

# Temporal and Unsupervised Learning

Lecture 5: From Sequences to Hidden Patterns (MSc Data Science)

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## Section 1

Introduction: A New Paradigm

# Slide 1: Course Overview and Transition

## Previous Lectures (L1-L4):

- L1-L2: Logistic Regression (supervised, static)
- L3: Ensemble Methods (supervised, static)
- L4: Neural Networks and XAI (supervised, static)

## Lecture 5 - Two New Dimensions:

- ① **Temporal:** Data with time ordering (sequences matter!)
- ② **Unsupervised:** No labels (find hidden structure)

**Key Shift:** From prediction to pattern discovery and forecasting

## Slide 2: Why Temporal Data is Different

**Static Data:** Each observation is independent

- Example: Predicting house prices from features

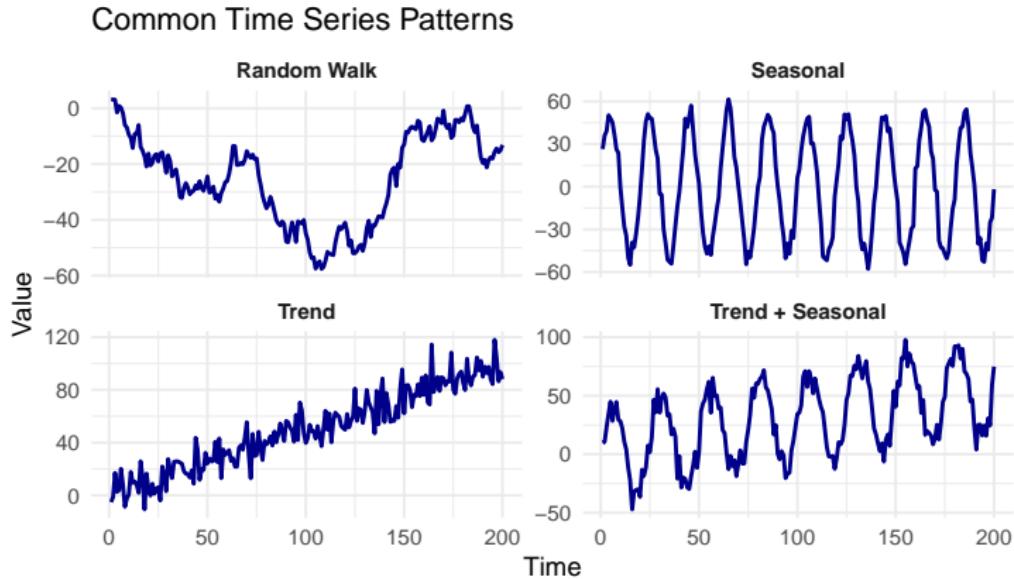
**Temporal Data:** Order matters, observations are dependent

- Example: Stock prices, temperature, heart rate

**Key Characteristics:**

- **Autocorrelation:** Values correlated with past values
- **Trends:** Long-term increases/decreases
- **Seasonality:** Regular periodic patterns
- **Non-stationarity:** Statistical properties change over time

# Slide 3: Time Series Examples



# Slide 4: Why Unsupervised Learning?

## Supervised Learning Limitations:

- Requires labeled data (expensive, time-consuming)
- Can't discover unknown patterns
- Limited to predefined categories

## Unsupervised Learning Goals:

- ① **Clustering:** Group similar observations
- ② **Dimensionality Reduction:** Find compact representations
- ③ **Association Rules:** Discover relationships
- ④ **Anomaly Detection:** Find unusual patterns

**Use Cases:** Customer segmentation, market basket analysis, exploratory data analysis

# Slide 5: Lecture 5 Roadmap

## Part I: Time Series Analysis (Slides 1-90)

- Time series components and decomposition
- Stationarity and transformations
- ARIMA models
- Forecasting techniques

## Part II: Unsupervised Learning (Slides 91-180)

- K-Means clustering
- Hierarchical clustering
- Association rule mining
- Practical applications

## Section 2

### Time Series Fundamentals

## Slide 6: What is a Time Series?

**Definition:** A sequence of observations recorded at successive time points

$$\{y_t : t = 1, 2, \dots, T\}$$

### Examples:

- Daily stock prices
- Monthly sales figures
- Hourly temperature readings
- Annual GDP growth

### Key Properties:

- **Temporal ordering:**  $t$  matters
- **Frequency:** Regular intervals (hourly, daily, monthly)

## Slide 7: Loading and Visualizing Time Series in R

```
# Create a time series object
# Example: Monthly airline passengers (1949-1960)
data(AirPassengers)

# View structure
str(AirPassengers)

## Time-Series [1:144] from 1949 to 1961: 112 118 132 129 121 ...
# Basic plot
plot(AirPassengers,
      main = "Monthly Airline Passengers",
      xlab = "Year",
      ylab = "Passengers (thousands)",
      col = "darkblue",
      lwd = 2)
```

## Slide 8: Time Series Components

**Additive Decomposition:**

$$Y_t = T_t + S_t + R_t$$

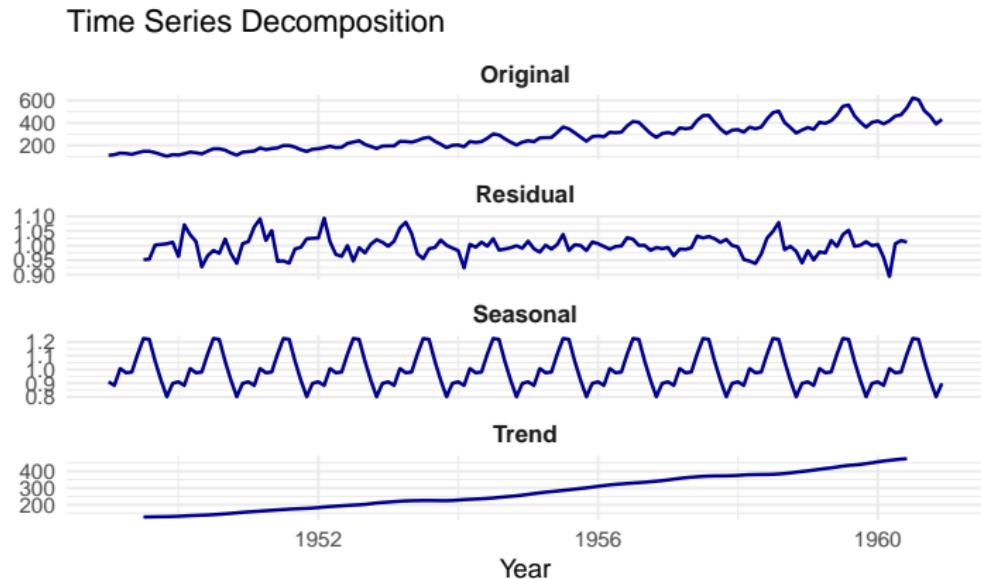
**Multiplicative Decomposition:**

$$Y_t = T_t \times S_t \times R_t$$

where:

- $T_t$  = **Trend** (long-term direction)
- $S_t$  = **Seasonal** (regular periodic variation)
- $R_t$  = **Residual/Irregular** (random noise)

# Slide 9: Visualizing Time Series Components



## Slide 10: Time Series Decomposition in R

```
# Multiplicative decomposition
decomp_mult <- decompose(AirPassengers,
                           type = "multiplicative")

# Additive decomposition
decomp_add <- decompose(AirPassengers,
                         type = "additive")

# Plot decomposition
plot(decomp_mult)

# Access components
trend <- decomp_mult$trend
seasonal <- decomp_mult$seasonal
random <- decomp_mult$random

# Remove seasonality
decomp_mult$seasonal <- 0
```

## Slide 11: Stationarity - The Foundation

**Definition:** A time series is **stationary** if its statistical properties don't change over time.

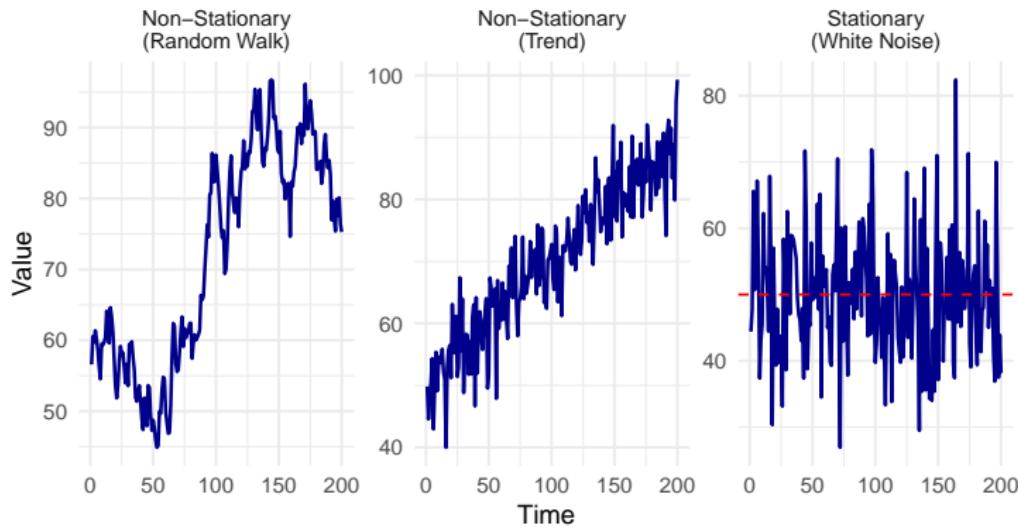
### Requirements:

- ① **Constant mean:**  $E[Y_t] = \mu$  for all  $t$
- ② **Constant variance:**  $Var(Y_t) = \sigma^2$  for all  $t$
- ③ **Constant autocovariance:**  $Cov(Y_t, Y_{t-k})$  depends only on  $k$ , not  $t$

**Why Important:** Most time series models (ARIMA) assume stationarity!

# Slide 12: Stationary vs Non-Stationary

## Stationary vs Non-Stationary Time Series



## Slide 13: Testing for Stationarity - Augmented Dickey-Fuller Test

**Null Hypothesis:** Series has a unit root (non-stationary)

**Alternative:** Series is stationary

**Decision Rule:**

- p-value < 0.05 → Reject null → Series is **stationary**
- p-value ≥ 0.05 → Fail to reject → Series is **non-stationary**

```
library(tseries)
```

```
# Test AirPassengers for stationarity  
adf.test(AirPassengers)
```

```
# Typical output:
```

```
# Dickey-Fuller = -1.6, p-value = 0.73  
# Conclusion: Non-stationary (p > 0.05)
```

## Slide 14: Making Series Stationary - Differencing

**First Differencing:**  $\Delta Y_t = Y_t - Y_{t-1}$

**Second Differencing:**  $\Delta^2 Y_t = \Delta Y_t - \Delta Y_{t-1}$

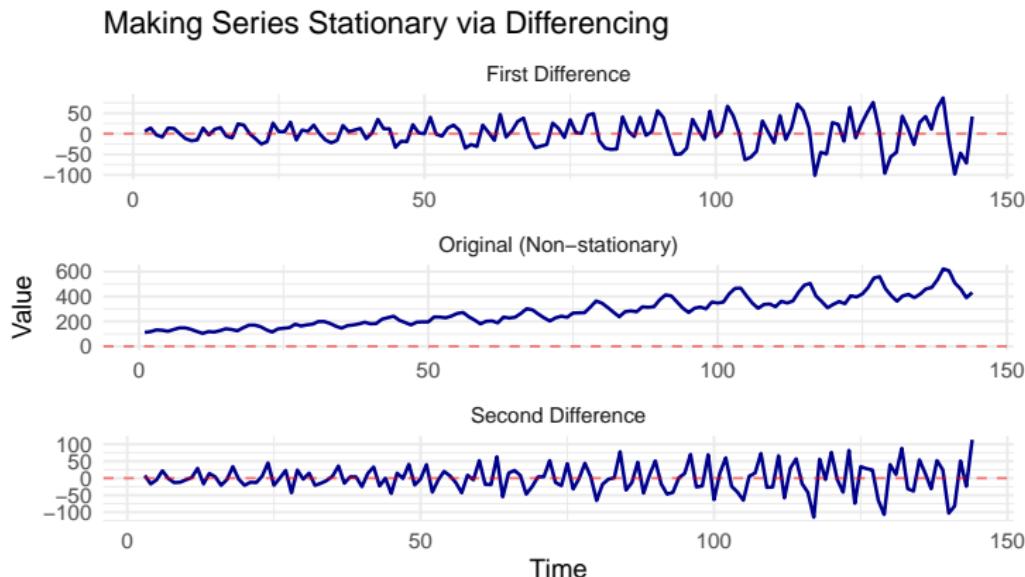
In R:

```
# First difference
diff1 <- diff(AirPassengers)
plot(diff1, main = "First Difference")

# Check stationarity
adf.test(diff1)

# Second difference (if needed)
diff2 <- diff(diff1)
plot(diff2, main = "Second Difference")
```

# Slide 15: Differencing Example



**After first differencing:** Series becomes stationary!

## Slide 16: Log Transformation for Variance Stabilization

**Problem:** Variance increases with level (heteroscedasticity)

**Solution:** Log transformation

$$Y'_t = \log(Y_t)$$

*# Log transformation*

```
log_series <- log(AirPassengers)
plot(log_series, main = "Log-transformed Series")
```

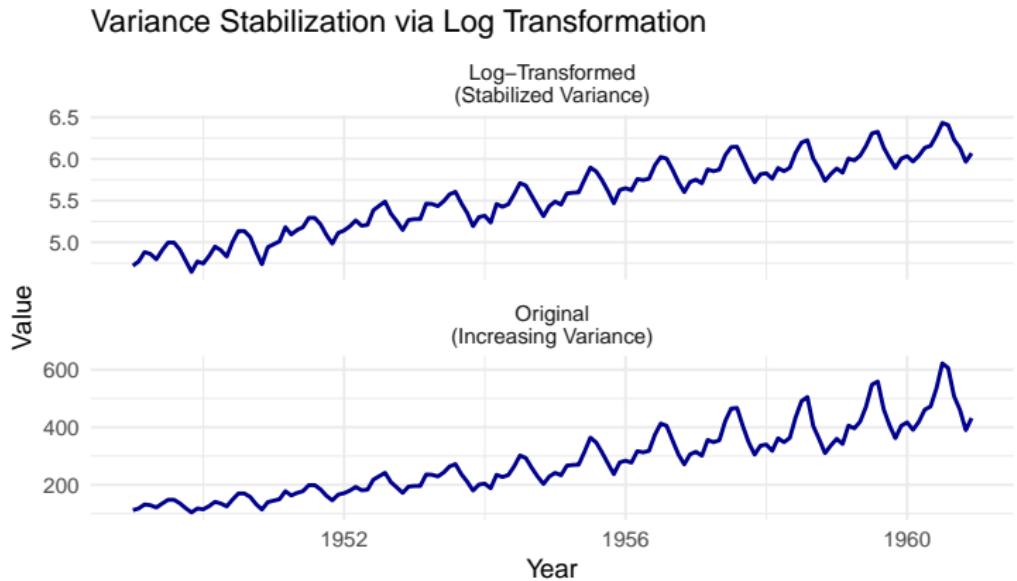
*# Compare variance*

```
var(AirPassengers)
var(log_series)
```

*# Often combine: log + differencing*

```
log_diff <- diff(log(AirPassengers))
plot(log_diff)
```

## Slide 17: Log Transformation Example



## Slide 18: Autocorrelation Function (ACF)

**Definition:** Correlation between  $Y_t$  and  $Y_{t-k}$  at different lags  $k$

$$\rho_k = \frac{Cov(Y_t, Y_{t-k})}{\sqrt{Var(Y_t)Var(Y_{t-k})}}$$

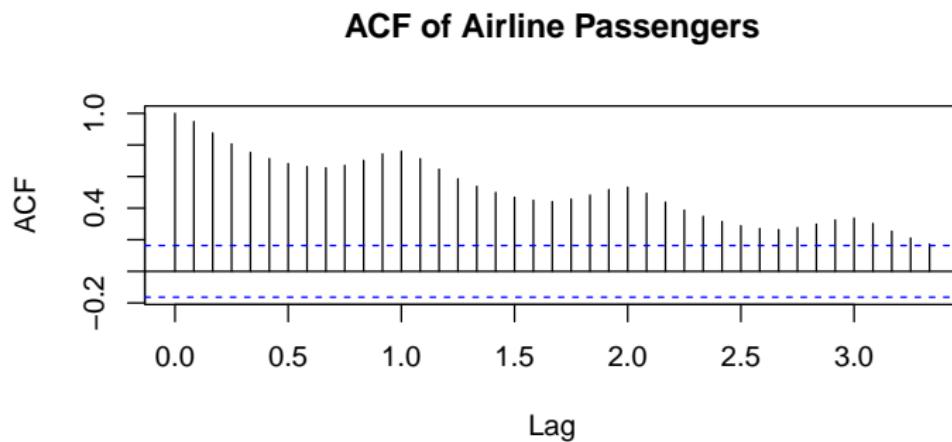
**ACF Plot:** Shows correlation at each lag

