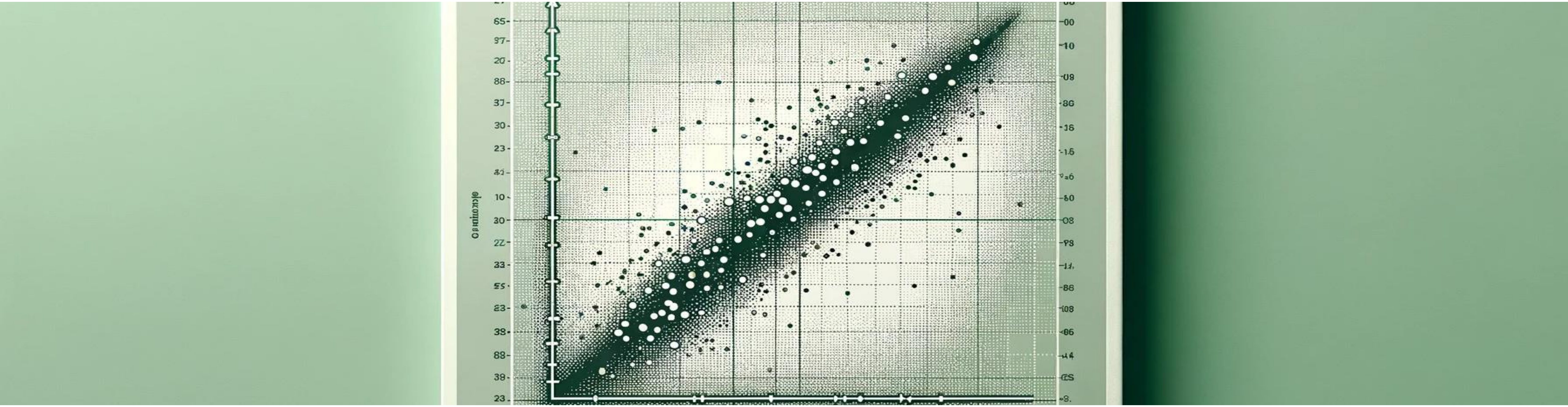
Hochschule Karlsruhe
University of
Applied Sciences

Fakultät für
Elektro- und
Informationstechnik

Linear Regression (1)



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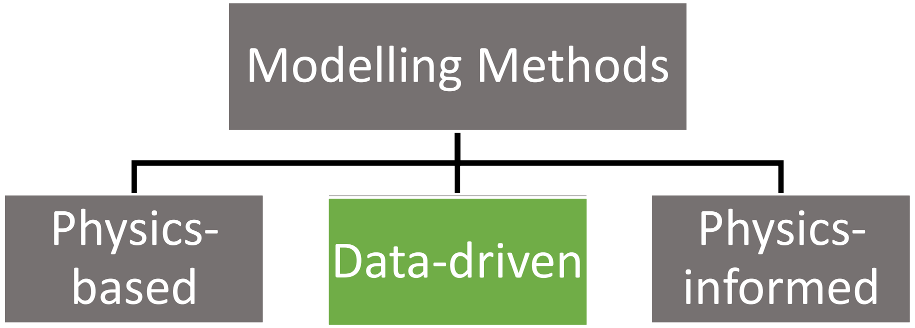
Kawther Aboalam

Linear Regression

Introduction and motivation

+ In fields such as engineering, economics, and medicine, there is a common task of exploring how a certain outcome (dependent variable) is influenced by one or several inputs (independent variables).
+ Classical modeling (Physics-based):
  - Analytical representation of the physical cause-effect relationships
  - Representation for example as block diagram
+ Regression model (Data-driven):
  - System under investigation is considered as a black box
  - Approach leads to mathematical model that describes the interaction of input and output variables
+ Hybrid model (Physics-informed):
  - It integrates data and available physical prior knowledge, even when partially understood



Linear Regression

Simple Linear Regression

+ Linear regression is a supervised algorithm. It is recognized as the most basic and most popular method for solving regression problems.
+ In general, the equation for linear regression is

$$y = \beta_0 + \beta_1 . x_1 + \beta_2 . x_2 + \ldots\ldots + \beta_m . x_m + \epsilon$$

y: the dependent variable to be predicted

x_i: the i^{th} independent variable

β_i: the i^{th} coefficient (weight) of the regression model

ϵ: the irreducible error in the model that represents the unmodeled data

+ By estimating the coefficients as $\hat{\beta}_i$, the dependent variable can be estimated as $\hat{y}$:

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 . x_1 + \hat{\beta}_2 . x_2 + \ldots\ldots + \hat{\beta}_m . x_m$$

+ The simple linear regression model predicts a dependent variable y as $\hat{y}$ by a function of one independent variable x and estimated coefficients ($\hat{\beta}_0$ & $\hat{\beta}_1$)

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 . x_1$$

Heating Load Dataset

WallArea (m^2)	HeatingLoad (W/m^2)
313.07	35.96
402.34	42.47
279.1	33.47
370.83	37.6
441.03	47.48
481.48	49.24
390.09	40.97
280.44	33.16
428.33	44.19
Feature	Target

Linear Regression

Simple Linear Regression

+ Data visualization by a scatter plot
+ There is a positive linear relationship between the Wall Area and the Heating Load
+ A simple linear regression model for the Heating Load that includes the independent variable "Wall Area" can be trained.
+ The equation of the linear model to be trained is

