

Lecture 5 Data Preprocessing & Model Tuning

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- Data Preparation
- Pipelining
- Hyperparameter Tuning
- Model Optimizing

Data Preparation

- Sampling
- Normalization
- Binning/Discretization
- Missing
- Duplicates
- Outliers
- Dimensionality Reduction



- Sampling is the main technique employed for data selection.
 - It is often used for both the preliminary investigation of the data and the final data analysis.
- Statisticians sample because obtaining the entire set of data of interest is too expensive or time consuming.
- Sampling is used in data mining because processing the entire set of data of interest is too expensive or time consuming.

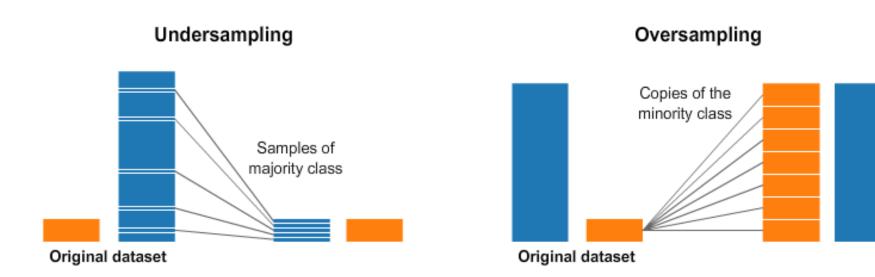


- The key principle for effective sampling is the following:
 - using a sample will work almost as well as using the entire data sets, if the sample is representative
 - A sample is representative if it has approximately the same property (of interest) as the original set of data



- Simple Random Sampling
 - equal probability of selecting any particular item
- Sampling without replacement
 - removed from the population
- Sampling with replacement (Bootstrap)
 - Objects are not removed from the population
- Stratified sampling
 - Split the data into several partitions; then draw random samples from each partition





Data Balancing: 2 classes

```
import numpy as np
import pandas as pd
majority = [[5.1, 3.5, 1.4, 0.2, 0],
             [4.9,3.0,1.4,0.2,0]
             [4.7,3.2,1.3,0.2,0],
             [4.6,3.1,1.5,0.2,0],
             [5.0,3.6,1.4,0.2,0],
             [5.4,3.9,1.7,0.4,0],
             [4,6,3,4,1,4,0,3,0],
             [5.0,3.4,1.5,0.2,0],
             [4.4,2.9,1.4,0.2,0],
             [4.9,3.1,1.5,0.1,0]]
minority = [[7.0, 3.2, 4.7, 1.4, 1],
             [6.4,3.2,4.5,1.5,1],
             [6.9,3.1,4.9,1.5,1],
             [5.5, 2.3, 4.0, 1.3, 1],
             [6.5, 2.8, 4.6, 1.5, 1]]
names = ['A1','A2','A3','A4','labels']
```



```
majority df = pd.DataFrame(majority,columns=names)
minority df = pd.DataFrame(minority,columns=names)
def balance data (majority df, minority df):
    fold=np.int32(np.floor(len(majority df)/len(minority df)))
    upsamples minority=minority df.copy()
    for i in range (0, fold):
        upsamples minority=pd.concat([upsamples minority, minority df])
    train data=pd.concat([majority df,upsamples minority])
    return train data
data = balance data(majority df, minority df)
data
```



- Synthetic Minority Oversampling TEchnique (SMOTE) was described by Nitesh Chawla, et al. (2002).
- SMOTE works by selecting examples that are close in the feature space, drawing a line between the examples in the feature space and drawing a new sample at a point along that line.
- SMOTE first selects a minority class instance a at random and finds its K nearest minority class neighbors.
- The synthetic instance is then created by choosing one of the K nearest neighbors b at random and connecting a and b to form a line segment in the feature space. The synthetic instances are generated as a convex combination of the two chosen instances a and b.

