dm25s1

Topic 06 : Data Modelling

Part 02 : Column Encoding Scaling

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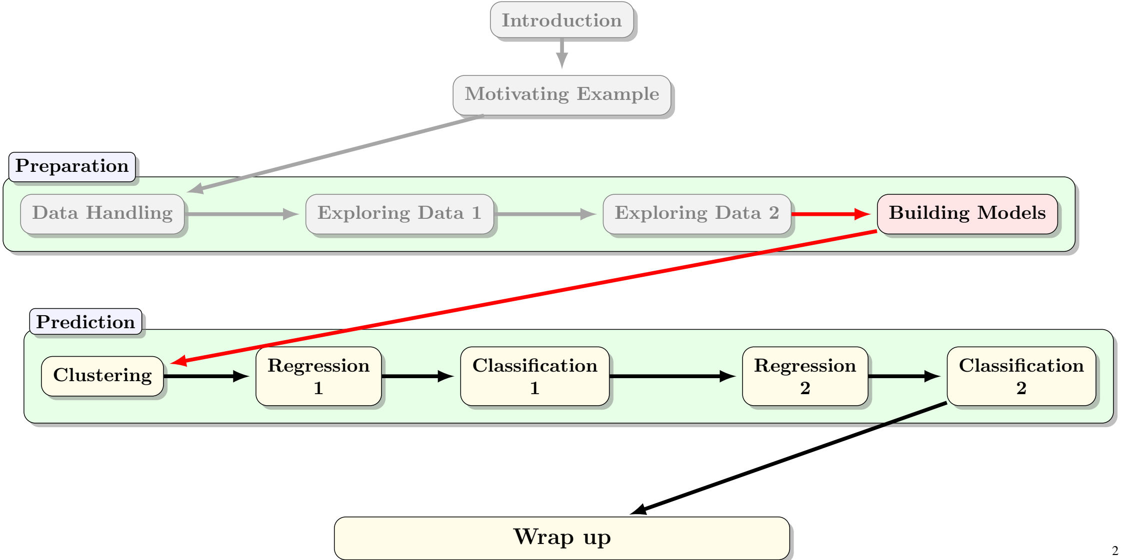
Outline

- Encoding categorical features, using pandas
- Scaling numeric features
- Looking ahead to feature preparation
- Overview of ML and what we have achieved

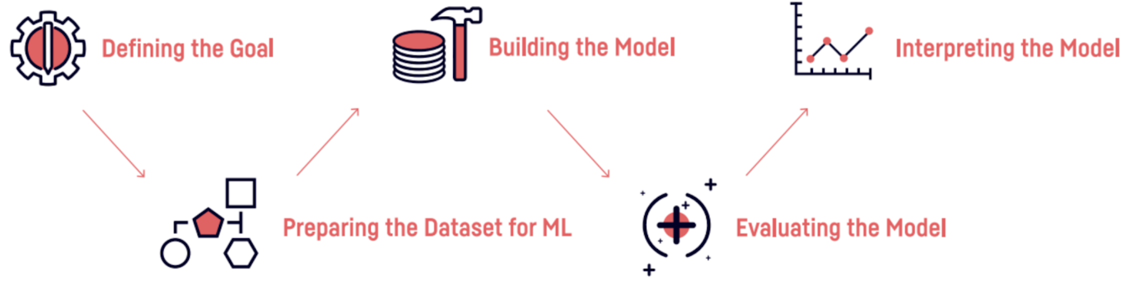
Data Mining (Week 6)



