THE UNIVERSITY OF MELBOURNE

Linear Regression

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Ling Luo

Outline

- Regression
- Parameter Estimation
  - Optimisation
  - Computing the Optimal Solution
  - Gradient Descent
- Application and Evaluation

Categorical Features and Classes

- For classification problems, classes are categorical
- Attributes can be categorical or continuous → discretise
- Continuous attributes lead to different methods or strategies, e.g. Naïve Bayes with continuous attributes

- What if the **class** were continuous?

Regression

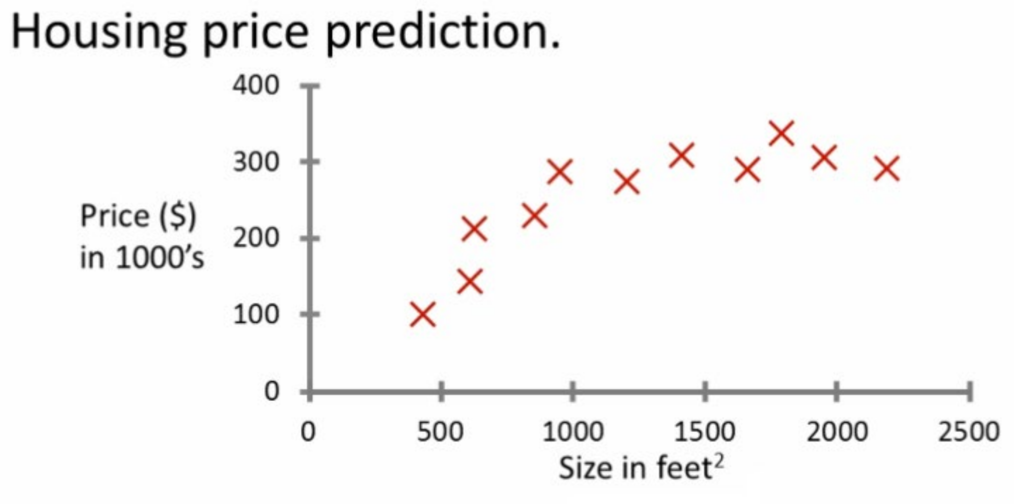
- Continuous attributes → continuous class
- Assuming a linear relationship between the attribute values a_k and the continuous class c, we have:

$$c = w_0 + \sum_{k=1}^{D} w_k a_k$$

where w_k is a weight corresponding to a_k

Regression

- Can we predict housing prices?
- A friend has a house which is 750 square feet. Can we estimate the price of this house?



