Features

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Learning Objectives

- Understand where a feature map sits in a machine learning pipeline.
- Understand that featurization/featuring mapping is inherently required to allow predictors to ingest many types of data.
- Understand how feature extraction can be used to extend the power of linear methods.
- Build pipelines with expanded feature spaces using the sklearn ecosystem.



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- \bullet Our general learning theory setup: no assumptions about ${\mathcal X}$
- But $\mathfrak{X} = \mathbf{R}^d$ for the specific methods we've developed:
 - Ridge regression
 - Lasso regression
 - Linear SVM

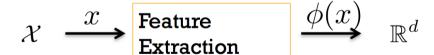
Feature Extraction

Definition

Mapping an input from \mathfrak{X} to a vector in \mathbb{R}^d is called **feature extraction** or **featurization**.

Raw Input

Feature Vector



- Two motivations for thinking about feature extraction:
 - Motivation 1 consuming inputs that are not natively in \mathbb{R}^d examples?

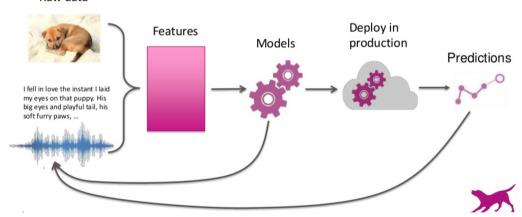
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 - Text documents
 - Image files
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 - DNA sequences
 - But everything in a computer is a sequence of numbers?
 - The *i*th entry of each sequence should have the same "meaning"
 - All the sequences should have the same length

The machine learning pipeline

Raw data



https://www.slideshare.net/AliceZheng3/understanding-feature-space-in-machine-learning

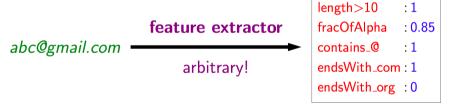


Example: Detecting Email Addresses

• Task: Predict whether a string is an email address

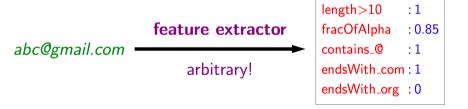
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- Task: Predict whether a string is an email address
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- But this was ad-hoc, and maybe we missed something.
- Could be more systematic?

From Percy Liang's "Lecture 3" slides from Stanford's CS221, Autumn 2014.

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Feature Templates

- Length greater than ____
- Last three characters equal ____
- Contains character ____

Feature Template: Last Three Characters Equal _ _ _

- Don't think about which 3-letter suffixes are meaningful...
- Just include them all.

Feature Template: Last Three Characters Equal

- Don't think about which 3-letter suffixes are meaningful...
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abc@gmail.com ----

endsWith_aaa : 0
endsWith_aab : 0
endsWith_aac : 0
...
endsWith_com : 1
...
endsWith_zzz : 0

From Percy Liang's "Lecture 3" slides from Stanford's CS221, Autumn 2014.

Feature Template: Last Three Characters Equal

- Don't think about which 3-letter suffixes are meaningful...
- Just include them all.

endsWith_aab: 0 endsWith aac : 0 abc@gmail.com endsWith.com:1 endsWith zzz : 0

• With regularization, our methods will not be overwhelmed.

endsWith_aaa : 0

```
fracOfAlpha: 0.85 contains_a : 0 ... contains_@ : 1 ...
```

Array representation (good for dense features):

Map representation (good for sparse features):

```
{"fracOfAlpha": 0.85, "contains_0": 1}
```

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- On "example string" we'd get {"endsWith_ing": 1}.
- Has overhead compared to arrays, so much slower for dense features.
- Question: if we have a sparse feature vector, what are the implications for preprocessing?

Feature Map – ingesting inputs not natively in \mathbb{R}^d

Example: Classifying documents from 20 newsgroups

• Context: The newsgroups dataset comprises around 18000 newsgroups posts on 20 topics.

