### **Features**

David S. Rosenberg and Ben Jakubowski

NYU

October 18, 2017

## 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.



## The Input Space $\mathfrak X$

 $\bullet$  Our general learning theory setup: no assumptions about  ${\mathcal X}$ 

## The Input Space $\mathfrak X$

- ullet Our general learning theory setup: no assumptions about  ${\mathfrak X}$
- But  $\mathfrak{X} = \mathbf{R}^d$  for the specific methods we've developed:

## The Input Space $\mathfrak X$

- $\bullet$  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

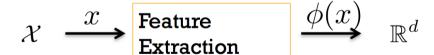
#### Feature Extraction

#### 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?

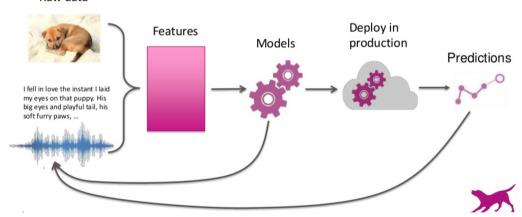
- Two motivations for thinking about feature extraction:
  - Motivation 1 consuming inputs that are not natively in  $\mathbb{R}^d$  examples?
    - Text documents
    - Image files
    - Sound recordings
    - DNA sequences

- Two motivations for thinking about feature extraction:
  - Motivation 1 consuming inputs that are not natively in  $\mathbb{R}^d$  examples?
    - Text documents
    - Image files
    - Sound recordings
    - DNA sequences
  - But everything in a computer is a sequence of numbers?

- Two motivations for thinking about feature extraction:
  - Motivation 1 consuming inputs that are not natively in  $\mathbf{R}^d$  examples?
    - Text documents
    - Image files
    - Sound recordings
    - 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

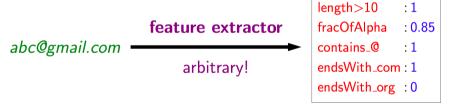


## Example: Detecting Email Addresses

• Task: Predict whether a string is an email address

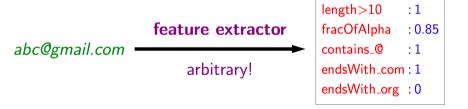
## Example: Detecting Email Addresses

- Task: Predict whether a string is an email address
- Could use domain knowledge and write down:



## Example: Detecting Email Addresses

- Task: Predict whether a string is an email address
- Could use domain knowledge and write down:



- 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.

#### Definition (informal)

A feature template is a group of features all computed in a similar way.

### Definition (informal)

A feature template is a group of features all computed in a similar way.

• Input: abc@gmail.com

### Definition (informal)

A feature template is a group of features all computed in a similar way.

• Input: abc@gmail.com

#### Feature Templates

Length greater than \_ \_ \_

### Definition (informal)

A feature template is a group of features all computed in a similar way.

• Input: abc@gmail.com

#### Feature Templates

- Length greater than \_\_\_\_
- Last three characters equal \_\_\_\_

### Definition (informal)

A feature template is a group of features all computed in a similar way.

• Input: abc@gmail.com

#### 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...
- Just include them all.

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}
```

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

- Arrays
  - assumed fixed ordering of the features

- Arrays
  - assumed fixed ordering of the features
  - appropriate when significant number of nonzero elements ("dense feature vectors")

- Arrays
  - assumed fixed ordering of the features
  - appropriate when significant number of nonzero elements ("dense feature vectors")
  - very efficient in space and speed (and you can take advantage of GPUs)

- Arrays
  - assumed fixed ordering of the features
  - appropriate when significant number of nonzero elements ("dense feature vectors")
  - very efficient in space and speed (and you can take advantage of GPUs)
- Map (a "dict" in Python)
  - best for sparse feature vectors (i.e. few nonzero features)

- Arrays
  - assumed fixed ordering of the features
  - appropriate when significant number of nonzero elements ("dense feature vectors")
  - very efficient in space and speed (and you can take advantage of GPUs)
- Map (a "dict" in Python)
  - best for sparse feature vectors (i.e. few nonzero features)
  - features not in the map have default value of zero

- Arrays
  - assumed fixed ordering of the features
  - appropriate when significant number of nonzero elements ("dense feature vectors")
  - very efficient in space and speed (and you can take advantage of GPUs)
- Map (a "dict" in Python)
  - best for sparse feature vectors (i.e. few nonzero features)
  - features not in the map have default value of zero
  - Python code for "ends with last 3 characters":

```
{\text{"endsWith}_{-} + x[-3:]: 1}.
```

- Arrays
  - assumed fixed ordering of the features
  - appropriate when significant number of nonzero elements ("dense feature vectors")
  - very efficient in space and speed (and you can take advantage of GPUs)
- Map (a "dict" in Python)
  - best for sparse feature vectors (i.e. few nonzero features)
  - features not in the map have default value of zero
  - Python code for "ends with last 3 characters":