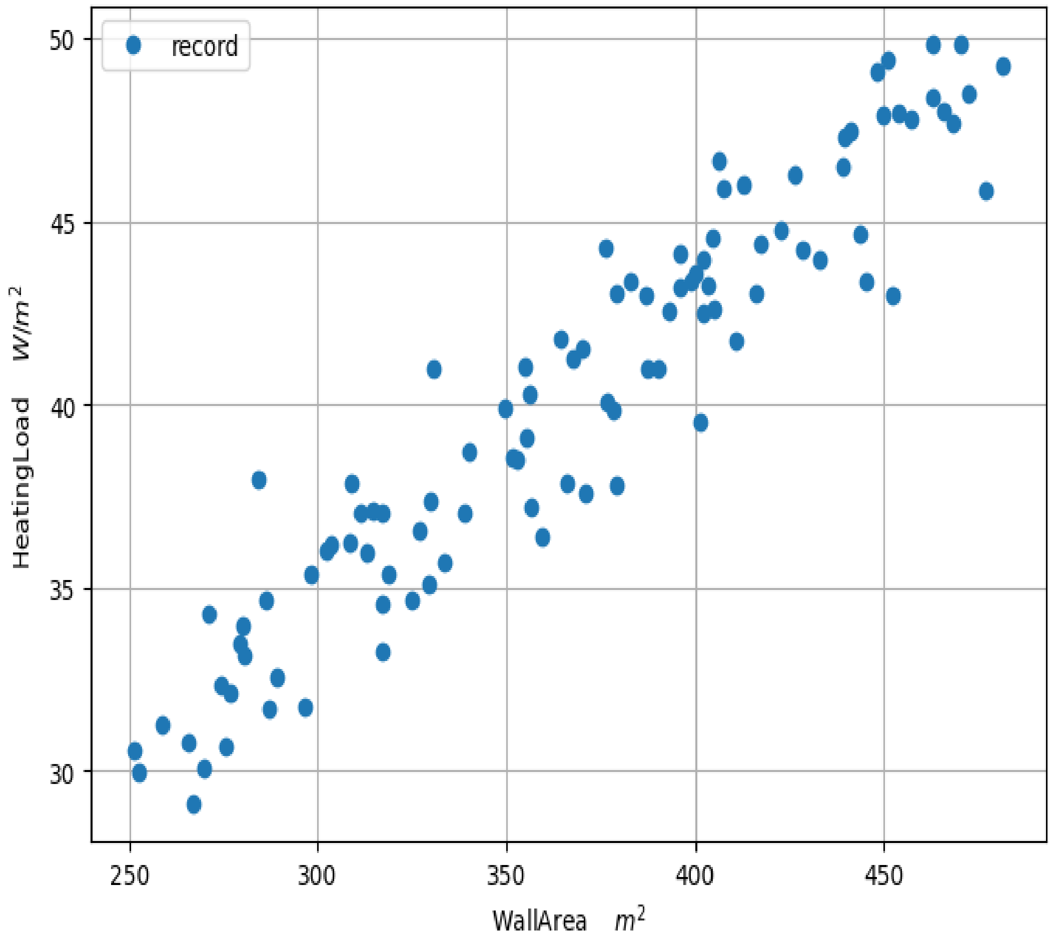
$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 . x_1$$

$\hat{y}$: estimated Heating Load (predicted target)

$\hat{\beta}_0$: intercept of the fit line

$\hat{\beta}_1$: slope of the fit line

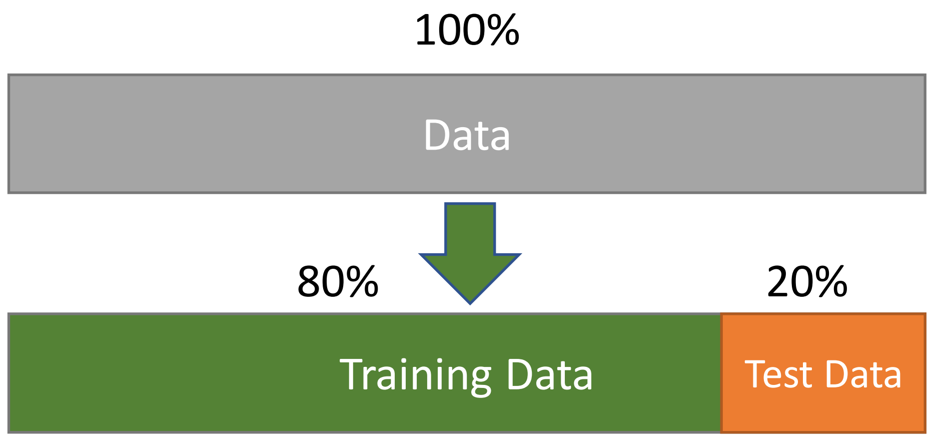
x_1 : Wall Area as a single feature



Linear Regression

Simple Linear Regression – Data Split

- Before model training, the dataset should be divided into training and testing subsets (later into training, validation, and testing subsets)
- Training set: a subset to train a model
- Test set: a subset to evaluate the performance of the trained model (unseen, holdout, can not be used during the training)
- Is there an ideal ratio between a training set and a test set?
- A common split for a dataset is 80% for training and 20% for testing.
- The motivation for using an 80 / 20 split is loosely driven by the Pareto principle (also called the 80–20 rule), which states that 80% of the effect is driven by 20% of causes, and vice versa.