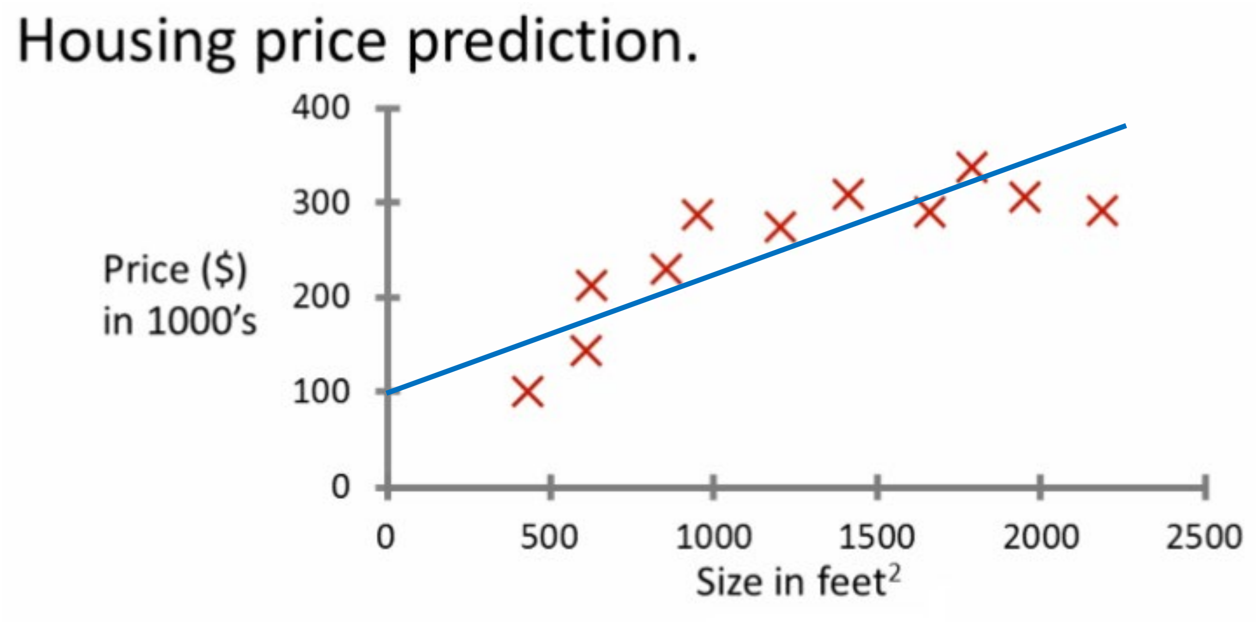
Linear Regression

- Linear regression captures a **linear relationship** between:
  - An **outcome variable** y (or called response variable, dependent variable, label) and
  - One or more **predictors** $x_1, \dots, x_D$ (or called independent variable, explanatory variable, feature)
- At its most basic, the relationship can be expressed as a *line*:

$$y = f(x) = \beta_0 + \beta_1 x_1 + \cdots + \beta_D x_D = \boldsymbol{\beta} \cdot \boldsymbol{x}$$

where $\boldsymbol{x} = [x_0, x_1, \dots, x_D], x_0 = 1$

Linear Regression



Linear Regression

- Linear functions capture changes in one variable that correlate linearly with changes in another variable.
- A simple assumption! They are less descriptive than non-linear functions, but permit simpler mathematical strategies.
- For some variables, this assumption makes sense.

  Example: The more umbrellas you sell, the more money you make. How much money you make is directly proportional to how many umbrellas you sell.

Training and Prediction

Training set: *N* examples

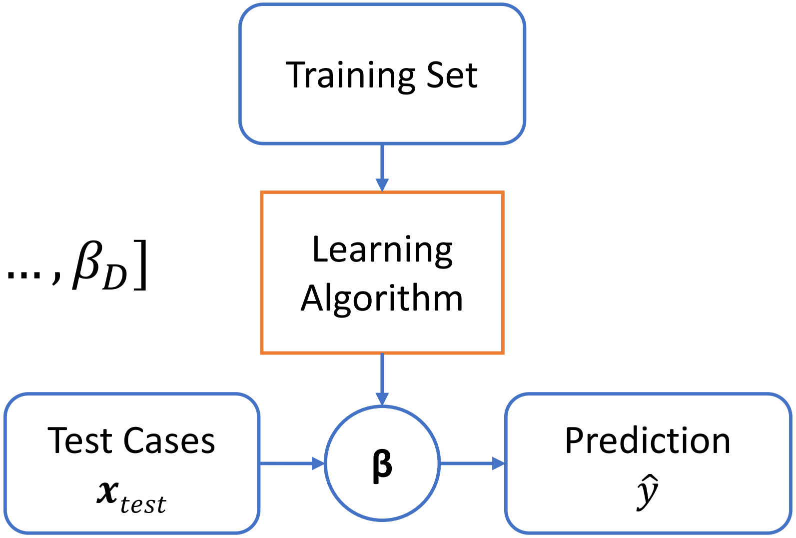
$(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_N, y_N),$

$\boldsymbol{x}_i = [x_{i0}, x_{i1}, x_{i2}, \ldots, x_{iD}]$

Find the optimal $\boldsymbol{\beta} = [\beta_0, \beta_1, \beta_2, \ldots, \beta_D]$

