

AIS477: S.T. in Artificial Intelligence

Lecture 4

# Feature Engineering, Transformation and Selection



# Welcome

# Feature Engineering



# Introduction to Preprocessing

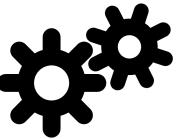
"Coming up with features is difficult, time-consuming, and requires expert knowledge. Applied machine learning often requires careful engineering of the features and dataset."

—Andrew Ng

### Outline

- Squeezing the most out of data
- The art of feature engineering
- Feature engineering process

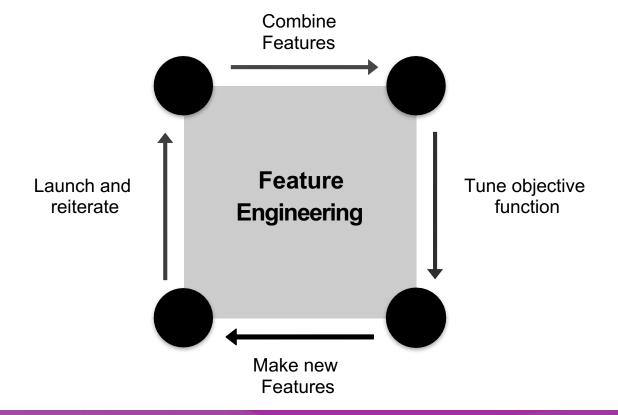




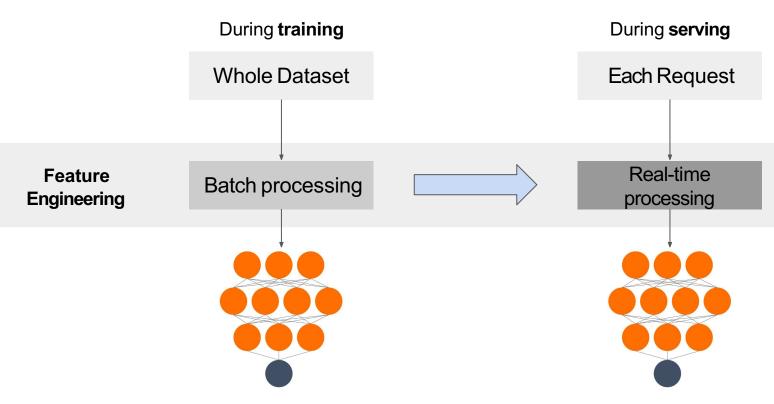
### Squeezing the most out of data

- Making data useful before training a model
- Representing data in forms that help models learn
- Increasing predictive quality
- Reducing dimensionality with feature engineering

### Art of feature engineering



## Typical ML pipeline



### Key points

- Feature engineering can be difficult and time consuming, but also very important to success
- Squeezing the most out of data through feature engineering enables models to learn better
- Concentrating predictive information in fewer features enables more efficient use of compute resources
- Feature engineering during training must also be applied correctly during serving

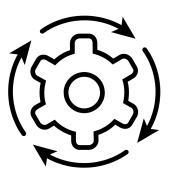
# Feature Engineering



# Preprocessing Operations

### Outline

- Main preprocessing operations
- Mapping raw data into features
- Mapping numeric values
- Mapping categorical values
- Empirical knowledge of data



### Main preprocessing operations











Data cleansing

Feature tuning

Representation transformation

Feature extraction

Feature construction

### Mapping raw data into features

#### **Raw Data**

```
0: {
  house_info : {
  num_rooms : 6
  num_bedrooms : 3
  street_name: "Shorebird Way"
  num_basement_rooms: -1
...
  }
  Raw data doesn't
  come to us as feature
  vectors
```

### **Feature Engineering**

#### **Feature Vector**

```
Process of creating features from raw data is feature engineering

9.321,
-2.20,
1.01,
0.0,
```

### Mapping categorical values

#### Street names

{'Charleston Road', 'North Shoreline Boulevard', 'Shorebird Way', 'Rengstorff Avenue'}

Raw Data

Feature Vector

```
0: {
  house_info : {
  num_rooms : 6
  num bedrooms : 3
  street_name: "Shorebird Way"
  num_basement_rooms: -1
...
  }
}
```

String Features can be handled with one-hot encoding

**Feature Engineering** 

#### **One-hot encoding**

This has a 1 for "Shorebird way" and 0 for all others

```
street_name feature=
[0,0, ..., 0, 1, 0, ..., 0]
```

### Categorical Vocabulary

```
# From a vocabulary list
vocabulary feature column = tf.feature column.categorical column with vocabulary list(
                            key=feature name,
                            vocabulary list=["kitchenware", "electronics", "sports"])
vocabulary feature column = tf.feature column.categorical column with vocabulary file(
                             key=feature name,
                             vocabulary file="product class.txt",
                             vocabulary size=3)
```

### Empirical knowledge of data



**Text** - stemming, lemmatization, TF-IDF, n-grams, embedding lookup



**Images** - clipping, resizing, cropping, blur, Canny filters, Sobel filters, photometric distortions

### Key points

- Data preprocessing: transforms raw data into a clean and training-ready dataset
- Feature engineering maps:
  - Raw data into feature vectors
  - Integer values to floating-point values
  - Normalizes numerical values
  - Strings and categorical values to vectors of numeric values
  - Data from one space into a different space

## Feature Engineering



# Feature Engineering Techniques

### Outline

- Feature Scaling
- Normalization and Standardization
- Bucketizing / Binning
- Other techniques

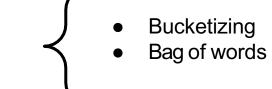


### Feature engineering techniques

Numerical Range 

• Scaling
• Normalizing
• Standardizing

Grouping



### Scaling

- Converts values from their natural range into a prescribed range
  - E.g. Grayscale image pixel intensity scale is [0,255] usually rescaled to [-1,1]

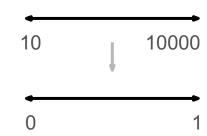
image = (image - 127.5) / 127.5

- Benefits
  - Helps neural nets converge faster
  - Do away with NaN errors during training
  - For each feature, the model learns the right weights

