Forest
- Gradient Boosting Regressor
- Epsilon-Support Vector Regressor SVR [3]

We observed that most promising results were produced by SVR and GBR models, where SVR out-performed that GBR with a small margin given a few different parameterizations. Given the limited amount of time allocated for this project, we decided to commit to SVR without any further analysis.

Evaluate model with different parameters and features

Engineering of Machine Learning course covers a broad set of tools to practise professional, production level ML system management. Tuning the parameters of a model is a tedious task, which fortunately can be automatized. We implemented a model tuning infrastructure on top of Optuna [4]. Optuna was left running for hours traversing in the parameter space towards (some) optimal set of parameters. Using an iterative process of alternately exploring feature engineering and running hyperparameter tuning in Optuna, we found an improved combination of features and hyperparameters.

Model validation

No experiments can be done without an adequate measure of model performance. We considered using either separate train-validation split or use cross-validation. After exploring both avenues, because of the benefits discussed in the IML textbook [5], we decided to move forward with cross-validation with five folds.

Report of Using Generative AI

ChatGPT was used to find information about saturation vapour pressure and to find some basic formulas what can be derived from a given set of features.

References

[1] "Box Cox Transformation: Definition, Examples," *Statistics How To*. Accessed: Dec. 05, 2024. [Online]. Available: https://www.statisticshowto.com/probability-and-statistics/normal-distributions/box-cox-transformation/

[2] kjytay, "The Box-Cox and Yeo-Johnson transformations for continuous variables," *Statistical Odds & Ends*. Feb. 2021. Accessed: Dec. 05, 2024. [Online]. Available: https://statisticaloddsandends.wordpress.com/2021/02/19/the-box-cox-and-yeo-johnson-transformations-for-continuous-variables/

[3] "SVR," *scikit-learn*. Accessed: Dec. 05, 2024. [Online]. Available: https://scikit-learn/stable/modules/generated/sklearn.svm.SVR.html

[4] "Optuna - A hyperparameter optimization framework," *Optuna*. Accessed: Dec. 05, 2024. [Online]. Available: https://optuna.org/

[5] G. James, D. Witten, T. Hastie, R. Tibshirani, and J. Taylor, *An Introduction to Statistical Learning: With Applications in Python*. in Springer Texts in Statistics. Cham: Springer International Publishing, 2023. doi: 10.1007/978-3-031-38747-0.