

# Machine Learning with Scikit-Learn

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

Material: http://bit.ly/sklsf

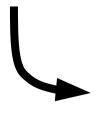
### Me













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





agramfort

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Jaques Grobler

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Kyle Kastner



bthirion bthirion



chrisfilo Chris Filo Gorgole...



cournape David Cournapeau



duchesnay



Duchesnay



David Warde-Farley



fabianp Fabian Pedregosa



kuantkid Wei LI





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pprett Peter Prettenhofer



robertlayton Robert Layton



ronw Ron Weiss



Satrajit Ghosh



sklearn-ci



Vlad Niculae





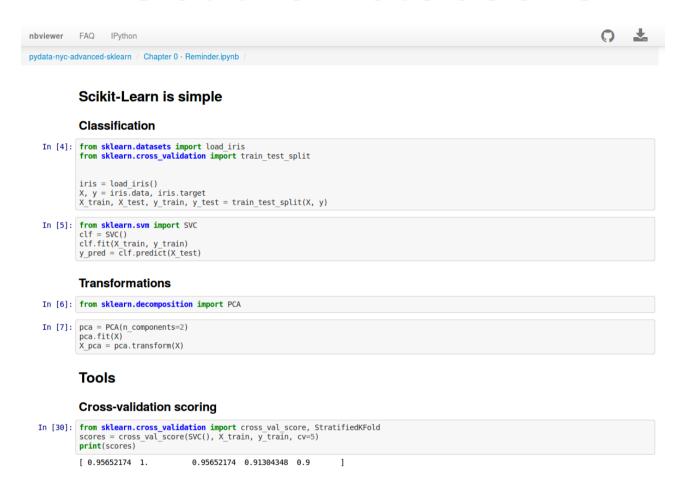
vmichel Vincent Michel



yarikoptic Yaroslav Halchenko



### Get the notebooks!



http://bit.ly/sklsf

#### 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.

#### Hi Andy,

I just received an email from the first tutorial speaker, presenting right before you, saying he's ill and won't be able to make it.

I know you have already committed yourself to two presentations, but is there anyway you could increase your tutorial time slot, maybe just offer time to try out what you've taught? Otherwise I have to do some kind of modern dance interpretation of Python in data :-)
-Leah

#### Hi Andreas,

I am very interested in your Machine Learning background. I work for X Recruiting who have been engaged by Z, a worldwide leading supplier of Y. We are expanding the core engineering team and we are looking for really passionate engineers who want to create their own story and help millions of people.

Can we find a time for a call to chat for a few minutes about this?

#### Hi Andy,

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I know you have a two presentations could increase you maybe just offer time to try out what you've taught? Otherwise I have to do some kind of modern dance interpretation of Python in data :-)
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Can we find a ti

for a few

### Doing Machine Learning With Scikit-Learn

```
      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

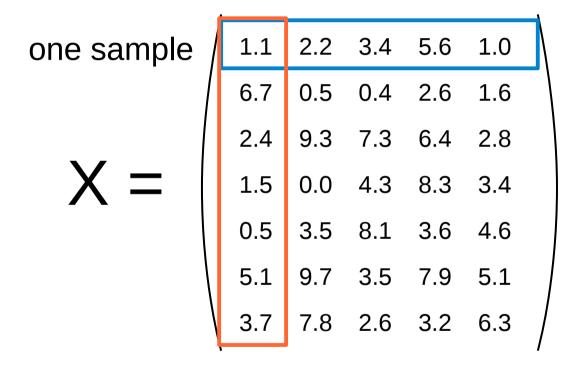
2.4 9.3 7.3 6.4 2.8

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

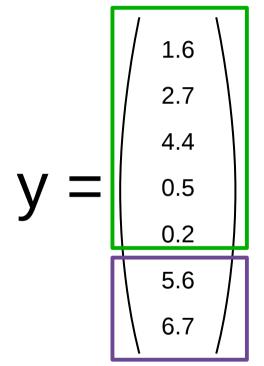
one feature

outputs / labels

## **Training and Testing Data**

## Training and Testing Data

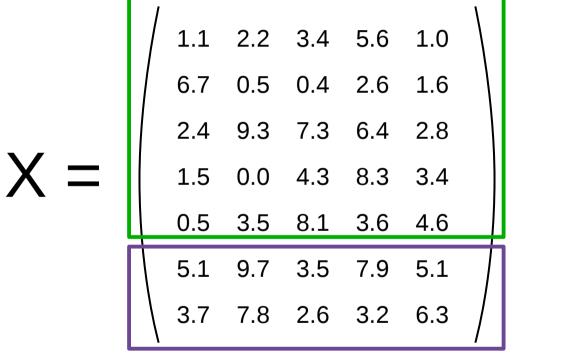
### training set

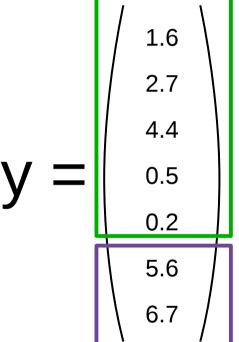


test set

# Training and Testing Data

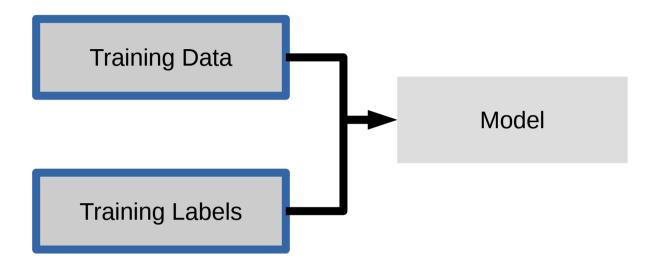
#### training set

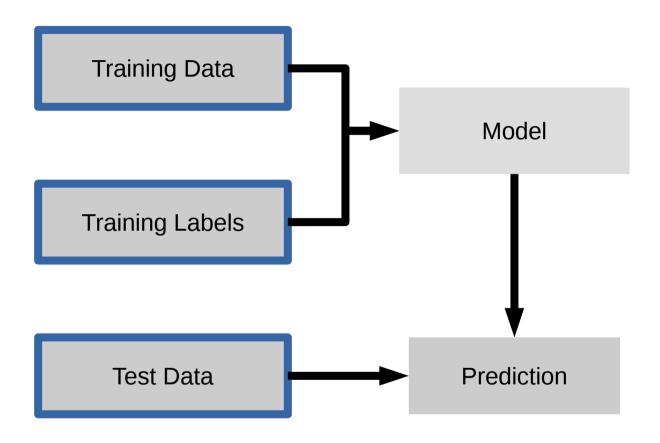


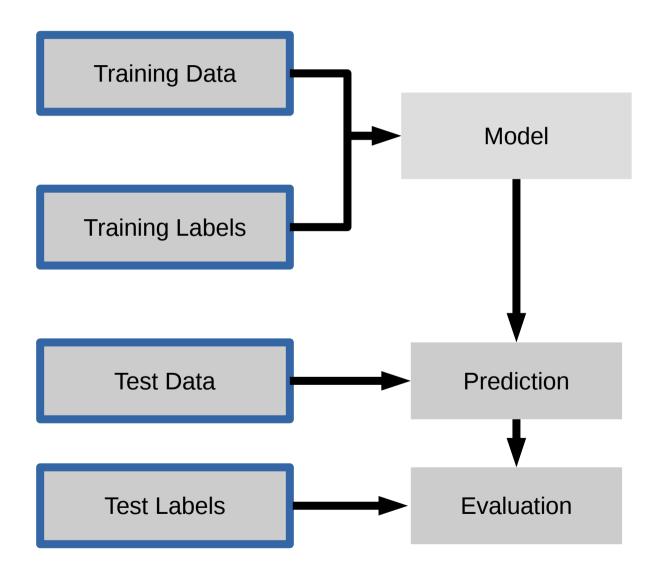


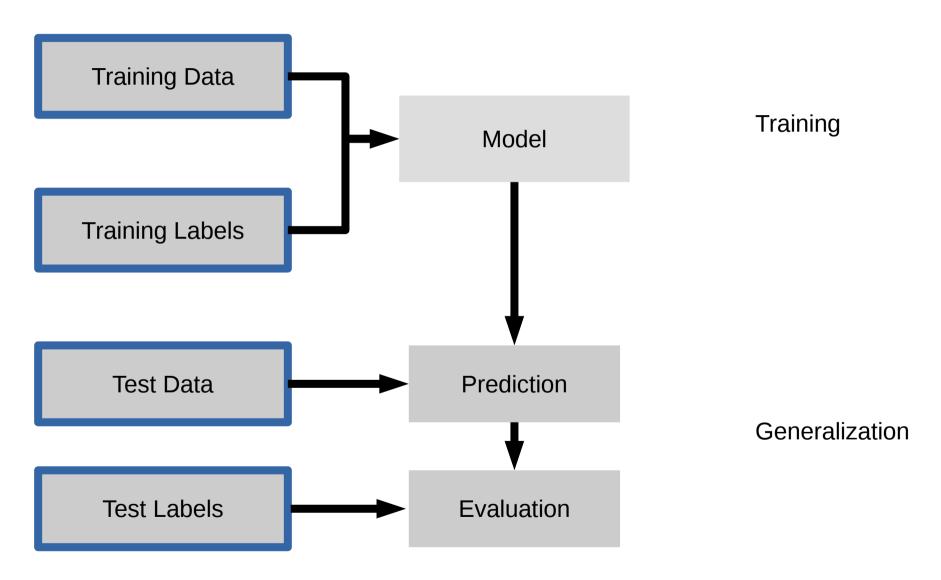
test set

from sklearn.cross\_validation import train\_test\_split
X\_train, X\_test, y\_train, y\_test = train\_test\_split(X, y)



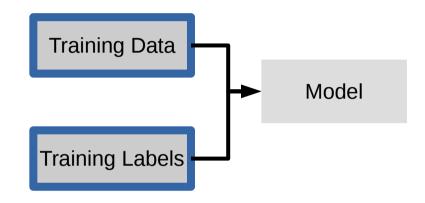






clf = RandomForestClassifier()

clf.fit(X\_train, y\_train)



clf = RandomForestClassifier()

clf.fit(X\_train, y\_train)

y\_pred = clf.predict(X\_test)

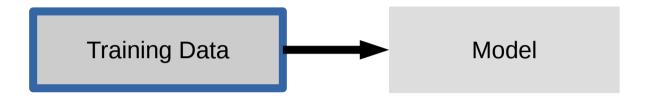
Training Data

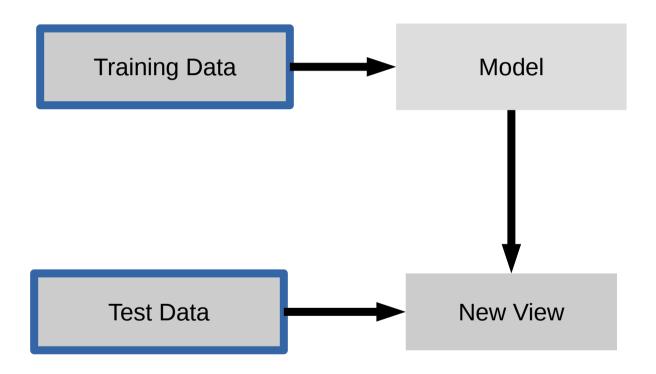
Training Labels

Prediction

clf = RandomForestClassifier() Training Data clf.fit(X\_train, y\_train) Model Training Labels y\_pred = clf.predict(X\_test) Test Data Prediction clf.score(X\_test, y\_test) Test Labels **Evaluation** 

### IPython Notebook: Part 1 - Introduction to Scikit-learn





## **Unsupervised Transformations**

