Data Wrangling

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Course Outline

Model Building Process

1. **Assemble** a modeling sample.
2. **Create** the target variable.
3. **Create** attributes.
4. **Explore** data (EDA).
5. **Transform** attributes (trim, impute, etc.).
6. **Select** attributes (aka Feature Selection).
7. **Train** and **test** the model.
8. **Select** the best model.
9. **Validate** the model.
10. ...

DATA PREPARATION

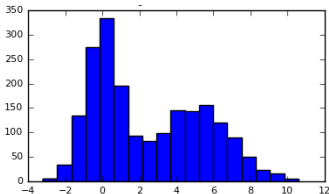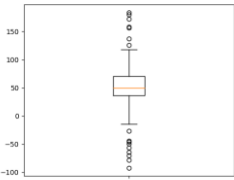**DATA WRANGLING**

DATA MUNGING

FEATURE ENGINEERING
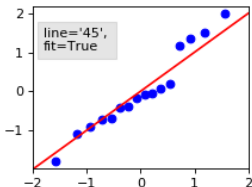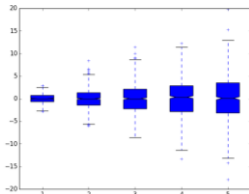
Summary Statistics
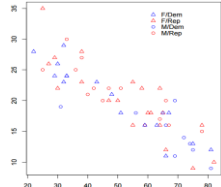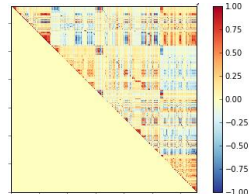
For each **numeric** variable in the training data set, calculate the following statistics:

1. Mean,
2. Median,
3. Mode,
4. Min and max,
5. Standard deviation,
6. Percentile values (1st, 2nd, 98th, 99th),
7. Cardinality (number of distinct values),
8. Kurtosis, and
9. Percent missing values (% of training data set that contain missing).

For each **categorical** variable in the training data set, calculate the following:

1. Cardinality (number of distinct values)
2. Count of records (rows) within each level (value) of the categorical variable,
3. Percent of records within each level, and
4. Target even rate for each level.

Exploratory Data Analysis (EDA)

	Univariate	Multivariate

Non-Graphical	o Categorical: Tabulated frequencies
	o Quantitative:
	    o Central tendency: mean, median, mode
	    o Spread: Standard deviation, inter-quartile range
	    o Skewness and kurtosis
		o Cross-tabulation
		o Univariate statistics by category
		o Correlation matrices

Graphical	o Histograms o Box plots, stem-and-leaf plots o Quantile-normal plots 	o Univariate graphs by category (e.g., side-by-side box-plots) o Scatterplots o Correlation matrix plots

Trimming

○ Variable trimming can help improve model stability by reducing the influence of extreme values the data.

○ To decide which variables contain extreme values, you can use **kurtosis**. A high kurtosis value suggests **flat tail(s)** in the distribution.

○ Steps for trimming:

1. From the descriptive statistics of all numeric variables, identify variables that have a kurtosis value **higher than 10**[†], and apply trimming and/or capping on those variables as explained in the next steps.
2. **Capping**: Replace extremely high values – i.e., values that exceed the variable's **99th percentile**[†] value – with the **99th percentile**[†] value.
3. **Flooring**: If the variable contains extreme negative values, and if a negative value exceeds the variable's **1st percentile**[†] value, then replace the extreme negative value with the **1st percentile**[†] value.

[†]These are suggested threshold values; change these values as needed.

Missing Values

1. Some statistical methods and data mining algorithms (e.g., linear regression, Support Vector Machines) are **unable to handle** missing values.

2. Missing data introduces **complications** in analyzing and processing (imputing) missing values.

3. Improper handling of missing values may introduce **bias** in the analysis.

Reasons for Missing data

1. **Not applicable**

   o Data usage for telecom customers who are voice-only users

   o Loan balance amount for a customer who never had a loan

2. **Not reported or provided**

   o Information not provided in the application form (e.g., race, ethnicity)

3. **Undefined**

   o Division by zero

4. **Not available**

   o Unknown reason

Sometimes missing data are denoted by specific (usually extreme) values. Each value indicates a different reason for why the data is missing.

Example: Total number of trades with derogatory occurred in the last 12 months including collections:
{**0-90**: valid values, **99**: No trade including collections, **97**: No trade reported within timeframe required}

Missing Data Mechanisms

Random

Missing Completely at Random (MCAR)

Missing at Random (MAR)

Non-random

Missingness depends on unobserved predictors

Missingness depends on missing value itself

Missing Completely at Random (MCAR)

The reason for missing values

is **completely independent**

of all other features.

In other words,

the probability of missing value

is the same for all records in the dataset.

This is an unlikely scenarios for most real-world datasets.

Missing (Conditionally) at Random (MAR)

Missingness is **dependent** on

other available features.

In practice, this is hard to know.

If you know which features the missingness is dependent on[†],

then including those features in the model

would eliminate the potential bias.

[†] One could model this process as a logistic regression model, where the target variable is 1 for missing cases and 0 otherwise.

Missing Not at Random: MNAR I

Missingness is **dependent** on

unobserved (unavailable) features.

