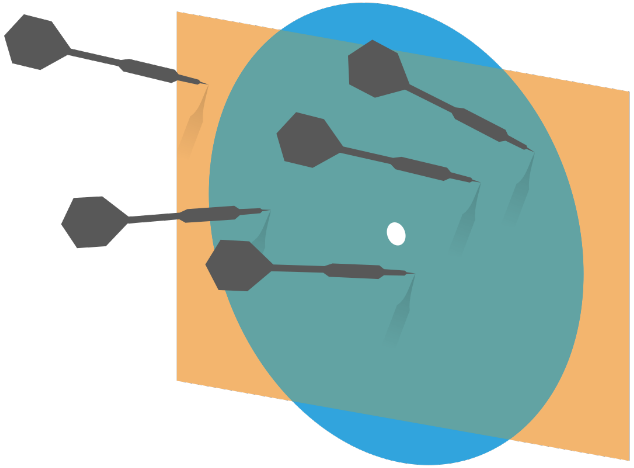
Probability and Statistics for Computer Science



Credit: wikipedia

"All models are wrong, but some models are useful"--- George Box

Hongye Liu, Teaching Assistant Prof, CS361, UIUC, 11.17.2020

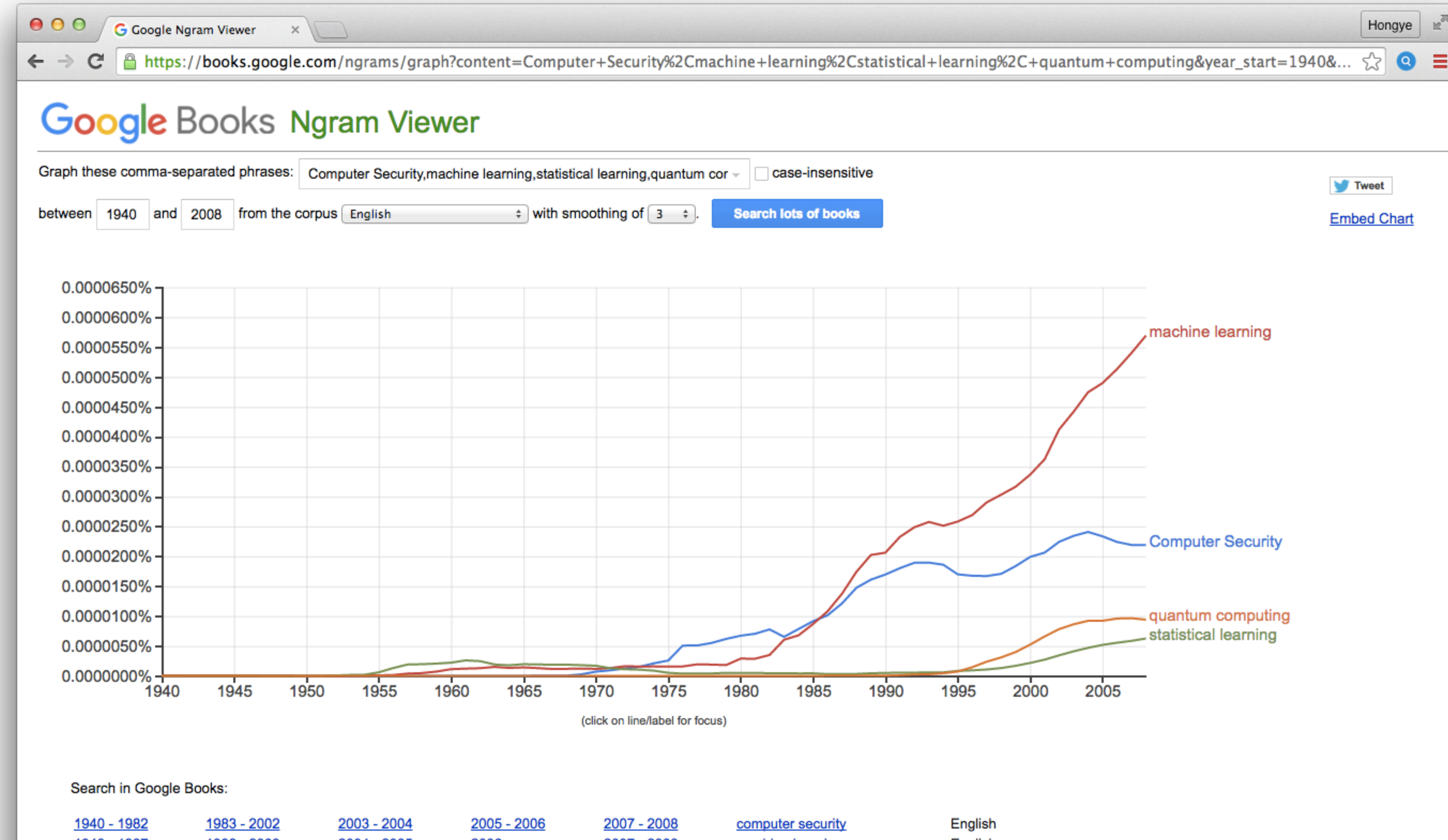
Last time

- Stochastic Gradient Descent
- Naïve Bayesian Classifier

Objectives

- Linear regression
  - The problem
  - The least square solution
  - The training and prediction
  - The R-squared for the evaluation of the fit.

Some popular topics in Ngram



Regression models are Machine learning methods

- Regression models have been around for a while
- Dr. Kelvin Murphy's Machine Learning book has 3+ chapters on regression

Wait, have we seen the linear regression before?

It's about *Relationship* between data features

- Example: does the Height of people relate to people's weight?

