MS&E 125: Intro to Applied Statistics

Feature Engineering

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Management Science and Engineering
Stanford

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Announcements

Outline

Linear models

To fit a linear model (= linear in parameters β)

- pick a transformation $\phi : \mathcal{X} \to \mathbf{R}^p$
- predict y using a linear function of $\phi(x)$

$$h(x) = \phi(x)^T \beta = \sum_{i=1}^{p} \beta_i (\phi(x))_i$$

- we want $h(x_i) \approx y_i$ for every $i = 1, \ldots, n$

Feature engineering

How to pick $\phi : \mathcal{X} \to \mathbf{R}^d$?

- so response y will depend linearly on $\phi(x)$
- so p is not too big

Feature engineering

How to pick $\phi : \mathcal{X} \to \mathbf{R}^d$?

- so response y will depend linearly on $\phi(x)$
- so d is not too big

if you think this looks like a hack: you're right

Feature engineering

examples:

- adding offset
- standardizing features
- polynomial fits
- products of features
- autoregressive models
- transforming Booleans
- transforming ordinals
- transforming nominals
- transforming images
- transforming text
- handling missing values
- concatenating data
- all of the above

`https://xkcd.com/2048/`

Outline

Feature engineering

Polynomial transformations

Boolean, nominal, ordinal

Missing values

Nonlinear transformations

Location

Text, images, . . .

Adding offset

- $\mathcal{X} = \mathbf{R}^{d-1}$
- let $\phi(x) = (x, 1)$
- now $h(x) = w^T \phi(x) = w_{1:d-1}^T x + w_d$

Fitting a polynomial

- $\mathcal{X} = \mathbf{R}$
- let
$$\phi(x) = (1, x, x^2, x^3, \ldots, x^{d-1})$$
be the vector of all monomials in x of degree $< d$
- now $h(x) = w^T \phi(x) = w_1 + w_2 x + w_3 x^2 + \cdots + w_d x^{d-1}$

Demo: crime

https://colab.research.google.com/github/stanford-mse-125/demos/blob/main/crime.ipynb

Model evaluation

how should we measure how good a model is?

- (root) mean squared error (RMSE)
- mean absolute error (MAE)
- coefficient of determination (R^2)

Mean square error

mean square error is minimized by the least squares estimator

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

equal to the sum of the residuals squared

Root mean square error

root mean square error is the square root of the mean square error

$$\hat{\sigma}^2 = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

(the residual standard error is similar, but normalizes by the **residual degrees of freedom** $n - p - 1$ instead of n)

Mean absolute error

mean absolute error is the mean of the absolute value of the residuals

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n} |y_i - \hat{y}_i|$$

often makes more sense than RMSE when we care about quality of the predictions
(e.g., if we will pay a linear penalty for being wrong)

Coefficient of determination

coefficient of determination $R^{@} \in [0,1]$ is the fraction of the variance in the data that is explained by the model

$$R^2 = 1 - \frac{\sum_i = 1^n (y_i - \hat{y}_i)^2}{\sum_i = 1^n (y_i - \bar{y})^2} = 1 - \frac{\mathsf{MSE}}{\mathsf{Var}(y)} = 1 - \frac{\mathsf{SSR}}{\mathsf{SST}}$$

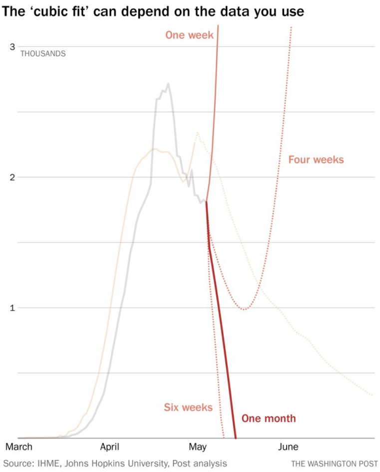
lingo:

- SSR is the **sum of squares of the residuals**
- SST is the **total sum of squares**

for a model with an intercept, R^2 is the square correlation between the predicted and true values of y

$$R^2 = [\rho(y, \hat{y})]^2$$

IMHE and the cubic fit



https://www.washingtonpost.com/politics/2020/05/05/
white-houses-self-serving-approach-estimating-deadliness-

Fitting a multivariate polynomial

- $\mathcal{X} = \mathbf{R}^2$
- pick a maximum degree k
- let

  $$\phi(x) = (1, x_1, x_2, x_1^2, x_1x_2, x_2^2, x_1^3, x_1^2x_2, x_1x_2^2, x_2^3 \ldots, x_2^k)$$

  be the vector of all monomials in x_1 and x_2 of degree $\leq k$
- now $h(x) = w^T\phi(x)$ can fit any polynomial of degree $\leq k$ in $\mathcal{X}$

