Overfitting and Underfitting

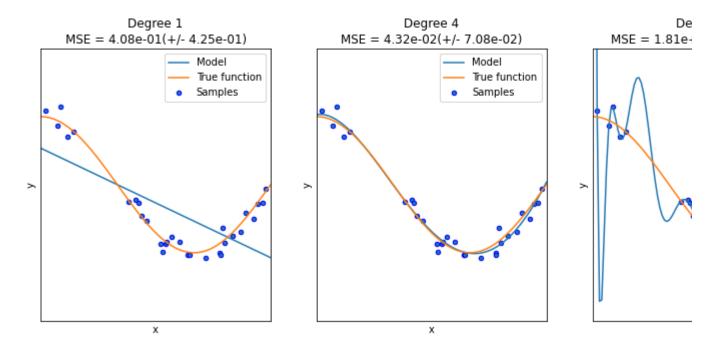
https://scikit-

<u>learn.org/stable/auto_examples/model_selection/plot_underfitting_o</u> verfitting.html

Program for understanding Overfitting and Underfitting

```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear model import LinearRegression
from sklearn.model_selection import cross_val_score
def true fun(X):
    return np.cos(1.5 * np.pi * X)
np.random.seed(0)
n \text{ samples} = 30
degrees = [1, 4, 15]
X = np.sort(np.random.rand(n_samples))
y = true fun(X) + np.random.randn(n samples) * 0.1
plt.figure(figsize=(14, 5))
for i in range(len(degrees)):
    ax = plt.subplot(1, len(degrees), i + 1)
    plt.setp(ax, xticks=(), yticks=())
    polynomial features = PolynomialFeatures(degree=degrees[i], include bias=False)
    linear_regression = LinearRegression()
    pipeline = Pipeline(
            ("polynomial_features", polynomial_features),
            ("linear_regression", linear_regression),
    pipeline.fit(X[:, np.newaxis], y)
```

```
# Evaluate the models using crossvalidation
    scores = cross_val_score(
        pipeline, X[:, np.newaxis], y, scoring="neg_mean_squared_error", cv=10
    )
    X \text{ test} = \text{np.linspace}(0, 1, 100)
    plt.plot(X_test, pipeline.predict(X_test[:, np.newaxis]), label="Model")
    plt.plot(X_test, true_fun(X_test), label="True function")
    plt.scatter(X, y, edgecolor="b", s=20, label="Samples")
    plt.xlabel("x")
    plt.ylabel("y")
    plt.xlim((0, 1))
    plt.ylim((-2, 2))
    plt.legend(loc="best")
    plt.title(
        "Degree {}\nMSE = {:.2e}(+/- {:.2e})".format(
            degrees[i], -scores.mean(), scores.std()
plt.show()
```



Overfitting (Printing accuracy at different steps)

