Supervised Learning
Regression

Regression vs Classification
Business applications (by task, by sector)
Terminology: from variable to grid search
Mathemical explanation. Linear and Non-linear
Data requirements for core regression models
The process: initiation - evaluation - fine-tuning
Python code for each stage of the process

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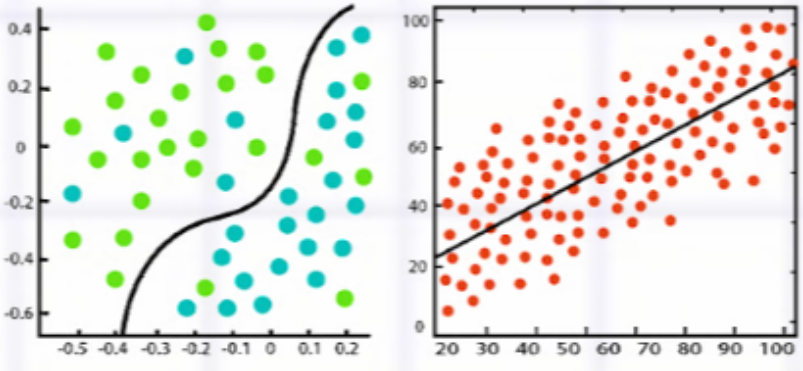
Supervised Learning Models

Regression

Prediction of a continuous value - number or quantity.
Key questions: "How much?", "What will the value be?"
Popular applications: sales forecast, budget changes, pricing

Classification

Assignment of a probability or a category to an observation.
Key questions: "Which group?", "How likely?", “Is it A or B?”
Popular applications: churn prediction, recommender systems



Classification Regression

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Business Applications

Areas

🧩 **Value Creation**: demand forecasting, market research (“synthetic consumer”).

💰 **Revenue Model**: promo efficiency, price elasticity, customer lifetime value (CLV).

🔍 **Market Opportunity**: market size forecast, pockets of growth, stores or leads potential.

🛒 **Go-to-Market**: omnichannel strategies marketing effectiveness, trade fundamentals (price, promo).

🏬 **Operations**: inventory and stocks optimization, transportation cost modeling, demand forecasts, stock disruptions, customerservice (virtual assistants).

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Business Applications

Consumer sectors

🛍️ **FMCG and Mass Fashion**: demand forecasting, marketing mix optimization, price and promo modeling.

🛒 **Retail:** revenue forecasting, footfall projection, customer spend prediction, basket size modeling.

🚗 **Durables:** replacement cycle forecasting, warranty prediction, price elasticity, cross-sell.

✈️ **Travel:** occupancy rates prediction, personalized offers, dynamic pricing.

💰 **Banking and Insurance:** loan amount estimate, insurance claims forecasting, individual premiums calculation, customer lifetime value.

📶 **Telecom:** data usage modeling, ARPU (average revenue per user) prediction, customer lifetime value.

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Business Applications

Business-to-Business sector

🏭 **Industrial products and services**: sales opportunity and market potential modeling, customer lifetime value.

💻 **SaaS**: Subscription revenue forecast, usage prediction e.g., storage, computing.

📽️ **Free platforms and search engines**: Ad revenue forecasting, user engagement projection (time, views).

🏠 **Sharing and Gig economy. Marketplaces:** ride-share demand, occupancy rate prediction, e.g., Uber, Airbnb.

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Terminology

Foundations of Regression

- **Dependent variable**: the outcome we aim to predict (e.g., sales revenue, temperature). Target. Output.
- **Independent variable**: the input(s) used to predict the dependent variable (e.g., ad spend, time of year).
- **Constant (Alpha, α, intercept):** the baseline value of the dependent variable when all independent variables are set to zero.Y-intercept of the regression line.
- **Coefficient (Beta, β, slope):** describes how much the dependent variable changes per unit increase in an independent variable. Positive or negative signs indicate the relationship's direction.

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Terminology

Evaluating Model Fit

- **Redisual**: The difference between the observed and predicted dependent variable values (aka "error").
- **Square Sum of Errors (SSE)**: the sum of squared residuals. Measures the total error. Low SSE indicates a better model fit.
- **R^2 (Coefficient of Determination):** indication of how much of the variance in dependent variable is explained by independent variables. Range: 0 (no fit) - 1 (perfect fit).
- **Cost function:** a formula to measure error across all predictions. MAE, MSE, RSME, MAPE (see: Evaluation).