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- Context: The newsgroups dataset comprises around 18000 newsgroups posts on 20 topics.
- We'll restrict ourselves to classifying posts within 4 topics:
 - 'alt.atheism'
 - 'soc.religion.christian'
 - 'comp.graphics'
 - 'sci.med'.
- Thanks to the sklearn team for this worked example (at http://scikit-learn.org/stable/tutorial/text_analytics/working_with_text_data.html).

Example Document:

```
From: sd345@citv.ac.uk (Michael Collier)
Subject: Converting images to HP LaserJet III?
Nntp-Posting-Host: hampton
Organization: The City University
Lines: 14
Does anyone know of a good way (standard PC application/PD utility) to
convert tif/img/tga files into LaserJet III format. We would also like to
do the same, converting to HPGL (HP plotter) files.
Please email any response.
Is this the correct group?
Thanks in advance. Michael.
Michael Collier (Programmer)
                                             The Computer Unit,
Email: M.P.Collier@uk.ac.city
                                             The City University,
Tel: 071 477-8000 x3769
                                             London,
```

EC1V OHB.

Fax: 071 477-8565

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17 / 61

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- What feature maps could we apply over these sorts of documents?
- A simple approach bag-of-words (BOW).
 - Assign a fixed integer id to each word occurring in any document of the training set.
 - For each document i, count the number of occurrences of each word w and store it (sparsely) as $doc_i[w] = j_w ==$ count of word w in document i.
 - The BOW representation implies that $n_{features}$ is the number of distinct words in the corpus.
 - What is the feature map $\phi(x)$?

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Here's the classifier we'll fit (note we're adding the TfidfTransformer to scale by inverse
document frequency, since it improves performance on this task – if you're not familiar
with TF-IDF see the docs).

• Which named steps in this Pipeline comprise our feature map ϕ ?

soc.religion.christian

avg / total

```
predicted = text_clf.predict(docs_test)
np.mean(predicted == twenty test.target)
0.9127829560585885
from sklearn import metrics
print(metrics.classification_report(twenty_test.target, predicted,
      target names=twenty test.target names))
                        precision
                                     recall
                                              f1-score
                                                         support
           alt.atheism
                                                  0.87
                             0.95
                                        0.81
                                                             319
         comp.graphics
                             0.88
                                        0.97
                                                  0.92
                                                             389
               sci.med
                             0.94
                                        0.90
                                                  0.92
                                                             396
```

• Key takeaway: need feature map ϕ when dealing with inputs not natively in \mathbb{R}^d .

0.90

0.92

0.95

0.91

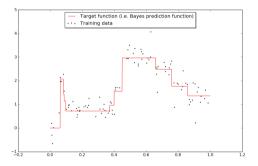
0.93

0.91

398

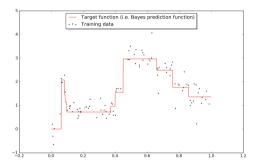
1502

- Two motivations for thinking about feature extraction:
 - Motive 2 Improving performance. Think about HW2.



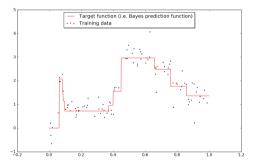
• What was our feature map $\phi(x)$? $\phi(x) \in \mathbb{R}^k$ for what k?

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- What was our feature map $\phi(x)$? $\phi(x) \in \mathbb{R}^k$ for what k?
- $\phi(x) = \left[\mathbb{1}(x \geqslant \frac{1}{400}), \dots, \mathbb{1}(x \geqslant \frac{399}{400}) \right]$

- Two motivations for thinking about feature extraction:
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• Why did we use this feature map instead of just learning a prediction function $y \sim x$?

- Two motivations for thinking about feature extraction:
 - Motive 2 Improving performance. Toy Example:

```
Boston House Prices dataset
Notes
Data Set Characteristics:
    :Number of Instances: 506
    :Number of Attributes: 13 numeric/categorical predictive
    :Median Value (attribute 14) is usually the target
```

- Two motivations for thinking about feature extraction:
 - Motive 2 Improving performance. Toy Example:

```
from sklearn.linear_model import ElasticNetCV
en = ElasticNetCV(cv = 5)

en.fit(np.log(train_X[['LSTAT']]), train_y)
en.score(np.log(test_X[['LSTAT']]), test_y)
0.74651286928253746

en.fit(train_X[['LSTAT']], train_y)
en.score(test_X[['LSTAT']], test_y)
0.57894475666257272
```