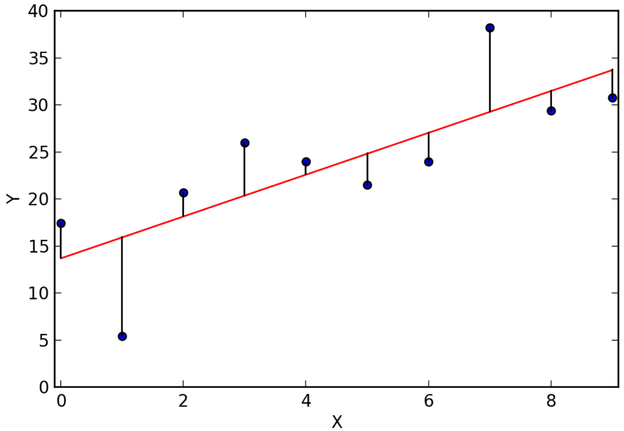
Predict a continuous valued output

$$\hat{y} = \boldsymbol{\beta} \cdot \boldsymbol{x}_{test}$$



Fitting the Model

- We want to choose the *best line*
  - Operationally, the line that minimises the *distance* between all points and the line.
  - Recall Euclidean distance: $d(A,B) = \sqrt{\sum_{k=1}^{D}(a_k - b_k)^2}$



Fitting the Model

- **Least squares method**: find the line that minimises the sum of the squares of the vertical distances between predicted $\hat{y}$ and actual y.
- **Minimise** the Mean Squared Error (MSE) of N data points

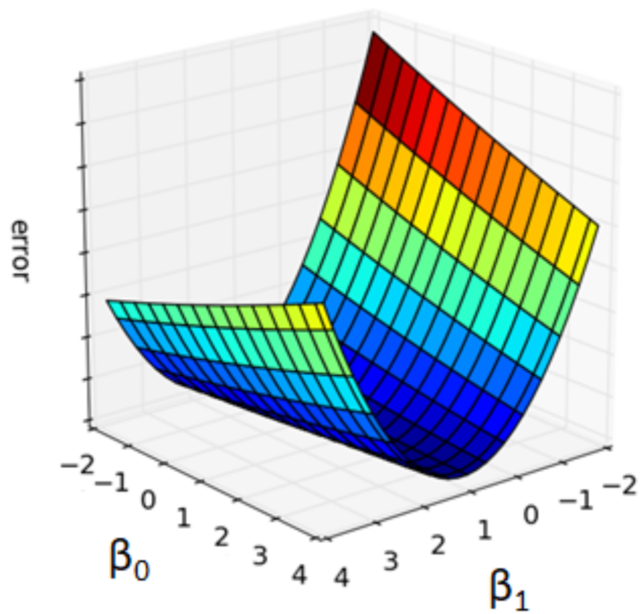
$$MSE = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2 = \frac{1}{N}\sum_{i=1}^{N}(y_i - \boldsymbol{\beta} \cdot \boldsymbol{x}_i)^2$$

$$\widehat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \mathrm{MSE}$$

loss function

Fitting the Model

- Good news! MSE is convex, the local minimum is a global minimum



Fitting the Model

- **Solution:** calculate partial derivatives of the loss function, with respect to $\boldsymbol{\beta}$, for N instances and D attributes
- Set $\frac{\partial}{\partial \beta_0}$ and all $\frac{\partial}{\partial \beta_k}$ to 0, and solve D+1 equations with D+1 unknowns

$\frac{1}{N}\sum_{i=1}^{N}(y_i - \underbrace{(\beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k)}^{\hat{y_i}})^2$

$[\beta_0, \cdots \beta_k] \cdot [1, x_1, \cdots x_k]$

closed form solution

$$\widehat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \frac{1}{N}\sum_{i=1}^{N}(y_i - \boldsymbol{\beta} \cdot \boldsymbol{x}_i)^2$$

$$\frac{\partial}{\partial \beta_0} = -\frac{2}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i) \qquad \frac{\partial}{\partial \beta_k} = -\frac{2}{N}\sum_{i=1}^{N}x_{ik}(y_i - \hat{y}_i)$$

Parameter Estimation

- Optimisation
- Computing the Optimal Solution
- Gradient Descent

Optimisation

- Learning can be viewed as an **optimisation** problem
- Given an evaluation metric M (like Accuracy or Error), a dataset T, a feature representation $F(T)$, and a learner L with parameters θ
  - Maximise or minimise $M\big(\theta; L, F(T)\big)$, where learner L and dataset $F(T)$ are fixed
  - If M is error rate,

$$\hat{\theta} = \arg\min_{\theta \in \Theta} Error\ (\theta; L, F(T))$$

- Learning => finding parameters that optimise some criterion M for model L and feature representation $F(T)$