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and similarly for $\mathcal{X} = \mathbf{R}^d \ldots$

Outline

Notation: boolean indicator function

define

$$\mathbb{1}(\text{statement}) = \begin{cases} 1 & \text{statement is true} \\ 0 & \text{statement is false} \end{cases}$$

examples:

- $\mathbb{1}(1 < 0) = 0$
- $\mathbb{1}(17 = 17) = 1$

Boolean variables

- $\mathcal{X} = \{\text{true}, \text{false}\}$
- let $\phi(x) = \mathbb{1}(x)$

Boolean expressions

- $\mathcal{X} = \{\text{true}, \text{false}\}^2 = \{(\text{true}, \text{true}), (\text{true}, \text{false}), (\text{false}, \text{true}), (\text{false}, \text{false})\}$.
- let $\phi(x) = [\mathbb{1}(x_1), \mathbb{1}(x_2), \mathbb{1}(x_1 \text{ and } x_2), \mathbb{1}(x_1 \text{ or } x_2)]$
- equivalent: polynomials in $[\mathbb{1}(x_1), \mathbb{1}(x_2)]$ span the same space
- encodes logical expressions!

Nominal values: one-hot encoding

- nominal data: *e.g.*, $\mathcal{X} = \{\text{apple}, \text{orange}, \text{banana}\}$
- let

$$\phi(x) = [\mathbb{1}(x = \text{apple}), \mathbb{1}(x = \text{orange}), \mathbb{1}(x = \text{banana})]$$

- called **one-hot encoding**: only one element is non-zero

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extension: sets

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Nominal values: the long tail

- **problem:** too many nominal categories
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  - feature hashing
  - ... be creative!

Nominal values: look up features!

why not use other information known about each item?

- $\mathcal{X} = \{\text{apple}, \text{orange}, \text{banana}\}$
  - price, calories, weight, ...
- $\mathcal{X} = \text{zip code}$
  - average income, temperature in July, walk score, % residential, ...
- ...

database lingo: **join** tables on nominal value

Ordinal values: real encoding

- ordinal data: *e.g.*, $\mathcal{X} = \{\text{Stage I}, \text{Stage II}, \text{Stage III}, \text{Stage IV}\}$
- let

$$\phi(x) = \begin{cases} 1, & x = \text{Stage I} \\ 2, & x = \text{Stage II} \\ 3, & x = \text{Stage III} \\ 4, & x = \text{Stage IV} \end{cases}$$

- default encoding

Ordinal values: real encoding

- $\mathcal{X} = \{\text{Stage I}, \text{Stage II}, \text{Stage III}, \text{Stage IV}\}$
- $\mathcal{Y} = \mathbf{R}$, number of years lived after diagnosis
- use real encoding ϕ to transform ordinal data
- fit linear model with offset to predict y as $w\phi(x) + b$

Suppose model predicts a person diagnosed with Stage II cancer will survive 2 more years, and a person diagnosed with Stage I cancer will survive 4 more years.

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A. $b = 6$, $w = -2$

B. $b = 2$, $w = 0$

C. $b = 6$, $w = 2$

D. $b = 0$, $w = -2$

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B. 2 years

C. 0 years

D. -2 years

Ordinal values: boolean encoding

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A: can't say without more information

Outline

Missing values

handling missing values:

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Missing values

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- impute with mean, median, or mode
- fancier imputation methods (covered later in this class): matrix completion, copula models, deep learning, ...
- add new feature: Boolean indicator $\mathbb{1}$(data is missing)
  - can detect if missingness is informative
  - can complement imputation method
  - can use different indicators for different kinds of missingness (refused, missing, illegible response, ...)

Poll

In an ambulance dataset (data taken by instruments on board an ambulance), we want to predict if the patient died. The variable “heart rate” is sometimes missing. Is missingness

A. informative?

B. uninformative?

Poll

In a weather dataset, the batteries in the instruments occasionally run out before the experimenter can replace them, leaving missing data for eg temperature, humidity, or barometric pressure. Is missingness

A. informative?

B. uninformative?

Talk to your neighbor

Can you think of a dataset in which missing values would be

- informative?
- uninformative?

Outline

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sometimes data is easy to predict with a simple but **non**linear relation, e.g.