```
pca = PCA()
pca.fit(X_train)
                                         Training Data
                                                           Model
X_new = pca.transform(X_test)
                                                        Transformation
                                          Test Data
```

### IPython Notebook: Part 2 – Unsupervised Transformers

### **Basic API**

estimator.fit(X, [y])

estimator.predict

estimator.transform

Classification

Preprocessing

Regression

Dimensionality reduction

Clustering

Feature selection

Feature extraction

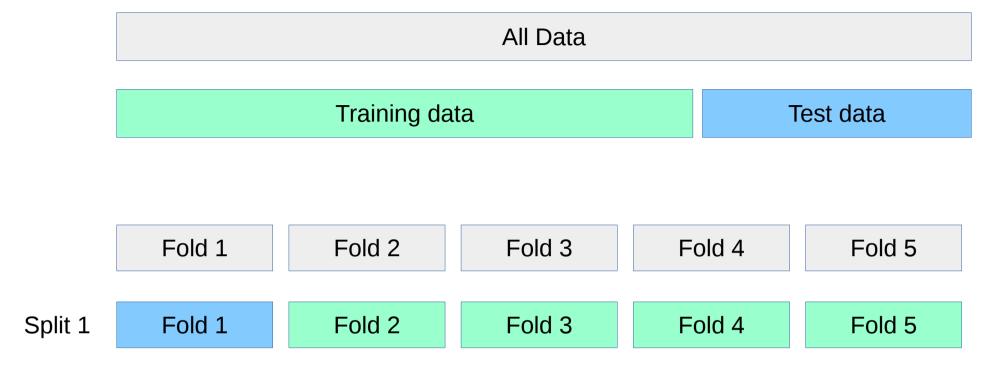
All Data	
Training data	Test data

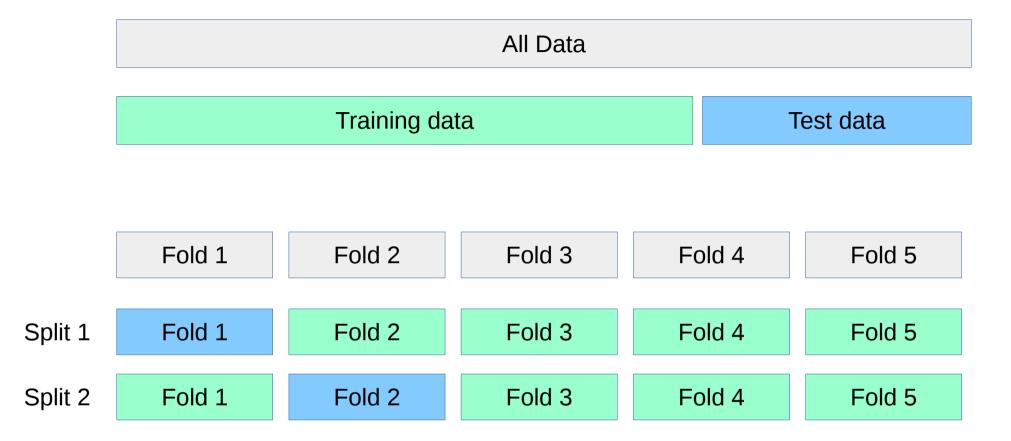
All Data

Training data

Test data

Fold 1 Fold 2 Fold 3 Fold 4 Fold 5





	All Data						
	Training data				Test data		
	Fold 1	Fold 2	Fold 3	Fol	d 4	Fold 5	
Split 1	Fold 1	Fold 2	Fold 3	Fol	d 4	Fold 5	
Split 2	Fold 1	Fold 2	Fold 3	Fol	d 4	Fold 5	
Split 3	Fold 1	Fold 2	Fold 3	Fol	d 4	Fold 5	
Split 4	Fold 1	Fold 2	Fold 3	Fold 4		Fold 5	
Split 5	Fold 1	Fold 2	Fold 3	Fol	d 4	Fold 5	

### IPython Notebook: Part 3 - Cross-validation