Data Normalization

Range Normalization or MaxMin Scaler: to [new_minA, new_maxA]

$$v' = \frac{v - min_A}{max_A - min_A} (new_max_A - new_min_A) + new_min_A$$

- Ex. Let income range \$12,000 to \$98,000 normalized to [0.0, 1.0]. Then \$73,600 is mapped to $\frac{73,600-12,000}{98,000-12,000}(1.0-0)+0=0.716$
- Z-score normalization (μ: mean, σ: standard deviation) or StandardScaler:

$$v' = \frac{v - \mu_A}{\sigma_A}$$

 \Box Ex. Let $\mu = 54,000$, $\sigma = 16,000$. Then

$$\frac{73,600 - 54,000}{16,000} = 1.225$$

Normalization by decimal scaling

$$v' = \frac{v}{10^{j}}$$
 where j is the smallest integer such that Max(|v'|) < 1

sklearn.preprocessing.MinMaxScaler(feature_range=(0, 1), copy=True)

Parameters:

feature_range: tuple (min, max), default=(0, 1)Desired range of transformed data.

copy: boolean, optional, default TrueSet to False to perform inplace row normalization and avoid a copy (if the input is already a numpy array). min_: ndarray, shape (n_features,)
Per feature adjustment for minimum. Equivalent to min X.min(axis=0) * self.scale_
scale_: ndarray, shape (n_features,)
Per feature relative scaling of the data. Equivalent to(max min) / (X.max(axis=0) - X.min(axis=0))
New in version 0.17: scale_ attribute.
data_min_: ndarray, shape (n_features,)
Per feature minimum seen in the data
New in version 0.17: data_min_
data_max_: ndarray, shape (n_features,)
Per feature maximum seen in the data
New in version 0.17: data_max_
data_range_: ndarray, shape (n_features,)

Per feature range (data max - data min) seen in the data

New in version 0.17: data range

MinMaxScaler MaxScaler

- fit(self, X[, y]) Compute the minimum and maximum to be used for later scaling.
- fit_transform(self, X[, y]) Fit to data, then transform it.
- get_params(self[, deep]) Get parameters for this estimator.
- inverse_transform(self, X) Undo the scaling of X according to feature_range.
- partial_fit(self, X[, y])
 Online computation of min and max on X for later scaling.
- set_params(self, **params) Set the parameters of this estimator.
- transform(self, X) Scaling features of X according to feature_range.



```
from sklearn.preprocessing import MinMaxScaler
data = [[-1, 2], [-0.5, 6], [0, 10], [1, 18]]
scaler = MinMaxScaler()
print(scaler.fit(data))
print(scaler.data_max_)
print(scaler.transform(data))
print(scaler.transform([[2, 2]]))
```

StandardScaler

sklearn.preprocessing.StandardScaler(copy=True, with_mean=True, with_std=True)

copy: boolean, optional, default True

If False, try to avoid a copy and do inplace scaling instead. This is not guaranteed to always work inplace; e.g. if the data is not a NumPy array or scipy.sparse CSR matrix, a copy may still be returned.

with_mean : boolean, True by default

Parameters: If True, center the data before scaling

If True, center the data before scaling. This does not work (and will raise an exception) when attempted on sparse matrices, because centering them entails building a dense matrix which in common use cases is likely to be too large to fit in memory.

with_std : boolean, True by default

If True, scale the data to unit variance (or equivalently, unit standard deviation).

scale_: *ndarray or None, shape (n_features,)*Per feature relative scaling of the data. This is calculated using np.sqrt(var_). Equal to Nonewhen with_std=False. *New in version 0.17: scale_* **mean_**: *ndarray or None, shape (n_features,)*The mean value for each feature in the training set. Equal to None when with mean=False.

Attributes:

var_ : ndarray or None, shape (n_features,)
The variance for each feature in the training set. Used to
compute scale_. Equal to Nonewhen with_std=False.
n_samples_seen_ : int or array, shape (n_features,)
The number of samples processed by the estimator for
each feature. If there are not missing samples,
the n_samples_seen will be an integer, otherwise it will
be an array. Will be reset on new calls to fit, but
increments across partial_fit calls.

