

Feature Selection and Feature Engineering

And why it Matters

My answer

Feature Selection and Feature Engineering matter.

Let me demonstrate why.

I literally grew up in a machine shop. Consequentially, I developed a curiosity re optimization of workflows and minimizing of waste.

My journey took me into aerospace, where I formalized this passion by acquiring a Lean Six Sigma Black Belt Certification.




After transitioning into Data Science, this passion did not change and naturally, I was curious about:

Where is the time best spend when working on a typical Data Science project or Machine Learning pipeline?

Consequently, I spend some time (about 200 hours) exploring this question.

This is my answer.

Who am I?

- Dirk Biesinger  [linkedin.com/in/dirkbiesinger/](https://www.linkedin.com/in/dirkbiesinger/)  [@Saravji](https://twitter.com/Saravji)
- Interested in AI and intelligence in general
- Lived and worked in Germany, Canada, USA
- Industries: Technology, Aerospace, Oil and Gas, Banking, Food, Manufacturing, Telecommunications, Consulting
- Sr. Data Scientist Consultant at Unify Consulting, focusing on ML
- teaching at UW Continuum College (Data Science and Python)
- creating educational materials:  saravji.github.io/saravjis_hut

Syllabus

Welcome

Links

Methodology used

Dataset used

Feature Selection

Feature Engineering

Don't trust me – trust these:

The algorithms we used are very standard for Kagglers. [...] We spent most of our efforts in feature engineering.

— Xavier Conort, on “[Q&A with Xavier Conort](#)” on winning the Flight Quest challenge on Kaggle

Actually the success of all Machine Learning algorithms depends on how you present the data.

— Mohammad Pezeshki, answer to “[What are some general tips on feature selection and engineering that every data scientist should know?](#)”

Basically, xgboost or lightgbm and Neural Nets are the algorithms used in Kaggle competitions. Feature Selection and Creative Feature Engineering decides which Teams will win.

— Anthony Goldbloom (CEO Kaggle), during a conversation.

you have to turn your inputs into things the algorithm can understand

— Shayne Miel, answer to “[What is the intuitive explanation of feature engineering in machine learning?](#)”

...some machine learning projects succeed and some fail. What makes the difference? Easily the most important factor is the features used.

— Pedro Domingos, in “[A Few Useful Things to Know about Machine Learning](#)”

Links

- This presentation: [github.com/Saravji/.../Art Feature Selection and Engineering.pdf](https://github.com/Saravji/.../Art%20Feature%20Selection%20and%20Engineering.pdf)
- Demo Feature Selection: [github.com/Saravji/.../Demo Notebook Feature Selection.ipynb](https://github.com/Saravji/.../Demo%20Notebook%20Feature%20Selection.ipynb)
- Demo Feature Engineering: [github.com/Saravji/.../Demo Notebook Feature Engineering.ipynb](https://github.com/Saravji/.../Demo%20Notebook%20Feature%20Engineering.ipynb)
- boruta_py feature selection method: [Boruta all-relevant feature selection method](#)
- boruta_py implementation (Daniel Homola): [Related blog post](#)
- boruta_py conda package: anaconda.org/Saravji/boruta
- MADELON Dataset: archive.ics.uci.edu/ml/datasets/madelon

Introducing the Methodology used:

- To assess the impact of individual components, each need to be assessed individually.
- To create a neutral picture, I selected randomly one ML algorithm out of the ML groupings in scikit-learn.
- Unless tuning of algorithms is part of the assessment, the default settings are used.
- The only exception is the seed, which is set to ensure repeatability (and make the results comparable)

Introducing the Dataset used: MADELON

The dataset used for the demonstrations is a synthetic dataset created by Isabelle Guyon (Prof. for DS @ Université Paris-Saclay; inventor of SVM-RFE) for the purpose of demonstrating feature selection and feature engineering.

It consists of 2000 training observations, 500 features with integers in the range 0...1000 and a target of -1 or 1 (equally distributed).

Further, 600 test observations in the same manner.