**Interpretation:**

- High ACF at lag  $k \rightarrow$  Strong relationship with past  $k$  periods
- ACF cuts off  $\rightarrow$  MA process
- ACF decays slowly  $\rightarrow$  AR process or non-stationary

## Slide 19: ACF in R

```
# Compute and plot ACF  
acf(AirPassengers,  
    main = "ACF of Airline Passengers",  
    lag.max = 40)
```



```
# Blue dashed lines = significance bounds  
# Values outside bounds = significant correlation
```

## Slide 20: Partial Autocorrelation Function (PACF)

**Definition:** Correlation between  $Y_t$  and  $Y_{t-k}$  after removing effects of intermediate lags

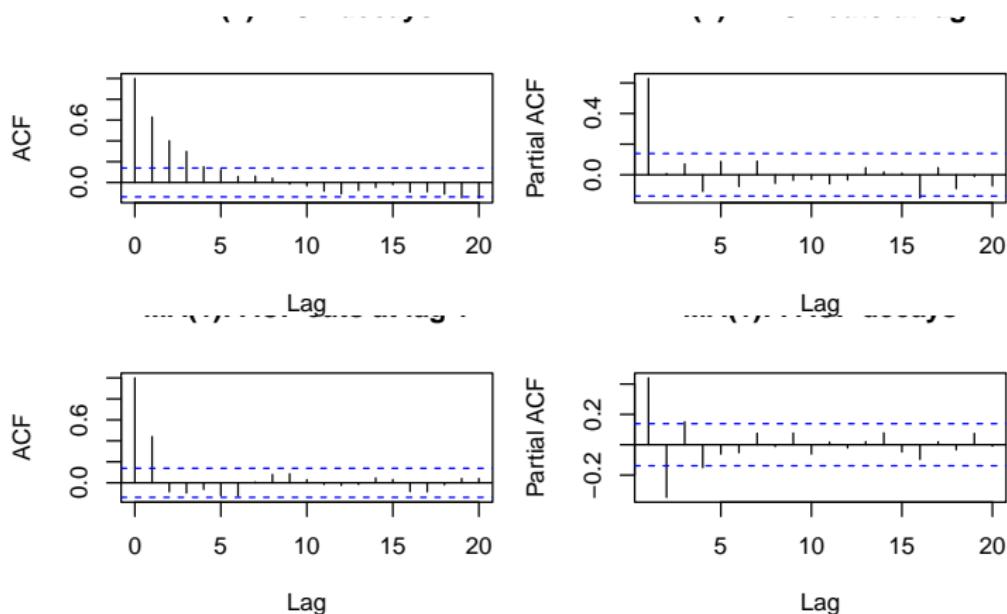
**Use Case:** Identify order of AR process

**Interpretation:**

- PACF cuts off at lag  $p \rightarrow \text{AR}(p)$  process
- PACF decays gradually  $\rightarrow \text{MA}$  process

```
# Compute and plot PACF
pacf(AirPassengers,
      main = "PACF of Airline Passengers",
      lag.max = 40)
```

## Slide 21: ACF vs PACF - Model Identification



## Slide 22: White Noise - The Baseline

**Definition:** Series with no autocorrelation

$$Y_t \sim N(0, \sigma^2), \quad \text{all } t$$

**Properties:**

- Mean = 0 (or constant)
- Constant variance
- No correlation between observations
- Unpredictable (best forecast = mean)

**Test:** Ljung-Box test

- H<sub>0</sub>: Series is white noise
- p-value < 0.05 → Reject null → Has structure (predictable)

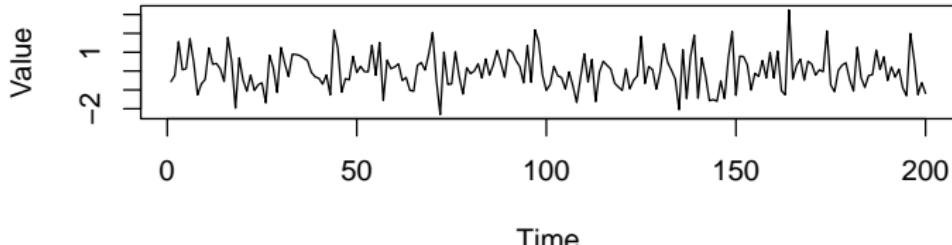
## Slide 23: Testing for White Noise

```
set.seed(123)

# Generate white noise
white_noise <- rnorm(200, mean = 0, sd = 1)

# Plot
plot(white_noise, type = "l",
      main = "White Noise Example",
      ylab = "Value", xlab = "Time")
```

**White Noise Example**



## Slide 24: Random Walk - The Simplest Non-Stationary Process

**Definition:** Current value = previous value + random shock

$$Y_t = Y_{t-1} + \epsilon_t, \quad \epsilon_t \sim N(0, \sigma^2)$$

**Properties:**

- Non-stationary (variance increases over time)
- Best forecast = current value
- Common in financial data (stock prices)

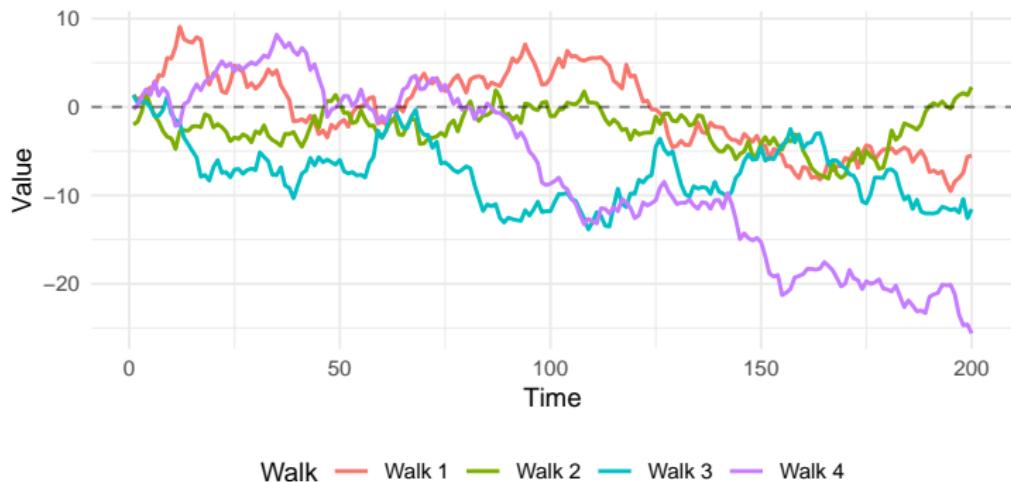
**Make stationary:** First differencing

$$\Delta Y_t = Y_t - Y_{t-1} = \epsilon_t \quad (\text{white noise!})$$

# Slide 25: Random Walk Visualization

Random Walks: Same Process, Different Realizations

Demonstrates non-stationarity: variance increases over time



## Slide 26: Autoregressive (AR) Models

**AR( $p$ ) Model:** Current value depends on  $p$  past values

$$Y_t = c + \phi_1 Y_{t-1} + \phi_2 Y_{t-2} + \cdots + \phi_p Y_{t-p} + \epsilon_t$$

**Example - AR(1):**

$$Y_t = c + \phi_1 Y_{t-1} + \epsilon_t$$

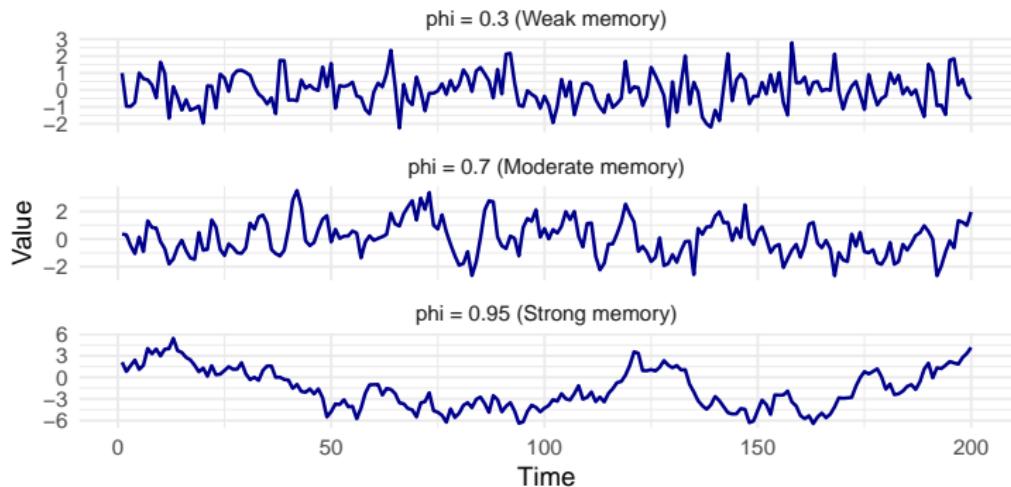
**Stationarity Condition:**  $|\phi_1| < 1$

**Interpretation:** If  $\phi_1 = 0.7$ , then 70% of previous value carries forward

# Slide 27: AR(1) Process Examples

## AR(1) Process with Different Coefficients

Higher coefficient = stronger dependence on past



## Slide 28: Moving Average (MA) Models

**MA( $q$ ) Model:** Current value depends on past  $q$  error terms

$$Y_t = \mu + \epsilon_t + \theta_1 \epsilon_{t-1} + \theta_2 \epsilon_{t-2} + \cdots + \theta_q \epsilon_{t-q}$$

**Example - MA(1):**

$$Y_t = \mu + \epsilon_t + \theta_1 \epsilon_{t-1}$$

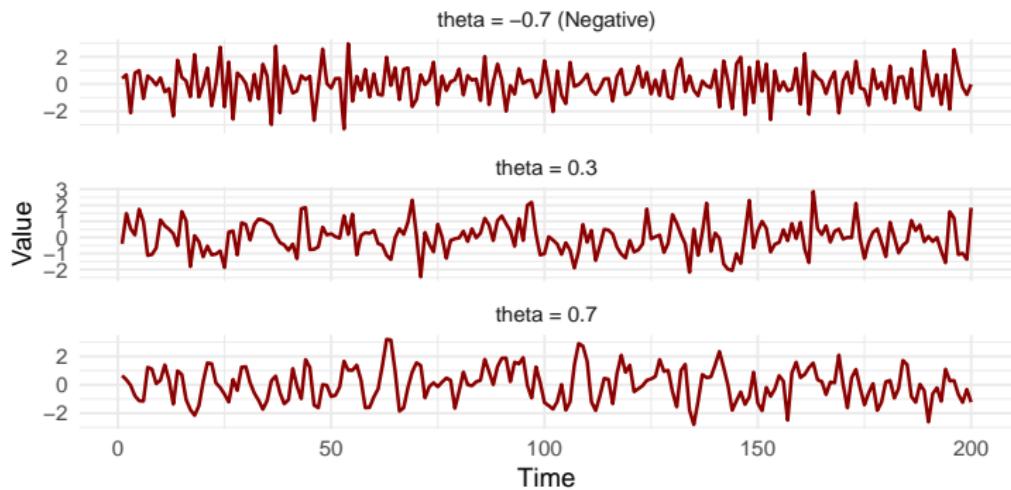
**Key Difference from AR:**

- AR: Depends on past **values**
- MA: Depends on past **errors**

## Slide 29: MA(1) Process Examples

### MA(1) Process with Different Coefficients

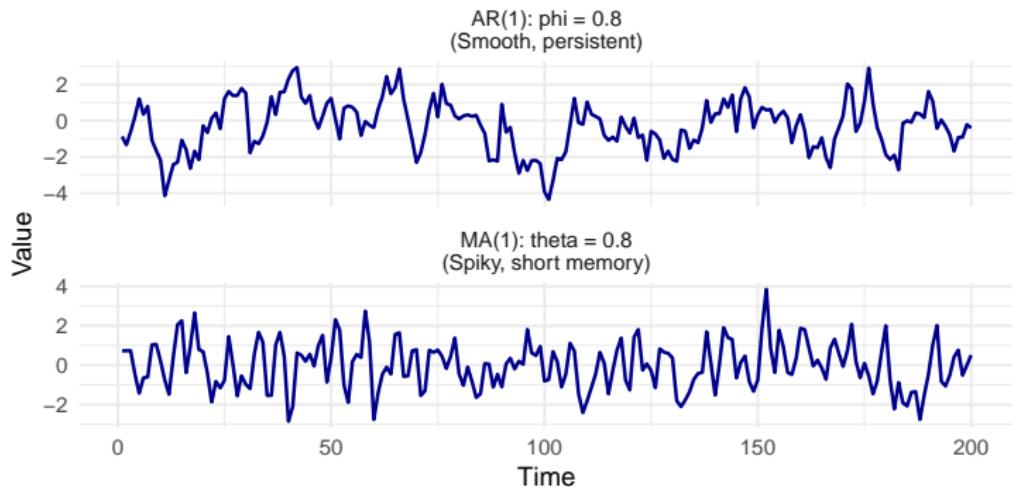
Negative theta creates oscillating pattern



# Slide 30: AR vs MA - Visual Comparison

## AR vs MA Processes

AR: smoother, longer memory | MA: spikier, short memory





## Section 3

### ARIMA Models

## Slide 31: Combining AR and MA - ARMA Models

**ARMA(p,q) Model:** Combines AR(p) and MA(q)

$$Y_t = c + \phi_1 Y_{t-1} + \cdots + \phi_p Y_{t-p} + \epsilon_t + \theta_1 \epsilon_{t-1} + \cdots + \theta_q \epsilon_{t-q}$$

### Why Combine?

- More flexible than pure AR or MA
- Often need fewer parameters
- Better fits real-world data

### Example - ARMA(1,1):

$$Y_t = c + \phi_1 Y_{t-1} + \epsilon_t + \theta_1 \epsilon_{t-1}$$

## Slide 32: ARIMA - Adding Integration

### ARIMA(p,d,q) Model:

- **p**: Order of AR component
- **d**: Degree of differencing (Integration)
- **q**: Order of MA component

### Process:

- ① Difference the series  $d$  times to achieve stationarity
- ② Fit ARMA(p,q) to the differenced series

### Common Models:

- ARIMA(1,0,0) = AR(1)
- ARIMA(0,1,1) = Random walk + MA(1) shock
- ARIMA(1,1,1) = Most common in practice

# Slide 33: ARIMA Model Selection - The Box-Jenkins Method

## Iterative 4-Step Process:

### ① Identification: Determine p, d, q

- Check stationarity (ADF test)
- Plot ACF/PACF
- Choose candidate models

### ② Estimation: Fit model parameters

### ③ Diagnostic Checking: Validate residuals

- Should be white noise
- Check ACF of residuals

### ④ Forecasting: Use the validated model

# Slide 34: Step 1 - Model Identification Guide

## ARIMA Model Identification Rules

ACF	PACF	Model
Cuts off at lag q	Decays gradually	MA(q)
Decays gradually	Cuts off at lag p	AR(p)
Decays gradually	Decays gradually	ARMA(p,q)

'Cuts off' = drops to zero after lag k

'Decays' = gradually approaches zero

## Slide 35: Determining d - Differencing Order

### Strategy:

- ① Plot the series
- ② Run ADF test
- ③ If  $p\text{-value} > 0.05 \rightarrow$  Apply first difference ( $d=1$ )
- ④ Test again
- ⑤ Repeat if needed (rarely  $d > 2$ )

```
# Test original series
adf.test(AirPassengers) # p-value = 0.01 (non-stationary)

# First difference
diff1 <- diff(AirPassengers)
adf.test(diff1) # p-value = 0.01 (stationary!)

# Conclusion: d = 1
```

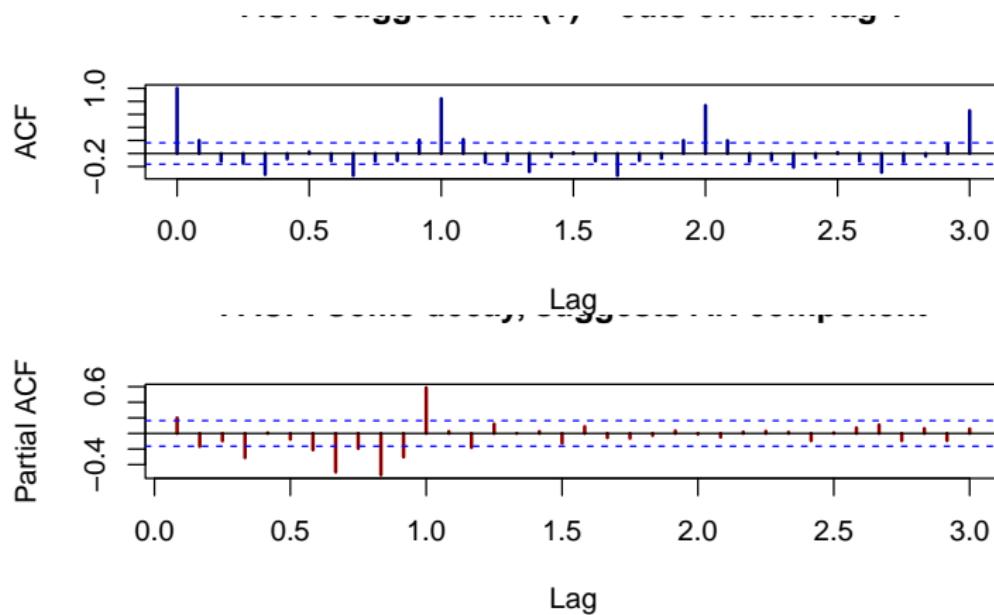
## Slide 36: Determining p and q - ACF/PACF Analysis

```
# After differencing, examine ACF/PACF
diff_series <- diff(log(AirPassengers))

par(mfrow = c(2, 1))
acf(diff_series, lag.max = 40,
     main = "ACF of Differenced Series")
pacf(diff_series, lag.max = 40,
      main = "PACF of Differenced Series")

# Look for:
# - ACF: Significant spike at lag q → MA(q)
# - PACF: Significant spike at lag p → AR(p)
# - Both: ARMA(p, q)
```

