POLITECNICO DI TORINO

Regression Analysis: Fundamentals

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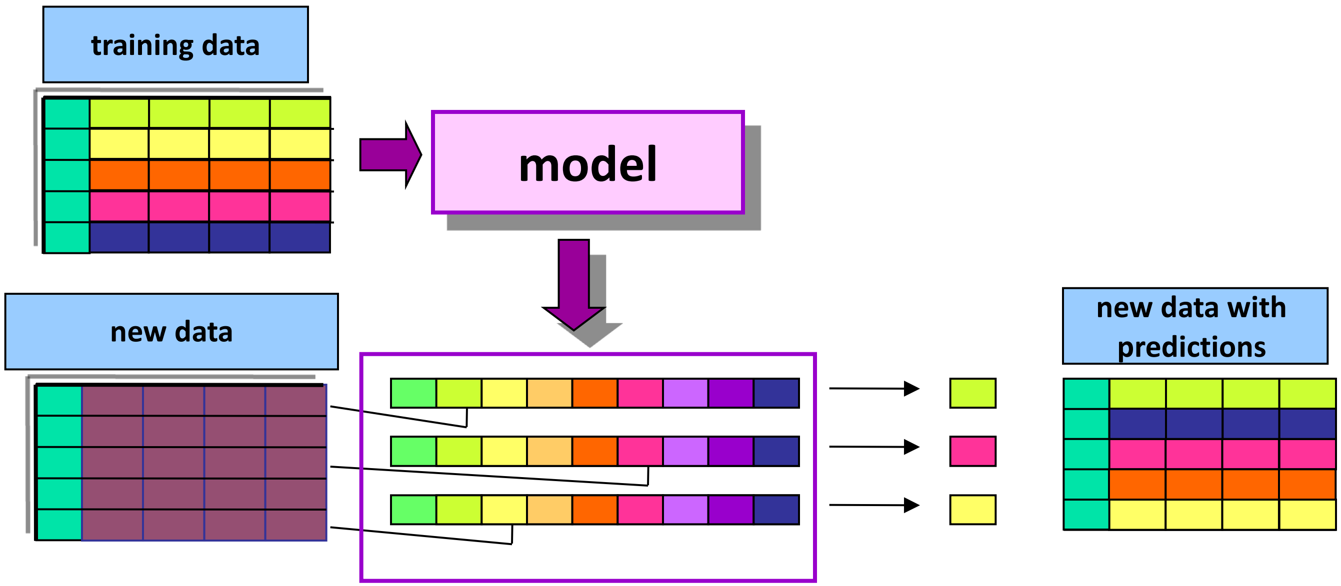
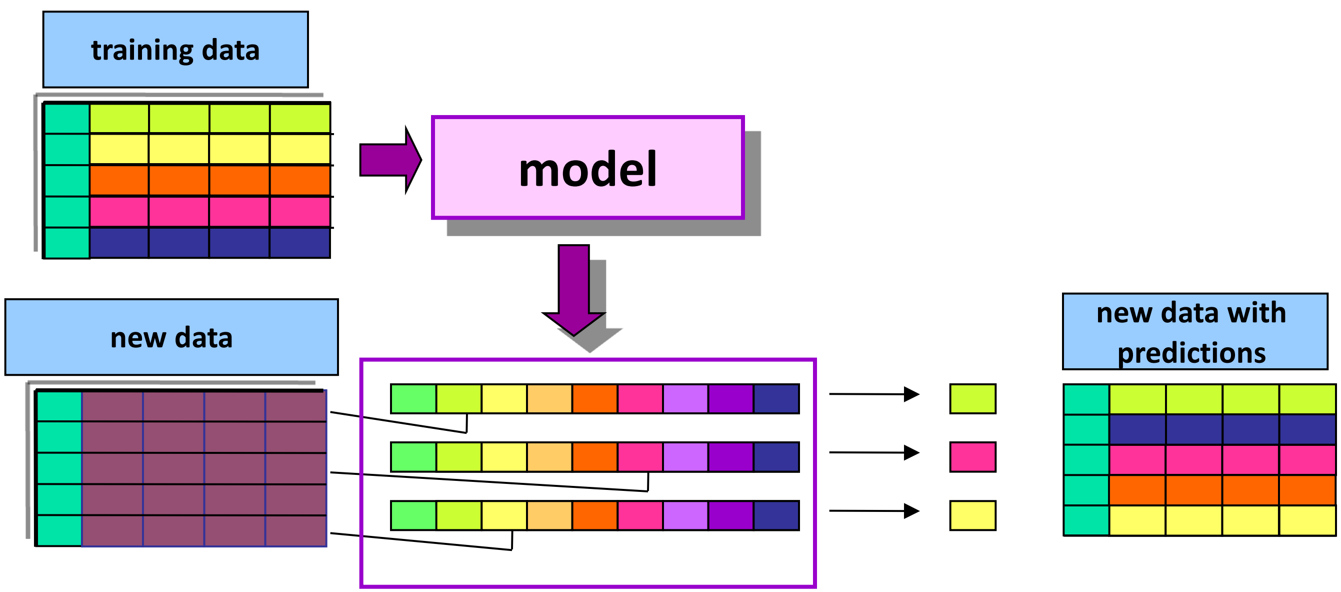
Introduction to the regression analysis

- Objectives
  - Prediction of a **numerical target variable**
  - Definition of a **model** of a given phenomenon