Details: <http://archive.ics.uci.edu/ml/datasets/madelon>

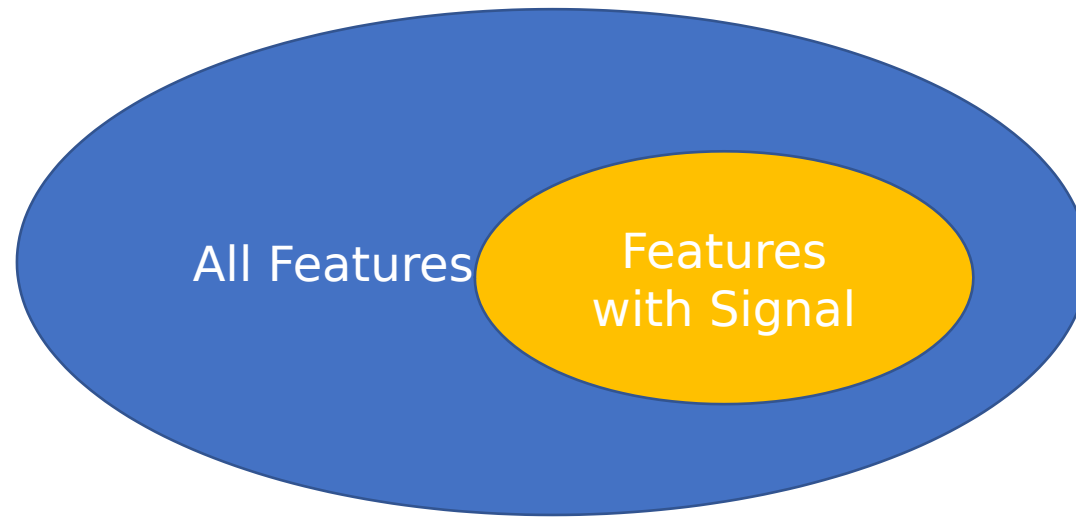
Feature Selection and Feature Engineering

And why it Matters

Feature Selection. Why?

- The Intuition behind feature selection is to only provide features supporting the signal to an ML algorithm and suppress the features adding noise.
- Feature Selection is fundamentally different from feature elimination and dimensionality reduction:
 - Feature elimination eliminates the feature that adds the least value while examining against the remainder of features.
 - Dimensionality reduction does not eliminate any data, but alters the composition of the data in a mathematical way. The original data can be reconstructed out of the result.
 - Feature Selection selects the features that add value.

Feature Selection. Why?



Feature Selection. Is it necessary?

- Would a ML algorithm not disregard the unimportant features no matter what?
 - No. The intuition behind each ML algorithm is to fit to the data presented. This includes all the noise presented as well. The result is a model fitting to the data plus noise presented during training. Provisions in the algorithm can only limit the adverse effects to a degree, but not eliminate them.
 - Especially vulnerable are boosted algorithms, as these can't learn basic and learnable combinations of weak hypotheses when presented with random noise.
- Can tuning, cross-validation, train-test-validate split compensate for this?
 - To a certain extend. But it is computationally expensive to achieve small gains.

Feature Selection. How?

- One method is to add one feature out of all not included features at a time and evaluate which one results in the biggest improvement. Repeat until no further improvement can be achieved. (Forward Selection)
- One method is to subtract one feature out of all remaining features at a time and evaluate which one results in no or the least reduction in the result. Repeat until no feature can be removed without effecting the results. (Backward Elimination)
- Both these approaches have the negative effect of being effected by the actual data (overfitting), the sequence (of adding / subtracting features), the evaluation method used and the remainder of features.

Feature Selection. Then How?

- One method evaluates each feature against itself:
 - The feature to be evaluated is being copied as additional (shadow) feature into the same dataset.
 - The sequence of the values in this feature gets randomized.
 - The importance of the original feature and the shadow feature gets evaluated after several model runs. If the shadow feature has a higher or equal importance then the original feature, the original feature does not add value.
 - Repeat for each feature.

Feature Selection. Demo Notebook

Feature Selection. The Results:

Using MCC as evaluation metric

- Naïve approach: (using all data and default models): Best: 0.51 in 45 sec.
- Brute Force: (all data, parameter tuning in models): Best 0.72 in 99 hrs. (4 days, 3hrs.)
- Univariate Feature Selection: (selective data and default models): Best 0.63, in < 10 sec.
- Recursive Feature Elimination: (reducing data and default models): Best 0.61, in < 15 sec.
- Dimensionality Reduction: (modified data and default models): Best 0.55, in < 10 sec.
- Selecting important features: (selective data and default models): Best 0.60, in < 10 sec.
- Feature Selection: (only selection of data and default models): Best 0.77, in < 2 min.

Note: only deviation from default model is setting a random state for reproducibility and fair comparison

Feature Selection and Feature Engineering

And why it Matters

Feature Engineering. Why?