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hints that your data might benefit from a nonlinear transform:

- y is positive and heavy-tailed? try $y \leftarrow \log(y)$
- residuals $r = y - x_i^T \beta$ are skewed (not normal)
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useful nonlinear transforms:

- log, exp, quantile, ...

more systematic ways to handle nonlinearities:
copula models, deep learning

Log transform

Q: what happens if x increases by 1 in the model

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A: $\log(y)$ increases by β_1, so y increases by $\exp(\beta_1)$

$$\begin{aligned} \log(y) = \beta_0 + \beta_1 x \quad &\Longrightarrow \quad y = \exp(\beta_0 + \beta_1 x) \\ \log(y') = \beta_0 + \beta_1(x+1) \quad &\Longrightarrow \quad y' = \exp(\beta_0 + \beta_1(x+1)) = \exp(\beta_0 \end{aligned}$$

A convenient approximation

- for small x, $\exp(x) \approx 1 + x$,
- *e.g.*, $\exp(0.01) \approx 1.01$
- if x increases by 1%, then y increases by factor of $\exp(\beta_1/100)$
- so if x increases by 1%, then y increases by factor of $\approx \beta_1/100 = \beta_1\%$

Log transformations of covariates

if we instead log transform x, $\hat{y}$ increases by $\beta_1/100$ for each 1% increase in x.

- *e.g.*, if $\beta_1 = 3$, $\hat{y}$ increases by 3/100=0.03 units for every 1% increase in x.

if we instead log transform both x and y, $\hat{y}$ increases by β_1% for each 1% increase in x.

- *e.g.*, if $\beta_1 = 3$, $\hat{y}$ increases by 3% for every 1% increase in x.

log transformation results in **multiplicative** increases (rather than **additive**)

Outline

Location

can be given as

- latitude, longitude
- zip code
- neighborhood, county, state, country

can be transformed between these!

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which makes sense for your problem?

- does nearness matter?
- are there sharp boundaries?
- are other properties of the location (eg, mean house price or crime rate) more important?

Outline

Text

$\mathcal{X}$ = sentences, documents, tweets, ...

- **bag of words** model (one-hot encoding):
  - pick set of words $\{w_1, \ldots, w_d\}$
  - $\phi(x) = [\mathbb{1}(x \text{ contains } w_1), \ldots, \mathbb{1}(x \text{ contains } w_d)]$
  - ignores order of words in sentence

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  - ignores order of words in sentence
- **pre-trained neural networks**:
  - sentiment analysis: `https://medium.com/@b.terryjack/nlp-pre-trained-sentiment-analysis-1eb52a9d742c`
  - Universal Sentence Encoder (USE) embedding: `https://colab.research.google.com/github/tensorflow/hub/blob/master/examples/colab/semantic_similarity_with_tf_hub_universal_encoder.ipynb`
  - lots of others: `https://modelzoo.co/`

Neural networks: whirlwind primer

$$\mathrm{NN}(x) = \sigma(W_1\sigma(W_2 \ldots \sigma(W_\ell x))))$$

- σ is a nonlinearity applied elementwise to a vector, *e.g.*
  - ReLU: $\sigma(x) = \max(x, 0)$
  - sigmoid: $\sigma(x) = \log(1 + \exp(x))$
- each W is a matrix
- trained on very large datasets, *e.g.*, Wikipedia, YouTube

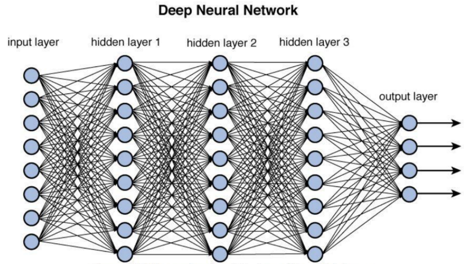
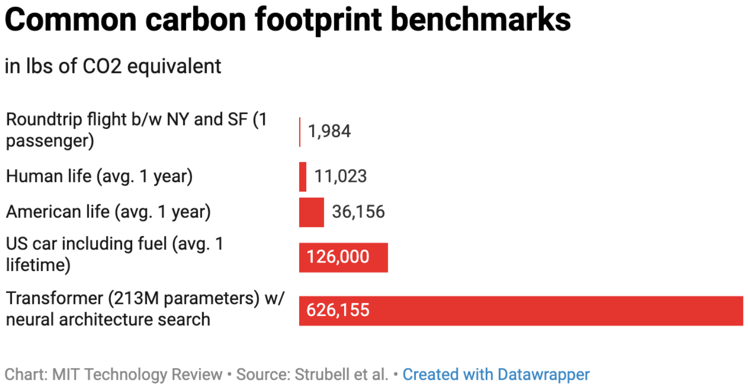


Figure 12.2 Deep network architecture with multiple layers.

Why not use deep learning?



towards a solution: `https://arxiv.org/abs/1907.10597`

Review

- linear models are linear in the **parameters** β
- can fit many different models by picking feature mapping $\phi : \mathcal{X} \to \mathbf{R}^d$