Computing the Optimal Solution

How to find the optimal solution?

$$\hat{\theta} = \arg\min_{\theta \in \Theta} Error\,(\theta; L, F(T))$$

- Analytic solution
- Exhaustive solution
- Grid search
- Iterative approximation

Computing the Optimal Solution

$$\hat{\theta} = \arg\min_{\theta \in \Theta} Error\,(\theta; L, F(T))$$

Analytic Solution

- closed form, can be computed exactly
- requires solving a system of equations

$$\frac{\partial(Error)}{\partial\theta_1} = 0, \frac{\partial(Error)}{\partial\theta_2} = 0, \ldots, \frac{\partial(Error)}{\partial\theta_D} = 0$$

- e.g. for linear regression, $\hat{\boldsymbol{\beta}} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$
- challenges: derivatives can be undefined or not calculable

Computing the Optimal Solution

$$\hat{\theta} = \arg\min_{\theta \in \Theta} Error\,(\theta; L, F(T))$$

Exhaustive solution not for continuous values ~~&~~ discrete

- For each $\theta \in \{k_1, k_2, \ldots, k_n\}$, calculate $Error\,(\theta; L, F(T))$
- For M parameters, each taking N **unique** values, it requires N^M train-evaluate cycles all comb: N^M
- Works for methods with a small number of hyperparameters, taking a small number of values, e.g. KNN
  - Similarity measure: Euclidean, Manhattan, cosine,…
  - Voting strategy: majority, ID, ILD,… inverse distance → inverse
  - Number of neighbours: 1, 2, 3, …

Computing the Optimal Solution

$$\hat{\theta} = \arg\min_{\theta \in \Theta} Error\ (\theta; L, F(T))$$

Grid Search numeric

- For each numerical $\theta \in R$
  - Identify boundaries of range R_-, R_+
  - Divide range $[R_-, R_+]$ into equal-width samples select step size
  - calculate $Error\ (\theta; L, F(T))$ for each sample
- More samples: closer to optimal estimate, but more time required

small step size more time

large step size miss the optimal estimate

Computing the Optimal Solution

$$\hat{\theta} = \arg\min_{\theta \in \Theta} Error\,(\theta; L, F(T))$$

Iterative approximation

1. **Initialisation**: set $iter = 0$, guess θ^0
2. **Evaluate**: compute $Error\,(\theta^{iter}; L, F(T))$
3. **Termination**: decide whether to stop
4. **Update**: compute θ^{iter+1} based on θ^{iter}; increase

$$iter := iter + 1$$

5. **Repeat**: Go to Step 2

efficient

Gradient Descent

$$\hat{\theta} = \arg\min_{\theta \in \Theta} Error\ (\theta; L, F(T))$$

Gradient Descent

$$\theta^{iter+1} := \theta^{iter} - \alpha \nabla Error(\theta^{iter}; L, F(T))$$

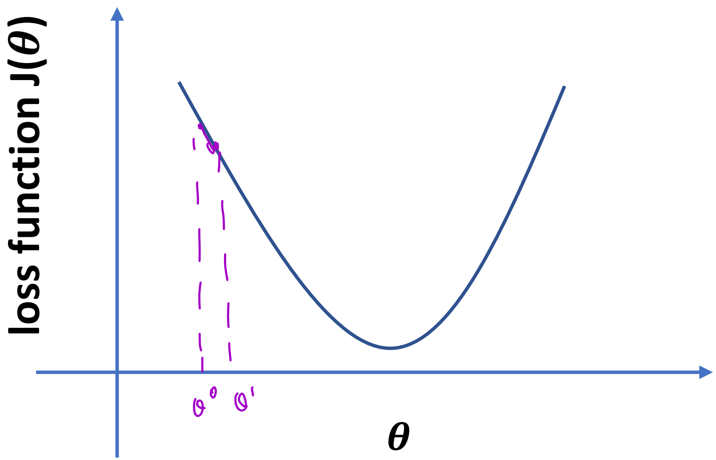
$$\theta_k^{iter+1} := \theta_k^{iter} - \alpha \frac{\partial\ Error(\theta_k^{iter})}{\partial \theta_k^{iter}}$$