Outline

The Pipeline Metaphor

Model Building Pipeline



Source: Dataiku

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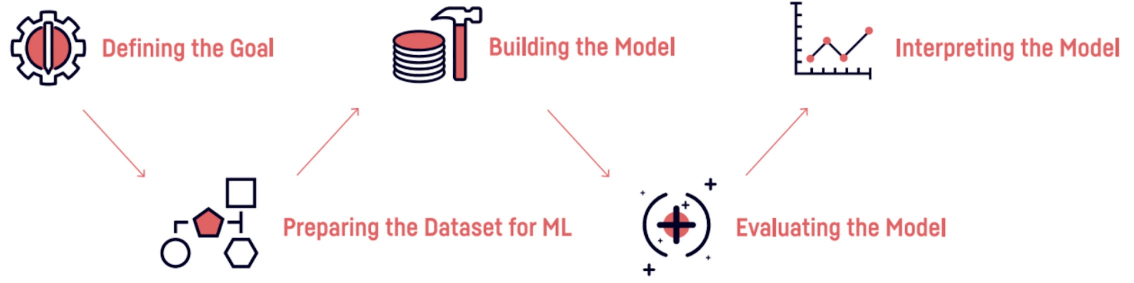

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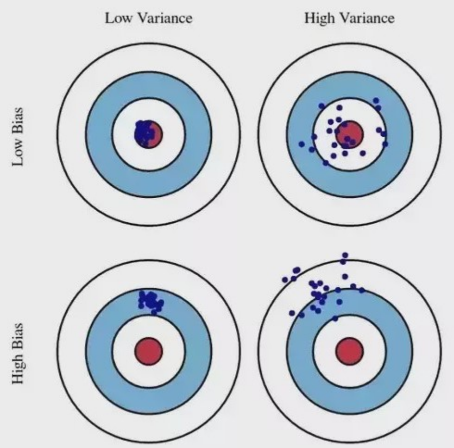
Comments

- We saw the first two stages in previous weeks
- This week we look at the remaining stages
- Of course this pipeline is a simplification. In reality it is iterative.

Bias-Variance and Total Error



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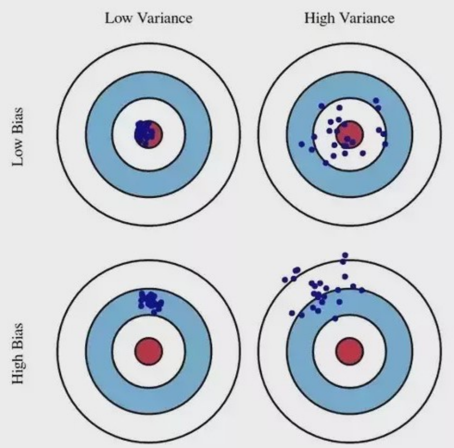

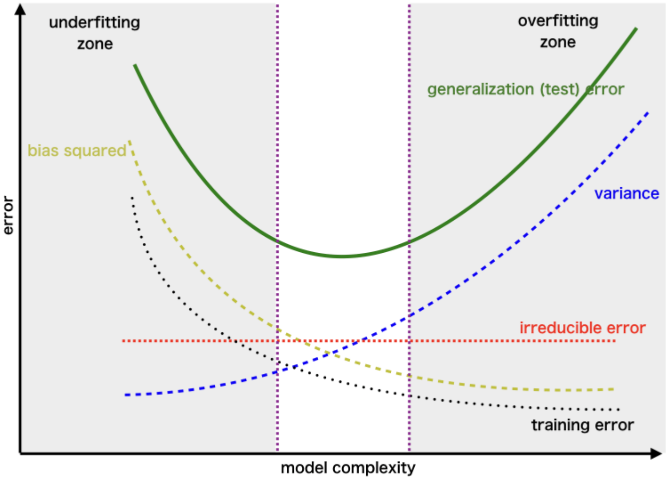

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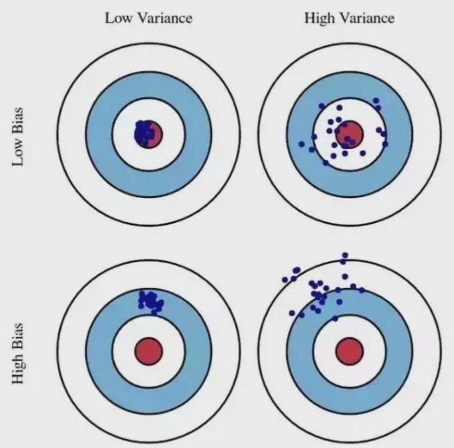