Linear Regression

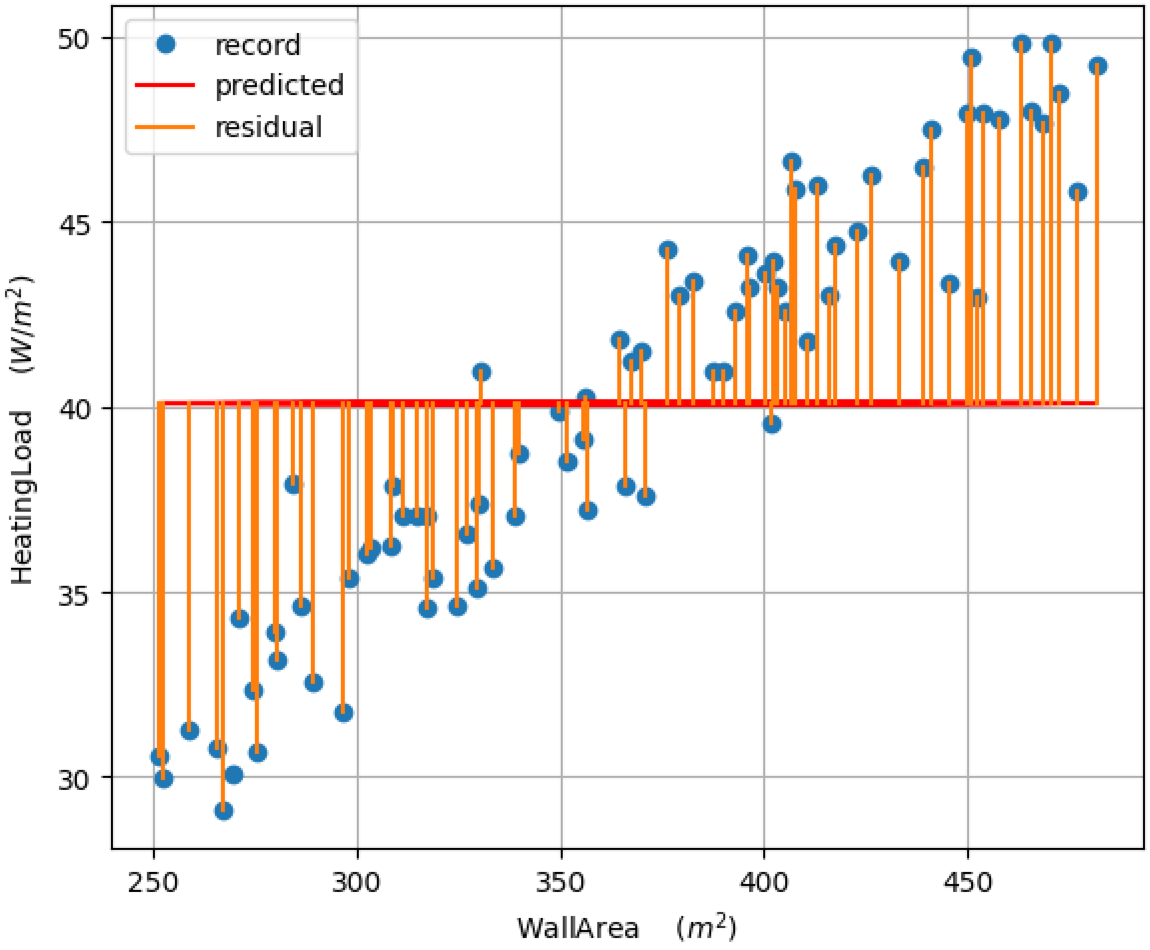
Simple Linear Regression – Model Training

+ During the model training, the best combination of $(\hat{\beta}_0$ & $\hat{\beta}_1)$ is determined
+ Selecting different values of $(\hat{\beta}_0$ & $\hat{\beta}_1)$ results in generating different fit lines
+ Try to choose some combinations and evaluate the model performance by measuring the error (residual) between the predicted target and the true values in the dataset:

1. $(\hat{\beta}_0 = \bar{Y}$ & $\hat{\beta}_1 = 0)$

$\bar{Y}$: the mean value of the target vector of the trainings examples

Training Subset



Linear Regression

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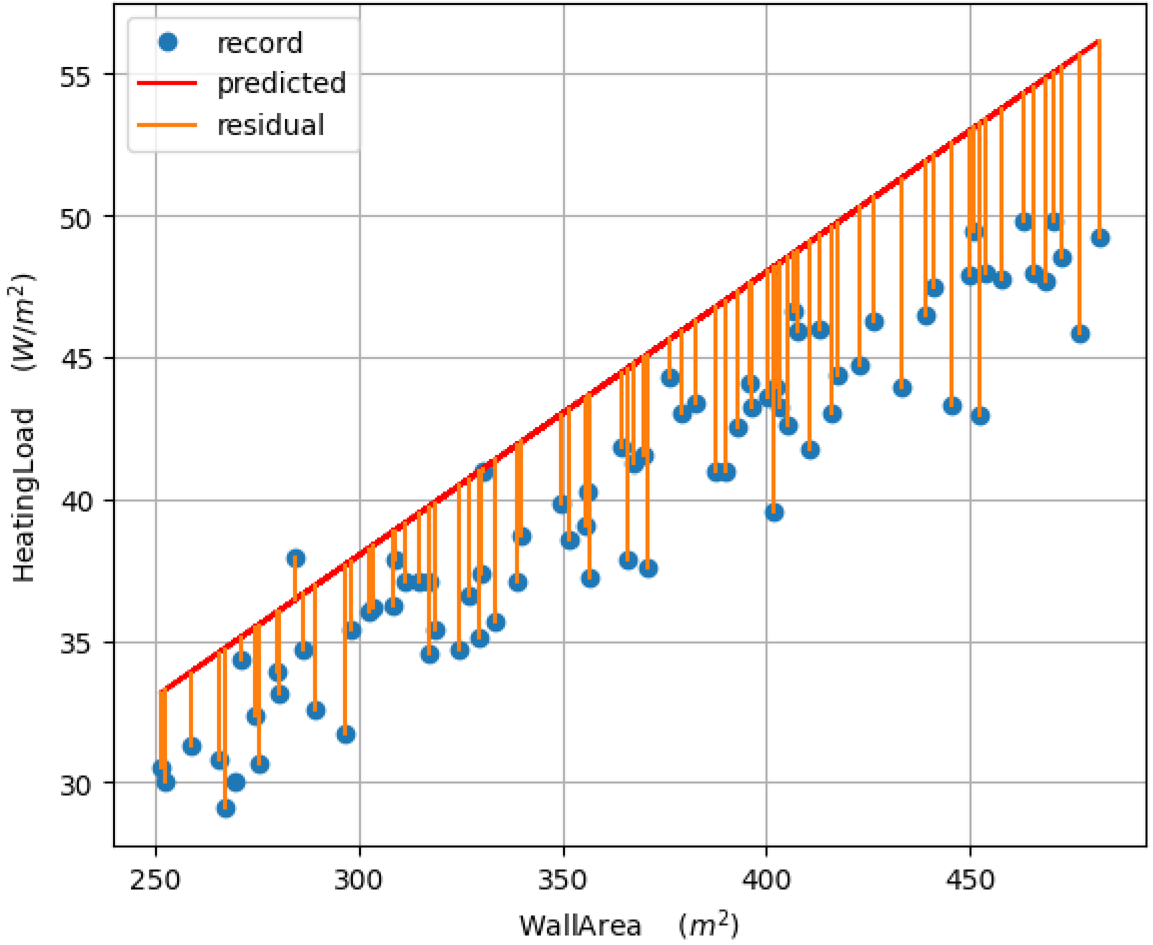
2. ($\hat{\beta}_0 = 8.0$ & $\hat{\beta}_1 = 0.1$)