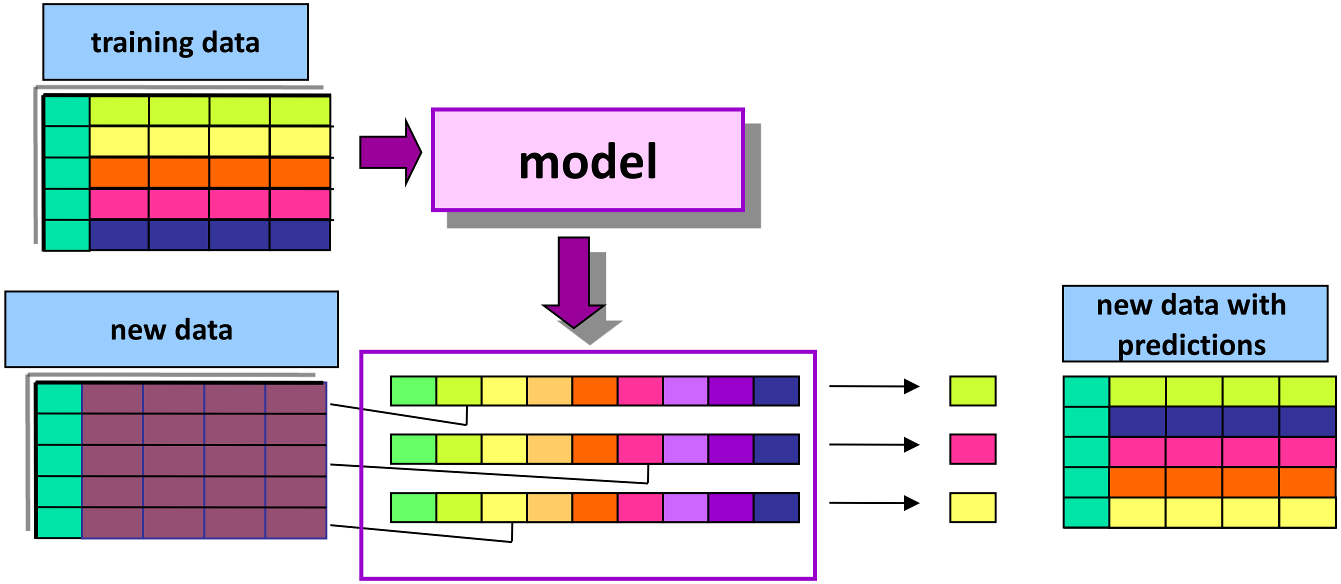
Introduction to the regression analysis

- Approach discussed in this set of slides
  - **Linear regression**
  - **SVMs (SVR)**
- Other approaches
  - k-Nearest Neighbours
  - Decision trees
  - ..



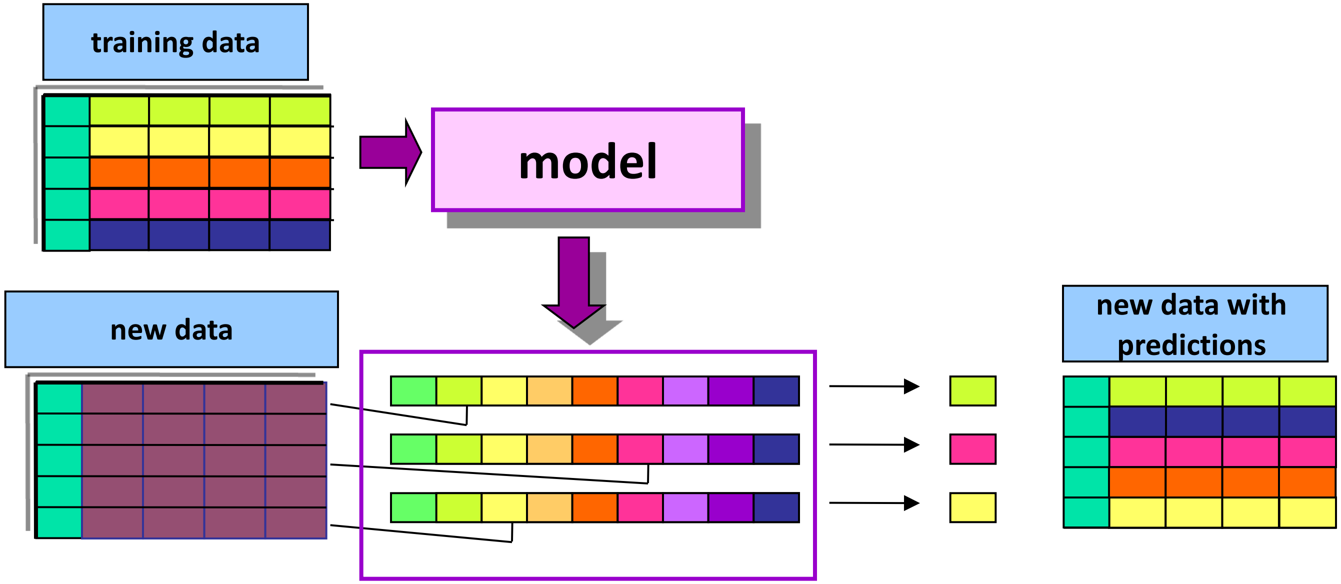
Introduction to the regression analysis

- Requirements
  - **accuracy**
  - interpretability
  - scalability
  - **noise and outlier management**



Introduction to the regression analysis

- Applications
  - Estimating the cost of a house
  - Estimating the remaining useful life (RUL) of an industrial equipment
  - Industrial Vehicle Usage Predictions
  - Predicting the Number of Free Floating Car Sharing Vehicles within Urban Areas
  - …



