

DL_01

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Deep Learning

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1 Neurônio simples

Um neurônio artificial do tipo **perceptron** faz uma combinação linear de entradas e aplica uma função de ativação como a função *sign*, *tanh* ou *relu* para produzir uma saída.

$$f(X) = \text{sign}(w_0 + w_1x_1 + \dots + w_nx_n)$$

O treinamento do neurônio é feito ajustando-se os pesos w_n de acordo com base em uma função de custo (por exemplo uma medida do erro e predição) obtido para se estimar a saída $f(X) \cong y$.

$$\min_W \sum ||f(X) - y||$$

Desse modo, você pode entender o aprendizado de um neurônio como um problema de otimização.

2 Redes neurais

Um único neurônio entretanto tem uma capacidade bastante limitada de aprendizado, restringindo-se a problemas de separação linear. Desse modo, por exemplo, ele não consegue aprender uma função como a função **XOR**.

Função $XOR(X) \rightarrow y$:

X	y
0 0	0
0 1	1
1 0	1
1 1	0

que é não linearmente separável.

Para resolver essa limitação podemos então trabalhar com múltiplos neurônios em camadas. As saídas dos neurônios de uma camada são então empregadas como entradas para a camada seguinte.

As camadas entre a camada inicial de neurônios (de entrada) e a camada final (de saída) constituem as camadas ocultas da rede.

O treinamento da rede segue o mesmo princípio, embora mais complexo, ajustando os pesos w_n de acordo com o erro de predição obtido para se estimar a saída $f(X) \cong y$.

$$\min_W \sum ||f(X) - y||$$

Chamamos esse aprendizado de *backpropagation* ou *retropropagação*.

Acesse agora <http://playground.tensorflow.org/> para uma demonstração.

3 Esquema Geral para Modelos Supervisionados e MLP

Modelos de Aprendizado Supervisionado seguem todos um esquema bastante geral no `scikit learn` e em muitos frameworks. Modelos Supervisionados de *Redes Neurais* podem ser implementados com o `scikit learn` e seguem a mesma estrutura.

4 Toy-example: Remain or Leave?

Abaixo um *toy-example*, um conjunto de dados de notas de alunos, de 0 a 5, para as disciplinas A, B, C, D e se o aluno R (*remain*) permanece no curso no final do semestre ou L (*leave*) deixa o curso.

Apesar de um exemplo simples, muitos outros problemas interessam se encaixam nessa mesma tipologia como problemas de *churn* de clientes, *fraud/non-fraud*, *credit/non-credit*, *defect/not-defect*, *benign/malign* etc.

Fig. 1. Esquema Geral para Modelos Supervisionados, aqui empregando uma Árvore de Decisão.

5 Obtenção dos Dados

```
[1]: import pandas as pd
students = pd.DataFrame({'A':[3, 5, 1, 1, 4, 2, 1, 5, 2, 4, 4, 2, 2, 2, 5, 5,
    ↪3, 4, 5, 4],
                        'B':[1, 1, 4, 5, 2, 4, 2, 3, 2, 1, 4, 3, 5, 2, 4, 1,
    ↪3, 2, 3, 2],
                        'C':[2, 1, 5, 3, 3, 1, 3, 4, 1, 4, 2, 4, 4, 1, 4, 1,
    ↪5, 1, 4, 3],
                        'D':[2, 3, 3, 1, 1, 2, 3, 4, 2, 4, 3, 5, 4, 2, 3, 1,
    ↪2, 2, 3, 2],
                        'status':['R', 'L', 'R', 'L', 'L', 'L', 'L', 'R', 'R', 'L',
    ↪'R', 'L', 'R', 'R', 'L', 'L', 'L', 'R', 'L', 'L', 'L']})
print(students)
new_students = pd.DataFrame({'A':[5, 4, 4, 3],
                             'B':[1, 4, 1, 3],
                             'C':[1, 1, 2, 3],
```

```

'D':[2, 4, 1, 3],
'status':['?', '?', '?', '?']})

print(new_students)

