Records and embedding

Raw data

- *raw data* pairs are (u, v), with $u \in \mathcal{U}$, $v \in \mathcal{V}$
- $\mathcal{U}$ is set of all possible input values
- $\mathcal{V}$ is set of all possible output values
- each u is called a *record*
- typically a record is a tuple, or list, $u = (u_1, u_2, \ldots, u_r)$
- each u_i is a *field* or *component*, which has a *type*, *e.g.*, real number, Boolean, categorical, ordinal, word, text, audio, image, parse tree (more on this later)
- *e.g.*, a record for a house for sale might consist of

$$(\text{address}, \text{photo}, \text{description}, \text{house/apartment?}, \text{lot size}, \ldots, \#\ \text{bedrooms})$$

Feature map

- learning algorithms are applied to (x, y) pairs,

$$x = \phi(u), \qquad y = \psi(v)$$

- $\phi : \mathcal{U} \to \mathbf{R}^d$ is the *feature map* for u
- $\psi : \mathcal{V} \to \mathbf{R}^m$ is the *feature map* for v
- feature maps transform *records* into *vectors*
- feature maps usually work on each field separately,

$$\phi(u_1, \ldots, u_r) = (\phi_1(u_1), \ldots, \phi_r(u_r))$$

- ϕ_i is an *embedding* of the type of field i into a vector

Embeddings

- embedding puts the different field types on an equal footing, *i.e.*, vectors
- some embeddings are simple, *e.g.*,
  - for a number field ($\mathcal{U} = \mathbf{R}$), $\phi_i(u_i) = u_i$
  - for a Boolean field, $\phi_i(u_i) = \begin{cases} 1 & u_i = \text{TRUE} \\ -1 & u_i = \text{FALSE} \end{cases}$
  - color to (R, G, B)
- others are more sophisticated
  - text to TFIDF histogram
  - `word2vec` (maps words into vectors)
  - pre-trained neural network for images (maps images into vectors)

(more on these later)

Faithful embeddings

a *faithful* embedding satisfies

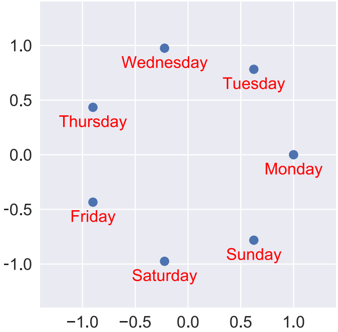
- $\phi(u)$ is near $\phi(\tilde{u})$ when u and $\tilde{u}$ are 'similar'
- $\phi(u)$ is not near $\phi(\tilde{u})$ when u and $\tilde{u}$ are 'dissimilar'

- lefthand concept is *vector distance*
- righthand concept depends on field type, application

- interesting examples: names, professions, companies, countries, languages, ZIP codes, cities, songs, movies
- we will see later how such embeddings can be constructed

Examples

- geolocation data: $\phi(u)$ =(Lat,Long) in $\mathbf{R}^2$ or embed in $\mathbf{R}^3$ (if data points are spread over planet)
- day of week (each day is 'similar' to the day before and day after)

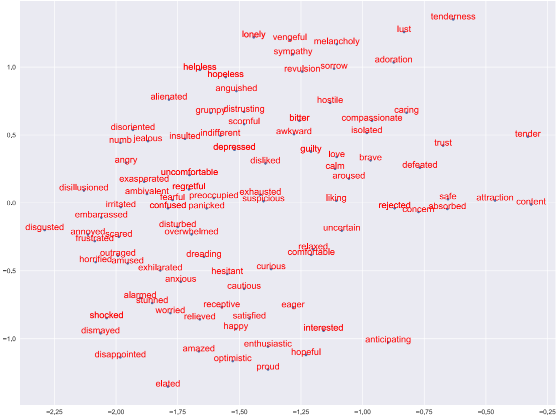


Example: word2vec

- word2vec maps a dictionary of 3 million words (and short phrases) into $\mathbf{R}^{300}$
- developed from a data set from Google News containing 100 billion words
- assigns words that frequently appear near each other in Google News to nearby vectors in $\mathbf{R}^{300}$