### Normalization

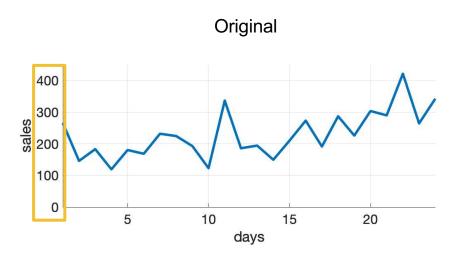
$$X_{\text{norm}} = \frac{X - X_{\min}}{X_{\max} - X_{\min}}$$

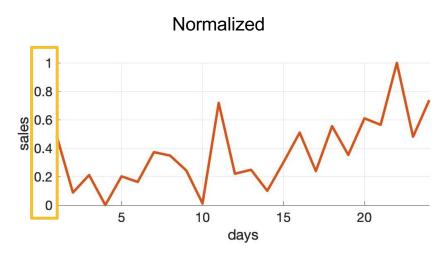
$$X_{\text{norm}} \in [0, 1]$$



Normalization works well for data that is not normally distributed

### Normalization

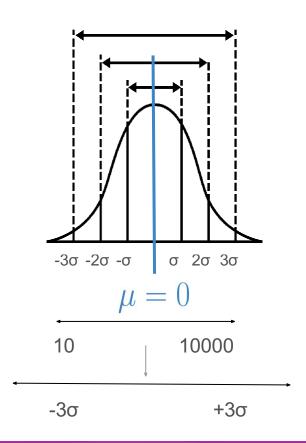




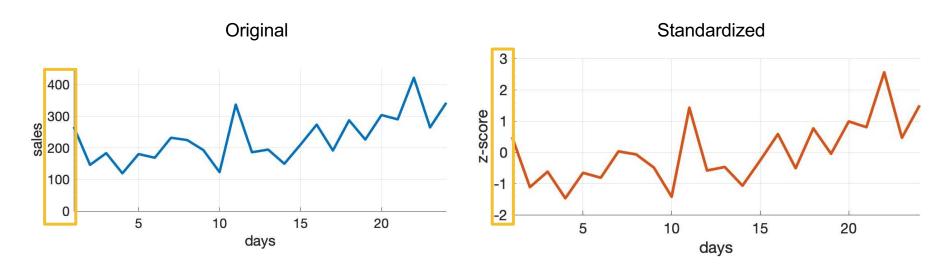
### Standardization (z-score)

- Z-score relates the number of standard deviations away from the mean
- Example:

$$X_{
m std} = rac{X - \mu}{\sigma}$$
 (z-score)  $X_{
m std} \sim \mathcal{N}(0,\sigma)$ 

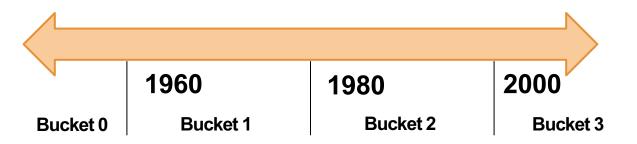


### Standardization (z-score)



Standardization works well for data that is normally distributed

## Bucketizing / Binning



Date Range	Represented as
< 1960	[1, 0, 0, 0]
>= 1960 but < 1980	[0, 1, 0, 0]
>= 1980 but < 2000	[0, 0, 1, 0]
>= 2000	[0, 0, 0, 1]

### Other techniques

Dimensionality reduction in embeddings

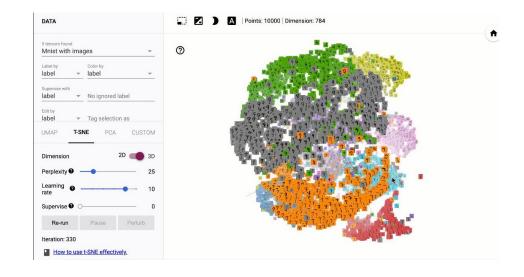


- t-Distributed stochastic neighbor embedding (t-SNE)
- Uniform manifold approximation and projection (UMAP)

Feature crossing

### TensorFlow embedding projector

- Intuitive exploration of high-dimensional data
- Visualize & analyze
- Techniques
  - PCA
  - o t-SNE
  - UMAP
  - Custom linear projections
- Ready to play
  - @projector.tensorflow.org



### Key points

- Feature engineering:
  - Prepares, tunes, transforms, extracts and constructs features.
- Feature engineering is key for model refinement
- Feature engineering helps with ML analysis