Introduction to regression

- The term "regression" was coined by **Francis Galton** in 1877 to describe a biological phenomenon
  - the heights of descendants of tall ancestors tend to regress down towards a normal average (i.e, regression toward the mean)
- Father of regression **Carl F. Gauss** (1777-1855)

Definition

- Given
  - A numerical target attribute
  - A collection of data objects also characterized by the target attribute

- The regression task finds a model that allows predicting the target variable value of new objects through
  - $y=f(x_1, x_2, \ldots x_n)$

Regression analysis

- Regression analysis can be classified based on
  - **Number of explanatory variables**
    - Simple regression: single explanatory variable
    - Multiple regression: includes any number of explanatory variables
  - **Types of relationship**
    - Linear regression: straight-line relationship
    - Non-linear: implies curved relationships (e.g., logarithmic relationships)
  - **Temporal dimension**
    - Cross Sectional: data gathered from the same time period
    - Time Series: involves data observed over equally spaced points in time

Simple linear regression

$$y = \beta_0 + \beta_1 x$$

- The regression line provides an **interpretable model** of the phenomenon under analysis
  - y: **estimated** (or predicted) **value**
  - β_0 : estimation of the **regression intercept**
    - The intercept represents the estimated value of y when x assumes 0
  - β_1 : estimation of the **regression slope**
  - x: **independent variable**

Simple linear regression

$$y = \beta_0 + \beta_1 x$$

- *Least squares method*
  - β_0 and β_1 can be obtained by **minimizing the Residual sum of squares (RSS)** that is the sum of the squared residuals
    - differences between actual values (y) and estimated ones $(\hat{y})$

$$min\, RSS = min \sum_i (y_i - \hat{y}_i)^2 =$$

$$min \sum_i (y_i - (\beta_0 + \beta_1 x_i))^2$$

Estimation of the parameters by least squares

$$y = \beta_0 + \beta_1 x$$

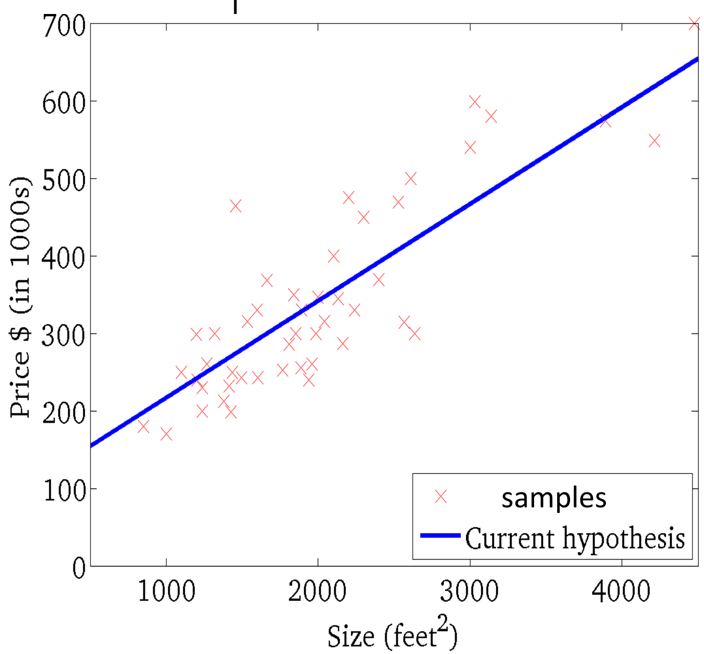
$$\beta_1 = \frac{\Sigma_i (x_i - \bar{x})(y_i - \bar{y})}{\Sigma_i (x_i - \bar{x})^2}$$

$$\beta_0 = \bar{y} - \beta_1 \bar{x}$$

- where $\bar{y} = \frac{1}{n}\sum_i y_i$ and $\bar{x} = \frac{1}{n}\sum_i x_i$ are the sample means

Simple linear regression: example

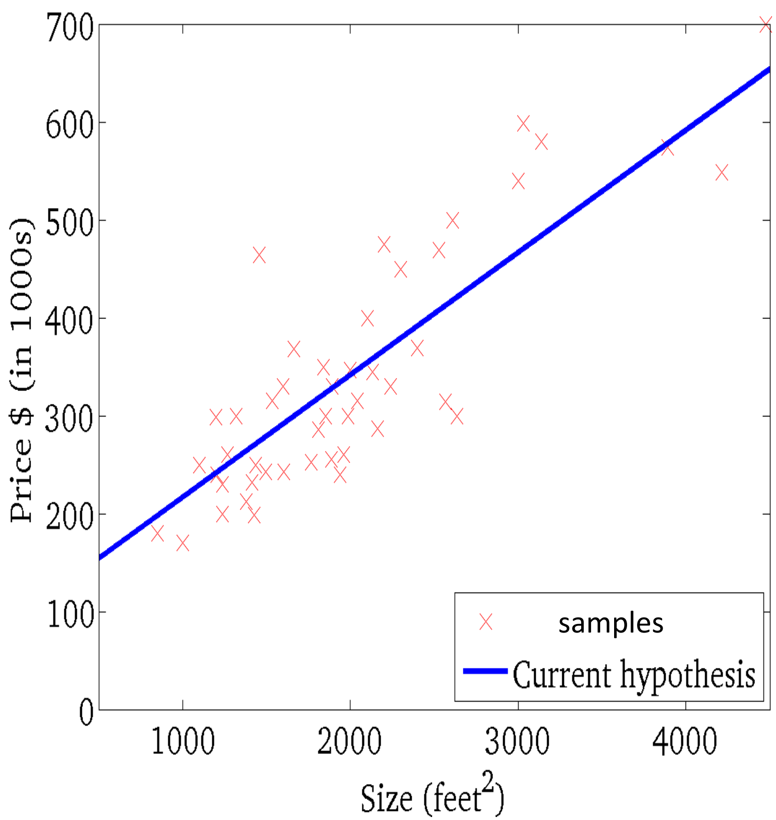
Size in feet^2	Price ($) in 1000's
2104	460
1416	232
1534	315
852	178
…	…