```
In [2]: clf = SVC()
  clf.fit(X_train, y_train)
  y_pred = clf.predict(X_test)
```

All Data			
Training data	Test data		

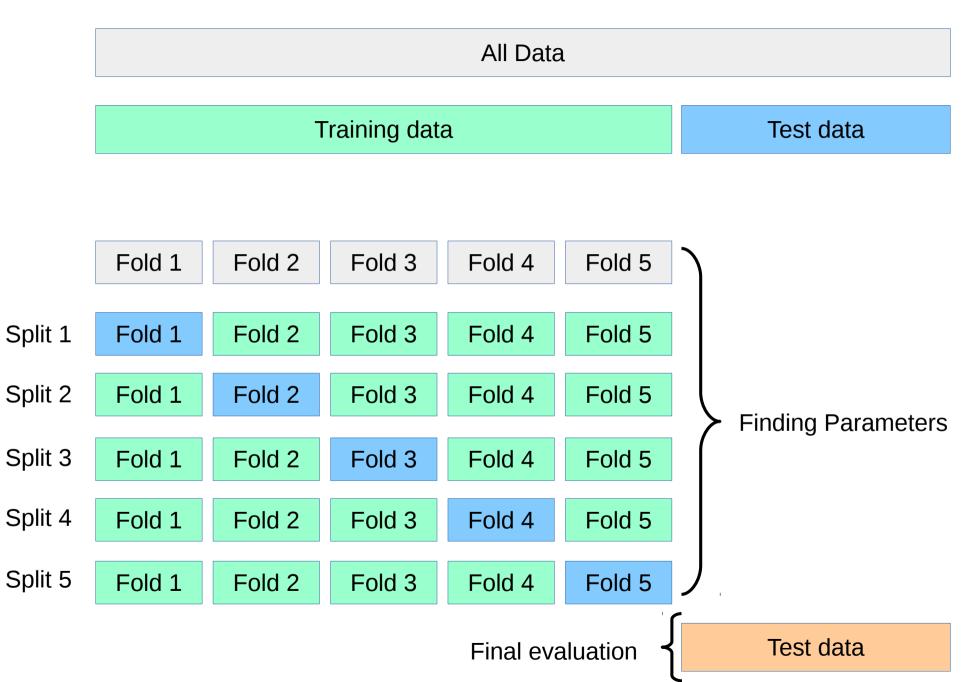
#### All Data

#### 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



SVC(C=0.001, gamma=0.001)

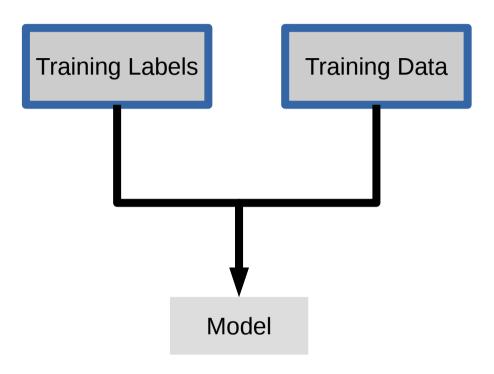
SVC(C=0.001, SVC(C=0.01, SVC(C=0.1, SVC(C=1, SVC(C=10, gamma=0.001) gamma=0.001) gamma=0.001) gamma=0.001)

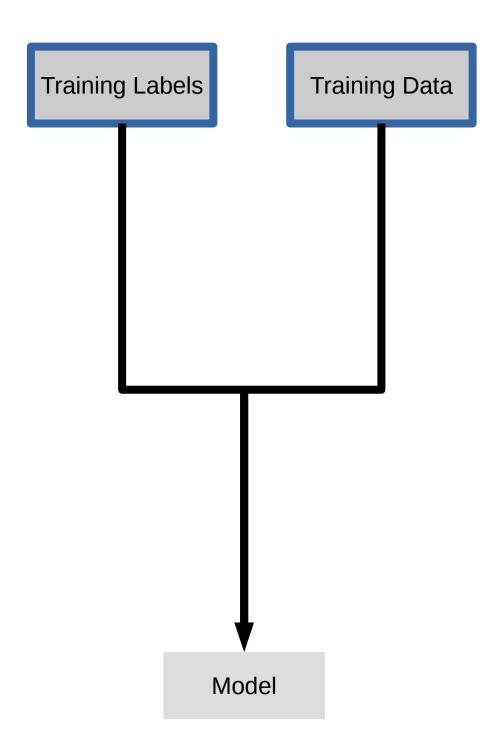
SVC(C=0.001,	SVC(C=0.01,	SVC(C=0.1,	SVC(C=1,	SVC(C=10,
gamma=0.001)	gamma=0.001)	gamma=0.001)	gamma=0.001)	gamma=0.001)
SVC(C=0.001, gamma=0.01)	SVC(C=0.01,	SVC(C=0.1,	SVC(C=1,	SVC(C=10,
	gamma=0.01)	gamma=0.01)	gamma=0.01)	gamma=0.01)

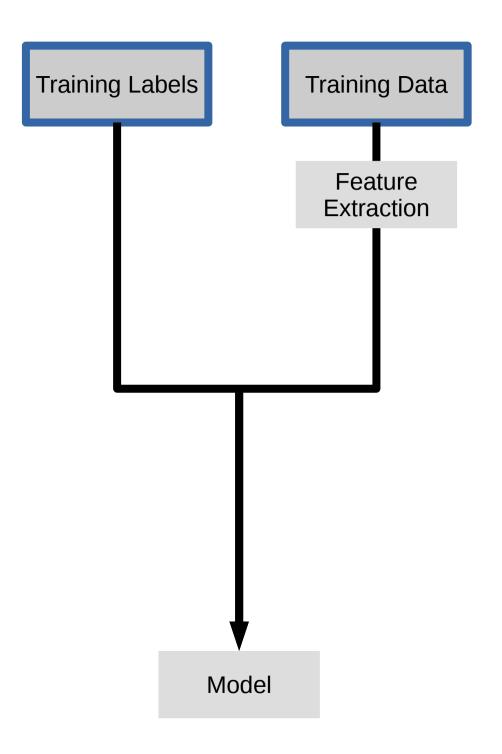
SVC(C=0.001,	SVC(C=0.01,	SVC(C=0.1,	SVC(C=1,	SVC(C=10,
gamma=0.001)	gamma=0.001)	gamma=0.001)	gamma=0.001)	gamma=0.001)
SVC(C=0.001,	SVC(C=0.01,	SVC(C=0.1,	SVC(C=1,	SVC(C=10,
gamma=0.01)	gamma=0.01)	gamma=0.01)	gamma=0.01)	gamma=0.01)
SVC(C=0.001,	SVC(C=0.01, gamma=0.1)	SVC(C=0.1,	SVC(C=1,	SVC(C=10,
gamma=0.1)		gamma=0.1)	gamma=0.1)	gamma=0.1)

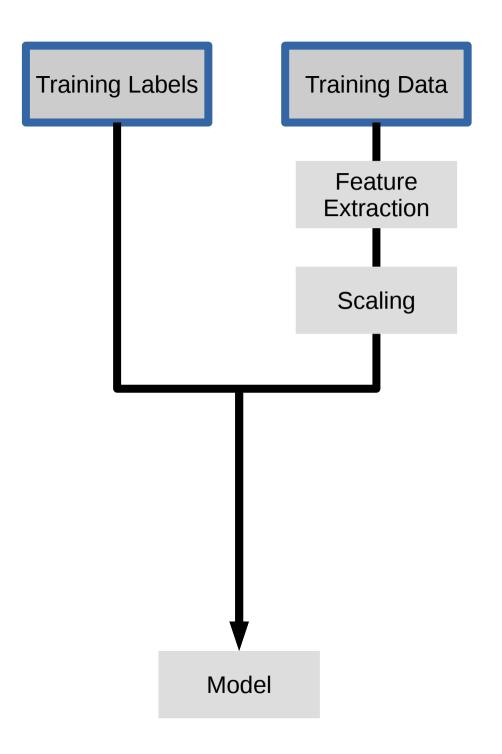
SVC(C=0.001,	SVC(C=0.01,	SVC(C=0.1,	SVC(C=1,	SVC(C=10,
gamma=0.001)	gamma=0.001)	gamma=0.001)	gamma=0.001)	gamma=0.001)
SVC(C=0.001,	SVC(C=0.01,	SVC(C=0.1,	SVC(C=1,	SVC(C=10,
gamma=0.01)	gamma=0.01)	gamma=0.01)	gamma=0.01)	gamma=0.01)
SVC(C=0.001,	SVC(C=0.01,	SVC(C=0.1,	SVC(C=1,	SVC(C=10,
gamma=0.1)	gamma=0.1)	gamma=0.1)	gamma=0.1)	gamma=0.1)
SVC(C=0.001, gamma=1)	SVC(C=0.01,	SVC(C=0.1,	SVC(C=1,	SVC(C=10,
	gamma=1)	gamma=1)	gamma=1)	gamma=1)
SVC(C=0.001,	SVC(C=0.01,	SVC(C=0.1,	SVC(C=1,	SVC(C=10,
gamma=10)	gamma=10)	gamma=10)	gamma=10)	gamma=10)

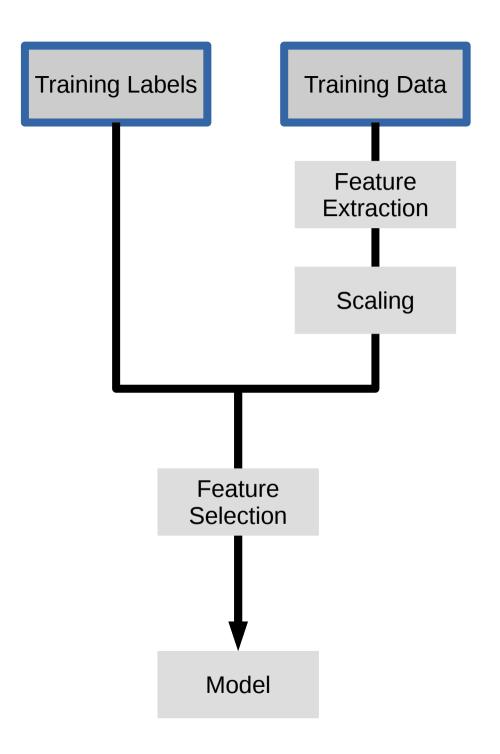
#### IPython Notebook: Part 4 – Grid Searches

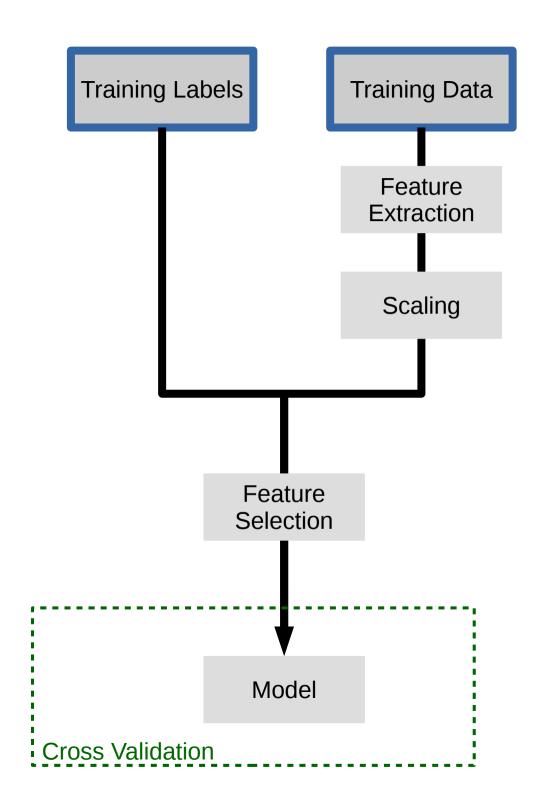


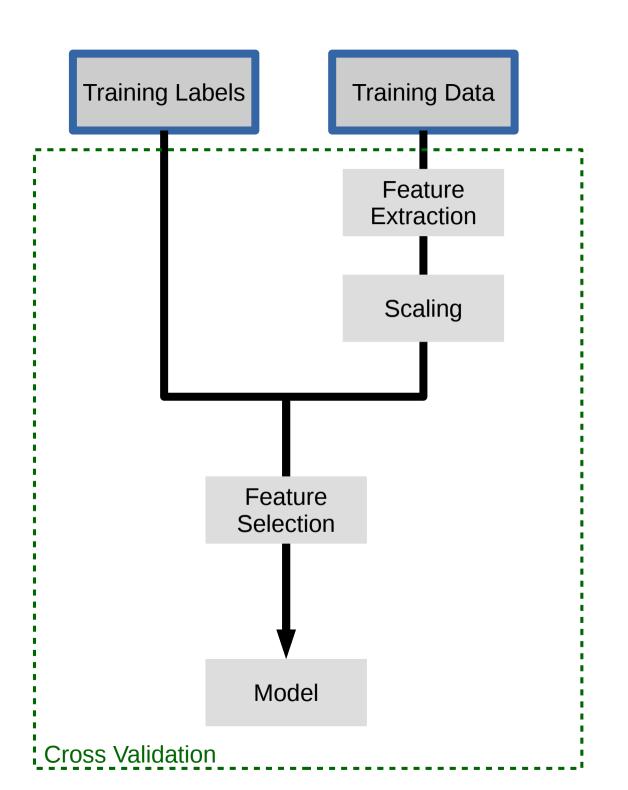












# **Pipelines**

# Pipelines

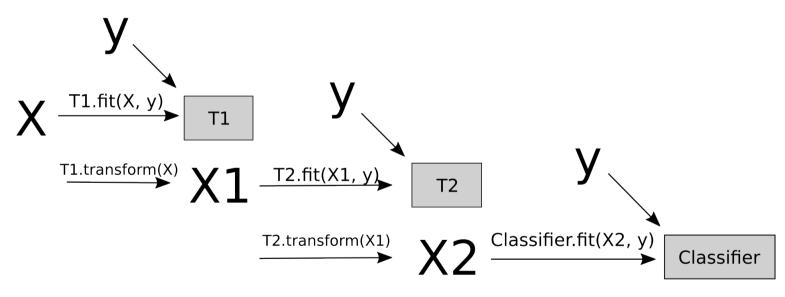
pipe = make\_pipeline(T1(), T2(), Classifier())

T1

T2

Classifier

pipe.fit(X, y)



pipe.predict(X)

$$X' \xrightarrow{\text{T1.transform(X)}} X' 1 \xrightarrow{\text{T2.transform(X1)}} X' 2 \xrightarrow{\text{Classifier.predict(X'2)}} y'$$

# IPython Notebook: Part 5 - Preprocessing and Pipelines

Do cross-validation over all steps jointly. Keep a separate test set until the very end. 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']

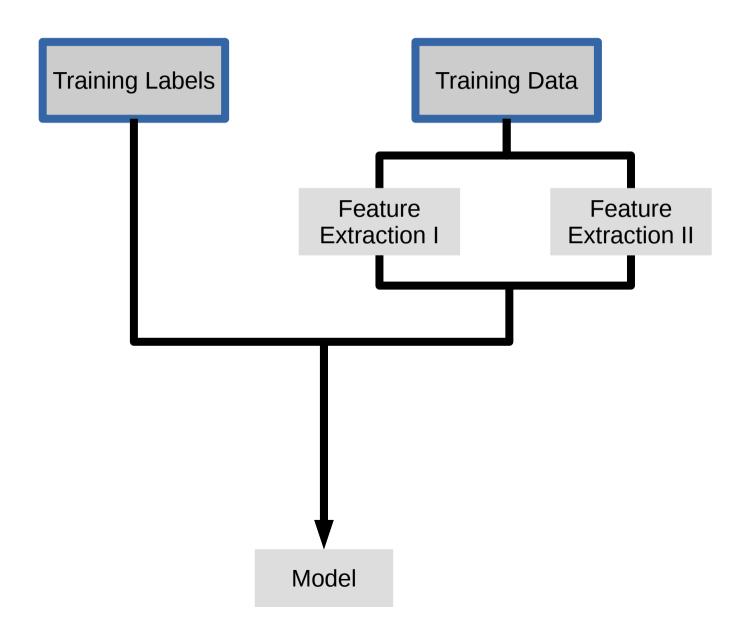
Build a vocabulary over all documents

['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]
```