https://machinelearningmastery.com/overfitting-machine-learning-models/

evaluate decision tree performance on train and test sets with different tree depths
from sklearn.datasets import make_classification

```
from sklearn.model selection import train test split
from sklearn.metrics import accuracy score
from sklearn.tree import DecisionTreeClassifier
from matplotlib import pyplot
# define dataset
X, y = make classification(n samples=10000, n features=20, n informative=5, n redundant=15, r
# summarize the dataset
print(X.shape, y.shape)
     (10000, 20) (10000,)
# split into train test sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3)
# summarize the shape of the train and test sets
print(X_train.shape, X_test.shape, y_train.shape, y_test.shape)
     (7000, 20) (3000, 20) (7000,) (3000,)
train scores, test scores = list(), list()
# define the tree depths to evaluate
values = [i for i in range(1, 31)]
# evaluate a decision tree for each depth
for i in values:
    # configure the model
    model = DecisionTreeClassifier(max depth=i)
    # fit model on the training dataset
    model.fit(X train, y train)
    # evaluate on the train dataset
    train_yhat = model.predict(X_train)
    train acc = accuracy score(y train, train yhat)
    train scores.append(train acc)
    # evaluate on the test dataset
    test yhat = model.predict(X test)
    test_acc = accuracy_score(y_test, test_yhat)
    test scores.append(test acc)
    # summarize progress
    print('>%d, train: %.3f, test: %.3f' % (i, train_acc, test_acc))
     >1, train: 0.763, test: 0.767
     >2, train: 0.804, test: 0.805
     >3, train: 0.871, test: 0.868
     >4, train: 0.906, test: 0.890
     >5, train: 0.924, test: 0.901
     >6, train: 0.937, test: 0.912
     >7, train: 0.947, test: 0.917
     >8, train: 0.956, test: 0.914
     >9, train: 0.966, test: 0.917
```

```
>10, train: 0.975, test: 0.911
>11, train: 0.981, test: 0.913
>12, train: 0.985, test: 0.909
>13, train: 0.990, test: 0.909
>14, train: 0.993, test: 0.907
>15, train: 0.995, test: 0.905
>16, train: 0.996, test: 0.910
>17, train: 0.997, test: 0.908
>18, train: 0.998, test: 0.904
>19, train: 0.999, test: 0.905
>20, train: 0.999, test: 0.903
>21, train: 1.000, test: 0.902
>22, train: 1.000, test: 0.905
>23, train: 1.000, test: 0.903
>24, train: 1.000, test: 0.901
>25, train: 1.000, test: 0.901
>26, train: 1.000, test: 0.906
>27, train: 1.000, test: 0.905
>28, train: 1.000, test: 0.900
>29, train: 1.000, test: 0.900
>30, train: 1.000, test: 0.908
```

Cross-validation

https://scikit-learn.org/stable/modules/cross_validation.html

Basic method to compute score

```
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.4, random_state=0)
```

Estimate the accuracy by splitting the data, computing the score 5 consecutive times (with different splits each time)

Using the different scoring parameter

```
from sklearn import metrics

scores = cross_val_score(
    clf, X, y, cv=5, scoring='f1_macro')
scores

array([0.96658312, 1. , 0.96658312, 0.96658312, 1. ])
```

Specified multiple metrics of predefined scorer names

```
from sklearn.model selection import cross validate
```

Calculate cross validation score by passing a cross validation iterator

```
from sklearn.model_selection import ShuffleSplit
n_samples = X.shape[0]
cv = ShuffleSplit(n_splits=5, test_size=0.3, random_state=0)
cross_val_score(clf, X, y, cv=cv)
array([0.97777778, 0.97777778, 1. , 0.95555556, 1. ])
```

▼ Use an iterable yielding (train, test) splits as arrays of indices

- ▼ Different type of Cross validation iterators
- ▼ K-fold

```
import numpy as np
from sklearn.model_selection import KFold
```

```
X = ["a", "b", "c", "d"]
kf = KFold(n_splits=2)
for train, test in kf.split(X):
    print("%s %s" % (train, test))

[2 3] [0 1]
    [0 1] [2 3]
```

Repeated K-Fold

```
import numpy as np
from sklearn.model_selection import RepeatedKFold

X = np.array([[1, 2], [3, 4], [1, 2], [3, 4]])
random_state = 12883823

rkf = RepeatedKFold(n_splits=2, n_repeats=2, random_state=random_state)
for train, test in rkf.split(X):
    print("%s %s" % (train, test))

[2 3] [0 1]
    [0 1] [2 3]
    [0 2] [1 3]
    [1 3] [0 2]
```

▼ Leave One Out (LOO)

```
from sklearn.model_selection import LeaveOneOut

X = [1, 2, 3, 4]
loo = LeaveOneOut()
for train, test in loo.split(X):
    print("%s %s" % (train, test))

       [1 2 3] [0]
       [0 2 3] [1]
       [0 1 3] [2]
       [0 1 2] [3]
```

▼ Random permutations cross-validation a.k.a. Shuffle & Split

```
from sklearn.model_selection import ShuffleSplit
```

```
X = np.arange(10)
ss = ShuffleSplit(n_splits=5, test_size=0.25, random_state=0)
for train_index, test_index in ss.split(X):
    print("%s %s" % (train_index, test_index))

[9 1 6 7 3 0 5] [2 8 4]
    [2 9 8 0 6 7 4] [3 5 1]
    [4 5 1 0 6 9 7] [2 3 8]
    [2 7 5 8 0 3 4] [6 1 9]
    [4 1 0 6 8 9 3] [5 2 7]
```