```
{\text{"endsWith}_{-}} + x[-3:]: 1.
```

• On "example string" we'd get {"endsWith\_ing": 1}.

- Arrays
  - assumed fixed ordering of the features
  - appropriate when significant number of nonzero elements ("dense feature vectors")
  - very efficient in space and speed (and you can take advantage of GPUs)
- Map (a "dict" in Python)
  - best for sparse feature vectors (i.e. few nonzero features)
  - features not in the map have default value of zero
  - Python code for "ends with last 3 characters":

```
{\text{"endsWith}_{-}} + x[-3:]: 1.
```

- 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.

## Example: Classifying documents from 20 newsgroups

- 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

```
From: sd345@city.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.

• What feature maps could we apply over these sorts of documents?

17 / 61

```
From: sd345@city.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.
```

- 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  $\phi(x)$ ?

Please email any response.

```
From: sd345@city.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.
```

- 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  $\phi(x)$ ?

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  $\phi$ ?

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  $\phi$  when dealing with inputs not natively in  $\mathbb{R}^d$ .

0.90

0.92

0.95

0.91

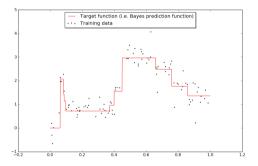
0.93

0.91

398

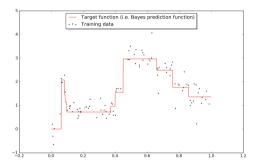
1502

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



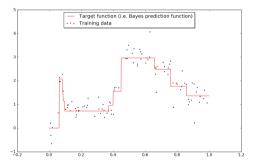
• What was our feature map  $\phi(x)$ ?  $\phi(x) \in \mathbb{R}^k$  for what k?

- 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?
- $\phi(x) = \left[ \mathbb{1}(x \geqslant \frac{1}{400}), \dots, \mathbb{1}(x \geqslant \frac{399}{400}) \right]$