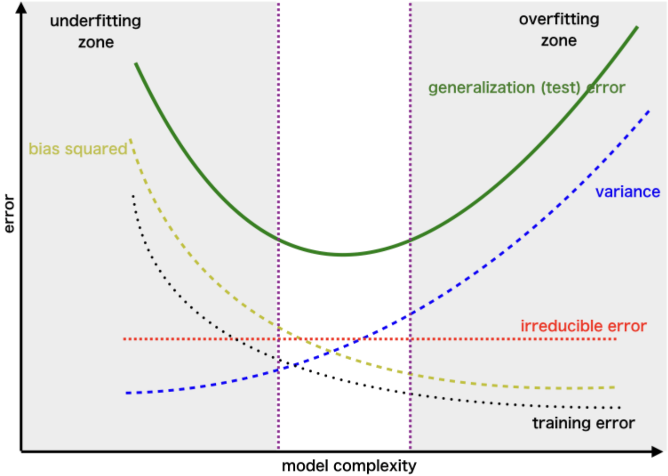

Look for parameters ***a*** that minimise the generalization error (estimated using the test set that was not used during training)

Example Model Types

Model	Applications	Concerns
Logistic Regression	X-ray classification	Regression with transformed variable
Fully connected networks	Classification	Classical ANN: choose encoding and size
Convolutional Neural Networks	Image processing	deep learning - choose segmentation
Recurrent Neural Networks	Voice recognition	ANN with feedback - how much?
Random Forest	Fraud Detection	Ensemble method - how many?
Reinforcement Learning	Learning by trial and error	Choose goal and penalties
Generative Models	Text, Image creation	Choose parameters
K-means	Segmentation	Choose distance function and k
k-Nearest Neighbors	Recommendation systems	Choose distance function and k
Bayesian Classifiers	Spam and noise filtering	Deal with imbalances

Outline

Using Categorical Features in (Logistic) Regression

How can Categorical-valued features participate in linear models?

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Given the following fragment of a dataset, where the goal is to predict the salary of employees in a large organisation:

```
df = pd.read_csv('data/team.csv',\
        index_col="Name")
df
```

	Role	Skilled	Salary
Name			
Alice	Designer	Yes	40000
Bob	Programmer	No	25000
Carol	Tester	No	30000

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How can this data be represented by a linear model, where all quantities must take numeric values?

Using pandas .getdummies() on a binary-valued column

```
dfSkilledDummies = pd.get_dummies(df['Skilled'],\
        prefix='Skilled',\
        dtype=int)
dfSkilledDummies
```

	Skilled_No	Skilled_Yes
Name		
Alice	0	1
Bob	1	0
Carol	1	0

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Note that a binary-valued column becomes 2 dummy columns

Reducing redundancy (by 1) in 2 dummy columns

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dfSkilledIndicators = pd.get_dummies(df['Skilled'],\
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	IsSkilled
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dfSkilledIndicators
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	IsSkilled
Name	
Alice	1
Bob	0
Carol	0

A single indicator column can replace a group of 2 dummy columns

Using pandas .getdummies() on a multi-valued column

```
dfRoleDummies = pd.get_dummies(df['Role'],\
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        dtype=int)
dfRoleDummies
```

	Role_Designer	Role_Programmer	Role_Tester
Name			
Alice	1	0	0
Bob	0	1	0
Carol	0	0	1

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```

	Role_Designer	Role_Programmer	Role_Tester
Name			
Alice	1	0	0
Bob	0	1	0
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Note that an n-valued column becomes n dummy columns

Reducing redundancy (by 1) in n dummy columns

```
dfRoleIndicators = pd.get_dummies(df['Role'],\
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        .rename(columns={\
        "Role_Programmer": "IsProgrammer",\
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dfRoleIndicators
```