▼ Group k-fold

Double-click (or enter) to edit

```
from sklearn.model_selection import GroupKFold
X = [0.1, 0.2, 2.2, 2.4, 2.3, 4.55, 5.8, 8.8, 9, 10]
y = ["a", "b", "b", "b", "c", "c", "c", "d", "d", "d"]
groups = [1, 1, 1, 2, 2, 2, 3, 3, 3, 3]
gkf = GroupKFold(n_splits=3)
for train, test in gkf.split(X, y, groups=groups):
    print("%s %s" % (train, test))

[0 1 2 3 4 5] [6 7 8 9]
    [0 1 2 6 7 8 9] [3 4 5]
    [3 4 5 6 7 8 9] [0 1 2]
```

GroupShuffleSplit

```
from sklearn.model_selection import GroupShuffleSplit

X = [0.1, 0.2, 2.2, 2.4, 2.3, 4.55, 5.8, 0.001]
y = ["a", "b", "b", "c", "c", "c", "a"]
groups = [1, 1, 2, 2, 3, 3, 4, 4]
gss = GroupShuffleSplit(n_splits=4, test_size=0.5, random_state=0)
for train, test in gss.split(X, y, groups=groups):
    print("%s %s" % (train, test))

    [0 1 2 3] [4 5 6 7]
    [2 3 6 7] [0 1 4 5]
    [2 3 4 5] [0 1 6 7]
    [4 5 6 7] [0 1 2 3]
```

Validation curve

https://keeeto.github.io/blog/bias_variance/

https://scikit-learn.org/stable/modules/learning_curve.html

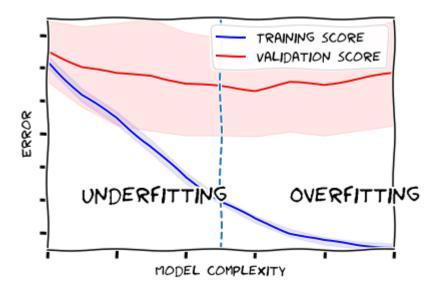
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from sklearn.ensemble import RandomForestClassifier
from sklearn.model selection import GridSearchCV
from sklearn.model_selection import cross_val_score, learning_curve, validation_curve
df_train = pd.read_csv('train.csv')
df test = pd.read csv('test.csv')
df_comb = df_train.append(df_test)
X = pd.DataFrame()
def encode sex(x):
    return 1 if x == 'female' else 0
def family_size(x):
    size = x.SibSp + x.Parch
    return 4 if size > 3 else size
X['Sex'] = df_comb.Sex.map(encode_sex)
X['Pclass'] = df comb.Pclass
X['FamilySize'] = df_comb.apply(family_size, axis=1)
fare_median = df_train.groupby(['Sex', 'Pclass']).Fare.median()
fare median.name = 'FareMedian'
```

```
age mean = df train.groupby(['Sex', 'Pclass']).Age.mean()
age mean.name = 'AgeMean'
def join(df, stat):
    return pd.merge(df, stat.to frame(), left on=['Sex', 'Pclass'], right index=True, how='le
X['Fare'] = df comb.Fare.fillna(join(df comb, fare median).FareMedian)
X['Age'] = df comb.Age.fillna(join(df comb, age mean).AgeMean)
def quantiles(series, num):
    return pd.qcut(series, num, retbins=True)[1]
def discretize(series, bins):
    return pd.cut(series, bins, labels=range(len(bins)-1), include_lowest=True)
X['Fare'] = discretize(X.Fare, quantiles(df_comb.Fare, 10))
X['Age'] = discretize(X.Age, quantiles(df_comb.Age, 10))
X_train = X.iloc[:df_train.shape[0]]
X test = X.iloc[df train.shape[0]:]
y_train = df_train.Survived
clf 1 = RandomForestClassifier(n estimators=100, bootstrap=True, random state=0)
clf 1.fit(X train, y train)
# Number of folds for cross validation
num folds = 7
def plot_curve(ticks, train_scores, test_scores):
    train_scores_mean = -1 * np.mean(train_scores, axis=1)
    train_scores_std = -1 * np.std(train_scores, axis=1)
    test_scores_mean = -1 * np.mean(test_scores, axis=1)
    test_scores_std = -1 * np.std(test_scores, axis=1)
    plt.figure()
    plt.fill between(ticks,
                     train_scores_mean - train_scores_std,
                     train scores mean + train scores std, alpha=0.1, color="b")
    plt.fill_between(ticks,
                     test_scores_mean - test_scores_std,
                     test scores mean + test scores std, alpha=0.1, color="r")
    plt.plot(ticks, train_scores_mean, 'b-', label='Training score')
    plt.plot(ticks, test scores mean, 'r-', label='Validation score')
    plt.legend(fancybox=True, facecolor='w')
```

return plt.gca()