Training Subset



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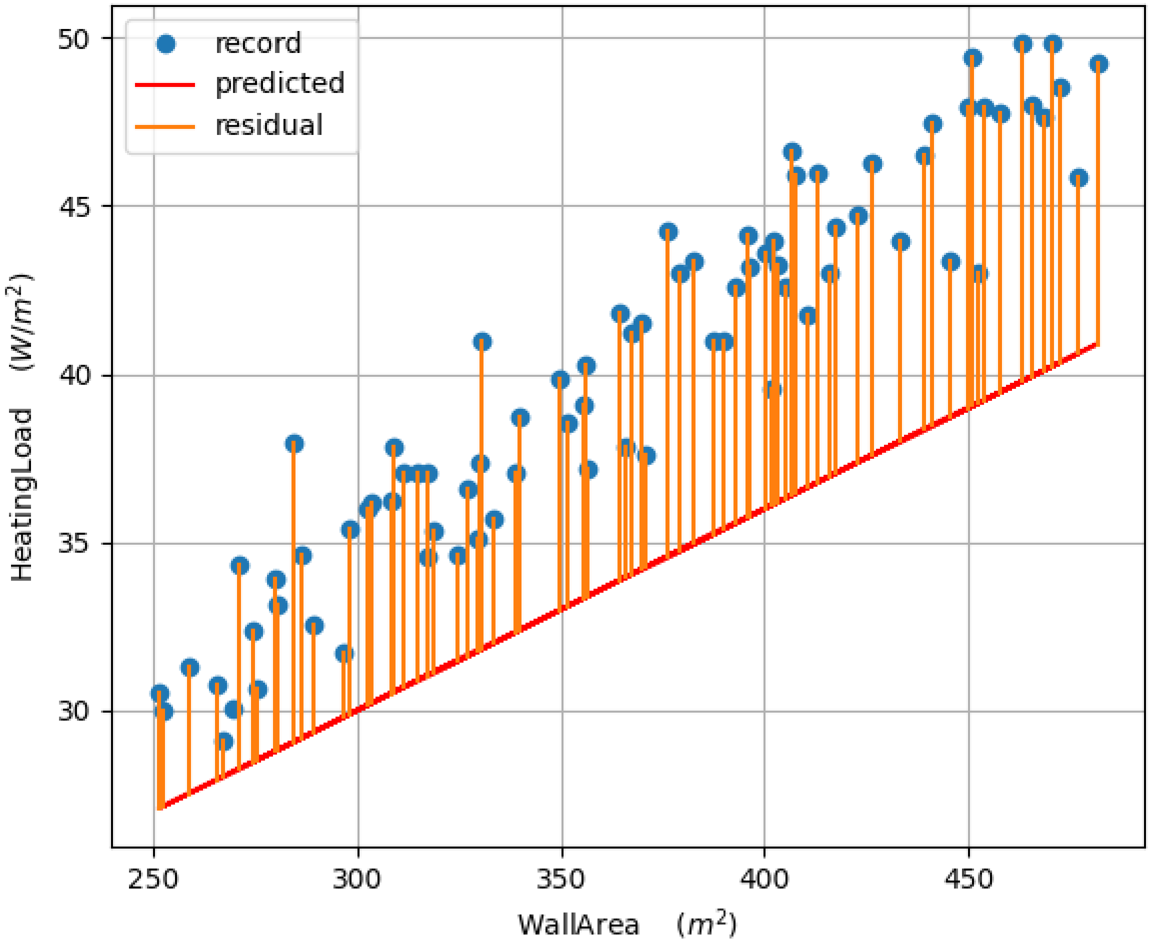
$\bar{Y}$: the mean value of the target vector of the trainings example

2. ($\hat{\beta}_0 = 8.0$ & $\hat{\beta}_1 = 0.1$)
3. ($\hat{\beta}_0 = 12.0$ & $\hat{\beta}_1 = 0.06$)

Training Subset



Linear Regression

Simple Linear Regression – Model Training – Finding best ($\hat{\beta}_0$ & $\hat{\beta}_1$)