- Goal of a **real estate agency**
  - Estimate the selling price of a home based on the value of size in square feet
- Simple linear regression finds **a linear model** of the problem
  - x = Size in feet^2
  - y = Price ($) in 1000's

$$y = \beta_0 + \beta_1 x$$

Simple linear regression: example



- β_0: The **intercept** represents the estimated value of y when x assumes 0
  - No house had 0 square feet, but β_0 is the portion of house price not explained by square feet
- β_1: the **slope** measures the estimated change in the y value as for every one-unit change in x
  - The average value of a square foot of size

Multiple linear regression

$$y = f(\mathbf{x}) = \beta_0 + \beta_1 \mathbf{x_1} + \beta_2 \mathbf{x_2} + \beta_3 \mathbf{x_3} + \ldots + \beta_n \mathbf{x_n} + \xi$$

- **Dependant variable** (y): the single variable being explained/predicted by the regression model
- **Independent or explanatory variables** (x_i): The variables used to predict/explain the dependant variable
- **Coefficients** (β_i): values, computed by the regression task, reflecting explanatory to dependent variable relationships
- **Residuals** (ξ): the portion of the dependent variable that is not explained by the model
  - The model performs under or over predictions

Interpretating regression coefficients

- Uncorrelated predictors
  - Each coefficient can be estimated and tested separately
  - Interpretation: a unit change in x_i is associated with a β_i change in y, white all the other variables stay fixed
    - β_i represents the average effect on y of a one unit increase in x_i, holding all other predictors fixed
- Correlation among predictors cause problems
  - The variance of all coefficients tends to increase, sometimes dramatically
  - Interpretations become complex: when x_j changes, everything else changes
- The claim of causality should be avoided for the observational data

Feature selection

- In case of a high dimensional data set, in terms of number of dependent variables, **some of the variables** might provide **redundant information**.
- Feature selection and removal (correlation-based approach)
  - simplifying the model computation
  - improving the model performance
  - Enhancing the model interpretation (i.e., better explainability of the dependent variables)
- Variable/feature selection
  - Driven by the business understanding and domain knowledge
  - Feature selection based on correlation test
    - Features highly-correlated with other attributes could be discarded from the analysis
    - having dependence or association in any statistical relationship, whether causal or not

Polynomial regression

- The polynomial models can be used in those situations where the **relationship** between dependent and explanatory variables is **curvilinear**.
- Polynomial regression consists of**:**
  - Computing new **features** that are power functions of the input features
  - Applying **linear** regression on these new features

$$y = \beta + \beta_1 x + \beta_2 x^2 + \varepsilon$$

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \varepsilon$$

  - The above models are also linear (i.e., A model is linear when it is linear in parameters)
  - They are the second order polynomials in one and two variables respectively.
- Sometimes a nonlinear relationship in a small range of explanatory variables can also be modeled by polynomials.