	IsProgrammer	**IsTester**
Name		
Alice	0	0
Bob	1	0
Carol	0	1

Reducing redundancy (by 1) in n dummy columns

```
dfRoleIndicators = pd.get_dummies(df['Role'],\
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```

	IsProgrammer	**IsTester**
Name		
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$n-1$ indicator columns can replace a group of n dummy columns

Deriving and using dummy/indicator features

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- Build the model using the features in F.

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But what about. . .

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3. How do we handle data (that includes categocial columns) that is split into training and test?
4. How can we reverse the operation (i.e., return from (0,1)-valued columns to categorical columns)?

Outline

Training, test and valuation subsets: 3-way Holdout

Why Split?

Hold back some data to check how the model is doing.

- Training data is sample used to fit the model parameters.
- Test data is sample used to test the final model fitted to the training data.
- Validation data is sample used to test each interim model while tuning it.

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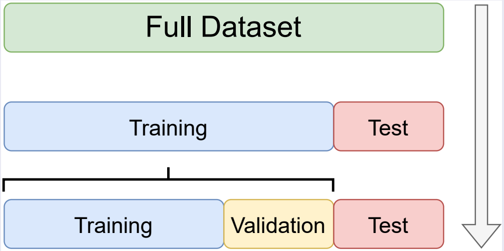
Typical Splits



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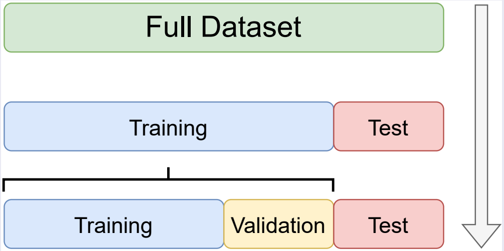
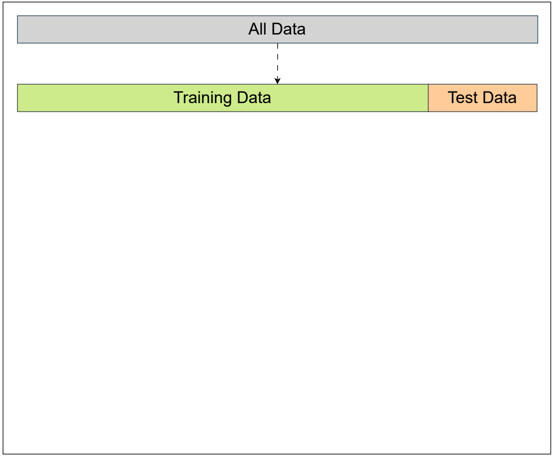


sklearn example