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



• 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)
```

David S. Rosenberg and Ben Jakubowski (NYU)

0.57894475666257272

- 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:

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

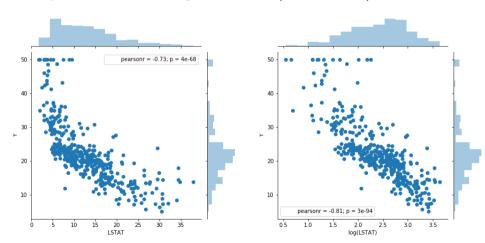
• The sum of squares of residuals, also called the residual sum of squares:

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

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

# Example Task: Predicting Health

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

### Issues for Linear Predictors

• For linear predictors, it's important how features are added

### Issues for Linear Predictors

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

### Issues for Linear Predictors

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

• Feature Map:  $\phi(x) = [1, temperature(x)]$ 

- Feature Map:  $\phi(x) = [1, temperature(x)]$
- Action: Predict health score  $y \in \mathbf{R}$  (positive is good)

- Feature Map:  $\phi(x) = [1, temperature(x)]$
- Action: Predict health score  $y \in \mathbf{R}$  (positive is good)
- $\bullet \ \, \mathsf{Hypothesis} \ \mathsf{Space} \ \mathcal{F} \! = \! \{ \mathsf{affine} \ \mathsf{functions} \ \mathsf{of} \ \mathsf{temperature} \}$

- Feature Map:  $\phi(x) = [1, temperature(x)]$
- Action: Predict health score  $y \in \mathbf{R}$  (positive is good)
- $\bullet \ \ \mbox{Hypothesis Space } {\mathfrak F} \, = \, \{\mbox{affine functions of temperature}\}$
- Issue:

- Feature Map:  $\phi(x) = [1, temperature(x)]$
- Action: Predict health score  $y \in \mathbf{R}$  (positive is good)
- $\bullet \ \, \mathsf{Hypothesis} \ \mathsf{Space} \ \mathcal{F} \! = \! \{ \mathsf{affine} \ \mathsf{functions} \ \mathsf{of} \ \mathsf{temperature} \}$
- Issue:
  - Health is not an affine function of temperature.

- Feature Map:  $\Phi(x) = [1, \text{temperature}(x)]$
- Action: Predict health score  $y \in \mathbb{R}$  (positive is good)
- Hypothesis Space  $\mathcal{F} = \{affine functions of temperature\}$
- 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.

29 / 61

• Transform the input:

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

where 37 is "normal" temperature in Celsius.

• Transform the input:

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

where 37 is "normal" temperature in Celsius.

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

• Think less, put in more:

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

• Think less, put in more:

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

• More expressive than Solution 1.

• Think less, put in more:

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

• More expressive than Solution 1.

#### General Rule

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

• Setting: Find products relevant to user's query

- Setting: Find products relevant to user's query
- Input: Product x
- Action: Score the relevance of x to user's query

- Setting: Find products relevant to user's query
- Input: Product x
- Action: Score the relevance of x to user's query
- Feature Map:

$$\phi(x) = [1, N(x)],$$

where N(x) = number of people who bought x.

- Setting: Find products relevant to user's query
- Input: Product x
- Action: Score the relevance of x to user's query
- Feature Map:

$$\phi(x) = [1, N(x)],$$

where N(x) = number of people who bought x.

• 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?

#### 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:

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

## Saturation: Solve with nonlinear transform

• Smooth nonlinear transformation:

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

ullet log  $(\cdot)$  good for values with large dynamic ranges

## Saturation: Solve with nonlinear transform

• Smooth nonlinear transformation:

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

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

• Discretization (a discontinuous transformation):

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

• Discretization (a discontinuous transformation):

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

Sometimes we might prefer one-sided buckets

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

Why?

• Discretization (a discontinuous transformation):

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

Sometimes we might prefer one-sided buckets

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

• Why? Hint: What's the effect of regularization on the parameters for rare buckets?

• Discretization (a discontinuous transformation):

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

Sometimes we might prefer one-sided buckets

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

- 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)
- Feature Map

$$\phi(x) = [\mathsf{height}(x), \mathsf{weight}(x)]$$

#### Interactions: The Issue

- Input: Patient information x
- Action: Health score  $y \in \mathbb{R}$  (higher is better)
- Feature Map

$$\phi(x) = [\mathsf{height}(x), \mathsf{weight}(x)]$$

• Issue: It's the weight relative to the height that's important.

#### Interactions: The Issue

- Input: Patient information x
- Action: Health score  $y \in \mathbf{R}$  (higher is better)
- Feature Map

$$\phi(x) = [\mathsf{height}(x), \mathsf{weight}(x)]$$

- 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"

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

$$\mathsf{weight}(\mathsf{kg}) = 52 + 1.9 \left[ \mathsf{height}(\mathsf{in}) - 60 \right]$$

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

$$\mathsf{weight}(\mathsf{kg}) = 52 + 1.9 \left[ \mathsf{height}(\mathsf{in}) - 60 \right]$$

• Make score square deviation between height(h) and ideal weight(w)

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

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

$$\mathsf{weight}(\mathsf{kg}) = 52 + 1.9 \left[ \mathsf{height}(\mathsf{in}) - 60 \right]$$

• Make score square deviation between height(h) and ideal weight(w)

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

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:

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

Just include all second order features:

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

• More flexible, no Google, no WolframAlpha.

Just include all second order features:

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

• More flexible, no Google, no WolframAlpha.

### General Principle

Simpler building blocks replace a single "smart" feature.

### Predicate Features and Interaction Terms

#### Definition

A **predicate** on the input space  $\mathcal{X}$  is a function  $P: \mathcal{X} \to \{\text{True}, \text{False}\}.$ 

### Predicate Features and Interaction Terms

#### **Definition**

A **predicate** on the input space  $\mathcal{X}$  is a function  $P: \mathcal{X} \to \{\text{True}, \text{False}\}.$ 

- Many features take this form:
  - $x \mapsto s(x) = 1$ (subject is sleeping)
  - $x \mapsto d(x) = 1$ (subject is driving)

### Predicate Features and Interaction Terms

#### Definition

A **predicate** on the input space  $\mathcal{X}$  is a function  $P: \mathcal{X} \to \{\text{True}, \text{False}\}.$ 

- 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:

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

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

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

• Linear in w? Yes.

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

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

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

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

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

- 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:

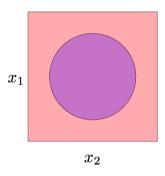
$$\mathcal{F} = \left\{ f(x) = w^T \varphi(x) \mid w \in \mathbb{R}^d \right\}.$$

- 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

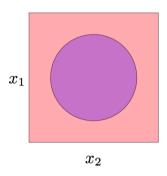
- Nonlinear f(x) is important for **expressivity**.
- f(x) linear in w and  $\varphi(x)$ : makes finding  $f^*(x)$  much easier

# Geometric Example: Two class problem, nonlinear boundary



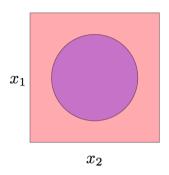
• With linear feature map  $\phi(x) = (x_1, x_2)$  and linear models, no hope

# 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

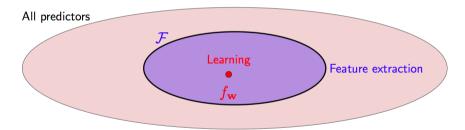
• Consider a linear hypothesis space with a feature map  $\phi: \mathfrak{X} \to \mathsf{R}^d$ :

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

# 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
```

#### 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']
```

45 / 61

• Feature map 1– looking at the code, what is the feature map  $\phi_1$ ?