E.g., if a particular medical treatment causes discomfort,

a patient is more likely to drop out of the study.

This missingness is not random,

unless the level of "discomfort" is measured and observed for all patients.

If missingness is not at random, it must be explicitly modeled,

or else you must accept some bias in your inferences.

Missing Not at Random: MNAR II

Missingness is **dependent** on *itself*.

E.g., people with high income are less likely to report their income.

If missingness is not random and is dependent on itself,

it can be explicitly modeled to reduce some of the bias.

Complete-case analysis

	A	B	C	D	E
1	5	3	4	4	
2	3	1	2	3	3
3	4		4	3	5
4	3	3	1	5	4
5	1	5	5	2	4

A direct and naïve approach is to exclude records that contain missing value(s).

NOT RECOMMENDED!

Instead, impute missing values.

Mean (or Median) Imputation

	A	B	C	D	E
1	5	3	4	4	**4**
2	3	1	2	3	3
3	4	**3**	4	3	5
4	3	3	1	5	4
5	1	5	5	2	4

Impute missing values with the mean (or median) of the observed values of that variable..

POTENTIAL ISSUES?

- Distorts the distribution of the imputed variable
- Usually, reduces the correlation with the target variable

Imputation Using Other Features

	Square Footage	# of Bedrooms
1	1,019	**3**
2	3,273	4
3	1,162	3
4	1,106	3
5	1,806	4

Impute missing values with the observed value from another, similar record ("hot deck" imputation).

POTENTIAL ISSUES?

- May propagate measurement errors
- May not be the optimal, "correct", imputation value

Multiple (Multivariate) Imputation

	A	C	D	E
1	5	4	4	?
2	3	2	3	3
3	4	4	3	5
4	3	1	5	4
5	1	5	2	4

$$X = \begin{bmatrix} 3 & 2 & 3 \\ 4 & 4 & 3 \\ 3 & 1 & 5 \\ 1 & 5 & 2 \end{bmatrix} \quad\quad y = \begin{bmatrix} 3 \\ 5 \\ 4 \\ 4 \end{bmatrix}$$

(Columns of X: A, C, D; column of y: E)

POTENTIAL ISSUES?

- Computationally intensive
- Dependent on how accurate the models are
- Difficult to put into production

Step 1 Build a model (e.g., regression) with all features that contain non-missing data as predictors and the feature that contain missing data as the target feature.

Step 2 Use this model to predict the missing value(s) for the target feature and use those predictions for imputation.

Missing Value Indicators

	A	B	C	D	E	B_Miss	E_Miss
1	5	3	4	4	4	0	1
2	3	1	2	3	3	0	0
3	4	3	4	3	5	1	0
4	3	3	1	5	4	0	0
5	1	5	5	2	4	0	0

Create missing value indicators for each variable that contain missing values: 1 if missing, 0 otherwise.

Autonomous Race Car Starts Test Lap, Immediately Slams Into Wall

And we mean immediately.

BY PETER HOLDERITH OCTOBER 29, 2020

[W]hile the team did code in many fail-safes in other areas of the application, it unfortunately only contained data validation on valid numbers—and as you recall, an `NaN` value is not a valid number, meaning that validation would not be performed on it.
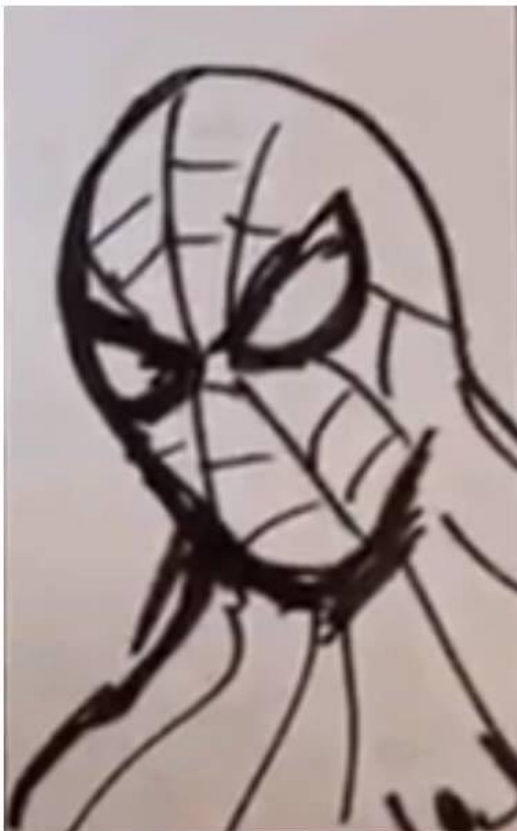
Standardize Features

O Attribute values are adjusted for differing level and spread.

  O E.g., standard (z) score: subtract the mean and divide by standard deviation

O Standardization does not impact the shape of the distribution.