Example: word2vec

(showing only x_1 and x_2, for a selection of words associated with emotion)



Imagenet embedding

- Imagenet is an open image database with 14m labeled images in 1000 classes
- vgg16 maps images u (224×224 pixels with R,G,B components) to $x \in \mathbf{R}^{4096}$
- vgg16 was originally developed to classify the image labels
- repurposed as general image feature mapping
- vgg16 has neural network form with 16 layers, with input u, output x

vgg16 embedding

1 2 3 4 5 6

- images u^i for $i = 1, 2, \ldots, 6$ are embedded to $x^i = \phi(u^i) \in \mathbf{R}^{4096}$
- matrix of pairwise distances $d_{ij} = ||x^i - x^j||_2$

$$d = \begin{bmatrix} 0 & 109.7 & 97.9 & 96.2 & 107.4 & 103.0 \\ & 0 & 63.9 & 71.6 & 109.4 & 109.2 \\ & & 0 & 69.4 & 101.5 & 101.4 \\ & & & 0 & 96.5 & 96.8 \\ & & & & 0 & 86.6 \\ & & & & & 0 \end{bmatrix}$$

Standardized embeddings

we usually assume that an embedding is *standardized*

- entries of $\phi(u)$ are centered around 0
- entries of $\phi(u)$ have RMS value around 1
- roughly speaking, entries of $\phi(u)$ range over ± 1

- with standardized embeddings, entries of feature map

$$\phi(u_1, \ldots, u_r) = (\phi_1(u_1), \ldots, \phi_r(u_r))$$

  are all comparable, *i.e.*, centered around zero, standard deviation around one
- $\mathrm{rms}(\phi(u) - \phi(\tilde{u}))$ is reasonable measure of how close records u and $\tilde{u}$ are

Standardization or z-scoring

- suppose $\mathcal{U} = \mathbf{R}$ (field type is real numbers)
- for data set $u^1, \ldots, u^n \in \mathbf{R}$

$$\bar{u} = \frac{1}{n}\sum_{i=1}^{n} u^i \qquad \mathrm{std}(u) = \left(\frac{1}{n}\sum_{i=1}^{n}(u^i - \bar{u})^2\right)^{\frac{1}{2}}$$

- the *z-score* or *standardization* of u is the embedding

$$x = \mathrm{zscore}(u) = \frac{1}{\mathrm{std}(u)}(u - \bar{u})$$

- ensures that embedding values are centered at zero, with standard deviation one
- z-scored features are very easy to interpret: $x = \phi(u) = +1.3$ means that u is 1.3 standard deviations above the mean value

Log transform

- old school rule-of-thumb: if field u is positive and ranges over wide scale, embed as $\phi(u) = \log u$ (or $\log(1+u)$ if u is sometimes zero), then standardize
- examples: web site visits, ad views, company capitalization
- interpretation as faithful embedding:
  - 20 and 22 are similar, as are 1000 and 1100
  - but 20 and 120 are not similar
  - *i.e.*, you care about fractional or relative differences between raw values

  (here, log embedding is faithful, affine embedding is not)
- can also apply to output or label field, *i.e.*, $y = \psi(v) = \log v$ if you care about percentage or fractional errors; recover $\hat{v} = \exp(\hat{y})$

Example: House price prediction

- we want to predict house selling price v from record $u = (u_1, u_2)$
  - $u_1 =$ area (sq. ft.)
  - $u_2 = \#$ bedrooms
- we care about relative error in price, so we embed v as $\psi(v) = \log v$ (and then standardize)
- we standardize fields u_1 and u_2

$$x_1 = \frac{u_1 - \mu_1}{\sigma_1}, \qquad x_2 = \frac{u_2 - \mu_2}{\sigma_2}$$

  - $\mu_1 = \bar{u}_1$ is mean area
  - $\mu_2 = \bar{u}_2$ is mean number of bedrooms
  - $\sigma_1 = \text{std}(u_1)$ is std. dev. of area
  - $\sigma_2 = \text{std}(u_2)$ is std. dev. of # bedrooms

  (means and std. dev. are over our data set)

Example: House price linear regression predictor

- predict $y = \log v$ (log of price) from standardized area and # bedrooms
- linear predictor: $\hat{y} = \theta_1 + \theta_2 x_1 + \theta_3 x_2$
- in terms of original raw data:

$$\hat{v} = \exp\left(\theta_1 + \theta_2 \frac{u_1 - \mu_1}{\sigma_1} + \theta_3 \frac{u_2 - \mu_2}{\sigma_2}\right)$$

- $\exp$ undoes log embedding of house price
- readily interpretable, *e.g.*, what does $\theta_2 = 0.7$ mean?