IDNO	BODYFAT	DENSITY	AGE	WEIGHT	HEIGHT
1	12.6	1.0708	23	154.25	67.75
2	6.9	1.0853	22	173.25	72.25
3	24.6	1.0414	22	154.00	66.25
4	10.9	1.0751	26	184.75	72.25
5	27.8	1.0340	24	184.25	71.25
6	20.6	1.0502	24	210.25	74.75
7	19.0	1.0549	26	181.00	69.75
8	12.8	1.0704	25	176.00	72.50
9	5.1	1.0900	25	191.00	74.00
10	12.0	1.0722	23	198.25	73.50

- x : HIGHT, y: WEIGHT

Chicago social economic census

- The census included 77 communities in Chicago
- The census evaluated the average hardship index of the residents
- The census evaluated the following parameters for each community:
  - PERCENT_OF_**HOUSING_CROWDED**
  - PERCENT_**HOUSEHOLD_BELOW_POVERTY**
  - PERCENT_**AGED_16p_UNEMPLOYED**
  - PERCENT_**AGED_25p_WITHOUT_HIGH_SCHOOL_DIPLOMA**
  - PERCENT_**AGED_UNDER_18_OR_OVER_64**
  - PER_CAPITA_**INCOME**

Given a new community and its parameters,
can you predict its average hardship index with all these parameters?

The regression problem

- Given a set of feature vectors x_i where each has a numerical label y_i, we want to train a model that can map unlabeled vectors to numerical values
- We can think of regression as fitting a line (or curve or hyperplane, etc.) to data
- Regression is like classification except that the prediction target is a number, not a class label. (Predicting class label can be considered a special case of regression)

Some terminology

- Suppose the dataset $\{(\mathbf{x}, y)\}$ consists of N labeled items $(\mathbf{x}_i, y_i)$
- If we represent the dataset as a table
  - The d columns representing $\{\mathbf{x}\}$ are called **explanatory variables** $\mathbf{x}^{(j)}$
  - The numerical column y is called the **dependent variable**

$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	y
1	3	0
2	3	2
3	6	5

Variables of the Chicago census

[1] "PERCENT_OF_HOUSING_CROWDED"
[2]"PERCENT_HOUSEHOLDS_BELOW_POVERTY"
[3] "PERCENT_AGED_16p_UNEMPLOYED"
[4]"PERCENT_AGED_25p_WITHOUT_HIGH_SCHOOL_DIPLOMA"
[5] "PERCENT_AGED_UNDER_18_OR_OVER_64"
[6]"PER_CAPITA_INCOME"
[7] "HardshipIndex"

Which is the dependent variable in the census example?

A. "PERCENT_OF_HOUSING_CROWDED"
B. "PERCENT_AGED_25p_WITHOUT_HIGH_SCHOOL_DIPLOMA”
C. "HardshipIndex”
D. "PERCENT_AGED_UNDER_18_OR_OVER_64"

Linear model

- We begin by modeling y as a linear function of $\mathbf{x}^{(j)}$ plus randomness

$$y = \mathbf{x}^{(1)}\beta_1 + \mathbf{x}^{(2)}\beta_2 + \ldots + \mathbf{x}^{(d)}\beta_d + \xi$$

Where ξ is a zero-mean random variable that represents model error

- In vector notation:

$$y = \mathbf{x}^T\boldsymbol{\beta} + \xi$$

Where $\boldsymbol{\beta}$ is the d-dimensional vector of coefficients that we train

$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	y
1	3	0
2	3	2
3	6	5

Each data item gives an equation

- The model: $y = \mathbf{x}^T \boldsymbol{\beta} + \xi = \mathbf{x}^{(1)} \beta_1 + \mathbf{x}^{(2)} \beta_2 + \xi$

Training data

$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	y
1	3	0
2	3	2
3	6	5

Which together form a matrix equation

- The model $y = \mathbf{x}^T \boldsymbol{\beta} + \xi = \mathbf{x}^{(1)}\beta_1 + \mathbf{x}^{(2)}\beta_2 + \xi$

Training data

$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	y
1	3	0
2	3	2
3	6	5

$$\begin{bmatrix} 0 \\ 2 \\ 5 \end{bmatrix} = \begin{bmatrix} 1 & 3 \\ 2 & 3 \\ 3 & 6 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{bmatrix}$$

Which together form a matrix equation

- The model $y = \mathbf{x}^T \boldsymbol{\beta} + \xi = \mathbf{x}^{(1)} \beta_1 + \mathbf{x}^{(2)} \beta_2 + \xi$

Training data

$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	y
1	3	0
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$$\begin{bmatrix} 0 \\ 2 \\ 5 \end{bmatrix} = \begin{bmatrix} 1 & 3 \\ 2 & 3 \\ 3 & 6 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{bmatrix}$$

$$\mathbf{y} = X \cdot \boldsymbol{\beta} + \mathbf{e}$$

Q. What's the dimension of matrix X?

A. $N \times d$
B. $d \times N$
C. $N \times N$
D. $d \times d$

Training the model is to choose β

- Given a training dataset $\{(\mathbf{x}, y)\}$, we want to fit a model $y = \mathbf{x}^T \boldsymbol{\beta} + \xi$

- Define $\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}$ and $X = \begin{bmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_N^T \end{bmatrix}$ and $\mathbf{e} = \begin{bmatrix} \xi_1 \\ \vdots \\ \xi_N \end{bmatrix}$

- To train the model, we need to choose $\boldsymbol{\beta}$ that makes $\mathbf{e}$ small in the matrix equation $\mathbf{y} = X \cdot \boldsymbol{\beta} + \mathbf{e}$

Training using least squares

- In the least squares method, we aim to minimize $\|\mathbf{e}\|^2$

$$\|\mathbf{e}\|^2 = \|\mathbf{y} - X\boldsymbol{\beta}\|^2 = (\mathbf{y} - X\boldsymbol{\beta})^T(\mathbf{y} - X\boldsymbol{\beta})$$

- Differentiating with respect to $\boldsymbol{\beta}$ and setting to zero

$$X^T X\boldsymbol{\beta} - X^T\mathbf{y} = 0$$

- If $X^T X$ is invertible, the least squares estimate of the coefficient is:

$$\widehat{\boldsymbol{\beta}} = (X^T X)^{-1} X^T \mathbf{y}$$

Derivation of least square solution

$$\|e\|^2 = (y - X\beta)^T (y - X\beta)$$

$$= y^T y - \beta^T X^T y - y^T X \beta + \beta^T X^T X \beta \qquad (1)$$

Useful derivatives involving vector/matrix

a, b are vectors

A is matrix

$$\frac{\partial (a^T A a)}{\partial a} = (A + A^T) a$$

$$\frac{\partial (b^T a)}{\partial a} = b$$

since $b^T a$ is scalar

$$\frac{\partial (b^T a)}{\partial a} = \frac{\partial (b^T a)^T}{\partial a} = \frac{\partial (a^T b)}{\partial a} = b$$