O Standardization makes the interpretation of coefficients easier in regression models.
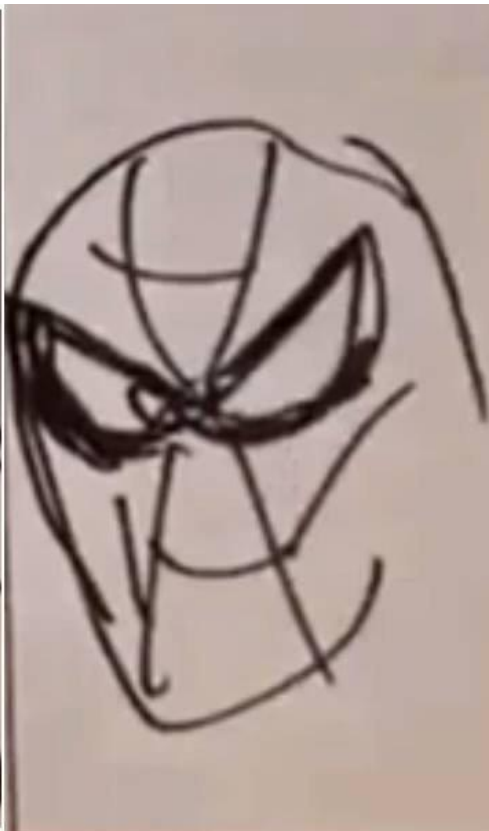
Box-Cox Transformations

○ Transformations may improve the linear correlations with the target

○ **Examples**: Log, inverse, root, square root

   ○ **Log:** Reduces right-skewness. Can be useful for diminishing-return type relationships.

   ○ **Inverse:** Drastic impact on distribution shape. Sometimes it improves interpretation (e.g., 'purchase frequency per year' becomes 'days between purchases')

   ○ **Root:** Reduces right-skewness. Unlike 'log', roots can be applied to zero.

   ○ **Square:** Reduces left-skewness. Can be used to fit a model with quadratic relationship, e.g., $y = \alpha + \beta_1 x + \beta_2 x^2$.

Kaggle Local Cross-validation — **Kaggle Public Leaderboard** — **Kaggle Private Leaderboard** — **Real World Unseen Data**

1. Not standardizing the features
2. Incorrect standardization approach
3. Improper handling of missing values
4. Insufficient handling of categorical data
5. **Lack of feature reduction (or selection)**
6. Wrong feature selection approach
7. Information leakage
8. Using the wrong training sample
9. Flawed target definition
10. Incorrect usage (or lack of) hold-out sample
11. Using the wrong accuracy measure to select the best model
12. Lack of Exploratory Data Analysis (EDA)
13. Lack of consultative approach

Feature Reduction

○ **Feature Reduction:** The process of selecting a subset of features to be used in model construction

   ○ Pre-processing of data in machine learning

   ○ Useful for both supervised and unsupervised learning problems

Art is the elimination of the unnecessary.

— Pablo Picasso

Why Not This?

1

```python
import pandas as pd


X = pd.read_csv('C:\train.csv')
y = X['target']
```

2

```python
from sklearn.linear_model import LogisticRegression

clf = LogisticRegression().fit(X.pop('target'), y)
```

The kitchen sink approach

Because...

- **True dimensionality $<<$ Observed dimensionality**
  - Redundant and irrelevant features are in abundance.
- **Curse of dimensionality**
  - With a fixed number of training samples, the predictive power reduces as the dimensionality increases. (Hughes phenomenon)
- **Goal of the Analysis**
  - Descriptive → Diagnostic → Predictive → Prescriptive

Hindsight	**Insight**	**Foresight**

- **Law of Parsimony** (Occam's Razor)
  - Other things being equal, simpler explanations are generally better than complex ones.
- **Overfitting** (The Bias-Variance trade-off)
- **Execution time** (Algorithm and data processing)
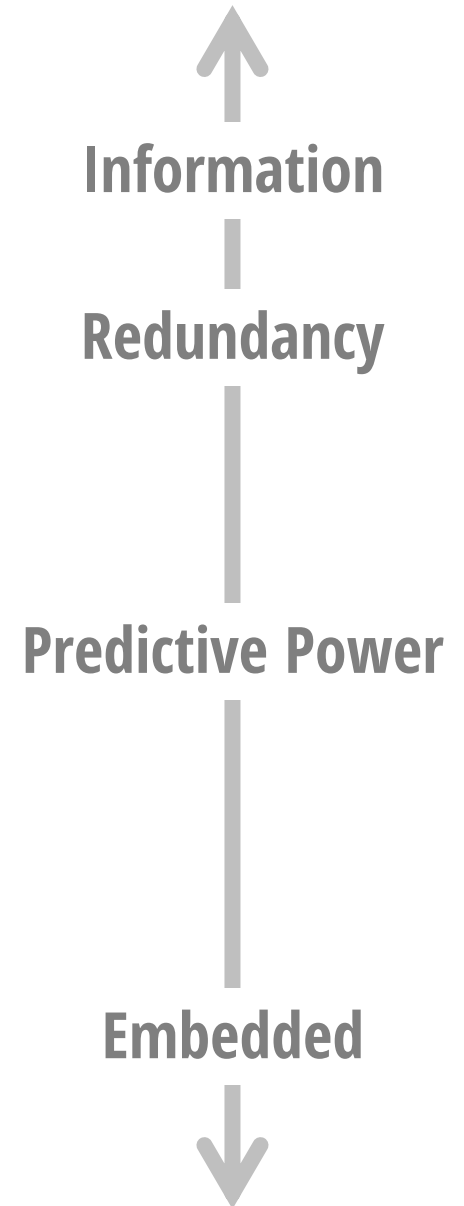- **Points of failure**