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Method of StandardScaler

- fit(self, X[, y]) Compute the mean and std to be used for later scaling.
- fit_transform(self, X[, y]) Fit to data, then transform it.
- get_params(self[, deep])Get parameters for this estimator.
- inverse_transform(self, X[, copy]) Scale back the data to the original representation
- partial_fit(self, X[, y]) Online computation of mean and std on X for later scaling.
- set_params(self, **params) Set the parameters of this estimator.
- transform(self, X[, copy]) Perform standardization by centering and scaling



```
from sklearn.preprocessing import StandardScaler
data = [[0, 0], [0, 0], [1, 1], [1, 1]]
scaler = StandardScaler()
print(scaler.fit(data))
print(scaler.mean_)
print(scaler.transform(data))
print(scaler.transform([[2, 2]]))
```

Discretization

- By Size: Each bin contains a user-defined number of examples.
- By Binning: Bins of equal range are automatically generated, the number of the values in different bins may vary.
- By Frequency: Bins of equal frequency are automatically generated, the range of different bins may vary.
- By Entropy: The boundaries of the bins are chosen so that the entropy is minimized in the induced partitions.

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 sklearn.preprocessing.KBinsDiscretizer(n_bins=5, encode='onehot', strategy='quantile')

n_bins: int or array-like, shape (n_features,) (default=5)
The number of bins to produce. Raises ValueError if n_bins < 2. **encode**: {'onehot', 'onehot-dense', 'ordinal'}, (default='onehot')
Method used to encode the transformed result.

Onehot Encode the transformed result with one-hot encoding and return a sparse matrix. Ignored features are always stacked to the right. onehot-dense Encode the transformed result with one-hot encoding and

Parameters: return a dense array. Ignored features are always stacked to the right.

Ordinal Return the bin identifier encoded as an integer value.

strategy : {'uniform', 'quantile', 'kmeans'}, (default='quantile')

Strategy used to define the widths of the bins.

Uniform All bins in each feature have identical widths.

Quantile All bins in each feature have the same number of points.

Kmeans Values in each bin have the same nearest center of a 1D kmeans cluster

Methods

fit(self, X[, y])	Fits the estimator.
<pre>fit_transform(self, X[, y])</pre>	Fit to data, then transform it.
<pre>get_params(self[, deep])</pre>	Get parameters for this estimator.
inverse_transform(self, Xt)	Transforms discretized data back to original feature space.
<pre>set_params(self, **params)</pre>	Set the parameters of this estimator.
transform(self, X)	Discretizes the data.

- Reasons for missing values
 - Information is not collected
 (e.g., people decline to give their age and weight)
 - Attributes may not be applicable to all cases
 (e.g., annual income is not applicable to children)
- Handling missing values
 - Remove Unused Values
 - Replace Missing Values
 - Impute Missing Values

 sklearn.impute.SimpleImputer(missing_values=nan, strategy='mean', fill_value=None, verbose=0, copy=True, add_indicator=False) missing_values : number, string, np.nan (default) or None

The placeholder for the missing values. All occurrences of missing_values will be imputed. **strategy**: *string*, *optional* (*default="mean"*)The imputation strategy.

- •If "mean", then replace missing values using the mean along each column. Can only be used with numeric data.
- •If "median", then replace missing values using the median along each column. Can only be used with numeric data.
- •If "most_frequent", then replace missing using the most frequent value along each column. Can be used with strings or numeric data.
- •If "constant", then replace missing values with fill_value. Can be used with strings or numeric data.

New in version 0.20: strategy="constant" for fixed value imputation.

fill_value: string or numerical value, optional (default=None)When strategy == "constant", fill_value is used to replace all occurrences of missing_values. If left to the default, fill_value will be 0 when imputing numerical data and "missing_value" for strings or object data types.

verbose: *integer, optional (default=0)* Controls the verbosity of the imputer.

copy: boolean, optional (default=True)If True, a copy of X will be created. If False, imputation will be done in-place whenever possible. Note that, in the following cases, a new copy will always be made, even if copy=False:

- •If X is not an array of floating values;
- If X is encoded as a CSR matrix;
- If add indicator=True.

add_indicator : boolean, optional (default=False)

If True, a <u>MissingIndicator</u> transform will stack onto output of the imputer's transform. This allows a predictive estimator to account for missingness despite imputation. If a feature has no missing values at fit/train time, the feature won't appear on the missing indicator even if there are missing values at transform/test time.