```
def plot_validation_curve(clf, X, y, param_name, param_range, scoring='roc_auc'):
   plt.xkcd()
   ax = plot_curve(param_range, *validation_curve(clf, X, y, cv=num_folds,
                                                   scoring=scoring,
                                                   param name=param name,
                                                   param_range=param_range, n_jobs=-1))
   ax.set title('')
   ax.set_xticklabels([])
   ax.set_yticklabels([])
   ax.set xlim(2,12)
   ax.set_ylim(-0.97, -0.83)
   ax.set ylabel('Error')
   ax.set_xlabel('Model complexity')
   ax.text(9, -0.94, 'Overfitting', fontsize=22)
   ax.text(3, -0.94, 'Underfitting', fontsize=22)
   ax.axvline(7, ls='--')
   plt.tight layout()
```

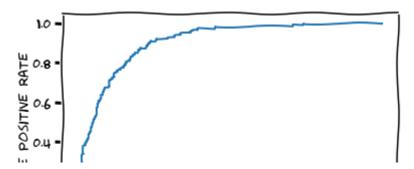
plot_validation_curve(clf_1, X_train, y_train, param_name='max_depth', param_range=range(2,13)



ROC

https://www.statology.org/plot-roc-curve-python/

```
import pandas as pd
import numpy as np
from sklearn.model selection import train test split
from sklearn.linear model import LogisticRegression
from sklearn import metrics
import matplotlib.pyplot as plt
#import dataset from CSV file on Github
url = "https://raw.githubusercontent.com/Statology/Python-Guides/main/default.csv"
data = pd.read csv(url)
#define the predictor variables and the response variable
X = data[['student', 'balance', 'income']]
y = data['default']
#split the dataset into training (70%) and testing (30%) sets
X_train,X_test,y_train,y_test = train_test_split(X,y,test_size=0.3,random_state=0)
#instantiate the model
log regression = LogisticRegression()
#fit the model using the training data
log regression.fit(X train,y train)
     LogisticRegression()
#define metrics
y_pred_proba = log_regression.predict_proba(X_test)[::,1]
fpr, tpr, = metrics.roc curve(y test, y pred proba)
#create ROC curve
plt.plot(fpr,tpr)
plt.ylabel('True Positive Rate')
plt.xlabel('False Positive Rate')
plt.show()
```



Task 1: Perform all of the above codes of Overfitting, Cross Validation, etc. with the help of the given reference link.

Task 2: Explain your analysis of the code. Make a detailed analysis that can also cover the following questions: (Submit the PDF of Report)

- 1) According to you, why do overfitting and underfitting occur, and how resolve them? What is the difference between them?
- 2) What kind of pattern did you analyze in the Train and Test score while running the code of overfitting?
- 3) What is cross-validation, and what did you analyze in a different type of validation that you performed?
- 4) Explain the analysis from generated ROC and validation curve and what they represent?

Task 3: Using the given Cross Validation iterators perform all types of Cross Validations we did in the task :

- 1) K-fold
- 2) Repeated K-Fold
- 3) Leave One Out (LOO)

Apart from this three, try to perform validation using three new iterators.

Task 4: With the help of the given code and references complete all of the following step:

- 1) Choose one new dataset. Train a overfitted model with the help of any machine learning technique, such as KNN, classification, regression.
- 2) Try to resolve the overfitting.
- Calculate the Validation score by any two or three given techniques and Validation iterators.
- 4) Generate the validation curve
- 5) Predict the output of testing data.
- 6) Generate the ROC curve using the predicted data and actual data.

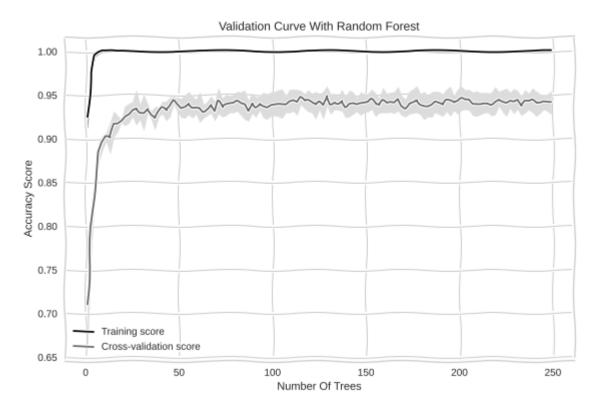
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression
from sklearn.model selection import cross val score
from sklearn.datasets import load diabetes
X, y = make_classification(n_samples=5000, n_features=20, n_informative=15)
from sklearn.model selection import train test split
X_train, X_test, y_train, y_test = train_test_split(
   X, y, test_size=0.2, shuffle=True)
print(len(X),len(X train),len(X test))
     5000 4000 1000
from sklearn.neighbors import KNeighborsClassifier
# Create KNN classifier
knn = KNeighborsClassifier(n_neighbors = 3)
```

```
# Fit the classifier to the data
knn.fit(X train,y train)
     KNeighborsClassifier(n_neighbors=3)
#show first 5 model predictions on the test data
knn.predict(X test)[0:5]
     array([0, 1, 1, 1, 1])
knn.score(X test, y test)
     0.934
from sklearn.model selection import ShuffleSplit
n samples = X.shape[0]
cv = ShuffleSplit(n_splits=5, test_size=0.3, random_state=0)
cross val score(clf, X, y, cv=cv)
     array([0.74066667, 0.73266667, 0.726 , 0.74866667, 0.72