- Find the direction: $\nabla Error(\theta)$ is a vector of partial derivative terms, which measures the slope (=gradient) of the function
- Each update reduces the error slightly

Gradient Descent

- α is learning rate, which defines how big a step to update θ_k^{iter}
  - If α is too small, the algorithm might be slow.
  - If α is too large, you might miss the minimum

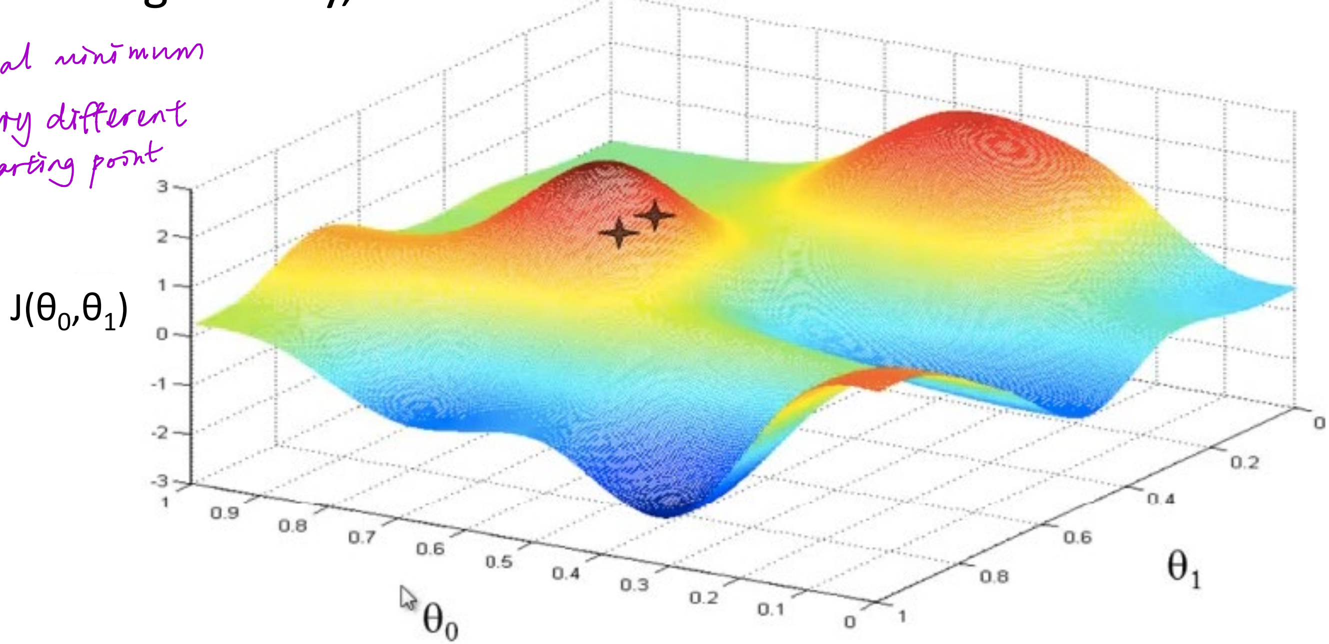
$\theta^{i+1} = \theta^{i} - a \cdot \frac{\partial J(\theta)}{\theta^{i}} \cdot J(\theta)$