+ Approach: Least Squares regression to minimize the Sum of Squared Errors (SSE) (Loss Function L)
+ Why minimize the sum of squared errors, and not the sum of errors?
  - positive and negative errors could indeed cancel each other out, potentially resulting in a sum of errors that is misleadingly close to zero.
+ The least squares method is to find the optimal values of $\hat{\beta}_0$ and $\hat{\beta}_1$ that minimizes

$$\mathrm{L}(\hat{\beta}_0, \hat{\beta}_1) = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$
$$= \sum_{i=1}^{n}(y_i - (\hat{\beta}_0 + \hat{\beta}_1 . x_{1i}))^2$$

where n is the number of the training examples

+ Taking partial derivatives of $\mathrm{L}(\hat{\beta}_0, \hat{\beta}_1)$ with respect to $\hat{\beta}_0$ & $\hat{\beta}_1$ we obtain

$$\left.\begin{aligned} \frac{\partial \mathrm{L}(\hat{\beta}_0, \hat{\beta}_1)}{\partial \hat{\beta}_0} &= -2\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 . x_{1i}) \overset{set}{=} 0 \\ \frac{\partial \mathrm{L}(\hat{\beta}_0, \hat{\beta}_1)}{\partial \hat{\beta}_1} &= -2\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 . x_{1i})x_{1i} \overset{set}{=} 0 \end{aligned}\right\} \quad \text{Solving for } \hat{\beta}_0 \,\&\, \hat{\beta}_1$$

Linear Regression

Simple Linear Regression – Model Training – Finding best ($\hat{\beta}_0$ & $\hat{\beta}_1$)

+ Solving for $\hat{\beta}_0$ and $\hat{\beta}_1$ using the last two equations resulting from the partial derivative of the loss function with respect to the two unknown free parameters gives:

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \overline{X_1} \qquad \text{and} \qquad \hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_{1i} - \overline{X_1})(y_i - \bar{Y})}{\sum_{i=1}^{n}(x_{1i} - \overline{X_1})^2}$$

where $\bar{Y}$: mean value of Y (the target vector of the trainings examples)

$\overline{X_1}$: mean value of X_1 (the input vector of the trainings examples)

Linear Regression

Simple Linear Regression – Model Training – Heating Load Example

+ The optimal values of $\hat{\beta}_0$ and $\hat{\beta}_1$ for the Heating Load example:

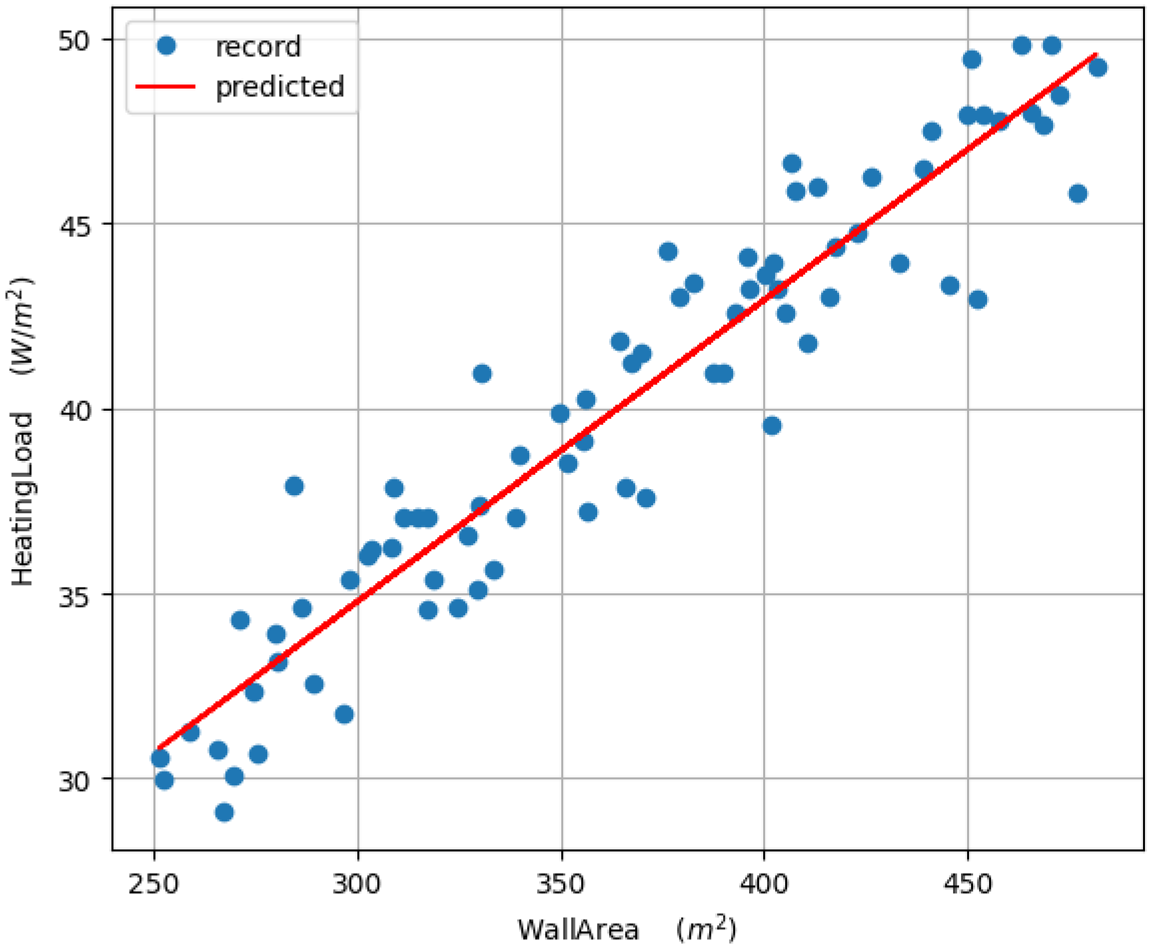
$$(\hat{\beta}_0 = 10.304 \quad \& \quad \hat{\beta}_1 = 0.082)$$