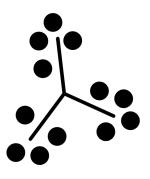
# Feature Engineering



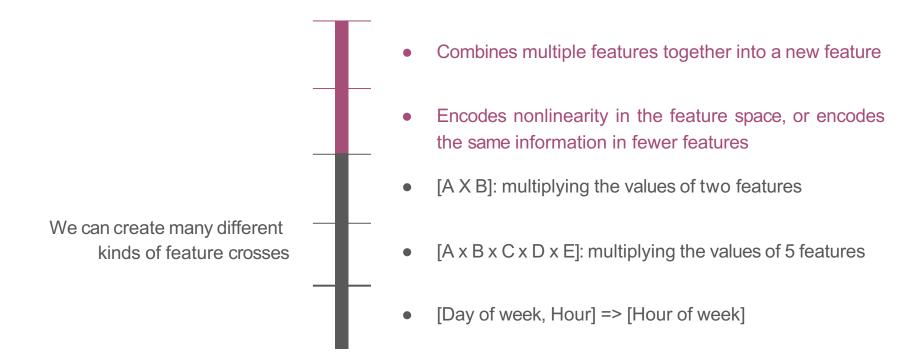
# Feature Crosses

### Outline

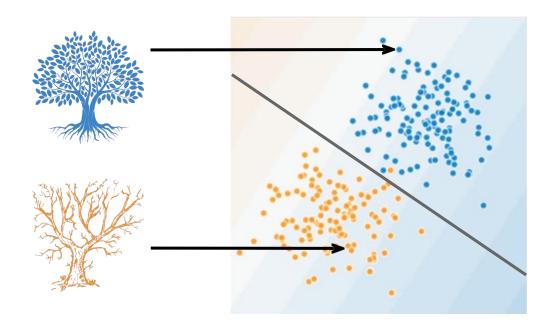
- Feature crosses
- Encoding features



### Feature crosses



### Encoding features

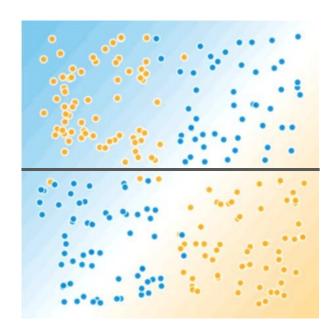


- healthy trees
- sick trees
- \_\_\_ Classification boundary

## Need for encoding non-linearity







- healthy trees
- sick trees
- \_\_\_ Classification boundary

### Key points

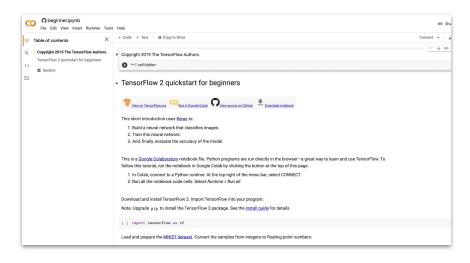
- Feature crossing: synthetic feature encoding nonlinearity in feature space.
- Feature coding: transforming categorical to a continuous variable.

### Feature Transformation At Scale



# Preprocessing Data At Scale

# Probably not ideal





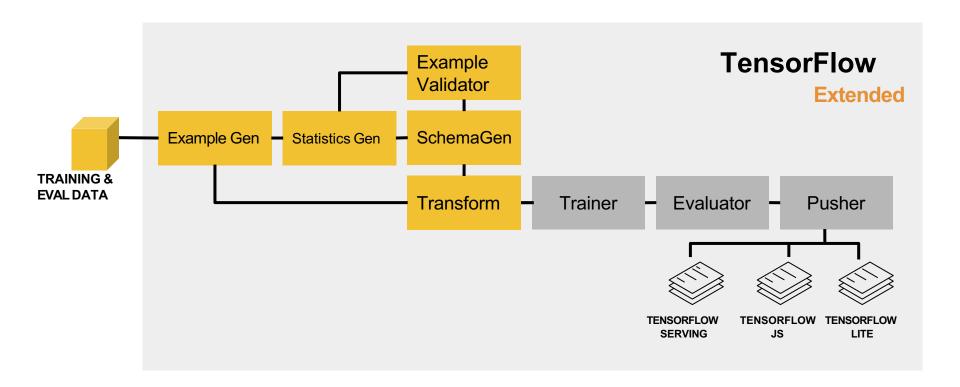


**Python** 



Java

# ML Pipeline



#### Outline

- Inconsistencies in feature engineering
- Preprocessing granularity
- Pre-processing training dataset
- Optimizing instance-level transformations
- Summarizing the challenges



# Preprocessing data at scale



Real-world models: terabytes of data



Large-scale data processing frameworks



Consistent transforms between training & serving

# Inconsistencies in feature engineering

Training & serving code paths are different Mobile (TensorFlow Lite) Diverse deployments scenarios Server (TensorFlow Serving) Web (TensorFlow JS) Risks of introducing training-serving skews Skews will lower the performance of your serving model

# Preprocessing granularity

Transformations		
Instance-level	Full-pass	
Clipping	Minimax	
Multiplying	Standard scaling	
Expanding features	Bucketizing	
etc.	etc.	

# When do you transform?

#### Pre-processing training dataset

Pros	Cons
Run-once	Transformations reproduced at serving
Compute on entire dataset	Slower iterations

#### How about 'within' a model?

#### Transforming within the model

Pros	Cons
Easy iterations	Expensive transforms
Transformation guarantees	Long model latency
	Transformations per batch: skew

# Why transform per batch?

- For example, normalizing features by their average per batch
- Access to a single batch of data, not the full dataset
- Ways to normalize per batch
  - Normalize by average within a batch
  - Precompute average and reuse it during normalization

## Optimizing instance-level transformations

- Indirectly affect training efficiency
- Typically accelerators sit idle while the CPUs transform
- Solution:
  - Prefetching transforms for better accelerator efficiency

# Summarizing the challenges

- Balancing predictive performance
- Full-pass transformations on training data
- Optimizing instance-level transformations for better training efficiency (GPUs, TPUs, ...)

# Key points

- Inconsistent data affects the accuracy of the results
- Need for scaled data processing frameworks to process large datasets in an efficient and distributed manner

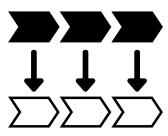
# Preprocessing Data At Scale



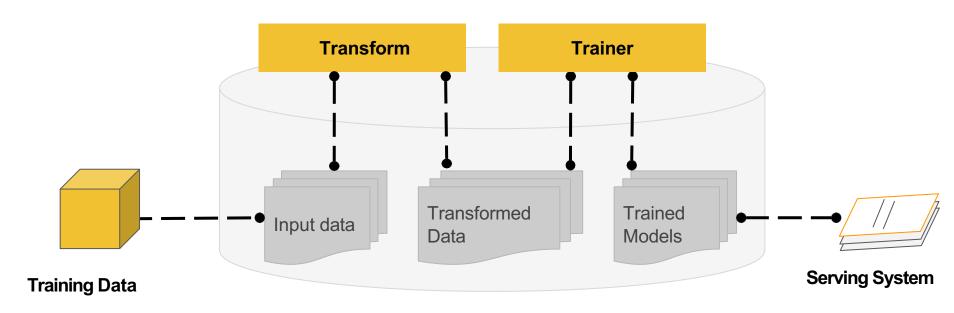
# TensorFlow Transform

#### Outline

- Going deeper
- Benefits of using TensorFlow Transform
- Applies feature transformations
- tf.Transform Analyzers