Gradient Descent

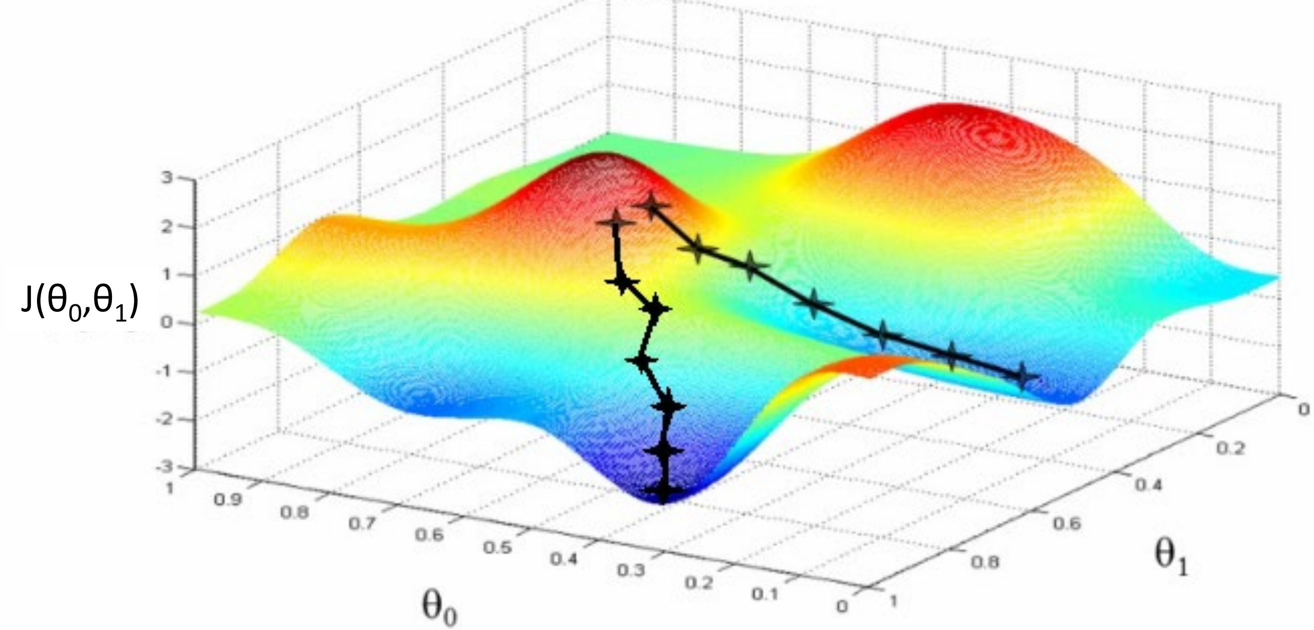
More generally, for non-convex loss function

local minimum
⇒ try different starting point



Gradient Descent

More generally, for non-convex loss function



Gradient Descent

For linear regression

$Error_i = (y_i - \beta x_i)^2$

$Error_{mean} = \frac{1}{N}\sum(y_i - \vec{\beta} x_i)^2$

$$\beta_k^{iter+1} := \beta_k^{iter} - \alpha \frac{\partial\, Error\left(\beta_k^{iter}\right)}{\partial \beta_k^{iter}} = \beta_k^{iter} + \frac{2\alpha}{N}\sum_{i=1}^{N} x_{ik}\left(y_i - \widehat{y_i^{iter}}\right)$$

$\frac{\partial\, Error}{\partial \beta} = \frac{2}{N}\sum_{i=1}^{N}(y_i - \beta x_i)\cdot x_{ik}$

Gradient descent steps for iteration $iter$

- Calculate prediction $\widehat{y_i^{iter}}$ for each training instance
- Compare prediction with actual value y_i
- Multiply by the corresponding attribute value x_{ik}
- Update weight β_k after all the training instances are processed

Application and Evaluation

Linear Regression Application

- Example on a dataset with more features

PRP = - 56.1 + 0.049 MYCT+ 0.015 MMIN+ 0.006 MMAX+ 0.630 CACH-
0.270 CHMIN+ 1.460 CHMAX

Table: CPU dataset

MYCT	MMIN	MMAX	CACH	CHMIN	CHMAX	PRP
125	256	6000	256	16	128	199
29	8000	32000	32	8	32	253
29	8000	32000	32	8	32	253
29	8000	32000	32	8	32	253
29	8000	16000	32	8	16	132
26	8000	32000	64	8	32	290
23	16000	32000	64	16	32	381
…	…	…	…	…	…	…

Categorical Attributes

- We can easily map nominal attributes onto numeric attributes through binarisation or one-hot encoder
- If we treat each resulting binary feature as continuous, we can use linear regression as it is

Evaluation

- It doesn't make sense to evaluate numeric prediction tasks in the same manner as classification tasks
  - true positive matches (direct hits) are an unreasonable expectation
  - regression can make use of the inherent ordering and scale of the outputs
- There are many scoring metrics for regression tasks, all of which are based on the **absolute or relative difference** between the predicted value $\hat{y}_i$ and actual y_i value of test instances

don't want to cancel + / -.