Parameters:



Methods

fit(self, X[, y])	Fit the imputer on X.
<pre>fit_transform(self, X[, y])</pre>	Fit to data, then transform it.
<pre>get_params(self[, deep])</pre>	Get parameters for this estimator.
<pre>set_params(self, **params)</pre>	Set the parameters of this estimator.
transform(self, X)	Impute all missing values in X.

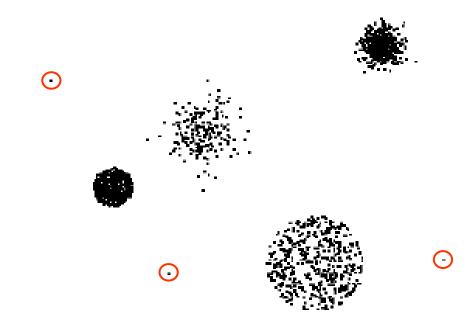
```
import numpy as np
from sklearn.impute import SimpleImputer
imp = SimpleImputer(missing_values=np.nan,
strategy='mean')
imp.fit([[1, 2], [np.nan, 3], [7, 6]])

X = [[np.nan, 2], [6, np.nan], [7, 6]]
print(imp.transform(X))
```

- Data set may include data objects that are duplicates, or almost duplicates of one another
 - Major issue when merging data from heterogeneous sources
- Examples:
 - Same person with multiple email addresses
- Data cleaning
 - Process of dealing with duplicate data issues



 Outliers are data objects with characteristics that are considerably different than most of the other data objects in the data set





Dimensionality Reduction

Purpose:

- Avoid curse of dimensionality
- Reduce amount of time and memory
- Allow data to be more easily visualized
- Eliminate irrelevant features or reduce noise

Techniques

- Principle Component Analysis (PCA)
- Independent Component Analysis (ICA)
- Singular Value Decomposition (SVD)
- t-distributed Stochastic Neighbor Embedding (TSNE)

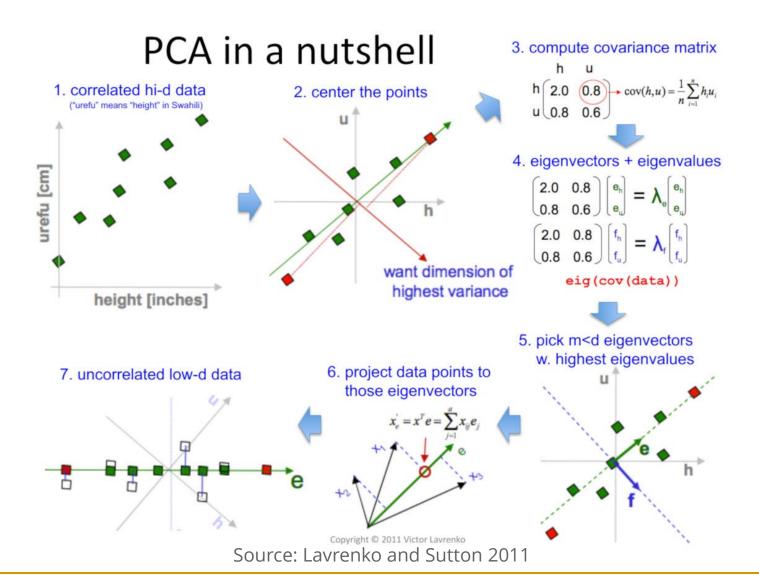


Principle Component Analysis (PCA)

- Principal component analysis (PCA) is the process of computing the principal components and using them to perform a change of basis on the data.
- PCA is used in exploratory data analysis and for making predictive models.
- We use only the first few principal components and ignore the rest, so it is used for dimension reduction.
- It is used for dimensionality reduction by projecting each data point onto only the first few principal components to obtain lower-dimensional data while preserving as much of the data's variation as possible.



