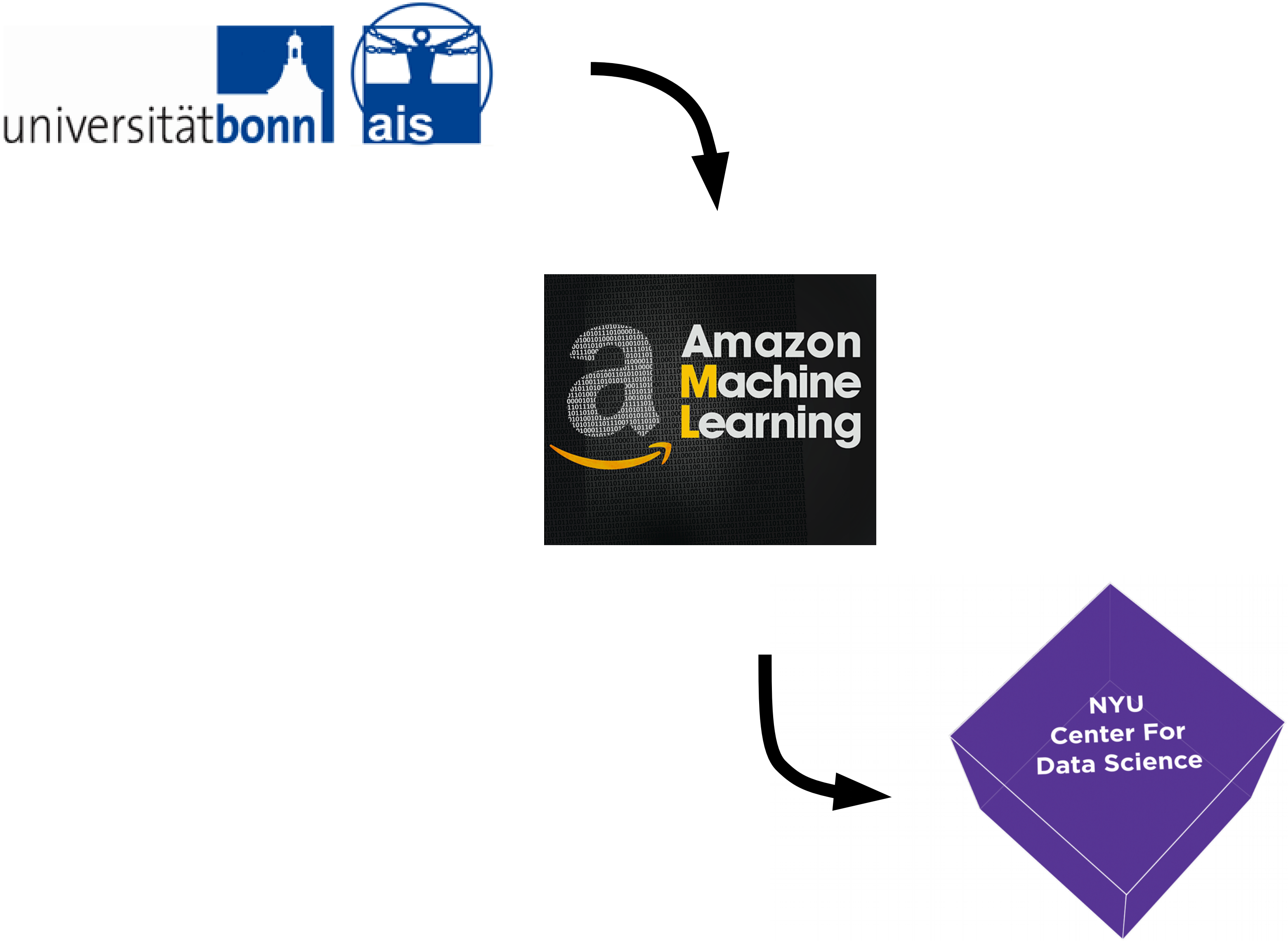
Advanced Scikit-Learn

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

Me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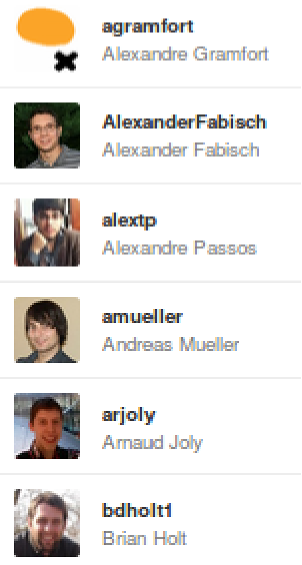
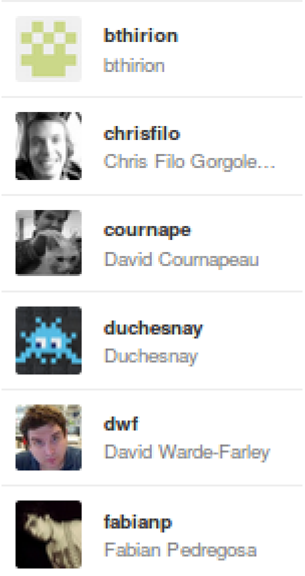
Amazon
Machine
Learning
NYU
Center For
Data Science

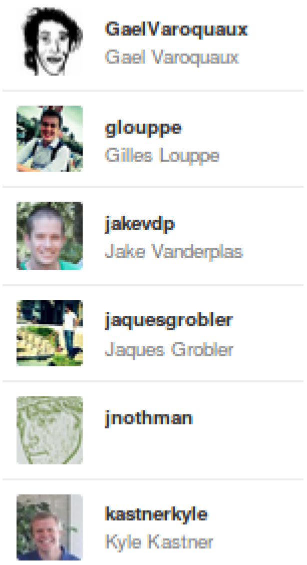


agramfort	Alexandre Gramfort
AlexanderFabisch	Alexander Fabisch
alextp	Alexandre Passos
amueller	Andreas Mueller
arjoly	Arnaud Joly
bdholt1	Brian Holt

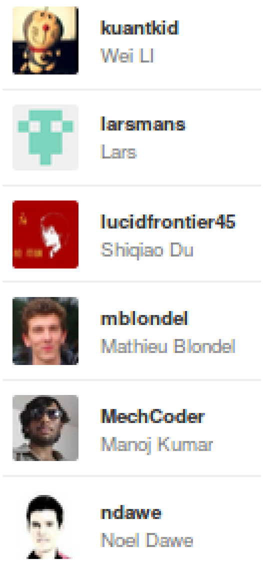


bthirion	bthirion
chrisfilo	Chris Filo Gorgole…
cournape	David Cournapeau
duchesnay	Duchesnay
dwf	David Warde-Farley
fabianp	Fabian Pedregosa

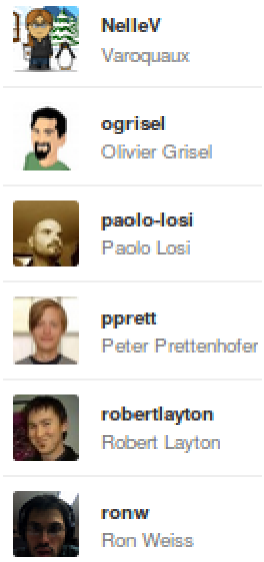
scikit learn



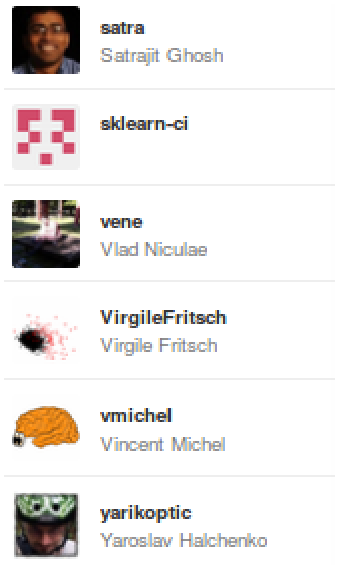
GaelVaroquaux	Gael Varoquaux
glouppe	Gilles Louppe
jakevdp	Jake Vanderplas
jaquesgrobler	Jaques Grobler
jnothman	
kastnerkyle	Kyle Kastner



kuantkid	Wei LI
larsmans	Lars
lucidfrontier45	Shiqiao Du
mblondel	Mathieu Blondel
MechCoder	Manoj Kumar
ndawe	Noel Dawe



NelleV	Varoquaux
ogrisel	Olivier Grisel
paolo-losi	Paolo Losi
pprett	Peter Prettenhofer
robertlayton	Robert Layton
ronw	Ron Weiss



satra	Satrajit Ghosh
sklearn-ci	
vene	Vlad Niculae
VirgileFritsch	Virgile Fritsch
vmichel	Vincent Michel
yarikoptic	Yaroslav Halchenko

Representing Data

$$X = \begin{pmatrix} 1.1 & 2.2 & 3.4 & 5.6 & 1.0 \\ 6.7 & 0.5 & 0.4 & 2.6 & 1.6 \\ 2.4 & 9.3 & 7.3 & 6.4 & 2.8 \\ 1.5 & 0.0 & 4.3 & 8.3 & 3.4 \\ 0.5 & 3.5 & 8.1 & 3.6 & 4.6 \\ 5.1 & 9.7 & 3.5 & 7.9 & 5.1 \\ 3.7 & 7.8 & 2.6 & 3.2 & 6.3 \end{pmatrix}$$

Representing Data

$$X = \begin{array}{r} \text{one sample} \\ \\ \\ \\ \\ \\ \\ \end{array} \left(\begin{array}{ccccc} \multicolumn{5}{c}{\boxed{1.1 \quad 2.2 \quad 3.4 \quad 5.6 \quad 1.0}} \\ 6.7 & 0.5 & 0.4 & 2.6 & 1.6 \\ 2.4 & 9.3 & 7.3 & 6.4 & 2.8 \\ 1.5 & 0.0 & 4.3 & 8.3 & 3.4 \\ 0.5 & 3.5 & 8.1 & 3.6 & 4.6 \\ 5.1 & 9.7 & 3.5 & 7.9 & 5.1 \\ 3.7 & 7.8 & 2.6 & 3.2 & 6.3 \end{array}\right)$$

Representing Data

$$X = \begin{array}{rccccc} \text{one sample} & 1.1 & 2.2 & 3.4 & 5.6 & 1.0 \\ & 6.7 & 0.5 & 0.4 & 2.6 & 1.6 \\ & 2.4 & 9.3 & 7.3 & 6.4 & 2.8 \\ & 1.5 & 0.0 & 4.3 & 8.3 & 3.4 \\ & 0.5 & 3.5 & 8.1 & 3.6 & 4.6 \\ & 5.1 & 9.7 & 3.5 & 7.9 & 5.1 \\ & 3.7 & 7.8 & 2.6 & 3.2 & 6.3 \\ & \text{one feature} & & & & \end{array}$$

Representing Data

one sample

$$X = \begin{pmatrix} 1.1 & 2.2 & 3.4 & 5.6 & 1.0 \\ 6.7 & 0.5 & 0.4 & 2.6 & 1.6 \\ 2.4 & 9.3 & 7.3 & 6.4 & 2.8 \\ 1.5 & 0.0 & 4.3 & 8.3 & 3.4 \\ 0.5 & 3.5 & 8.1 & 3.6 & 4.6 \\ 5.1 & 9.7 & 3.5 & 7.9 & 5.1 \\ 3.7 & 7.8 & 2.6 & 3.2 & 6.3 \end{pmatrix} \qquad y = \begin{pmatrix} 1.6 \\ 2.7 \\ 4.4 \\ 0.5 \\ 0.2 \\ 5.6 \\ 6.7 \end{pmatrix}$$

one feature

outputs / labels

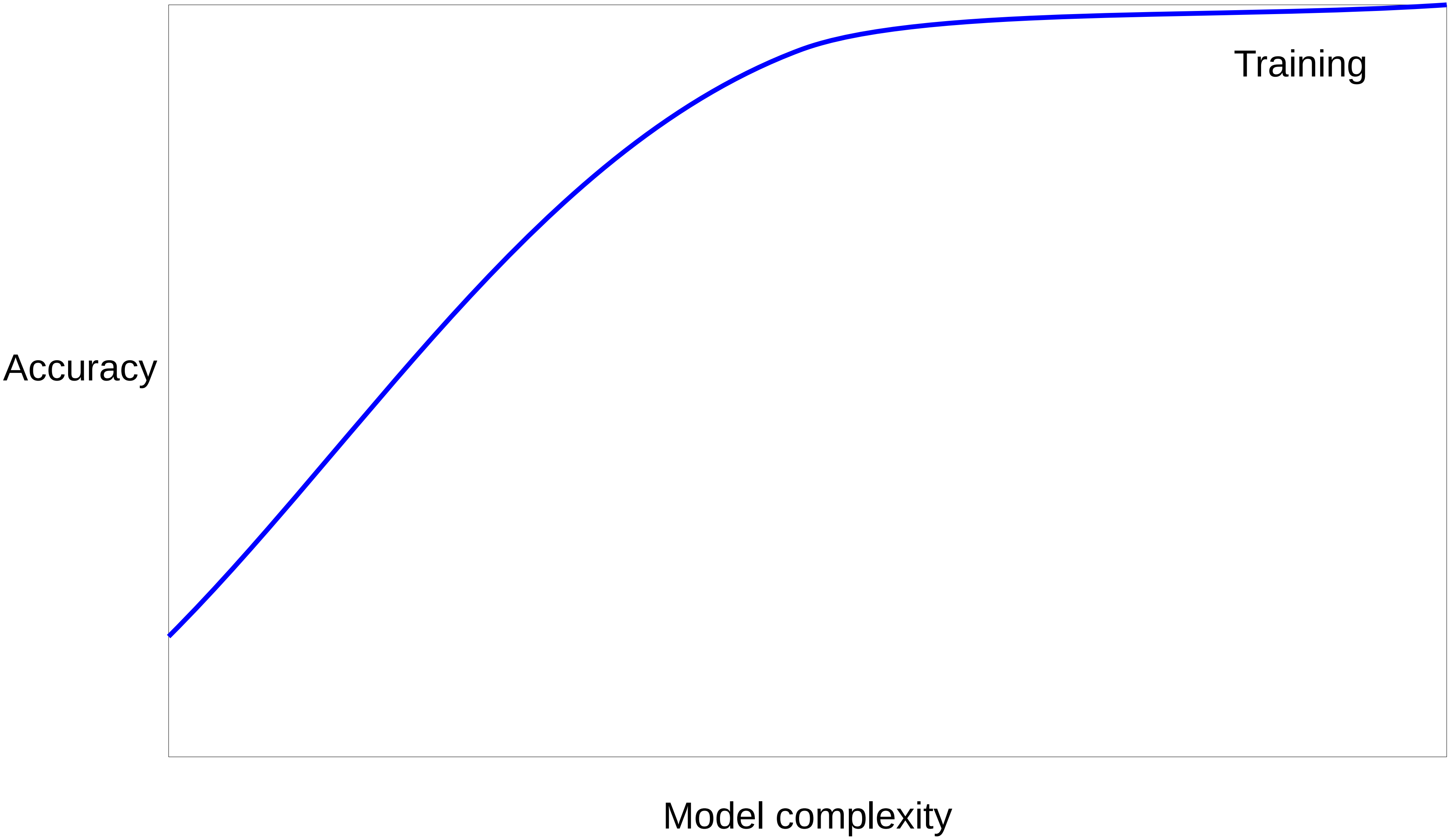
Basic API

```
estimator.fit(X, [y])
```