See https://github.com/davidrosenberg/mlcourse/blob/gh-pages/Notebooks/Features/simple_feature_transformations.ipynb

- We'll be looking at regression examples throughout this lab.
- Using Elastic Net in sklearn, the default score method returns the coefficient of determination R^2 of the prediction.
- Recall:

The total sum of squares (proportional to the variance of the data):

$$SS_{
m tot} = \sum_i (y_i - ar{y})^2,$$

• The regression sum of squares, also called the explained sum of squares:

$$SS_{ ext{reg}} = \sum_i (f_i - ar{y})^2,$$

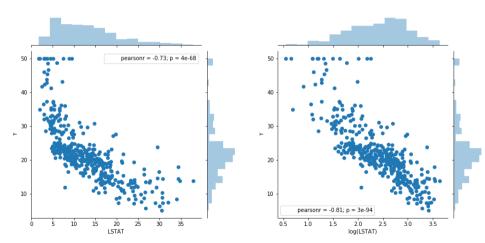
• The sum of squares of residuals, also called the residual sum of squares:

$$SS_{ ext{res}} = \sum_i (y_i - f_i)^2 = \sum_i e_i^2$$

The most general definition of the coefficient of determination is

$$R^2 \equiv 1 - rac{SS_{
m res}}{SS_{
m tot}}.$$

• Key idea: instead of using more flexible (i.e. non-linear) models, build better features.



Handling Nonlinearity with Linear Methods

Example Task: Predicting Health

• General Philosophy: Extract every feature that might be relevant

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- General Philosophy: Extract every feature that might be relevant
- Features for medical diagnosis
 - height
 - weight
 - body temperature
 - blood pressure
 - etc...

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- For linear predictors, it's important how features are added
- Three types of nonlinearities can cause problems:
 - Non-monotonicity
 - Saturation
 - Interactions between features

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- Feature Map: $\phi(x) = [1, temperature(x)]$
- Action: Predict health score $y \in \mathbf{R}$ (positive is good)
- Hypothesis Space $\mathcal{F} = \{affine \text{ functions of temperature}\}$
- Issue:
 - Health is not an affine function of temperature.
- Affine function can either say
 - Very high is bad and very low is good, or
 - Very low is bad and very high is good,
 - But here, both extremes are bad.

• Transform the input:

$$\phi(x) = \left[1, \{\text{temperature}(x) - 37\}^2\right],$$

where 37 is "normal" temperature in Celsius.

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- Ok, but this requires domain knowledge
 - Do we really need that?

• Think less, put in more:

$$\phi(x) = \left[1, \text{temperature}(x), \{\text{temperature}(x)\}^2\right].$$

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General Rule

Features should be simple building blocks that can be pieced together.

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• We expect a monotonic relationship between N(x) and relevance, but...

Is relevance linear in N(x)?

- Relevance score reflects confidence in relevance prediction.
- Are we 10 times more confident if N(x) = 1000 vs N(x) = 100?

Saturation: The Issue

Is relevance linear in N(x)?

- Relevance score reflects confidence in relevance prediction.
- Are we 10 times more confident if N(x) = 1000 vs N(x) = 100?
- Bigger is better... but not that much better.

Saturation: Solve with nonlinear transform

• Smooth nonlinear transformation:

$$\phi(x) = [1, \log\{1 + N(x)\}]$$

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• Smooth nonlinear transformation:

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- ullet log (\cdot) good for values with large dynamic ranges
- Does it matter what base we use in the log?

• Discretization (a discontinuous transformation):

$$\phi(x) = (1(5 \leqslant N(x) < 10), 1(10 \leqslant N(x) < 100), 1(100 \leqslant N(x)))$$

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- Why? Hint: What's the effect of regularization on the parameters for rare buckets?
- Small buckets allow quite flexible relationship

Interactions: The Issue

- Input: Patient information x
- Action: Health score $y \in \mathbb{R}$ (higher is better)
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$$\phi(x) = [\mathsf{height}(x), \mathsf{weight}(x)]$$

- Issue: It's the weight relative to the height that's important.
- Impossible to get with these features and a linear classifier.
- Need some interaction between height and weight.