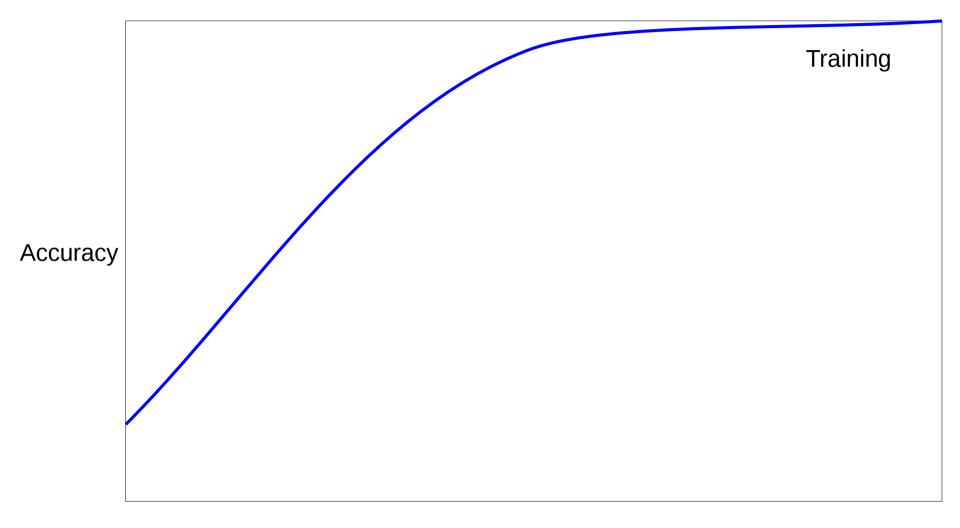
#### IPython Notebook: Part 6 - Working With Text Data