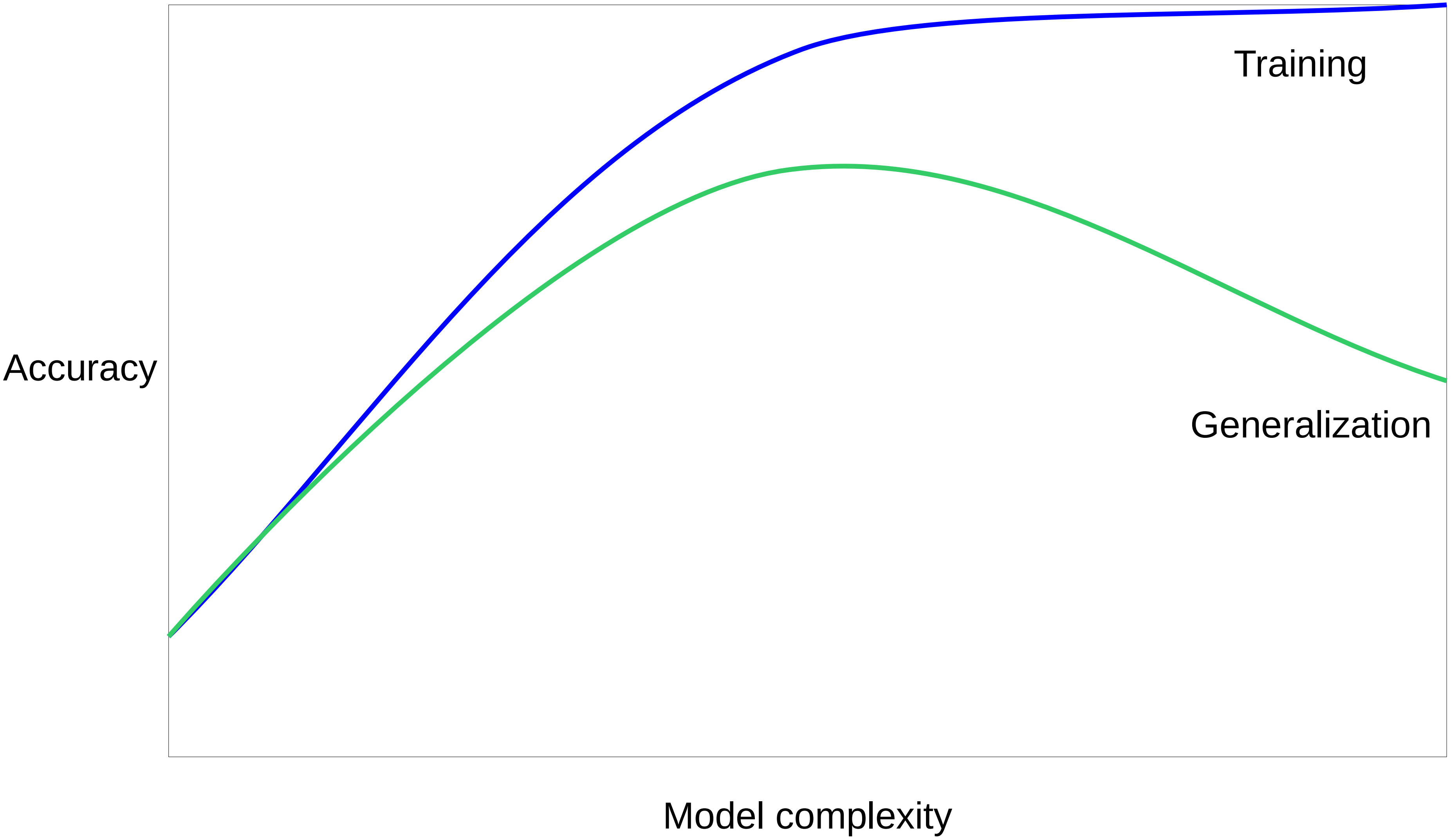
`estimator.predict`	`estimator.transform`
Classification	Preprocessing
Regression	Dimensionality reduction
Clustering	Feature selection
	Feature extraction

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

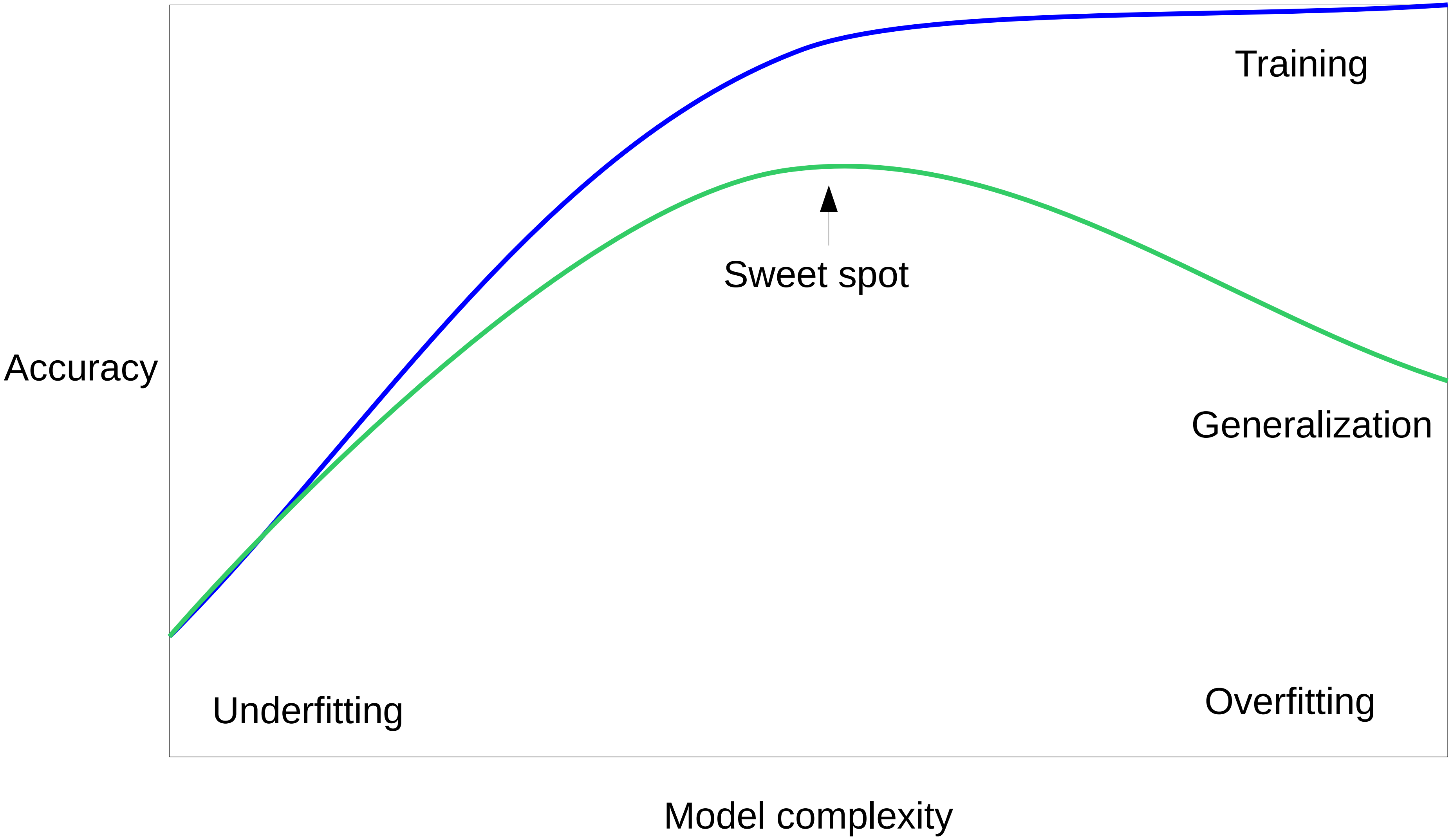
Overfitting and Underfitting



Overfitting and Underfitting



Overfitting and Underfitting



Cross-Validation

```
from sklearn.cross_validation import cross_val_score

scores = cross_val_score(SVC(), X, y, cv=5)
print(scores)

>> [ 0.92  1.    1.    1.    1.  ]
```

Cross-Validation

```
from sklearn.cross_validation import cross_val_score

scores = cross_val_score(SVC(), X, y, cv=5)
print(scores)

>> [ 0.92  1.    1.    1.    1.  ]

cv_ss = ShuffleSplit(len(X_train), test_size=.3,
                     n_iter=10)
scores_shuffle_split = cross_val_score(SVC(), X, y,
                                       cv=cv_ss)
```

Cross-Validation

```
from sklearn.cross_validation import cross_val_score

scores = cross_val_score(SVC(), X, y, cv=5)
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                     n_iter=10)
scores_shuffle_split = cross_val_score(SVC(), X, y,
                                       cv=cv_ss)

cv_labels = LabelKFold(labels, n_folds=5)
scores_pout = cross_val_score(SVC(), X, y, cv=cv_labels)
```

Cross-Validation

```
from sklearn.cross_validation import cross_val_score

scores = cross_val_score(SVC(), X, y, cv=5)
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>> [ 0.92  1.    1.    1.    1.  ]

cv_ss = ShuffleSplit(~~len(X_train),~~ test_size=.3,
                     n_iter=10)
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                                       cv=cv_ss)

cv_labels = LabelKFold(~~labels,~~ n_folds=5)
scores_pout = cross_val_score(SVC(), X, y, cv=cv_labels)
```
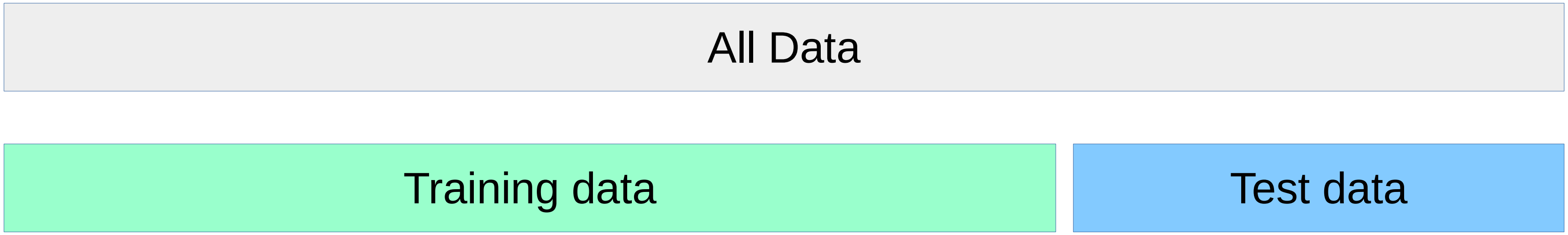
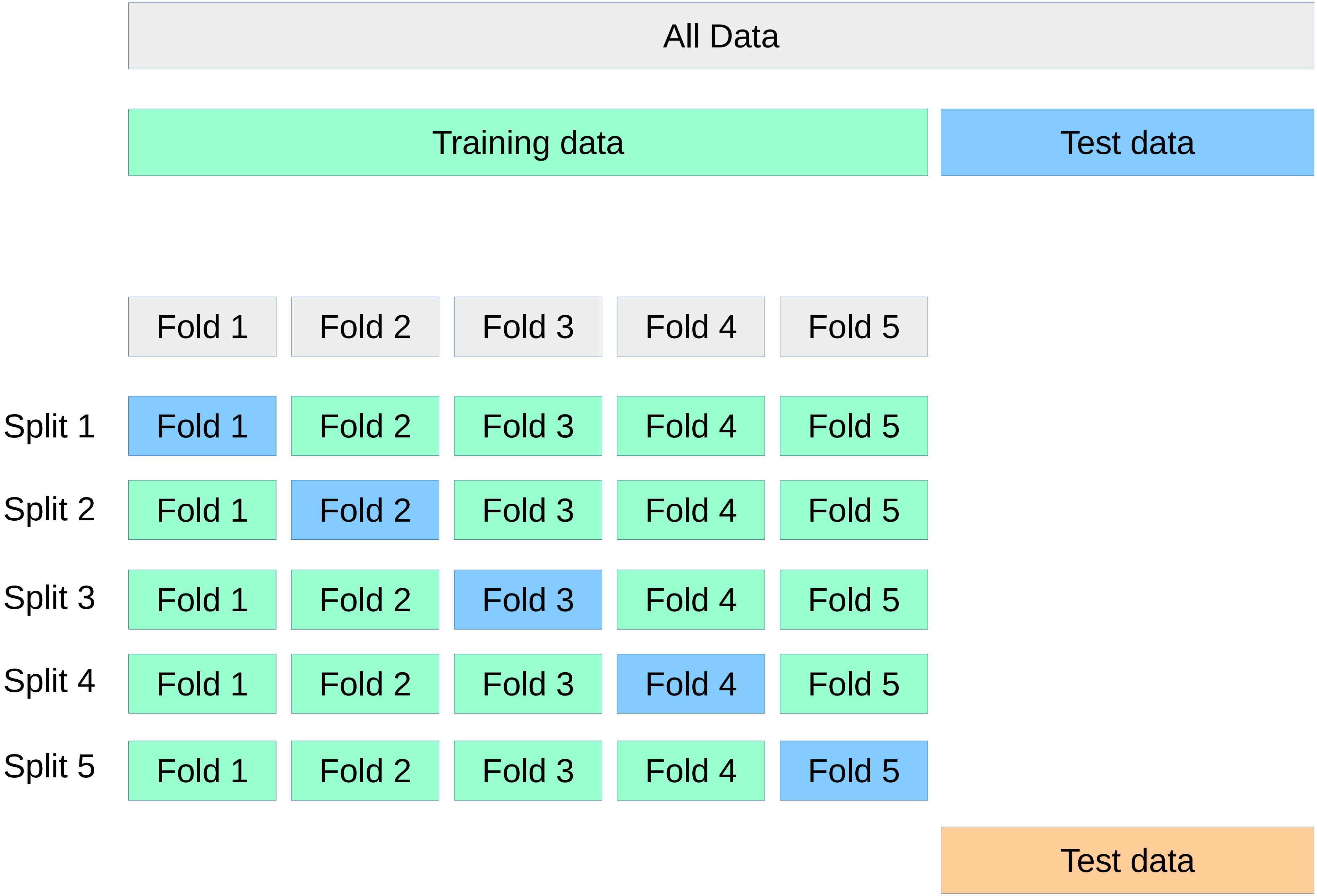



All Data

Training data

Test data

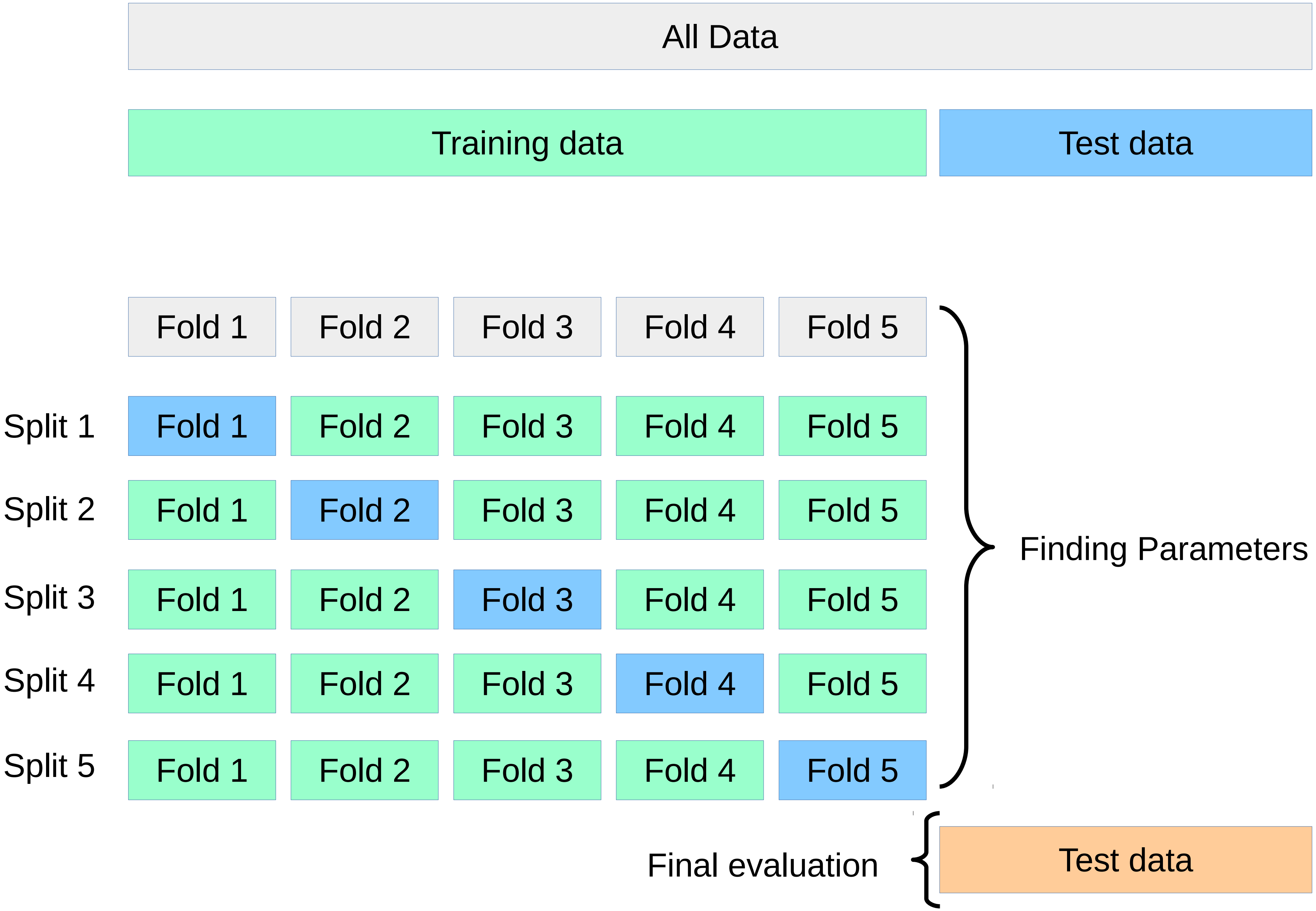


All Data

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



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

Finding Parameters

Final evaluation

Test data

Cross -Validated Grid Search

```
from sklearn.grid_search import GridSearchCV
from sklearn.cross_validation import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y)

param_grid = {'C': 10. ** np.arange(-3, 3),
              'gamma': 10. ** np.arange(-3, 3)}
grid = GridSearchCV(SVC(), param_grid=param_grid)
grid.fit(X_train, y_train)
grid.predict(X_test)
grid.score(X_test, y_test)
```