• Google "ideal weight from height"

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- J. D. Robinson's "ideal weight" formula (for a male):

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$$f(x) = (52 + 1.9 [h(x) - 60] - w(x))^{2}$$

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WolframAlpha for complicated Mathematics:

$$f(x) = 3.61h(x)^2 - 3.8h(x)w(x) - 235.6h(x) + w(x)^2 + 124w(x) + 3844$$

Just include all second order features:

$$\phi(x) = \left[1, h(x), w(x), h(x)^2, w(x)^2, \underbrace{h(x)w(x)}_{\text{cross term}}\right]$$

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General Principle

Simpler building blocks replace a single "smart" feature.

Predicate Features and Interaction Terms

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- Many features take this form:
 - $x \mapsto s(x) = 1$ (subject is sleeping)
 - $x \mapsto d(x) = 1$ (subject is driving)
- For predicates, interaction terms correspond to AND conjunctions:
 - $x \mapsto s(x)d(x) = 1$ (subject is sleeping AND subject is driving)

- Non-linear feature map $\phi: \mathcal{X} \to \mathbf{R}^d$
- Hypothesis space:

$$\mathcal{F} = \left\{ f(x) = w^T \varphi(x) \mid w \in \mathbf{R}^d \right\}.$$

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• Linear in w? Yes.

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- Linear in $\phi(x)$? Yes.

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$$\mathcal{F} = \left\{ f(x) = w^T \phi(x) \mid w \in \mathbf{R}^d \right\}.$$

- Linear in w? Yes.
- Linear in $\phi(x)$? Yes.
- Linear in x? No.
 - ullet Linearity not even defined unless ${\mathcal X}$ is a vector space

Key Idea: Non-Linearity

• Nonlinear f(x) is important for expressivity.

- Non-linear feature map $\phi: \mathcal{X} \to \mathbf{R}^d$
- Hypothesis space:

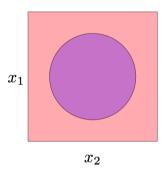
$$\mathcal{F} = \left\{ f(x) = w^T \varphi(x) \mid w \in \mathbb{R}^d \right\}.$$

- Linear in w? Yes.
- Linear in $\phi(x)$? Yes.
- Linear in x? No.
 - ullet Linearity not even defined unless ${\mathcal X}$ is a vector space

Key Idea: Non-Linearity

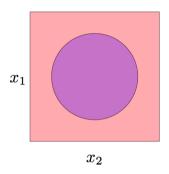
- Nonlinear f(x) is important for **expressivity**.
- f(x) linear in w and $\phi(x)$: makes finding $f^*(x)$ much easier

Geometric Example: Two class problem, nonlinear boundary



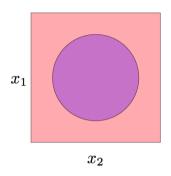
• With linear feature map $\phi(x) = (x_1, x_2)$ and linear models, no hope

Geometric Example: Two class problem, nonlinear boundary



- With linear feature map $\phi(x) = (x_1, x_2)$ and linear models, no hope
- With appropriate nonlinearity $\phi(x) = (x_1, x_2, x_1^2 + x_2^2)$, piece of cake.

Geometric Example: Two class problem, nonlinear boundary



- With linear feature map $\phi(x) = (x_1, x_2)$ and linear models, no hope
- With appropriate nonlinearity $\phi(x) = (x_1, x_2, x_1^2 + x_2^2)$, piece of cake.
- Video: http://youtu.be/3liCbRZPrZA

Expressivity of Hypothesis Space

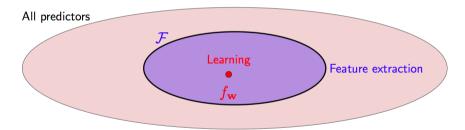
• Consider a linear hypothesis space with a feature map $\phi: \mathfrak{X} \to \mathsf{R}^d$:

$$\mathcal{F} = \left\{ f(x) = w^T \phi(x) \right\}$$

Expressivity of Hypothesis Space

• Consider a linear hypothesis space with a feature map $\phi: \mathfrak{X} \to \mathsf{R}^d$:

$$\mathcal{F} = \left\{ f(x) = w^T \phi(x) \right\}$$



Question: does \mathcal{F} contain a good predictor?