Feature Reduction Techniques

Filtering Approaches

1. Amount of variation
2. Percent missing values
3. Pairwise correlation
4. Multicolinearity
5. Principal Component Analysis (PCA)
6. Cluster analysis

Wrapper Approaches

7. Correlation (with the target)
8. Forward selection
9. Backward elimination
10. Stepwise selection
11. LASSO
12. Tree-based selection

Information

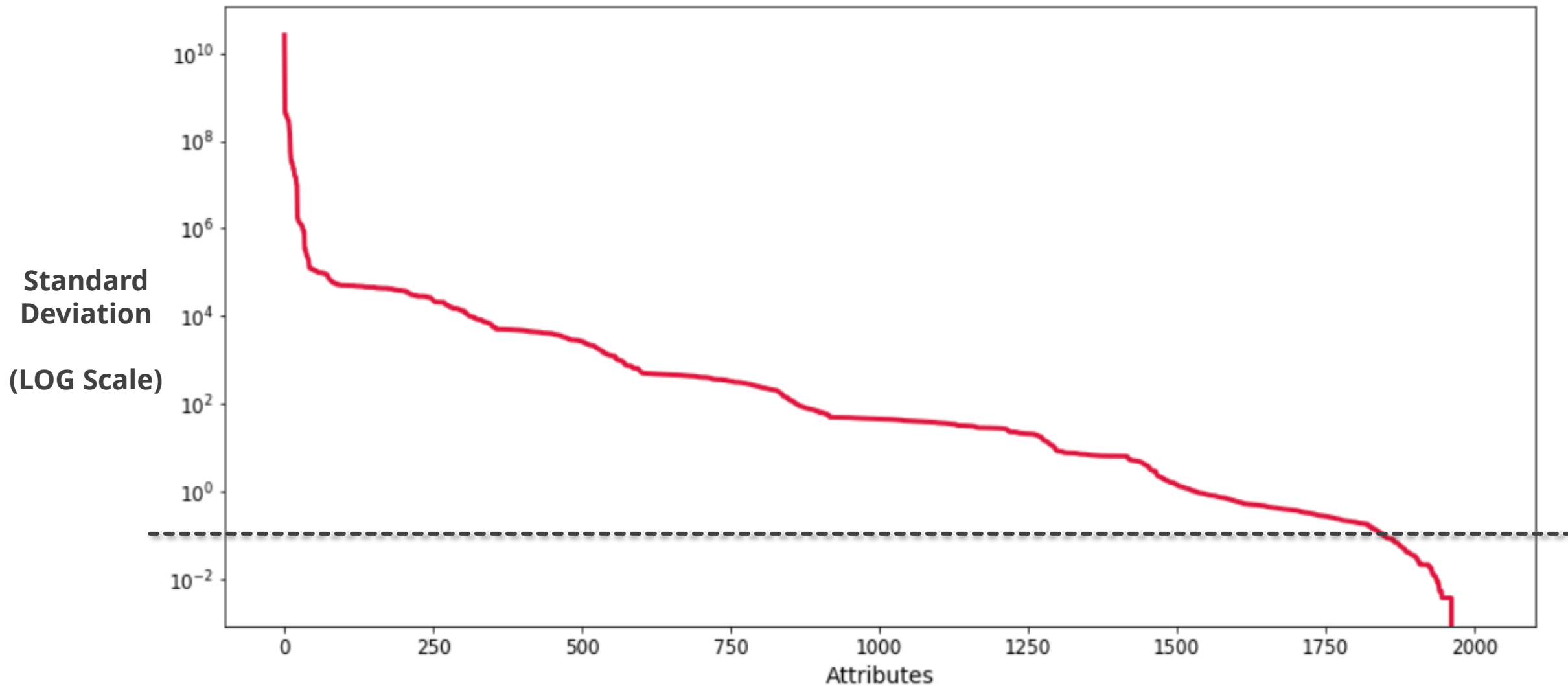Redundancy

Predictive Power

Embedded

○ Drop or review variables that have a **very low standard deviation**.

  ○ Drop variables with zero variation (unary variables), if any.

Standard Deviation

Less than 1

Drop features with zero variation

○ Drop variables that have a very **high % of missing values**.

    ○ Number of records with missing values / Number of total records

○ Create **binary indicators** to denote missing (or non-missing) values.

○ Review or visualize variables with high % of missing values.

○ Many variables are often correlated with each other, and hence one of them is possibly redundant.

○ If two variables are **highly correlated**, keeping only one will help reduce dimensionality without much loss of information.

○ **Which variable to keep?**

    ○ The one that has a higher correlation coefficient **with the target**.