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

Bag Of Word Representations

`CountVectorizer / TfidfVectorizer`

Bag Of Word Representations

`CountVectorizer / TfidfVectorizer`

`“This is how you get ants.”`

Bag Of Word Representations

CountVectorizer / TfidfVectorizer

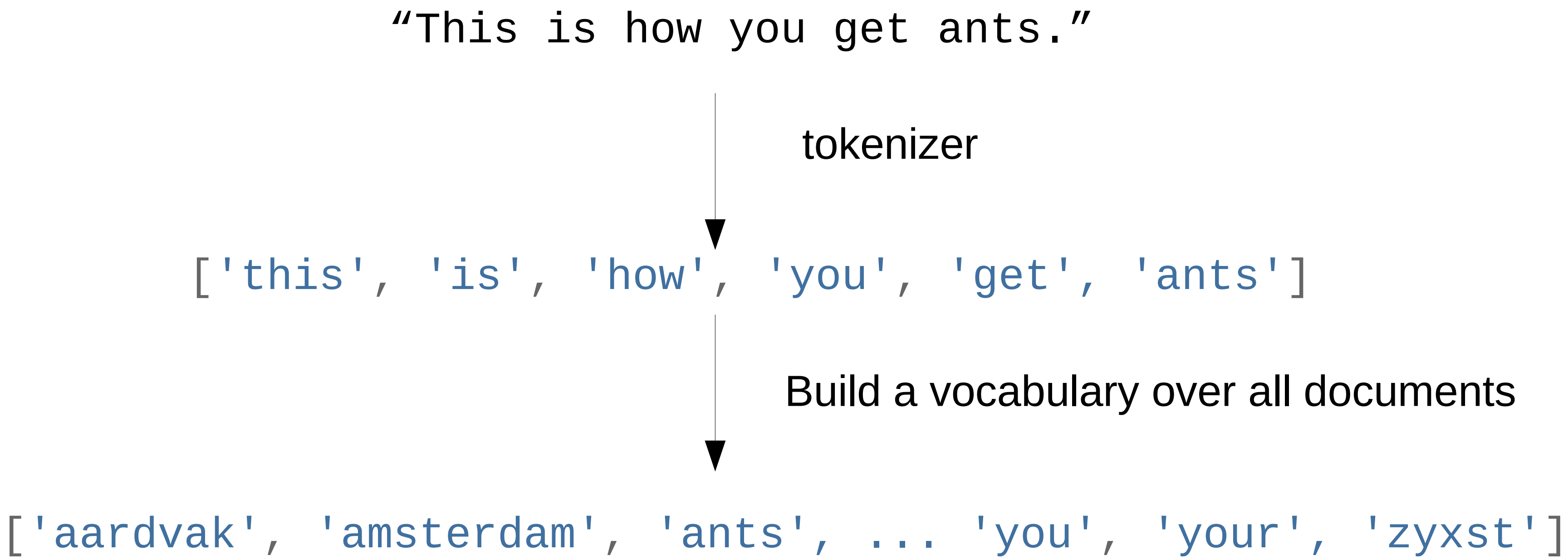
“This is how you get ants.”

tokenizer

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

Bag Of Word Representations

`CountVectorizer / TfidfVectorizer`



“This is how you get ants.”

tokenizer

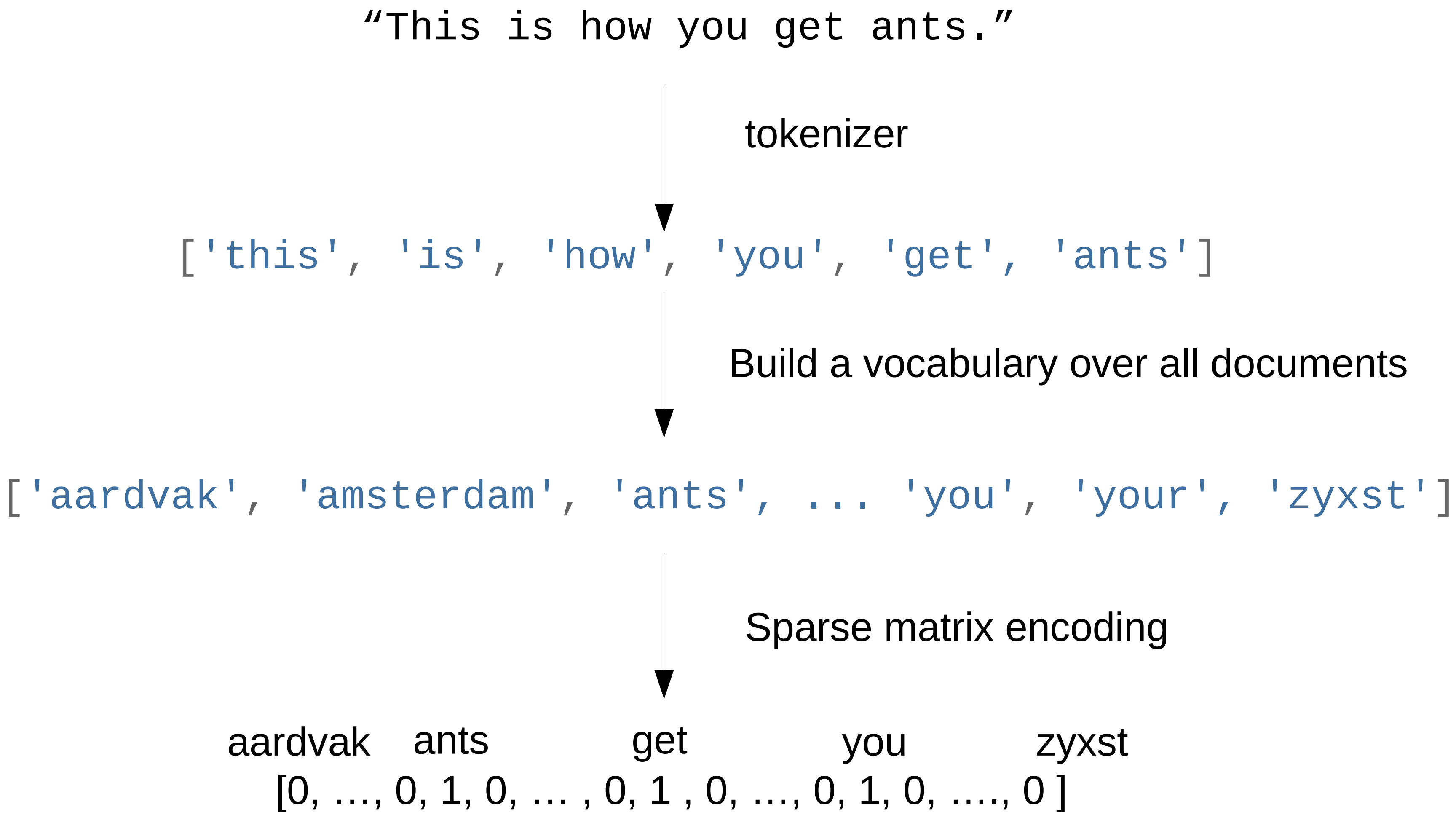
```
['this', 'is', 'how', 'you', 'get', 'ants']
```

Build a vocabulary over all documents

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

Bag Of Word Representations

`CountVectorizer / TfidfVectorizer`



“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)

`CountVectorizer` / `TfidfVectorizer`

N-grams (unigrams and bigrams)