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Terminology

Key Statistical Assumptions

- **Homoscedasticity**: the residuals have a constant variance across all levels of the independent variables. This means the spread of prediction errors doesn't change
- **Multicollinearity:** when two or more independent variables are highly correlated, it undermines their individual contributions to predicting the dependent.

Overfitting

- **Overfitting:** when a model is too complex and fits the noise in the training data, it performs poorly on new or unseen data (low generalizability).
- **Regularization L1 and L2**: techniques to reduce overfitting by penalizing large coefficients. L1 (Lasso) shrinks some coefficients to zero, L2 (Ridge) reduces their magnitude.

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Terminology

Optimization techniques

- **Gradient descent**: an iterative optimization algorithm that adjusts the model's coefficients to minimize the cost function (error). Steps are taken in the direction of steepest descent (negative gradient).
- **Grid search:** a process to optimize hyperparameters by systematically testing all possible combinations and selecting the best-performing set.

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Mathematical explanation

$$y = a + bx$$

Intercept Slope

Linear regression is setting the data (x) into a line (y).

y : Dependent variable (outcome, target)

x : Independent variable (input)

α : Intercept ß : Slope

Multifactor linear regression

$y = \alpha + ß1*x1 + ß2*x2 + ... + ß2*x2$

x1, ..., xn : independent variables

ß1, ..., ßn: coefficients estimating impact of each x on y

Visuals: www.FairlyNerdy.com

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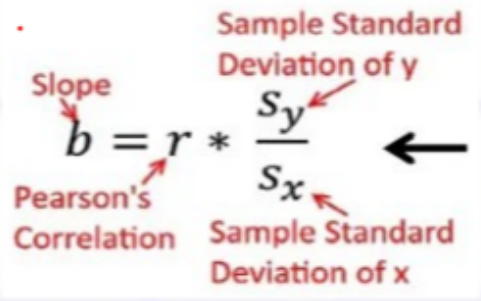
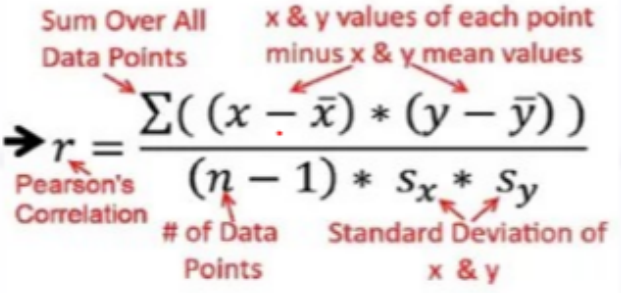
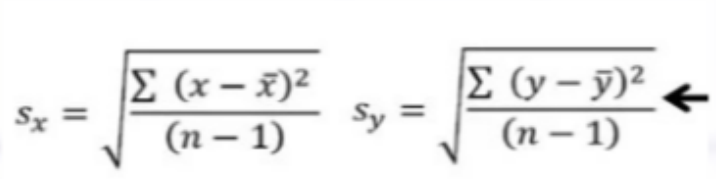
Mathematical explanation



Slope shows impact of x on y and depends on xy correlation and the difference in standard deviations.

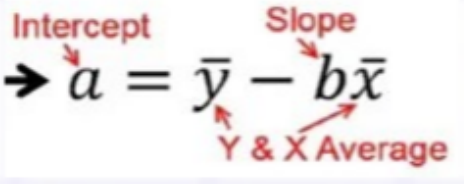
Correlation shows how much x and y change together. Can be positive and negative. Range [-1, 1].





Sample **standard deviations** show the spread of values around x and y means.

Intercept is the point where the line crosses y-axis (x is zero).



Visuals: www.FairlyNerdy.com

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Other types of regression

Polynomial

Fits a curve (e.g., quadradic, cubic) to data, not a straight line.

Business application: **stock price prediction, profit modeling**

$$\hat{y} = \beta_0 x^0 + \beta_1 x^1 + \beta_2 x^2 + \cdots + \beta_m x^m$$

n = number of $x_i y_i$ variable pairs in the data
m = order of the polynomial to be used for regression
$\beta_{(0-m)}$ = polynomial coefficient for each corresponding $x^{(0-m)}$
$\hat{y}$ = estimated y variable based on the polynomial regression calculations.