```
from sklearn.model_selection import train_test_split
trainVal, test = train_test_split(df, test_size=0.2, seed=42)
train, validation = train_test_split(trainVal, test_size=0.1)
```

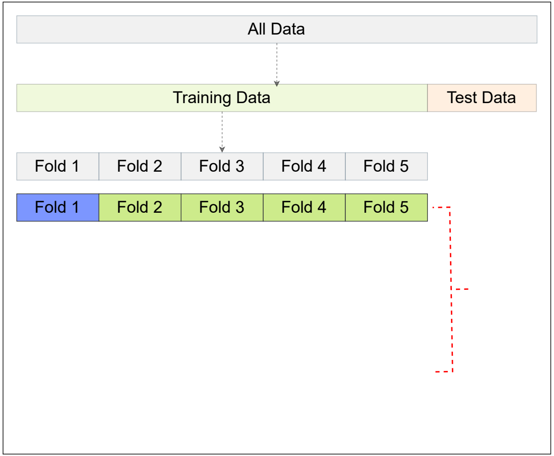
K-fold cross validation - preparation



Before Cross Validation

- Perform the train-test split
- Using the Training Set only
  - Perform 3-pass EDA
  - Encode the categorical features
  - Scale the numerical features
  - Other feature engineering steps. . .

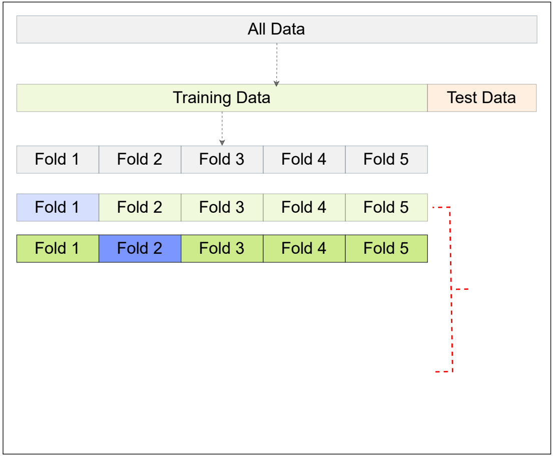
K-fold cross validation - initialise, pass 1



Initialise and perform first pass

- Randomly split the training set into K folds
- In the diagram, $K = 5$ but $K = 10$ is common
- In the first pass, set $i = 1$
- Fold $i = 1$ is held back for validation
- Folds $i = 2, \ldots, K$ are used to train a model, giving parameters $\boldsymbol{a}^{(1)}$.
- The model is evaluated against fold $i = 1$
- The distance between the actual and predicted targets is calculated and recorded as $d^{(1)}$.

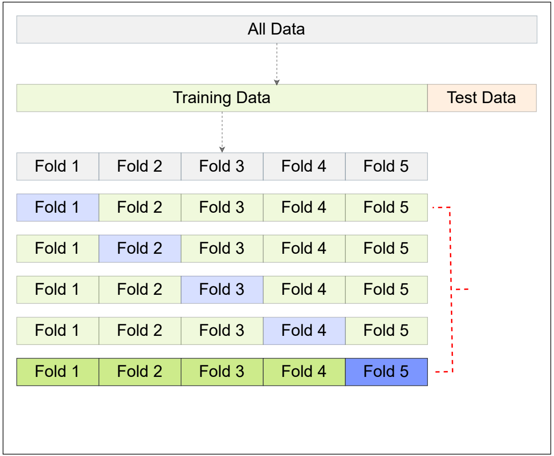
K-fold cross validation - initialise, pass 2



Perform second pass

- In the second pass, set $i = 2$
- Fold $i = 2$ is held back for validation
- Folds $i = 1, 3, \ldots, K$ are used to train a model, giving parameters $\boldsymbol{a}^{(2)}$.
- The model is evaluated against fold $i = 2$
- The distance between the actual and predicted targets is calculated and recorded as $d^{(2)}$.
- The parameters $\boldsymbol{a}^{(2)}$ and distance $d^{(2)}$ are recorded.

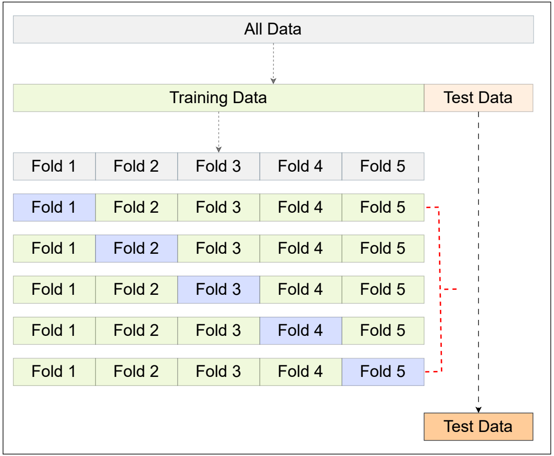
K-fold cross validation - initialise, pass $K = 5$



Perform last pass

- In the last pass, set $i = K$
- Fold $i = K$ is held back for validation
- Folds $i = 1, \ldots, K - 1$ are used to train a model, giving parameters $\boldsymbol{a}^{(\mathrm{K})}$.
- The model is evaluated against fold $i = K$
- The distance between the actual and predicted targets is calculated and recorded as $d^{(\mathrm{K})}$.
- The entire training set was used to learn the "average" parameters $\boldsymbol{a}$
- We also have an estimate of the distribution of the prediction error d, so can compare hyperparameters

K-fold cross validation - using the results



Finding and using the best model

- Typically cross validation is used to compare effects of hyperparameters
- Use the setting(s) with the lowest cross-validation error
- Given this "best" model, we can predict the test targets
- We can then compute the prediction error on the test set, as before

K-fold cross validation

sklearn example