## Slide 37: ACF/PACF for Model Selection



**Interpretation:** Try ARIMA(1,1,1) or ARIMA(0,1,1) as starting points

## Slide 38: Fitting ARIMA Models in R

```
library(forecast)

# Manual specification
model1 <- arima(AirPassengers, order = c(1, 1, 1))
summary(model1)

# Auto ARIMA (automated selection)
model_auto <- auto.arima(AirPassengers,
                           seasonal = TRUE,
                           stepwise = TRUE,
                           trace = TRUE)

summary(model_auto)

# Compare models
AIC(model1)
AIC(model_auto)
# I get AIC values for both
```

## Slide 39: Model Comparison - Information Criteria

### Akaike Information Criterion (AIC):

$$AIC = -2 \log(L) + 2k$$

### Bayesian Information Criterion (BIC):

$$BIC = -2 \log(L) + k \log(n)$$

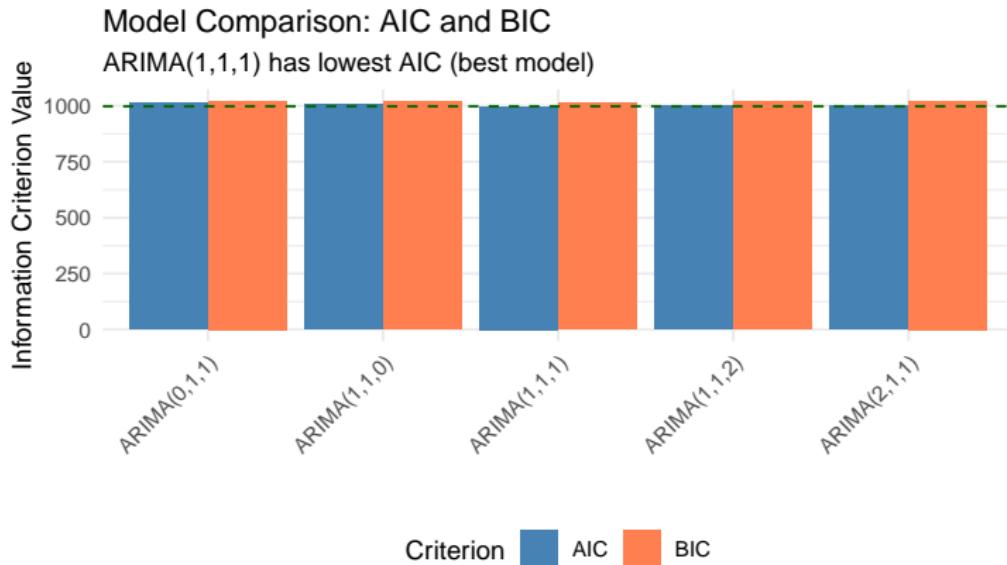
where:

- $L$  = likelihood
- $k$  = number of parameters
- $n$  = sample size

**Rule:** Lower is better (balances fit vs complexity)

**BIC:** Penalizes complexity more heavily than AIC

# Slide 40: Model Comparison Example



## Slide 41: Diagnostic Checking - Residual Analysis

After fitting, check residuals should be white noise:

- ① Plot residuals: No patterns
- ② ACF of residuals: No significant lags
- ③ Ljung-Box test: p-value > 0.05
- ④ Normality: QQ-plot

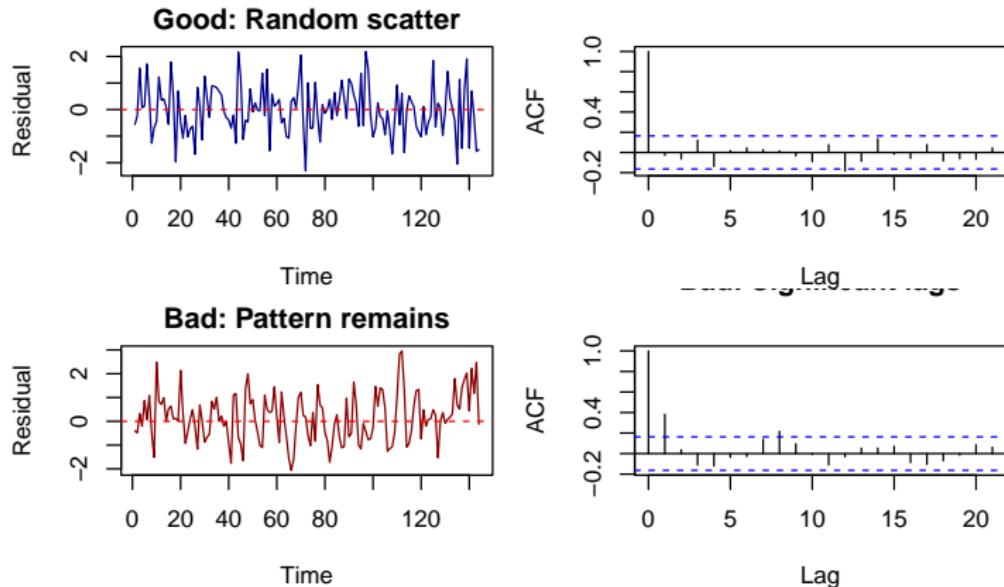
```
# Fit model
model <- arima(AirPassengers, order = c(1, 1, 1))

# Extract residuals
residuals <- residuals(model)

# Diagnostic plots
tsdiag(model)

# Ljung-Box test
Box.test(residuals, lag = 20, type = "Ljung-Box")
# p > 0.05 → Residuals are white noise (good!)
```

# Slide 42: Residual Diagnostics Visualization



## Slide 43: Complete ARIMA Workflow Example

```
library(forecast)

# 1. Load and visualize data
data(AirPassengers)
plot(AirPassengers)

# 2. Check stationarity
adf.test(AirPassengers) # Non-stationary

# 3. Transform and difference
log_ap <- log(AirPassengers)
diff_ap <- diff(log_ap)
adf.test(diff_ap) # Stationary!

# 4. Examine ACF/PACF
acf(diff_ap)
pacf(diff_ap)
```

## Slide 44: Forecasting with ARIMA

**Point Forecast:** Expected future value

$$\hat{Y}_{T+h} = E[Y_{T+h}|Y_1, \dots, Y_T]$$

**Prediction Interval:** Uncertainty around forecast

- 80% interval: 80% chance true value falls within
- 95% interval: 95% chance true value falls within

**Key Property:** Intervals widen as horizon  $h$  increases (more uncertainty)

## Slide 45: Generating Forecasts in R

```
# Fit model
model <- auto.arima(AirPassengers)

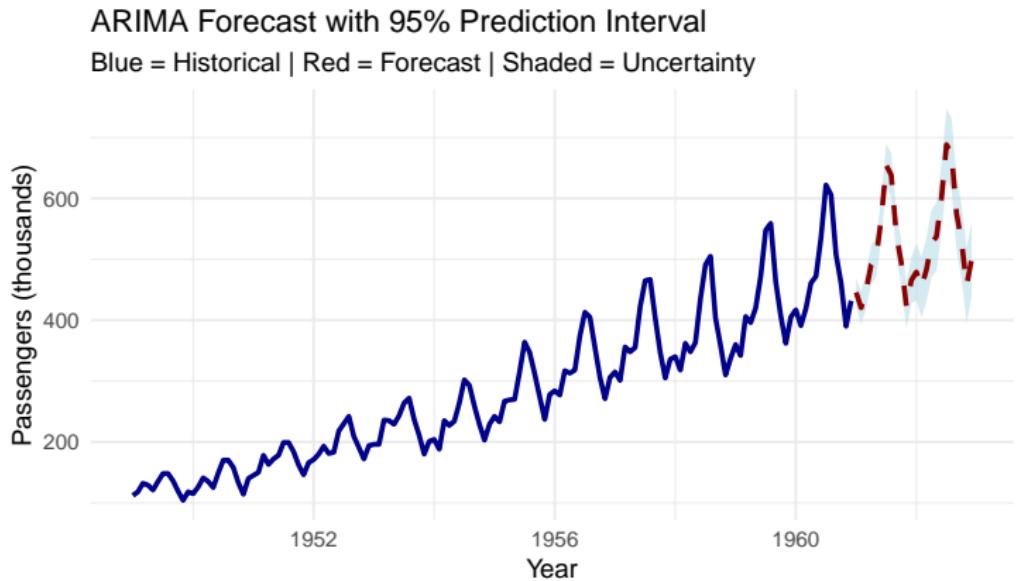
# Forecast 24 months ahead
forecasts <- forecast(model, h = 24)

# View forecasts
print(forecasts)

# Plot forecast with prediction intervals
plot(forecasts,
      main = "24-Month Forecast",
      xlab = "Year",
      ylab = "Passengers")

# Dark gray = 80% interval
# Light gray = 95% interval
```

## Slide 46: Forecast Visualization



## Slide 47: Forecast Accuracy Metrics

**Mean Absolute Error (MAE):**

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

**Root Mean Squared Error (RMSE):**

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

**Mean Absolute Percentage Error (MAPE):**

$$MAPE = \frac{100}{n} \sum_{i=1}^n \left| \frac{y_i - \hat{y}_i}{y_i} \right|$$

**Lower is better** for all metrics

## Slide 48: Cross-Validation for Time Series

### Time Series Cross-Validation (Rolling Origin):

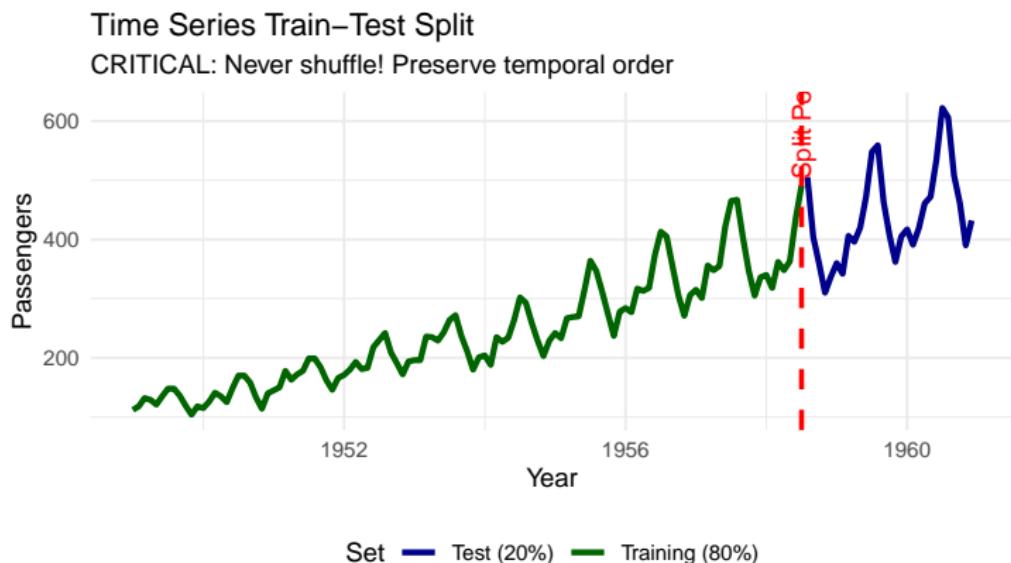
- ① Train on data up to time  $t$
- ② Forecast next period(s)
- ③ Compare with actual
- ④ Move origin forward, repeat

```
# Time series cross-validation
cv_results <- tsCV(AirPassengers,
                     forecastfunction = function(x, h) {
                       forecast(auto.arima(x), h = h)
                     },
                     h = 1) # 1-step ahead forecast

# Compute accuracy
mae <- mean(abs(cv_results), na.rm = TRUE)
rmse <- sqrt(mean(cv_results^2, na.rm = TRUE))

cat("MAE:", mae, "\n")
```

## Slide 49: Train-Test Split for Time Series



**Warning:** Never shuffle time series data!

## Slide 50: Seasonal ARIMA (SARIMA)

### SARIMA(p,d,q)(P,D,Q)s Model:

- Lowercase: Non-seasonal components
- Uppercase: Seasonal components
- $s$ : Seasonal period (e.g., 12 for monthly, 4 for quarterly)

**Example:** SARIMA(1,1,1)(1,1,1)

- Regular ARIMA(1,1,1)
- Seasonal ARIMA(1,1,1) with period 12

**Use Case:** Data with strong seasonal patterns (AirPassengers!)

## Slide 51: SARIMA Model Equation

### Full SARIMA Equation:

$$\phi(B)\Phi(B^s)(1 - B)^d(1 - B^s)^D Y_t = \theta(B)\Theta(B^s)\epsilon_t$$

where:

- $B$  = Backshift operator:  $BY_t = Y_{t-1}$
- $\phi(B)$  = Non-seasonal AR polynomial
- $\Phi(B^s)$  = Seasonal AR polynomial
- $\theta(B)$  = Non-seasonal MA polynomial
- $\Theta(B^s)$  = Seasonal MA polynomial

**Don't panic!** R handles this complexity automatically

## Slide 52: Fitting SARIMA in R

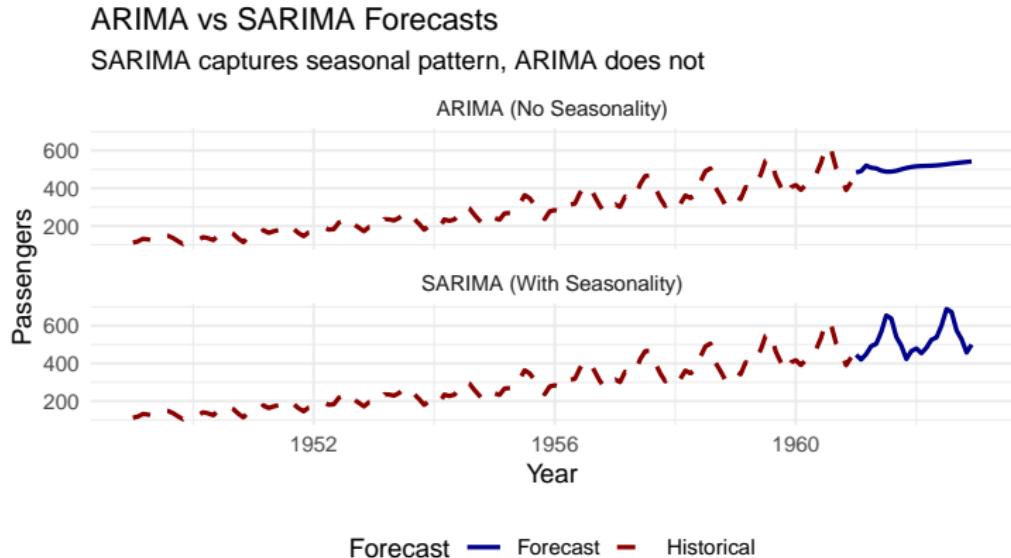
```
# Manual SARIMA specification
# SARIMA(1,1,1)(1,1,1)[12]
sarima_model <- arima(AirPassengers,
                      order = c(1, 1, 1),
                      seasonal = list(order = c(1, 1, 1),
                                      period = 12))

summary(sarima_model)

# Auto SARIMA
auto_sarima <- auto.arima(AirPassengers,
                           seasonal = TRUE,
                           stepwise = FALSE,
                           approximation = FALSE)

summary(auto_sarima)
# Typically finds: ARIMA(0,1,1)(0,1,1)[12]
```