```

	A	B	C	D	status
0	3	1	2	2	R
1	5	1	1	3	L
2	1	4	5	3	R
3	1	5	3	1	L
4	4	2	3	1	L
5	2	4	1	2	L
6	1	2	3	3	R
7	5	3	4	4	R
8	2	2	1	2	L
9	4	1	4	4	R
10	4	4	2	3	L
11	2	3	4	5	R
12	2	5	4	4	R
13	2	2	1	2	L
14	5	4	4	3	L
15	5	1	1	1	L
16	3	3	5	2	R
17	4	2	1	2	L
18	5	3	4	3	L
19	4	2	3	2	L

	A	B	C	D	status
0	5	1	1	2	?
1	4	4	1	4	?
2	4	1	2	1	?
3	3	3	3	3	?

6 Definição das Variáveis Preditoras X e Dependente y

Neste ponto é esperado que os dados já estejam prontos para a aplicação do modelo tendo sido analisados e transformados nas fases de Entendimento e Preparação dos Dados (tratamento de nulos, hot encode, normalização e outras transformações necessárias).

```

[2]: X = students[['A', 'B', 'C', 'D']]
      y = students.status

```

7 Separação dos Conjuntos de Treinamento e Teste X_train, X_test, y_train, y_test

```
[3]: from sklearn.model_selection import train_test_split
seed = 1984

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
↳stratify=y, random_state=seed)
```

8 Declaração do Modelo clf

```
[4]: from sklearn.tree import DecisionTreeClassifier

clf = DecisionTreeClassifier(criterion='gini',
                             max_depth=None,
                             random_state=seed)
```

9 Treinamento do modelo fit()

```
[5]: clf.fit(X_train, y_train)
```

```
[5]: DecisionTreeClassifier(random_state=1984)
```

10 Predição do Conjunto de Teste predict()

```
[6]: y_pred = clf.predict(X_test)
```

11 Avaliação das métricas do modelo

Dependente do tipo de modelo. Aqui empregamos apenas a acuracidade.

```
[7]: from sklearn.metrics import accuracy_score

accuracy = accuracy_score(y_pred, y_test)
print(f'Accuracy: {accuracy :0.3f} %')
```

Accuracy: 1.000 %

12 Predição dos novos casos

```
[8]: X_new = new_students[['A', 'B', 'C', 'D']]

y_pred = clf.predict(X_new)

print(y_pred)
```

```
['L' 'R' 'L' 'R']
```

Nota O esquema apresentado é aqui é um esquema introdutório com propósitos unicamente didáticos e é, portanto, um modelo bastante simplificado. Particularmete ele não leva em consideração múltiplas execuções dos modelos ou técnicas como Cross Validation e também emprega uma única métrica de resultados, a acuracidade. O seguimento desse tema deveria incluir o Cross Validation e outras métricas (ROC, F1-score, recall, overfitting etc.).

13 Esquema Geral Completo

Colocando todas as células em um único código temos o seguinte:

```
[9]: from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score

from sklearn.tree import DecisionTreeClassifier

seed = 1984

X = students[['A', 'B', 'C', 'D']]
y = students.status

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
↳stratify=y, random_state=seed)

clf = DecisionTreeClassifier(criterion='gini',
                             max_depth=None,
                             random_state=seed)

#
# Por exemplo, alternativamente, poderíamos empregar um outro modelo como um
↳SVC no lugar a Árvore de Decisão
#
# from sklearn import svm
# clf = svm.SVC()
#
# Todos as demais instruções, poderiam ser mantidas sem qualquer alteração.
#
```

```

clf.fit(X_train, y_train)

y_pred = clf.predict(X_test)

accuracy = accuracy_score(y_pred, y_test)
print(f'Accuracy: {accuracy :0.3f} %')

X_new = new_students[['A', 'B', 'C', 'D']]

y_pred = clf.predict(X_new)

print(y_pred)

```

```

Accuracy: 1.000 %
['L' 'R' 'L' 'R']

```

Note que

```

“ from sklearn.tree import DecisionTreeClassifier clf = DecisionTreeClassi-
fier(criterion='gini', max_depth=None, random_state=seed)

```

Poderia ser substituído por qualquer outro modelo, por exemplo uma Support Vector Machine:

```

>'''
from sklearn import svm
clf = svm.SVC()

```

Com todas as demais instruções mantidas sem qualquer mudança.

14 Mais Métricas (opcional)

```

[10]: from sklearn.metrics import confusion_matrix
from sklearn.metrics import classification_report
from sklearn.metrics import accuracy_score

y_pred = clf.predict(X_test)

cm = confusion_matrix(y_pred, y_test)
print(cm)

accuracy = accuracy_score(y_pred, y_test)
print(accuracy)

print(classification_report(y_pred,y_test))

```

```

[[4 0]
 [0 2]]
1.0

precision    recall  f1-score   support


```

L	1.00	1.00	1.00	4
R	1.00	1.00	1.00	2
accuracy			1.00	6
macro avg	1.00	1.00	1.00	6
weighted avg	1.00	1.00	1.00	6

Alternativamente

```
[11]: clf.score(X_test, y_test)
```

```
[11]: 1.0
```

15 Exercício

Altere o esquema geral apresentado para aplicação de um modelo de rede neural [MLP](#).

```
from sklearn.neural_network import MLPClassifier
```

```
clf = MLPClassifier(solver='lbfgs',
                    alpha = ...,
                    max_iter = ...,
                    hidden_layer_sizes = ...,
                    random_state = ...)
```

Nota

Função de Ativação: * `activation`{'identity', 'logistic', 'tanh', 'relu'}, default='relu'

Solvers: * L-BFGS: Use para pequenos conjuntos de dados. * Adam: Use para grandes conjuntos de dados (default). * SGD: Gradiente estocástico, requer definir corretamente parâmetros como taxa de aprendizado, momentum etc.

```
[12]: from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score

from sklearn.neural_network import MLPClassifier

seed = 1984

X = students[['A', 'B', 'C', 'D']]
y = students.status

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
→stratify=y, random_state=seed)

clf = MLPClassifier(solver='lbfgs',
```

```

        alpha = 0.01,
        max_iter = 100,
        hidden_layer_sizes = (2,2),
        random_state = seed)

clf.fit(X_train, y_train)

y_pred = clf.predict(X_test)

accuracy = accuracy_score(y_pred, y_test)
print(f'Accuracy: {accuracy :0.3f} %')

X_new = new_students[['A', 'B', 'C', 'D']]

y_pred = clf.predict(X_new)

print(y_pred)

```

```

Accuracy: 1.000 %
['L' 'L' 'L' 'R']

```

```

/home/pbraga/.local/lib/python3.8/site-
packages/sklearn/neural_network/_multilayer_perceptron.py:471:
ConvergenceWarning: lbfgs failed to converge (status=1):
STOP: TOTAL NO. of ITERATIONS REACHED LIMIT.

```

Increase the number of iterations (max_iter) or scale the data as shown in:
<https://scikit-learn.org/stable/modules/preprocessing.html>
self.n_iter_ = _check_optimize_result("lbfgs", opt_res, self.max_iter)

16 Exibindo os pesos da MLP

Este código executará sobre o modelo o exercício anterior (clf).

```

[13]: import numpy as np

print(f'\nCamadas : ')
for i in range(len(clf.coefs_)):
    print(np.shape(clf.coefs_[i]))

for i in range(len(clf.coefs_)):
    print(f'\nW{i}: ')
    print(clf.coefs_[i])
    print(f'\nB{i}: ')
    print(clf.intercepts_[i])

```

```
Camadas :
```


(4, 2)
(2, 2)
(2, 1)

W0:

```
[[ 1.0703103 -0.27709637]
 [ 1.53423257 -0.42054466]
 [-1.0931328  0.30892174]
 [-1.50550167  0.46162624]]
```

B0:

```
[1.16101666 0.33004816]
```

W1:

```
[[ 2.66789684e+00  7.15011937e-04]
 [-7.21939314e-01 -3.02613406e-02]]
```

B1:

```
[ 0.41857034 -0.8053998 ]
```

W2:

```
[[ -2.77532442]
 [ -0.03938361]]
```

B2:

```
[10.97377198]
```

17 Exercício

Neste exercício você fará a predição de diagnóstico de câncer de mama a partir de features já extraídas de imagens para diagnóstico. Você pode usar os dados pré-formatados [aqui](#), evitando assim empregar os dados brutos da fonte original.

Decision Tree Model in the Diagnosis of Breast Cancer

[Breast Cancer Data]([https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+\(Diagnostic\)](https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+(Diagnostic)))

Analise os dados e, antes de criar seu modelo neural, verifique a necessidade tratamentos prévios dos dados como:

- *Feature selection* com a exclusão de atributos para o treinamento ()
- Tratamento dos dados faltantes ()
- *Hot encode* para conversão de dados categóricos ()
- Normalização dos dados ()

Apresente os resultados de acuracidade do seu modelo para as variáveis preditoras normalizadas e não normalizadas. Qual a sua conclusão?

```
[101]: import pandas as pd
breast = pd.read_csv('http://meusite.mackenzie.br/rogerio/DLA2021S1/
↳breast_cancer.csv')
breast.head()
```

```
[101]:
```

	id	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean	\
0	842302	M	17.99	10.38	122.80	1001.0	
1	842517	M	20.57	17.77	132.90	1326.0	
2	84300903	M	19.69	21.25	130.00	1203.0	
3	84348301	M	11.42	20.38	77.58	386.1	
4	84358402	M	20.29	14.34	135.10	1297.0	

	smoothness_mean	compactness_mean	concavity_mean	concave	points_mean	\
0	0.11840	0.27760	0.3001		0.14710	
1	0.08474	0.07864	0.0869		0.07017	
2	0.10960	0.15990	0.1974		0.12790	
3	0.14250	0.28390	0.2414		0.10520	
4	0.10030	0.13280	0.1980		0.10430	

...	radius_worst	texture_worst	perimeter_worst	area_worst	\
0	...	25.38	17.33	184.60	2019.0
1	...	24.99	23.41	158.80	1956.0
2	...	23.57	25.53	152.50	1709.0
3	...	14.91	26.50	98.87	567.7
4	...	22.54	16.67	152.20	1575.0

	smoothness_worst	compactness_worst	concavity_worst	concave	points_worst	\
0	0.1622	0.6656	0.7119		0.2654	
1	0.1238	0.1866	0.2416		0.1860	
2	0.1444	0.4245	0.4504		0.2430	
3	0.2098	0.8663	0.6869		0.2575	
4	0.1374	0.2050	0.4000		0.1625	

	symmetry_worst	fractal_dimension_worst
0	0.4601	0.11890
1	0.2750	0.08902
2	0.3613	0.08758
3	0.6638	0.17300
4	0.2364	0.07678

[5 rows x 32 columns]

```
[84]: # Seu código

# Mapeando a feature 'diagnosis' para '0' ou '1'
diag = {"M":0, "B":1}
breast['diagnosis'] = breast['diagnosis'].map(diag)
```

```
[85]: breast.head()
```

```
[85]:
```

	id	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean	\
0	842302	0	17.99	10.38	122.80	1001.0	
1	842517	0	20.57	17.77	132.90	1326.0	
2	84300903	0	19.69	21.25	130.00	1203.0	
3	84348301	0	11.42	20.38	77.58	386.1	
4	84358402	0	20.29	14.34	135.10	1297.0	

	smoothness_mean	compactness_mean	concavity_mean	concave	points_mean	\
0	0.11840	0.27760	0.3001		0.14710	
1	0.08474	0.07864	0.0869		0.07017	
2	0.10960	0.15990	0.1974		0.12790	
3	0.14250	0.28390	0.2414		0.10520	
4	0.10030	0.13280	0.1980		0.10430	

	...	radius_worst	texture_worst	perimeter_worst	area_worst	\
0	...	25.38	17.33	184.60	2019.0	
1	...	24.99	23.41	158.80	1956.0	
2	...	23.57	25.53	152.50	1709.0	
3	...	14.91	26.50	98.87	567.7	
4	...	22.54	16.67	152.20	1575.0	

	smoothness_worst	compactness_worst	concavity_worst	concave	points_worst	\
0	0.1622	0.6656	0.7119		0.2654	
1	0.1238	0.1866	0.2416		0.1860	
2	0.1444	0.4245	0.4504		0.2430	
3	0.2098	0.8663	0.6869		0.2575	
4	0.1374	0.2050	0.4000		0.1625	

	symmetry_worst	fractal_dimension_worst
0	0.4601	0.11890
1	0.2750	0.08902
2	0.3613	0.08758
3	0.6638	0.17300
4	0.2364	0.07678

[5 rows x 32 columns]

```
[86]: breast.corr().style.background_gradient().set_precision(2)
```

```
[86]: <pandas.io.formats.style.Styler at 0x7f60aa1badf0>
```

```
[87]: fList=[]
      for i in breast:
          fList.append(i)
```

```
[88]: # Removendo features com correlação menor que [.1]
```

```
cVal=0
for j in fList:
    cVal = breast['diagnosis'].corr(breast[j])
    if cVal < 0:
        cVal*=-1
    if cVal < 0.1:
        breast = breast.drop([j], axis = 1)
```

```
[89]: breast.head()
```

```
[89]:
```

	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean	\
0	0	17.99	10.38	122.80	1001.0	
1	0	20.57	17.77	132.90	1326.0	
2	0	19.69	21.25	130.00	1203.0	
3	0	11.42	20.38	77.58	386.1	
4	0	20.29	14.34	135.10	1297.0	

	smoothness_mean	compactness_mean	concavity_mean	concave points_mean	\
0	0.11840	0.27760	0.3001	0.14710	
1	0.08474	0.07864	0.0869	0.07017	
2	0.10960	0.15990	0.1974	0.12790	
3	0.14250	0.28390	0.2414	0.10520	
4	0.10030	0.13280	0.1980	0.10430	

	symmetry_mean	...	radius_worst	texture_worst	perimeter_worst	\
0	0.2419	...	25.38	17.33	184.60	
1	0.1812	...	24.99	23.41	158.80	
2	0.2069	...	23.57	25.53	152.50	
3	0.2597	...	14.91	26.50	98.87	
4	0.1809	...	22.54	16.67	152.20	

	area_worst	smoothness_worst	compactness_worst	concavity_worst	\
0	2019.0	0.1622	0.6656	0.7119	
1	1956.0	0.1238	0.1866	0.2416	
2	1709.0	0.1444	0.4245	0.4504	
3	567.7	0.2098	0.8663	0.6869	
4	1575.0	0.1374	0.2050	0.4000	

	concave points_worst	symmetry_worst	fractal_dimension_worst
0	0.2654	0.4601	0.11890
1	0.1860	0.2750	0.08902
2	0.2430	0.3613	0.08758
3	0.2575	0.6638	0.17300
4	0.1625	0.2364	0.07678

```
[5 rows x 26 columns]
```

```
[94]: from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score

from sklearn.neural_network import MLPClassifier

seed = 1984

X = breast.loc[:, breast.columns != 'diagnosis']
y = breast.loc[:, breast.columns == 'diagnosis']

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
↳stratify=y, random_state=seed)

clf = MLPClassifier(solver='lbfgs',
                    alpha = 0.01,
                    max_iter = 100,
                    hidden_layer_sizes = (2,2),
                    random_state = seed)

clf.fit(X_train, y_train)

y_pred = clf.predict(X_test)

accuracy = accuracy_score(y_pred, y_test)
print(f'Accuracy: {accuracy :0.3f} %')
```

Accuracy: 0.626 %

/home/pbraga/.local/lib/python3.8/site-packages/sklearn/utils/validation.py:72:
DataConversionWarning: A column-vector y was passed when a 1d array was
expected. Please change the shape of y to (n_samples,), for example using
ravel().
return f(**kwargs)

```
[91]: # Normalizando os dados
from sklearn.preprocessing import MinMaxScaler

# create a scaler object
scaler = MinMaxScaler()
# fit and transform the data
breastNorm = pd.DataFrame(scaler.fit_transform(breast), columns=breast.columns)
```

```
[96]: X = breastNorm.loc[:, breastNorm.columns != 'diagnosis']
y = breastNorm.loc[:, breastNorm.columns == 'diagnosis']

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
↳stratify=y, random_state=seed)
```

```

clf = MLPClassifier(solver='lbfgs',
                    alpha = 0.01,
                    max_iter = 100,
                    hidden_layer_sizes = (2,2),
                    random_state = seed)

clf.fit(X_train, y_train)

y_pred = clf.predict(X_test)

accuracy = accuracy_score(y_pred, y_test)
print(f'Accuracy: {accuracy :0.3f} %')

```

Accuracy: 0.959 %

/home/pbraga/.local/lib/python3.8/site-packages/sklearn/utils/validation.py:72:
DataConversionWarning: A column-vector y was passed when a 1d array was
expected. Please change the shape of y to (n_samples,), for example using
ravel().

```

    return f(**kwargs)
/home/pbraga/.local/lib/python3.8/site-
packages/sklearn/neural_network/_multilayer_perceptron.py:471:
ConvergenceWarning: lbfgs failed to converge (status=1):
STOP: TOTAL NO. of ITERATIONS REACHED LIMIT.

```

Increase the number of iterations (max_iter) or scale the data as shown in:

```

https://scikit-learn.org/stable/modules/preprocessing.html
self.n_iter_ = _check_optimize_result("lbfgs", opt_res, self.max_iter)

```

Após a normalização dos dados a precisão do preditor melhora consideravelmente pois as features são colocadas em uma mesma escala.

18 Aplicando Cross-Validation

Este código executará sobre o modelo e conjuntos de dados do exercício anterior (clf, X_train, y_train, X_test, y_test).

```

[97]: from sklearn.model_selection import cross_val_score

cv = cross_val_score(clf, X_train, y_train, cv=10)
test_score = clf.fit(X_train, y_train).score(X_test, y_test)

print('CV accuracy score: %0.3f' % np.mean(cv))
print('Test accuracy score: %0.3f' % (test_score))

```

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```

CV accuracy score: 0.932

Test accuracy score: 0.959

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```

19 Vários Modelos Comparados (opcional)

```
[98]: models = [ ]

from sklearn.tree import DecisionTreeClassifier
clf = DecisionTreeClassifier(criterion='gini',
```

```

                                max_depth=None,
                                random_state=seed)
models.append(['Decision Tree', clf])

from sklearn import neighbors
n_neighbors = 5
clf = neighbors.KNeighborsClassifier(n_neighbors)

models.append(['Knn', clf])

from sklearn.naive_bayes import GaussianNB, BernoulliNB
clf = BernoulliNB()

models.append(['Naive Bayes', clf])

from sklearn.ensemble import RandomForestClassifier
clf = RandomForestClassifier(n_estimators=10)

models.append(['Random Forest', clf])

from sklearn import svm
clf = svm.SVC()

models.append(['Support Vector Machines', clf])

from sklearn.neural_network import MLPClassifier

clf = MLPClassifier(solver='lbfgs',
                    alpha = 1e-5,
                    max_iter = 10000,
                    hidden_layer_sizes = (3, 10, 2),
                    random_state = seed)

models.append(['MLP Neural Network', clf])

from sklearn.metrics import accuracy_score
for model in models:
    clf = model[1]
    clf.fit(X_train, y_train)
    y_pred = clf.predict(X_test)
    accuracy = accuracy_score(y_pred, y_test)
    print('Model ' + model[0] + ' accuracy: {:.3f} %'.format(accuracy))

```

Model Decision Tree accuracy: 0.906 %
 Model Knn accuracy: 0.971 %
 Model Naive Bayes accuracy: 0.632 %
 Model Random Forest accuracy: 0.947 %

Model Support Vector Machines accuracy: 0.965 %

Model MLP Neural Network accuracy: 0.626 %

```
<ipython-input-98-2b59bc4d4739>:43: DataConversionWarning: A column-vector y was
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```
    clf.fit(X_train, y_train)
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