Principle Component Analysis (PCA)





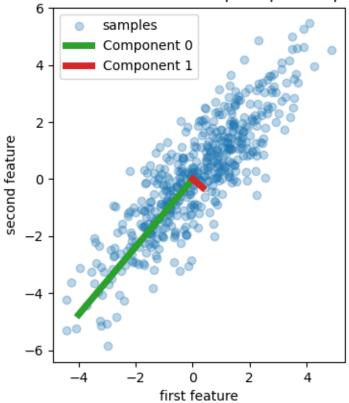
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
rng = np.random.RandomState(0)
n_samples = 500
cov = [[3, 3], [3, 4]]
X = rng.multivariate_normal(mean=[0, 0], cov=cov, size=n_samples)
pca = PCA(n_components=2).fit(X)
plt.scatter(X[:, 0], X[:, 1], alpha=0.3, label="samples")
```



```
for i, (comp, var) in enumerate(
    zip(pca.components , pca.explained variance )):
    comp = comp*var #scale component by its variance explanation power
    plt.plot(
        [0, comp[0]],
        [0, comp[1]],
        label=f"Component {i}",
        linewidth=5,
        color=f"C{i + 2}",
plt.gca().set(
    aspect="equal",
    title="2-dimensional dataset with principal components",
    xlabel="first feature",
    ylabel="second feature",
plt.legend()
plt.show()
```



2-dimensional dataset with principal components





Independent component analysis (ICA)

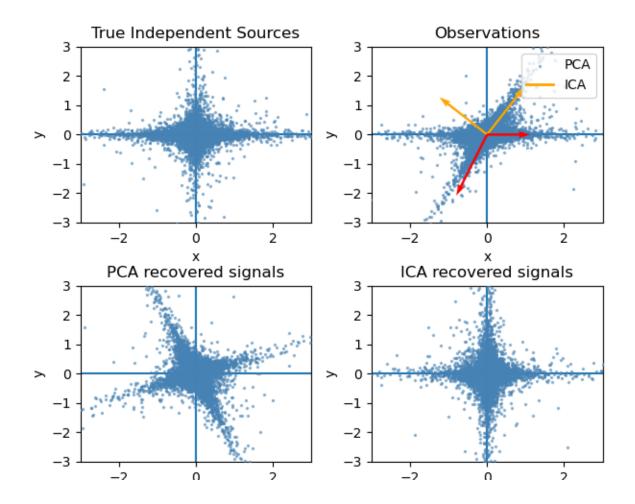
- Independent component analysis (ICA) is a statistical and computational technique for revealing hidden factors that underlie sets of random variables, measurements, or signals.
- ICA defines a generative model for the observed multivariate data, which is typically given as a large database of samples.
- In the model, the data variables are assumed to be linear mixtures of some unknown latent variables, and the mixing system is also unknown.
- The latent variables are assumed non-gaussian and mutually independent, and they are called the independent components of the observed data.
- These independent components, also called sources or factors, can be found by ICA.



Independent Component Analysis (ICA)

The data are represented by the observed random vector $\boldsymbol{x}=(x_1,\ldots,x_m)^T$ and the hidden components as the random vector $\boldsymbol{s}=(s_1,\ldots,s_n)^T$. The task is to transform the observed data \boldsymbol{x} , using a linear static transformation \boldsymbol{W} as $\boldsymbol{s}=\boldsymbol{W}\boldsymbol{x}$, into a vector of maximally independent components \boldsymbol{s} measured by some function $F(s_1,\ldots,s_n)$ of independence.