                                                                       1)
def custom cv 2folds(X):
   n = X.shape[0]
   i = 1
   while i <= 2:
        idx = np.arange(n * (i - 1) / 2, n * i / 2, dtype=int)
       yield idx, idx
        i += 1
custom cv = custom cv 2folds(X)
cross_val_score(clf, X, y, cv=custom_cv)
     array([0.748 , 0.7364])
import numpy as np
from sklearn.model_selection import KFold
X = ["a", "b", "c", "d"]
kf = KFold(n splits=2)
for train, test in kf.split(X):
     print("%s %s" % (train, test))
     [2 3] [0 1]
     [0 1] [2 3]
import numpy as np
from sklearn.model selection import RepeatedKFold
X = np.array([[1, 2], [3, 4], [1, 2], [3, 4]])
```

```
random state = 12883823
rkf = RepeatedKFold(n splits=2, n repeats=2, random state=random state)
for train, test in rkf.split(X):
   print("%s %s" % (train, test))
     [2 3] [0 1]
     [0 1] [2 3]
     [0 2] [1 3]
     [1 3] [0 2]
import matplotlib.pyplot as plt
import numpy as np
from sklearn.datasets import load diabetes
from sklearn.ensemble import RandomForestClassifier
from sklearn.model selection import validation curve
diabetes = load diabates()
# Create feature matrix and target vector
X, y = diabetes.data, diabetes.target
train_scores, test_scores = list(), list()
# define the tree depths to evaluate
values = [i for i in range(1, 31)]
for i in values:
   # configure the model
   model = RandomForestClassifier(max depth=i)
   # fit model on the training dataset
   model.fit(X train, y train)
   # evaluate on the train dataset
   train yhat = model.predict(X train)
   train acc = accuracy score(y train, train yhat)
   train scores.append(train acc)
   # evaluate on the test dataset
   test yhat = model.predict(X test)
   test_acc = accuracy_score(y_test, test_yhat)
   test scores.append(test acc)
   # summarize progress
   print('>%d, train: %.3f, test: %.3f' % (i, train acc, test acc))
   plt.show()
     >1, train: 0.903, test: 0.893
     >2, train: 0.922, test: 0.909
     >3, train: 0.984, test: 0.960
     >4, train: 0.996, test: 0.980
```

```
>5, train: 0.998, test: 0.987
     >6, train: 0.999, test: 0.993
     >7, train: 1.000, test: 0.993
     >8, train: 1.000, test: 0.993
     >9, train: 1.000, test: 0.996
     >10, train: 1.000, test: 0.996
     >11, train: 1.000, test: 0.993
     >12, train: 1.000, test: 0.993
     >13, train: 1.000, test: 0.996
     >14, train: 1.000, test: 0.991
     >15, train: 1.000, test: 0.991
     >16, train: 1.000, test: 0.993
     >17, train: 1.000, test: 0.991
     >18, train: 1.000, test: 0.991
     >19, train: 1.000, test: 0.993
     >20, train: 1.000, test: 0.987
     >21, train: 1.000, test: 0.993
     >22, train: 1.000, test: 0.989
     >23, train: 1.000, test: 0.996
     >24, train: 1.000, test: 0.993
     >25, train: 1.000, test: 0.996
     >26, train: 1.000, test: 0.996
     >27, train: 1.000, test: 0.993
     >28, train: 1.000, test: 0.996
     >29, train: 1.000, test: 0.993
     >30, train: 1.000, test: 0.991
param range = np.arange(1, 250, 2)
# Calculate accuracy on training and test set using range of parameter values
train scores, test scores = validation curve(RandomForestClassifier(),
                                             Χ,
                                             у,
                                             param_name="n_estimators",
                                             param range=param range,
                                             cv=3,
                                             scoring="accuracy",
                                             n jobs=-1
# Calculate mean and standard deviation for training set scores
train mean = np.mean(train scores, axis=1)
train std = np.std(train scores, axis=1)
# Calculate mean and standard deviation for test set scores
test_mean = np.mean(test_scores, axis=1)
test std = np.std(test scores, axis=1)
# Plot mean accuracy scores for training and test sets
plt.plot(param range, train mean, label="Training score", color="black")
plt.plot(param_range, test_mean, label="Cross-validation score", color="dimgrey")
# Plot accurancy bands for training and test sets
plt.fill_between(param_range, train_mean - train_std, train_mean + train_std, color="gray")
plt.fill_between(param_range, test_mean - test_std, test_mean + test_std, color="gainsboro")
```

```
# Create plot
plt.title("Validation Curve With Random Forest")
plt.xlabel("Number Of Trees")
plt.ylabel("Accuracy Score")
plt.tight_layout()
plt.legend(loc="best")
plt.show()
```



from sklearn.datasets import load_diabetes
diabetes = load_diabetes()

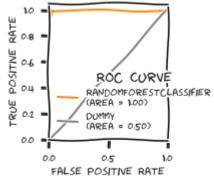
```
from sklearn.naive_bayes import GaussianNB
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(diabetes.data, diabetes.target)
clf = GaussianNB()
clf.fit(X_train, y_train)
```

GaussianNB()

```
predicted = clf.predict(X_test)
expected = y_test
print(predicted)
```

from sklearn import datasets from sklearn.linear model import LogisticRegression from sklearn.metrics import roc_curve, roc_auc_score from sklearn.model_selection import train_test_split import matplotlib.pyplot as plt dataset = datasets.load diabetes() X = dataset.data y = dataset.target Double-click (or enter) to edit from sklearn import datasets, ensemble, metrics, model selection, dummy import matplotlib.pyplot as plt diabetes = datasets.load_diabetes() # First we work only on sevens: sevens = (diabetes.target == 7) classifier = ensemble.RandomForestClassifier() most frequent = dummy.DummyClassifier(strategy='most frequent') X train, X test, y train, y test = model selection.train test split(diabetes.data, sevens, random state=0) y score = classifier.fit(X train, y train).predict proba(X test) most frequent score = most frequent.fit(X train, y train).predict proba(X test) fpr, tpr, _ = metrics.roc_curve(y_test, y_score[:, 1]) roc auc = metrics.auc(fpr, tpr) fpr_dummy, tpr_dummy, _ = metrics.roc_curve(y_test, most frequent score[:, 1])

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