Vector embeddings

Vector embeddings for real field

- we can embed a field u into a vector $x = \phi(u) \in \mathbf{R}^k$
- useful even when $\mathcal{U} = \mathbf{R}$ (real field)
- polynomial embedding:
$$\phi(u) = (1, u, u^2, \ldots, u^d)$$
- piecewise linear embedding:
$$\phi(u) = (1, (u)_-, (u)_+)$$
where $(u)_- = \min(u, 0)$, $(u)_+ = \max(u, 0)$
- linear predictor with these features yield polynomial and piecewise linear predictors of raw features

Categorical data

- data field is *categorical* if it only takes a finite number of values
- *i.e.*, $\mathcal{U}$ is a finite set $\{\alpha_1, \ldots, \alpha_k\}$; α_i are *category labels*
- we often use category labels $1, \ldots, k$, and refer to 'category i'
- examples:
  - TRUE/FALSE (two values, also called Boolean)
  - APPLE, ORANGE, BANANA (three values)
  - MONDAY, . . . , SUNDAY (seven values)
  - ZIP code (around 40000 values)
  - countries (around 185 values)
  - languages (several thousand spoken by large numbers of people)

One-hot embedding for categoricals

- $\mathcal{U} = \{1, \ldots, k\}$
- *one-hot embedding*: $\phi(i) = e_i \in \mathbf{R}^k$
- examples:
  - $\phi(\textsc{apple}) = (1,0,0), \quad \phi(\textsc{orange}) = (0,1,0), \quad \phi(\textsc{banana}) = (0,0,1)$
  - $\phi(\textsc{true}) = (1,0), \quad \phi(\textsc{false}) = (0,1)$ (another embedding of Boolean, into $\mathbf{R}^2$)
  - $\phi(\textsc{Mandarin}) = e_1$, $\phi(\textsc{English}) = e_2$, $\phi(\textsc{Hindi}) = e_3$, $\ldots$, $\phi(\textsc{Azeri}) = e_{55}$, $\ldots$
- standardizing these features handles *unbalanced* data

Reduced one-hot embedding for categoricals

- $\mathcal{U} = \{1, \ldots, k\}$
- one-hot embedding maps $\mathcal{U}$ to $\mathbf{R}^k$; *reduced one-hot embedding* maps $\mathcal{U}$ to $\mathbf{R}^{k-1}$
- choose one value, say $i = k$, as the *default* or *nominal* value
- $\phi(k) = 0 \in \mathbf{R}^{k-1}$, *i.e.*, map the default value to (vector) 0
- $\phi(i) = e_i \in \mathbf{R}^{k-1}$, $i = 1, \ldots, k-1$
- example: $\mathcal{U} = \{\textsc{True}, \textsc{False}\}$ with $\textsc{False}$ as default

  $$\phi(\textsc{true}) = 1, \qquad \phi(\textsc{false}) = 0$$

  (a common embedding of Booleans into $\mathbf{R}$)

Ordinal data

- ordinal data is categorical, with an order
- example: *Likert scale*, with values

  STRONGLY DISAGREE, DISAGREE, NEUTRAL, AGREE, STRONGLY AGREE

- can embed into $\mathbf{R}$ with values $-2, -1, 0, 1, 2$
- or treat as categorical, with one-hot embedding into $\mathbf{R}^5$
- example: number of bedrooms in house
  - can be treated as a real number
  - or as an ordinal with (say) values $1, \ldots, 6$