```python
from sklearn.model_selection import cross_val_score
# clf is some classifier, X and y are the features and target of the training set
scores = cross_val_score(clf, X, y, cv=5)
```

- `scores` is a $k = 5$ element array, can be used to estimate the prediction error (or other score) while building a model
- Details of cross validation are hidden...

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Featuring engineering 1: Scaling of numerical variables

Scaling - what it does

- If numeric features have different scales, e.g. [-0.005, -0.003] and [10000, 10001] some terms dominate, others are "lost"
- Better: transfer the scaling from the feature to the model parameter
- A min-max scaling is often a good choice:

$$\tilde{X} = \frac{X - X_{\text{min}}}{X_{\text{max}} - X_{\text{min}}}$$

- Note that X is in the range $[X_{\text{min}}, X_{\text{max}}]$ but $\tilde{X}$ is in the range $[0, 1]$.
- Other options include StandardScaler (subtract mean and divide by standard deviation) and a max-abs scaler (scales to [-1,1])

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sklearn example

```
from sklearn.preprocessing import MinMaxScaler
# df is a dataframe with numeric features
scaler = MinMaxScaler()
dfScaled = scaler.fit(df))
```

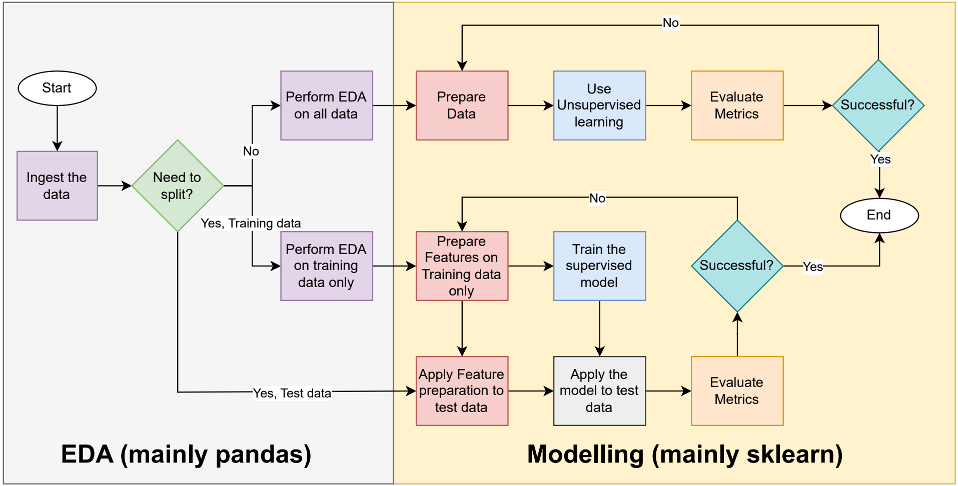
`dfScaled` can be used instead of `df` with the advantage that the fitted parameters are more accurate.

Feature Engineering 2: Choice of Features

- How many to include? Use metrics to decide. Will see some when considering regression and classification.
- How do we handle different feature types? Need to encode categorical variables.
- Can we derive new numeric features? Yes, $f' = \log(f)$ etc. is possible

