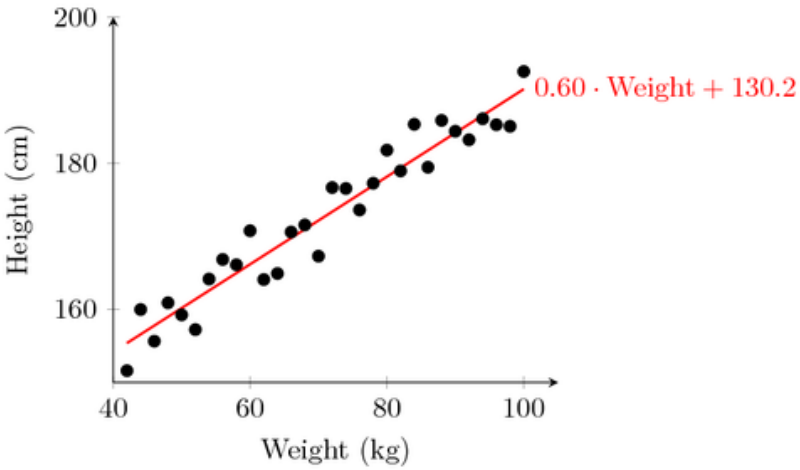
1 Linear regression (for regression)

Model a scalar target with one or more quantitative features.
Although regression computes a linear combination, features can be transformed by nonlinear functions if relationships are known or can be guessed.



Example of prediction using a linear regression model

1.1 Univariate linear regression

- Description

  Simple linear regression is a statistical method that studies the relationship between two variables:
  - x: the predictor, explanatory, independent variable,
  - y: the response, outcome, dependent variable.

- Model's hypothesis

  $h(x) = \theta_0 + \theta_1 * x = \hat{y}$

- Model's parameters (# 2)
  - θ_0
  - θ_1

- Cost function (in this case, the squared error function)

  $J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(\hat{y}^i - y^{(i)}\right)^2$

- Goal

  $minimize_{\theta_0, \theta_1} J(\theta_0, \theta_1)$

- Algorithm
  - gradient descent
    - start with some initial values for θ_0 and θ_1 (usually zero)
    - keep changing θ_0 and θ_1 to reduce $J(\theta_0, \theta_1)$
      - $\theta_0 = \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \theta_0 - \alpha \left(\frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^i - y^{(i)}\right) \right)$
      - $\theta_1 = \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) = \theta_1 - \alpha \left(\frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^i - y^{(i)}\right) \cdot x^{(i)} \right)$
  - directly use the following **formulas**
    - $\theta_1 = \frac{\sum_{i=1}^{m} (x^{(i)} - \bar{x})(y^{(i)} - \bar{y})}{\sum_{i=1}^{m} (x^{(i)} - \bar{x})^2}$

    - $\theta_0 = \bar{y} - \theta_1 \bar{x}$

- Notations
    - x: the independent variable
    - y: the dependent variable
    - m: the number of training examples
    - $x^{(i)}$: the input value of the i^{th} training example
    - $y^{(i)}$: the target value of the i^{th} training example
    - $\hat{y}^{(i)}$: the prediction made on the i^{th} training example by the current hypothesis function
    - α: the learning rate; determines how big steps we take when updating the θ parameters

- Hyperparameters:
    - α: if too small, slow gradient descent; if too large, gradient descent may fail to converge

- Problems:
    - gradient descent may converge to a local minimum

1.2 Multivariate linear regression

- Description

  Multivariate linear regression is a statistical method that studies the relationship between multiple variables:
    - n variables $x = \{x_1, x_2, \ldots, x_n\}$: the predictor, explanatory, independent variables,
    - one y variable: the response, outcome, dependent variable.