+ The trained model can be represented by the following straight line equation below

$$\hat{y} = 10.304 + 0.082 * x_1$$

The straight line is drawn in the diagram

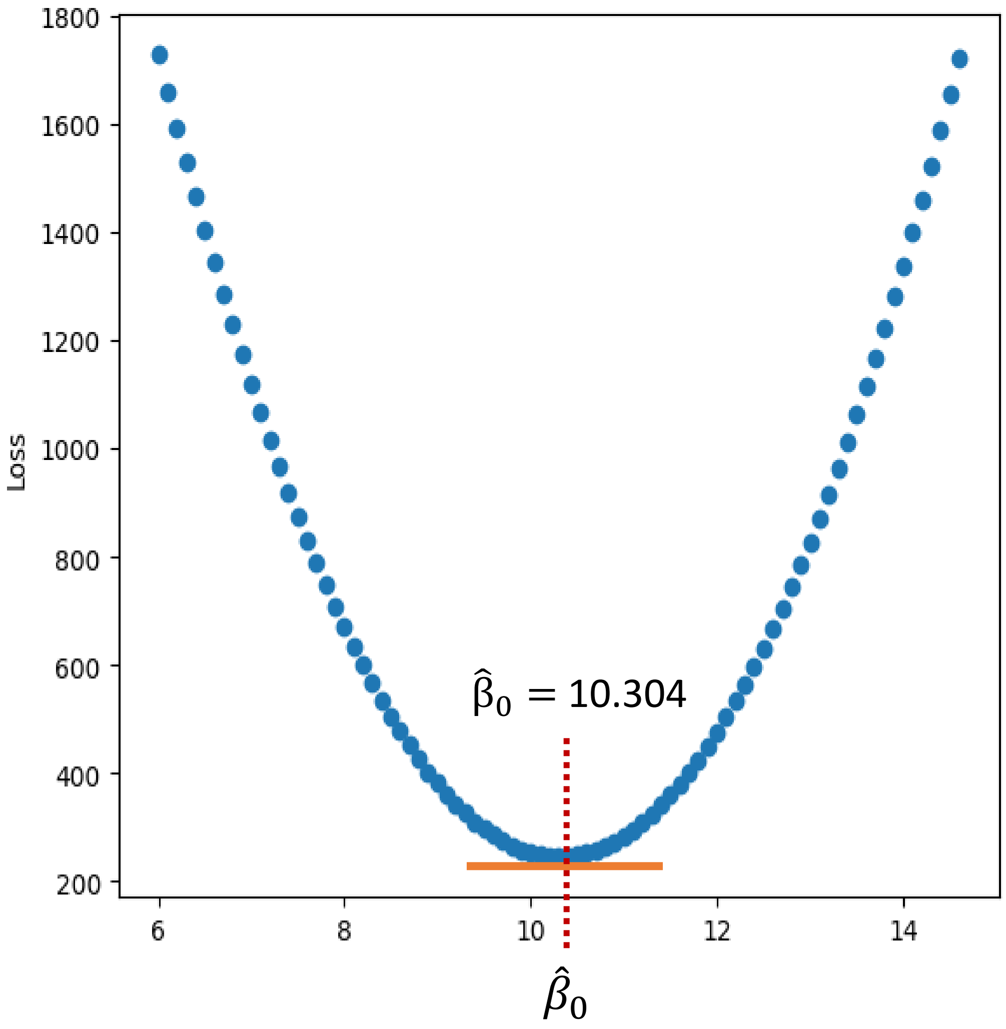
Training Subset



Linear Regression

Simple Linear Regression – Model Training – Heating Load Example

+ Is ($\hat{\beta}_0 = 10.304$ & $\hat{\beta}_1 = 0.082$) the exact solution?
+ Let's check that graphically
    - Fix the value of $\hat{\beta}_1 = 0.082$ and vary the value of $\hat{\beta}_0$ in a range [6,15]
    - Draw the loss function $L(\hat{\beta}_0, \hat{\beta}_1)$ with respect to $\hat{\beta}_0$
+ The partial derivatives of $L(\hat{\beta}_0, \hat{\beta}_1)$ with respect to $\hat{\beta}_0$ is the slope of the curve
+ The slope equals zero at the bottom of the curve that is the most minimum value of the loss with ($\hat{\beta}_0 = 10.304$)