Quantile

Predicts specific quantiles (e.g., median). Estimates conditional quantile relationships. Better for skewed, non-normal distributions.

Business application: **healthcare median costs.**

Poisson

Models count data or event rates.

Business application: **call center events, purchase frequency modeling.**

Visuals: Wikipedia

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Data Requirements

	Linear Regression	Non-Linear Regression
Linearity	🔴	🟡
Normal distribution	🟡	🟡
No outliers *	🟡	🟡
Independence of errors	🟡	🟡
Constant spread of errors	🔴	🟡 (polynomial)
Independence of features	🔴	🔴

Legend:

🔴 Must-Have: essential for the method to give valid results.

🟡 Desirable: desirable for better performance or interpretation.

* If outliers are legit (not errors), data scientist decides whether to keep. E.g., having a 20 room villa in a sample of 2 bedroom apartments might disturb house prices modeling.

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The process

Pre-requisites

- Business question is understood and formulated as
  - **S**pecific (problem to solve)
  - **M**easurable (success criteria)
  - **A**chievable (data and capabilities in place)
  - **R**elevant (answers will lead to action)
  - **T**ime-bound (stakeholders and deadline are known).
- Data meets requirements and is pre-processed.
  See here how to prepare the data.

Modeling process

- This covers only modeling process, not production. End point: deployment or decision to increase model complexity.
  1. Initial model set up
  2. First evaluation
  3. If meets evaluation criteria → check overfit
     If overfit → try regularization
  4. If the model don't meet criteria at initial evaluation or after regularization doesn't help → check pre-processing (incl. feature engineering)
  5. If doen't help → increase model complexity (Decision Tree or SVR)

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1. Model initialization

Objectives

1. Import necessary libraries
2. Loading the dataset
3. Split the dataset into training and testing sets so the model can learn from one part (training – 80% of the dataset) and be evaluated on another unseen part (testing – 20% of the dataset) to ensure reliable performance.

```
# Step 1: Import libraries and load data
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error, mean_absolute_error, r2_score

# Load the dataset
data = pd.read_csv('your_file.csv')  # Replace 'your_file.csv' with the actual file path

X = data.drop(columns='target')  # Features
y = data['target']  # Target variable

# Split into training and testing sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)

# Explanation:
# Setting random_state=42 ensures consistent results across runs by fixing the randomness.
# Without it, splits will be random each time, leading to potential inconsistencies in results.
```

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2. Initial run and evaluation

Objectives

1. Modeling (here: linear regression)
2. Evaluating model performance. See here which evaluation metric to choose

```
# Step 2: Fit the model and make predictions
model = LinearRegression()  # Initialize the linear regression model
model.fit(X_train, y_train)  # Train the model on the training data

# Predictions
y_pred = model.predict(X_test)  # Make predictions on the test data

# Function for MAPE (Mean Absolute Percentage Error)
def mean_absolute_percentage_error(y_true, y_pred):
    return 100 * (abs((y_true - y_pred) / y_true).mean())

# Initial evaluation. Set the most relevant evaluation metric
mae = mean_absolute_error(y_test, y_pred)  # Mean Absolute Error
mse = mean_squared_error(y_test, y_pred)  # Mean Squared Error
rmse = mse ** 0.5  # Root Mean Squared Error
mape = mean_absolute_percentage_error(y_test, y_pred)  # Mean Absolute Percentage Error
r2 = r2_score(y_test, y_pred)  # R² Score

# Print evaluation metrics
print(f"MAE: {mae:.2f}, MSE: {mse:.2f}, RMSE: {rmse:.2f}, MAPE: {mape:.2f}%, R²: {r2:.2f}")

# Explanation:
# - MAE (Mean Absolute Error): Average of absolute differences between true and predicted values.
# - MSE (Mean Squared Error): Average of squared differences. Penalizes large errors.
# - RMSE (Root Mean Squared Error): Square root of MSE, same unit as the target.
# - MAPE (Mean Absolute Percentage Error): Percentage-based error to assess relative accuracy.
# - R² (R-squared): Explains the proportion of variance captured by the model (closer to 1 is best).
```