#### **Feature Union**



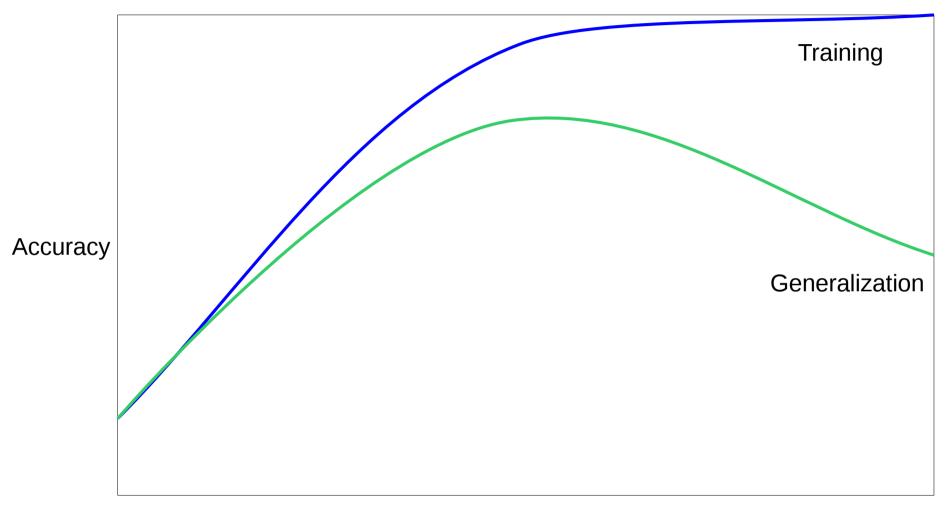
#### IPython Notebook: Part 7 – FeatureUnion