1 Identify pairs of highly correlated variables.

	x_1	x_2	x_3	x_4
x_1	1.00	0.15	0.85	0.01
x_2		1.00	0.45	0.60
x_3			1.00	0.17
x_4				1.00

Correlation tolerance ≈ 0.85

1 Identify pairs of highly correlated variables

	x_1	x_2	x_3	x_4
x_1	1.00	0.15	0.85	0.01
x_2		1.00	0.45	0.60
x_3			1.00	0.17
x_4				1.00

Correlation tolerance ≈ 0.85

2 Discard variable that has a weaker correlation with the target

	y
x_1	0.67
x_2	0.82
x_3	0.38
x_4	0.25

1 Identify pairs of highly correlated variables.

2 Discard variable that has a weaker correlation with the target.

	x_1	x_2	x_3	x_4
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x_4				1.00

Correlation tolerance ≈ 0.85

	y
x_1	0.67
x_2	0.82
x_3	0.38
x_4	0.25

Keep x_1, Discard x_3

○ When two **or more** variables are highly correlated with each other.

○ Dropping one or more variables should help reduce dimensionality without a substantial loss of information.

○ Which variable(s) to drop?

  ○ Use Condition Index.

Eigenvalue Decomposition

	x_1	x_2	x_3	x_4
x_1	1.00	0.15	0.85	0.01
x_2		1.00	0.45	0.60
x_3			1.00	0.17
x_4				1.00

Condition Index	x_1	x_2	x_3	x_4
$u_1 = 1.0$	0.01	0.05	0.00	0.16
$u_2 = 16.5$	0.03	0.12	0.01	0.19
$u_3 = 28.7$	0.05	0.02	0.13	0.25
$u_4 = 97.1$	0.93	0.91	0.98	0.11

Condition Index tolerance ≈ 30

	x_1	x_2	x_3	x_4
x_1	1.00	0.15	0.85	0.01
x_2		1.00	0.45	0.60
x_3			1.00	0.17
x_4				1.00

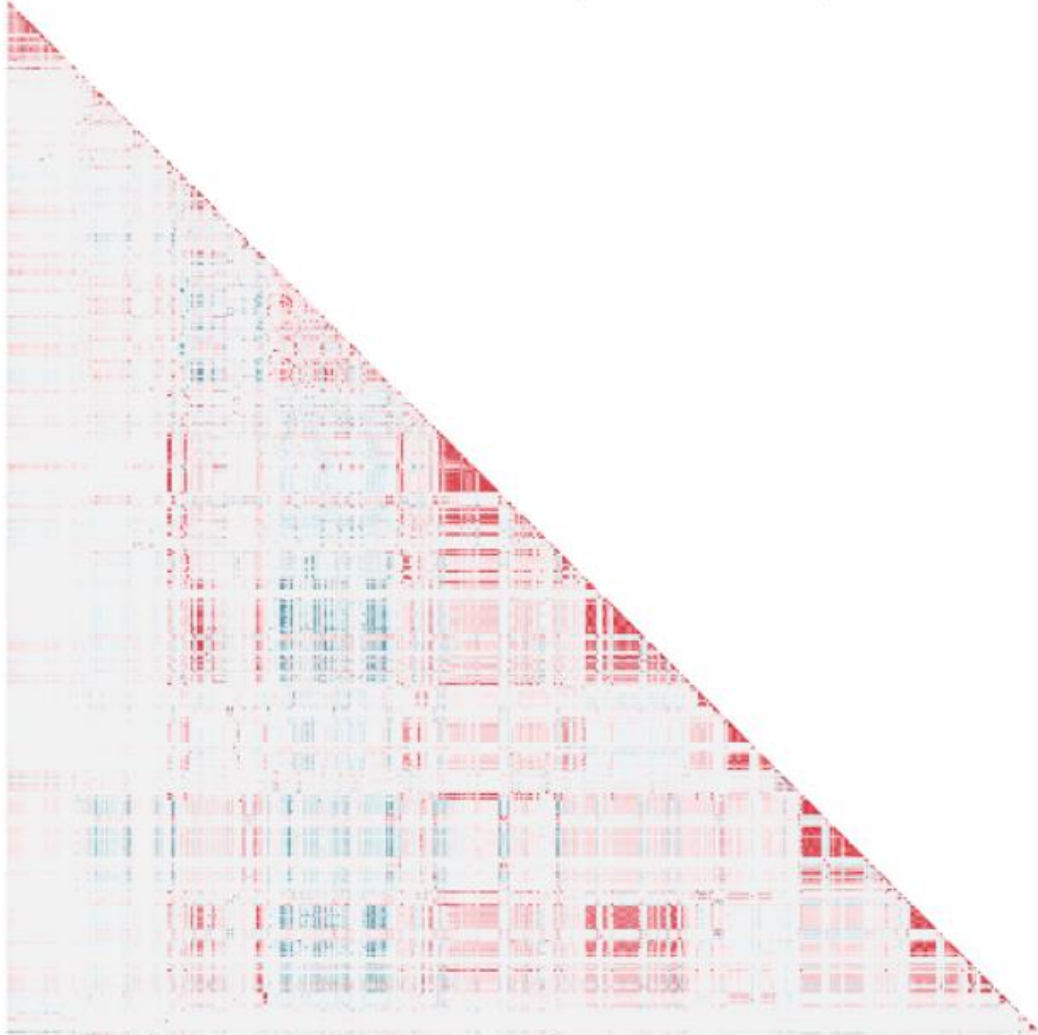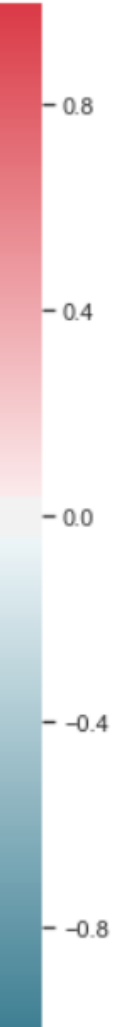| Condition Index	x_1	x_2	x_3	x_4
$u_1 = 1.0$	0.01	0.05	0.00	0.16
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$u_3 = 28.7$	0.05	0.02	0.13	0.25
$u_4 = 97.1$	0.93	0.91	0.98	0.11