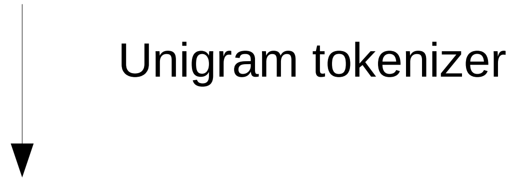
`CountVectorizer / TfidfVectorizer`

`“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']
```

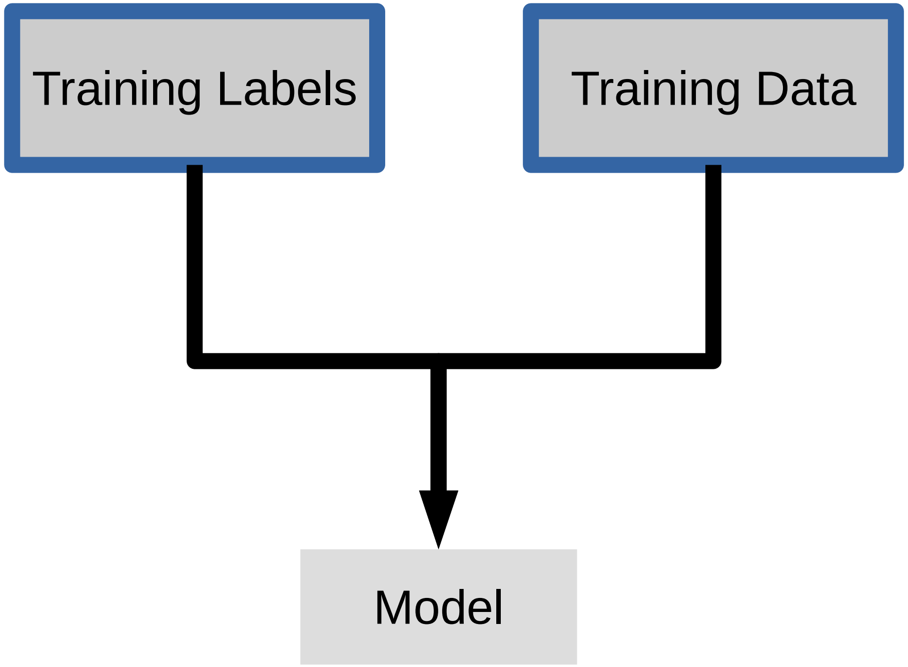
`“This is how you get ants.”`

Bigram tokenizer

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

Notebook Working With Text Data

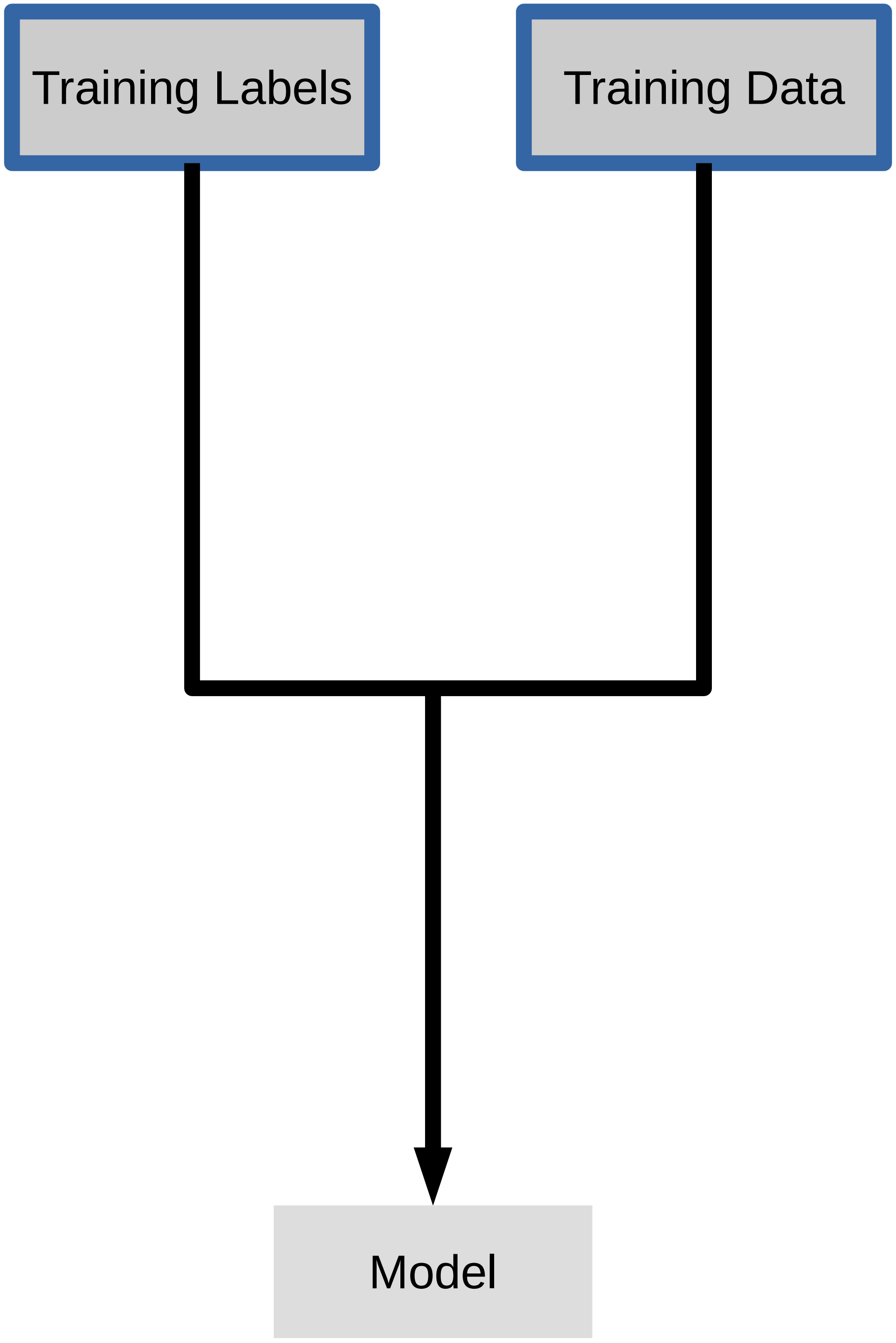
Pipelines



Training Labels

Training Data

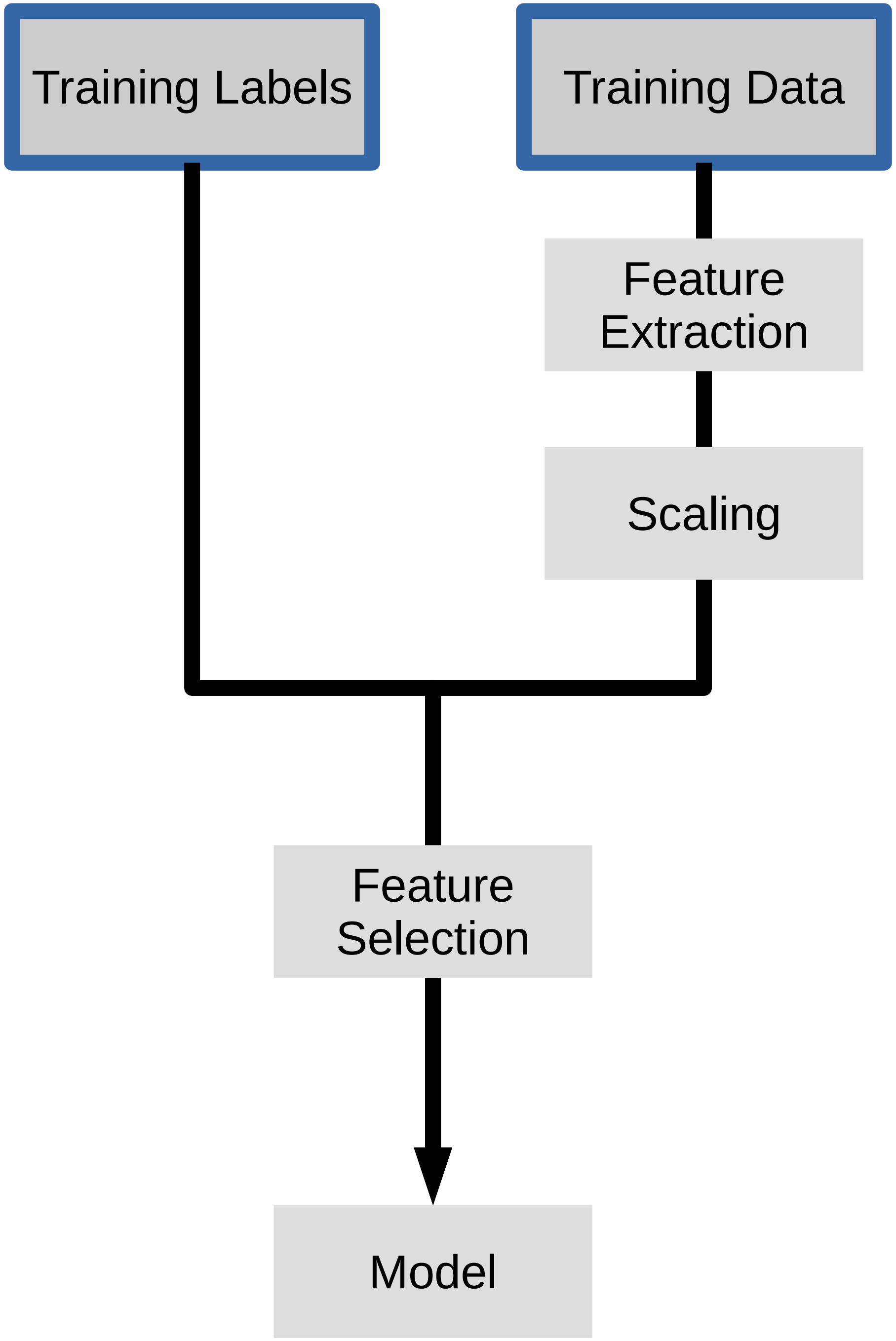
Model



Training Labels

Training Data

Model



Training Labels

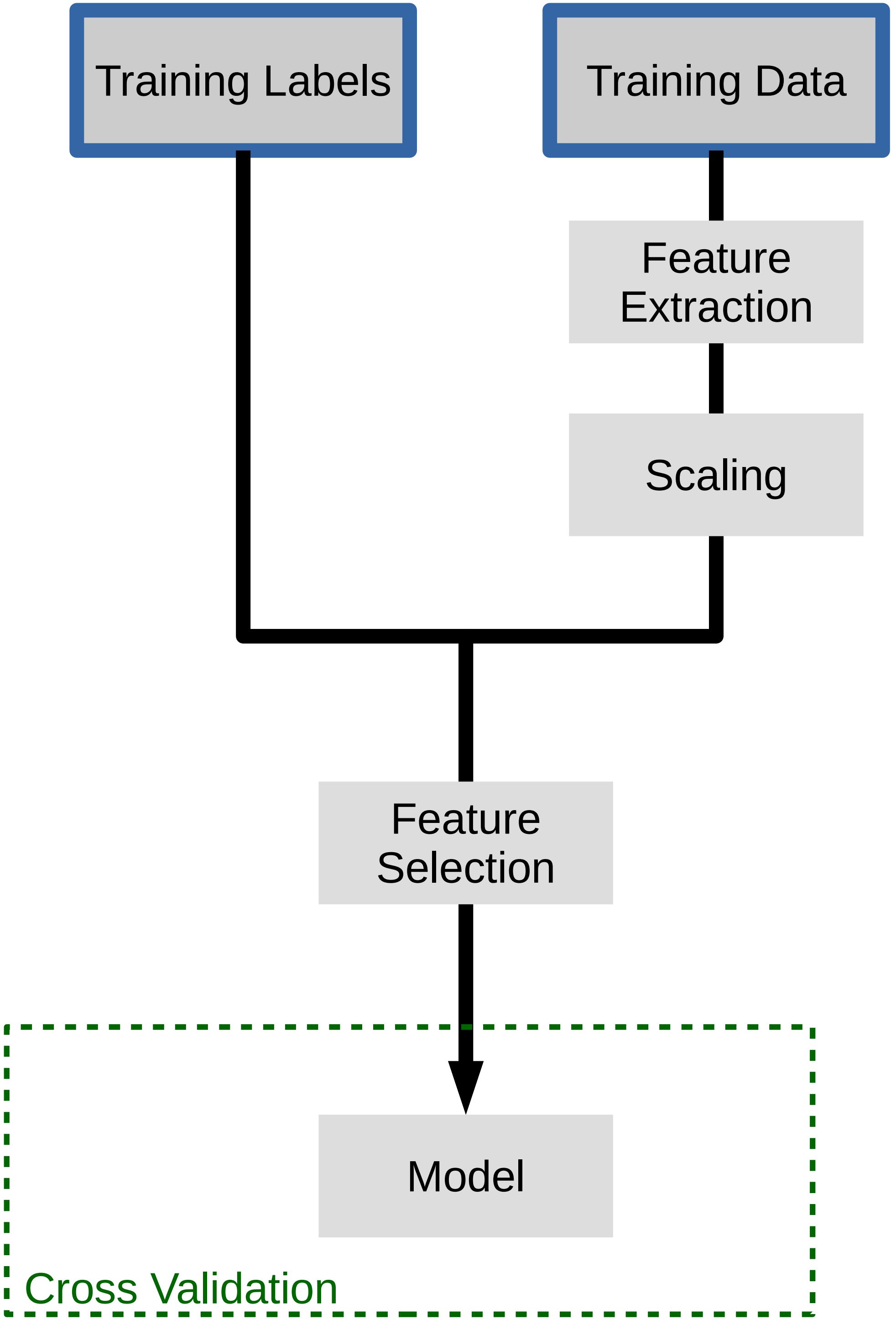
Training Data

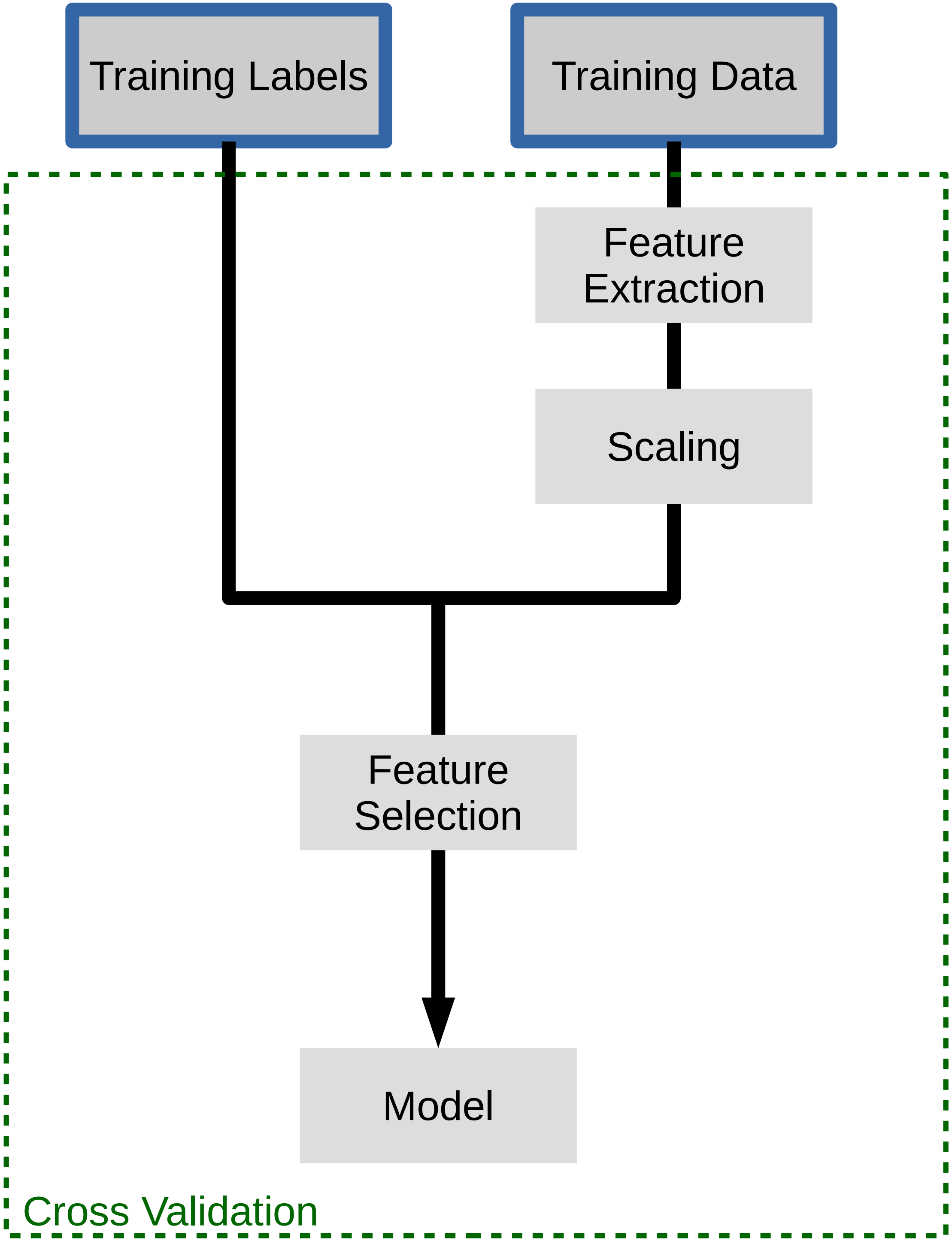
Feature Extraction

Scaling

Feature Selection

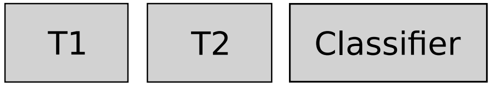
Model


Training Labels
Training Data
Feature Extraction
Scaling
Feature Selection
Model
Cross Validation


Training Labels
Training Data
Feature Extraction
Scaling
Feature Selection
Model
Cross Validation

Pipelines

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

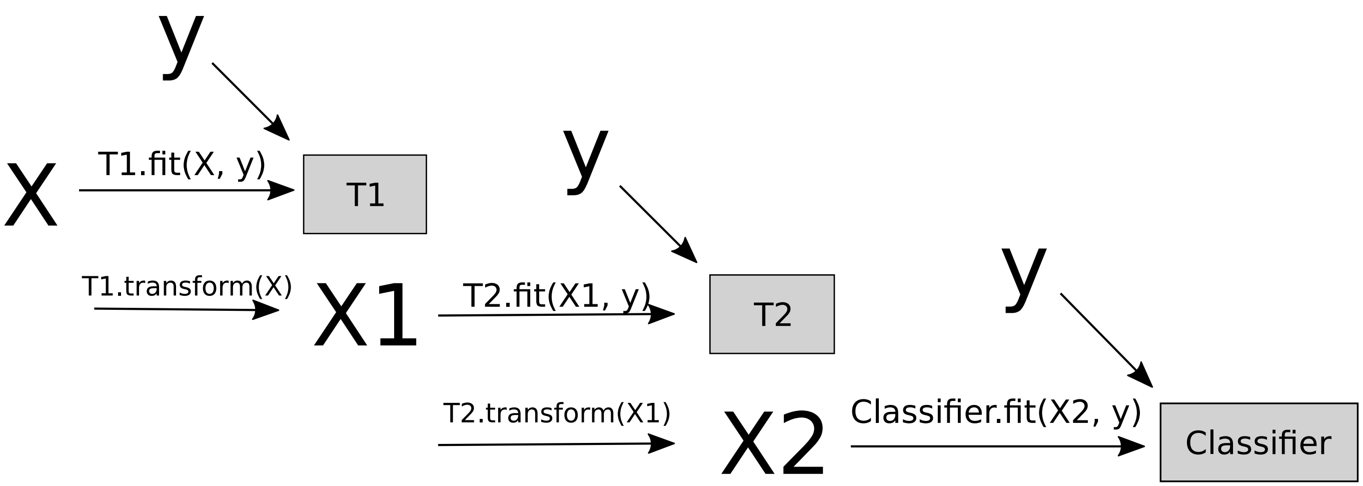


T1

T2

Classifier

pipe.fit(X, y)



y

X

T1.fit(X, y)

T1

y

T1.transform(X)

X1

T2.fit(X1, y)

T2

y

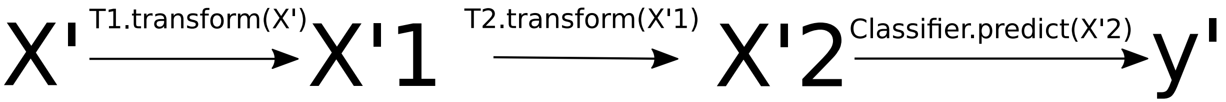
T2.transform(X1)

X2

Classifier.fit(X2, y)

Classifier

pipe.predict(X')



X'

T1.transform(X')

X'1

T2.transform(X'1)

X'2

Classifier.predict(X'2)

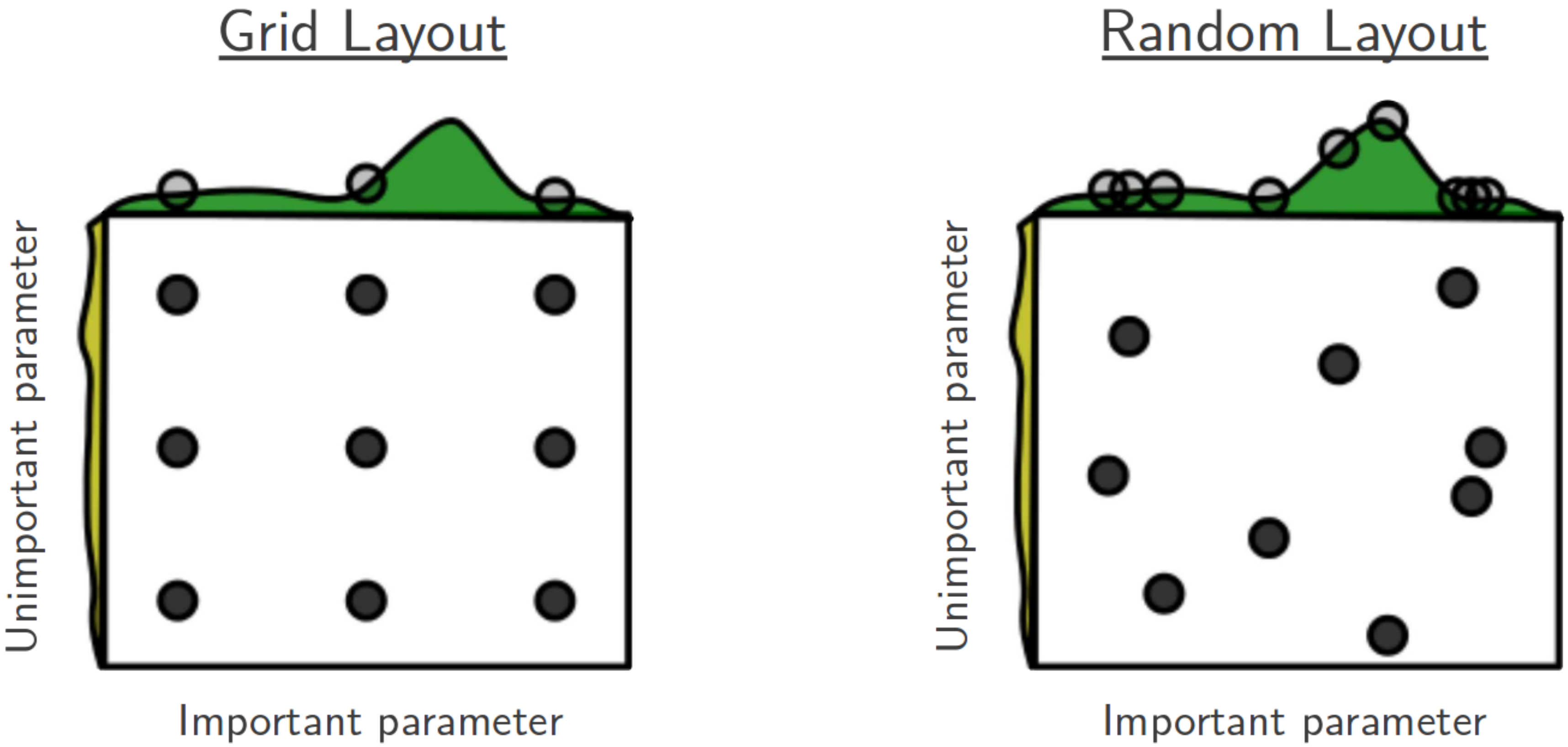
y'

Pipelines