We can grow the linear hypothesis space $\mathcal F$ by adding more features.

Example 1: Boston housing and Abalone

- Let's revisit the Boston housing dataset from the start of lab.
- We're going to be predicting the median house values in Boston suburbs.
- We'll build our feature map using sklearn and sklearn_pandas

```
import pandas as pd
import numpy as np
from sklearn.base import TransformerMixin
from sklearn.preprocessing import OneHotEncoder,LabelEncoder
from sklearn_pandas import DataFrameMapper
from sklearn.pipeline import Pipeline
from sklearn.linear_model import ElasticNetCV
from sklearn.model selection import train test split
from sklearn.preprocessing import PolynomialFeatures
import seaborn as sns
import matplotlib.pyplot as plt
%matplotlib inline
```

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• Set up data:

```
from sklearn.datasets import load_boston
data = load_boston()
df = data.data
cols = ['CRIM','ZN','INDUS','CHAS','NOX',
        'RM', 'AGE', 'DIS', 'RAD', 'TAX',
        'PTRATIO', 'B', 'LSTAT']
df = pd.DataFrame(df, columns=cols)
train_X, test_X, train_y, test_y = train_test_split(df, data.target,
                                                      test_size=0.2.
                                                      random_state = 2142018)
categorical = ['CHAS', 'RAD']
numeric = ['CRIM','ZN','INDUS','NOX','RM',
        'AGE', 'DIS', 'TAX', 'PTRATIO', 'B',
        'LSTAT']
```

See https://github.com/davidrosenberg/mlcourse/blob/gh-pages/Notebooks/Features/polynomial_feature_comparison.ipynb

• Feature map 1– looking at the code, what is the feature map ϕ_1 ?

```
mapper = DataFrameMapper(
    [(col, None) for col in numeric] + \
    [(col, OneHotStrings()) for col in categorical])
pipe = Pipeline([
    ('mapper', mapper),
    ('clf', ElasticNetCV(cv=10,
                         l1_ratio=[.5, .7, .9, .95, .99, 1],
                         normalize=True))
1)
pipe.fit(train X. train v)
print('Train score: ',pipe.score(train_X, train_y))
print('Test score: '.pipe.score(test X, test v))
Train score: 0.762945577283
```

Test score: 0.645054949322

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• Feature map 1– looking at the code, what is the feature map ϕ_1 ?

```
mapper = DataFrameMapper(
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Train score: 0.762945577283
```

Test score: 0.645054949322

• $\phi_1(X)$ dummy encodes categoricals and passes numeric features untouched.

Boston Housing

• Feature map 2– looking at the code, what is the feature map ϕ_2 ?

```
mapper2 = DataFrameMapper(
    [(numeric, PolynomialFeatures(degree=2))] + \
    [(col, OneHotStrings()) for col in categorical])
pipe2 = Pipeline([
    ('mapper', mapper2),
    ('clf', ElasticNetCV(cv=10,
                         l1_ratio=[.1, .5, .7, .9, .95, .99, 1],
                         normalize=True))
1)
pipe2.fit(train_X, train v)
print('Train score: ',pipe2.score(train_X, train_y))
print('Test score: '.pipe2.score(test X, test v))
```

Train score: 0.879364391327 Test score: 0.816386882677

Boston Housing

• Feature map 2– looking at the code, what is the feature map ϕ_2 ?

```
mapper2 = DataFrameMapper(
    [(numeric, PolynomialFeatures(degree=2))] + \
    [(col, OneHotStrings()) for col in categorical])
pipe2 = Pipeline([
    ('mapper', mapper2),
    ('clf', ElasticNetCV(cv=10,
                         l1_ratio=[.1, .5, .7, .9, .95, .99, 1],
                         normalize=True))
1)
pipe2.fit(train X, train v)
print('Train score: ',pipe2.score(train_X, train_y))
print('Test score: '.pipe2.score(test X, test v))
Train score: 0.879364391327
Test score: 0.816386882677
```

• $\phi_2(X)$ dummy encodes categoricals and maps numeric features to polynomial features of degree $d \leq 2$.

Abalone

- Here we are using the abalone dataset predicting the number of rings on an abalone (a kind of shellfish).
- Set up data:

```
df = pd.read csv('http://archive.ics.uci.edu/ml/machine-learning-databases/' +
                 'abalone/abalone.data'.
                 header=None)
df = df.rename(columns={
    0: 'sex', 1: 'length', 2: 'diameter', 3: 'height',
    4: 'whole_weight', 5: 'shucked_weight', 6: 'viscera_weight',
    7: 'shell weight', 8: 'rings'
1)
categorical = ['sex']
numeric = ['length', 'diameter', 'height',
        'whole weight', 'shucked weight',
        'shell weight'l
train_X, test_X, train_y, test_y = train_test_split(df.drop('rings', axis=1),
                                                     df['rings'].
                                                      random state=42)
```

See https://github.com/davidrosenberg/mlcourse/blob/gh-pages/Notebooks/Features/polynomial_feature_comparison.ipynb

Abalone

 \bullet $\phi_1(X)$ dummy encodes categoricals and passes numeric features untouched.

```
mapper = DataFrameMapper(
    [(col, None) for col in numeric] + \
    [(col. OneHotStrings()) for col in categorical])
pipe = Pipeline([
    ('mapper', mapper),
    ('clf', ElasticNetCV(cv=10.
                         l1_ratio=[.1, .5, .7, .9, .95, .99, 1].
                         normalize=True))
pipe.fit(train X, train v)
print('Train score: ',pipe.score(train_X, train_y))
print('Test score: '.pipe.score(test X, test v))
Train score: 0.528393673016
Test score: 0.534127249172
```

Abalone

• $\phi_2(X)$ dummy encodes categoricals and maps numeric features to polynomial features of degree $d \leq 2$.

```
poly_mapper = DataFrameMapper(
    [(numeric, PolynomialFeatures(degree=2))] + \
    [(col, OneHotStrings()) for col in categorical])
pipe_poly = Pipeline([
    ('mapper', poly_mapper),
    ('clf', ElasticNetCV(cv=10.
                         l1_ratio=[.1, .5, .7, .9, .95, .99, 1],
                         normalize=True))
pipe_poly.fit(train_X, train_y)
print('Train score: ',pipe_poly.score(train_X, train_y))
print('Test score: '.pipe_poly.score(test_X, test_y))
Train score: 0.559442492704
Test score: 0.554318625419
```

• Why did the performance improve much more for the Boston Housing dataset versus the Abalone dataset when we used map 2?

• Why did the performance improve much more for the Boston Housing dataset versus the Abalone dataset when we used map 2?

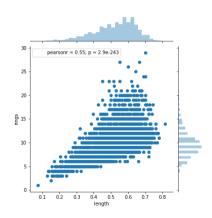
 What is the Bayes prediction function for square loss?

• Why did the performance improve much more for the Boston Housing dataset versus the Abalone dataset when we used map 2?

- What is the Bayes prediction function for square loss?
- If E[Y|X] is linear in $\phi_1(X)$, will we improve performance using $\phi_2(X)$?

• Why did the performance improve much more for the Boston Housing dataset versus the Abalone dataset when we used map 2?

- What is the Bayes prediction function for square loss?
- If E[Y|X] is linear in $\phi_1(X)$, will we improve performance using $\phi_2(X)$?
- Do we typically know in advance the structure of E[Y|X]?



Example 2: Two moons data



- From Alice Zheng and Amanda Casari's Feature Engineering for Machine Learning.
- What feature maps might be helpful for this problem?

See https://github.com/davidrosenberg/mlcourse/blob/gh-pages/Notebooks/Features/vector_quantization.ipynb



- From Alice Zheng and Amanda Casari's Feature Engineering for Machine Learning.
- What feature maps might be helpful for this problem?
- We'll try binning data instances using k-means let's look at the transformers (in notebook).