# Slide 53: SARIMA vs ARIMA Comparison



## Slide 54: Identifying Seasonal Components

**Check for seasonality:**

- ① **Visual inspection:** Regular peaks/valleys
- ② **Seasonal subseries plot:** Compare same periods
- ③ **ACF:** Spikes at seasonal lags (12, 24, 36...)

```
# Seasonal subseries plot
monthplot(AirPassengers,
           main = "Seasonal Subseries Plot")

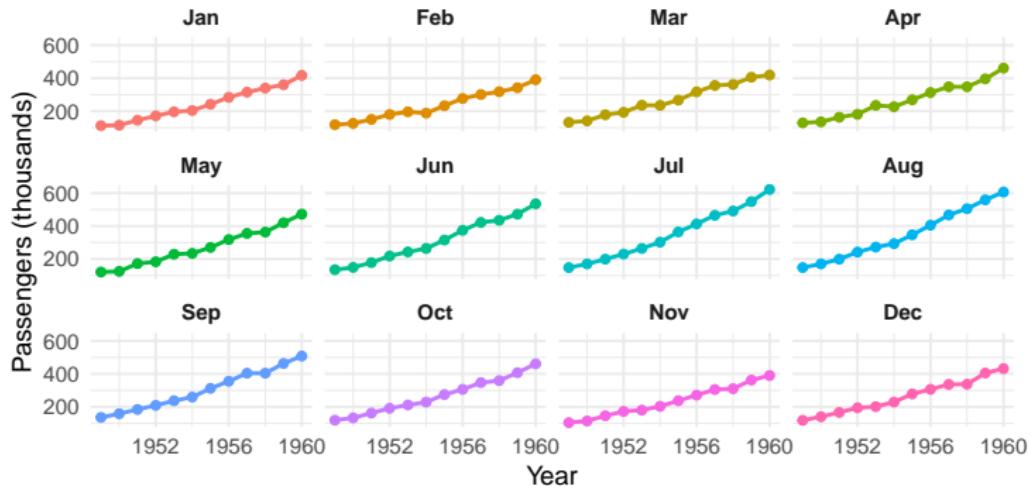
# ACF shows seasonal pattern
acf(AirPassengers, lag.max = 48)
# Look for spikes at lags 12, 24, 36...

# Seasonal decomposition
decompose_result <- decompose(AirPassengers)
plot(decompose_result)
```

# Slide 55: Seasonal Subseries Plot

## Seasonal Subseries Plot: Airline Passengers

Each panel = one month across years. Clear upward trend in all months



# Slide 56: Advanced Forecasting - Exponential Smoothing

## Alternative to ARIMA: Exponential Smoothing

- **Simple:** No trend, no seasonality
- **Holt:** With trend
- **Holt-Winters:** With trend and seasonality

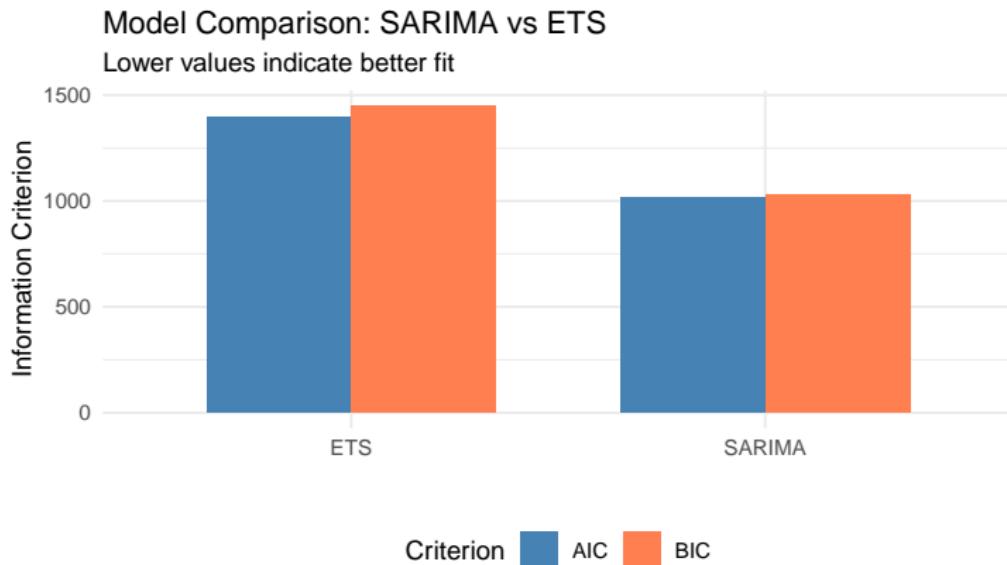
**Advantage:** Often more robust, easier to understand

**ETS (Error, Trend, Seasonal) Framework:**

```
# Automatic ETS model selection
ets_model <- ets(AirPassengers)
summary(ets_model)

# Forecast
ets_forecast <- forecast(ets_model, h = 24)
plot(ets_forecast)
```

# Slide 57: ETS vs ARIMA



**Conclusion:** Try both, compare performance on validation set!

## Slide 58: Forecast Combination

**Ensemble Forecasting:** Average multiple forecasts

$$\hat{Y}_{combined} = w_1 \hat{Y}_{ARIMA} + w_2 \hat{Y}_{ETS} + w_3 \hat{Y}_{others}$$

**Benefits:**

- Reduces forecast variance
- Often outperforms individual models
- Robust to model misspecification

```
# Generate multiple forecasts
fc1 <- forecast(auto.arima(AirPassengers), h = 24)
fc2 <- forecast(ets(AirPassengers), h = 24)
```

```
# Simple average
combined_forecast <- (fc1$mean + fc2$mean) / 2
```

```
# Plot
```

# Slide 59: Dealing with Multiple Seasonality

**Problem:** Data with multiple seasonal patterns

- Daily data: Weekly (7) + Yearly (365) seasonality
- Hourly data: Daily (24) + Weekly (168) seasonality

**Solution: TBATS Model**

- Trigonometric
- Box-Cox transformation
- ARMA errors
- Trend
- Seasonal components

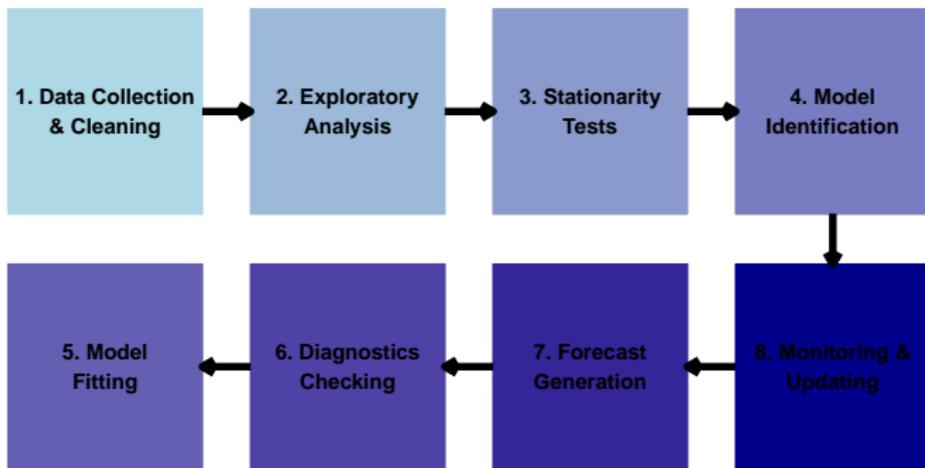
```
# Fit TBATS model
tbats_model <- tbats(time_series_data)

# Forecast
tbats_forecast <- forecast(tbats_model, h = 100)
plot(tbats_forecast)
```

# Slide 60: Real-World Forecasting Workflow

## Complete Time Series Forecasting Workflow

Iterative process: If diagnostics fail, return to step 4





## Section 4

Advanced Time Series Topics

# Slide 61: Handling Missing Values in Time Series

## Common Approaches:

- ① **Linear Interpolation:** Connect neighboring points
- ② **Spline Interpolation:** Smooth curve fitting
- ③ **Last Observation Carried Forward (LOCF)**
- ④ **Model-based Imputation:** Use ARIMA to predict missing values

```
library(zoo)

# Introduce missing values (for demo)
ts_with_na <- AirPassengers
ts_with_na[c(10, 25, 50)] <- NA

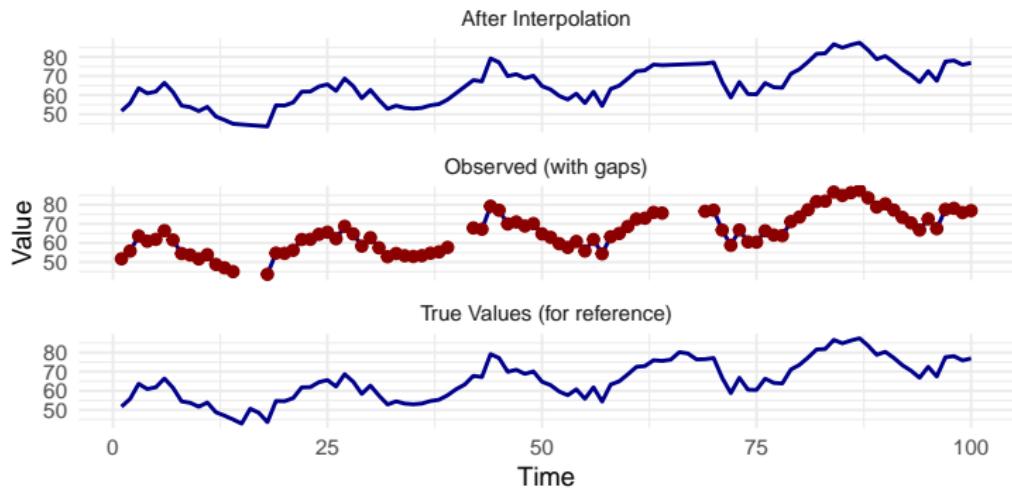
# Linear interpolation
ts_interpolated <- na.approx(ts_with_na)

# Spline interpolation
ts_spline <- na.spline(ts_with_na)
```

# Slide 62: Missing Value Imputation Visualization

## Missing Value Imputation in Time Series

Red points = observed data | Blue line = interpolated



# Slide 63: Outlier Detection in Time Series

## Methods:

- ① **Statistical:** Values beyond  $\text{mean} \pm 3$
- ② **IQR Method:** Beyond  $\text{Q1} - 1.5 \times \text{IQR}$  or  $\text{Q3} + 1.5 \times \text{IQR}$
- ③ **Model-based:** Residuals from fitted model

```
# Fit model
model <- auto.arima(AirPassengers)

# Extract residuals
residuals <- residuals(model)

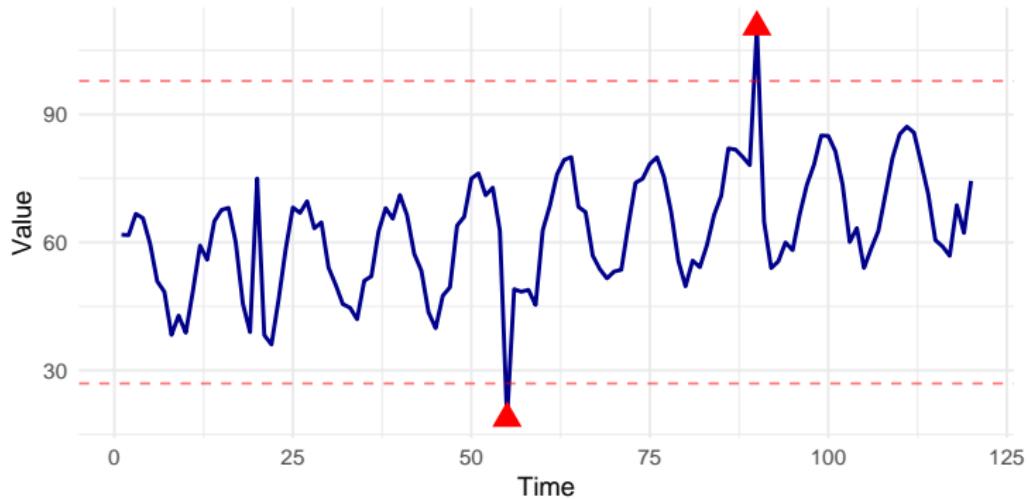
# Detect outliers ( $|residual| > 2.5 \text{ SD}$ )
threshold <- 2.5 * sd(residuals)
outliers <- which(abs(residuals) > threshold)

# Plot
plot(AirPassengers)
points(time(AirPassengers)[outliers])
```

## Slide 64: Outlier Detection Example

### Outlier Detection Using IQR Method

Red triangles = detected outliers | Dashed lines = bounds



## Slide 65: Multivariate Time Series - VAR Models

**Vector Autoregression (VAR):** Multiple time series that influence each other

$$\mathbf{Y}_t = \mathbf{c} + {}_1\mathbf{Y}_{t-1} + {}_2\mathbf{Y}_{t-2} + \cdots + {}_t$$

**Example:** Stock prices of related companies

- Apple stock → Microsoft stock
- Microsoft stock → Apple stock
- Mutual influence captured

```
library(vars)

# Create multivariate time series
data(Canada)

# Fit VAR model
var_model <- VAR(Canada, p = 2, type = "const")
```

## Slide 66: Granger Causality

**Question:** Does time series X “Granger-cause” Y?

**Definition:** X Granger-causes Y if past values of X help predict Y beyond what Y's own past values provide

**Test:**

- $H_0$ : X does not Granger-cause Y
- p-value < 0.05 → Reject  $H_0$  → X Granger-causes Y

```
library(lmtest)

# Test if x Granger-causes y
grangertest(y ~ x, order = 2)

# Bidirectional test
grangertest(x ~ y, order = 2)
```

# Slide 67: Structural Breaks in Time Series

**Structural Break:** Permanent change in time series behavior

**Examples:**

- Policy changes (new regulations)
- Economic shocks (2008 financial crisis)
- Technology adoption (internet boom)

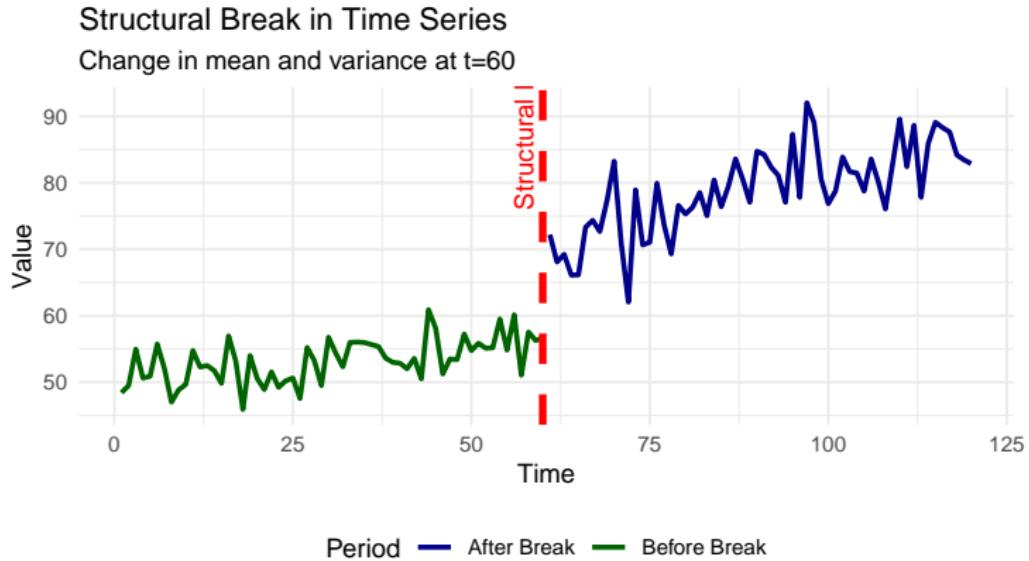
**Detection:**

```
library(strucchange)

# Test for structural breaks
bp_test <- breakpoints(AirPassengers ~ time(AirPassengers))
summary(bp_test)

# Plot breaks
plot(bp_test)
plot(AirPassengers)
```

# Slide 68: Structural Break Visualization



## Slide 69: GARCH Models - Volatility Modeling

**GARCH (Generalized AutoRegressive Conditional Heteroskedasticity):**

Models time-varying variance (volatility clustering)

$$\sigma_t^2 = \omega + \alpha\epsilon_{t-1}^2 + \beta\sigma_{t-1}^2$$

**Use Case:** Financial returns

- Periods of high volatility cluster together
- Periods of low volatility cluster together

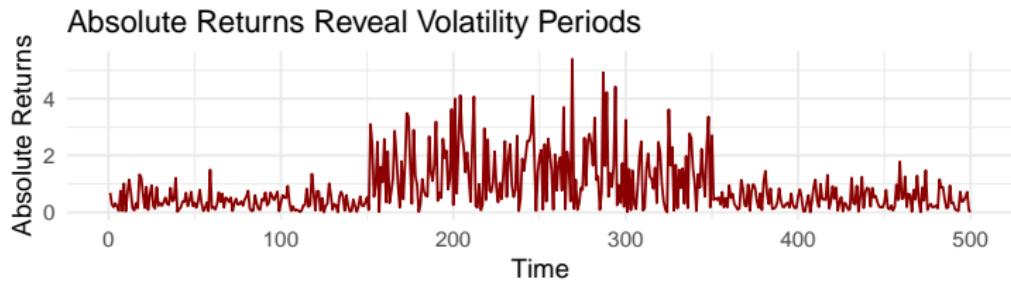
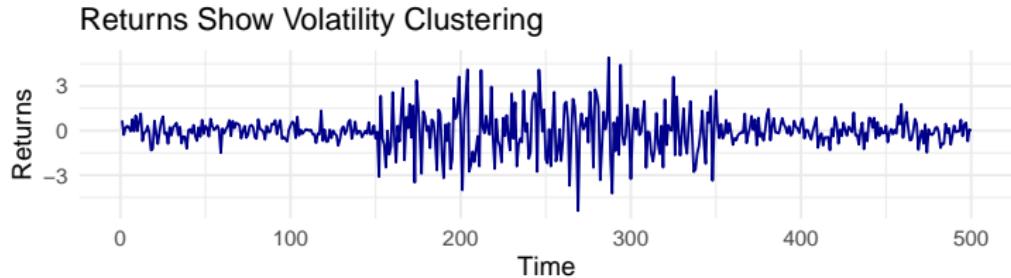
```
library(rugarch)
```

```
# Specify GARCH(1,1) model
```

```
spec <- ugarchspec(variance.model = list(model = "sGARCH",
                                         garchOrder = c(1, 1)))
```

```
# Fit model
```