- Equalizing the signal strength between features to establish equal importance between features.
- Amplifying signal in features
- Abstracting timeless meaning to allow application of past configurations to current configurations
- Creating additional amplitude or distinction out of existing features
- Creating additional dimensionality
- Reducing dimensionality

Feature Engineering. Is it necessary?

More often than not, the data has features that have implicit meaning easily comprehensible to humans. But: ML algorithms don't have these capabilities (yet).

It is important to complement the implicit data with these explicit features to **ENABLE** the ML algorithms to utilize this information.

Feature Engineering is a vast field only limited by imagination. There are innumerable possibilities.

The following slides will be limited to a few basic approaches and ideas that can be used as starting points.

Feature Engineering. Is it necessary?

- If an important features is not presented, it can't be fitted.
- If one feature dwarfs other features with its numbers, it may dominate.
- If the signal is barely noticeable, it might not get picked up.
- If the meaning is hidden within data presented, but not extracted, it will not get picked up.

Feature Engineering. How?

Intuitive Approaches to Feature Engineering:

- Normalizing or standardizing features to eliminate range imbalances. Example: house price forecast (number bedrooms vs. sq.ft. house)
- Abstracting features to counter drift over time. Example: Harddrives / SSD in laptops, stock prices after stock split
- Amplifying values to pronounce importance of a signal. Example: analyzing faint radio signals or background noise in audio / visual data.
- Creating features out of existing data. Example: Creating Day-of-Week out of date for weekly pattern
- Creating additional dimensionality. Example: volume out of three dimensions
- Reducing dimensionality. Example: grouping data by region or grouping languages by family.

Feature Engineering. How?

Creative Approaches to Feature Engineering:

- Combining existing numerical features mathematically
- Chaining existing categorical features
- Grouping categories in dependence of available observations and additional dimensionality
- Creating categories based on statistically inferred threshold values in available data
- Combining categorical features to create a matrix of occurring combinations
- Use ML algorithm output based on a sub-selection of features as additional feature for a second stage (be wary of data leakage)

Complimentary Approaches to Feature Engineering:

- Add external data

Feature Engineering. Demo Notebook:

Feature Engineering. Results:

Using MCC as evaluation metric and selected Features

- Baseline: (default models): Best: 0.763 in < 2 min.
- Deep Dive: (modified feature selection, default models): Best 0.793 in < 10 sec.
- Standard Scaler: (modified feature selection, default models): Best 0.860, in < 10 sec.
- MinMax Scaler: (modified feature selection, default models): Best 0.834, in < 10 sec.
- PCA: (modified feature selection, default models): Best 0.777, in < 10 sec.
- Std Scaler plus PCA: (modified feature selection, default models): Best 0.857, in < 10 sec.
- MinMax Scaler plus PCA: (modified feature selection, default models): Best 0.824, in < 10 sec.
- Std Scaler, PCA, Std Scaler: (modified feature selection, tuned models): Best 0.863, in < 15 sec.

The results of 0.86 and 0.863 mean: 43 and 41 incorrectly classified observations or an error rate of 7.167% and 6.83% respectively (relative to the target which has deliberately flipped labels)

Note: only deviation from default model is setting a random state for reproducibility and fair comparison

Feature Engineering: Remarks

- The Boruta package utilized for Feature Selection is a convenient shortcut. The paper it is based on has a few shortcomings which result in inconsistent - and depending on the dataset unintentional - results. The implementation does not follow the paper and is at best a rough approximation on some of the core principles. Use cautiously and verify results.
- As demonstrated, a better feature selection is available.
- As demonstrated, Feature Selection and Feature Engineering outperform algorithm tuning by a wide margin, especially when combined.
- On this dataset, it is hard and taxed with significant effort to get two (2) observations more correctly classified.

Overall Results:

Using MCC as evaluation metric

- Naïve approach: (using all data and default models): Best: 0.51 in 45 sec.
- Brute Force: (all data, parameter tuning in models): Best 0.72 in 99 hrs. (4 days, 3 hrs.)
- Feature Selection: (default models): Best: 0.763 in < 2 min.
- Deep Dive: (modified feature selection, default models): Best 0.793 in < 10 sec.
- Standard Scaler: (modified feature selection, default models): Best 0.860, in < 10 sec.

Significant effort required to tune the parameters:

- Std Sclr, PCA, Std Sclr: (modified feature selection, tuned models): Best 0.863, in < 15 sec.

The Art of Feature Selection and Engineering

It Matters.

Thank you.