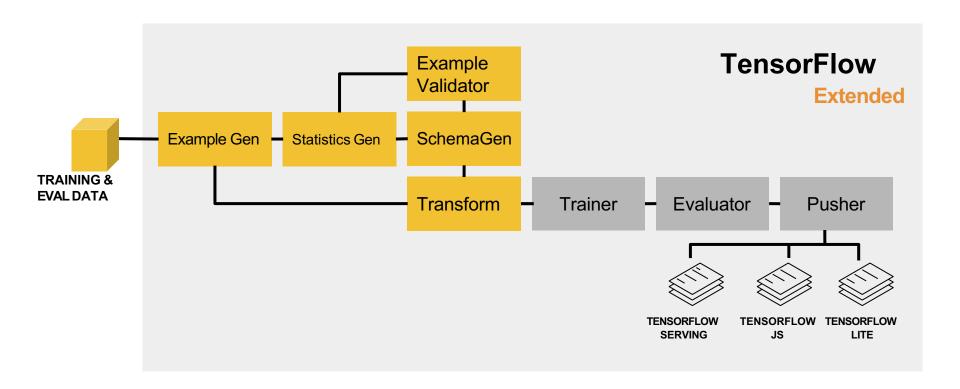


#### Enter tf. Transform



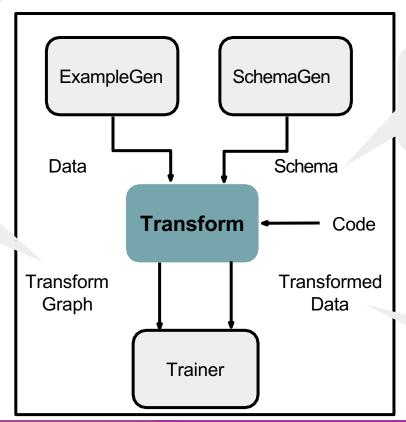
PIPELINE + METADATA STORAGE

#### Inside TensorFlow Extended



#### tf.Transform layout

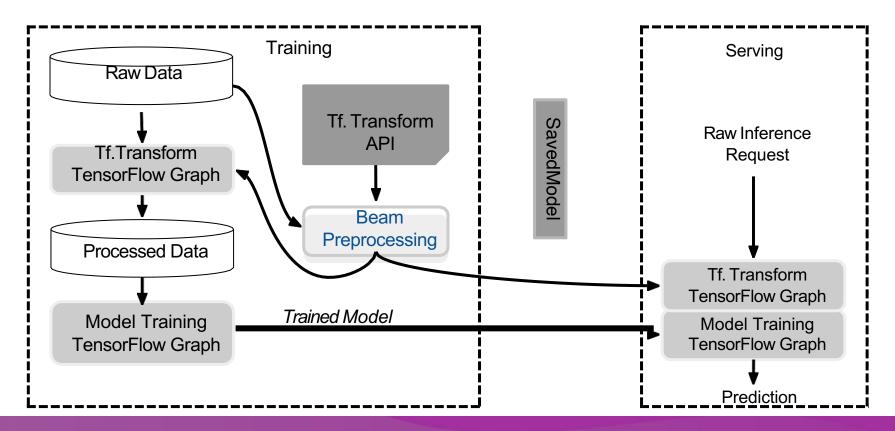
- Applied during training
- Embedded during serving



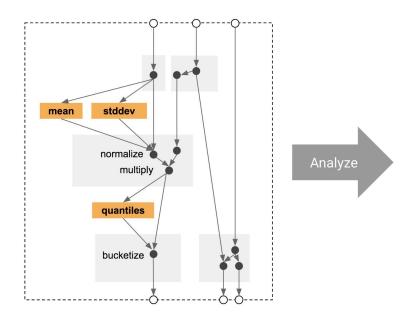
- User-provided transform (tf.Transform)
- **Schema** for parsing

Performance optimizations

## tf. Transform: Going deeper



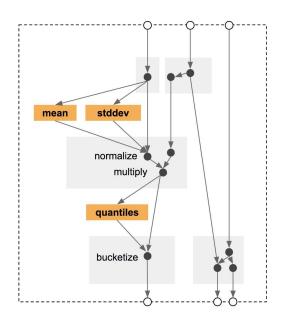
## tf.Transform Analyzers



They behave like TensorFlow Ops, but run only once during training

For example: tft.min computes the minimum of a tensor over the training dataset

#### How Transform applies feature transformations

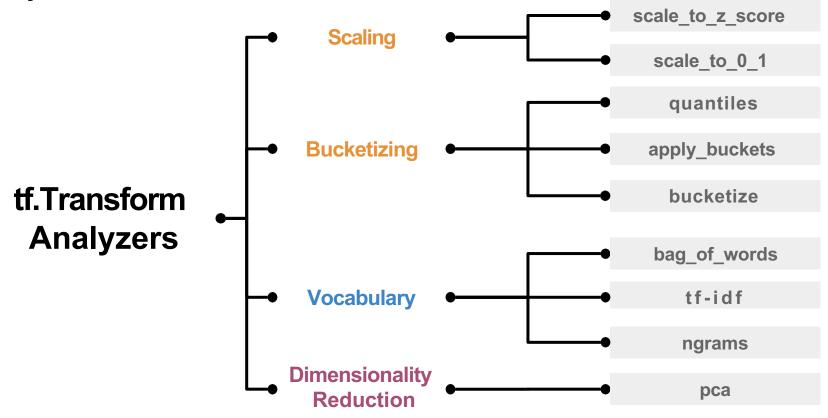




## Benefits of using tf. Transform

- Emitted tf.Graph holds all necessary constants and transformations
- Focus on data preprocessing only at training time
- Works in-line during both training and serving
- No need for preprocessing code at serving time
- Consistently applied transformations irrespective of deployment platform

## Analyzers framework



# tf.Transform preprocessing\_fn

```
def preprocessing fn(inputs):
for key in DENSE FLOAT FEATURE KEYS:
     outputs[key] = tft.scale_to_z_score(inputs[key])
for key in VOCAB FEATURE KEYS:
     outputs[key] = tft.vocabulary(inputs[key], vocab filename=key)
for key in BUCKET FEATURE KEYS:
  outputs[key] = tft.bucketize(inputs[key], FEATURE_BUCKET_COUNT)
```

# Commonly used imports

```
import tensorflow as tf
import apache_beam as beam
import apache_beam.io.iobase

import tensorflow_transform as tft
import tensorflow_transform.beam as tft_beam
```