Feature engineering

Feature engineering

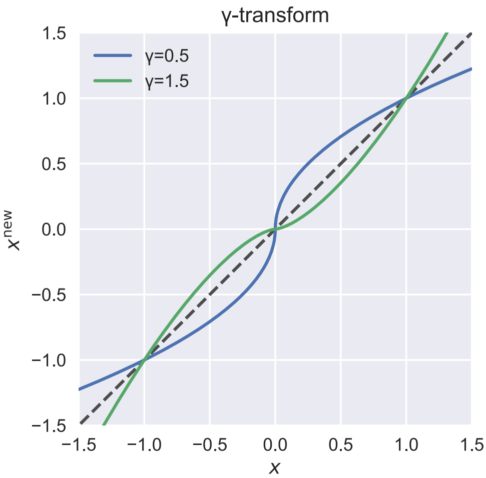
- basic idea:
  - start with some features
  - then process or transform them to produce new ('engineered') features
  - use these new features in your predictor
- was it a good idea? did it improve your predictor?
  - train your model with original features and validate performance
  - train your model with new features and validate performance
  - if performance with new features is better, your feature engineering was successful

Types of feature transforms

- *modify individual features*: replace original feature x_i with modified or transformed feature x_i^{new}
  - simple example: standardize, $x_i^{\text{new}} = (x_i - \mu_i)/\sigma_i$
- *create multiple features from each original feature*
  - simple example: powers, replace x_i with $(x_i, x_i^2, \ldots, x_i^q)$
- *create new features from multiple original features*
  - simple example: product, $x_i^{\text{new}} = x_k x_l$

Gamma-transform

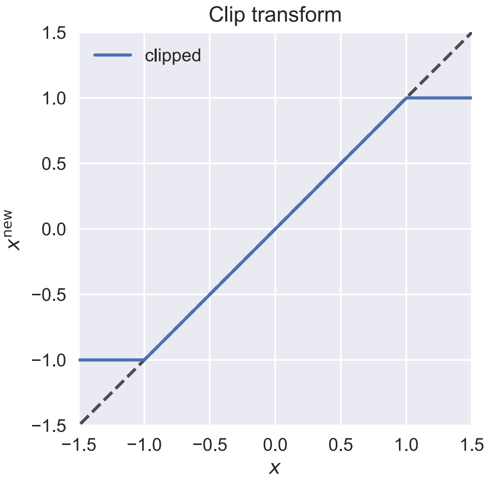
- *γ-transform*: $x_i^{\text{new}} = \text{sign}(x_i)|x_i|^{\gamma_i}$, $\gamma_i > 0$



Clipping

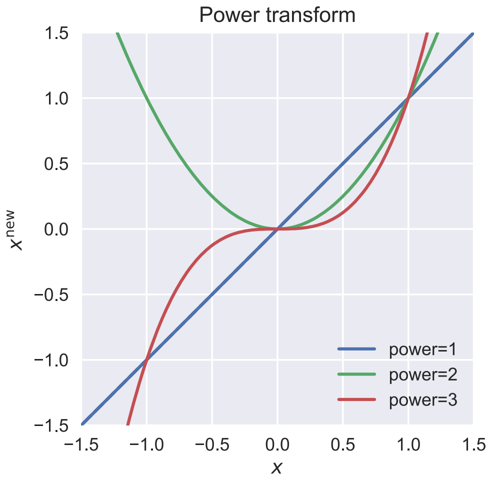
- *winsorize* or *clip* or *saturate* with lower and upper clip levels l_i, u_i

$$x_i^{\mathtt{new}} = \begin{cases} u_i & x_i > u_i \\ x_i & l_i \leq x_i \leq u_i \\ l_i & x_i < l_i \end{cases}$$



Powers

- replace x_i with $(x_i, x_i^2, \ldots, x_i^q)$

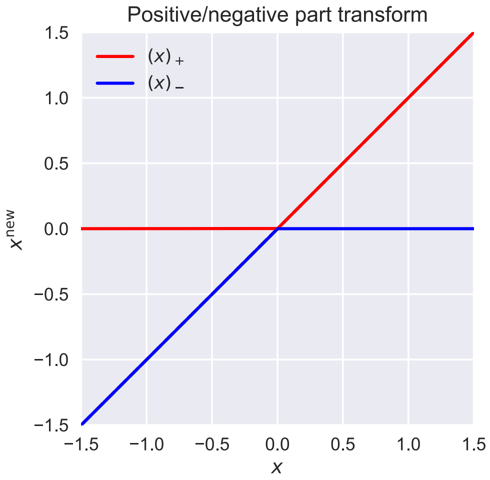


Split into positive and negative parts

- replace x_i with $((x_i)_+, (x_i)_-)$
- or, split into negative, middle, and high values: replace x_i with