Evaluation Metrics

- Mean Squared Error (MSE):

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

- Root Mean Squared Error (RMSE): scale down $\approx |y_i - \hat{y}_i|$

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

- Root Relative Squared Error (RRSE): relative to baseline $\bar{y} = \frac{1}{N}\sum y_i$

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

Evaluation Metrics

- Correlation Coefficient (Pearson's correlation): statistical correlation between predicted and actual values

strong positive correlation

→ accurate

$$r = \frac{S_{\hat{Y}Y}}{\sqrt{S_{\hat{Y}} S_Y}}$$

$$S_{\hat{Y}Y} = \frac{\sum_i (\hat{y}_i - \bar{\hat{y}})(y_i - \bar{y})}{N - 1}$$

$$S_{\hat{Y}} = \frac{\sum_i (\hat{y}_i - \bar{\hat{y}})^2}{N - 1}, S_Y = \frac{\sum_i (y_i - \bar{y})^2}{N - 1}$$

Evaluation Metrics

- Which metric to use?

  The relative ranking of methods across the different metrics is reasonably stable, such that the actual choice of metric isn't crucial

	A	B	C	D
RMSE	67.8	91.7	63.3	**57.4**
RRSE	42.2	57.2	39.4	**35.8**
CC	0.88	0.88	0.89	**0.91**

Beyond Linear Relationship

- Linear regression is an intuitive model, with relatively easy implementation
- But can we really expect a linear relationship between feature values and target variables?
- Other regression methods
  - regression trees
  - locally weighted linear regression
  - support vector regression
  - …

Beyond Linear Relationship

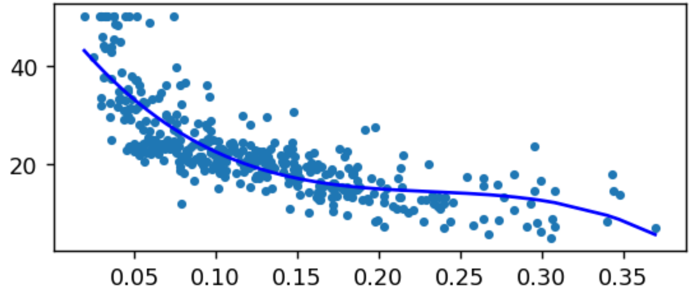
- Polynomial of x as input variables

$$\overrightarrow{\varphi(x)} = [1, x, x^2, x^3, \ldots, x^D]$$

$$\mathbf{z} = [z_0, z_1, z_2, z_3, \ldots, z_D]$$

$$\hat{y} = \boldsymbol{\beta} \cdot \boldsymbol{z}$$

- Can capture nonlinear relationship regarding x



Summary

- What is linear regression, and how does it operate?
- How is learning a type of optimisation? learning ~ optimisation
- What is gradient descent, and why is it used for linear regression?
- How can we evaluate regression tasks?

Question 3

0 / 1 pts

If a linear regression fits the training data perfectly, which of the following is true?

You Answered

- Fitness of test data is unrelated to the linear regression model
- It will never fit test data perfectly
- It will fit test data perfectly as well

Correct Answer

- None of the above

Fitness of the test data depends on how well the model fits the training data, as well as how well the test data is represented in the training data. If test data is represented perfectly, in another word, there is no noise in the test data, the model can fit test set perfectly. Otherwise, it won't.

Question 4

0 / 1 pts

Which of the following are correct about linear regression?

Correct!

- [x] The model should represent a line which minimises the MSE.

You Answered

- [x] The true relationship between the outcome variable and predictors is linear
- [ ] The predictors are estimated measurements with errors

Correct Answer

- [ ] Linear regression captures changes in one variable linearly with changes in another variable

In linear regression models, the predictors are features, which are accurate measurements, and outcome/response values are estimations. The true relationship between the outcome variable and predictors may not be linear.