```
from sklearn.pipeline import make_pipeline

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

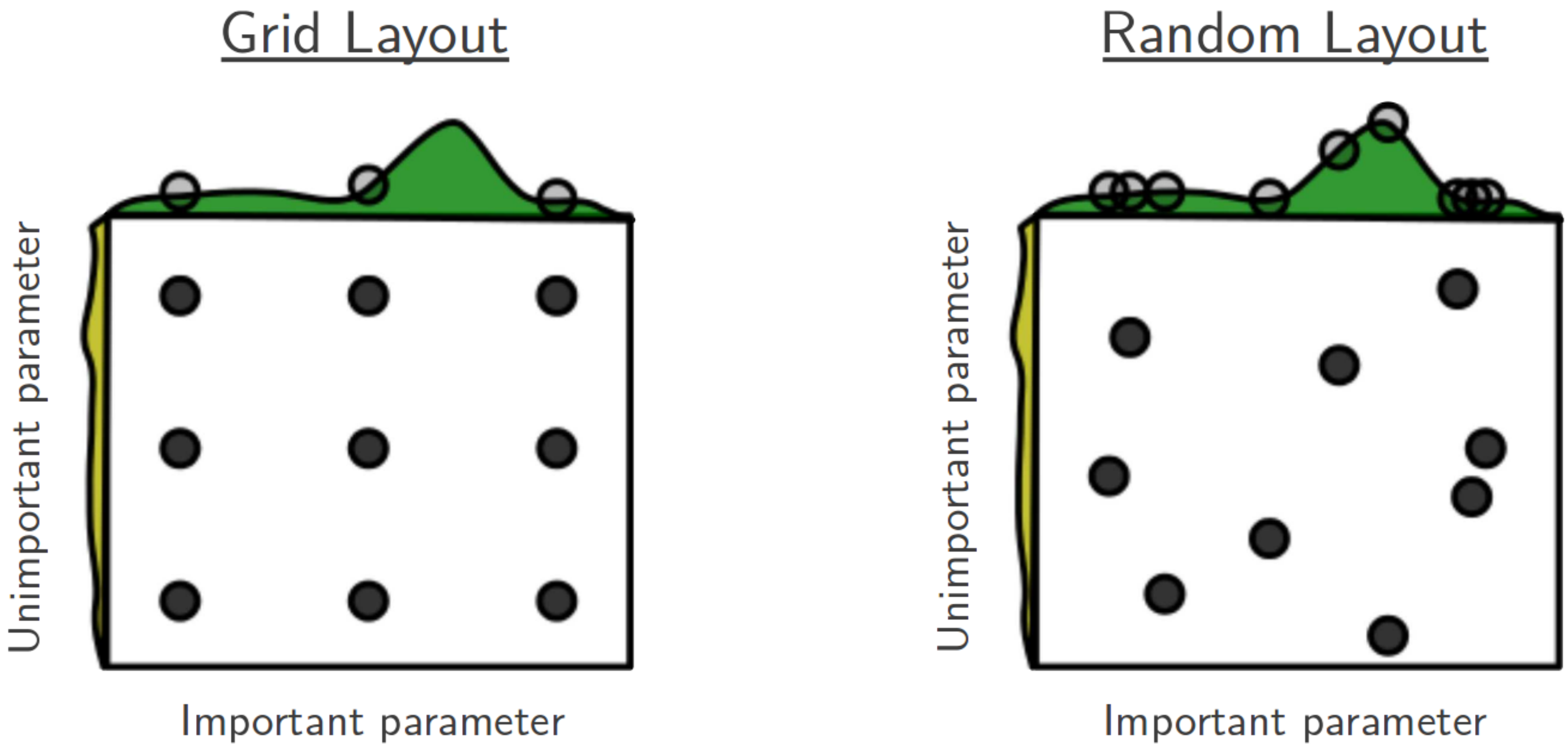
Randomized Parameter Search

Randomized Parameter Search



Source: Bergstra and Bengio

Randomized Parameter Search



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

Source: Bergstra and Bengio

Randomized Parameter Search

```
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': 10. ** np.arange(-3, 3)}
```

Randomized Parameter Search

```
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()}
```

Randomized Parameter Search

```
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          'featureunion__countvectorizer-2__ngram_range':
          [(1, 1), (1, 2), (2, 2)],
          'linearsvc__C': expon()}
```
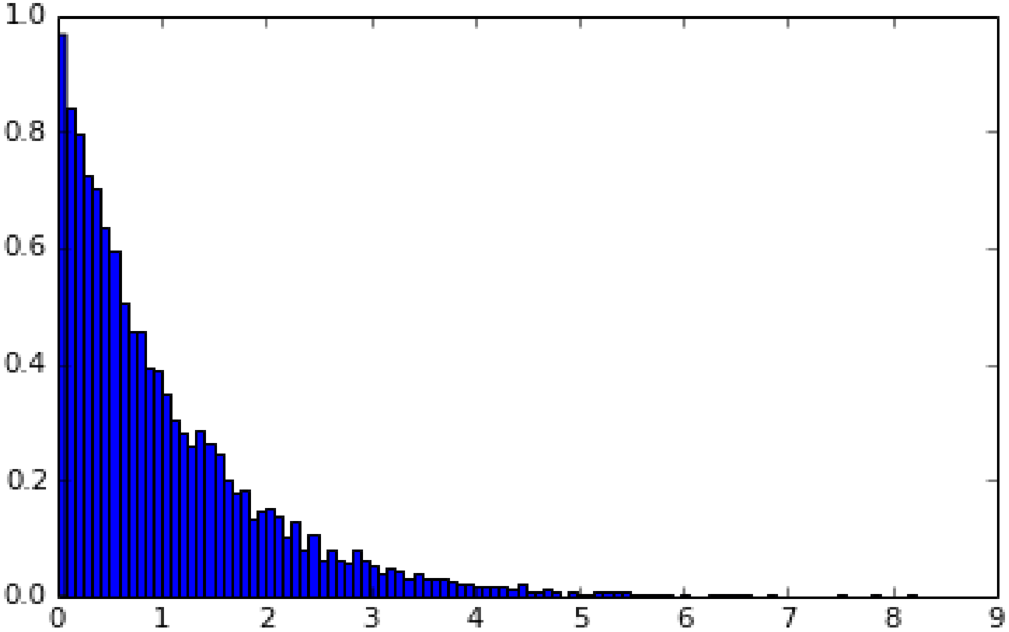
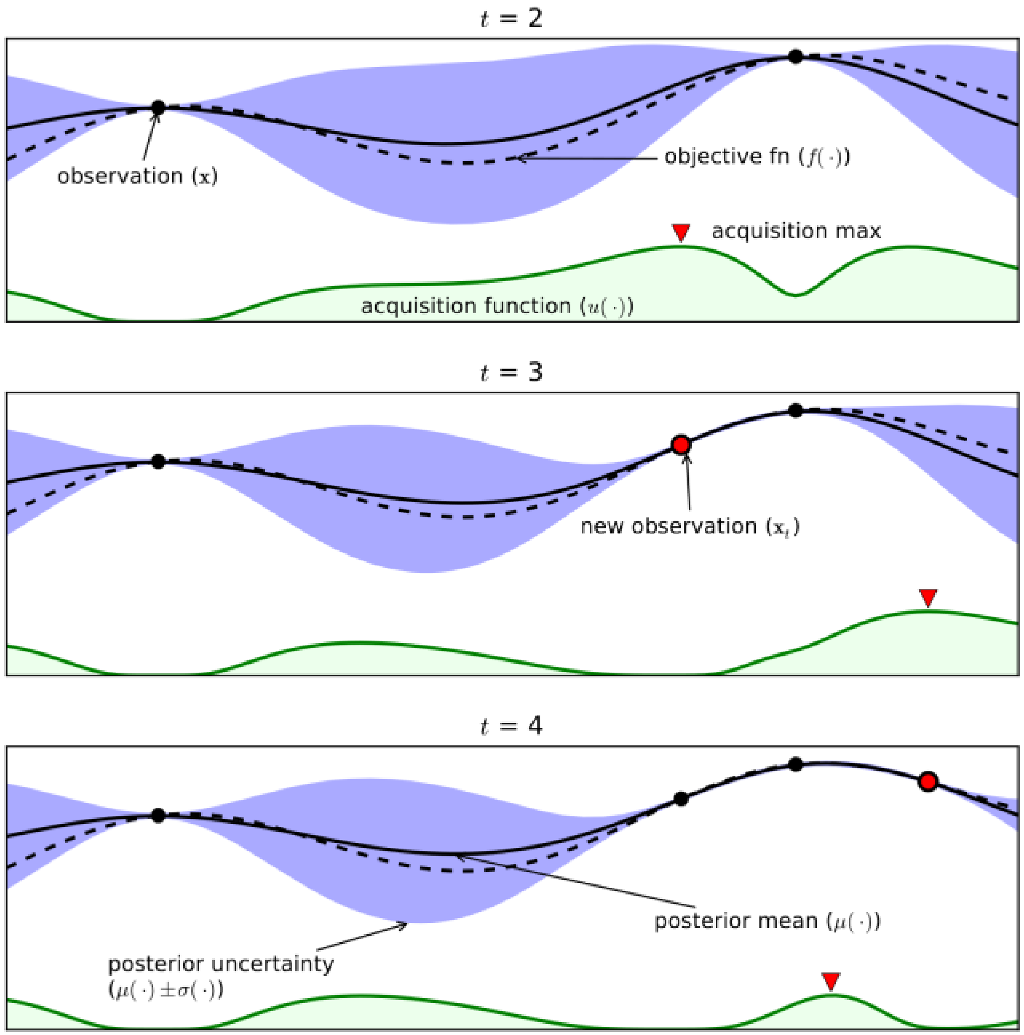



```
rs = RandomizedSearchCV(text_pipe,
   param_distributions=param_distributins, n_iter=50)
```

Randomized Parameter Search

- 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

Scoring Functions

GridSeachCV
RandomizedSearchCV
cross_val_score
...CV

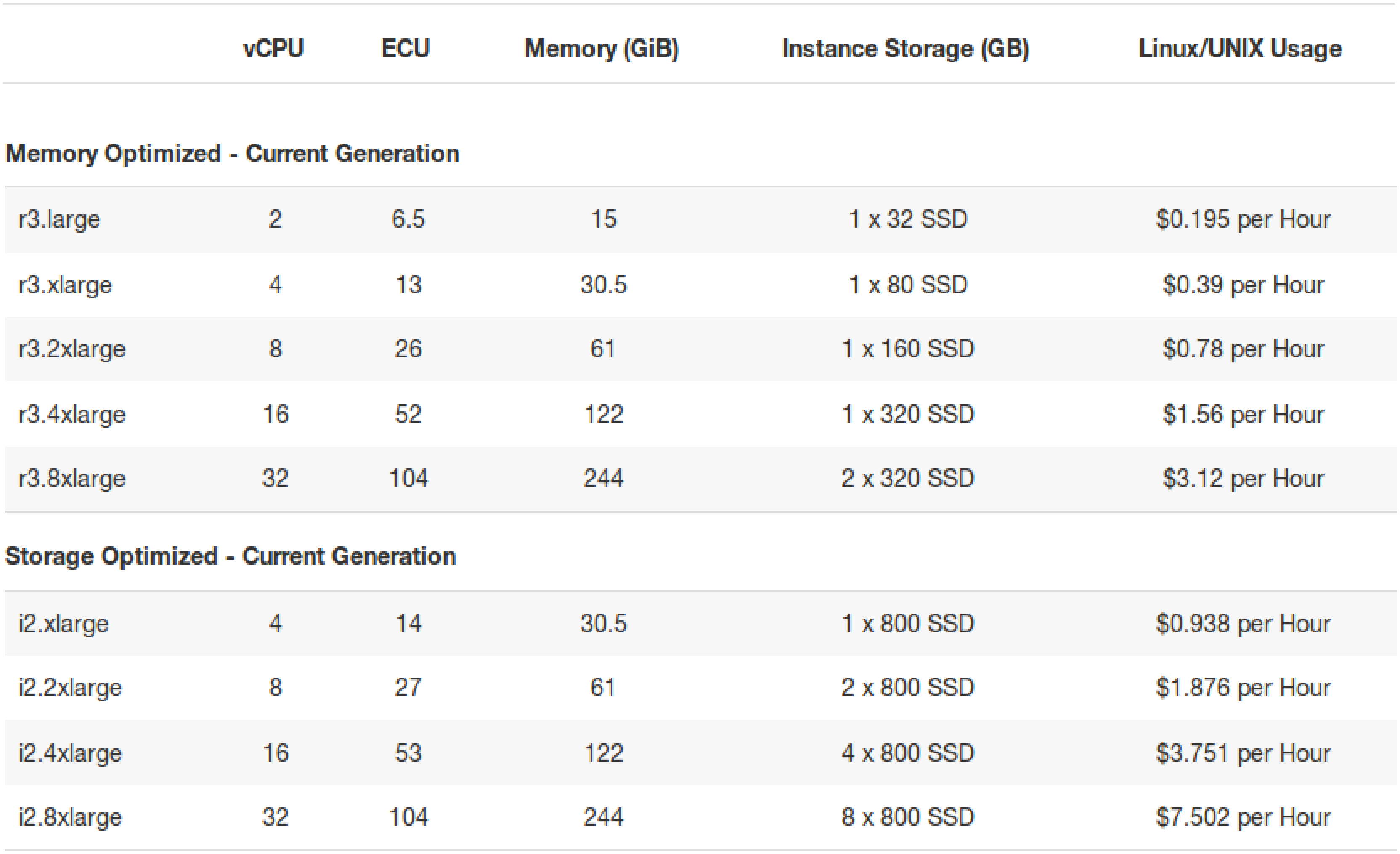
Default:
Accuracy (classification)
R2 (regression)