$$((x_i + 1)_-, \mathsf{sat}(x_i), (x_i - 1)_+)$$

$\mathsf{sat}(a) = \min(1, \max(x, -1))$ is the *saturation function*



Creating new features from multiple original features

- can be used to model *interactions* among features
- examples: for $i < j$
  - maximum: $\max(x_i, x_j)$
  - product: $x_i x_j$
- example: all monomials up to degree 3 of (x_1, x_2):

$$(x_1,\ x_2,\ x_1^2,\ x_1x_2,\ x_2^2,\ x_1^3,\ x_1^2x_2,\ x_1x_2^2,\ x_2^3)$$

  linear model with these features gives arbitrary degree 3 polynomial of (x_1, x_2)

Interpreting products of features as interactions

- suppose x_i are Boolean, with values 0, 1, for $i = 1, \ldots, d$, *e.g.*, representing patient symptoms
- create new 'interaction' features $x_i x_j$, for $i < j$, of which there are $d(d-1)/2$
- linear regression model (for $d = 3$) is

$$\theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \theta_{12} x_1 x_2 + \theta_{13} x_1 x_3 + \theta_{23} x_2 x_3$$

  - θ_1 is the amount our prediction goes up when $x_1 = 1$
  - θ_3 is the amount our prediction goes up when $x_3 = 1$
  - θ_{13} is the amount our prediction goes up when x_1 *and* x_3 are both 1 (in addition to $\theta_1 + \theta_3$)
  - *e.g.*, with θ_{13} large, the simultaneous presence of symptoms 1 *and* 3 makes our estimate go up a lot

Quantizing

- specify *bin boundaries* $b_1 < b_2 < \cdots < b_k$
- partitions into *bins* or *buckets* $(-\infty, b_1]$, $(b_1, b_2]$, $\ldots$ $(b_{k-1}, b_k]$, (b_k, ∞)
- common choice of bin boundaries: quantiles of x_i, *e.g.*, deciles
- replace x_i with

$$\begin{cases} e_1 & x_i \leq b_1 \\ e_2 & b_1 < x_i \leq b_2 \\ \vdots & \\ e_k & b_{k-1} < x_i \leq b_k \\ e_{k+1} & b_k < x_i \end{cases}$$

i.e., x_i maps to e_l, if x_i is in bin l

Feature engineering pipeline

- feature transformations can be done multiple times
- start by embedding original record u into vector feature $x^0 \in \mathbf{R}^{d_0}$ using $\tilde{\phi}$, $x^0 = \tilde{\phi}(u)$
- superscript 0 in x^0 and d^0 means starting point for feature engineering
- transform x^0 using a feature engineering transform $\mathcal{T}^1$, to get $x^1 = \mathcal{T}^1(x^0) \in \mathbf{R}^{d_1}$
- superscript 1 in x^1 and d^1 means 'first step' of feature engineering
- repeat M times to get final embedding $x = x^M = \varphi^M(x^{M-1})$
- final feature map is a composition:

$$\phi = \mathcal{T}^M \circ \mathcal{T}^{M-1} \circ \cdots \circ \mathcal{T}^1 \circ \tilde{\phi}$$

- called *feature engineering pipeline*

Automatic feature generation

Hand crafted versus automatic features

- features and feature engineering described above generally done by hand, using experience
- can also develop feature mappings automatically, directly from some data
- examples: word2vec, vgg16 were developed automatically (from very large data sets)
- we'll later see some of these methods (PCA, neural nets, ...)

Summary

Summary

- raw features are mapped to vectors for subsequent processing
- feature maps can range from simple to complex
- use validation to choose among different candidate feature maps
- sometimes the original feature map is followed by subsequent transformations, called feature engineering
- we'll see later how feature mappings can be derived from data, as opposed to by hand