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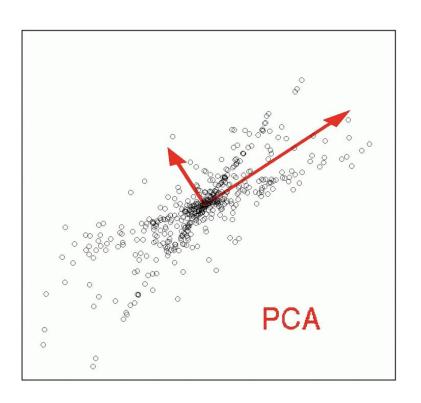


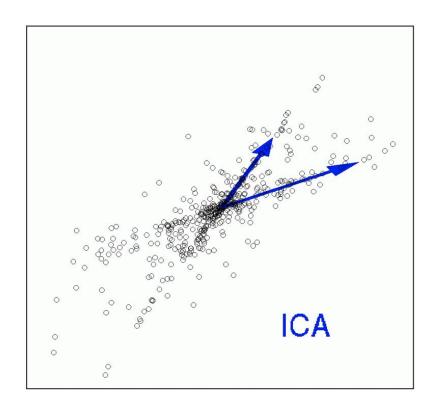
PCA:

- Find projections to minimize reconstruction error
 - Variance of projected data is as large as possible
- 2. 2nd-order statistics needed (cov(x))

ICA:

- Find "interesting" projections
 - Projected data look as non-Gaussian, independent as possible
- Higher-order statistics needed to measure degree of independence

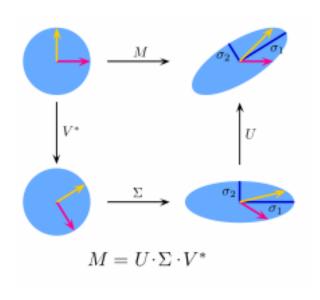




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ngular Value Decomposition (SVD)

- The singular value decomposition (SVD) is a factorization of a real or complex matrix.
- It generalizes the eigendecomposition of a square normal matrix with an orthonormal eigenbasis to any n × n matrix.
- It is related to the polar decomposition.



SVD Calculation

An eigenvector of a square matrix $\bf A$ is a vector $\bf v$ such that $\bf A$ only changes the magnitude of $\bf v$

- ▶ I.e. $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$ for some $\lambda \in \mathbb{R}$
- Such λ is an eigenvalue of A

The eigendecomposition of **A** is $\mathbf{A} = \mathbf{Q} \Delta \mathbf{Q}^{-1}$

- ▶ The columns of **Q** are the eigenvectors of **A**
- ightharpoonup Matrix Δ is a diagonal matrix with the eigenvalues

Not every (square) matrix has eigendecomposition

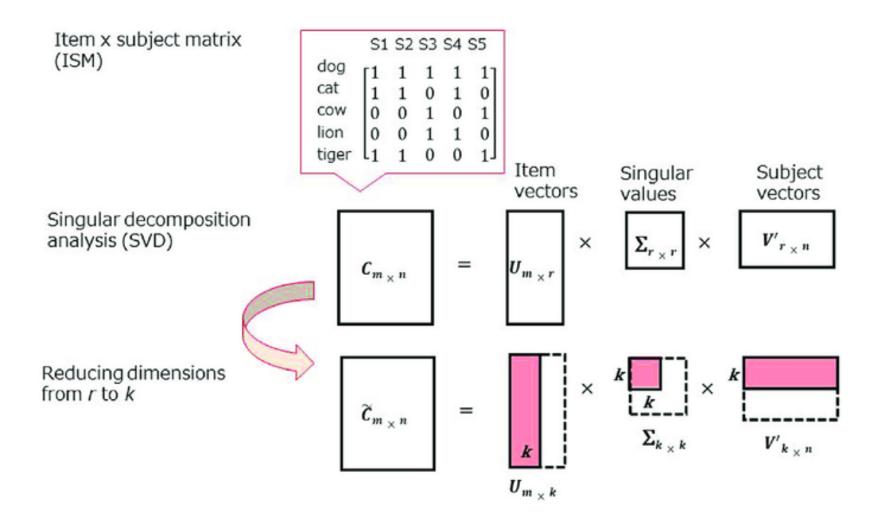
▶ If A is of form BB^T , it always has eigendecomposition

The SVD of **A** is closely related to the eigendecompositions of $\mathbf{A}\mathbf{A}^T$ and $\mathbf{A}^T\mathbf{A}$

- ► The left singular vectors are the eigenvectors of AA^T
- ► The right singular vectors are the eigenvectors of A^TA
- The singular values are the square roots of the eigenvalues of both $\mathbf{A}\mathbf{A}^T$ and $\mathbf{A}^T\mathbf{A}$



SVD for Dimension Reduction





t-distributed Stochastic Neighbor Embedding (TSNE)

- A method for visualizing high-dimensional data by giving each datapoint a location in a two or three-dimensional map.
- It is based on Stochastic Neighbor Embedding originally developed by Sam Roweis and Geoffrey Hinton, where Laurens van der Maaten proposed the t-distributed variant.