Notebook scoring metrics

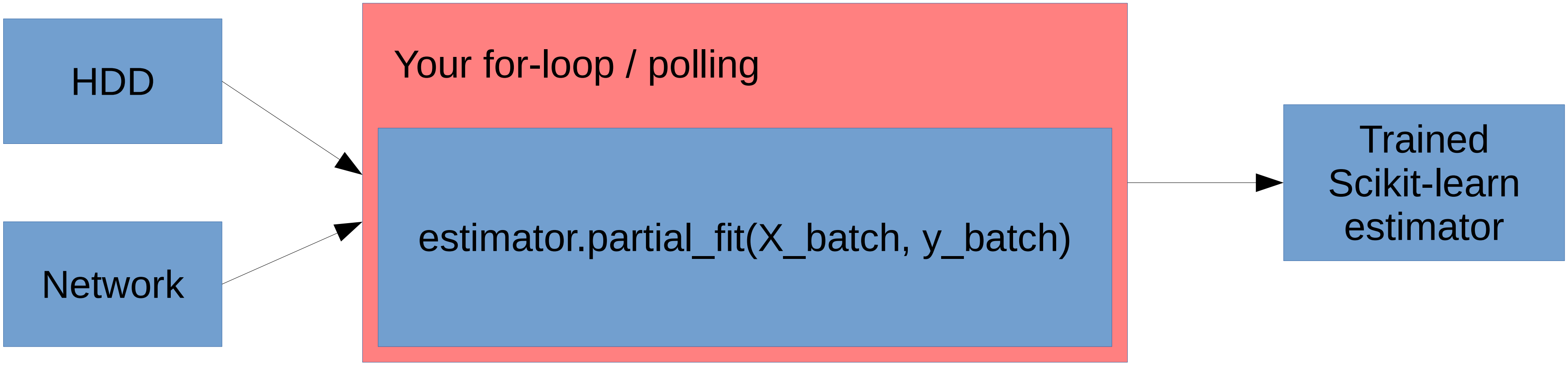
Out of Core Learning

Three regimes of data

- Fits in RAM
- Fits on a Hard Drive
- Doesn't fit on a single PC



	vCPU	ECU	Memory (GiB)	Instance Storage (GB)	Linux/UNIX Usage
Memory Optimized - 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 Optimized - Current 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



HDD

Network

Your for-loop / polling

estimator.partial_fit(X_batch, y_batch)

Trained Scikit-learn estimator

Supported Algorithms

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

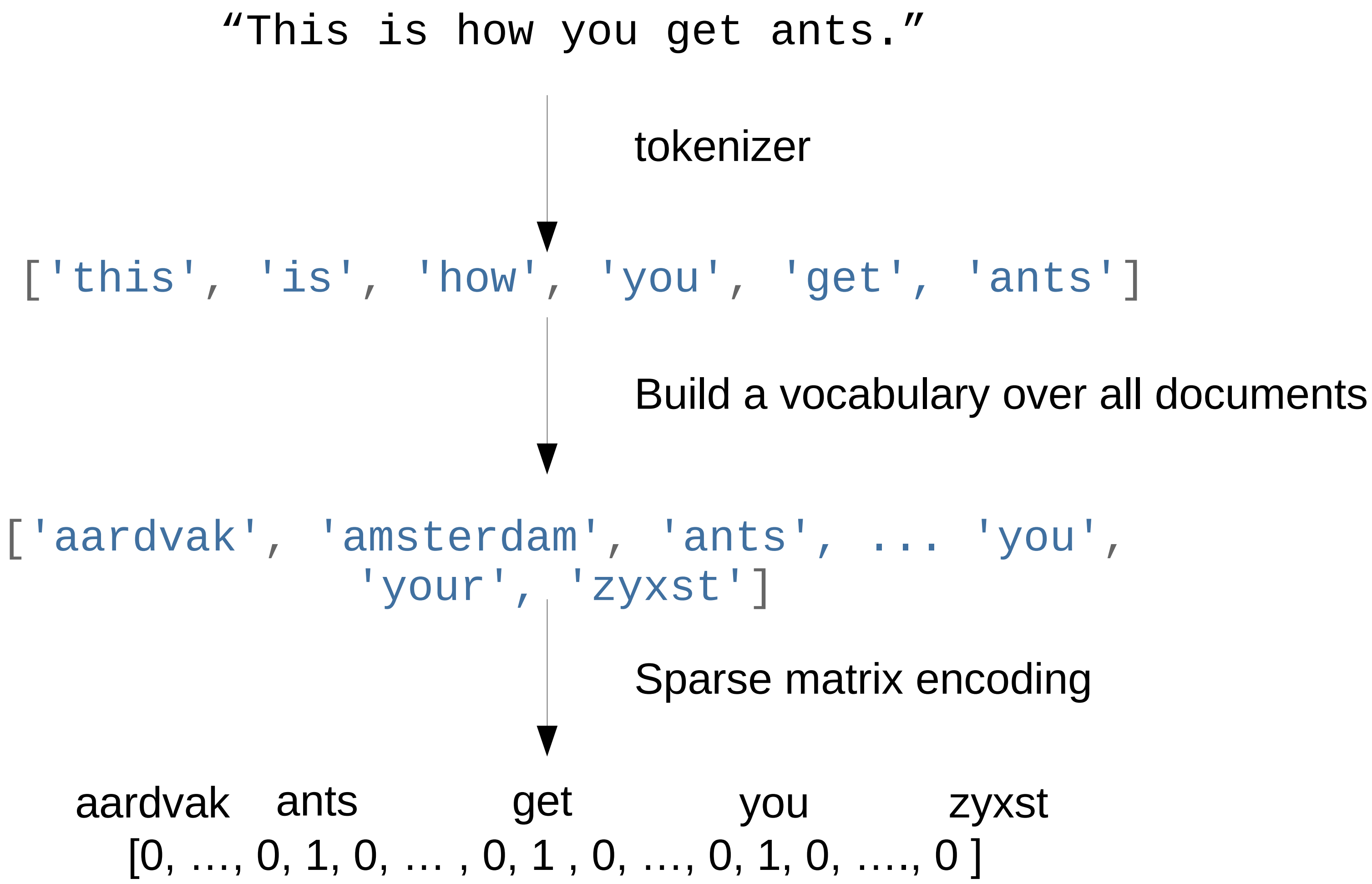
Out of Core Learning

```
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']

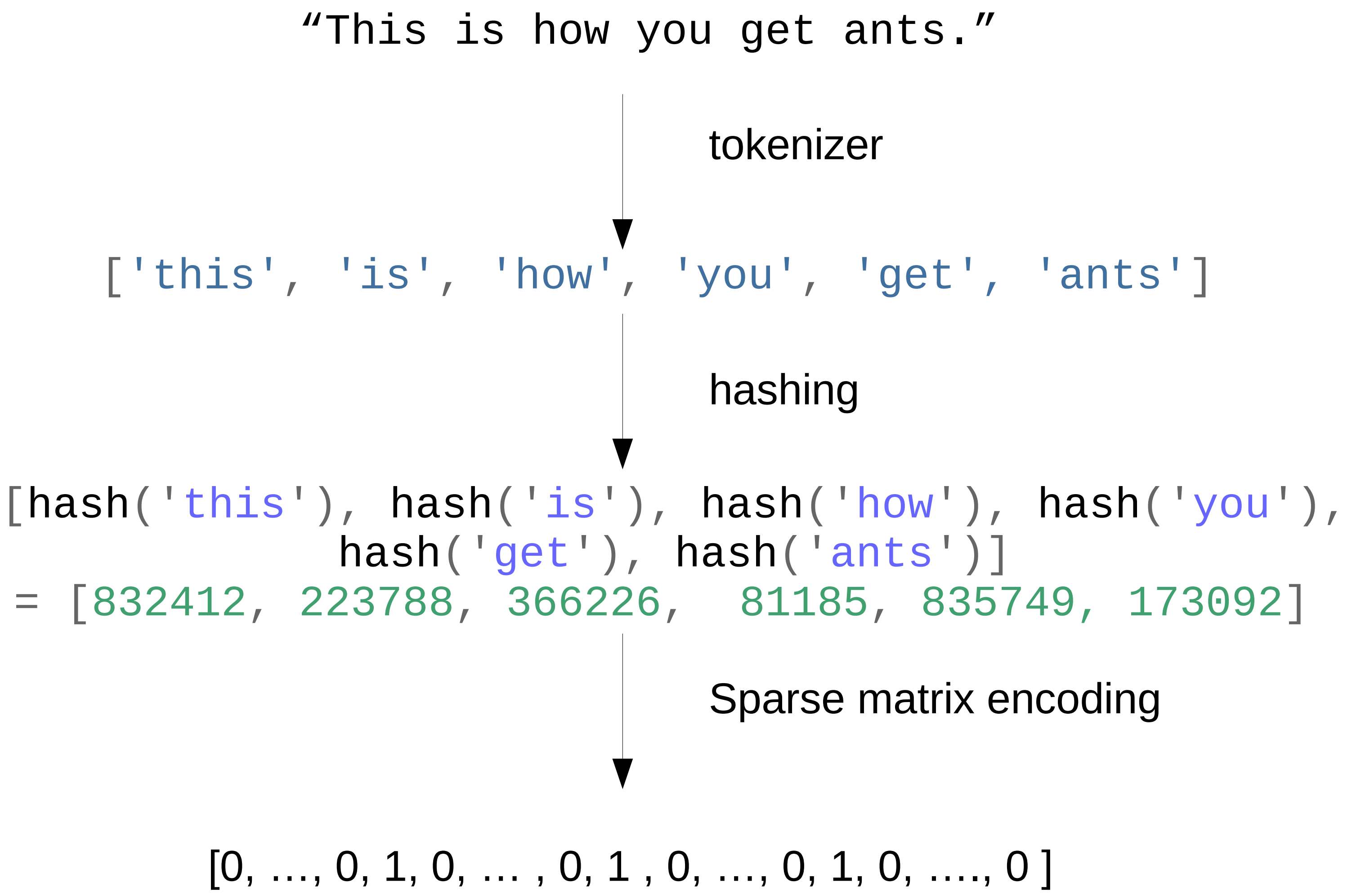
Build a vocabulary over all documents

['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']
```

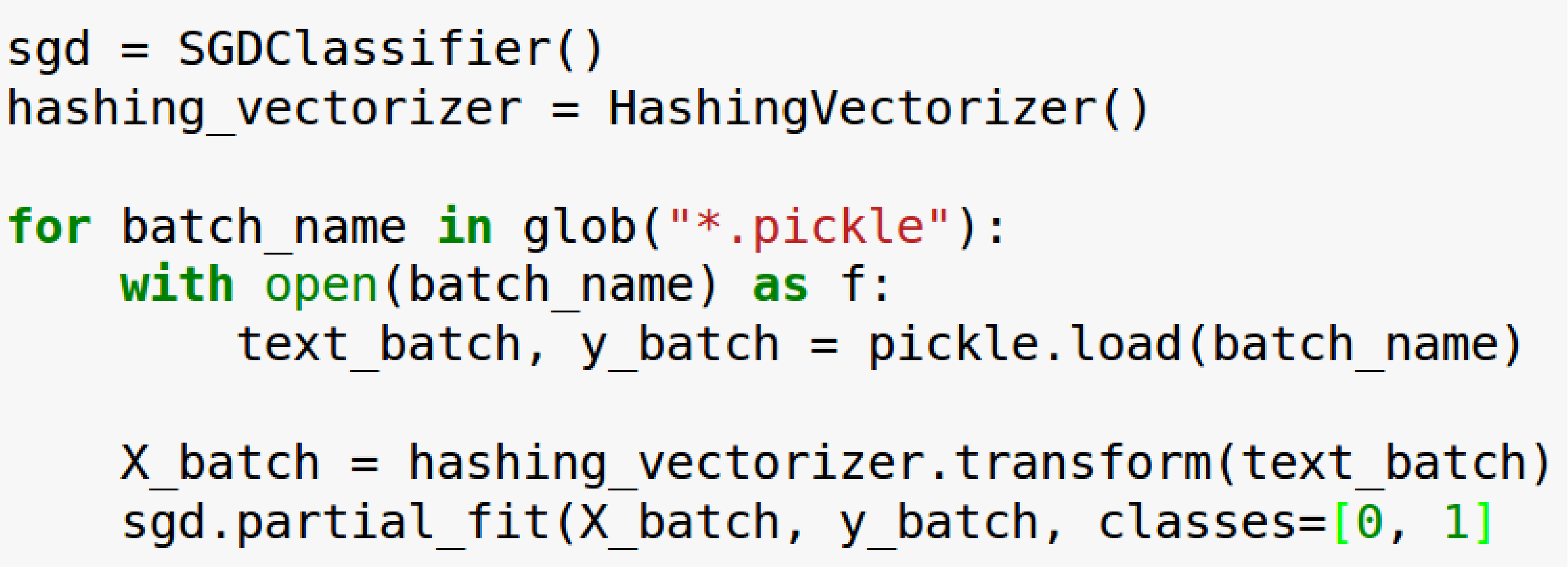
hashing

```
[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]

Text Classification: Hashing Trick



```python
sgd = SGDClassifier()
hashing_vectorizer = HashingVectorizer()

for batch_name in glob("*.pickle"):
    with open(batch_name) as f:
        text_batch, y_batch = pickle.load(batch_name)