Note $\|e\|^2$ is scalar, all items in (1) are scalar.

$$\frac{\partial \|e\|^2}{\partial \beta} = 0 - X^T y - X^T y + 2 X^T X \beta = 0$$

$$\Rightarrow \quad X^T X \beta = X^T y$$

$$\Rightarrow \quad \beta = (X^T X)^{-1} X^T y$$

Convex set and convex function

- If a set is convex, any line connecting two points in the set is completely included in the set

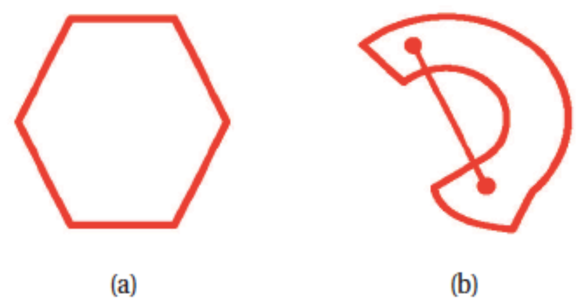
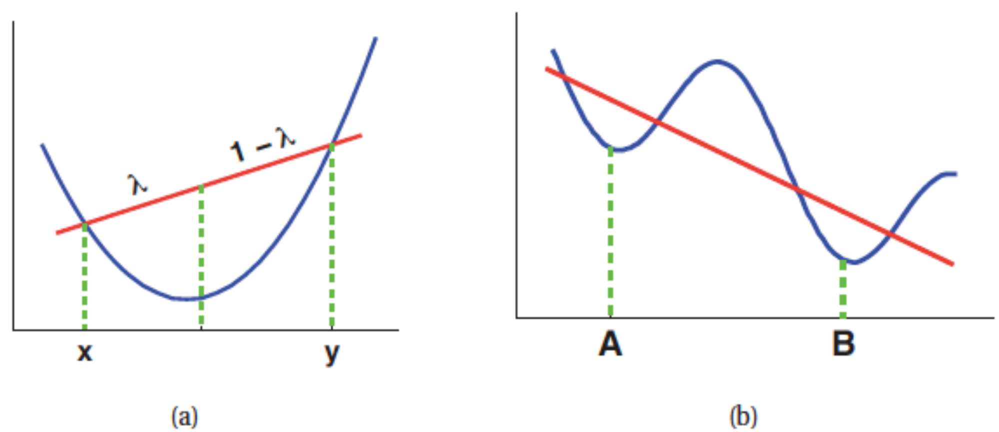


Figure 7.4 (a) Illustration of a convex set. (b) Illustration of a nonconvex set.

- A convex function: the area above the curve is convex

$$f(\lambda x + (1-\lambda)y) < \lambda f(x) + (1-\lambda)f(y)$$



- The least square function is **convex**

Credit: Dr. Kelvin Murphy

What's the dimension of matrix $X^T X$?

A. $N \times d$
B. $d \times N$
C. $N \times N$
D. $d \times d$

Is this statement true?

If the matrix $\mathbf{X}^T\mathbf{X}$ does NOT have zero valued eigenvalues, it is invertible.

A. TRUE
B. FALSE

Training using least squares example

- Model: $y = \mathbf{x}^T \boldsymbol{\beta} + \xi = \mathbf{x}^{(1)} \beta_1 + \mathbf{x}^{(2)} \beta_2 + \xi$

$$\widehat{\boldsymbol{\beta}} = (X^T X)^{-1} X^T \mathbf{y} = \begin{bmatrix} 2 \\ -\frac{1}{3} \end{bmatrix}$$

Training data

$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	y
1	3	0
2	3	2
3	6	5

$$\widehat{\boldsymbol{\beta}}_1 = 2$$
$$\widehat{\boldsymbol{\beta}}_2 = -\frac{1}{3}$$

Prediction

- If we train the model coefficients $\widehat{\boldsymbol{\beta}}$, we can predict y_0^p from $\mathbf{x}_0$

$$y_0^p = \mathbf{x}_0^T \widehat{\boldsymbol{\beta}}$$

- In the model $y = \mathbf{x}^{(1)}\beta_1 + \mathbf{x}^{(2)}\beta_2 + \xi$ with $\widehat{\boldsymbol{\beta}} = \begin{bmatrix} 2 \\ -\frac{1}{3} \end{bmatrix}$

  - The prediction for $\mathbf{x}_0 = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$ is y_0^p
  - The prediction for $\mathbf{x}_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ is y_0^p

A linear model with constant offset

- The problem with the model $y = \mathbf{x}^{(1)}\beta_1 + \mathbf{x}^{(2)}\beta_2 + \xi$ is:it always predicts y_0^p = 0 if the input vector $\mathbf{x}_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

- Let's add a constant offset β_0 to the model

$$y = \beta_0 + \mathbf{x}^{(1)}\beta_1 + \mathbf{x}^{(2)}\beta_2 + \xi$$

Training and prediction with constant offset

- The model $y = \beta_0 + \mathbf{x}^{(1)}\beta_1 + \mathbf{x}^{(2)}\beta_2 + \xi = \mathbf{x}^T\boldsymbol{\beta} + \xi$

- Training data:

$$\begin{bmatrix} 1 & x^{(1)} & x^{(2)} \end{bmatrix}$$

1	$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	y
1	1	3	0
1	2	3	2
1	3	6	5

$$\widehat{\boldsymbol{\beta}} = (X^T X)^{-1} X^T \mathbf{y} = \begin{bmatrix} -3 \\ 2 \\ \frac{1}{3} \end{bmatrix}$$

- For $\mathbf{x}_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

$$y_0^p = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} -3 \\ 2 \\ \frac{1}{3} \end{bmatrix} = -3$$

Variance of the linear regression model

- The least squares estimate satisfies this property

$$var(\{y_i\}) = var(\{\mathbf{x}_i^T \widehat{\boldsymbol{\beta}}\}) + var(\{\xi_i\})$$

- The random error is uncorrelated to the least square solution of linear combination of explanatory variables.