#### Feature Transformation At Scale



# Hello World with tf.Transform

#### Hello world with tf. Transform

1 — 2 — 3 — 4

Data Define metadata Transform Constant graph

Collect raw data

Prepare metadata for the dataset using

DatasetMetadata

Define the preprocessing function with tf.Transform analyzers

Generate a constant graph with the required transformations

## Collect raw samples (Data)

```
{'x': 1, 'y': 1, 's': 'hello'},
{'x': 2, 'y': 2, 's': 'world'},
{'x': 3, 'y': 3, 's': 'hello'}
```

# Inspect data and prepare metadata (Data)

```
from tensorflow transform.tf metadata import (
    dataset metadata, dataset schema)
raw data metadata = dataset metadata.DatasetMetadata(
    dataset schema.from feature spec({
    'y': tf.io.FixedLenFeature([], tf.float32),
        'x': tf.io.FixedLenFeature([], tf.float32),
        's': tf.io.FixedLenFeature([], tf.string)
    }))
```

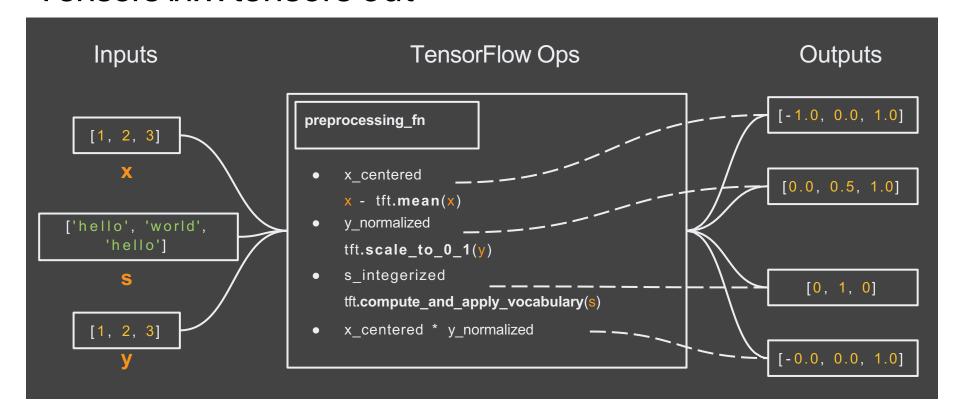
## Preprocessing data (Transform)

```
def preprocessing fn(inputs):
"""Preprocess input columns into transformed columns."""
   x, y, s = inputs['x'], inputs['y'], inputs['s']
   x centered = x - tft.mean(x)
   y normalized = tft.scale_to_0_1(y)
   s_integerized = tft.compute_and_apply_vocabulary(s)
   x centered times y normalized = (x centered * y normalized)
```

## Preprocessing data (Transform)

```
return {
  'x centered': x centered,
 'y normalized': y normalized,
 's integerized': s integerized,
 'x centered times y normalized': x centered times y normalized,
```

#### Tensors in... tensors out



#### Running the pipeline

## Running the pipeline

```
transformed data, transformed metadata = transformed dataset
  print('\nRaw data:\n{}\n'.format(pprint.pformat(raw data)))
  print('Transformed data:\n{}'.format(pprint.pformat(transformed data)))
if __name__ == ' __main__':
  main()
```

## Before transforming with tf.Transform

```
# Raw data:
[{'s': 'hello', 'x': 1, 'y': 1},
{'s': 'world', 'x': 2, 'y': 2},
{'s': 'hello', 'x': 3, 'y': 3}]
```

## After transforming with tf.Transform

```
# After transform
[{'s integerized': 0,
 'x centered': -1.0,
  'x centered times y normalized': -0.0,
 'y normalized': 0.0},
 {'s integerized': 1,
  'x centered': 0.0,
  'x centered times y normalized': 0.0,
  'y normalized': 0.5},
 {'s_integerized': 0,
  'x centered': 1.0,
  'x centered times y normalized': 1.0,
  'y normalized': 1.0}]
```

# Key points

- tf.Transform allows the pre-processing of input data and creating features
- tf.Transform allows defining pre-processing pipelines and their execution using large-scale data processing frameworks
- In a TFX pipeline, the Transform component implements feature engineering using TensorFlow Transform

## **Feature Selection**



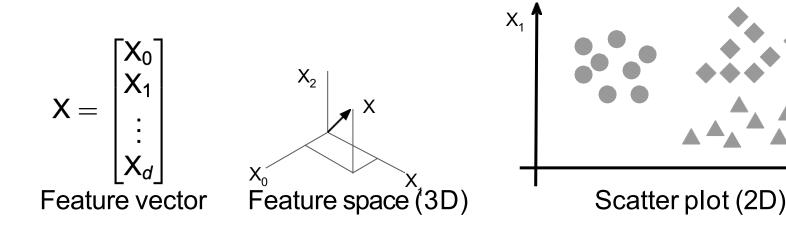
# Feature Spaces

#### Outline

- Introduction to Feature Spaces
- Introduction to Feature Selection
- Filter Methods
- Wrapper Methods
- Embedded Methods

# Feature space

- N dimensional space defined by your N features
- Not including the target label



# Feature space

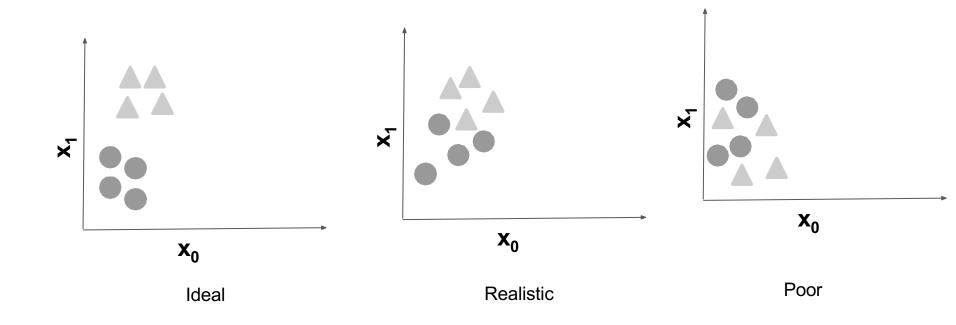


No. of Rooms $X_0$	Area X <sub>1</sub>	Locality $old X_2$	Price Y	
5	1200 sq. ft	New York	\$40,000	
6	1800 sq. ft	Texas	\$30,000	