    X_batch = hashing_vectorizer.transform(text_batch)
    sgd.partial_fit(X_batch, y_batch, classes=[0, 1]
```

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

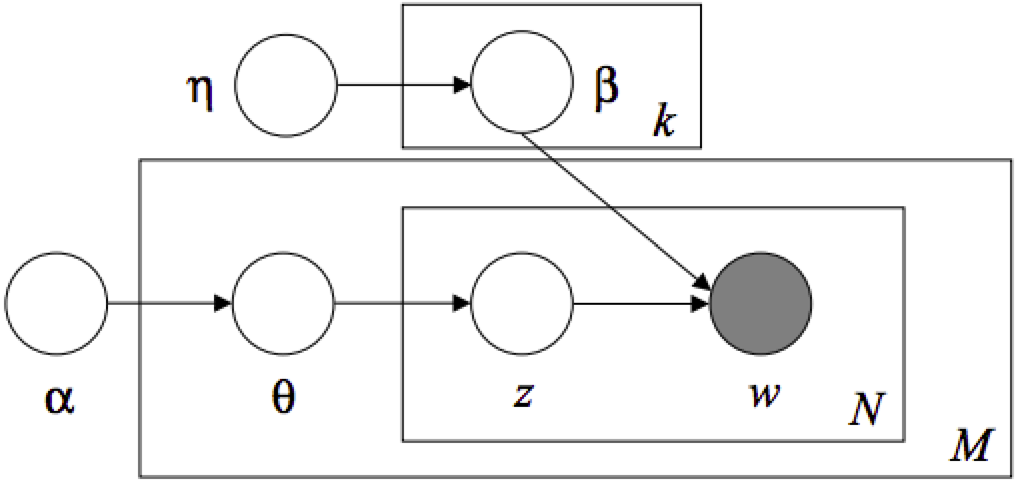
See the “build your own estimator” docs!

Notebook Building your own estimator

What's new in 0.17

Latent Dirichlet Allocation

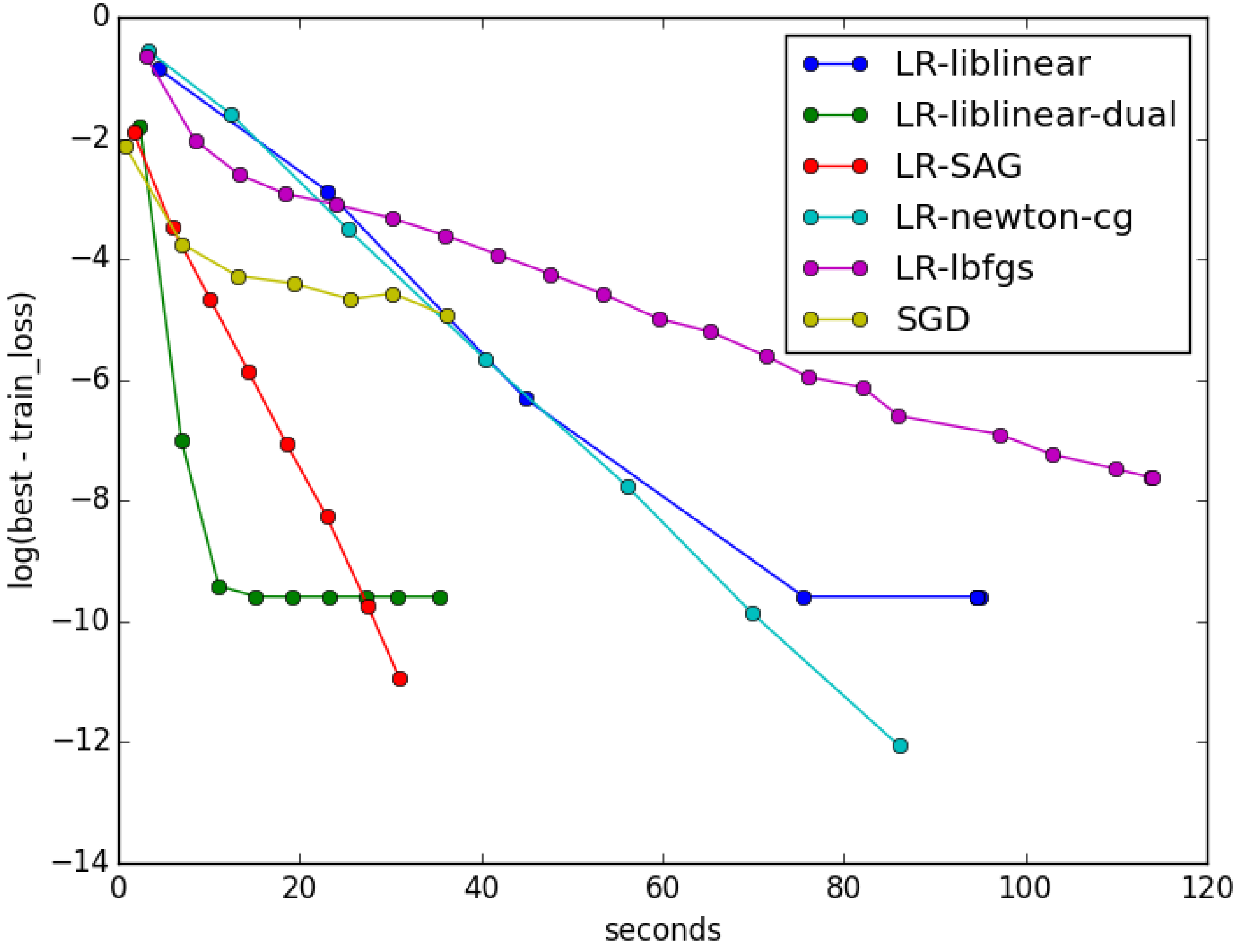
using online variational inference



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 ll
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



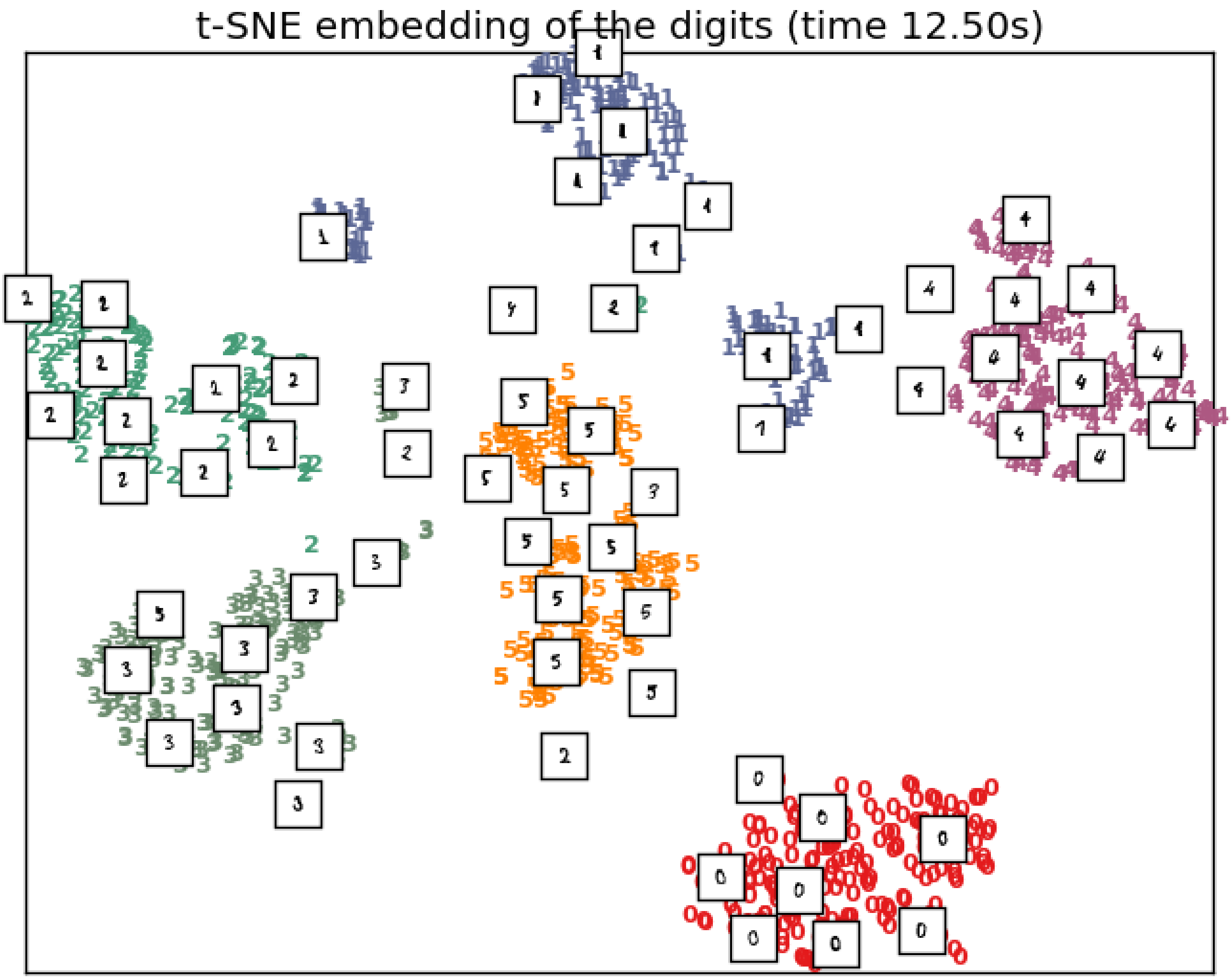
By Danny Sullivan and Tom Dupre la Tour

Coordinate Descent Solver for Non-Negative Matrix Factorization

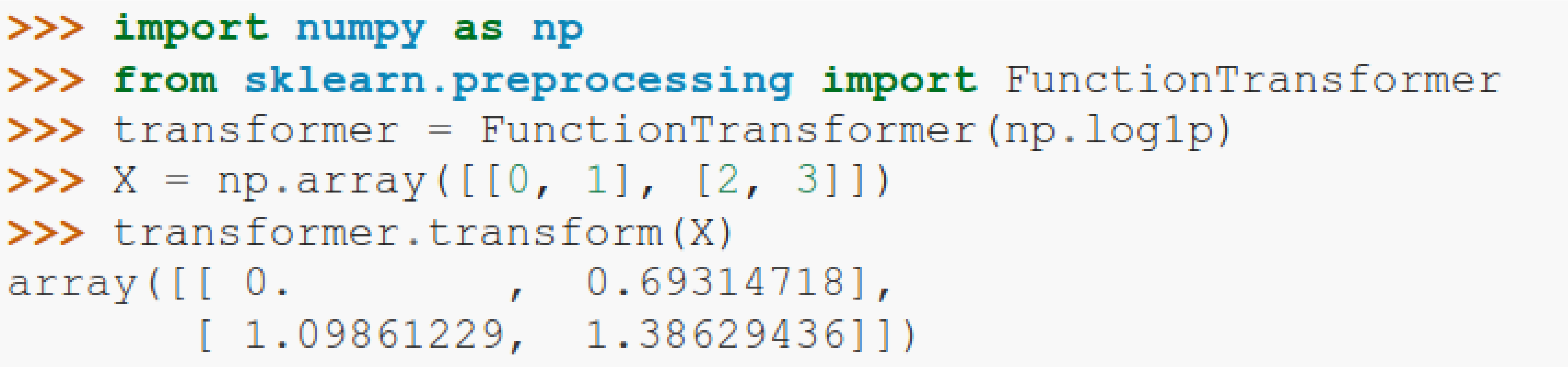
```
Topics in NMF model:
Topic #0:
don people just like think know time good right ve make say want did really way new use going said
Topic #1:
windows file dos files window program use running using version ms problem server pc screen ftp run application os software
Topic #2:
god jesus bible christ 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
```

By Tom Dupre la Tour and Mathieu Blondel

Barnes-Hut Approximation for T-SNE manifold learning



FunctionTransformer



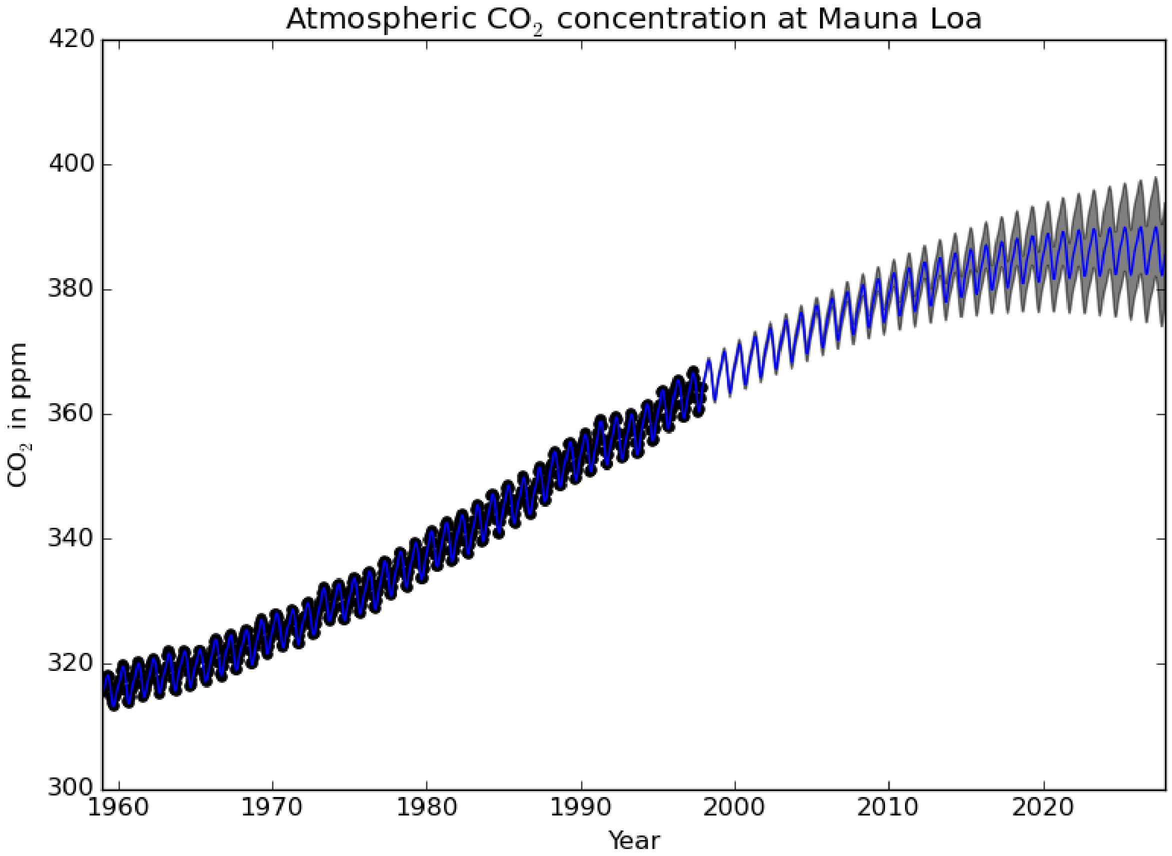
```
>>> import numpy as np
>>> from sklearn.preprocessing import FunctionTransformer
>>> transformer = FunctionTransformer(np.log1p)
>>> X = np.array([[0, 1], [2, 3]])
>>> transformer.transform(X)
array([[ 0.        ,  0.69314718],
       [ 1.09861229,  1.38629436]])
```

VotingClassifier

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

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

What the future will bring (0.18)

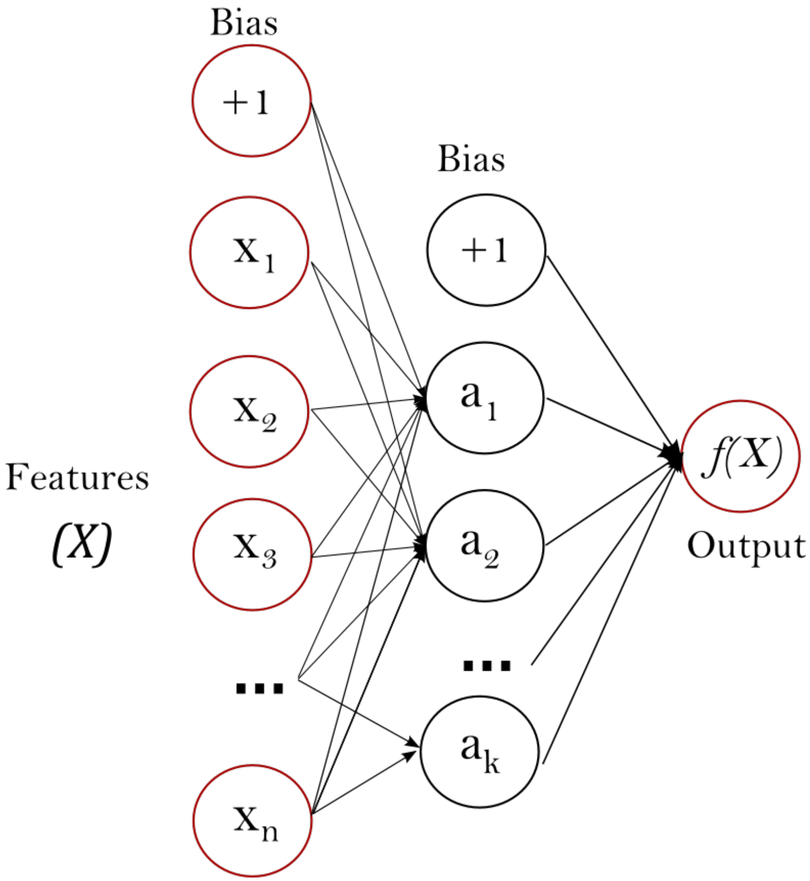
Gaussian Process Rewrite

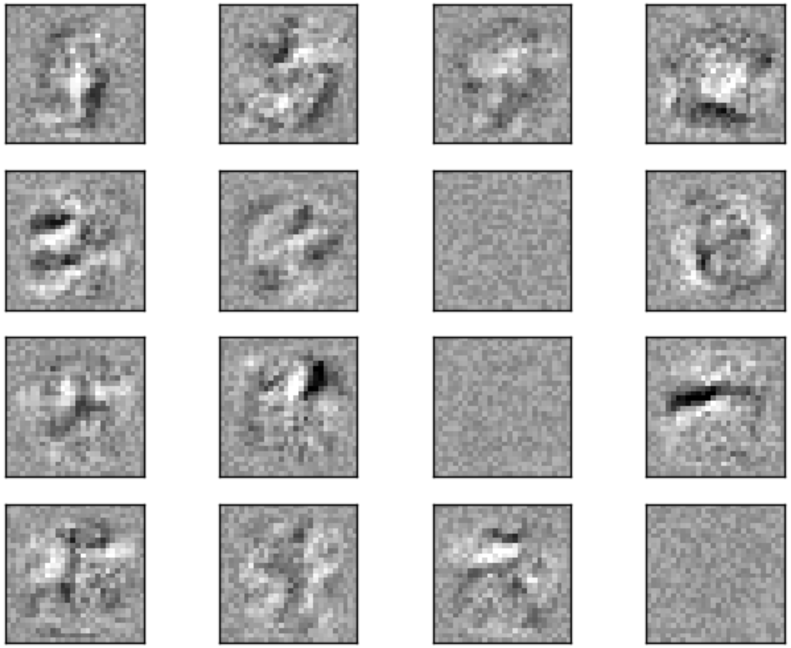