Variance of the linear regression model: proof

- The least squares estimate satisfies this property

$$var(\{y_i\}) = var(\{\mathbf{x}_i^T \widehat{\boldsymbol{\beta}}\}) + var(\{\xi_i\})$$

Proof:

$$y = \mathbf{X} \cdot \hat{\boldsymbol{\beta}} + \mathbf{e}$$

$$var[y] = (1/N)(y - \overline{y})^T (y - \overline{y})$$

$$var[y] = (1/N)([X\hat{\beta} - \overline{X\hat{\beta}}] + [\mathbf{e} - \overline{\mathbf{e}}])^T ([X\hat{\beta} - \overline{X\hat{\beta}}] + [\mathbf{e} - \overline{\mathbf{e}}])$$

Variance of the linear regression model: proof

- The least squares estimate satisfies this property

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Proof:

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$$var[y] = (1/N)([X\hat{\beta} - \overline{X\hat{\beta}}]^T[X\hat{\beta} - \overline{X\hat{\beta}}] + 2[\mathbf{e} - \overline{\mathbf{e}}]^T[X\hat{\beta} - \overline{X\hat{\beta}}] + [\mathbf{e} - \overline{\mathbf{e}}]^T[\mathbf{e} - \overline{\mathbf{e}}])$$

Variance of the linear regression model: proof

- The least squares estimate satisfies this property

$$var(\{y_i\}) = var(\{\mathbf{x}_i^T \widehat{\boldsymbol{\beta}}\}) + var(\{\xi_i\})$$

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$$var[y] = (1/N)([X\hat{\beta} - \overline{X\hat{\beta}}]^T[X\hat{\beta} - \overline{X\hat{\beta}}] + 2[\mathbf{e} - \overline{\mathbf{e}}]^T[X\hat{\beta} - \overline{X\hat{\beta}}] + [\mathbf{e} - \overline{\mathbf{e}}]^T[\mathbf{e} - \overline{\mathbf{e}}])$$

Because $\overline{\mathbf{e}} = 0$; $\mathbf{e}^T X\widehat{\boldsymbol{\beta}} = 0$; $\mathbf{e}^T\mathbf{1} = 0$

Variance of the linear regression model: proof

- The least squares estimate satisfies this property

$$var(\{y_i\}) = var(\{\mathbf{x}_i^T\widehat{\boldsymbol{\beta}}\}) + var(\{\xi_i\})$$

Proof:

$$var[y] = (1/N)([X\hat{\beta} - \overline{X\hat{\beta}}] + [\mathbf{e} - \overline{\mathbf{e}}])^T([X\hat{\beta} - \overline{X\hat{\beta}}] + [\mathbf{e} - \overline{\mathbf{e}}])$$

$$var[y] = (1/N)([X\hat{\beta} - \overline{X\hat{\beta}}]^T[X\hat{\beta} - \overline{X\hat{\beta}}] + 2[\mathbf{e} - \overline{\mathbf{e}}]^T[X\hat{\beta} - \overline{X\hat{\beta}}] + [\mathbf{e} - \overline{\mathbf{e}}]^T[\mathbf{e} - \overline{\mathbf{e}}])$$

Because $\overline{\mathbf{e}} = 0$; $\mathbf{e}^T X\widehat{\boldsymbol{\beta}} = 0$ and $\mathbf{e}^T\mathbf{1} = 0$ ← Due to Least square minimized

$$var[y] = (1/N)([X\hat{\beta} - \overline{X\hat{\beta}}]^T[X\hat{\beta} - \overline{X\hat{\beta}}] + [\mathbf{e} - \overline{\mathbf{e}}]^T[\mathbf{e} - \overline{\mathbf{e}}])$$

Variance of the linear regression model: proof

- The least squares estimate satisfies this property

$$var(\{y_i\}) = var(\{\mathbf{x}_i^T\widehat{\boldsymbol{\beta}}\}) + var(\{\xi_i\})$$

Proof:

$$var[y] = (1/N)([X\hat{\beta} - \overline{X\hat{\beta}}] + [\mathbf{e} - \overline{\mathbf{e}}])^T([X\hat{\beta} - \overline{X\hat{\beta}}] + [\mathbf{e} - \overline{\mathbf{e}}])$$

$$var[y] = (1/N)([X\hat{\beta}-\overline{X\hat{\beta}}]^T[X\hat{\beta}-\overline{X\hat{\beta}}]+2[\mathbf{e}-\overline{\mathbf{e}}]^T[X\hat{\beta}-\overline{X\hat{\beta}}]+[\mathbf{e}-\overline{\mathbf{e}}]^T[\mathbf{e}-\overline{\mathbf{e}}])$$

Because $\overline{\mathbf{e}} = 0$; $\mathbf{e}^T X\widehat{\boldsymbol{\beta}} = 0$ and $\mathbf{e}^T\mathbf{1} = 0$ ← Due to Least square minimized

$$var[y] = (1/N)([X\hat{\beta} - \overline{X\hat{\beta}}]^T[X\hat{\beta} - \overline{X\hat{\beta}}] + [\mathbf{e} - \overline{\mathbf{e}}]^T[\mathbf{e} - \overline{\mathbf{e}}])$$

$$var[y] = var[X\widehat{\beta}] + var[\mathbf{e}]$$

Evaluating models using R-squared

- The least squares estimate satisfies this property

$$var(\{y_i\}) = var(\{\mathbf{x}_i^T \widehat{\boldsymbol{\beta}}\}) + var(\{\xi_i\})$$

- This property gives us an evaluation metric called R-squared

$$R^2 = \frac{var(\{\mathbf{x}_i^T \widehat{\boldsymbol{\beta}}\})}{var(\{y_i\})}$$