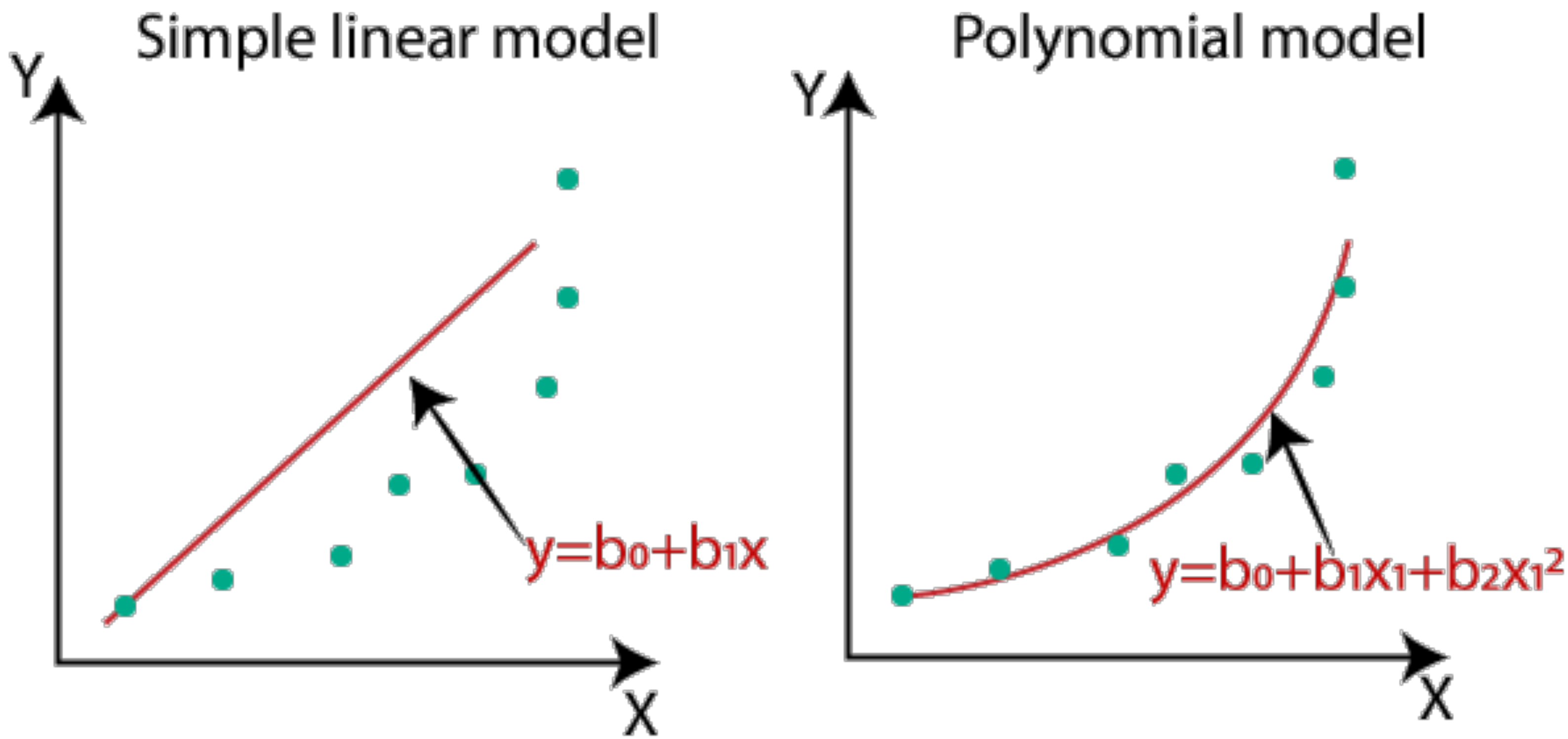
Polynomial model in one variable

- The k[th] order polynomial model in one variable is given by
$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_k x^k + \varepsilon$$
- It is included in the linear regression model below
$$y = X\beta + \varepsilon$$
- Techniques for fitting linear model can be used for fitting the polynomial regression model
- For example, $y = \beta_0 + \beta_1 x + \beta_2 x^2$
  - Is a polynomial regression model in one variable and is called as **second order model** or **quadratic model**, where the coefficients
    - β_1 is the linear effect parameter
    - β_2 is the quadratic effect parameter
- The polynomial models can be used to approximate a complex nonlinear relationship

Polynomial model in one variable

Example.

Second order model or quadratic model



Polynomial regression: considerations in case of one variable

- Order of the model
  - Keep the order of the polynomial model as low as possible
    - Up to the **second order** polynomial
    - If necessary, you should apply some **data transformations**
  - Arbitrary fitting of higher order polynomials can be a serious abuse of regression analysis.
    - Data overfitting issue
- Different model building strategies do not necessarily lead to the same model
  - **Forward selection procedure**: to successively fit the models in increasing order and test the significance of regression coefficients at each step of model fitting.
    - Keep the order increasing until t-test for the highest order term is nonsignificant
    - The significance of highest order term is tested through the null hypothesis
  - **Backward elimination:** to fit the appropriate highest order model and then delete terms one at a time starting with highest order. This is continued until the highest order remaining term has a significant t-test
- The first and second order polynomials are mostly used in practice.

Polynomial models in two or more variables

- The techniques of fitting of polynomial model in one variable can be extended to fitting of polynomial models in two or more variables.
- A second order polynomial is more used in practice and its model is specified by

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \varepsilon$$

- This is also called **response surface**.

Strong and weak points of Polynomial Regression

- Advantages of using Polynomial Regression:
  - **Broad range of function** can be fit under it.
  - Polynomial basically fits **wide range of curvature**.
  - Polynomial usually provides the **best approximation** of the relationship between dependent and independent variable.
- Disadvantages of using Polynomial Regression
  - They are **too sensitive to the outliers**.
    - The presence of a few outliers in the data can seriously affect the results of a nonlinear analysis.
  - Higher polynomial degree means **higher flexibility** of your model, but also **data overfitting**
    - Overfitting occurs in those cases when you have a few samples and a model that has high flexibility
    - It is always possible for a polynomial of order (n-1) to pass through n points so that a polynomial of sufficiently high degree can always be found that provides a "good" fit to the data.
    - Those models **never enhance the understanding** of the unknown function and they are **never good predictors**.

To avoid data overfitting

- Use more training data (if possible)
- Use lower model complexity
- Use regularization techniques
  - e.g., Ridge and Lasso

RIDGE and LASSO

- Regression analysis methods that perform both **variable selection** and **regularization** in order to enhance the prediction **accuracy** and **interpretability** of the statistical model it produces.
- Useful **to reduce model complexity** and **prevent overfitting** when
  - The number of variables describing each observation exceeds the number of observations
  - The number of variables does not exceed the number of observations, but the learned model suffers from poor generalization.
- Techniques of training a linear regression (or a linear regression with polynomial features)
  - They try to assign values **closer to zero (RIDGE) or zero (LASSO)** to the coefficients assigned to features that are not useful for the regression
  - The effect is the **decreasing of the complexity of the model**

Regularization: RIDGE and LASSO

Cost function

Linear regression

$$\text{RSS} = \sum_i (y_i - \hat{y}_i)^2 = \sum_i \left(y_i - \beta_0 - \sum_{j=}^{p} \beta_j x_{ij}\right)^2$$

Ridge regression

$$RSS + \lambda \sum_{j=1}^{p} \beta_j^2$$

Lasso regression

$$RSS + \lambda \sum_{j=1}^{p} |\beta_j|$$

Penalty term λ → amount of shrinkage (or constraint)

Regularization

Ridge regression

- It adds L2 as the penalty
- L2 is the sum of the square of the magnitude of beta coefficients

$$RSS + \lambda \sum_{j=1}^{p} \beta_j^2$$

This is equivalent to minimizing the RSS under the condition

$$For\ c > 0, \sum_{j=1}^{p} \beta_j^2 < c$$

- Penalty term λ → amount of shrinkage (or constraint)
  - Regularizes the coefficients, penalizing coefficients taking large values