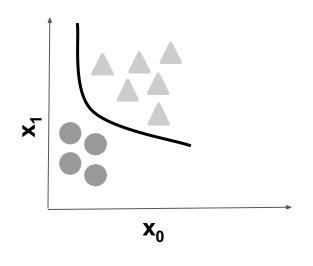
$$Y = f(X_0, X_1, X_2)$$

f is your ML model acting on feature space X<sub>0</sub>, X<sub>1</sub>, X<sub>2</sub>

# 2D Feature space - Classification



# Drawing decision boundary



Model learns decision boundary

Boundary used to classify data points

# Feature space coverage

- Train/Eval datasets representative of the serving dataset
  - Same numerical ranges
  - Same classes
  - Similar characteristics for image data
  - Similar vocabulary, syntax, and semantics for NLP data

# Ensure feature space coverage

- Data affected by: seasonality, trend, drift.
- Serving data: new values in features and labels.
- Continuous monitoring, key for success!

## **Feature Selection**



# **Feature Selection**

#### Feature selection

#### **All Features**



Feature selection



**Useful features** 



- Identify features that best represent the relationship
- Remove features that don't influence the outcome
- Reduce the size of the feature space
- Reduce the resource requirements and model complexity

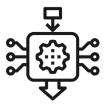
# Why is feature selection needed?





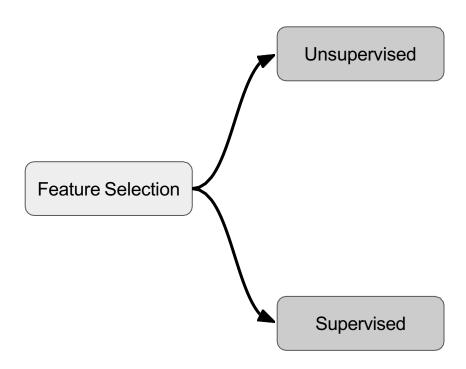
Reduce storage and I/O requirements





Minimize training and inference costs

#### Feature selection methods



# Unsupervised feature selection

#### 1. Unsupervised

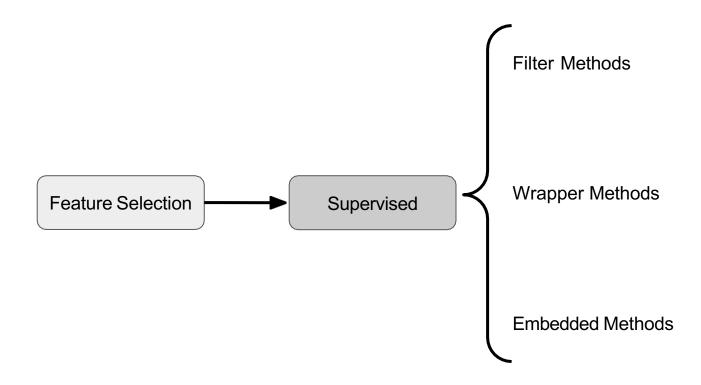
- Features-target variable relationship not considered
- Removes redundant features (correlation)

# Supervised feature selection

#### 2. Supervised

- Uses features-target variable relationship
- Selects those contributing the most

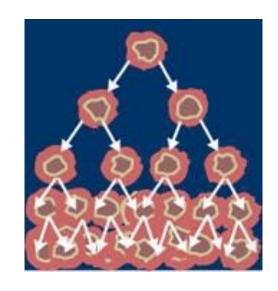
# Supervised methods



# Practical example

Feature selection techniques on Breast Cancer Dataset (Diagnostic)

Predicting whether tumour is benign or malignant.



# Feature list

id	diagnosis	radius-mean	texture_mea n	perimeter_ mean	area_mean	smoothness _mean	compactnes s_mean	
842302	М	17.99	10.38	122.8	1001.0	0.1184	0.2776	
concavity_m ean	concavepoin ts_mean	symmetry_ mean	fractal_dime nsion_mean	radius_se	texture_se	perimeter_s e	area_se	Irrelevant
0.3001	0.1471	0.2419	0.07871	1.095	0.9053	8.589	153.4	features
smoothness _se	compactnes s_se	concavity_se	concavepoint s_se	symmetry_ se	fractal_dime nsion_se	radius-wors t	texture_wor st	
0.0064	0.049	0.054	0.016	0.03	0.006	25.38	17.33	
perimeter_w orst	area_worst	smoothness _worst	compactness _worst	concavity_ worst	concavepoin ts_worst	symmetry_ worst	fractal_dime nsion_worst	Unnamed:3 2
184.6	2019.0	0.1622	0.6656	0.7119	0.2654	0.4601	0.1189	NaN

#### Performance evaluation

We train a **RandomForestClassifier** model in sklearn.ensemble on selected features

#### **Metrics** (sklearn.metrics):

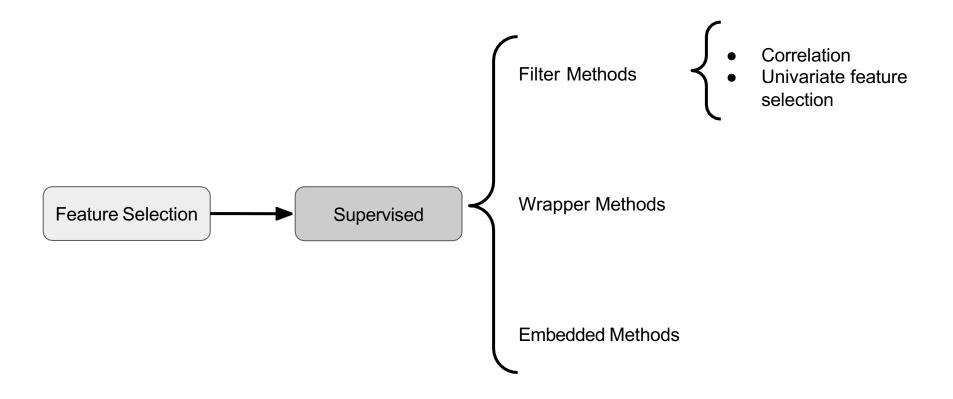
Method	Feature Count	Accuracy	AUROC	Precision	Recall	F1 Score
All Features	30	0.967262	0.964912	0.931818	0.97619	0.953488

## **Feature Selection**



# Filter Methods

#### Filter methods



#### Filter methods

- Correlated features are usually redundant
  - Remove them!