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3a. Overfit check

Objectives

If the model performs much worse on test data than on training data, this is a signal of overfit. Click here to learn about overfit.

```
# Step 2: Fit the model and make predictions
model = LinearRegression()  # Initialize the linear regression model
model.fit(X_train, y_train)  # Train the model on the training data

# Predictions
y_pred = model.predict(X_test)  # Make predictions on the test data

# Function for MAPE (Mean Absolute Percentage Error)
def mean_absolute_percentage_error(y_true, y_pred):
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rmse = mse ** 0.5  # Root Mean Squared Error
mape = mean_absolute_percentage_error(y_test, y_pred)  # Mean Absolute Percentage Error
r2 = r2_score(y_test, y_pred)  # R² Score

# Print evaluation metrics
print(f"MAE: {mae:.2f}, MSE: {mse:.2f}, RMSE: {rmse:.2f}, MAPE: {mape:.2f}%, R²: {r2:.2f}")

# Explanation:
# - MAE (Mean Absolute Error): Average of absolute differences between true and predicted values.
# - MSE (Mean Squared Error): Average of squared differences. Penalizes large errors.
# - RMSE (Root Mean Squared Error): Square root of MSE, same unit as the target.
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```

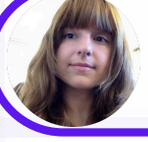

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3a. Regularization

Objectives

Try L1 and L2 regularization. Re-evaluate the model to see whether overfit decreases. Click here to learn about regularization.

```
# Step 3aa: Address overfitting with regularization. Compare training and test MSE.

from sklearn.linear_model import Ridge, Lasso

# 1. Train the original model (for comparison)
original_train_mse = mean_squared_error(y_train, model.predict(X_train))
original_test_mse = mean_squared_error(y_test, y_pred)

print("Original Model:")
print(f"Training MSE: {original_train_mse:.2f}")
print(f"Test MSE: {original_test_mse:.2f}")

# 2. Ridge Regularization (L2)
ridge_model = Ridge(alpha=1.0)  # Alpha is the regularization strength
ridge_model.fit(X_train, y_train)

ridge_train_mse = mean_squared_error(y_train, ridge_model.predict(X_train))
ridge_test_mse = mean_squared_error(y_test, ridge_model.predict(X_test))

print("\nRidge Regularization:")
print(f"Training MSE: {ridge_train_mse:.2f}")
print(f"Test MSE: {ridge_test_mse:.2f}")

# 3. Lasso Regularization (L1)
lasso_model = Lasso(alpha=0.1)  # Alpha is the regularization strength
lasso_model.fit(X_train, y_train)

lasso_train_mse = mean_squared_error(y_train, lasso_model.predict(X_train))
lasso_test_mse = mean_squared_error(y_test, lasso_model.predict(X_test))

print("\nLasso Regularization:")
print(f"Training MSE: {lasso_train_mse:.2f}")
print(f"Test MSE: {lasso_test_mse:.2f}")

# Explanation:
# - Look for reduced gap between training and test MSE after each regularization.
# - Choose the regularization (if any) that optimizes generalization (i.e., reduces overfitting).
# - Alpha can be tuned further for better performance.
```

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3 and 4. Pre-processing?

Objectives

Check residual for randomness. If residuals are not random, go back to pre-processing and check whether model assumptions are met (next slide).

```
import matplotlib.pyplot as plt
import scipy.stats as stats
import numpy as np

# Step 3ab: Check residuals for randomness
# Residuals are calculated as the difference between true and predicted values
residuals = y_test - model.predict(X_test)

# 1. Visualization: Residual Plot
plt.figure(figsize=(8, 6))
plt.scatter(model.predict(X_test), residuals, alpha=0.7, edgecolor='k')
plt.axhline(0, color='red', linestyle='--', linewidth=1)
plt.xlabel("Predicted Values")
plt.ylabel("Residuals")
plt.title("Residual Plot")
plt.show()

# 2. Statistical Test: Test for randomness using the Durbin-Watson statistic
from statsmodels.stats.stattools import durbin_watson

dw_stat = durbin_watson(residuals)
print(f"Durbin-Watson Statistic: {dw_stat:.2f}")

# Interpretation:
# - Residuals should ideally be scattered randomly around the horizontal line at zero.
# - Durbin-Watson Statistic ≈ 2 indicates no autocorrelation (random residuals).
# - Stat < 2: Positive autocorrelation (residuals are not independent).
# - Stat > 2: Negative autocorrelation.
```

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3 and 4. Assumption check

Objectives

Check assumptions for linear regression: linearity, no outliers, heteroscedasticity, no multicollinearity.