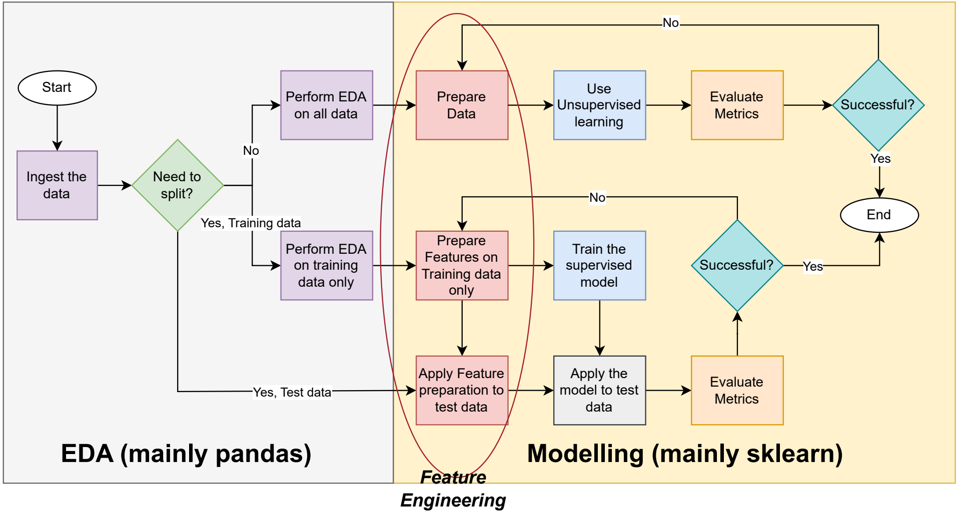
Outline

An overview of Machine Learning



On first glance, this might seem overwhelming, but note that the boxes are colour-coded, so that related operations share the same colour.

Where feature preparation fits. . .



NB: Feature preparation is informed by EDA *but is not part of EDA*.

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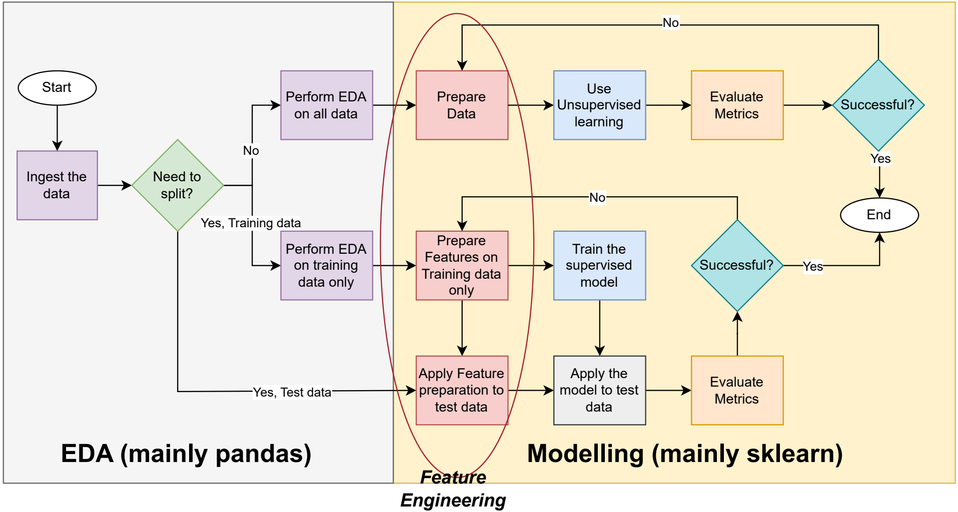

NB: Feature preparation is informed by EDA *but is not part of EDA*. So, not part of your EDA assignment!

Feature Engineering more generally

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- Can also rescale numerical columns, or encode more exotic columns (other datatypes, computed columns, . . .)
- As seen in the schematic, if an ML procedure is unsuccessful, more feature engineering should be considered - it can help.

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- In subsequent weeks we will put this theory into practice.

Outline

Resources

- **A Summary of the Basic Machine Learning Models**
  towardsdatascience.com/a-summary-of-the-basic-machine-learning-models-e0a65627ecbe

- **Train-Test Split for Evaluating Machine Learning Algorithms**
  https://machinelearningmastery.com/train-test-split-for-evaluating-machine-learning-algorithms
  This week I have focused on the theory rather than its (python) implementation. This is a nice article that covers the implementation side of things.

- **Cross-Validation: Estimator Evaluator**
  medium.com/swlh/cross-validation-estimator-evaluator-897d28afb4ff
  Nice article that covers cross-validation in a lot more detail — we will be using many of these variants in later weeks, especially k-fold stratified.