# Slide 70: Volatility Clustering Example



## Slide 71: Time Series Case Study - Retail Sales Forecasting

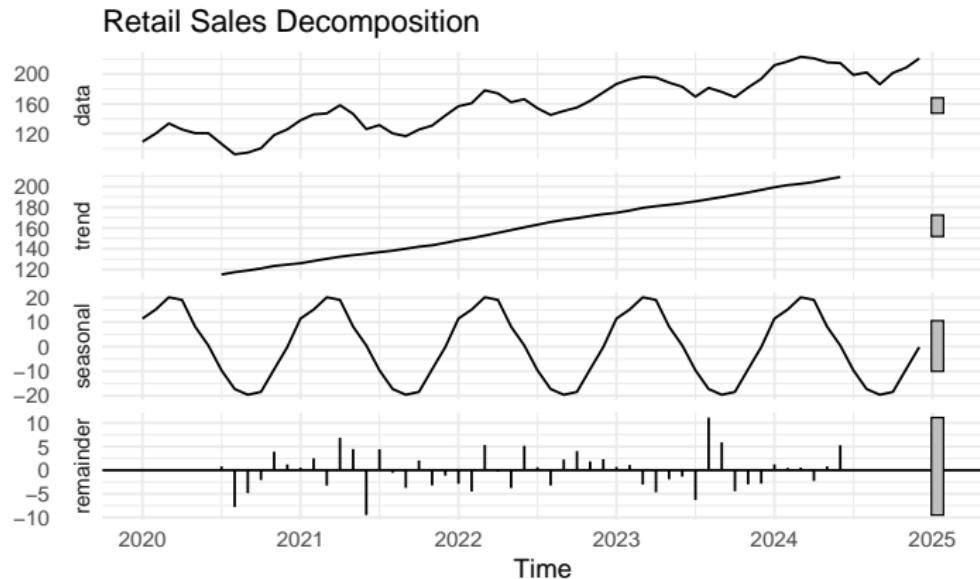
**Business Problem:** Predict next quarter's sales for inventory planning

**Data:** Monthly retail sales (5 years)

**Approach:**

- ① EDA: Identify trend and seasonality
- ② Transform: Log + seasonal differencing
- ③ Model: SARIMA(1,0,1)(1,1,1)
- ④ Validate: MAPE = 3.2% on test set
- ⑤ Deploy: Generate rolling forecasts

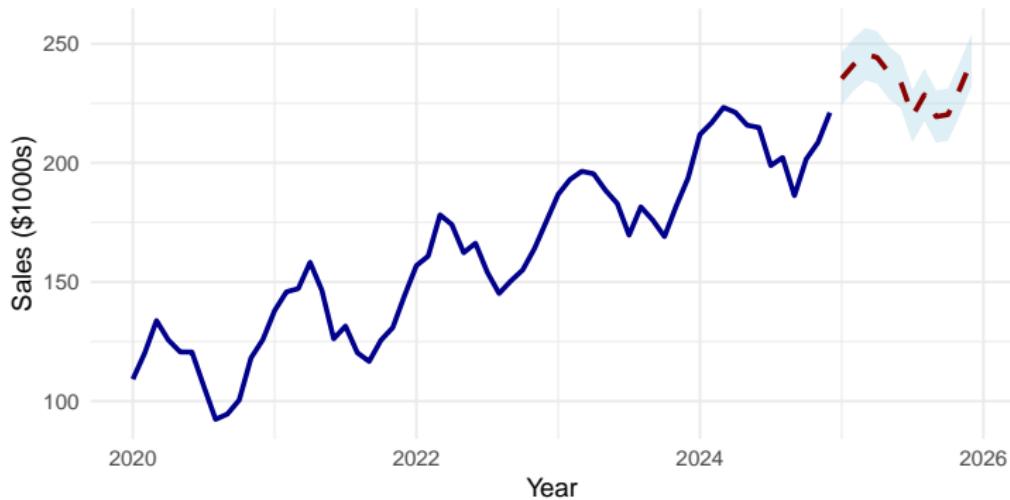
## Slide 72: Retail Sales - Data Exploration



## Slide 73: Retail Sales - Model and Forecast

Retail Sales Forecast: Next 12 Months

MAPE on validation set: 3.2%



## Slide 74: Time Series Forecast Intervals - Interpretation

### Key Points:

- ① **80% PI:** 80% chance true value falls within
- ② **95% PI:** 95% chance true value falls within
- ③ **Wider intervals = More uncertainty**

### Factors Affecting Width:

- Forecast horizon (longer = wider)
- Model uncertainty
- Historical volatility
- Structural breaks

**Business Use:** Risk management and scenario planning

# Slide 75: Common Time Series Pitfalls

## Top 10 Mistakes:

- ① **Ignoring stationarity** → Spurious results
- ② **Over-differencing** → Destroys information
- ③ **Forgetting seasonality** → Poor forecasts
- ④ **Using future data** → Data leakage
- ⑤ **Not checking residuals** → Model inadequacy
- ⑥ **Extrapolating too far** → Unreliable forecasts
- ⑦ **Ignoring structural breaks** → Model misspecification
- ⑧ **Wrong frequency** → Seasonal pattern mismatch
- ⑨ **Not updating models** → Performance degradation
- ⑩ **Assuming stationarity** → Wrong inference

## Slide 76: Time Series Checklist

### Before Forecasting:

- Plot the series (visual inspection)
- Check for missing values
- Identify trend component
- Identify seasonal component
- Test for stationarity (ADF test)
- Apply transformations if needed
- Split into train/test sets
- Check for outliers
- Examine ACF/PACF plots
- Consider external events

## Production Forecasting:

- ① **Monitor performance:** Track forecast errors continuously
- ② **Update regularly:** Retrain as new data arrives
- ③ **Document assumptions:** Record transformations, parameters
- ④ **Maintain baselines:** Compare against naive forecasts
- ⑤ **Communicate uncertainty:** Always show prediction intervals
- ⑥ **Version control:** Track model changes
- ⑦ **A/B testing:** Compare model versions
- ⑧ **Human oversight:** Expert review of forecasts

# Slide 78: Transitioning to Unsupervised Learning

## From Time Series to Clustering:

### Time Series Focus:

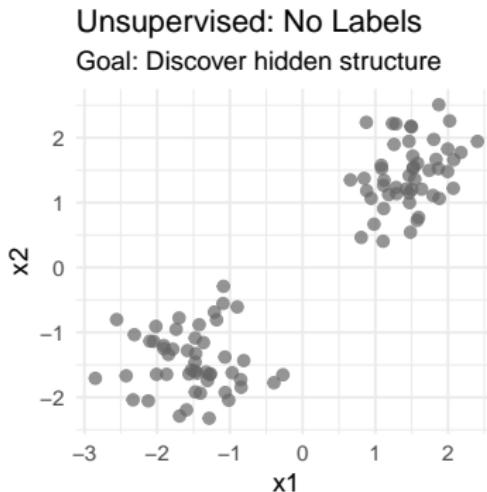
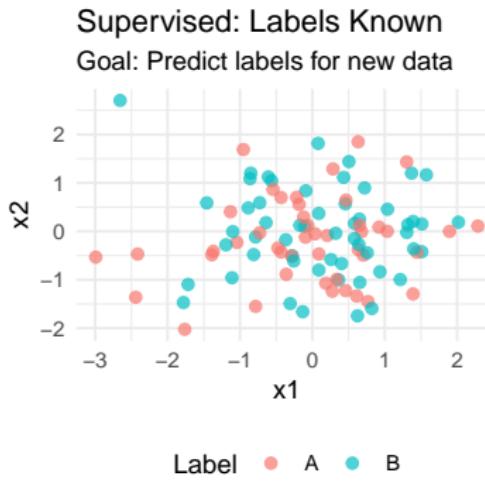
- Temporal dependence
- Forecasting future values
- Understanding trends/seasonality

### Unsupervised Learning Focus:

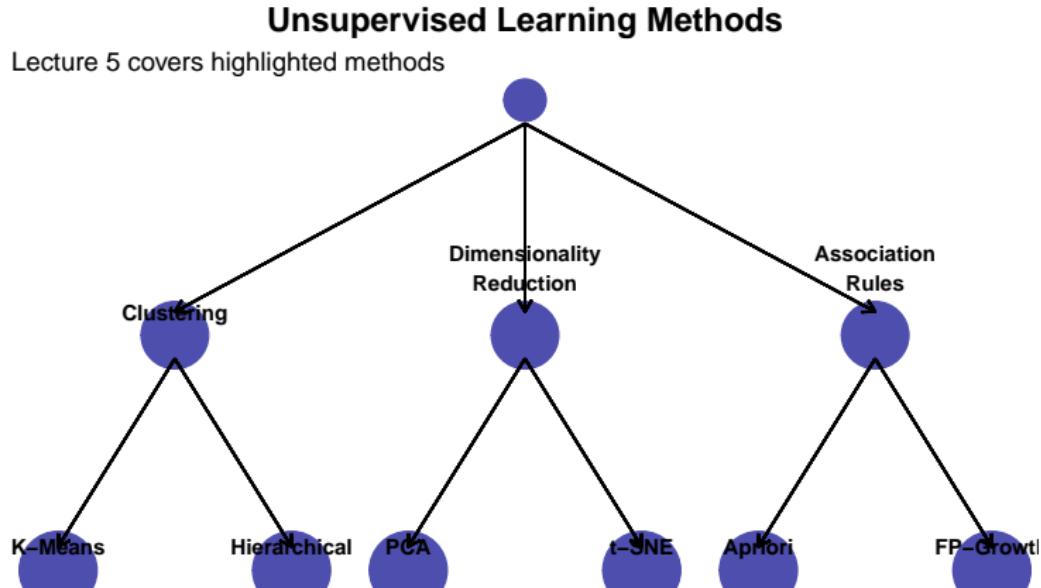
- Finding hidden patterns
- Grouping similar observations
- Dimensionality reduction
- **No labels needed!**

# Slide 79: Why Unsupervised Learning?

## Motivation:



# Slide 80: Unsupervised Learning Taxonomy



## Section 5

### Introduction to Clustering

# Slide 81: What is Clustering?

**Definition:** Grouping data points so that:

- Points in the same cluster are **similar**
- Points in different clusters are **dissimilar**

**No ground truth labels!**

**Applications:**

- Customer segmentation
- Document categorization
- Image compression
- Anomaly detection
- Gene expression analysis

# Slide 82: Clustering Example - Customer Segmentation



# Slide 83: Distance Metrics - Measuring Similarity

## Common Distance Measures:

### ① Euclidean Distance (L2):

$$d(x, y) = \sqrt{\sum_{i=1}^n (x_i - y_i)^2}$$

### ② Manhattan Distance (L1):

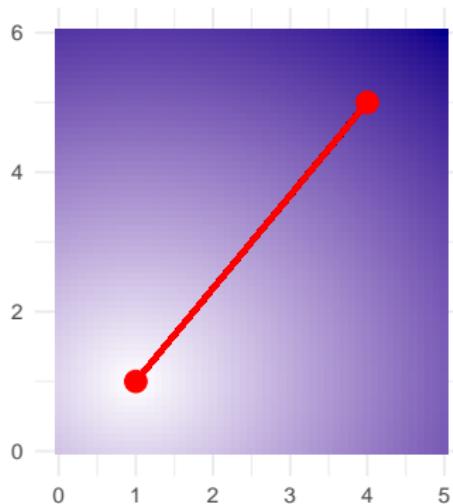
$$d(x, y) = \sum_{i=1}^n |x_i - y_i|$$

### ③ Cosine Similarity:

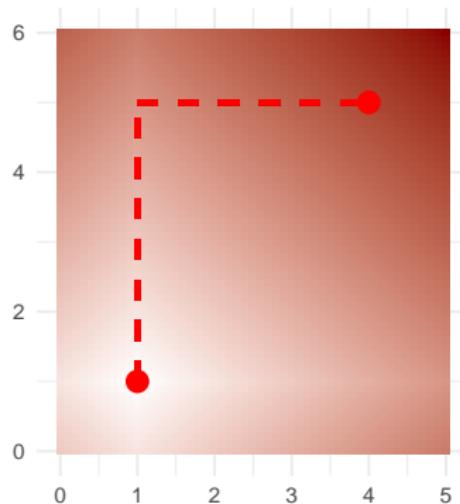
$$\text{sim}(x, y) = \frac{x \cdot y}{\|x\|\|y\|}$$

## Slide 84: Distance Metrics Visualization

Euclidean Distance



Manhattan Distance



## Slide 85: Feature Scaling - Critical for Clustering

**Problem:** Features on different scales dominate distance calculations

**Example:**

- Income: \$20,000 - \$200,000
- Age: 18 - 65

Income will dominate the distance!

**Solution: Standardization**

$$z = \frac{x - \mu}{\sigma}$$

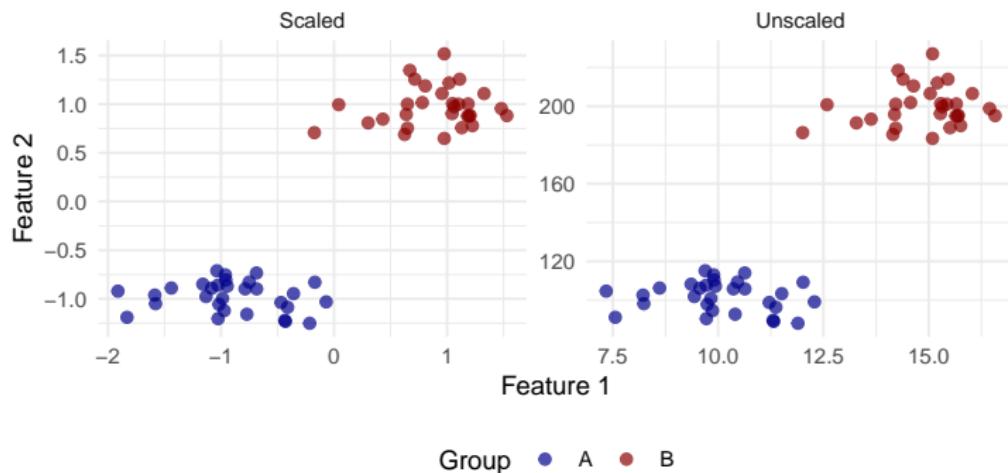
```
# Standardize features  
data_scaled <- scale(data)
```

```
# Alternative: Min-Max scaling [0, 1]  
data_minmax <- apply(data, 2, function(x) {  
  (x - min(x)) / (max(x) - min(x))})
```

# Slide 86: Impact of Scaling on Clustering

## Impact of Feature Scaling

Left: Feature2 dominates | Right: Balanced features



## Slide 87: K-Means Algorithm - Overview

**Goal:** Partition  $n$  observations into  $k$  clusters

**Algorithm:**

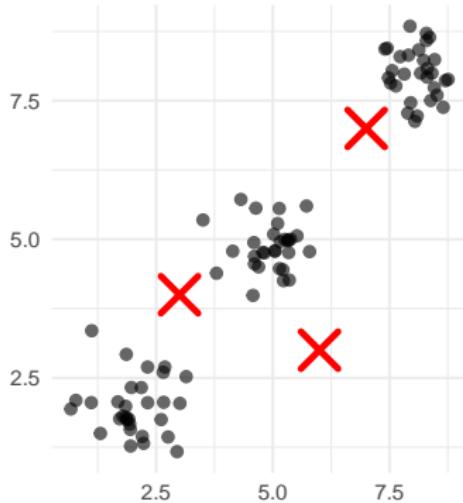
- ① **Initialize:** Randomly select  $k$  cluster centers
- ② **Assignment:** Assign each point to nearest center
- ③ **Update:** Recalculate centers as mean of assigned points
- ④ **Repeat:** Until convergence (centers don't change)

**Objective:** Minimize within-cluster sum of squares (WCSS)

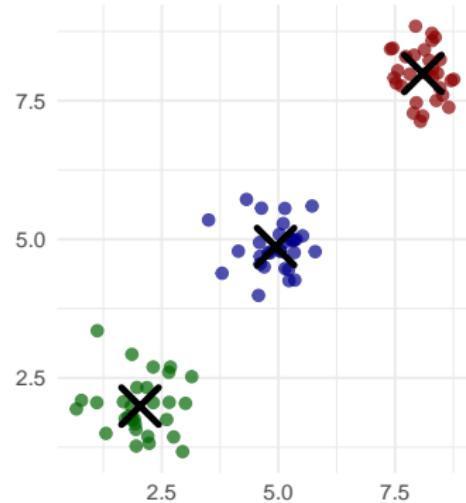
$$WCSS = \sum_{i=1}^k \sum_{x \in C_i} \|x - \mu_i\|^2$$

# Slide 88: K-Means Step-by-Step Visualization

Step 1: Random Centers



Step 4: Converged



## Slide 89: K-Means in R

```
# Load and prepare data
data(iris)
iris_features <- iris[, 1:4]

# Scale features
iris_scaled <- scale(iris_features)

# Fit K-Means with k=3
set.seed(123)
kmeans_result <- kmeans(iris_scaled,
                         centers = 3,
                         nstart = 25) # Try 25 random starts

# View results
kmeans_result$centers      # Cluster centers
kmeans_result$cluster       # Cluster assignments
kmeans_result$size          # Cluster sizes
```

# Slide 90: Choosing K - The Elbow Method

**Problem:** How many clusters?

**Elbow Method:**

- ① Run K-Means for different values of  $k$
- ② Plot WCSS vs  $k$
- ③ Look for “elbow” (point of diminishing returns)

```
# Compute WCSS for k = 1 to 10
wcss <- numeric(10)

for (k in 1:10) {
  kmeans_fit <- kmeans(data_scaled, centers = k, nstart = 25)
  wcss[k] <- kmeans_fit$tot.withinss
}

# Plot elbow curve
plot(1:10, wcss, type = "b",
      xlab = "Number of Clusters (k)"
```

## Slide 91: Mining Association Rules - Complete Example

```
library(arules)
library(arulesViz)

# Load grocery transactions
data("Groceries")

# Summary statistics
summary(Groceries)
# Output: 9835 transactions, 169 items

# Item frequency plot
itemFrequencyPlot(Groceries, topN = 20,
                  type = "absolute",
                  main = "Top 20 Most Frequent Items")

# Mine rules
rules <- apriori(Groceries,
```

## Slide 92: Silhouette Analysis - Alternative to Elbow

**Silhouette Coefficient:** Measures how well each point fits its cluster

$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}$$

where: -  $a(i)$  = average distance to points in same cluster -  $b(i)$  = average distance to points in nearest other cluster

**Range:** -1 (wrong cluster) to +1 (perfect fit)

**Rule:** Choose  $k$  that maximizes average silhouette score

## Slide 93: Silhouette Score Calculation

```
library(cluster)

# Compute silhouette scores for different k
silhouette_scores <- numeric(9)

for (k in 2:10) {
  kmeans_fit <- kmeans(data_scaled, centers = k, nstart = 25)

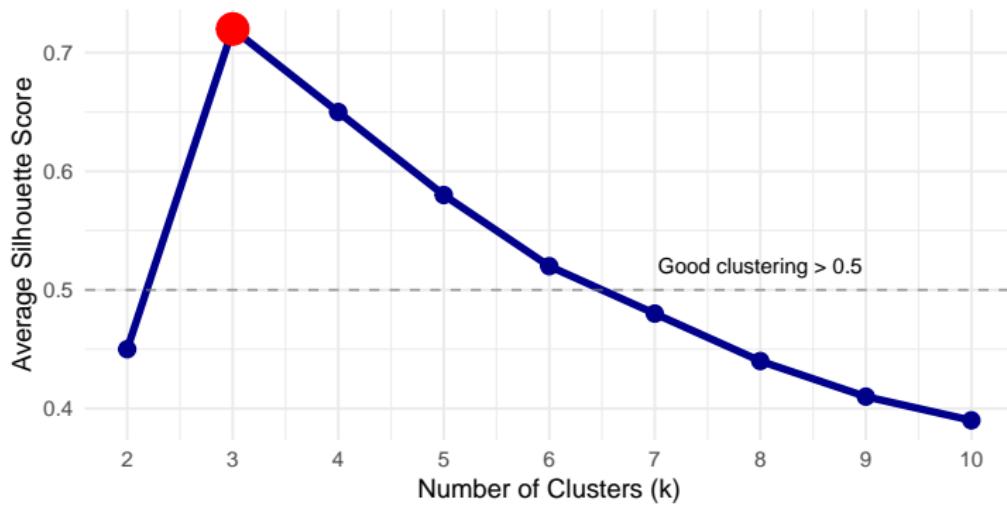
  # Calculate silhouette
  sil <- silhouette(kmeans_fit$cluster, dist(data_scaled))
  silhouette_scores[k-1] <- mean(sil[, 3])
}

# Plot
plot(2:10, silhouette_scores, type = "b",
      xlab = "Number of Clusters (k)",
      ylab = "Average Silhouette Score",
      main = "Silhouette Scores")
```

# Slide 94: Silhouette Plot Visualization

## Silhouette Analysis for Optimal K

Peak at k=3: Best cluster separation



## Slide 95: K-Means Limitations

### Major Drawbacks:

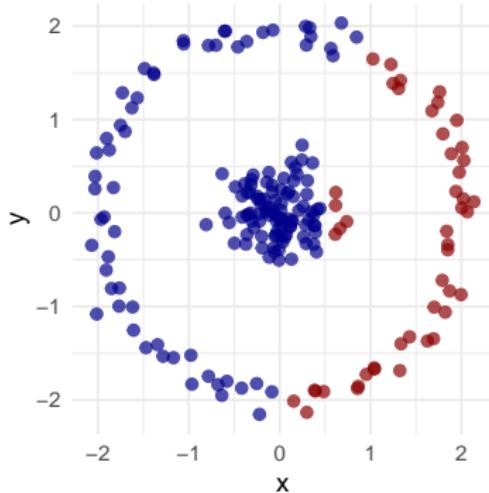
- ① Must specify K in advance (chicken-egg problem)
- ② Sensitive to initialization (local minima)
- ③ Assumes spherical clusters (equal variance)
- ④ Sensitive to outliers (means get pulled)
- ⑤ Hard to interpret in high dimensions

**When K-Means Fails:** - Non-convex shapes (crescents, rings) - Different cluster densities - Different cluster sizes

## Slide 96: When K-Means Fails - Examples

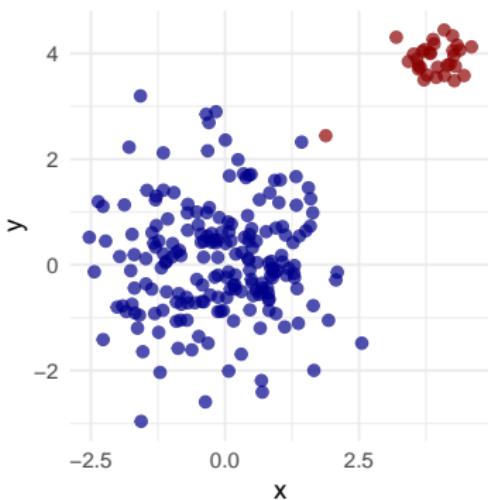
Failure: Concentric Circles

K-Means can't handle non-convex shapes



Failure: Different Sizes

K-Means splits large cluster incorrect



## Slide 97: K-Means++ Initialization

**Problem:** Random initialization can lead to poor results

**K-Means++ Solution:** Smart initialization

- ① Choose first center randomly
- ② For each remaining center:
  - Choose point with probability proportional to distance from nearest existing center
  - Favors points far from current centers

**Result:** Better initial centers → faster convergence, better clusters

```
# K-Means++ is default in R
kmeans_result <- kmeans(data,
                           centers = 3,
                           nstart = 25, # Multiple random starts
                           algorithm = "Lloyd")
```

## Slide 98: Mini-Batch K-Means for Large Data

**Problem:** Standard K-Means slow on large datasets

### Mini-Batch K-Means:

- ① Sample random mini-batch of data
- ② Assign points to nearest center
- ③ Update centers based on mini-batch only
- ④ Repeat

**Advantages:** - Much faster (suitable for millions of points) - Similar quality to standard K-Means - Scalable to streaming data

## Slide 99: K-Means Case Study - Customer Segmentation

**Business Problem:** E-commerce company wants to segment 10,000 customers

**Features:** - Recency (days since last purchase) - Frequency (number of purchases) - Monetary (total spending)

**Approach:** RFM Analysis with K-Means

## Slide 100: RFM Segmentation Implementation

```
# Load customer data
# customers <- read.csv("customer_data.csv")

# Create RFM features
rfm_data <- customers %>%
  group_by(customer_id) %>%
  summarise(
    Recency = as.numeric(max(purchase_date) - Sys.Date()),
    Frequency = n(),
    Monetary = sum(purchase_amount)
  )

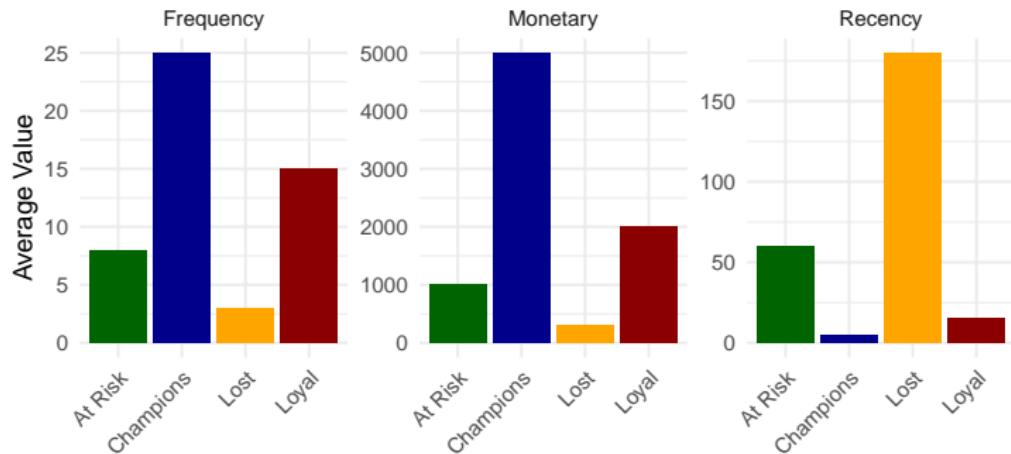
# Scale features
rfm_scaled <- scale(rfm_data[, 2:4])

# Determine optimal k using elbow method
# ... (see previous slides)
```

# Slide 101: RFM Segments Interpretation

## Customer Segments: RFM Analysis

Champions: High value | Lost: Need re-engagement



## Slide 102: Business Actions from Segmentation

### Segment-Specific Strategies:

Segment	Characteristics	Action
<b>Champions</b>	Recent, frequent, high \$	VIP treatment, early access
<b>Loyal</b>	Regular buyers	Loyalty rewards, referrals
<b>At Risk</b>	Haven't bought recently	Win-back campaigns
<b>Lost</b>	Inactive, low value	Minimal marketing spend

**ROI:** Targeted campaigns → 3x conversion vs. mass marketing

## Section 6

### Hierarchical Clustering

# Slide 103: Introduction to Hierarchical Clustering

## Key Difference from K-Means:

- **K-Means:** Flat partitioning (must choose K)
- **Hierarchical:** Creates tree structure (dendrogram)

## Two Approaches:

### ① Agglomerative (Bottom-Up):

- Start: Each point is its own cluster
- Iteratively merge closest clusters
- End: One cluster containing all points

### ② Divisive (Top-Down):

- Start: All points in one cluster
- Iteratively split clusters
- End: Each point in its own cluster

## Slide 104: Agglomerative Clustering Algorithm

### Algorithm:

- ① **Initialize:** Treat each point as a cluster ( $n$  clusters)
- ② **Repeat:**
  - Find two closest clusters
  - Merge them
  - Update distance matrix
- ③ **Stop:** When desired number of clusters reached (or all merged)

**Output:** Dendrogram showing merge history

**Advantage:** Don't need to specify K upfront!

# Slide 105: Linkage Methods - Measuring Cluster Distance

**How to measure distance between clusters?**

① **Single Linkage (MIN):**

$$d(C_i, C_j) = \min_{x \in C_i, y \in C_j} d(x, y)$$

② **Complete Linkage (MAX):**

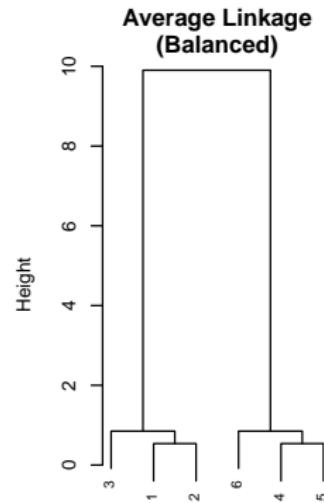
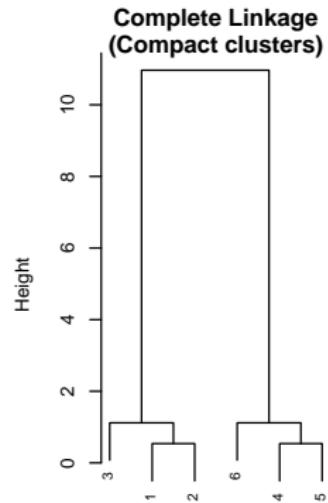
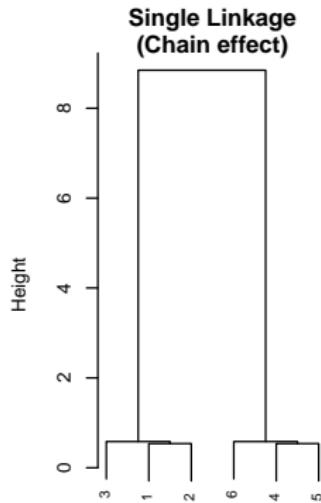
$$d(C_i, C_j) = \max_{x \in C_i, y \in C_j} d(x, y)$$

③ **Average Linkage:**

$$d(C_i, C_j) = \frac{1}{|C_i||C_j|} \sum_{x \in C_i} \sum_{y \in C_j} d(x, y)$$

④ **Ward's Method:** Minimize within-cluster variance

# Slide 106: Linkage Methods Comparison



## Slide 107: Hierarchical Clustering in R

```
# Prepare data
iris_features <- iris[, 1:4]
iris_scaled <- scale(iris_features)

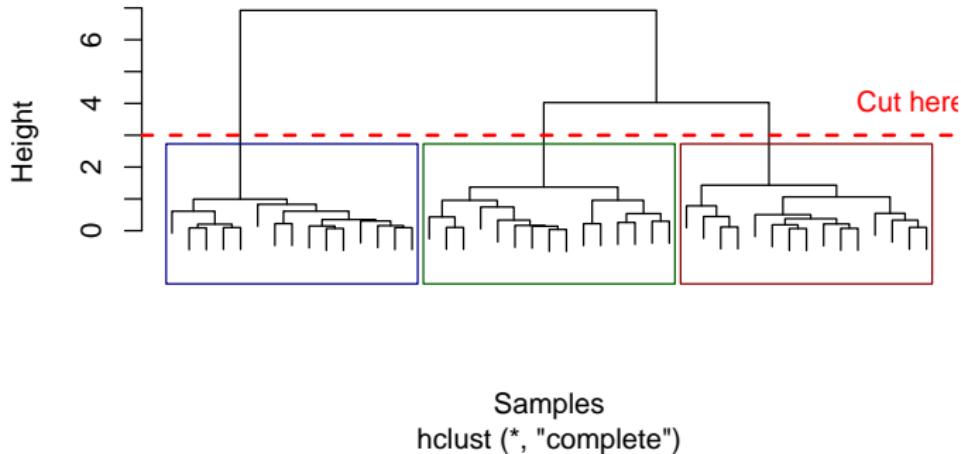
# Compute distance matrix
dist_matrix <- dist(iris_scaled, method = "euclidean")

# Perform hierarchical clustering
hc_result <- hclust(dist_matrix, method = "complete")

# Plot dendrogram
plot(hc_result,
      main = "Hierarchical Clustering Dendrogram",
      xlab = "Sample Index",
      ylab = "Distance",
      cex = 0.6)
```

# Slide 108: Dendrogram Interpretation

Dendrogram with Cut Height



**Reading the Dendrogram:** - Height = dissimilarity between merged clusters - Lower merges = more similar - Horizontal line = choose number of clusters

## Slide 109: Cutting the Dendrogram

```
# Method 1: Cut at specific height
clusters_height <- cutree(hc_result, h = 5)

# Method 2: Specify number of clusters
clusters_k <- cutree(hc_result, k = 3)

# Compare cluster assignments
table(clusters_k, iris$Species)

# Visualize clusters
pairs(iris[, 1:4],
      col = clusters_k,
      pch = 19,
      main = "Hierarchical Clustering Results")
```

## Slide 110: Hierarchical vs K-Means Comparison

Aspect	K-Means	Hierarchical
<b>K Selection</b>	Must specify upfront	Can decide later from dendrogram
<b>Scalability</b>	Fast (linear)	Slow (quadratic)
<b>Cluster Shape</b>	Spherical only	Any shape
<b>Deterministic</b>	No (random init)	Yes
<b>Memory</b>	Low	High (distance matrix)
<b>Interpretation</b>	Hard	Easy (dendrogram)

**Rule of Thumb:** -  $n < 5,000 \rightarrow$  Hierarchical -  $n > 5,000 \rightarrow$  K-Means

## Slide 111: Hierarchical Clustering Case Study - Gene Expression

**Problem:** Cluster genes based on expression patterns

**Data:** Gene expression levels across different conditions

**Goal:** Identify co-regulated genes (similar expression patterns)

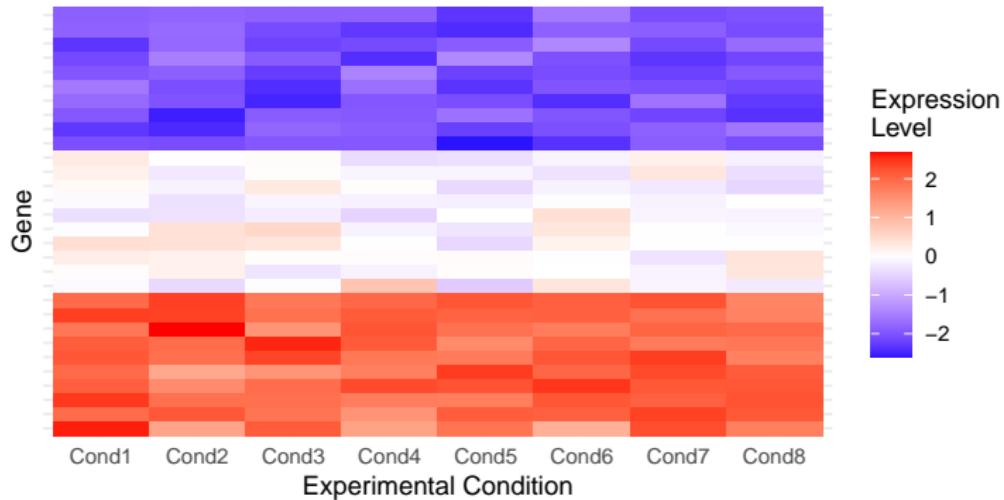
**Approach:**

- ① Compute correlation between gene expression profiles
- ② Convert correlation to distance:  $d = 1 - |r|$
- ③ Hierarchical clustering with average linkage
- ④ Visualize with heatmap + dendrogram

# Slide 112: Gene Expression Heatmap

Gene Expression Heatmap with Clustering

Rows ordered by hierarchical clustering



## Section 7

### Association Rule Mining

## Slide 113: Introduction to Association Rules

**Goal:** Find interesting relationships in transaction data

**Classic Example:** Market Basket Analysis

- Transaction: {Bread, Milk, Eggs}
- Rule: {Bread, Milk} → {Eggs}
- Interpretation: “Customers who buy bread and milk also buy eggs”

**Applications:**

- Retail: Product recommendations
- Web: Clickstream analysis
- Healthcare: Symptom → disease associations

## Slide 114: Association Rule Terminology

### Key Concepts:

- **Itemset:** Set of items, e.g., {Bread, Milk}
- **Transaction:** A collection of items purchased together
- **Rule:** Implication of the form  $X \rightarrow Y$

### Example Transaction Database:

TID	Items
1	{Bread, Milk}
2	{Bread, Diaper, Beer, Eggs}
3	{Milk, Diaper, Beer, Cola}
4	{Bread, Milk, Diaper, Beer}
5	{Bread, Milk, Diaper, Cola}

## Slide 115: Support, Confidence, and Lift

### Three Key Metrics:

- ① **Support:** Frequency of itemset

$$\text{Support}(X) = \frac{\text{number of transactions containing } X}{\text{total number of transactions}}$$

- ② **Confidence:** Conditional probability

$$\text{Confidence}(X \rightarrow Y) = \frac{\text{Support}(X \cup Y)}{\text{Support}(X)}$$

- ③ **Lift:** Independence measure

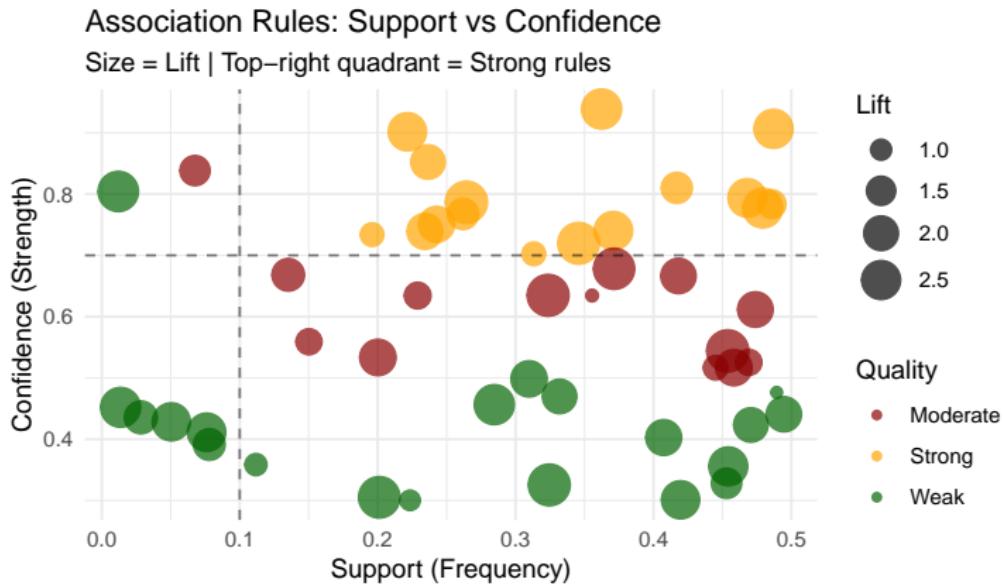
$$\text{Lift}(X \rightarrow Y) = \frac{\text{Confidence}(X \rightarrow Y)}{\text{Support}(Y)}$$

## Slide 116: Interpreting Support, Confidence, Lift

**Support = 0.4 (40%):** - Rule occurs in 40% of transactions - High support = frequent pattern

**Confidence = 0.8 (80%):** - 80% of customers who buy X also buy Y - High confidence = strong rule

# Slide 117: Support-Confidence Framework



## Slide 118: The Apriori Algorithm

**Problem:** Exponential search space ( $2^n$  possible itemsets)

**Apriori Principle:** If an itemset is frequent, all its subsets must be frequent

**Algorithm:**

- ① Find all frequent 1-itemsets (support  $\geq \text{min\_support}$ )
- ② Generate candidate 2-itemsets from frequent 1-itemsets
- ③ Prune candidates using Apriori principle
- ④ Count support, keep frequent 2-itemsets
- ⑤ Repeat for  $k=3, 4, \dots$  until no more frequent itemsets

# Slide 119: Apriori Algorithm Illustration

## Apriori Algorithm: Level-wise Search

Level 1: {A}, {B}, {C}, {D}, {E}

Prune: {E} (support < threshold)

Level 2: {A,B}, {A,C}, {A,D}, {B,C}, {B,D}, {C,D}

Prune: {A,D}, {C,D} (support < threshold)

Level 3: {A,B,C}, {A,B,D}, {B,C,D}

Prune: {B,C,D} (C,D not frequent in Level 2)

Final: {A,B,C}, {A,B,D}

## Slide 120: Association Rules in R - arules Package

```
library(arules)

# Load example data
data("Groceries")

# Inspect transactions
inspect(Groceries[1:5])

# Mine frequent itemsets
frequent_items <- apriori(Groceries,
                            parameter = list(
                                support = 0.01,      # Min 1% support
                                target = "frequent itemsets"
                            ))
                            ))

# Mine association rules
rules <- apriori(Groceries,
```

## Slide 121: Mining Association Rules - Complete Example

```
library(arules)
library(arulesViz)

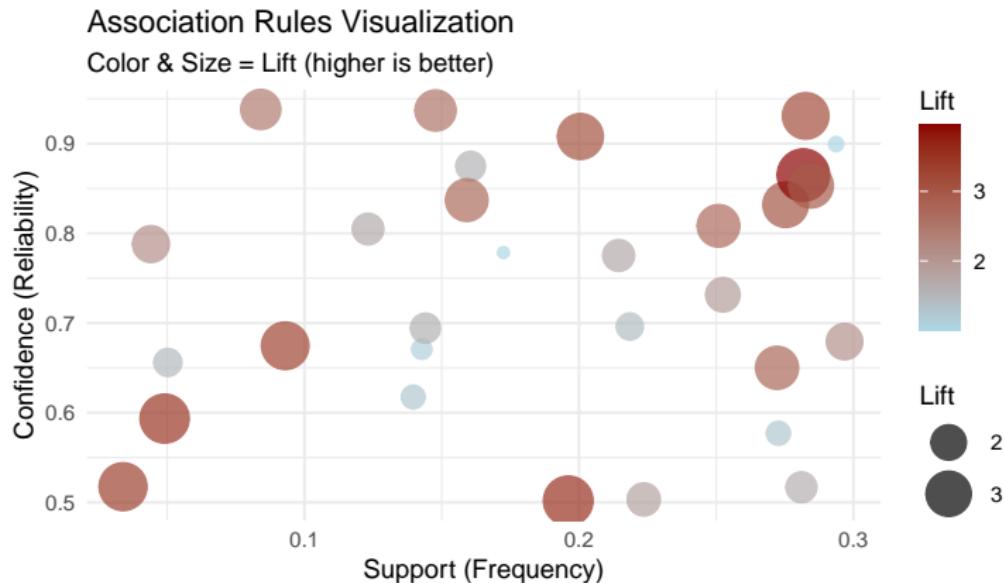
# Load grocery transactions
data("Groceries")

# Summary statistics
summary(Groceries)
# 9835 transactions, 169 items

# Item frequency plot
itemFrequencyPlot(Groceries, topN = 20,
                  type = "absolute",
                  main = "Top 20 Most Frequent Items")

# Mine rules
rules <- apriori(Groceries,
```

# Slide 122: Visualizing Association Rules



**Interactive visualization:** Use `arulesViz::plot(rules, method="graph")`

## Slide 123: Redundant Rules and Pruning

**Problem:** Many rules are redundant

**Example:** -  $\{\text{Milk}\} \rightarrow \{\text{Bread}\}$  [conf=0.8] -  $\{\text{Milk, Eggs}\} \rightarrow \{\text{Bread}\}$  [conf=0.8]

If second rule has same confidence, it's **redundant**

**Pruning Strategy:**

```
# Remove redundant rules
rules_pruned <- rules[!is.redundant(rules)]  
  
# Compare
length(rules)           # Before: 463 rules
length(rules_pruned)    # After: 231 rules  
  
# Significant rules only (high lift)
significant_rules <- subset(rules_pruned, lift > 2)
inspect(significant_rules)
```

## Slide 124: Closed and Maximal Itemsets

**Closed Itemset:** No superset with same support

**Maximal Itemset:** No superset is frequent

### Why Use Them?

- Reduce redundancy
- Faster mining
- More compact representation

```
# Mine closed frequent itemsets
closed <- apriori(Groceries,
                    parameter = list(
                      support = 0.01,
                      target = "closed frequent itemsets"
                    ))
```

```
# Mine maximal frequent itemsets
maximal <- apriori(Groceries,
```

## Slide 125: Sequential Pattern Mining

**Extension:** Consider order of purchases over time

**Example Sequence:** - Week 1: {Bread, Milk} - Week 2: {Eggs} - Week 3: {Butter}

**Sequential Rule:** {Bread, Milk} → {Eggs} → {Butter}

**Applications:** - Customer journey analysis - Web navigation patterns - DNA sequence analysis

```
library(arulesSequences)

# Read sequential data
sequences <- read_baskets("sequences.txt",
                           info = c("sequenceID", "eventID"))

# Mine sequential patterns
seq_rules <- cspade(sequences,
                     parameter = list(support = 0.01))
```

# Slide 126: Association Rules Case Study - Retail Recommendations

**Business Goal:** Increase average basket size through recommendations

**Dataset:** 100,000 grocery transactions over 6 months

## Analysis:

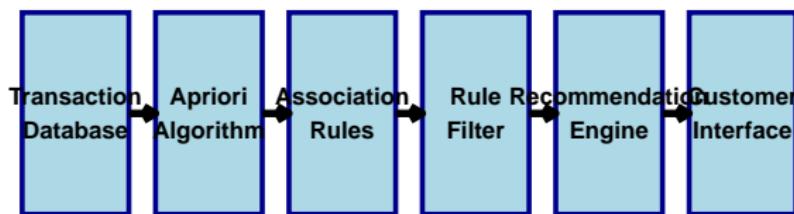
- ① Mine rules (support 0.01, confidence 0.6)
- ② Filter by lift > 2 (strong associations)
- ③ Remove redundant rules
- ④ Deploy top 50 rules to recommendation engine

## Results:

- 15% increase in basket size
- 8% increase in revenue
- Most effective rule: {Pasta, Tomato Sauce} → {Parmesan Cheese}

# Slide 127: Recommendation System Architecture

## Real-Time Recommendation System Architecture



## Section 8

### Density-Based Clustering

**Key Idea:** Clusters are dense regions separated by sparse regions

### Advantages over K-Means:

- ① No need to specify number of clusters
- ② Can find arbitrarily shaped clusters
- ③ Robust to outliers
- ④ Identifies noise points

### Parameters:

- **(epsilon):** Neighborhood radius
- **minPts:** Minimum points to form dense region

### Three Types of Points:

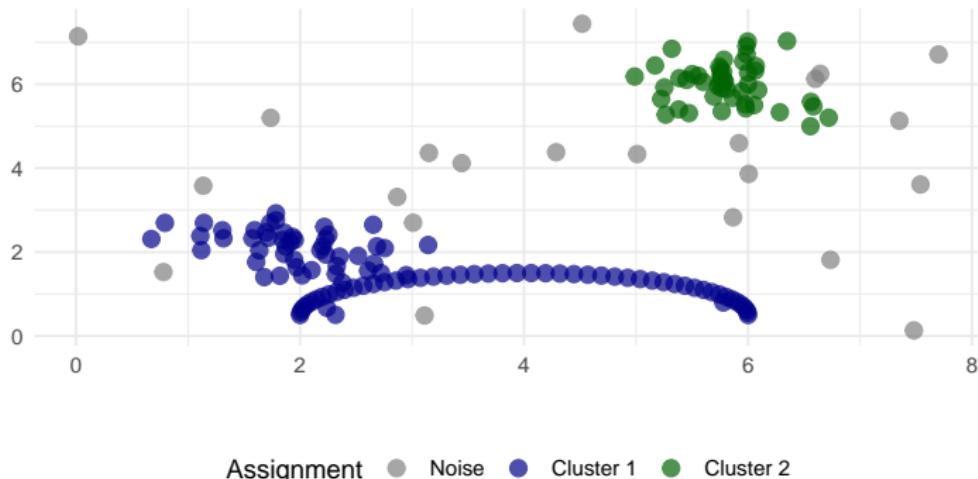
- ① **Core Point:** Has  $\text{minPts}$  within
- ② **Border Point:** Within  $\epsilon$  of a core point, but not core itself
- ③ **Noise Point:** Neither core nor border

**Density-Connected:** Two points are in same cluster if connected through chain of core points

# Slide 130: DBSCAN Visual Intuition

DBSCAN: Finds Arbitrary Shapes + Noise

Gray points = noise (outliers)



# Slide 131: DBSCAN Algorithm

## Algorithm:

- ① **Mark all points** as unvisited
- ② **For each unvisited point p:**
  - Mark as visited
  - Find neighborhood  $N$  (points within  $\epsilon$ )
  - If  $|N| < \text{minPts}$ : Mark as **noise**
  - Else:
    - Create new cluster
    - Add p to cluster
    - **Expand cluster** from p's neighbors
- ③ **Repeat** until all points visited

## Slide 132: DBSCAN in R

```
library(dbscan)

# Prepare data
data_scaled <- scale(data)

# Run DBSCAN
db_result <- dbscan(data_scaled,
                      eps = 0.5,           # Neighborhood radius
                      minPts = 5)          # Min points for core

# View results
db_result$cluster # Cluster assignments (0 = noise)
table(db_result$cluster)

# Visualize
plot(data_scaled,
      col = db_result$cluster + 1,
```

## Slide 133: Choosing DBSCAN Parameters

### (epsilon) Selection:

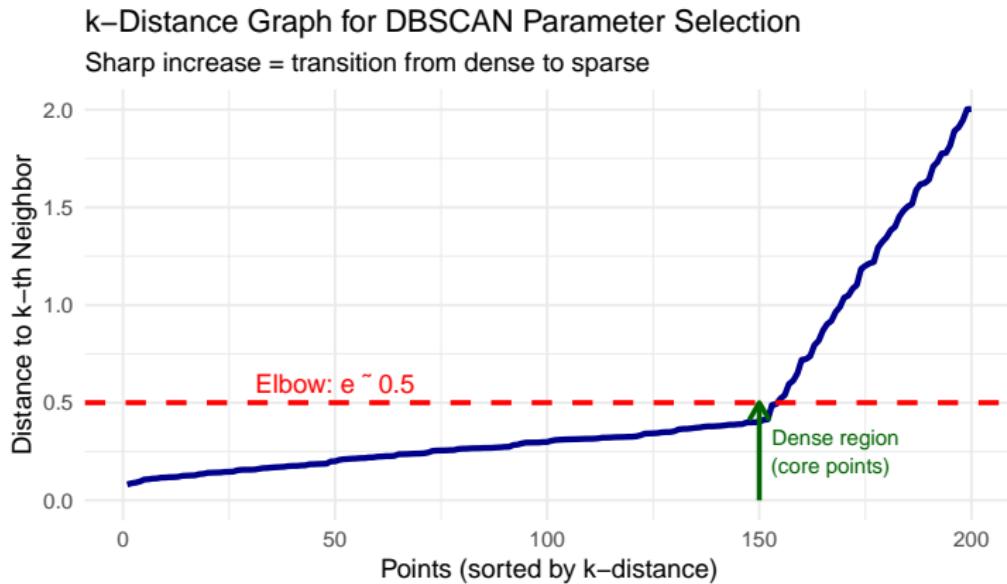
Use **k-distance graph** (elbow method for DBSCAN)

- ① For each point, compute distance to k-th nearest neighbor
- ② Sort distances
- ③ Plot sorted k-distances
- ④ Look for “elbow” → optimal

```
# Compute k-nearest neighbor distances
k <- 5 # Same as minPts
knn_dist <- kNNdist(data_scaled, k = k)

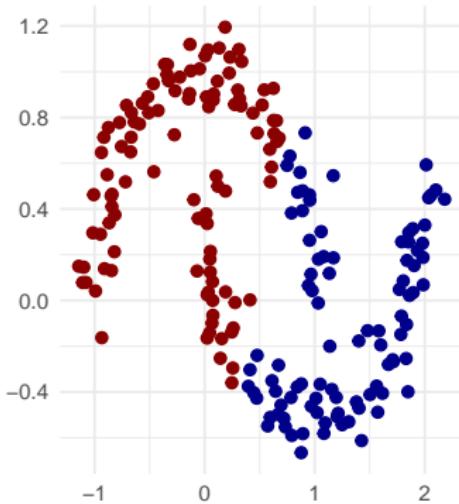
# Sort and plot
knn_sorted <- sort(knn_dist)
plot(knn_sorted,
     type = "l",
     xlab = "Points (sorted)",
     ylab = "k-NN Distance",
```

# Slide 134: k-Distance Graph for Parameter Selection

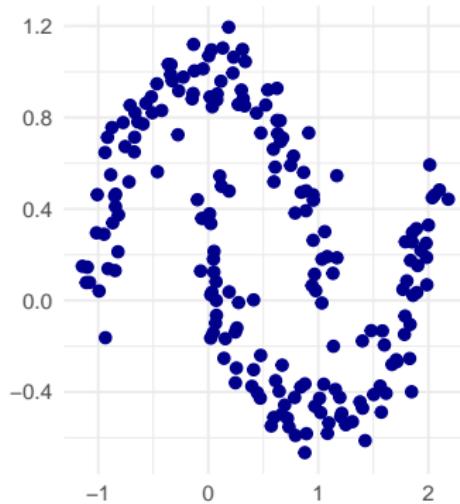


## Slide 135: DBSCAN vs K-Means Comparison

K-Means: Fails on Non-Convex Data



DBSCAN: Handles Arbitrary Shapes



## Slide 136: HDBSCAN - Hierarchical DBSCAN

**Problem with DBSCAN:** Single doesn't work for varying densities

**HDBSCAN Solution:** Hierarchy of DBSCAN results

### Advantages:

- Automatically selects for each cluster
- Handles varying density clusters
- More robust parameter selection (only minPts)

```
library(dbSCAN)

# Run HDBSCAN
hdb_result <- dbSCAN(data_scaled, minPts = 5)

# View cluster tree
plot(hdb_result, show_flat = TRUE)

# Extract flat clustering
```

## Section 9

### Dimensionality Reduction

## Slide 137: The Curse of Dimensionality

**Problem:** As dimensions increase:

- ① **Distance loses meaning:** All points become equidistant
- ② **Sparsity:** Data points spread thin
- ③ **Computation:** Exponential time/space
- ④ **Visualization:** Can't plot beyond 3D

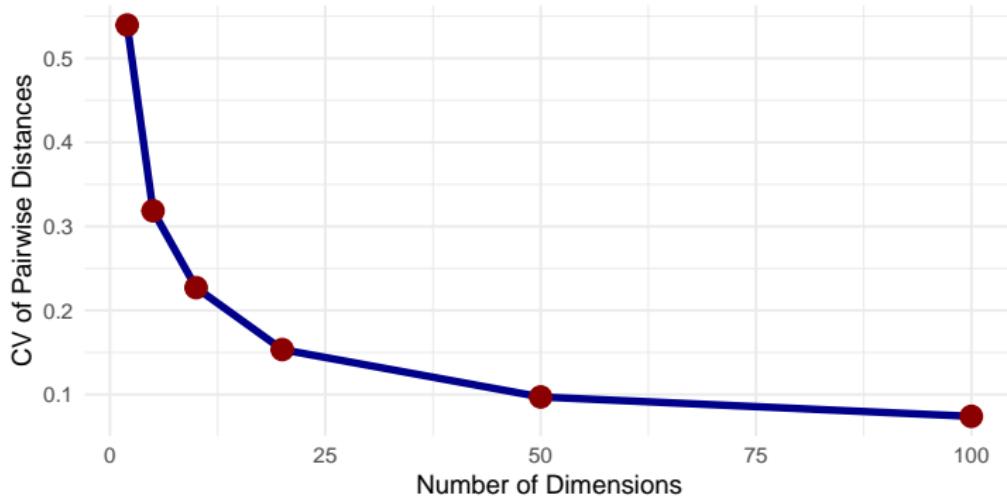
**Example:** 100 features  $\rightarrow 2^{100}$  possible feature combinations!

**Solution:** Reduce dimensions while preserving information

## Slide 138: Distance Concentration in High Dimensions

Curse of Dimensionality: Distance Loses Meaning

Coefficient of Variation decreases: distances become similar



## Slide 139: Principal Component Analysis (PCA)

**Goal:** Find directions of maximum variance

**Key Idea:**

- ① Center the data
- ② Compute covariance matrix
- ③ Find eigenvectors (principal components)
- ④ Project data onto top k eigenvectors

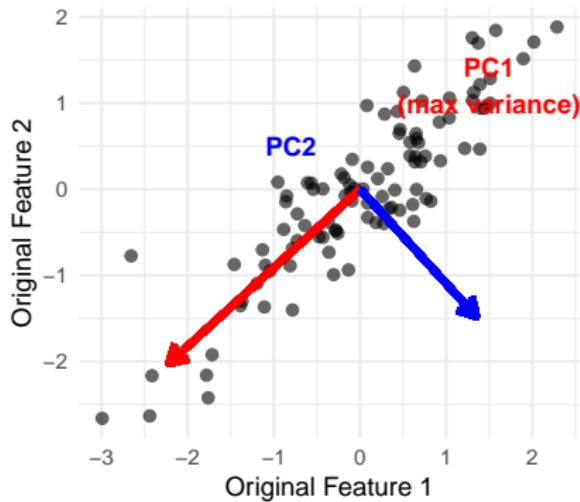
**Result:** New uncorrelated features (PC1, PC2, ...)

- PC1: Direction of maximum variance
- PC2: Direction of maximum variance perpendicular to PC1
- ...

# Slide 140: PCA Visualization - 2D Example

PCA: Finding Principal Components

Red = PC1 (captures most variance)



## Slide 141: PCA in R - Complete Workflow

```
# Load and prepare data
data(iris)
iris_features <- iris[, 1:4]

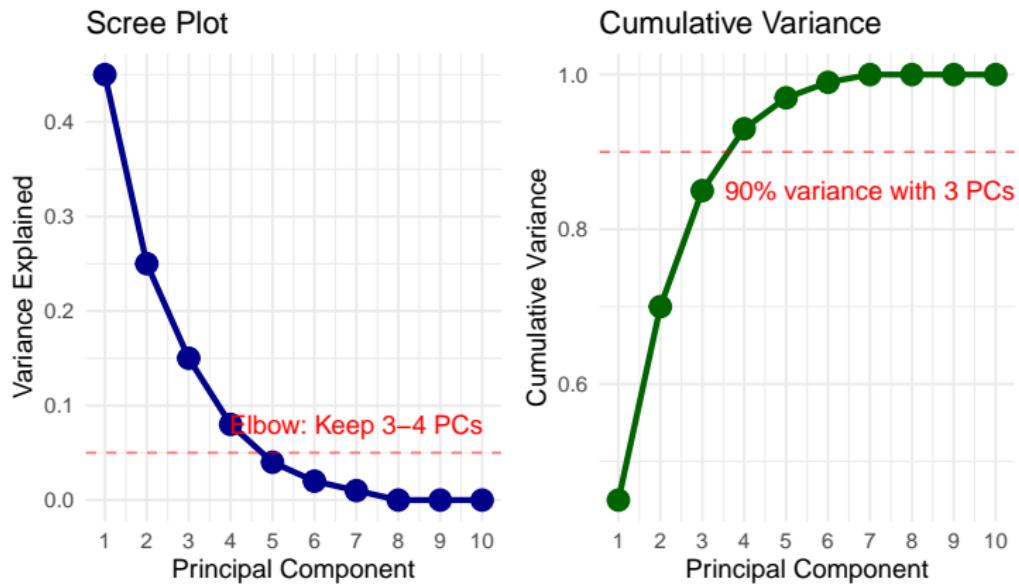
# Perform PCA (important: center and scale)
pca_result <- prcomp(iris_features,
                      center = TRUE,
                      scale. = TRUE)

# Summary
summary(pca_result)

# Variance explained
pca_var <- pca_result$sdev^2 / sum(pca_result$sdev^2)
cumsum(pca_var) # Cumulative variance

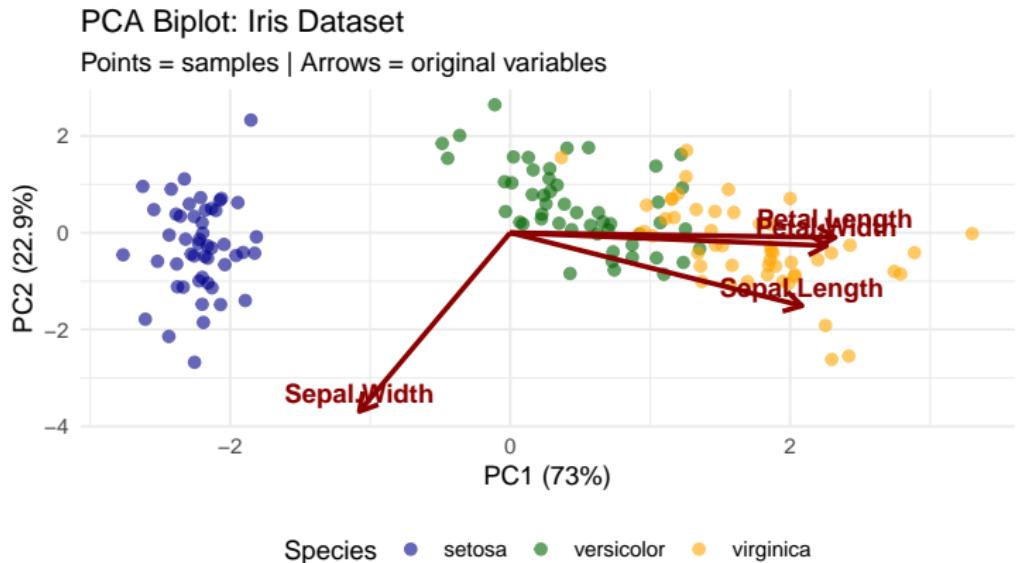
# Scree plot
```

## Slide 142: Scree Plot - Choosing Number of Components



**Rule of Thumb:** Keep PCs that explain  $\geq 80 - 90\%$  cumulative variance

# Slide 143: PCA Biplot - Variables and Observations



## Slide 144: Interpreting PCA Results

### PC Loadings Interpretation:

- High positive loading: Variable increases with PC
- High negative loading: Variable decreases with PC
- Near-zero loading: Variable uncorrelated with PC

### Example - Iris Dataset:

- **PC1:** Overall size (all measurements positively correlated)
- **PC2:** Contrast between sepal and petal measurements

### Use Cases:

- Data visualization ( $3D \rightarrow 2D$ )
- Noise reduction
- Feature extraction for ML
- Multicollinearity reduction

## Slide 145: PCA Limitations and Alternatives

### PCA Limitations:

- ① **Linear:** Only finds linear combinations
- ② **Variance Information:** Max variance best features
- ③ **Sensitive to scaling:** Must standardize first
- ④ **Not interpretable:** PCs are abstract combinations

### Alternatives:

- **t-SNE:** Nonlinear, preserves local structure (visualization)
- **UMAP:** Faster than t-SNE, preserves global + local
- **Autoencoders:** Deep learning approach (nonlinear)
- **Factor Analysis:** Assumes latent factors

## Slide 146: t-SNE for Visualization

### t-Distributed Stochastic Neighbor Embedding

**Key Idea:** Preserve pairwise similarities in lower dimensions

**Advantages:** - Excellent for visualization - Reveals cluster structure - Handles nonlinear relationships

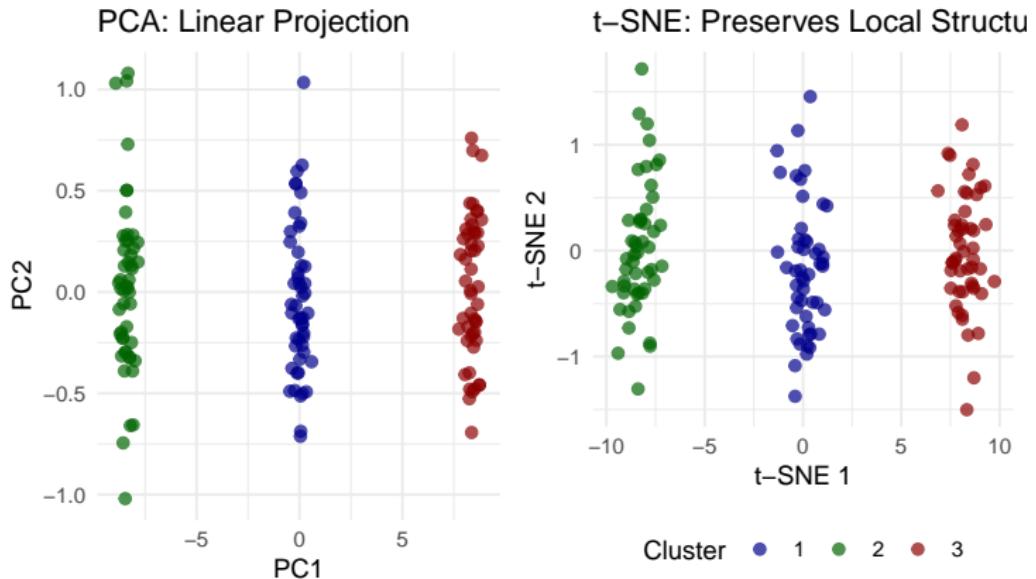
**Limitations:** - Slow (not for >10k points) - Non-deterministic (different runs → different results) - Only for visualization (not feature extraction)

```
library(Rtsne)

# Prepare data
data_scaled <- scale(data)

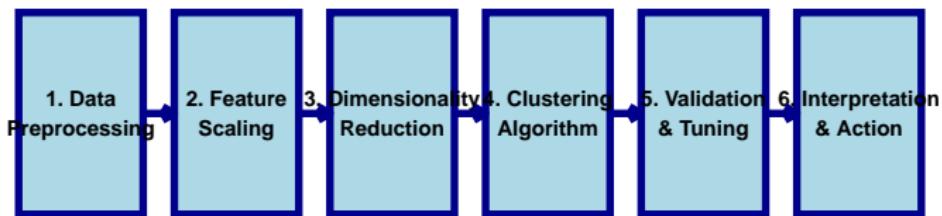
# Run t-SNE
tsne_result <- Rtsne(data_scaled,
                       dims = 2,
                       perplexity = 30,
```

## Slide 147: PCA vs t-SNE Comparison



# Slide 148: Complete Unsupervised Learning Pipeline

## Unsupervised Learning Pipeline



*Iterative Process: May need to revisit earlier steps*

## Slide 149: Clustering Validation Metrics

### Internal Metrics (no ground truth):

- ① **Silhouette Score:**  $[-1, 1]$ , higher better
- ② **Davies-Bouldin Index:** Lower better
- ③ **Calinski-Harabasz Index:** Higher better

### External Metrics (with ground truth):

- ① **Adjusted Rand Index (ARI):**  $[-1, 1]$ , 1 = perfect
- ② **Normalized Mutual Information (NMI):**  $[0, 1]$ , 1 = perfect
- ③ **Purity:**  $[0, 1]$ , 1 = perfect

```
library(clusterCrit)
```

```
# Internal validation
```

```
silhouette_score <- intCriteria(data, clusters, "Silhouette")
davies_bouldin <- intCriteria(data, clusters, "Davies_Bouldin")
```

```
# External validation (if labels available)
```

## Slide 150: Final Project Ideas - Unsupervised Learning

**Project 1: Customer Segmentation Dashboard** - RFM clustering on transaction data - Interactive visualization with Shiny - Automated segment reports

**Project 2: Anomaly Detection System** - DBSCAN on sensor/log data - Real-time outlier alerts - