

Advanced Scikit-Learn

Andreas Mueller (NYU Center for Data Science, scikit-learn)

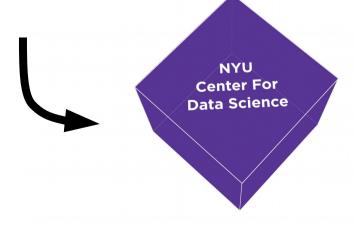
Me











Classification Regression Clustering Semi-Supervised Learning **Feature Selection Feature Extraction** Manifold Learning **Dimensionality Reduction Kernel Approximation** Hyperparameter Optimization **Evaluation Metrics** Out-of-core learning





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Jake Vanderplas

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Jaques Grobler

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kastnerkyle

Kyle Kastner



bthirion bthirion



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cournape David Cournapeau



duchesnay



Duchesnay



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NelleV Varoquaux



ogrisel Olivier Grisel



paolo-losi Paolo Losi



pprett Peter Prettenhofer



robertlayton Robert Layton



ronw Ron Weiss



Satrajit Ghosh



sklearn-ci



Vlad Niculae





vmichel Vincent Michel



yarikoptic Yaroslav Halchenko

Overview

- Reminder: Basic scikit-learn concepts
- Working with text data
- Model building and evaluation:
 - Pipelines
 - Randomized Parameter Search
 - Scoring Interface
- Out of Core learning
 - Feature Hashing
 - Kernel Approximation
- New stuff in 0.17 and 0.18-dev
 - Overview
 - Calibration

Documentation of scikit-learn 0.17

Quick Start

learn

A very short introduction into machine learning problems and how to solve them using scikit-learn. Introduced basic concepts and conventions.

User Guide

The main documentation. This contains an in-depth description of all algorithms and how to apply them.

Other Versions

- scikit-learn 0.18 (development)
- scikit-learn 0.17 (stable)
- scikit-learn 0.16
- scikit-learn 0.15

Tutorials

Useful tutorials for developing a feel for some of scikit-learn's applications in the machine learning field.

API

The exact API of all functions and classes, as given by the docstrings. The API documents expected types and allowed features for all functions, and all parameters available for the algorithms.

Additional Resources

Talks given, slide-sets and other information relevant to scikit-learn.

Contributing

Information on how to contribute. This also contains useful information for advanced users, for example how to build their own estimators.

Flow Chart

A graphical overview of basic areas of machine learning, and guidance which kind of algorithms to use in a given situation.

FAQ

Frequently asked questions about the project and contributing.

```
      1.1
      2.2
      3.4
      5.6
      1.0

      6.7
      0.5
      0.4
      2.6
      1.6

      2.4
      9.3
      7.3
      6.4
      2.8

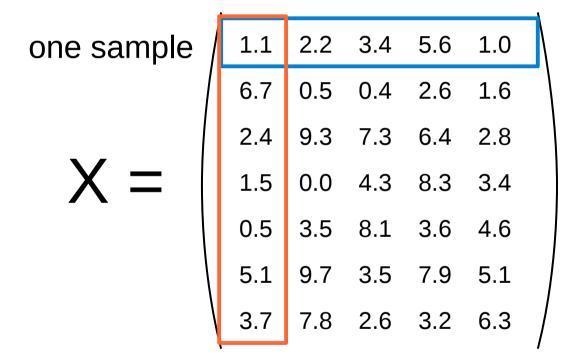
      1.5
      0.0
      4.3
      8.3
      3.4

      0.5
      3.5
      8.1
      3.6
      4.6

      5.1
      9.7
      3.5
      7.9
      5.1

      3.7
      7.8
      2.6
      3.2
      6.3
```

	,					•
one sample /	1.1	2.2	3.4	5.6	1.0	
	6.7	0.5	0.4	2.6	1.6	
	2.4	9.3	7.3	6.4	2.8	
X =	1.5	0.0	4.3	8.3	3.4	
	0.5	3.5	8.1	3.6	4.6	
	5.1	9.7	3.5	7.9	5.1	
	3.7	7.8	2.6	3.2	6.3	
	•					,



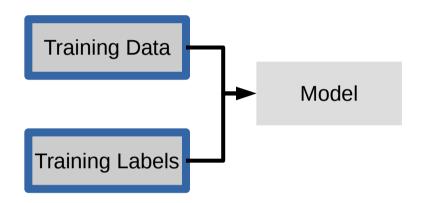
one feature

one feature

outputs / labels

Supervised Machine Learning

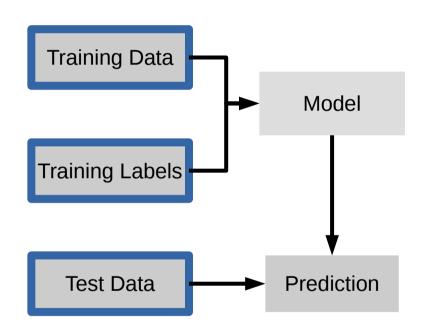
```
clf = RandomForestClassifier()
clf.fit(X_train, y_train)
```



Supervised Machine Learning

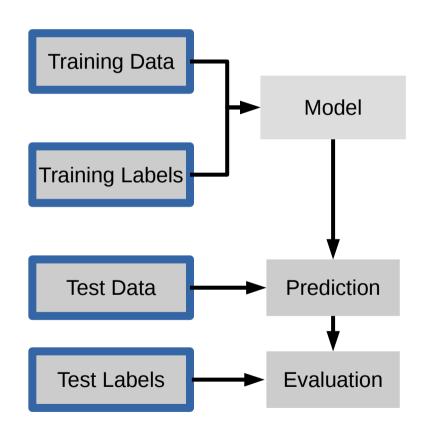
```
clf = RandomForestClassifier()
clf.fit(X_train, y_train)

y_pred = clf.predict(X_test)
```



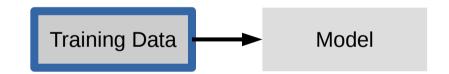
Supervised Machine Learning

```
clf = RandomForestClassifier()
clf.fit(X_train, y_train)
y_pred = clf.predict(X_test)
clf.score(X_test, y_test)
```



Unsupervised Transformations

```
pca = PCA(n_components=3)
```



Unsupervised Transformations

Basic API

estimator.fit(X, [y])

estimator.predict estimator.transform

Classification Preprocessing

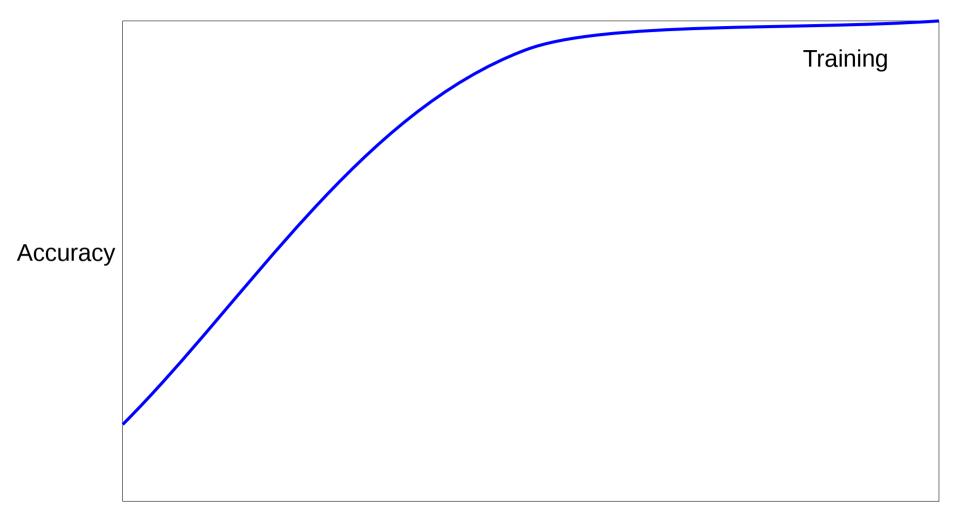
Regression Dimensionality reduction

Clustering Feature selection

Feature extraction

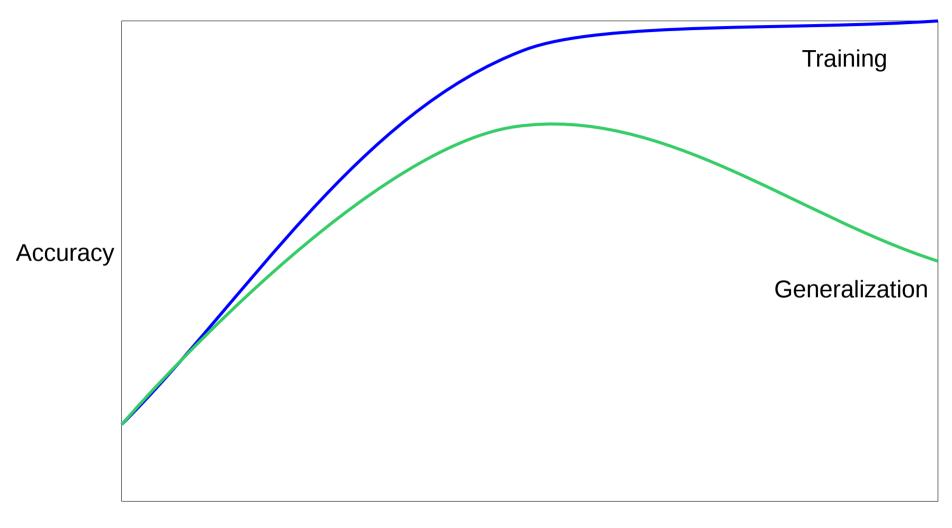
Model selection and model complexity (aka bias-variance tradeoff)

Overfitting and Underfitting



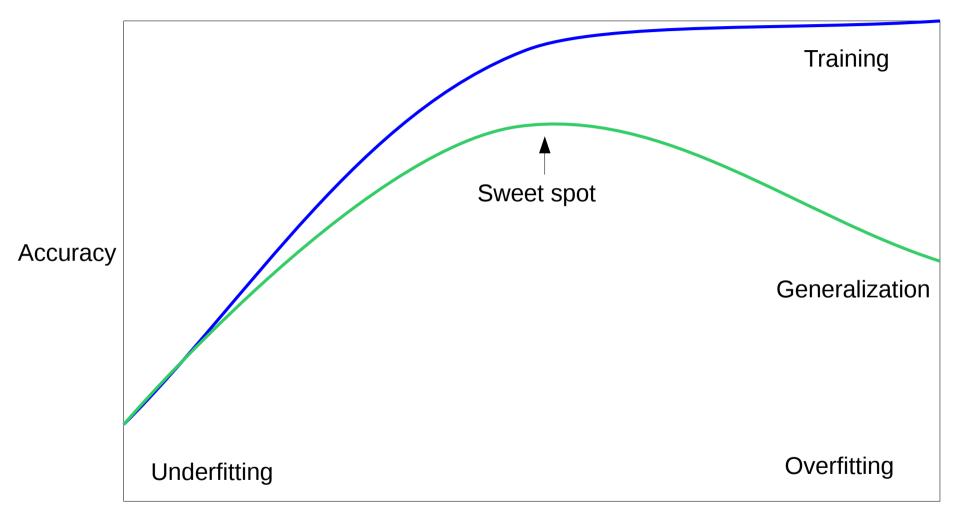
Model complexity

Overfitting and Underfitting



Model complexity

Overfitting and Underfitting



Model complexity

Cross-Validation

Cross-Validation

Cross-Validation

Cross -Validated Grid Search

All Data				
Training data	Test data			

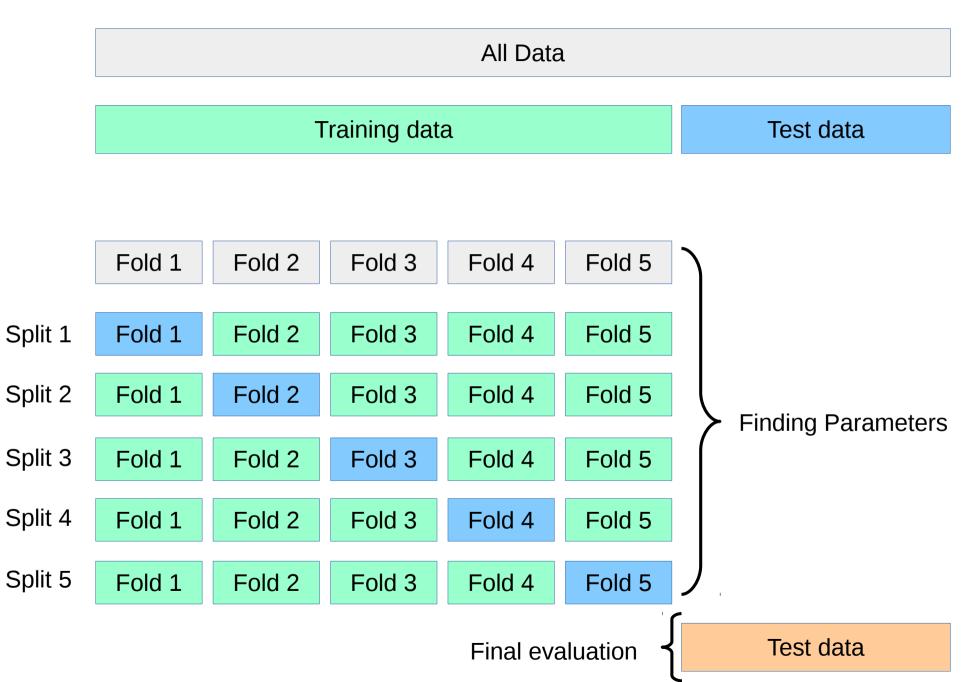
All Data

Training data

Test data

	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Split 1	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Split 2	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Split 3	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Split 4	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Split 5	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5

Test data



Cross -Validated Grid Search

Sample application: Sentiment Analysis

IMDB Movie Reviews Data

Review:

One of the worst movies I've ever rented. Sorry it had one of my favorite actors on it (Travolta) in a nonsense role. In fact, anything made sense in this movie.

Who can say there was true love between Eddy and Maureen? Don't you remember the beginning of the movie?

Is she so lovely? Ask her daughters. I don't think so.

Label: negative

Training data: 12500 positive, 12500 negative

CountVectorizer / TfidfVectorizer

"This is how you get ants."

```
"This is how you get ants."

tokenizer

['this', 'is', 'how', 'you', 'get', 'ants']
```

```
"This is how you get ants."

tokenizer

['this', 'is', 'how', 'you', 'get', 'ants']

Build a vocabulary over all documents

['aardvak', 'amsterdam', 'ants', ... 'you', 'your', 'zyxst']
```

```
"This is how you get ants."
                                  tokenizer
        ['this', 'is', 'how', 'you', 'get', 'ants']
                                 Build a vocabulary over all documents
['aardvak', 'amsterdam', 'ants', ... 'you', 'your', 'zyxst']
                                  Sparse matrix encoding
          aardvak ants get you zyxst
            [0, ..., 0, 1, 0, ..., 0, 1, 0, ..., 0, 1, 0, ..., 0]
```

N-grams (unigrams and bigrams)

N-grams (unigrams and bigrams)

CountVectorizer / TfidfVectorizer

"This is how you get ants."

N-grams (unigrams and bigrams)

CountVectorizer / TfidfVectorizer

```
"This is how you get ants."

Unigram tokenizer

['this', 'is', 'how', 'you', 'get', 'ants']
```

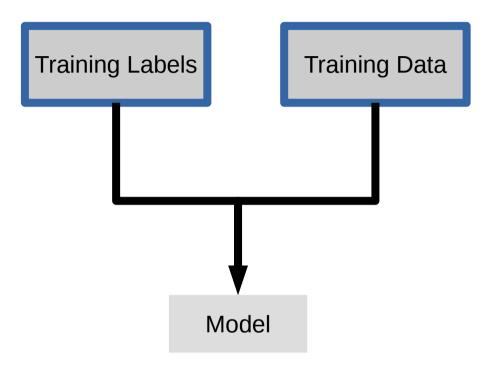
N-grams (unigrams and bigrams)

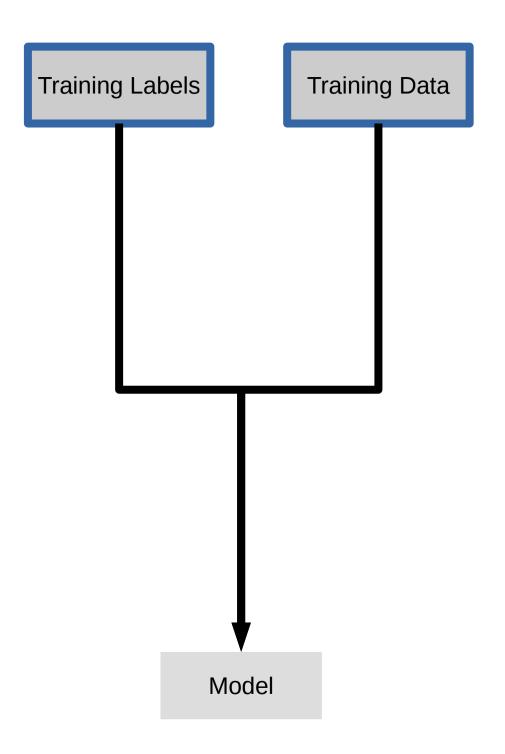
CountVectorizer / TfidfVectorizer

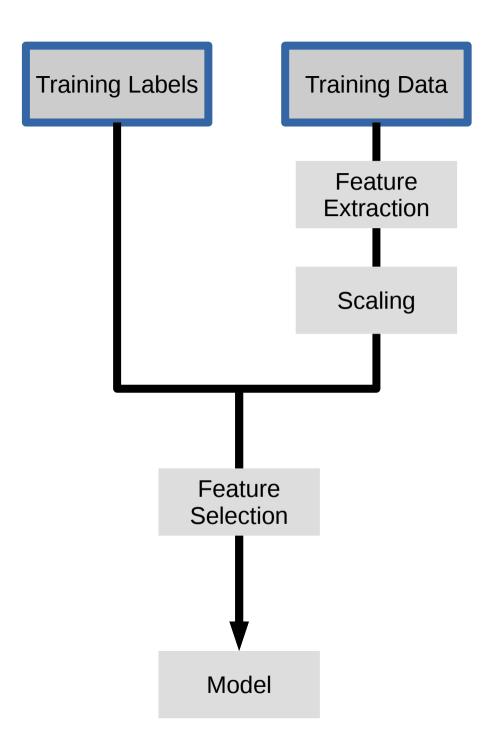
```
"This is how you get ants."
                              Unigram tokenizer
      ['this', 'is', 'how', 'you', 'get', 'ants']
               "This is how you get ants."
                              Bigram tokenizer
['this is', 'is how', 'how you', 'you get', 'get ants']
```

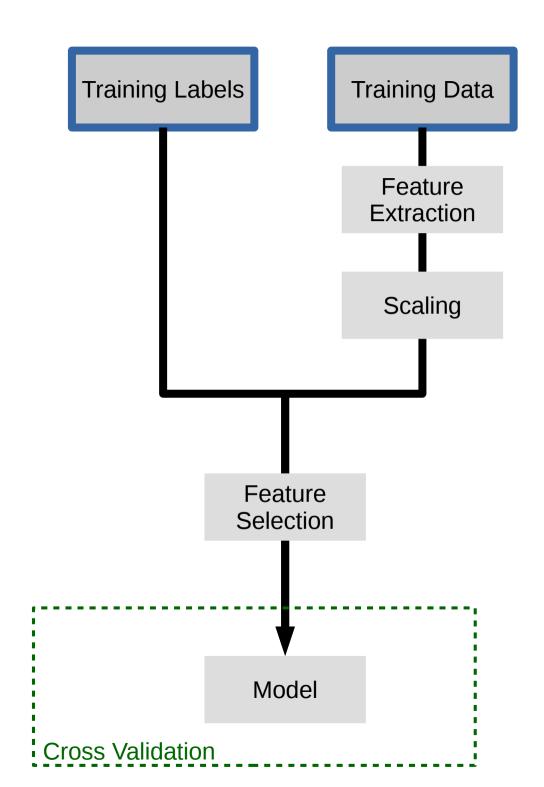
Notebook Working With Text Data

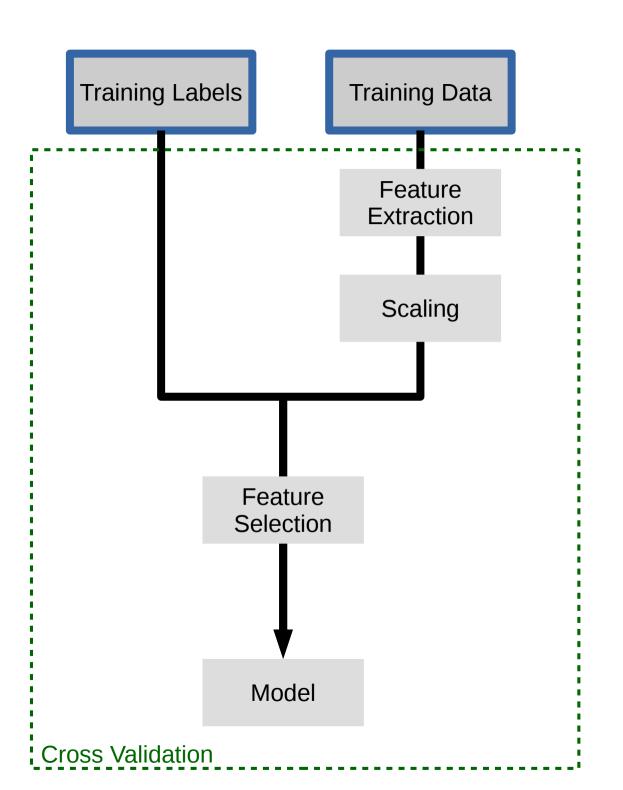
Pipelines









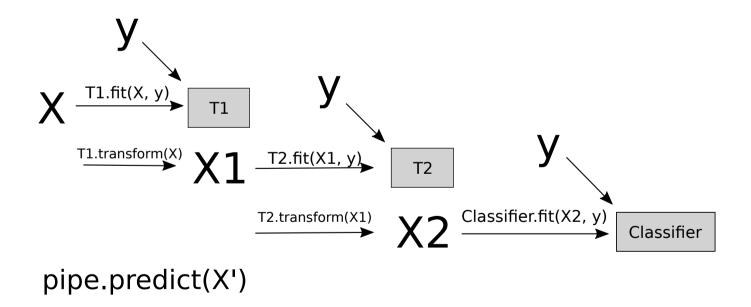


Pipelines

pipe = make_pipeline(T1(), T2(), Classifier())

T1 T2 Classifier

pipe.fit(X, y)



$$X^{\text{T1.transform}(X')}X^{\text{1}} \xrightarrow{\text{T2.transform}(X'1)} X^{\text{2}} \xrightarrow{\text{Classifier.predict}(X'2)} Y^{\text{1}}$$

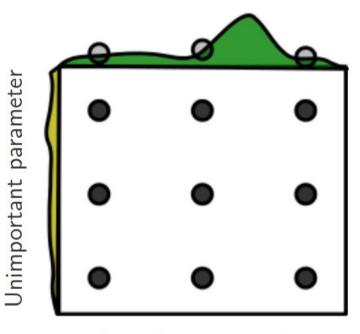
Pipelines

```
from sklearn.pipeline import make_pipeline

pipe = make_pipeline(StandardScaler(), SVC())
pipe.fit(X_train, y_train)
pipe.predict(X_test)
```

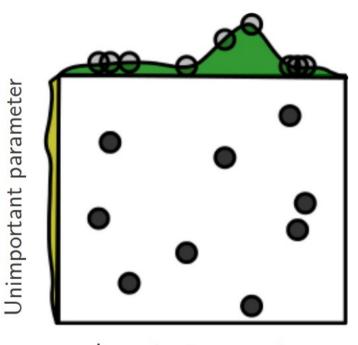
Continue Notebook Working with Text Data

Grid Layout



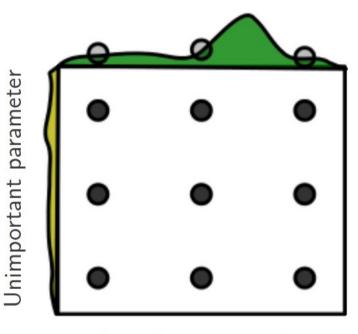
Important parameter

Random Layout



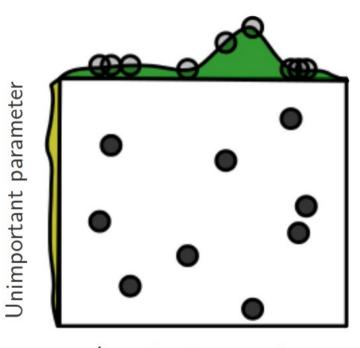
Important parameter

Grid Layout



Important parameter

Random Layout



Important parameter

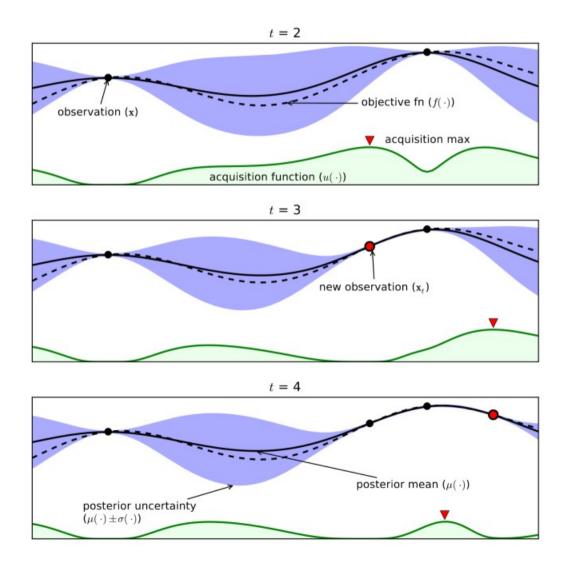
Step-size free for continuous parameters Decouples runtime from search-space size Robust against irrelevant parameters

```
params = { 'featureunion countvectorizer-1 ngram range':
          [(1, 3), (1, 5), (2, 5)],
          'featureunion__countvectorizer-2__ngram_range':
          [(1, 1), (1, 2), (2, 2)],
          'linearsvc__C': expon()}
       1.0
       0.8
       0.6
       0.2
```

```
rs = RandomizedSearchCV(text_pipe,
    param_distributions=param_distributins, n_iter=50)
```

- Always use distributions for continuous variables.
- Don't use for low dimensional spaces.

GP based parameter optimization (coming soon)



From Eric Brochu, Vlad M. Cora and Nando de Freitas

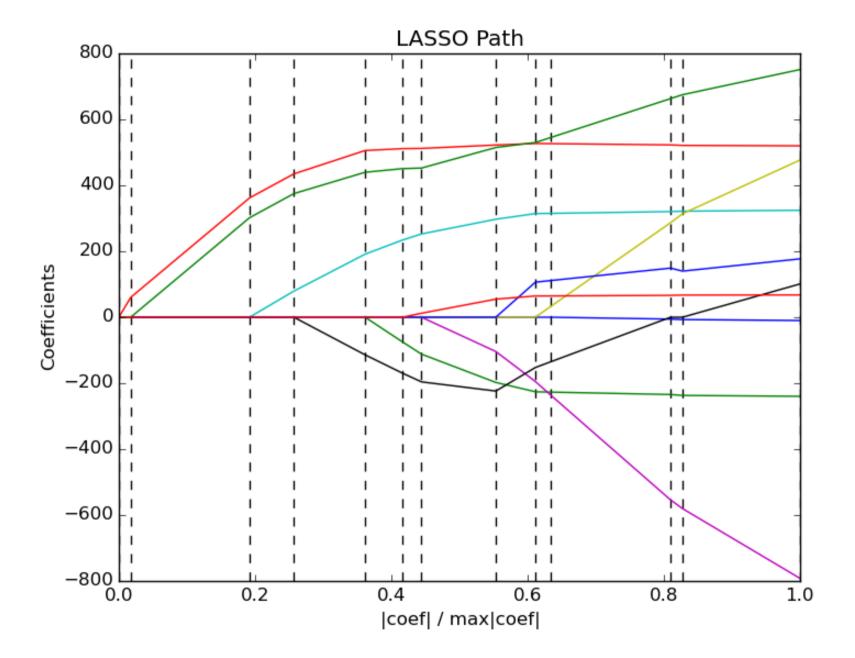
Efficient Parameter Search and Path Algorithms

rfe = RFE(LogisticRegression())

```
rfe = RFE(LogisticRegression())
param_grid = {'n_features_to_select': range(1, n_features)}
gridsearch = GridSearchCV(rfe, param_grid)
grid.fit(X, y)
```

```
rfecv = RFECV(LogisticRegression())
```

```
rfecv = RFECV(LogisticRegression())
rfecv.fit(X, y)
```



Linear Models	Feature Selection	Tree-Based models [possible]
LogisticRegressionCV [new]	RFECV	[DecisionTreeCV]
RidgeCV		[RandomForestClassifierCV]
RidgeClassifierCV		[GradientBoostingClassifierCV]
LarsCV		
ElasticNetCV 		

Notebook Efficient Parameter Search

Scoring Functions

GridSeachCV RandomizedSearchCV cross_val_score ...CV

Default: Accuracy (classification) R2 (regression)

Notebook scoring metrics

Out of Core Learning

 Large Scale – "Out of core: Fits on a hard disk but in RAM" Large Scale – "Out of core: Fits on a hard disk but in RAM"

Non-linear – because real-world problems are not.

 Large Scale – "Out of core: Fits on a hard disk but in RAM"

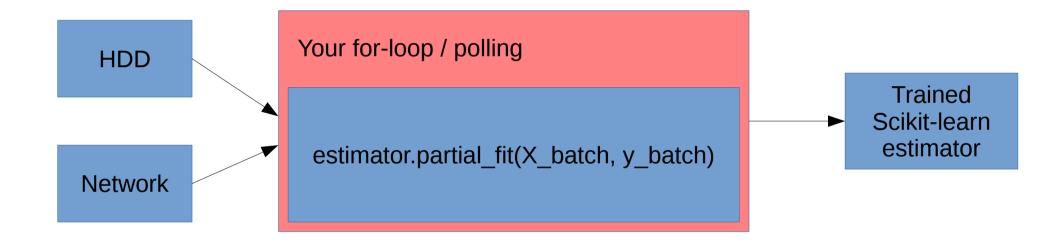
Non-linear – because real-world problems are not.

 Single CPU – Because parallelization is hard (and often unnecessary)

Think twice!

- Old laptop: 4GB Ram
- 1073741824 float32
- Or 1mio data points with 1000 features
- EC2: 256 GB Ram
- 68719476736 float32
- Or 68mio data points with 1000 features

	vCPU	ECU	Memory (GiB)	Instance Storage (GB)	Linux/UNIX Usage
Memory Optimiz	ed - Current (Generation			
r3.large	2	6.5	15	1 x 32 SSD	\$0.195 per Hour
r3.xlarge	4	13	30.5	1 x 80 SSD	\$0.39 per Hour
r3.2xlarge	8	26	61	1 x 160 SSD	\$0.78 per Hour
r3.4xlarge	16	52	122	1 x 320 SSD	\$1.56 per Hour
r3.8xlarge	32	104	244	2 x 320 SSD	\$3.12 per Hour
Storage Optimize	ed - Current C	Generation			
i2.xlarge	4	14	30.5	1 x 800 SSD	\$0.938 per Hour
i2.2xlarge	8	27	61	2 x 800 SSD	\$1.876 per Hour
i2.4xlarge	16	53	122	4 x 800 SSD	\$3.751 per Hour
i2.8xlarge	32	104	244	8 x 800 SSD	\$7.502 per Hour



Supported Algorithms

- All SGDClassifier derivatives
- Naive Bayes
- MinibatchKMeans
- IncrementalPCA
- MiniBatchDictionaryLearning
- MultilayerPerceptron (dev branch)
- Scalers

Out of Core Learning

```
sgd = SGDClassifier()

for i in range(9):
    X_batch, y_batch = cPickle.load(open("batch_%02d" % i))
    sgd.partial_fit(X_batch, y_batch, classes=range(10))
```

Possibly go over the data multiple times.

The hashing trick for text data

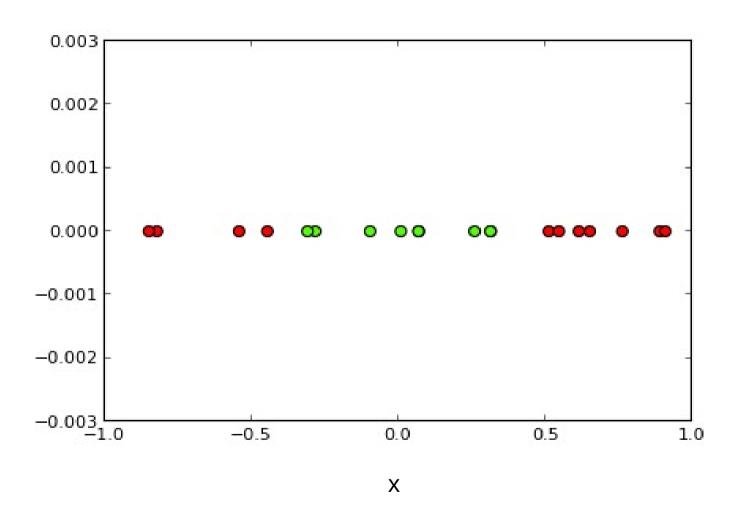
Text Classification: Bag Of Word

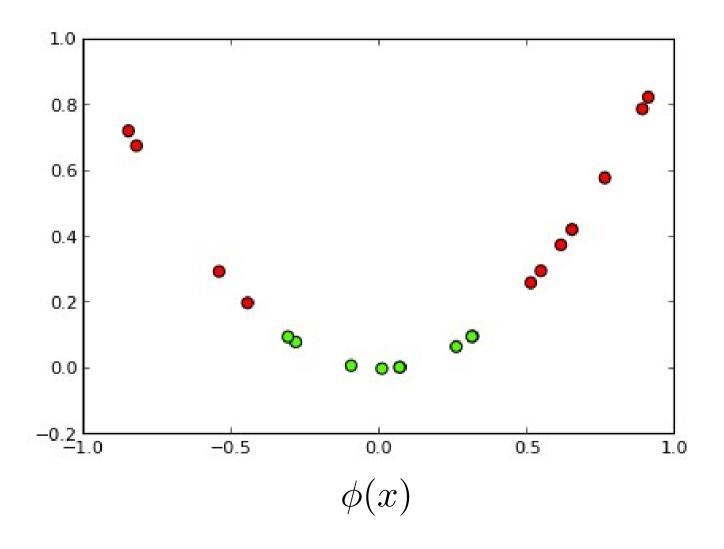
```
"This is how you get ants."
                           tokenizer
['this', 'is', 'how', 'you', 'get', 'ants']
                           Build a vocabulary over all documents
['aardvak', 'amsterdam', 'ants', ... 'you',
               'your', 'zyxst']
                           Sparse matrix encoding
   aardvak ants
                     get
                          you zyxst
     [0, ..., 0, 1, 0, ..., 0, 1, 0, ..., 0, 1, 0, ..., 0]
```

Text Classification: Hashing Trick

```
"This is how you get ants."
                              tokenizer
   ['this', 'is', 'how', 'you', 'get', 'ants']
                              hashing
[hash('this'), hash('is'), hash('how'), hash('you'),
              hash('get'), hash('ants')]
= [832412, 223788, 366226, 81185, 835749, 173092]
                              Sparse matrix encoding
        [0, ..., 0, 1, 0, ..., 0, 1, 0, ..., 0, 1, 0, ..., 0]
```

Kernel Approximations





Classifier linear → need only

$$\langle \phi(x_i), \phi(x_j) \rangle = k(x_i, x_j)$$

Classifier linear → need only

$$\langle \phi(x_i), \phi(x_j) \rangle = k(x_i, x_j)$$

Linear: $\langle x, x' \rangle$

Polynomial: $(\gamma \langle x, x' \rangle + r)^d$

RBF: $\exp(-\gamma |x - x'|^2)$

Sigmoid: $\tanh(\gamma \langle x, x' \rangle + r)$

Complexity

- Solving kernelized SVM:
 ~O(n samples ** 3)
- Solving linear (primal) SVM:
 ~O(n_samples * n_features)

n_samples large? Go primal!

Undoing the Kernel Trick

Kernel approximation:

$$\langle \hat{\phi}(x_i), \hat{\phi}(x_j) \rangle \approx k(x_i, x_j)$$

•
$$\mathbf{k} = \exp(-\gamma |x - x'|^2)$$

 $\hat{\phi} = \text{RBFSampler}$

Usage

```
sgd = SGDClassifier()
kernel_approximation = RBFSampler(gamma=.001, n_components=400)

for i in range(9):
    X_batch, y_batch = cPickle.load(open("batch_%02d" % i))
    if i == 0:
        kernel_approximation.fit(X_batch)
    X_transformed = kernel_approximation.transform(X_batch)
    sgd.partial_fit(X_transformed, y_batch, classes=range(10))
```

How (and why) to build your own estimator

Why?

GridSearchCV cross_val_score Pipeline

How

- "fit" method
- set_params and get_params (or inherit)
- Run check_estimator

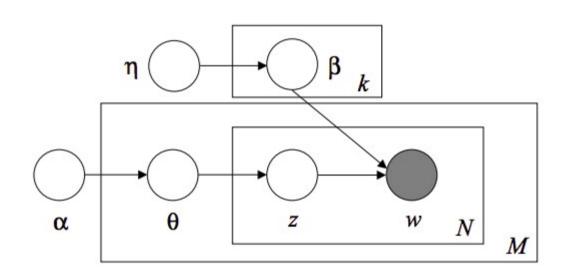
See the "build your own estimator" docs!

Notebook Building your own estimator

What's new in 0.17

Latent Dirichlet Allocation

using online variational inference



Topic #0:

government people mr law gun state president states public use right rights national new control american security encryption health united

Topic #1:

drive card disk bit scsi use mac memory thanks pc does video hard speed apple problem used data monitor software

Topic #2:

said people armenian armenians turkish did saw went came women killed children turkey told dead didn left started greek war

Topic #3:

year good just time game car team years like think don got new play games ago did season better II

Topic #4:

10 00 15 25 12 11 20 14 17 16 db 13 18 24 30 19 27 50 21 40 Topic #5:

windows window program version file dos use files available display server using application set edu motif package code ms software Topic #6:

edu file space com information mail data send available program ftp email entry info list output nasa address anonymous internet Topic #7:

ax max b8f g9v a86 pl 145 1d9 0t 34u 1t 3t giz bhj wm 2di 75u 2tm bxn 7ey

Topic #8:

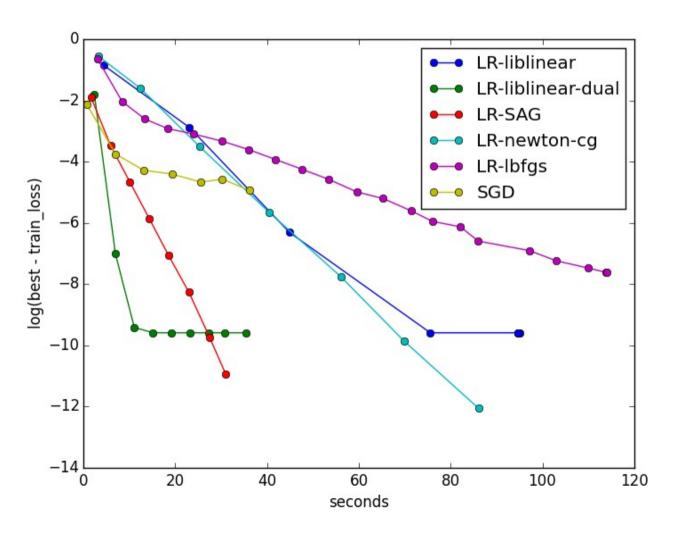
god people jesus believe does say think israel christian true life jews did bible don just know world way church

Topic #9:

don know like just think ve want does use good people key time way make problem really work say need

By Chyi-Kwei Yau, based on code by Matt Hoffman

SAG for Logistic Regression and Ridge Regression



By Danny Sullivan and Tom Dupre la Tour

Coordinate Descent Solver for Non-Negative Matrix Factorization

Topics in NMF model:

Topic #0:

don people just like think know time good right ve make say want did really way new use going said Topic #1:

windows file dos files window program use running using version ms problem server pc screen ftp run application os software Topic #2:

god jesus bible christ faith believe christians christian heaven sin hell life church truth lord say belief does existence man Topic #3:

geb dsl n3jxp chastity cadre shameful pitt intellect skepticism surrender gordon banks soon edu lyme blood weight patients medical probably

Topic #4:

key chip encryption clipper keys escrow government algorithm secure security encrypted public des nsa enforcement bit privacy law secret use

Topic #5:

drive scsi ide drives disk hard controller floppy hd cd mac boot rom cable internal tape bus seagate bios quantum Topic #6:

game team games players year hockey season play win league teams nhl baseball player detroit toronto runs pitching best playoffs

Topic #7:

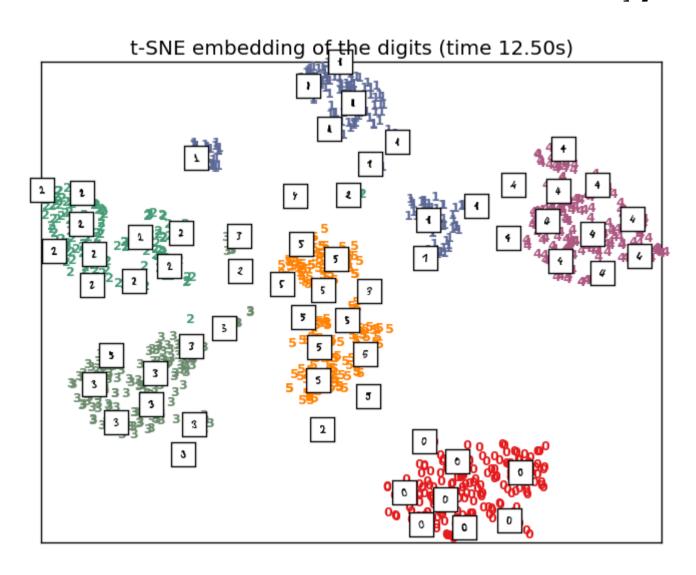
thanks mail does know advance hi info looking anybody address appreciated help email information send ftp post interested list appreciate

Topic #8:

card video monitor vga bus drivers cards color driver ram ati mode memory isa graphics vesa pc vlb diamond bit Topic #9:

00 sale 50 shipping 20 10 price 15 new 25 30 dos offer condition 40 cover asking 75 interested 01

Barnes-Hut Approximation for T-SNE manifold learning



FunctionTransformer

VotingClassifier

```
clf1 = LogisticRegression()
clf2 = RandomForestClassifier()
clf3 = GaussianNB()

eclf = VotingClassifier(
    estimators=[('lr', clf1), ('rf', clf2), ('gbn', clf3)],
    voting="hard")
```

Scalers

- RobustScaler
- MaxAbsScaler

Add Backlinks to Docs



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Google™ Custom Search

Search ×

Previous sklearn.ense

Up API Reference

This documentation is for scikit-learn version

0.18.dev0 — Other versions

If you use the software, please consider citing scikit-learn.

3.2.4.3.1.

sklearn.ensemble.RandomForestC lassifier

3.2.4.3.1.1. Examples using sklearn.ensemble.RandomForestClas sifier

3.2.4.3.1. sklearn.ensemble.RandomForestClassifier

class sklearn.ensemble.RandomForestClassifier(n_estimators=10, criterion='gini', max_depth=None, min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features='auto', max_leaf_nodes=None, bootstrap=True, oob_score=False, n_jobs=1, random_state=None, verbose=0, warm_start=False, class_weight=None)

[source]

A random forest classifier.

A random forest is a meta estimator that fits a number of decision tree classifiers on various sub-samples of the dataset and use averaging to improve the predictive accuracy and control over-fitting. The sub-sample size is always the same as the original input sample size but the samples are drawn with replacement if bootstrap=True (default).

Read more in the User Guide.

Parameters: n_estimators : integer, optional (default=10)

The number of trees in the forest.

criterion: string, optional (default="gini")

The function to measure the quality of a split. Supported criteria are "gini" for the Gini impurity and "entropy" for the information gain. Note: this parameter is tree-specific.

max features: int, float, string or None, optional (default="auto")

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Examples





Previous sklearn.ense m...

Up API Reference

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0.18.dev0 — Other versions

If you use the software, please consider citing scikit-learn.

3.2.4.3.1.

sklearn.ensemble.RandomForestC lassifier

3.2.4.3.1.1. Examples using sklearn.ensemble.RandomForestClas sifier

3.2.4.3.1. sklearn.ensemble.RandomForestClassifier

class sklearn.ensemble.RandomForestClassifier(n_estimators=10, criterion='gini', max_depth=None, min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features='auto', max_leaf_nodes=None, bootstrap=True, oob_score=False, n_jobs=1, random_state=None, verbose=0, warm_start=False, class_weight=None)

[source]

A random forest classifier.

A random forest is a meta estimator that fits a number of decision tree classifiers on various sub-samples of the dataset and use averaging to improve the predictive accuracy and control over-fitting. The sub-sample size is always the same as the original input sample size but the samples are drawn with replacement if bootstrap=True (default).

Parameters: n_estimators : integer, optional (default=10)

The number of trees in the forest.

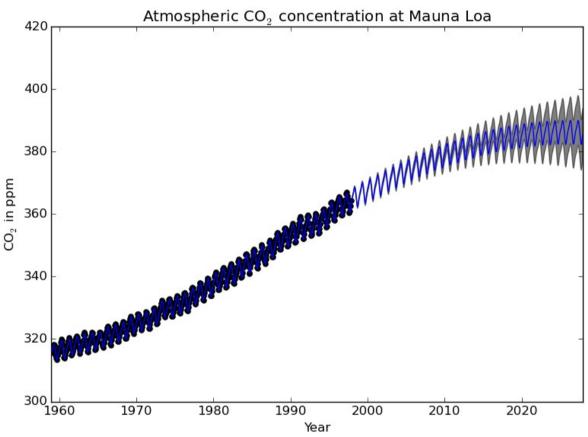
criterion: string, optional (default="gini")

The function to measure the quality of a split. Supported criteria are "gini" for the Gini impurity and "entropy" for the information gain. Note: this parameter is tree-specific.

max features: int, float, string or None, optional (default="auto")

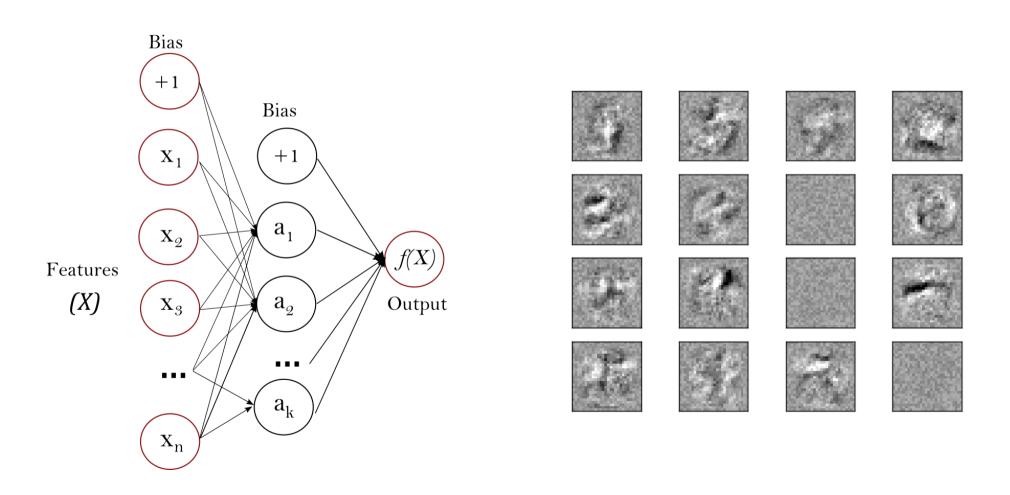
What the future will bring (0.18)

Gaussian Process Rewrite



By Jan Hendrik Metzen.

Neural Networks



By Jiyuan Qian and Issam Laradji

Improved Cross-Validation

current

```
>>> import numpy as np
>>> from sklearn.cross_validation import KFold

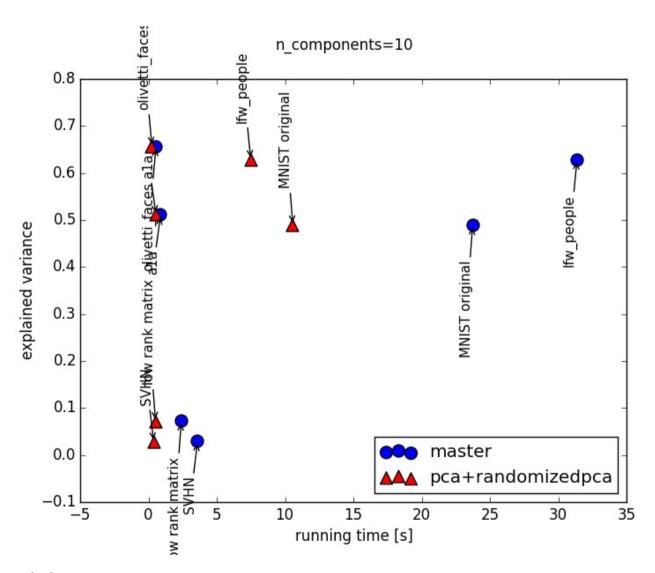
>>> kf = KFold(4, n_folds=2)
>>> for train, test in kf:
... print("%s %s" % (train, test))
[2 3] [0 1]
[0 1] [2 3]
```

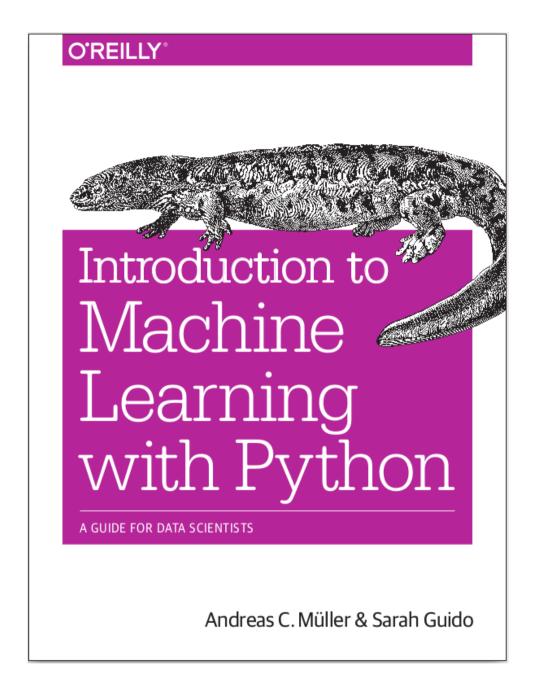
future

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

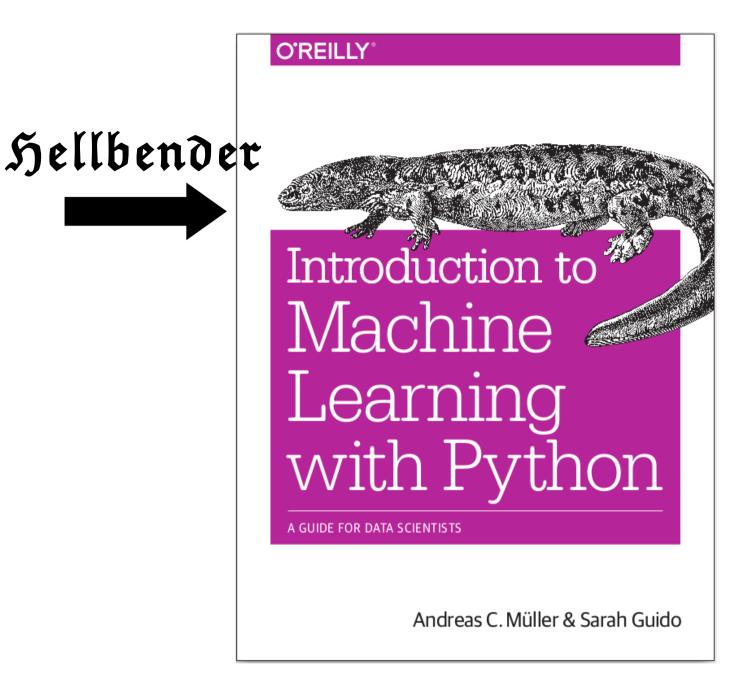
>>> X = ["a", "b", "c", "d"]
>>> kf = KFold(n_folds=2)
>>> for train, test in kf.split(X):
... print("%s %s" % (train, test))
[2 3] [0 1]
[0 1] [2 3]
```

Faster PCA





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Thank you!



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http://amueller.github.io