 $\textbf{See} \ \texttt{https://github.com/davidrosenberg/mlcourse/blob/gh-pages/Notebooks/Features/vector_quantization.ipynbulker.} \\$

- Here's the pipeline. First, notice the sklearn class FeatureUnion, which let's us easily apply multiple feature maps over an input array.
- What is the feature map $\phi(X)$? What will transformed.shape[1] equal?

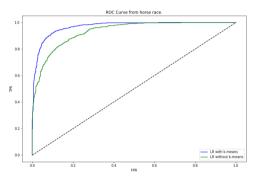
```
pipe = Pipeline([
    ('feats'.FeatureUnion([
        ('kmeans', KMeansFeaturizer(k=100,random_state=2052018)),
        ('ID', IdentityFeaturizer())
   1)),
   ('clf', LogisticRegressionCV())
pipe.fit(training_data, training_labels)
# Just to make sure it's clear what this does:
transformed = pipe.named steps['feats'].transform(training data)
transformed.shape
```

- Here's the pipeline. First, notice the sklearn class FeatureUnion, which let's us easily apply multiple feature maps over an input array.
- What is the feature map $\phi(X)$? What will transformed.shape[1] equal?

• $\phi(X) = [X_1, X_2, \mathbb{1}[(X_1, X_2) \text{ binned to centroid } 1], \dots, \mathbb{1}[(X_1, X_2) \text{ binned to centroid } 100]]$

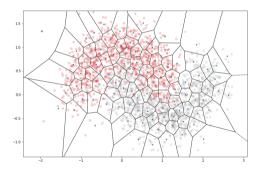
- Here's the pipeline. First, notice the sklearn class FeatureUnion, which let's us easily apply multiple feature maps over an input array.
- What is the feature map $\phi(X)$? What will transformed.shape[1] equal?

• Let's fit this pipe, and compare to a baseline logistic regression over just $\phi_I(X) = X$.

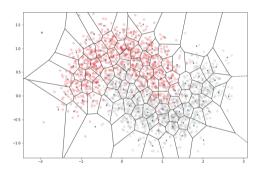


• We see performance improve.

• Here's the voronoi diagram after fitting the KMeansFeaturizer (fit in pipe.fit call).



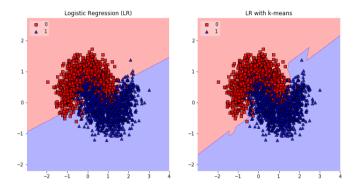
• Intuitively, why did this improve performance?



• Think back to the 1D discretization discussed earlier – which map is this analogous to?

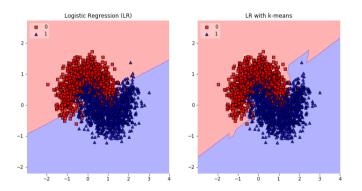
$$\begin{aligned} \Phi_2(x) &= (1(5 \leqslant N(x) < 10), 1(10 \leqslant N(x) < 100), 1(100 \leqslant N(x))) \\ \Phi_1(x) &= (1(5 \leqslant N(x)), 1(10 \leqslant N(x)), 1(100 \leqslant N(x))) \end{aligned}$$

• Here's a comparison of decision boundaries (note made using mlexend).

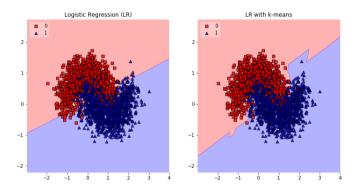


• What's with the plotted decision boundaries? I thought logistic regression was linear?

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• What's with the plotted decision boundaries? I thought logistic regression was linear?



Both decision boundaries are affine, but with k-means embedding it's affine in R^{102} .

Learning Objectives

- Understand where a feature map sits in a machine learning pipeline.
- Understand that featurization/featuring mapping is inherently required to allow predictors to ingest many types of data.
- Understand how feature extraction can be used to extend the power of linear methods.
- Build pipelines with expanded feature spaces using the sklearn ecosystem.