- It is a nonlinear dimensionality reduction technique wellsuited for embedding high-dimensional data for visualization in a low-dimensional space of two or three dimensions.
- It models each high-dimensional object by a two- or threedimensional point in such a way that similar objects are modeled by nearby points and dissimilar objects are modeled by distant points with high probability.

t-SNE

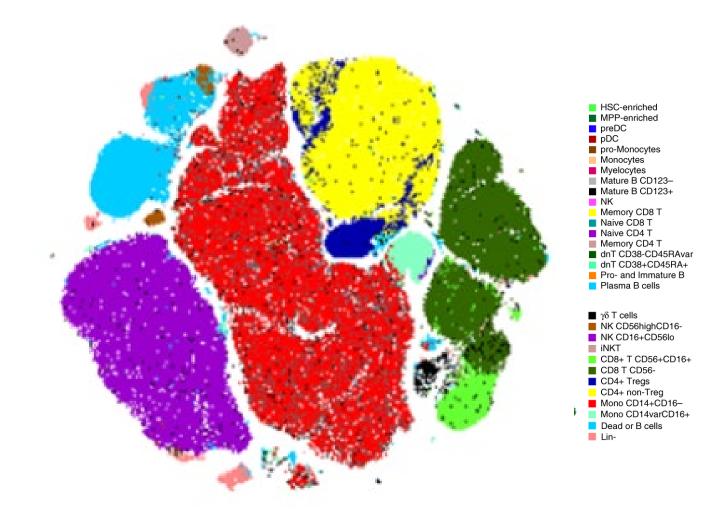
The t-SNE algorithm comprises two main stages.

■ 1st:

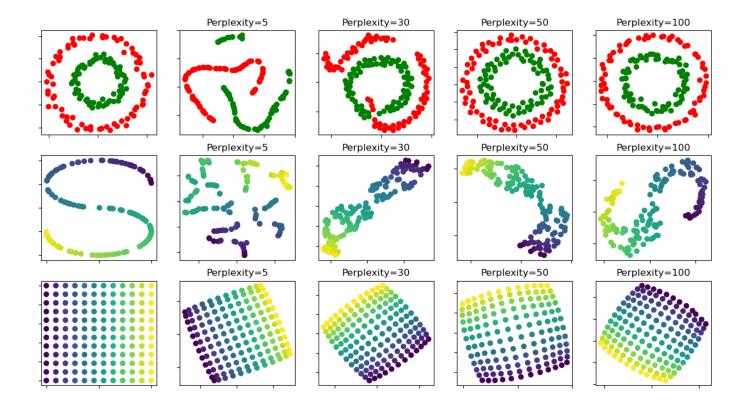
 t-SNE constructs a probability distribution over pairs of highdimensional objects in such a way that similar objects are assigned a higher probability while dissimilar points are assigned a lower probability.

2nd:

t-SNE defines a similar probability distribution over the points in the low-dimensional map, and it minimizes the Kullback–Leibler divergence (KL divergence) between the two distributions with respect to the locations of the points in the map.









Optimizing Parameters

sklearn.model_selection.GridSearchCV(estimator, param_grid, scoring=None, n_jobs=None, iid='warn', refit=True, cv='warn', verbose=0, pre_dispatch='2*n_jobs', error_score='raisedeprecating', return_train_score=False)



GridSearchCV

decision_function(self, X)	Call decision_function on the estimator with the best found parameters.
<pre>fit(self, X[, y, groups])</pre>	Run fit with all sets of parameters.
get_params(self[, deep])	Get parameters for this estimator.
inverse_transform(self, Xt)	Call inverse_transform on the estimator with the best found params.
predict(self, X)	Call predict on the estimator with the best found parameters.
<pre>predict_log_proba(self, X)</pre>	Call predict_log_proba on the estimator with the best found parameters.
<pre>predict_proba(self, X)</pre>	Call predict_proba on the estimator with the best found parameters.
score(self, X[, y])	Returns the score on the given data, if the estimator has been refit.
set_params(self, **params)	Set the parameters of this estimator.
transform(self, X)	Call transform on the estimator with the best found parameters.