#### Popular filter methods:

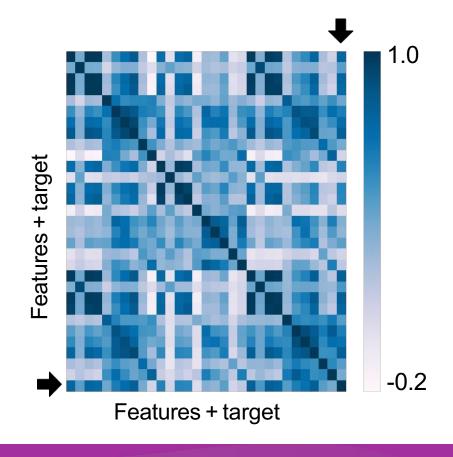
- Pearson Correlation
  - Between features, and between the features and the label
- Univariate Feature Selection

#### Filter methods



#### Correlation matrix

- Shows how features are related:
  - To each other (Bad)
  - And with target variable (Good)
- Falls in the range [-1, 1]
  - 1 High positive correlation
  - -1 High negative correlation



# Feature comparison statistical tests

- Pearson's correlation: Linear relationships
- Kendall Tau Rank Correlation Coefficient: Monotonic relationships & small sample size
- Spearman's Rank Correlation Coefficient: Monotonic relationships

#### Other methods:

- Mutual information
- F-Test
- Chi-Squared test

#### Determine correlation

```
1.0
cor = df.corr()
plt.figure(figsize=(20,20))
# Seaborn
                                                    -eatures
sns.heatmap(cor, annot=True, cmap=plt.cm.PuBu)
plt.show()
                                                            Features + target
```

## Selecting features

```
cor_target = abs(cor["diagnosis_int"])
# Selecting highly correlated features as potential features to eliminate
relevant_features = cor_target[cor_target>0.2]
```

## Performance table

Method	Feature Count	Accuracy	AUROC	Precision	Recall	F1 Score
All Features	30	0.967262	0.964912	0.931818	0.97619	0.953488
Correlation	21	0.974206	0.973684	0.953488	0.97619	0.964706

#### **Best Result**

#### Univariate feature selection in SKLearn

#### SKLearn Univariate feature selection routines:

- 1. SelectKBest
- 2. SelectPercentile
- 3. GenericUnivariateSelect

#### Statistical tests available:

- Regression: <u>f\_regression</u>, <u>mutual\_info\_regression</u>
- Classification: <u>chi2</u>, <u>f classif</u>, <u>mutual info classif</u>

# SelectKBest implementation

```
def univariate selection():
 X train, X test, Y train, Y test = train test split(X, Y,
                                               test size = 0.2, stratify=Y, random state = 123)
 X train scaled = StandardScaler().fit transform(X train)
 X test scaled = StandardScaler().fit transform(X test)
 min max scaler = MinMaxScaler()
 Scaled X = min max scaler.fit transform(X train scaled)
 selector = SelectKBest(chi2, k=20) # Use Chi-Squared test
 X new = selector.fit transform(Scaled X, Y train)
 feature idx = selector.get_support()
 feature_names = df.drop("diagnosis_int",axis = 1 ).columns[feature_idx]
 return feature names
```

## Performance table

	Method	Feature Count	Accuracy	AUROC	Precision	Recall	F1 Score
	All Features	30	0.967262	0.964912	0.931818	0.97619	0.953488
Γ	Correlation	21	0.974206	0.973684	0.953488	0.97619	0.964706
	Univariate (Chi²)	20	0.960317	0.95614	0.91111	0.97619	0.94252

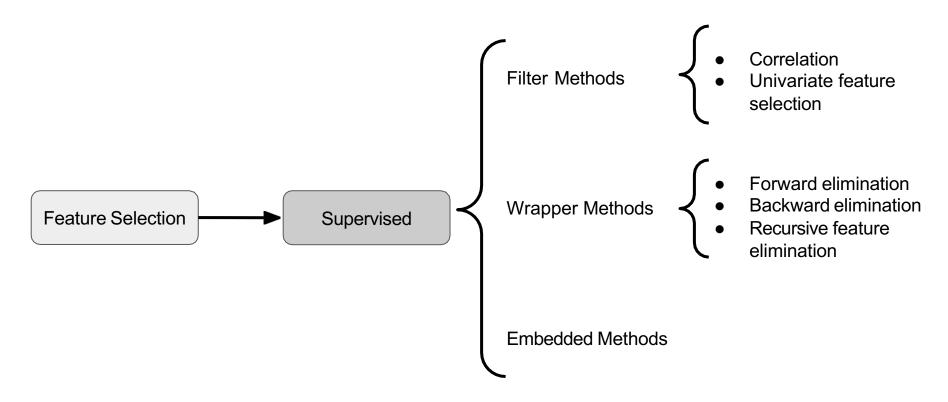
**Best Result** 

## **Feature Selection**

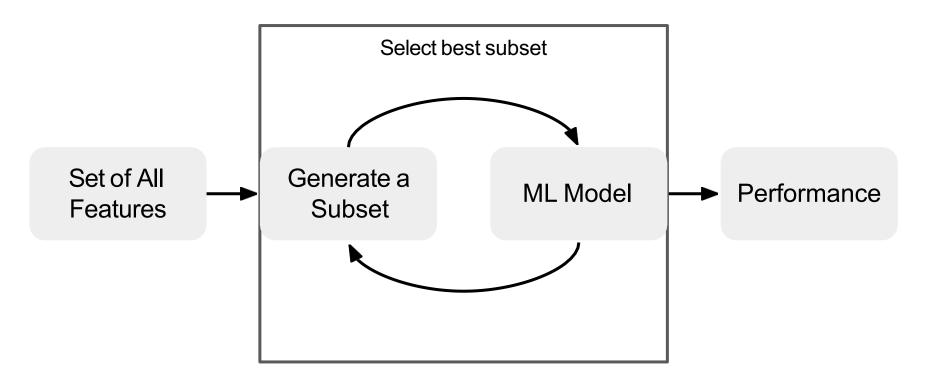


# Wrapper Methods

# Wrapper methods



# Wrapper methods



# Wrapper methods

#### Popular wrapper methods

- 1. Forward Selection
- 2. Backward Selection
- 3. Recursive Feature Elimination

#### Forward selection

- 1. Iterative, greedy method
- 2. Starts with 1 feature
- Evaluate model performance when adding each of the additional features, one at a time
- 4. Add next feature that gives the best performance
- 5. Repeat until there is no improvement

#### **Backward elimination**

- Start with all features
- 2. Evaluate model performance when **removing** each of the included features, one at a time
- 3. Remove next feature that gives the best performance
- 4. Repeat until there is no improvement

## Recursive feature elimination (RFE)

- 1. Select a model to use for evaluating feature importance
- 2. Select the desired number of features
- Fit the model
- Rank features by importance
- 5. Discard least important features
- 6. Repeat until the desired number of features remains

#### Recursive feature elimination

```
def run rfe():
  X train, X test, y train, y test = train test split(X,Y, test size = 0.2, random state = 0)
  X train scaled = StandardScaler().fit transform(X train)
  X test scaled = StandardScaler().fit transform(X test)
  model = RandomForestClassifier(criterion='entropy', random_state=47)
  rfe = RFE(model, 20)
  rfe = rfe.fit(X train scaled, y train)
  feature_names = df.drop("diagnosis_int",axis = 1 ).columns[rfe.get_support()]
  return feature names
rfe feature names = run rfe()
rfe eval df = evaluate model on features(df[rfe feature names], Y)
rfe_eval_df.head()
```

#### Performance table

Method	Feature Count	Accuracy	AUROC	Precision	Recall	F1 Score
All Features	30	0.96726	0.96491	0.931818	0.97619	0.953488
Correlation	21	0.97420	0.97368	0.9534883	0.97619	0.964705
Univariate (Chi²)	20	0.96031	0.95614	0.91111	0.97619	0.94252
Recursive Feature Elimination	20	0.97420	0.97368	0.953488	0.97619	0.964706

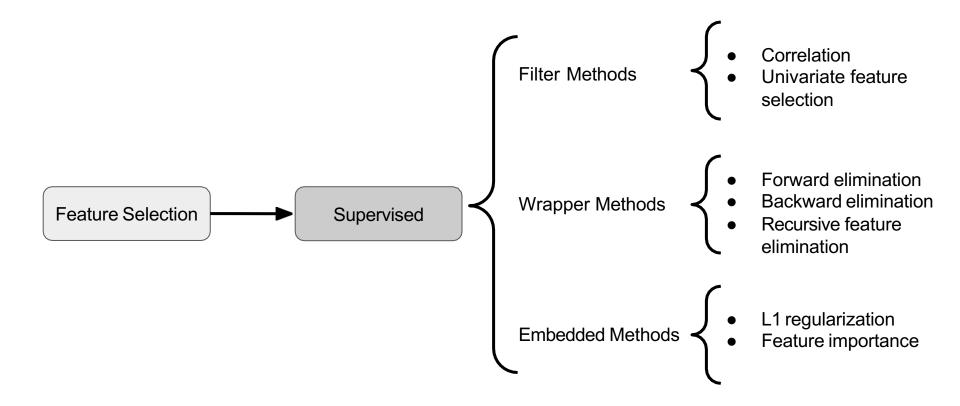
#### **Best Result**

#### **Feature Selection**



# **Embedded Methods**

#### **Embedded methods**



## Feature importance

- Assigns scores for each feature in data
- Discard features scored lower by feature importance

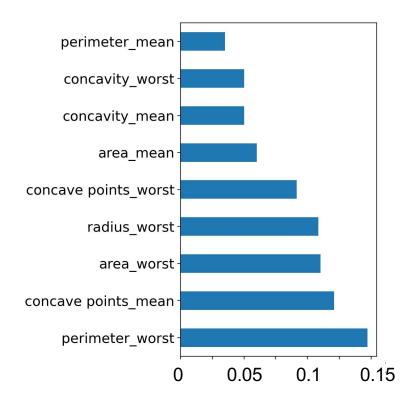
## Feature importance with SKLearn

- Feature Importance class is in-built in Tree Based Models (eg., RandomForestClassifier)
- Feature importance is available as a property feature\_importances\_
- We can then use SelectFromModel to select features from the trained model based on assigned feature importances.

### Extracting feature importance

```
def feature importances from tree based model ():
 X train, X test, Y train, Y test = train test split(X, Y, test size = 0.2,
                                               stratify=Y, random state = 123)
  model = RandomForestClassifier()
  model = model.fit(X train, Y train)
 feat importances = pd.Series(model.feature importances , index=X.columns)
  feat importances.nlargest(10).plot(kind='barh')
  plt.show()
 return model
```

# Feature importance plot



### Select features based on importance

```
def select features from model(model):
  model = SelectFromModel(model, prefit=True, threshold=0.012)
  feature idx = model.get support()
  feature names = df.drop("diagnosis int", 1).columns[feature idx]
 return feature names
```

# Tying together and evaluation

```
# Calculate and plot feature importances
model = feature importances from tree based model ()
feature_imp_feature_names = select_features_from_model(model)
```

#### Performance table

Method	Feature Count	Accuracy	ROC	Precision	Recall	F1 Score
All Features	30	0.96726	0.964912	0.931818	0.9761900	0.953488
Correlation	21	0.97420	0.973684	0.953488	0.9761904	0.964705
Univariate Feature Selection	20	0.96031	0.95614	0.91111	0.97619	0.94252
Recursive Feature Elimination	20	0.9742	0.973684	0.953488	0.97619	0.964706
Feature Importance	14	0.96726	0.96491	0.931818	0.97619	0.953488

#### **Best Result**

#### Review

- Intro to Preprocessing
- Feature Engineering
- Preprocessing Data at Scale
  - TensorFlow Transform
- Feature Spaces
- Feature Selection
  - Filter Methods
  - Wrapper Methods
  - Embedded Methods