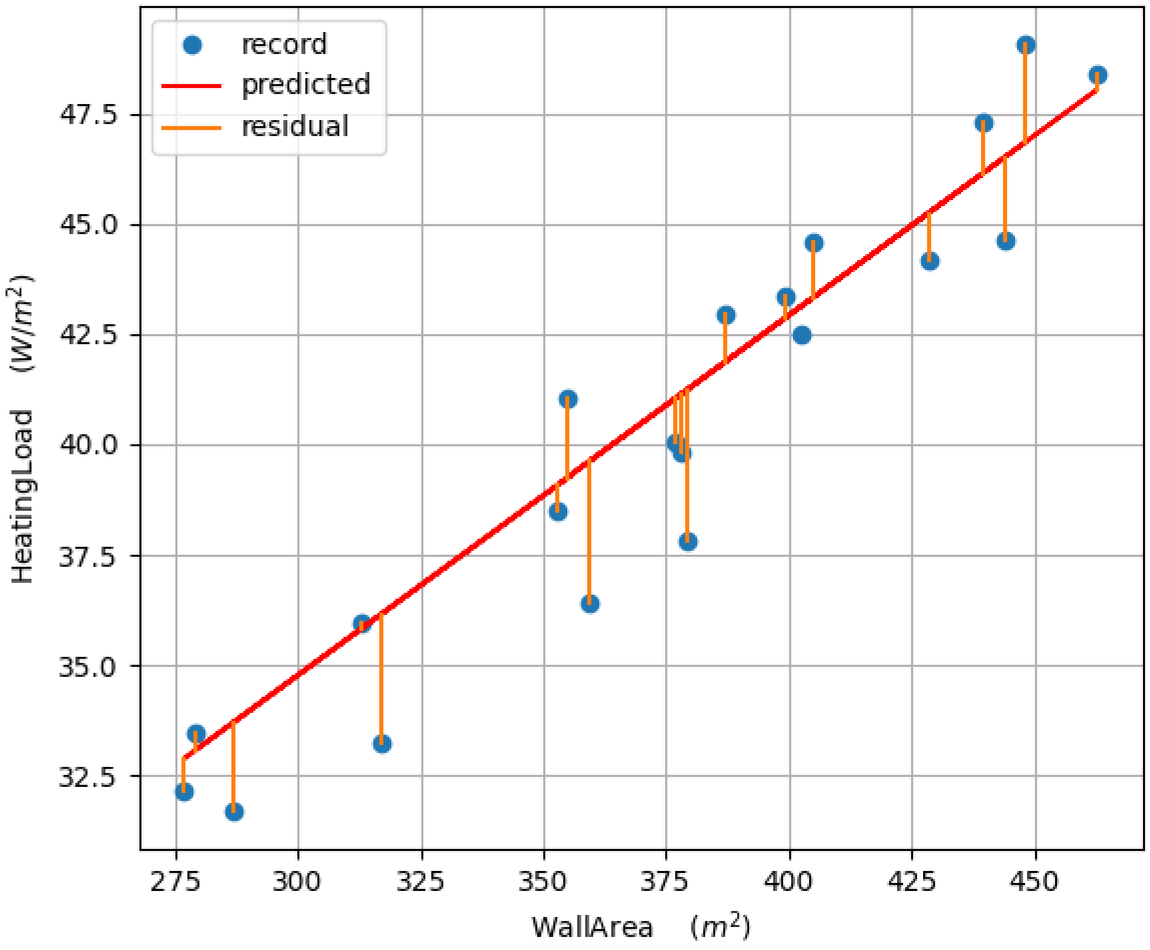
Linear Regression

Simple Linear Regression – Model Evaluation

+ The performance of the model is assessed by its evaluation on the test subset.

+ Regression evaluation metrics help us understand how well the model is making accurate predictions. Common metrics include:
  - Mean Absolute Error (MAE) = 1.38
  - Mean Squared Error (MSE) = 2.80
  - Root Mean Squared Error (RMSE) = 1.76
  - R-squared (R^2) = 0.90

Test Subset



Linear Regression

Simple Linear Regression – Evaluation Metrics

+ Mean Absolute Error (MAE): the average of the absolute differences between predicted and true values

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

- It gives a straightforward measure of prediction accuracy without direction (positive or negative errors don't cancel each other out).

+ Mean Squared Error (MSE): the average of the squared differences between predicted and true values

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

- MSE emphasizes larger errors more than smaller ones because it squares the errors before averaging, making it sensitive to outliers.

+ Root Mean Squared Error (RMSE): the square root of MSE. It is on the same scale as the original data and penalizes larger errors more heavily.