Discard x_3, Iterate

Condition Index tolerance ≈ 30

CORRELATION MATRIX (1667 FEATURES)

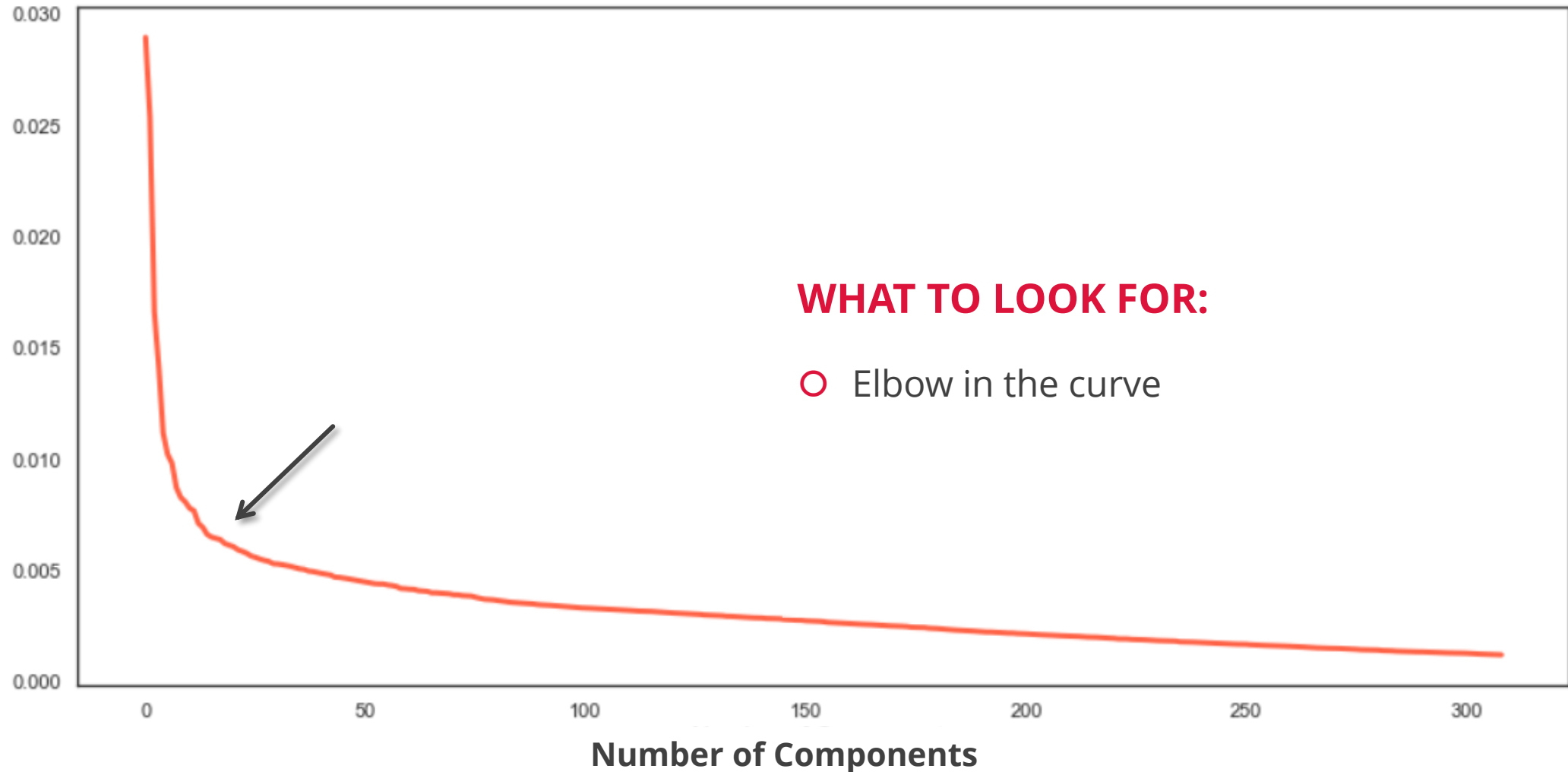CORRELATION MATRIX (309 FEATURES)

81% reduction in dimensionality!

○ A dimensionality reduction technique which emphasizes **variation**

○ Eliminates multicollinearity – but **explicability** is compromised.

○ Works independently from the (supervised) learning task.

○ When to use:

  ○ Excessive multicollinearity

  ○ Explanation of the predictors is not important.

  ○ A slight overhead in implementation is okay.