```
34.4**2 * RBF(length_scale=41.8)
+ 3.27**2 * RBF(length_scale=180)
   * ExpSineSquared(length_scale=1.44, periodicity=1)
+ 0.446**2 * RationalQuadratic(alpha=17.7, length_scale=0.957)
+ 0.197**2 * RBF(length_scale=0.138) +
WhiteKernel(noise_level=0.0336)
```

By Jan Hendrik Metzen.

Neural Networks

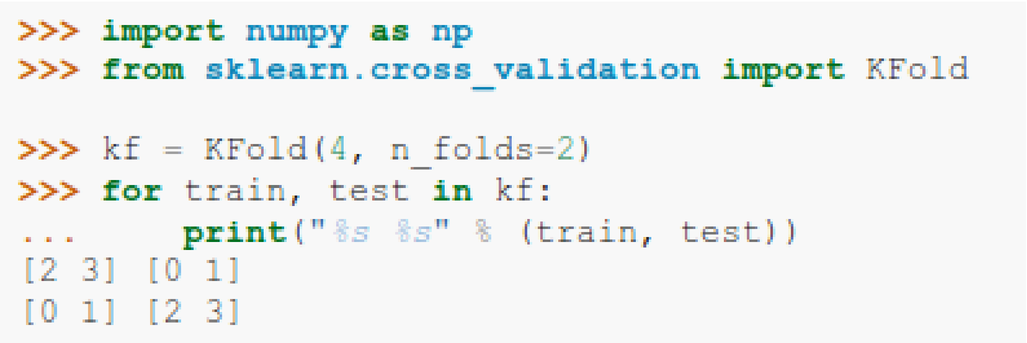




By Jiyuan Qian and Issam Laradji

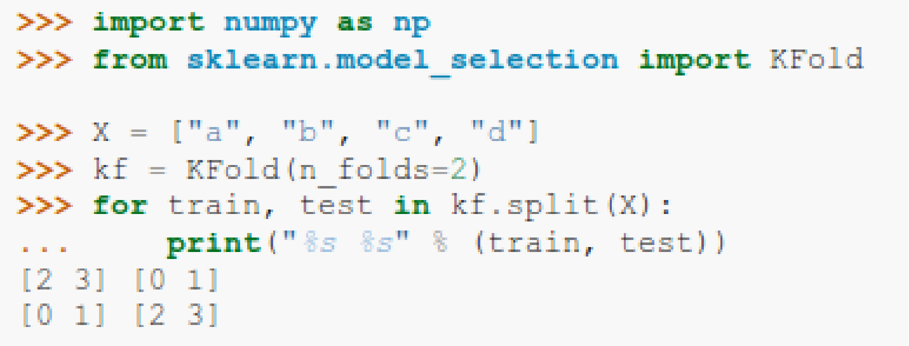
Improved Cross-Validation

current

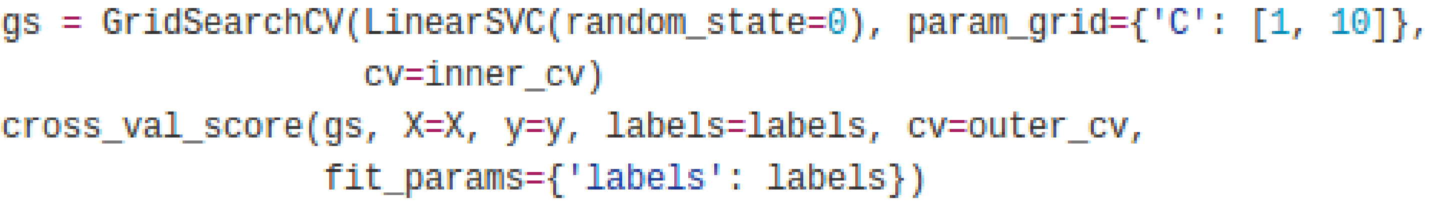


```
>>> import numpy as np
>>> from sklearn.cross_validation import KFold

>>> 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



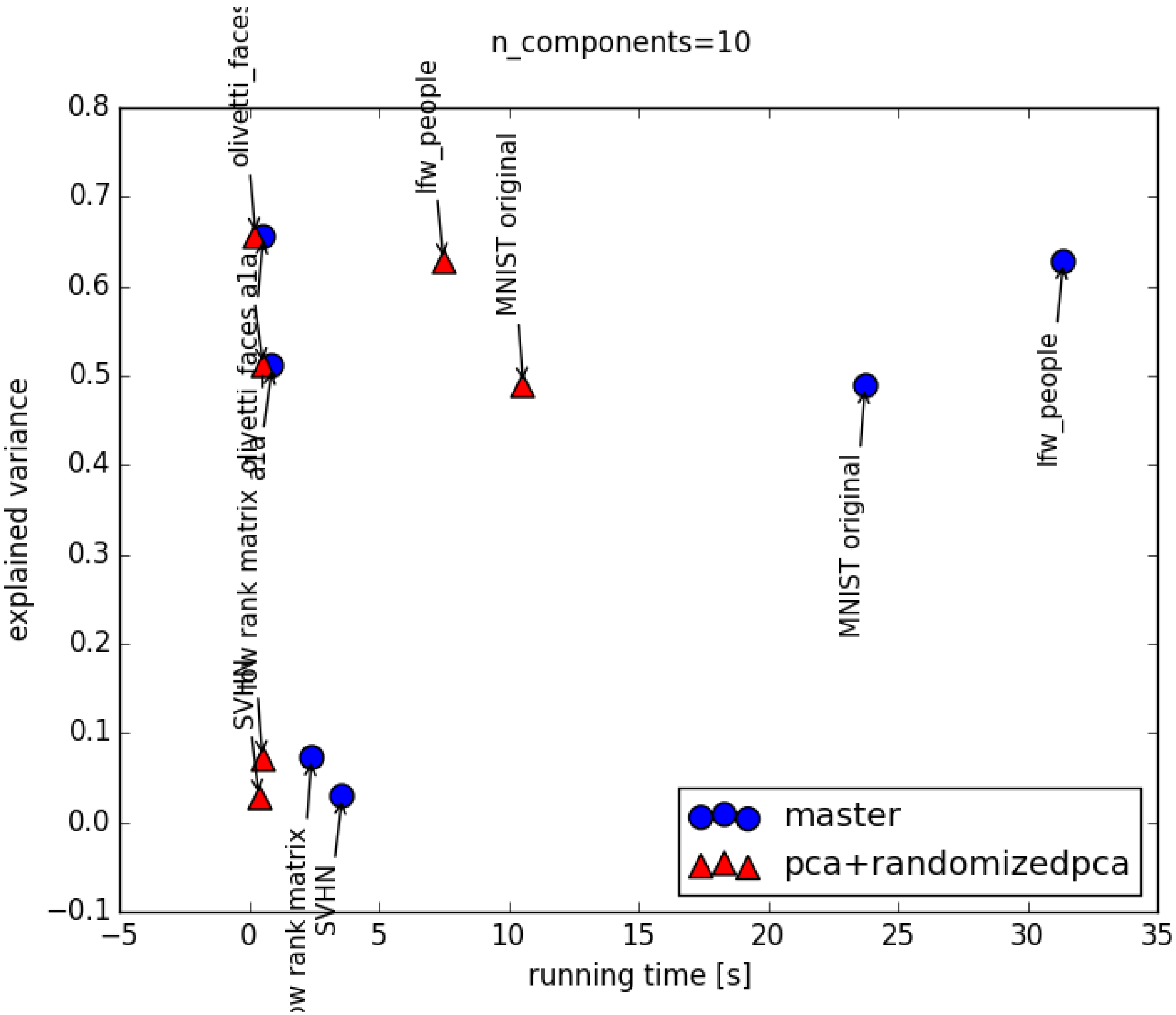
```
>>> import numpy as np
>>> from sklearn.model_selection import KFold

>>> 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]
```



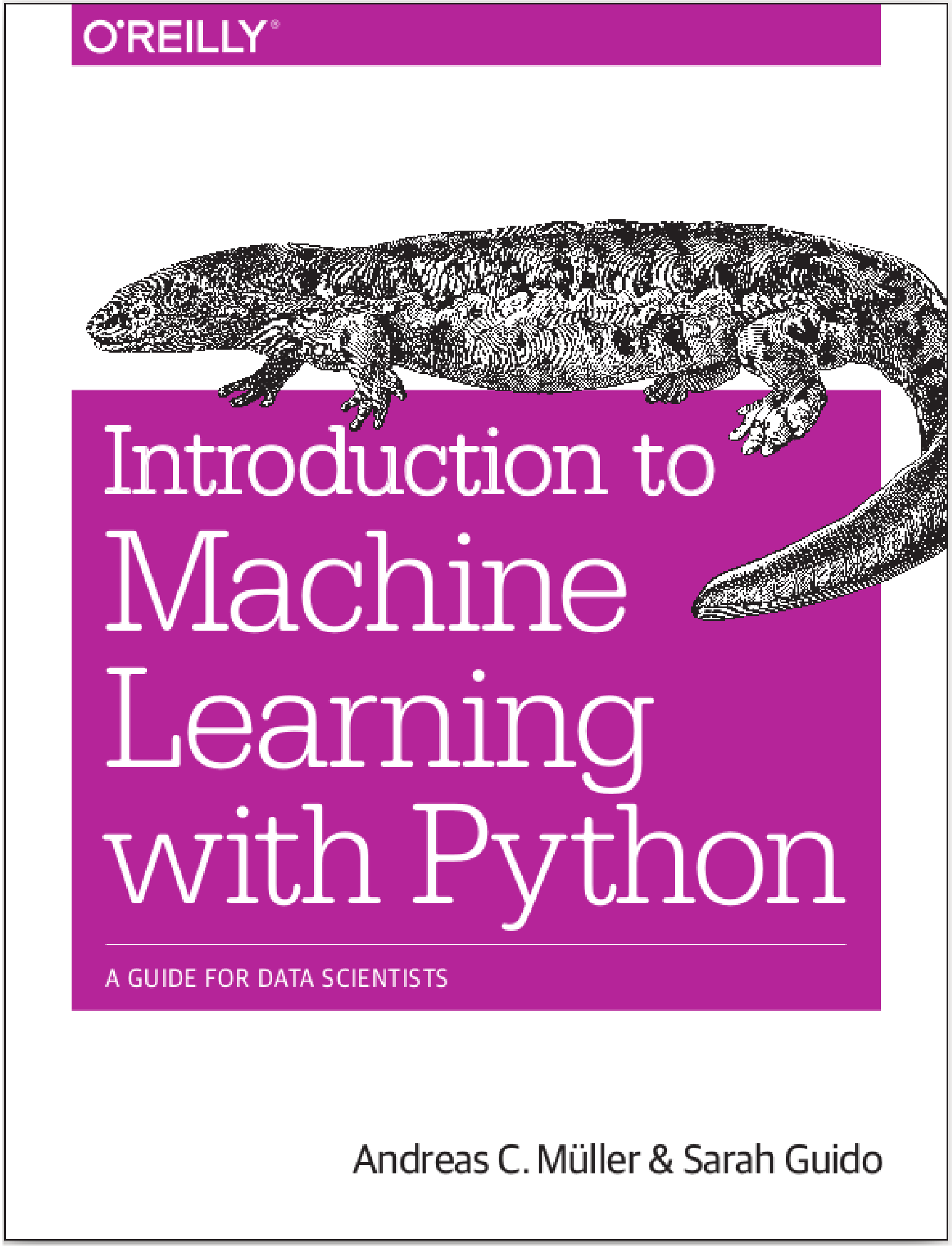
```
gs = GridSearchCV(LinearSVC(random_state=0), param_grid={'C': [1, 10]},
                  cv=inner_cv)
cross_val_score(gs, X=X, y=y, labels=labels, cv=outer_cv,
                fit_params={'labels': labels})
```

By Raghav RV

Faster PCA



By Giorgio Patrini



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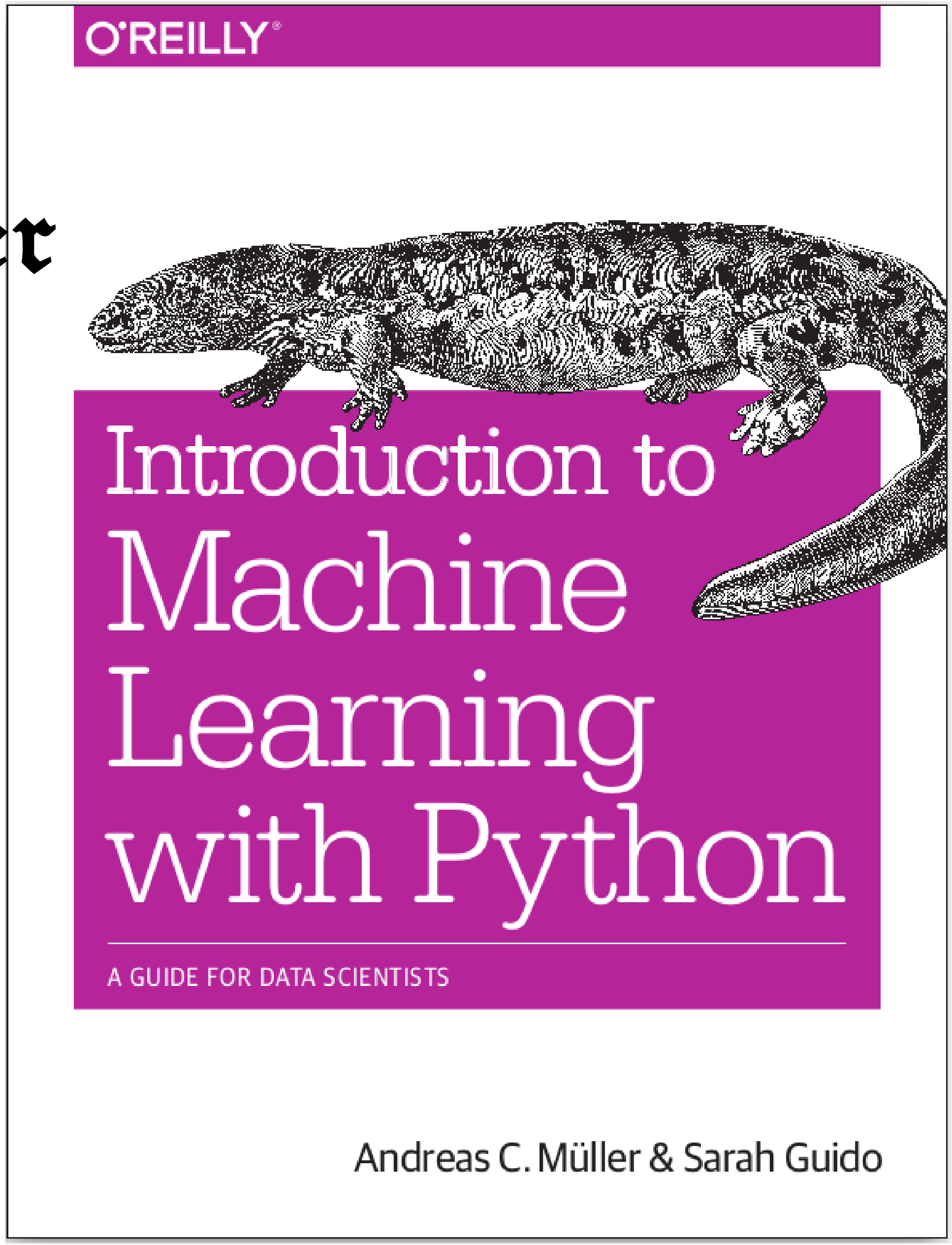
Andreas C. Müller & Sarah Guido

Release June 2016

Hellbender



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Thank you!

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