```python
# Visualize the relationship between predictors and the target
for feature in X.columns:
    plt.figure(figsize=(8, 6))
    plt.scatter(X[feature], y, alpha=0.7, edgecolor='k')
    plt.xlabel(feature)
    plt.ylabel("Target")
    plt.title(f"Scatter Plot: {feature} vs Target")
    plt.show()
```

```python
from sklearn.ensemble import IsolationForest

# Detect outliers using Isolation Forest (alternative: Z-score or IQR)
iso_forest = IsolationForest(contamination=0.05, random_state=42)
outlier_flags = iso_forest.fit_predict(X)  # -1 indicates an outlier

# Count detected outliers
print(f"Number of suspected outliers: {sum(outlier_flags == -1)}")
```

```python
# Breusch-Pagan test for heteroscedasticity
from statsmodels.stats.diagnostic import het_breuschpagan
import statsmodels.api as sm

lm_test = sm.OLS(residuals, sm.add_constant(model.predict(X_test))).fit()
bp_test = het_breuschpagan(lm_test.resid, lm_test.model.exog)
print(f"Breusch-Pagan p-value: {bp_test[1]:.3f}")

# Interpretation:
# - If p-value < 0.05, heteroscedasticity is present (non-constant residual variance).
```

```python
import seaborn as sns

# Plot a correlation matrix
cor_matrix = X.corr()
plt.figure(figsize=(10, 8))
sns.heatmap(cor_matrix, annot=True, cmap="coolwarm")
plt.title("Feature Correlation Matrix")
plt.show()

# Calculate Variance Inflation Factor (VIF) for multicollinearity
from statsmodels.stats.outliers_influence import variance_inflation_factor

vif_data = pd.DataFrame()
vif_data['Feature'] = X.columns
vif_data['VIF'] = [variance_inflation_factor(X.values, i) for i in range(X.shape[1])]
print(vif_data)

# Interpretation:
# - VIF > 5 (or 10) indicates significant multicollinearity.
```

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3 and 4. Feature engineering

Examples

Log transformation. Polynomial transformation. Feature removal and addition.

```
from sklearn.preprocessing import PolynomialFeatures
from numpy import log1p  # log1p(x) = log(1 + x), better for skewed data and values close to 0

# Log transformation of a skewed feature
X['log_feature'] = log1p(X['feature_to_transform'])

# Polynomial feature generation
poly = PolynomialFeatures(degree=2, include_bias=False)
X_poly = poly.fit_transform(X[['feature_to_transform']])  # Generates x, x²
print(f"Polynomial Features Shape: {X_poly.shape}")
```

```
# Drop irrelevant or problematic features
X = X.drop(columns=['feature_to_remove'])
print("Removed feature: feature_to_remove")
```

```
# Replace 'absolute price' with 'price index'
X['price_index_vs_brand_A'] = X['price'] / X['competitor_price']
X = X.drop(columns=['price'])  # Drop the original price column
print("Added 'price_index_vs_brand_A' and removed 'price'")
```

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5. Final model evaluation

Examples

Check whether changes have improved evaluation scores and whether the model meets evaluation criteria now. If not - consider increasing its complexity.

```
# Refit the transformed model
refined_model = LinearRegression()
refined_model.fit(X_train, y_train)

# Predictions and performance
original_y_pred = model.predict(X_test)
refined_y_pred = refined_model.predict(X_test)

# Calculate and compare metrics
original_mse = mean_squared_error(y_test, original_y_pred)
refined_mse = mean_squared_error(y_test, refined_y_pred)

print("Comparison of Model Performance:")
print(f"Original Model MSE: {original_mse:.2f}")
print(f"Refined Model MSE: {refined_mse:.2f}")

# Interpretation:
# - A lower MSE in the refined model suggests that the transformations improved performance.
```

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