- Model's hypothesis

  $h(x) = \theta_0 + \theta_1 * x_1 + \theta_2 * x_2 + \ldots + \theta_n * x_n = \hat{y}$

- Model's parameters (# $n + 1$)

  $\theta = \{\theta_0, \theta_1, \ldots, \theta_n\}$

- Cost function (in this case, the squared error function)

  $J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} \left(\hat{y}^{(i)} - y^{(i)}\right)^2$

- Goal

  $minimize_\theta J(\theta)$

- Algorithm
    - gradient descent
        - start with some initial values for θ_0, θ_1, ..., θ_n (usually 0)
        - keep changing θs to reduce $J(\theta)$
            - $\theta_0 = \theta_0 - \alpha \frac{\partial J}{\partial \theta_0} = \theta_0 - \alpha \left(\frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^i - y^{(i)}\right)\right)$
            - $\theta_1 = \theta_1 - \alpha \frac{\partial J}{\partial \theta_1} = \theta_1 - \alpha \left(\frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^i - y^{(i)}\right) \cdot x_1^{(i)}\right)$
            - ...
            - $\theta_n = \theta_n - \alpha \frac{\partial J}{\partial \theta_n} = \theta_n - \alpha \left(\frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^i - y^{(i)}\right) \cdot x_n^{(i)}\right)$

- Notations
    - x: the independent variables
    - y: the dependent variable
    - m: the number of training examples
    - n: the number of features representing each training example
    - $x^{(i)}$: the input values of the i^{th} training example
    - $x_j^{(i)}$: the value of the j^{th} feature of the i^{th} training example

- $y^{(i)}$: the target value of the i^{th} training example
- $\hat{y}^{(i)}$: the prediction made on the i^{th} training example by the current hypothesis function
- α: the learning rate; determines how big steps we take when updating the θ parameters

- Hyperparameters:
  - α
- Problems:
  - make sure features are on similar scales; gradient descent may be slow otherwise
    - rescaling: $x' = \frac{x - min(x)}{max(x) - min(x)}$
    - mean normalization: $x' = \frac{x - mean(x)}{max(x) - min(x)}$
    - standardization: $x' = \frac{x - mean(x)}{std(x)}$
  - make sure the gradient descent is working correctly
    - plot the value of the cost function J over the number of iterations (# $epochs$)
    - for a sufficiently small α, $J(\theta)$ should decrease on every iteration
    - if α is too small, the gradient descent can be slow to converge
    - if α is too large, $J(\theta)$ may not decrease on every iteration; may not converge
    - try values $\alpha \in \{\dots, 0.001, 0.01, 0.1, 1, \dots\}$
  - in case of **underfitting**
    - try adding new features
      - e.g, use a polynomial regression

        $\theta_0 + \theta_1 * x \quad \Rightarrow \quad \theta_0 + \theta_1 * x + \theta_2 * x^2 + \theta_3 * x^3$
  - in case of **overfitting**
    - reduce the number of features
      - manually select which features to keep
      - use a model-selection algorithm
    - use regularization
      - keep all the features, but reduce the magnitude of parameters θ;
        works well when working with a lot of features, each of which contributes a bit to predicting y
      - intuition: *shrink* model parameters in order to *smooth out* the decision boundary (generate a *simpler* hypothesis)
      - cost function with the *regularization term*

        $J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} \left(\hat{y}^{(i)} - y^{(i)}\right)^2 + \frac{\lambda}{2m} \sum_{j=1}^{n} \theta_j^2$
      - parameter update in gradient descent (for $j \in \{1, 2, \dots, n\}$)

        $\theta_j = \theta_j - \alpha \frac{\partial J}{\partial \theta_j} = \theta_j - \alpha \left(\frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^{i} - y^{(i)}\right) \cdot x_j^{(i)} + \frac{\lambda}{m} \theta_j\right) = \theta_j \left(1 - \alpha \frac{\lambda}{m}\right) - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^{i} - y^{(i)}\right) \cdot x_j^{(i)}$
      - λ is the *regularization parameter* and needs to be tuned;
        it controls the trade-off between the goal of fitting the training data well and the goal of keeping the parameters small