```
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

46 / 61

• Feature map 1– looking at the code, what is the feature map  $\phi_1$ ?

```
mapper = DataFrameMapper(
    [(col, None) for col in numeric] + \
    [(col, OneHotStrings()) for col in categoricall)
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

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

• Feature map 2– looking at the code, what is the feature map  $\phi_2$ ?

```
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

47 / 61

## Boston Housing

• Feature map 2– looking at the code, what is the feature map  $\phi_2$ ?

```
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'
})
categorical = ['sex']
numeric = ['length', 'diameter', 'height',
        'whole_weight', 'shucked_weight',
        'shell_weight'l
train X, test X, train v, test v = train test split(df.drop('rings', axis=1),
                                                     df['rings'].
                                                     random state=42)
```

#### **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?

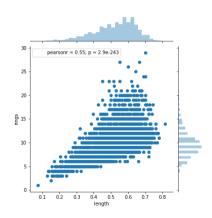
 What is the Bayes prediction function for square loss?

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

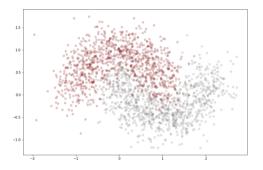
- What is the Bayes prediction function for square loss?
- If E[Y|X] is linear in  $\phi_1(X)$ , will we improve performance using  $\phi_2(X)$ ?

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

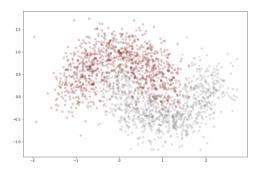
- What is the Bayes prediction function for square loss?
- If E[Y|X] is linear in  $\phi_1(X)$ , will we improve performance using  $\phi_2(X)$ ?
- Do we typically know in advance the structure of E[Y|X]?



Example 2: Two moons data



• What feature maps might be helpful for this problem?



- What feature maps might be helpful for this problem?
- We'll try binning data instances using k-means (and for fun random tree embeddings) let's look at the transformers (in notebook).

From Alice Zheng, Amanda Casari, Feature Engineering for Machine Learning

- 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?

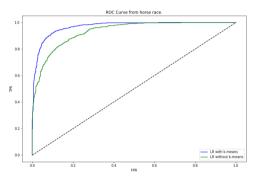
```
pipe = Pipeline([
    ('feats'.FeatureUnion([
        ('kmeans', KMeansFeaturizer(k=100,random_state=2052018)),
        ('ID', IdentityFeaturizer())
   1)),
   ('clf', LogisticRegressionCV())
pipe.fit(training_data, training_labels)
# Just to make sure it's clear what this does:
transformed = pipe.named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

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

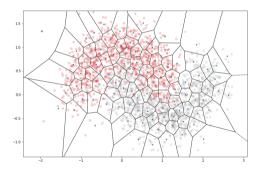
- Here's the pipeline. First, notice the sklearn class FeatureUnion, which let's us easily apply multiple feature maps over an input array.
- What is the feature map  $\phi(X)$ ? What will transformed.shape[1] equal?

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

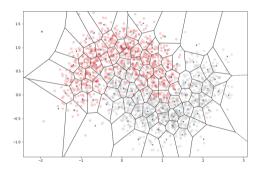


• We see performance improve.

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



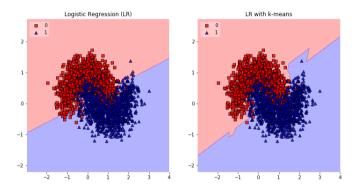
• Intuitively, why did this improve performance?



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

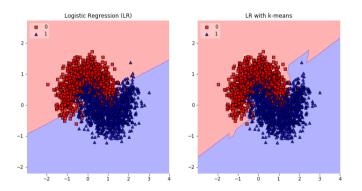
$$\begin{aligned} \varphi_2(x) &= (1(5 \leqslant \textit{N}(x) < 10), 1(10 \leqslant \textit{N}(x) < 100), 1(100 \leqslant \textit{N}(x))) \\ \varphi_1(x) &= (1(5 \leqslant \textit{N}(x)), 1(10 \leqslant \textit{N}(x)), 1(100 \leqslant \textit{N}(x))) \end{aligned}$$

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

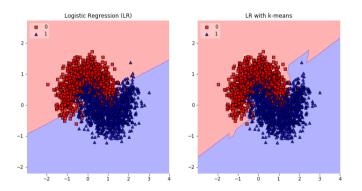


• What's with the plotted decision boundaries? I thought logistic regression was linear?

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



• 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.