LASSO

- LASSO means **Least Absolute Shrinkage and Selection Operator**
- Term coined by Robert Tibshirani in 1996, but it was originally introduced in geophysics literature 10 years before
- Lasso **regularization** was originally defined for **least squares**, but it is easily extended to a wide variety of statistical models in a straightforward fashion
  - E.g., generalized linear models
- The Lasso's **variable selection** relies on the form of the **constraint**
  - It forces the sum of the absolute value of the regression coefficients to be less than a fixed constraint, which forces some coefficients to be set to zero
  - The selected model is simpler since it does not include coefficients set to zero.
- It is similar to RIDGE regression but usually identifier a simpler model
  - **RIDGE** simplifies the model **by shrinking the size of some coefficients**, while **LASSO sets some coefficients to zero**.

Lasso regression

- It adds L1 the penalty
- L1 is the sum of the absolute value of the beta coefficients

$$RSS + \lambda \sum_{j=1}^{p} |\beta_j|$$

This is equivalent to minimizing the RSS under the condition

$$For\ c > 0, \sum_{j=1}^{p} |\beta_j| < c$$

The regularization (L1) can lead to zero coefficients

- i.e. some of the features are completely neglected for the evaluation
  It not only helps in reducing overfitting but also in feature selection

Simple linear regression vs Support Vector Regression

Recall that for linear regression, the parameters and the model can be derived by **minimizing the Residual sum of squares (RSS)**

$$min\,RSS = min \sum_i (y_i - \hat{y}_i)^2 =$$

We can instead be interested in reducing error to a certain degree

- errors within an acceptable range

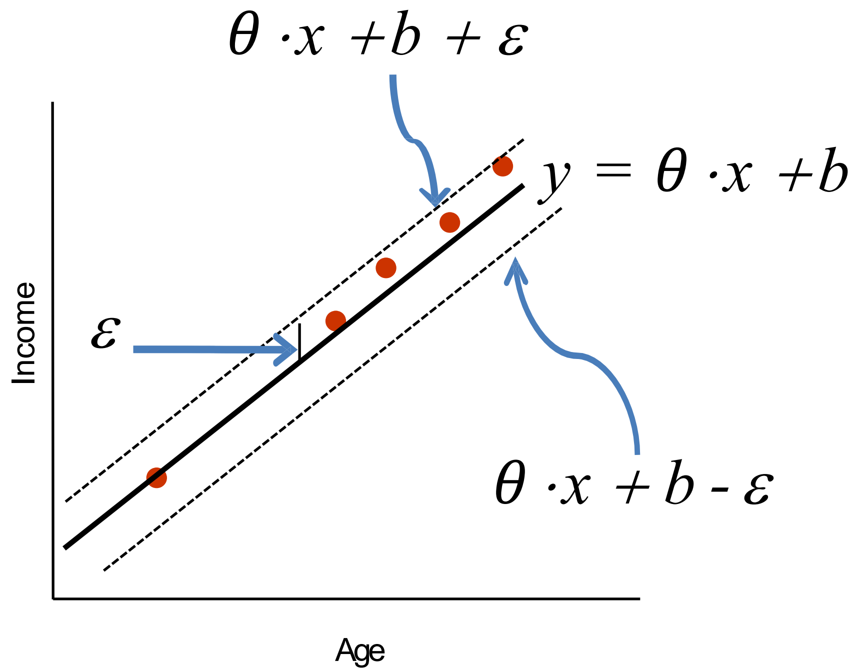
Support Vector Regression

- define how much error is acceptable in our model
- find an appropriate hyperplane to fit the data

Support Vector Machine – Regression

- Find a function, $f(x)$, that performs a prediction of the target attribute y with a maximum error equal to ε

We do not care about errors as long as they are less than ε



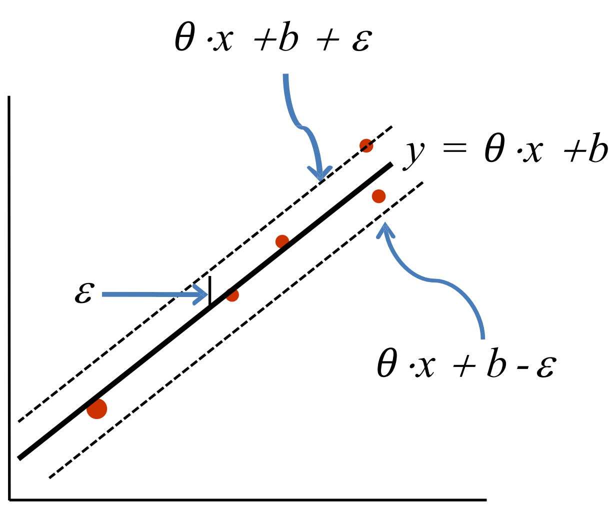
Support Vector Regression: linear model

- The (training) problem can be formulated as a convex optimization problem

$$\min \frac{1}{2} \| \theta \|^2$$

$$s.t. \quad y^i - \theta \cdot x^i - b \leq \varepsilon; \quad \theta \cdot x^i + b - y^i \leq \varepsilon$$