```
from sklearn import datasets
from sklearn.model selection import train test split
from sklearn.model selection import GridSearchCV
from sklearn.metrics import classification_report
from sklearn.svm import SVC
# Loading the Digits dataset
digits = datasets.load digits()
# To apply an classifier on this data, we need to flatten the image, to
# turn the data in a (samples, feature) matrix:
n samples = len(digits.images)
X = digits.images.reshape((n samples, -1))
y = digits.target
# Split the dataset in two equal parts
X train, X test, y train, y test = train test split(X, y, test size=0.5,
random_state=0)
```





```
for score in scores:
  print("# Tuning hyper-parameters for %s" % score)
  print()
  clf = GridSearchCV(SVC(), tuned parameters, scoring="%s macro" % score)
  clf.fit(X train, y train)
  print("Best parameters set found on development set:")
  print()
  print(clf.best params )
  print()
  print("Grid scores on development set:")
  print()
  means = clf.cv results ["mean test score"]
  stds = clf.cv results ["std test score"]
  for mean, std, params in zip(means, stds, clf.cv_results_["params"]):
     print("%0.3f (+/-%0.03f) for %r" % (mean, std * 2, params))
  print()
  print("Detailed classification report:")
  print()
  print("The model is trained on the full development set.")
  print("The scores are computed on the full evaluation set.")
  print()
  y true, y pred = y test, clf.predict(X test)
  print(classification report(y true, y pred))
  print()
```



- Pipeline of transforms with a final estimator.
- Sequentially apply a list of transforms and a final estimator.
- Intermediate steps of the pipeline must be 'transforms', that is, they must implement fit and transform methods.
- The final estimator only needs to implement fit. The transformers in the pipeline can be cached using memory argument.
- The purpose of the pipeline is to assemble several steps that can be cross-validated together while setting different parameters.



steps: *list*, List of (name, transform) tuples (implementing fit/transform) that are chained, in the order in which they are chained, with the last object an estimator.

Parameters:

memory: None, str or object with the joblib.Memory interface, optional Used to cache the fitted transformers of the pipeline. By default, no caching is performed. If a string is given, it is the path to the caching directory. Enabling caching triggers a clone of the transformers before fitting. Therefore, the transformer instance given to the pipeline cannot be inspected directly. Use the attribute named_steps or steps to inspect estimators within the pipeline. Caching the transformers is advantageous when fitting is time consuming.

verbose: boolean, optionallf True, the time elapsed while fitting each step will be printed as it is completed.

Attributes:

named_steps: bunch object, a dictionary with attribute accessRead-only attribute to access any step parameter by user given name. Keys are step names and values are steps parameters.



- decision_function(self, X) Apply transforms, and decision_function of the final estimator
- fit(self, X[, y]) Fit the model
- fit_predict(self, X[, y]) Applies fit_predict of last step in pipeline after transforms.
- fit_transform(self, X[, y]) Fit the model and transform with the final estimator
- get_params(self[, deep]) Get parameters for this estimator.
- predict(self, X, **predict_params) Apply transforms to the data, and predict with the final estimator
- predict_log_proba(self, X) Apply transforms, and predict_log_proba of the final estimator
- predict_proba(self, X) Apply transforms, and predict_proba of the final estimator
- score(self, X[, y, sample_weight]) Apply transforms, and score with the final estimator
- set_params(self, **kwargs) Set the parameters of this estimator.

from sklearn.svm import SVC from sklearn.preprocessing import StandardScaler from sklearn.datasets import make_classification from sklearn.model_selection import train_test_split from sklearn.pipeline import Pipeline

```
X, y = make_classification(random_state=101)
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=101)
pipe = Pipeline([('scaler', StandardScaler()), ('svc', SVC())])
# The pipeline can be used as any other estimator
# and avoids leaking the test set into the train set
pipe.fit(X_train, y_train)
pipe.score(X_test, y_test)
```