% Variance Explained

WHAT TO LOOK FOR:

○ Elbow in the curve

Number of Components

% Variance Explained

Cumulative % Variance Explained

WHAT TO LOOK FOR:

- Cumulative % Variance Explained
- Eigenvalue ≥ 1
- Number of components retained

Number of Components
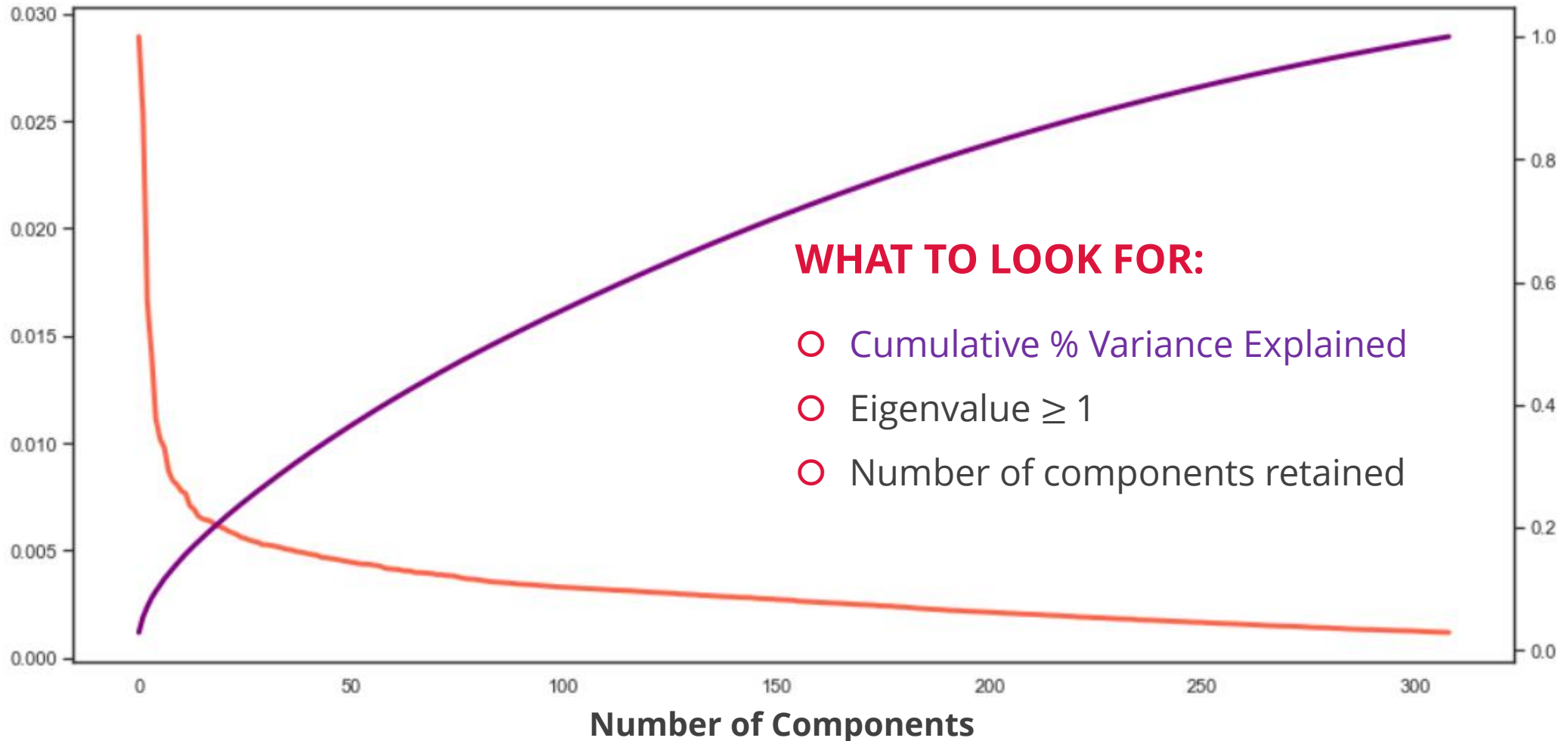
○ A dimensionality reduction technique which emphasizes **correlation** (or, similarity).

    ○ Identify groups of variables that are as correlated as possible among themselves and as uncorrelated as possible with variables in other clusters.

○ Reduces multicollinearity – and explicability is not compromised.

```python
from sklearn.cluster import FeatureAgglomeration

var_clus = FeatureAgglomeration(n_clusters=50)

X_clus = var_clus.fit_transform(X_scaled)
```

○ This returns a pooled value for each cluster (i.e., the centroids), which can then be used to build a supervised learning model.

○ You can choose one variable from each cluster that is the most representative of that cluster.