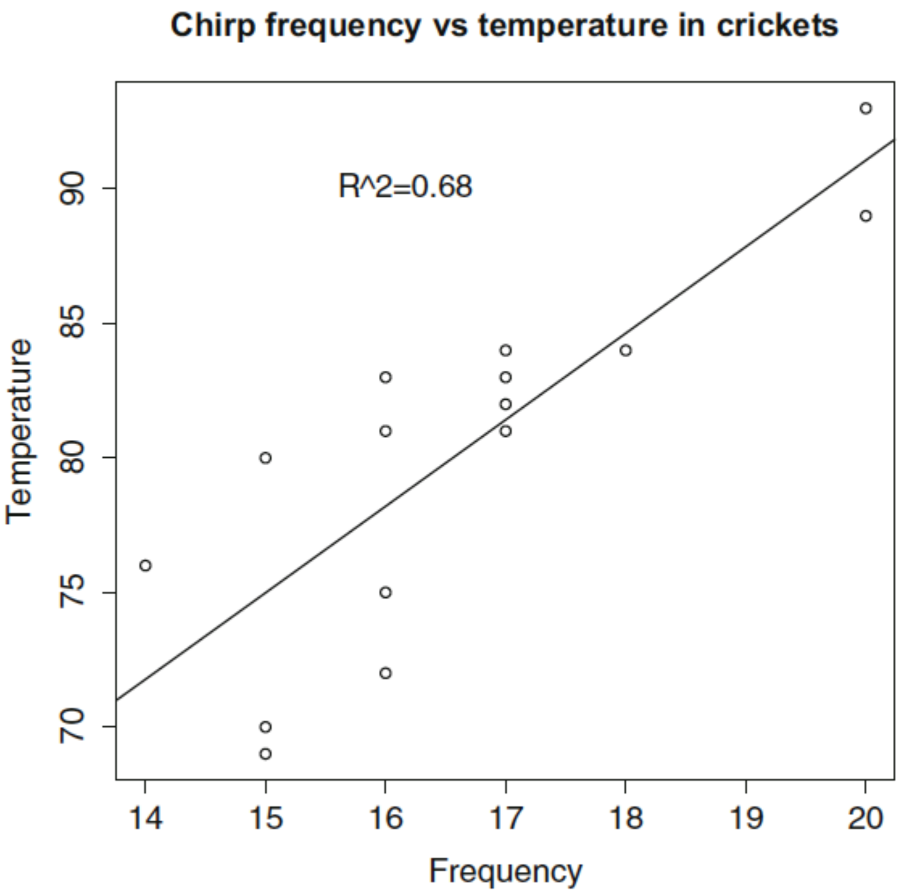
- We have $0 \leq R^2 \leq 1$ with a larger value meaning a better fit.

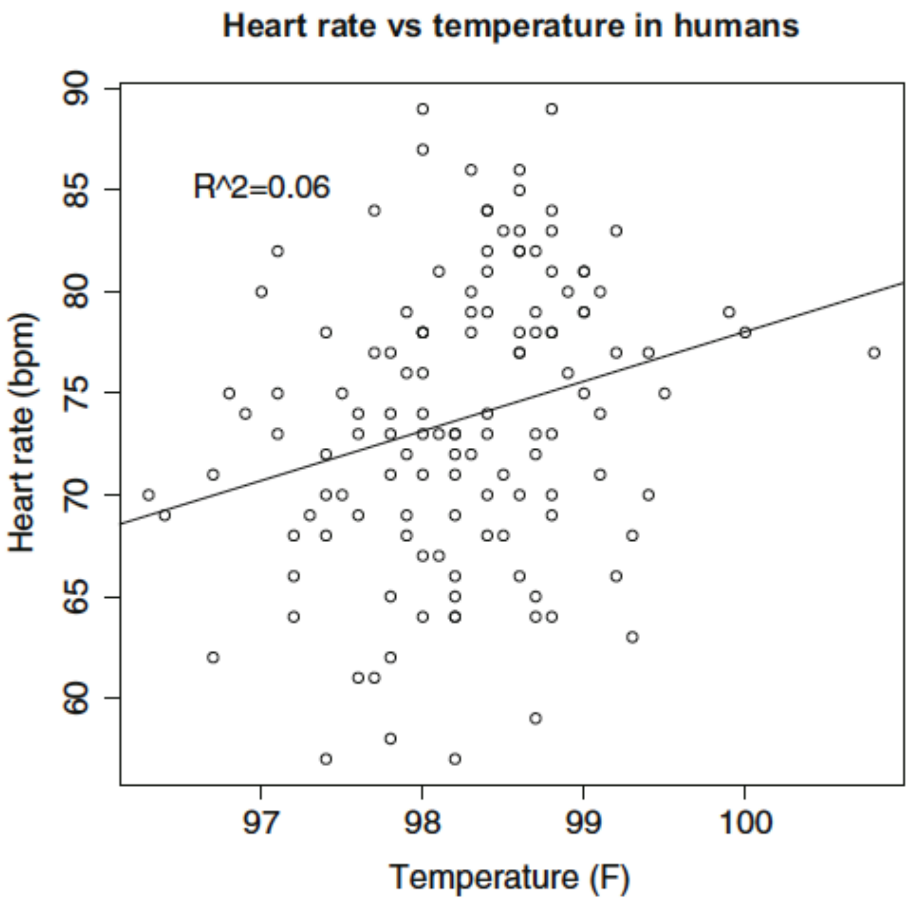
Q: What is R-squared if there is only one explanatory variable in the model?

Q: What is R-squared if there is only one explanatory variable in the model?

R-squared would be **the correlation coefficient squared** (textbook pgs 43-44)

R-squared examples





Comparing our example models

$$y = \mathbf{x}^{(1)}\beta_1 + \mathbf{x}^{(2)}\beta_2 + \xi$$

$$\widehat{\boldsymbol{\beta}} = \begin{bmatrix} 2 \\ -\frac{1}{3} \end{bmatrix}$$

$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	y	$\mathbf{x}^T\widehat{\boldsymbol{\beta}}$
1	3	0	1
2	3	2	3
3	6	5	4

$$y = \beta_0 + \mathbf{x}^{(1)}\beta_1 + \mathbf{x}^{(2)}\beta_2 + \xi$$

$$\widehat{\boldsymbol{\beta}} = \begin{bmatrix} -3 \\ 2 \\ \frac{1}{3} \end{bmatrix}$$

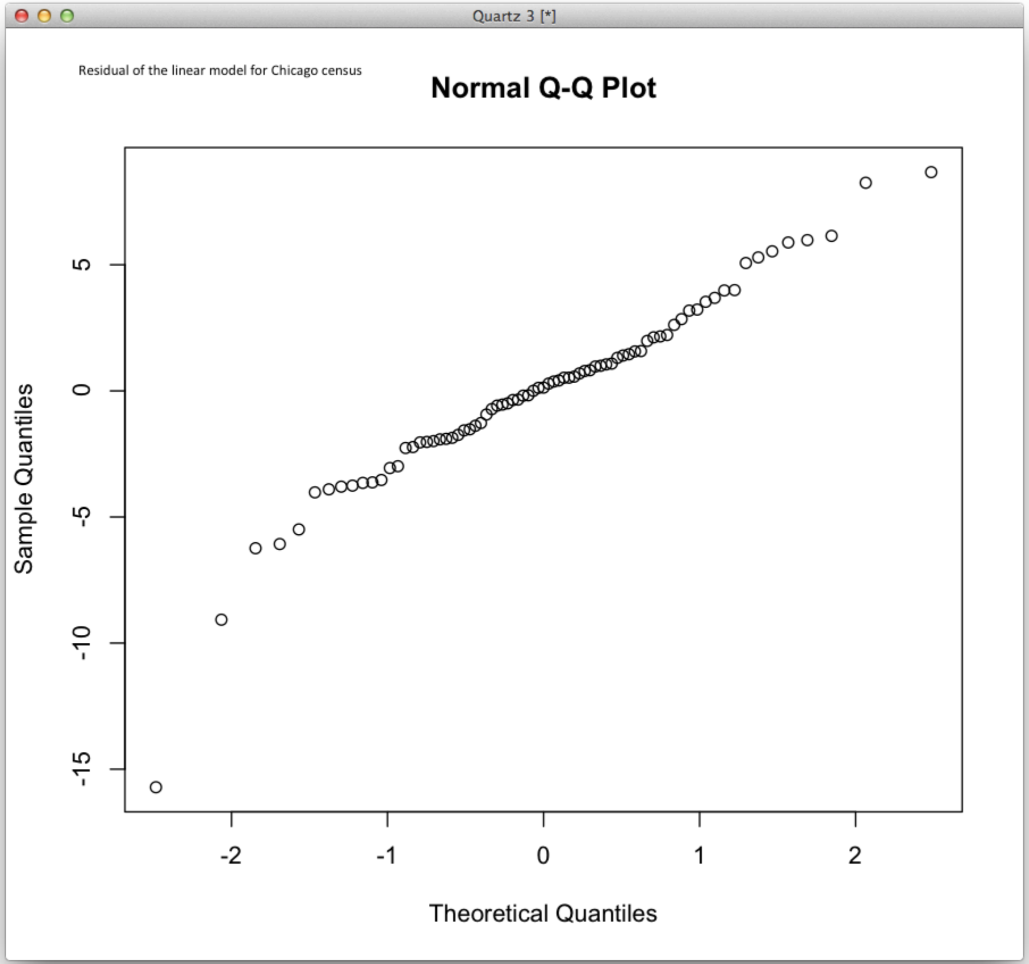
1	$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	y	$\mathbf{x}^T\widehat{\boldsymbol{\beta}}$
1	1	3	0	0
1	2	3	2	2
1	3	6	5	5

Linear regression model for the Chicago census data

```
Call:
lm(formula = HardshipIndex ~ ., data = dat)

Residuals:
     Min       1Q   Median       3Q      Max
-15.7157  -1.9230   0.1301   1.9810   8.6719

Coefficients:
                                             Estimate Std. Error t value Pr(>|t|)
(Intercept)                                  105.1394    37.3622   2.814 0.006346 **
PERCENT_OF_HOUSING_CROWDED                     0.7189     0.2753   2.612 0.011014 *
PERCENT_HOUSEHOLDS_BELOW_POVERTY               0.6665     0.0781   8.534 1.90e-12 ***
PERCENT_AGED_16p_UNEMPLOYED                    0.8023     0.1350   5.941 9.93e-08 ***
PERCENT_AGED_25p_WITHOUT_HIGH_SCHOOL_DIPLOMA   0.7751     0.1063   7.293 3.64e-10 ***
PERCENT_AGED_UNDER_18_OR_OVER_64               0.4807     0.1202   3.998 0.000156 ***
PER_CAPITA_INCOME                            -11.8819     3.1888  -3.726 0.000391 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 3.9 on 70 degrees of freedom
Multiple R-squared:  0.983, Adjusted R-squared:  0.9815
F-statistic: 673.9 on 6 and 70 DF,  p-value: < 2.2e-16
```

Residual is normally distributed?

The Q-Q plot of the residuals is roughly normal



Prediction for another community

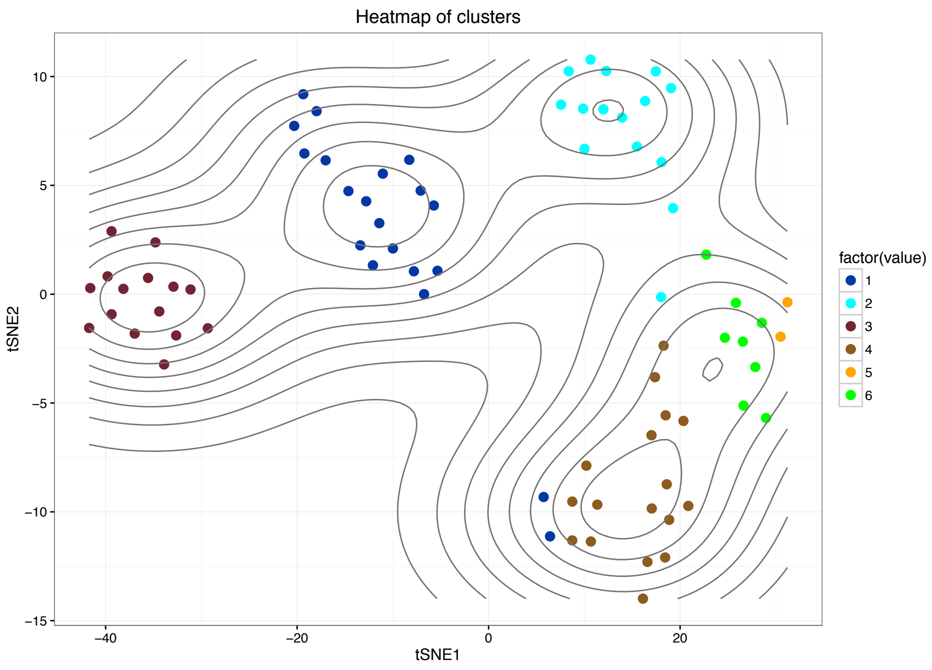
[1] "PERCENT_OF_HOUSING_CROWDED"	**4.7**
[2]"PERCENT_HOUSEHOLDS_BELOW_POVERTY"	**19.7**
[3] "PERCENT_AGED_16p_UNEMPLOYED"	**12.9**
[4]"PERCENT_AGED_25p_WITHOUT_HIGH_SCHOOL_DIPLOMA"	**19.5**
[5] "PERCENT_AGED_UNDER_18_OR_OVER_64"	**33.5**
[6]"PER_CAPITA_INCOME"	**Log(28202)**

Predicted hardship index: **41.46038**

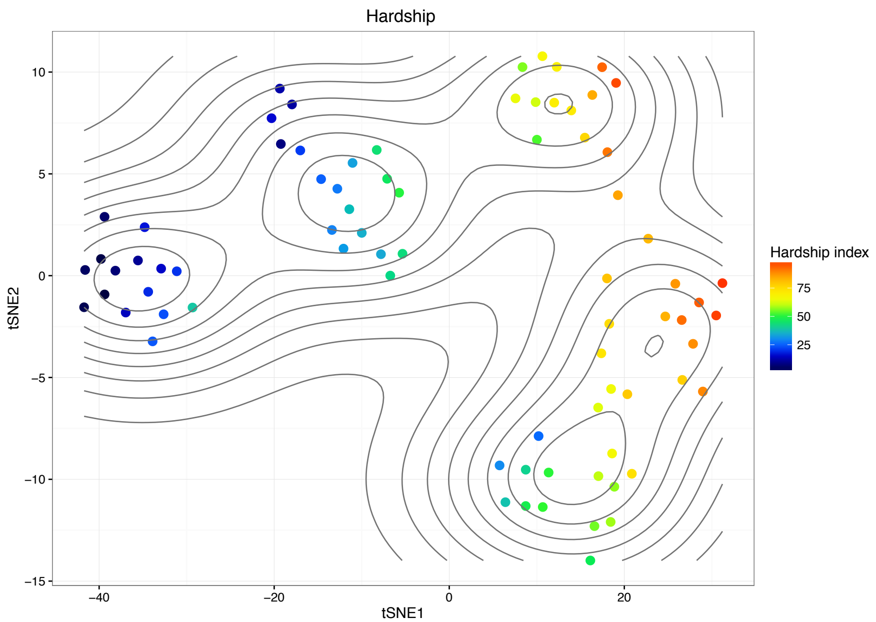
Note: maximum of hardship index in the training data is 98, minimum is 1

The clusters of the Chicago communities: clusters and hardship

Clusters of community

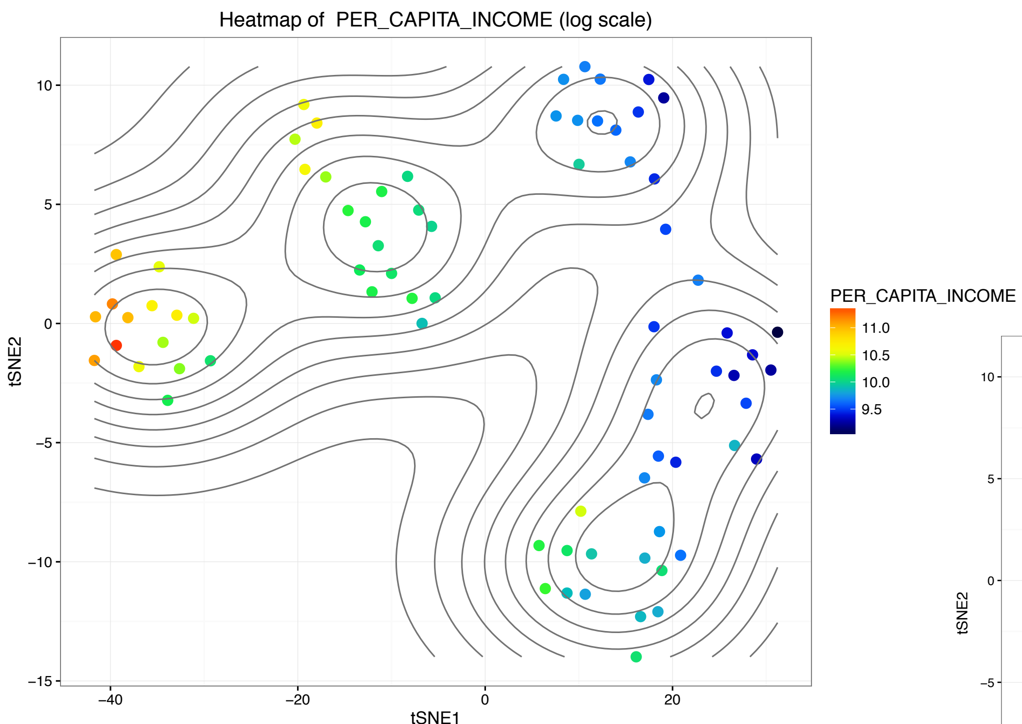


Hardship index of communities

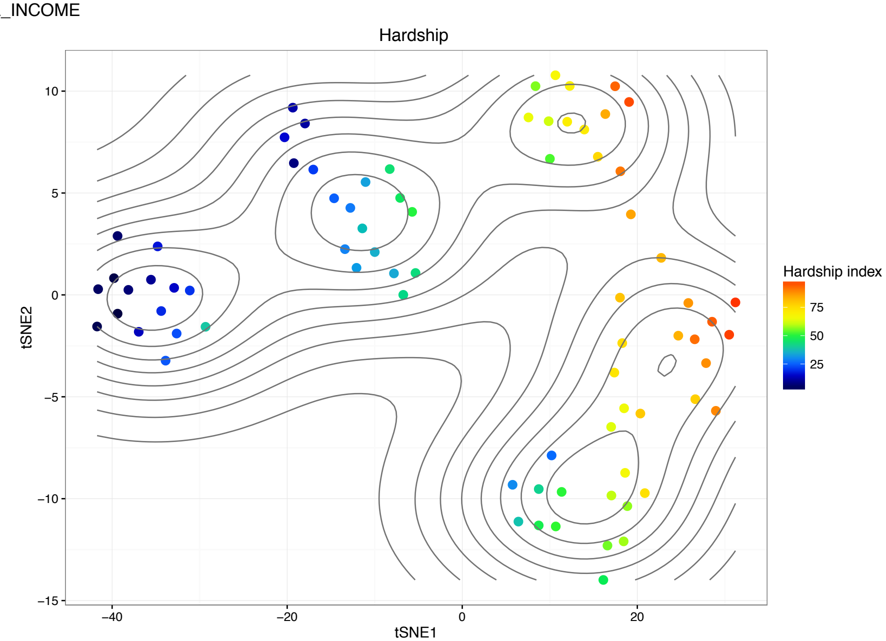


The clusters of the Chicago communities: per capital income and hardship

PER_CAPITAL_INCOME

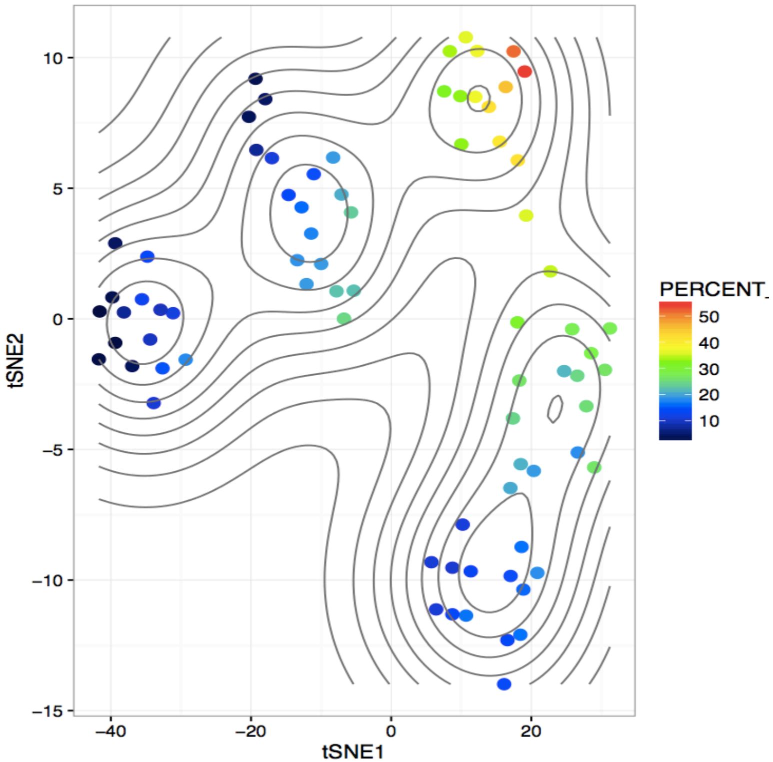


Hardship index of communities

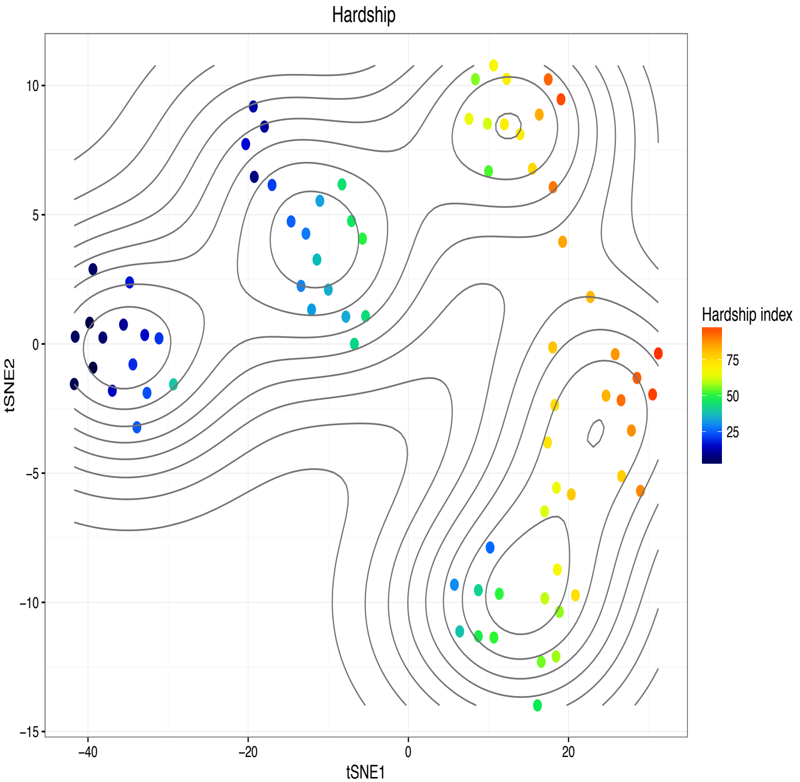


The clusters of the Chicago communities: without diploma and hardship

PERCENT_AGED_25p_WITHOUT _HIGH_SCHOOL_DIPLOMA



Hardship index of communities



Assignments

- Read Chapter 13 of the textbook
- Next time: More on linear regression

Additional References

- Robert V. Hogg, Elliot A. Tanis and Dale L. Zimmerman. “Probability and Statistical Inference”
- Kelvin Murphy, “Machine learning, A Probabilistic perspective”

See you next time

See You!