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

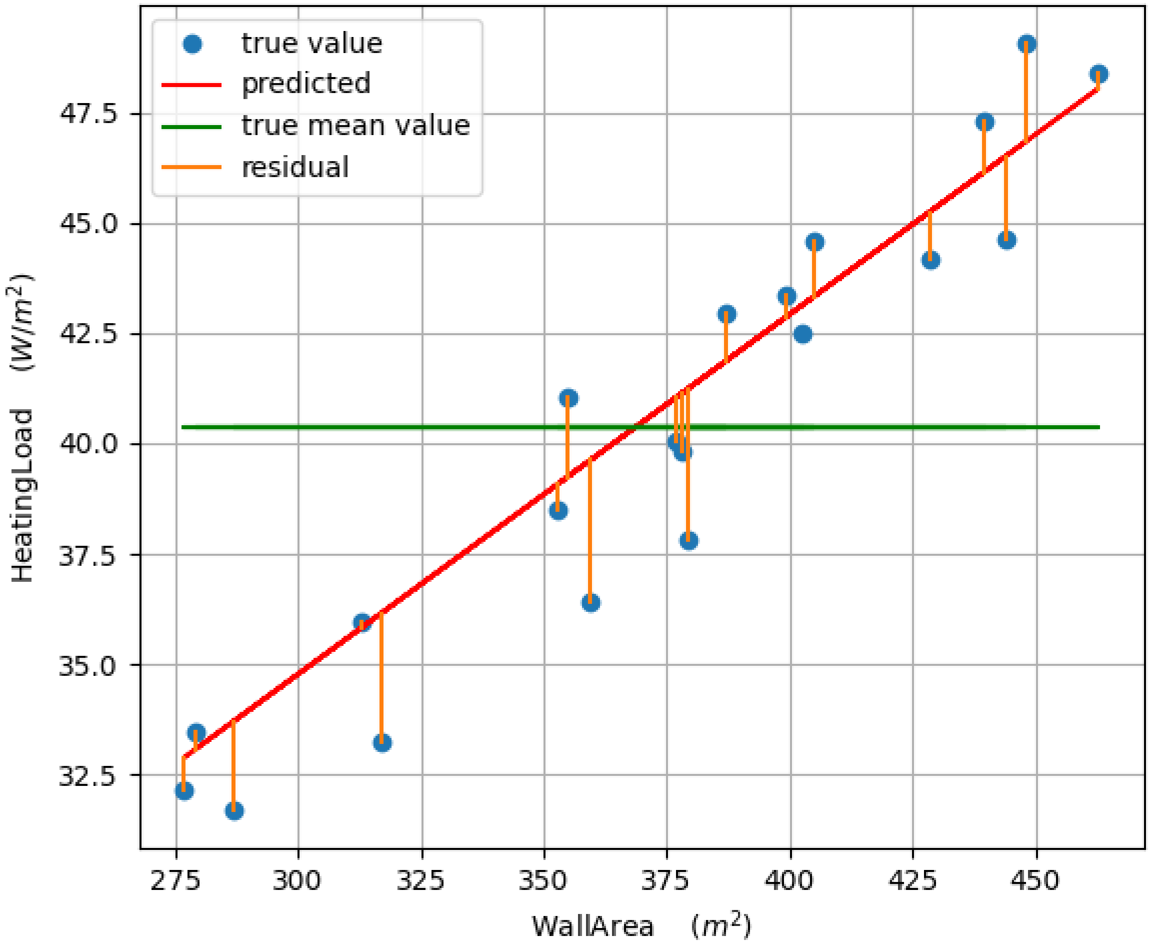
Linear Regression

Simple Linear Regression – Evaluation Metrics

+ R-squared (R^2): Measures the proportion of the variance in the dependent variable that is predictable from the independent variable(s).

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \widehat{y_i})^2}{\sum_{i=1}^{n}(y_i - \bar{Y})^2} = 1 - \frac{RSS}{TSS}$$

- Residual Sum of Squares: RSS= $\sum_{i=1}^{n}(y_i - \widehat{y_i})^2$
- Total Sum of Squares: TSS= $\sum_{i=1}^{n}(y_i - \bar{Y})^2$
- R^2 provides an indication of the goodness of fit of the model, with values closer to 1 indicating a better fit
- R^2=1, that means RSS=0 (zero sum squared error)
- R^2=0, that means RSS=TSS. In this case the model acts like the mean value of the data
- $R^2 < 0$, that means the mean value of the data represents it better than the model itself

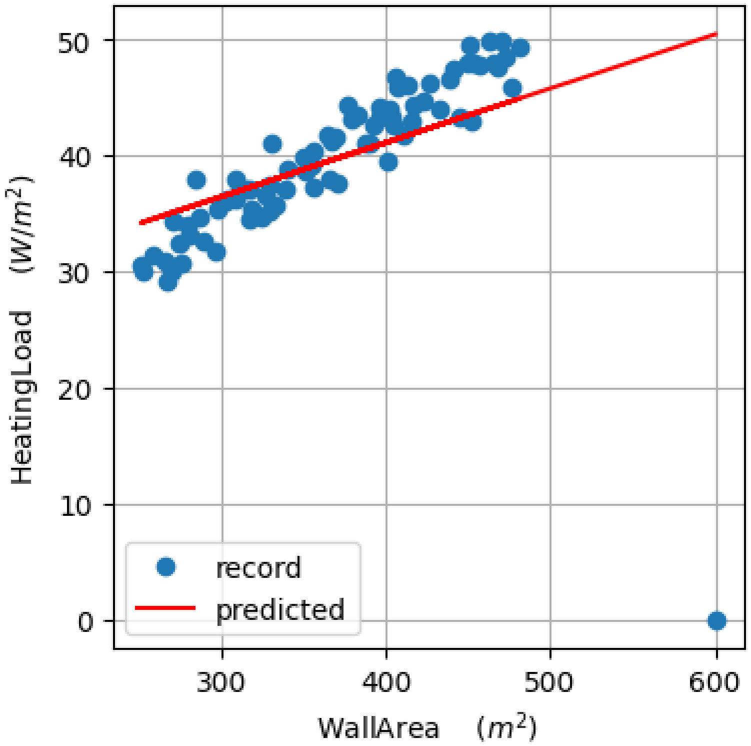


Linear Regression

Simple Linear Regression – Influence of Outlier

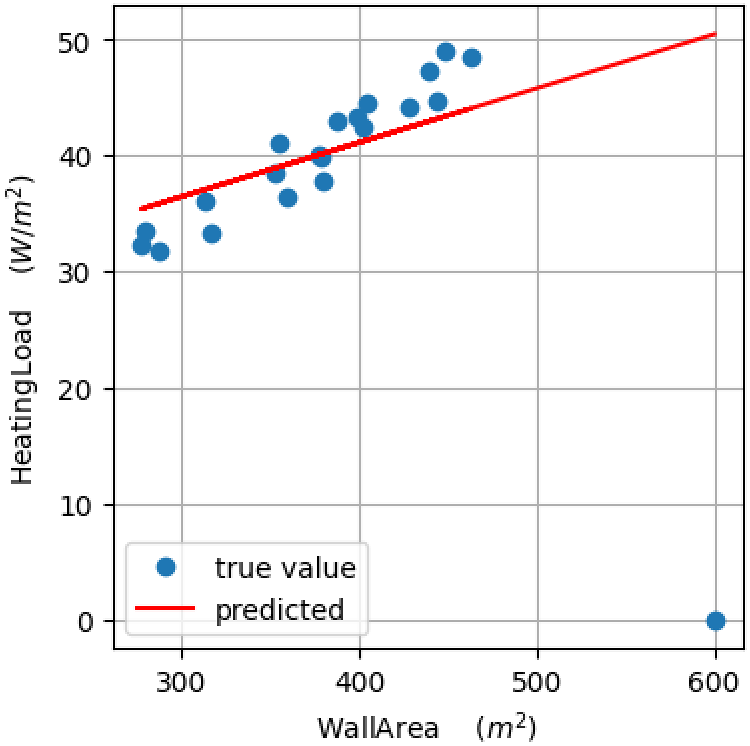
+ Outliers lead to larger residuals, indicating poor model fit

Train Subset



R^2 = 0.21, MAE = 3.04, MSE = 39.90

Test Subset



R^2 = -0.29, MAE = 4.74, MSE = 128.99

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