Constraints



y^i = value of the target attribute of the i^th training object

x^i = value of the predictive attributes of the i^th training object

θ and b = parameter of the regression model

Support Vector Regression: Soft margin

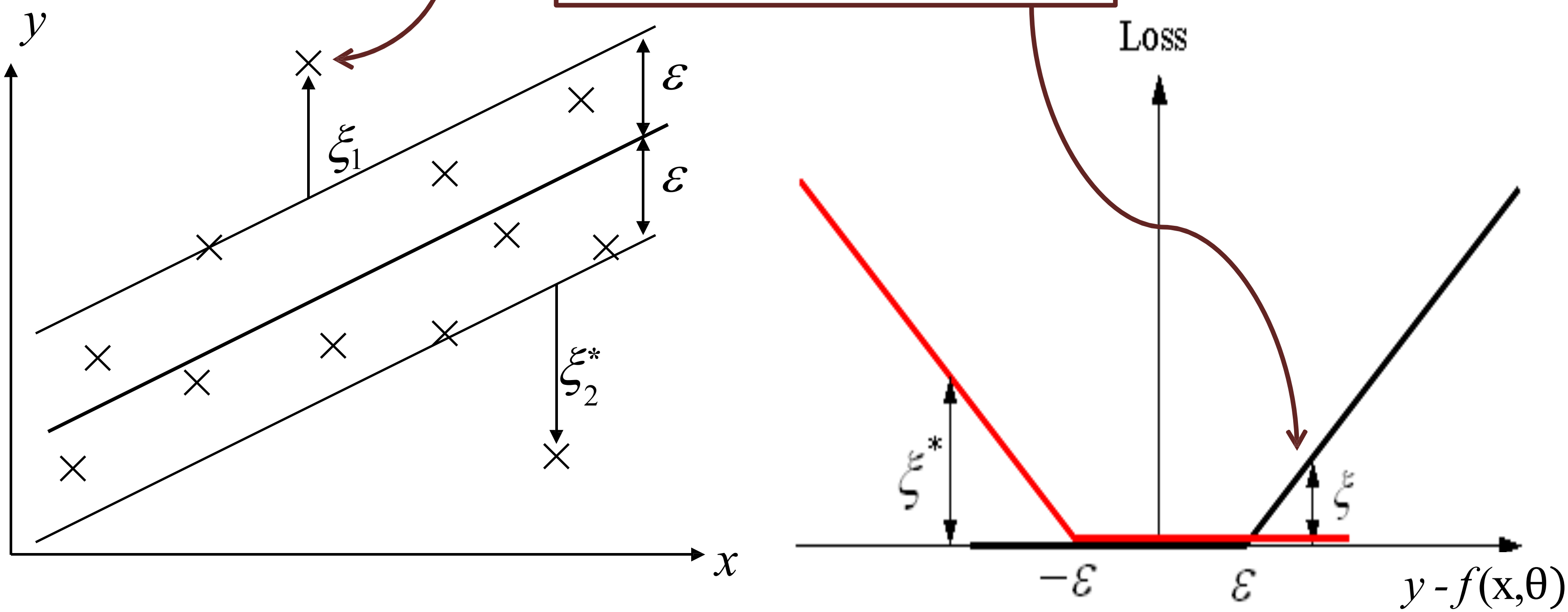
- Given a specific value of ε, the problem is not always feasible
- **Soft margin**
  - Reformulate the problem by considering the errors related to the predictions that do not satisfy the $\boldsymbol{\varepsilon}$ **maximum distance**

Support Vector Regression: Soft margin

Assume linear model

$$f(\mathrm{x},\theta) = \theta \cdot \mathrm{x} + b$$

Only the point outside the ε-region contribute to the final cost



For any value that falls outside of ε, we can denote its deviation from the margin as ξ

Support Vector Regression: Soft margin

- The (training) problem can be formulated as a convex optimization problem

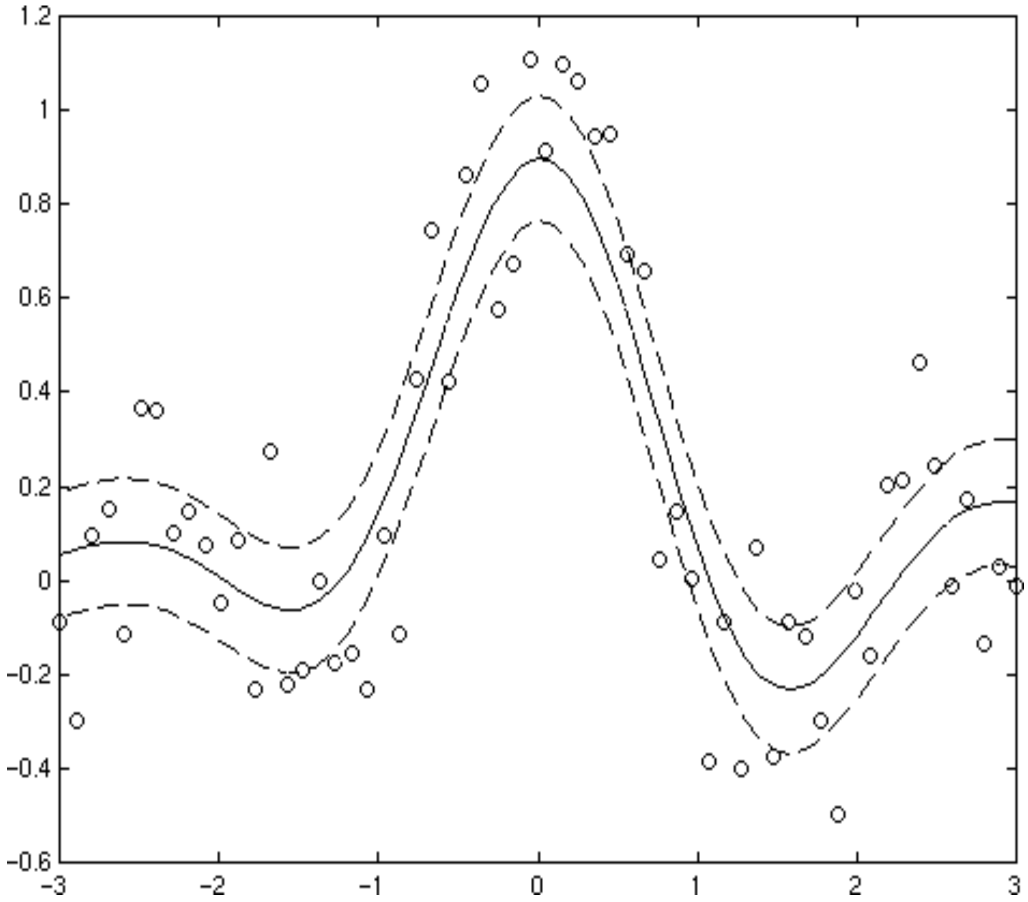
$$\min \frac{1}{2} \| \theta \|^2 + \quad C \sum_{i=1}^{m} (\xi_i + \xi_i^*)$$

$$\begin{aligned} s.t. \quad & y^i - \theta \cdot x^i - b \leq \varepsilon + \xi_i; \\ & \theta \cdot x^i + b - y^i \leq \varepsilon + \xi_i^* \\ & \xi_i, \xi_i^* \geq 0, i = 1, \ldots, m \end{aligned}$$

We minimize the deviation ξ from the margin
C: additional hyperparameter.

- As C increases, also the tolerance for points outside of ε increases

How about a non-linear case?



Linear versus Non-linear SVR

- Map the original features into a higher order dimensional space
- Apply a kernel transformation
  - Polynomial
  - Gaussian radial
  - …
- Transform the input data by means of the kernel function φ and then solve the previous problem

Linear versus Non-linear SVR

- φ maps the input data into a new dimensional space

$$\min \frac{1}{2} \| \theta \|^2 + C \sum_{i=1}^{m} (\xi_i + \xi_i^*)$$

$$\begin{aligned} s.t. \quad & y^i - \theta \cdot \phi(x^i) - b \le \varepsilon + \xi_i; \\ & \theta \cdot \phi(x^i) + b - y^i \le \varepsilon + \xi_i^* \\ & \xi_i, \xi_i^* \ge 0, i = 1, \ldots, m \end{aligned}$$

Evaluating regression

- Evaluation metrics for regression:
  - MAE (Mean Absolute Error)
  - MSE (Mean Squared Error)
  - RSE: Residual Standard Error
  - R^2
  - Adjusted R^2

- The evaluation is performed by comparing
  - y: the actual value (**ground truth**)
  - $\hat{y}$: the predicted value through the regression model

Evaluating regression

- MAE (Mean Absolute Error)
  - the average vertical distance between each real value and the predicted one

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

- MSE (Mean Squared Error)
  - the average of the squares of the errors
  - the average squared difference between the estimated values and the actual value.
  - MSE tends to penalize less errors close to 0

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

- MAE and MSE always > 0
  - The lower the values of MAE and MSE the better the model
  - It is mainly affected by the domains of data sample

Evaluating regression

- Overall accuracy of the model
  - RSE: Residual Standard Error

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

    - n is the number of samples
    - RSS is the residual sum of squares
  - RSE is always greater than 0
    - The lower the RSE value the better the regression model

Evaluating regression

- R^2: R−squared measures the goodness of fit of a model
  - how well the regression predictions approximate the real data points.
  - It estimates a normalized error

$$R^2 = \frac{TSS - RSS}{TSS} = 1 - \frac{RSS}{TSS}$$

  - RSS is the residual sum of squares $RSS = \sum_i (y_i - \hat{y}_i)^2$
  - TSS is the total sum of squares $TSS = \sum_i (y_i - \bar{y}_i)^2$
    with $\bar{y} = \frac{1}{n}\sum_i y_i$

Evaluating regression: R^2

$$R^2 = 1 - \frac{RSS}{TSS} = 1 - FVU$$

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

- R^2 represents the proportion of variance of y explained by variation in x
  - FVU means the fraction of variance unexplained
    - Ratio between the unexplained variance (variance of the model's errors) and the total variance

Evaluating regression: R^2

- R^2 value
  - $R^2 = 1$
    - A perfect linear relationship between x and y
    - 100% of the Y variation is explained by variation in x
  - R^2 close to 1
    - A very good linear relationship between x and y
    - Good predictions
  - $0 < R^2 << 1$
    - Weaker linear relationship between x and y
    - A portion of the variation in y is not explained by variation in x
  - $R^2 = 0$
    - No linear relationship between x and y
    - The value of y does not depend on the value of x
  - $R^2 < 0$
    - the model is predicting worse than the mean of the target values

Evaluating regression: R^2 adjusted

- Drawback of R^2
  - In the context of multiple linear regression, if new predictors (X_i) are added to the model, R^2 only increases or remains constant but it never decreases.
  - However, it is not always true that by increasing the complexity of regression model, the latter will be more accurate
- The Adjusted R-Squared is the modified form of R-Squared that has been adjusted to incorporate model's degree of freedom.
- It should be used to evaluate the quality of a multiple linear regression model

$$\bar{R}^2 = 1 - (1 - R^2)\frac{n-1}{n-p-1}$$

  - p = number of explanatory variables
  - n = number of samples

- The adjusted R-Squared only increases if the new term improves the model accuracy.