     ○ Use $1 - R^2$ ratio to select the most representative variable from each cluster.
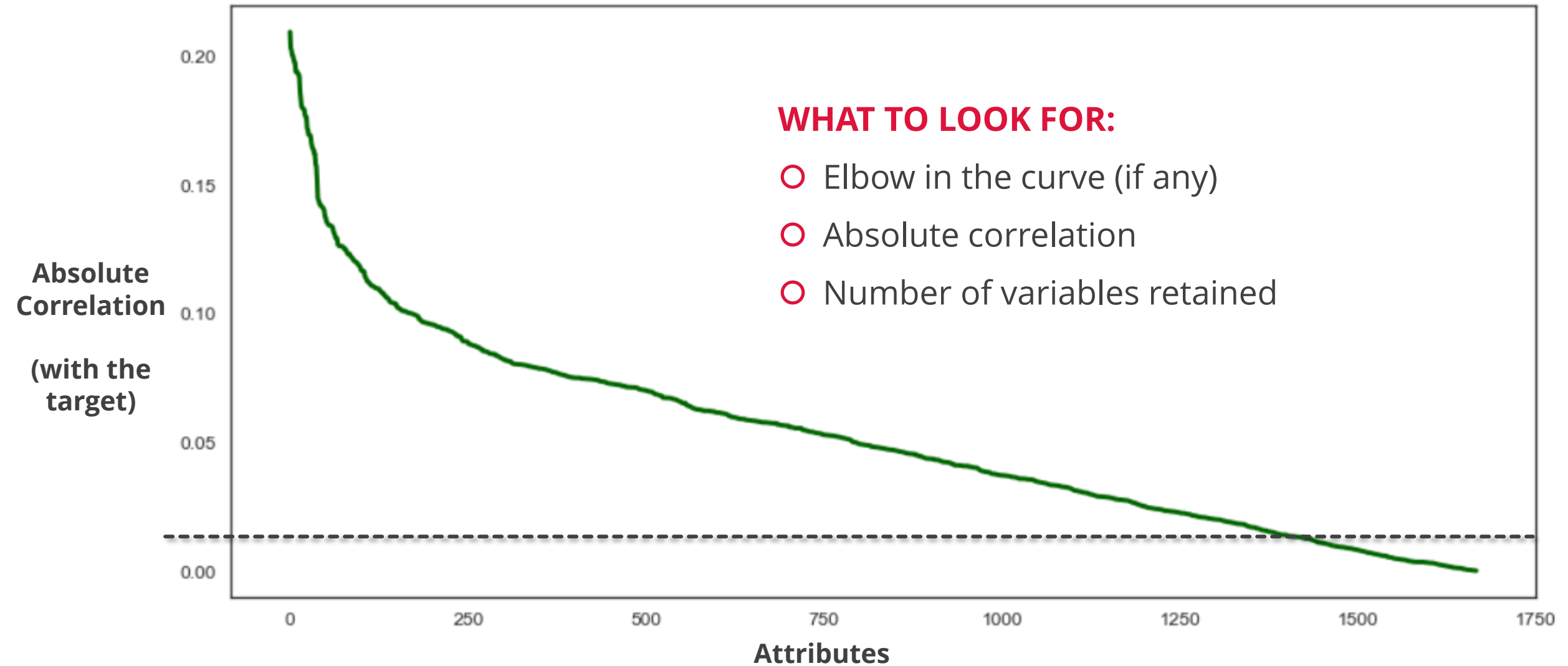
○ Drop variables that have a very low correlation with the target.

   ○ If a variable has a very low correction with the target, it's not going to useful for the model (prediction).

○ Caveat: **Linear** correlations

WHAT TO LOOK FOR:

○ Elbow in the curve (if any)

○ Absolute correlation

○ Number of variables retained

○ **Forward Selection**

1. Identify the **best** variable (e.g., based on model accuracy).

2. **Add** the next best variable into the model.

3. And so on until some predefined criterion is satisfied.

○ **Backward Elimination**

1. Start with **all** variables included in the model.

2. **Drop** the least useful variable (e.g., based on the smallest drop in model accuracy).

3. And so on until some predefined criterion is satisfied.

○ **Stepwise Selection**

○ Similar to forward selection process, but a variable can also be dropped if it's deemed as not useful anymore after some steps.

○ **L**east **A**bsolute **S**hrinkage and **S**election **O**perator

○ Two birds, one stone: Variable Selection + Regularization

```
lasso = LogisticRegression(C=1.0, penalty='l1', random_state=314)
```

OLS

$$\arg\min_{\beta} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

OLS

$$\arg\min_{\beta} \sum_{i=1}^{n} (y_i - (\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}))^2$$

LASSO

$$\arg\min_{\beta} \sum_{i=1}^{n} (y_i - (\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}))^2 + \lambda \sum_{j=1}^{p} |\beta_j|^2$$

λ controls the amount of (L_1) regularization.

LASSO

$$\underset{\beta}{\arg\min} \sum_{i=1}^{n} (y_i - (\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}))^2 + \lambda \sum_{j=1}^{p} |\beta_j|^2$$

- λ controls the amount of (L_1) **regularization**.

- If $\lambda = 0$ then the LASSO model is identical to OLS.

- If $\lambda > 1$ then a coefficient can increase only if it leads to a reduction in the Residual Sum of Squares (RSS for the OLS part).

- If $\lambda = 1$ then a coefficient can increase by a certain amount only if it leads to the same amount of reduction in the RSS.

- Making λ sufficiently large will result in some of coefficients exactly equal to zero, aka feature reduction!

○ Use a **forest** of trees to evaluate the importance of features.

○ Fit a number of randomized decision trees on various sub-samples of the dataset and use `_feature_importances` to select features.

FEARURE REDUCTION: WORKFLOW