# Overfitting and Underfitting



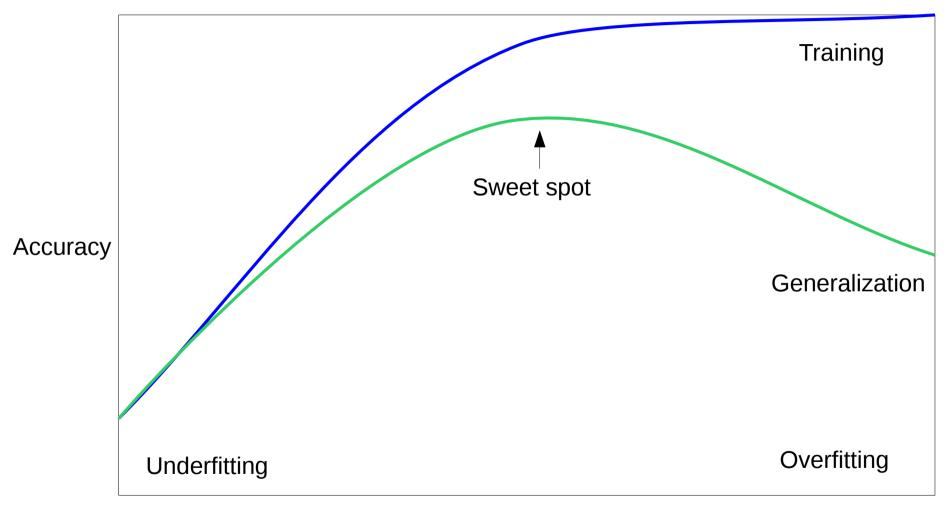
Model complexity

# Overfitting and Underfitting



Model complexity

# Overfitting and Underfitting



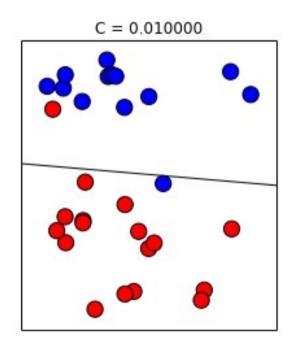
Model complexity

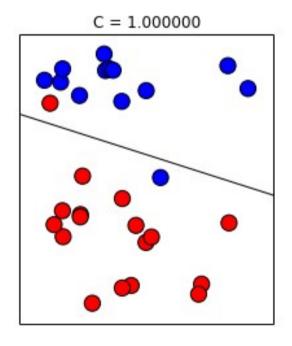
#### Linear SVM

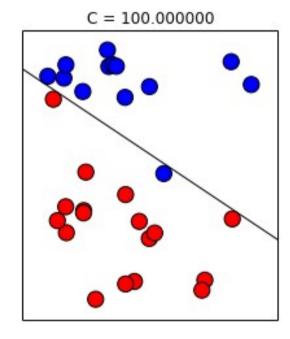
$$\hat{y} = \operatorname{sign}(w_0 + \sum_i w_i x_i)$$

#### Linear SVM

$$\hat{y} = \operatorname{sign}(w_0 + \sum_i w_i x_i)$$



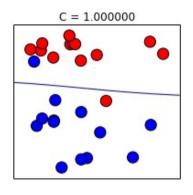


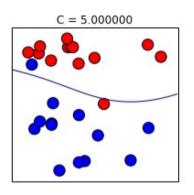


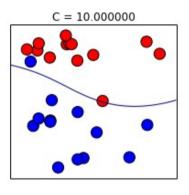
$$\hat{y} = \operatorname{sign}(\alpha_0 + \sum_j \alpha_j y_j k(\mathbf{x}^{(\mathbf{j})}, \mathbf{x}))$$

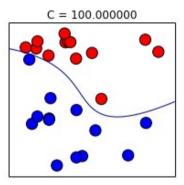
$$\hat{y} = \operatorname{sign}(\alpha_0 + \sum_j \alpha_j y_j k(\mathbf{x}^{(j)}, \mathbf{x}))$$
$$k(\mathbf{x}, \mathbf{x}') = \exp(-\gamma ||\mathbf{x} - \mathbf{x}'||^2)$$

$$\hat{y} = \operatorname{sign}(\alpha_0 + \sum_j \alpha_j y_j k(\mathbf{x}^{(j)}, \mathbf{x}))$$
$$k(\mathbf{x}, \mathbf{x}') = \exp(-\gamma ||\mathbf{x} - \mathbf{x}'||^2)$$

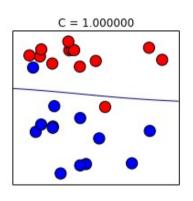


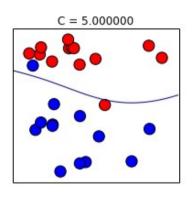


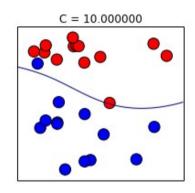


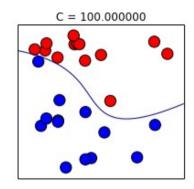


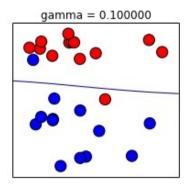
$$\hat{y} = \operatorname{sign}(\alpha_0 + \sum_j \alpha_j y_j k(\mathbf{x}^{(j)}, \mathbf{x}))$$
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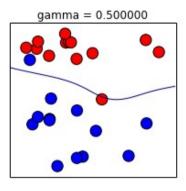


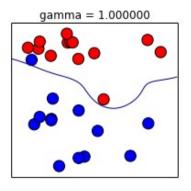


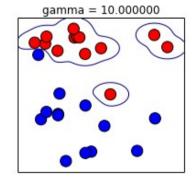


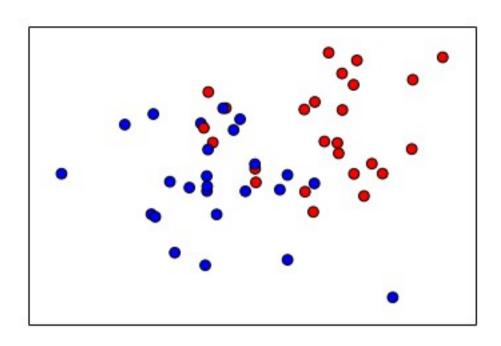


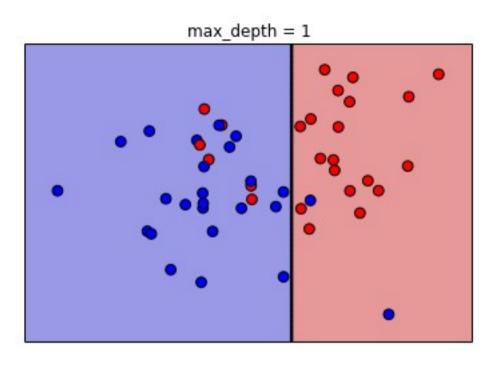


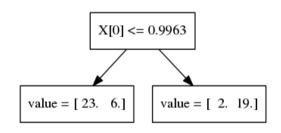


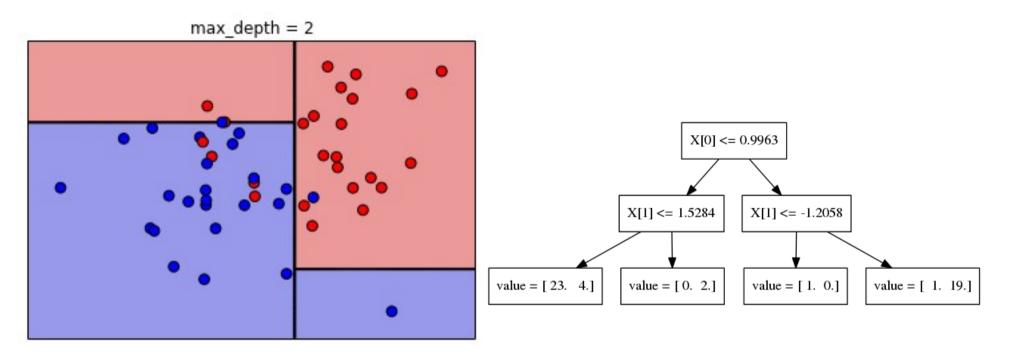


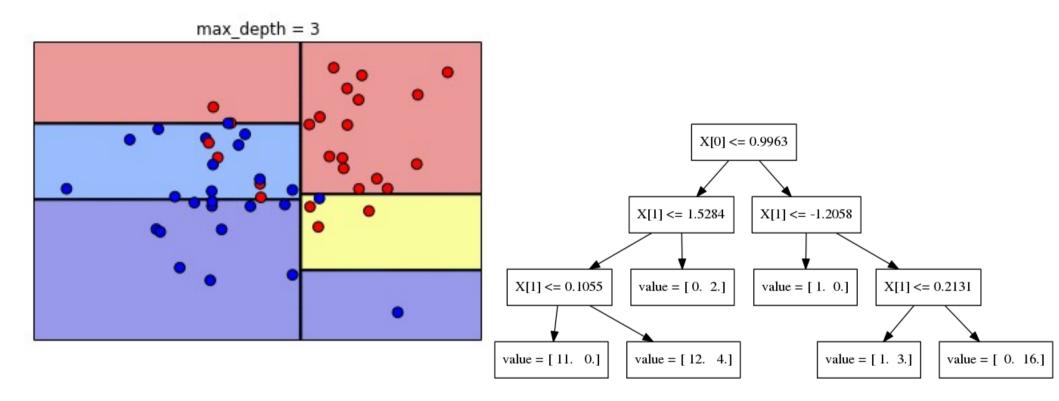


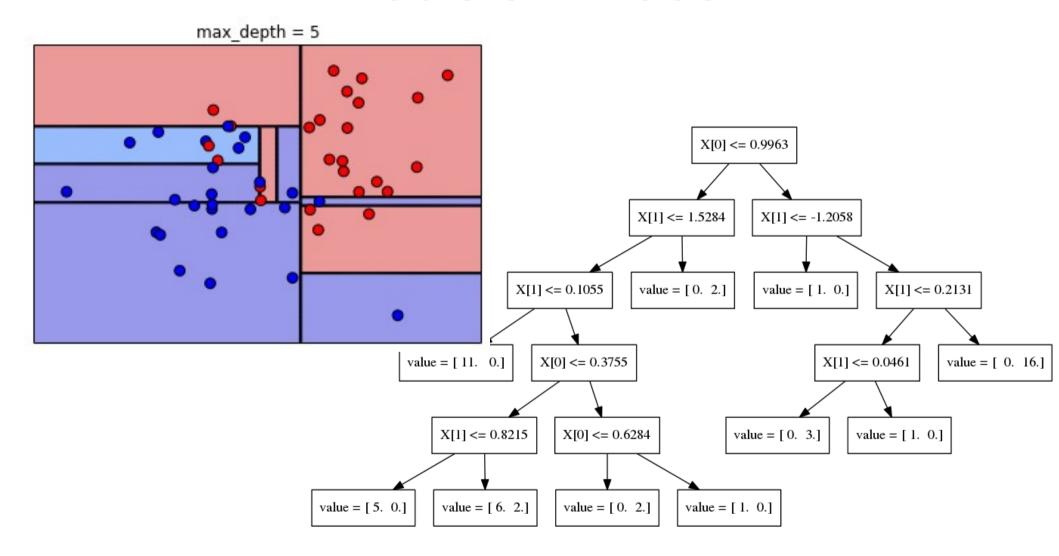


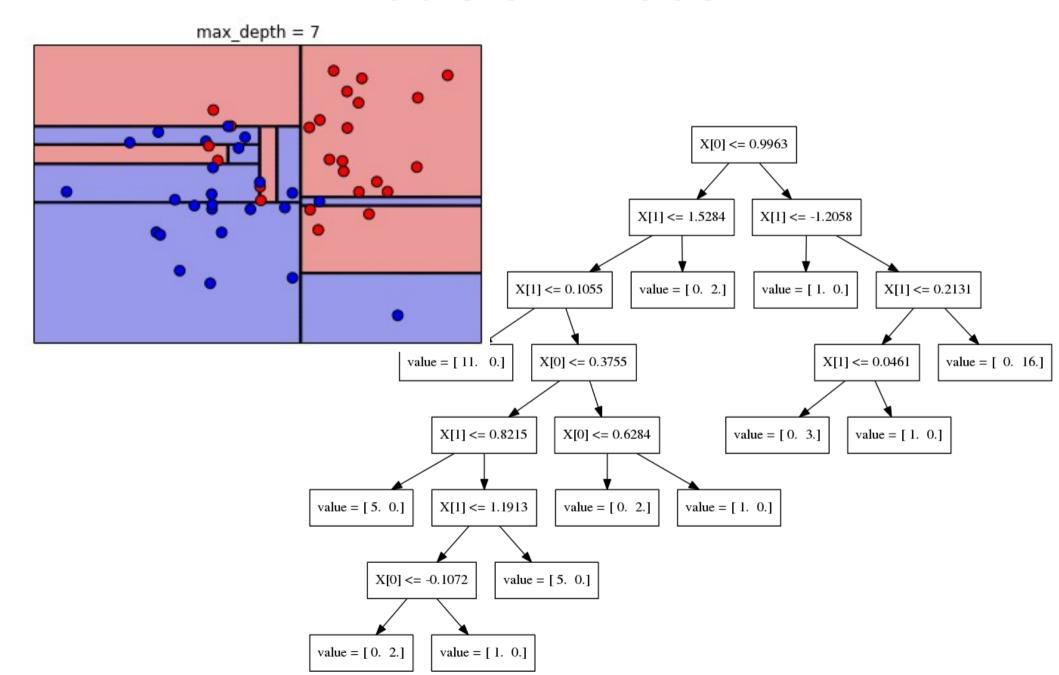




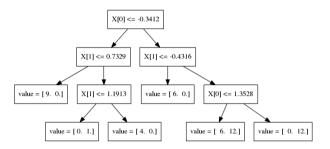




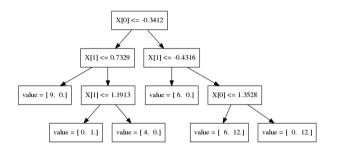


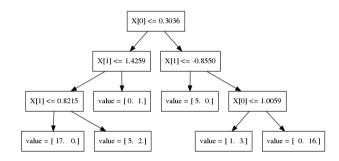


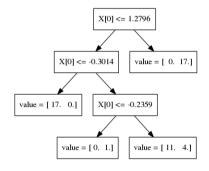
#### Random Forests



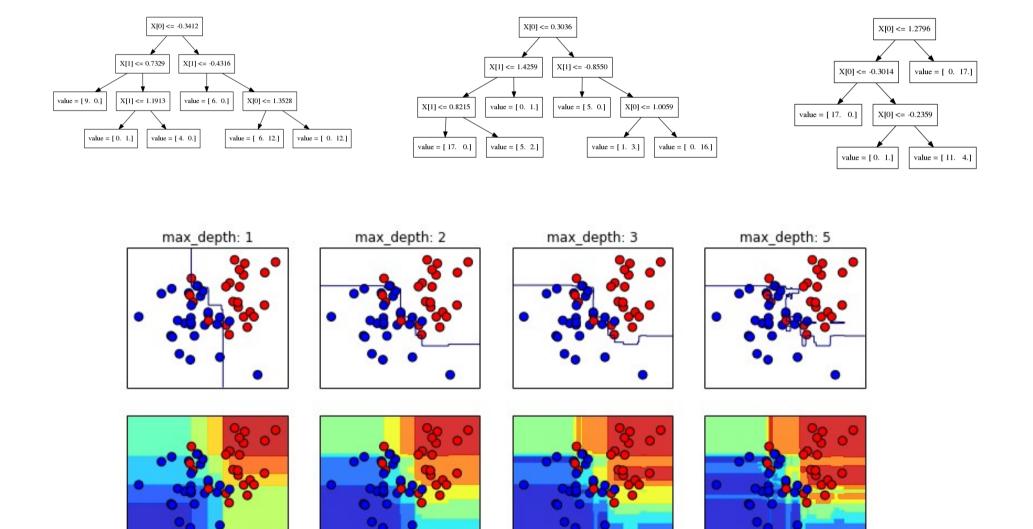
#### Random Forests



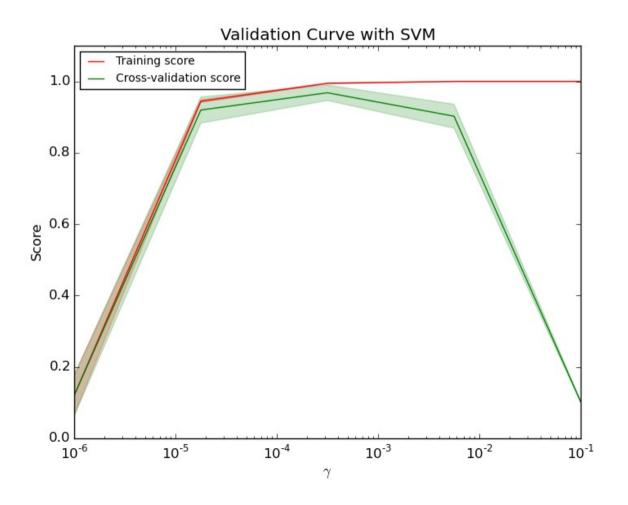




#### Random Forests



#### Validation Curves



## Scaling Up

## Three regimes of data

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

### Three regimes of data

- Fits in RAM (up to 256 GB?)
- Fits on a Hard Drive (up to 6TB?)
- Doesn't fit on a single PC

#### Nobody ever got fired for using Hadoop on a cluster

Antony Rowstron, Dushyanth Narayanan, Austin Donnelly, Greg O'Shea, and Andrew Douglas 10 April 2012

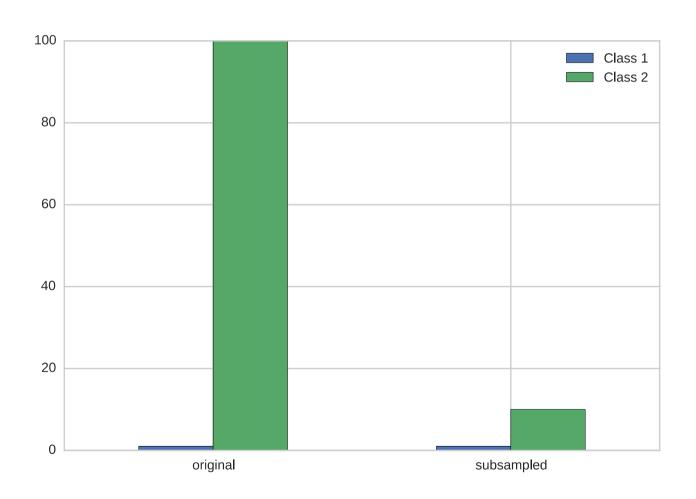
	vCPU	ECU	Memory (GiB)	Instance Storage (GB)	Linux/UNIX Usage
Memory Optimiz	zed - Current (	Generation			
r3.large	2	6.5	15	1 x 32 SSD	\$0.195 per Hour
r3.xlarge	4	13	30.5	1 x 80 SSD	\$0.39 per Hour
r3.2xlarge	8	26	61	1 x 160 SSD	\$0.78 per Hour
r3.4xlarge	16	52	122	1 x 320 SSD	\$1.56 per Hour
r3.8xlarge	32	104	244	2 x 320 SSD	\$3.12 per Hour
Storage Optimiz	zed - Current G	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

"256Gb ought to be enough for anybody." - me

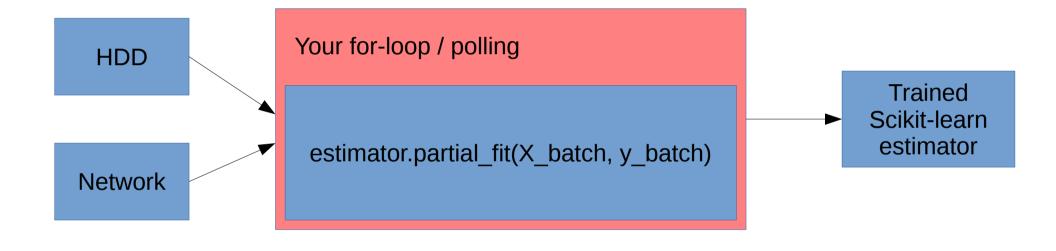
## "256Gb ought to be enough for anybody." - me

(for machine learning)

## Subsample!



#### The scikit-learn way



## Supported Algorithms

- All SGDClassifier derivatives
- Naive Bayes
- MinibatchKMeans
- Birch
- IncrementalPCA
- MiniBatchDictionaryLearning

#### IPython Notebook: Part 8 – Out Of Core Learning

#### Stateless Transformers

- Normalizer
- HashingVectorizer
- RBFSampler (and other kernel approx)

## 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]
```

## Hashing Trick

HashingVectorizer

```
"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
      aardvak ants
                        get
                             you zyxst
        [0, ..., 0, 1, 0, ..., 0, 1, 0, ..., 0, 1, 0, ..., 0]
```

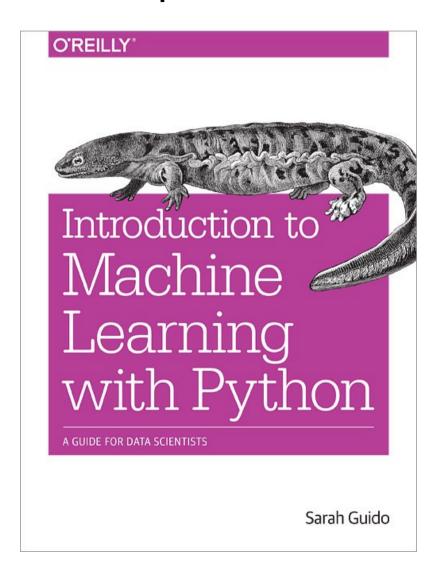
#### IPython Notebook: Part 9 – Out Of Core Learning for Text

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#### Thank you for your attention.



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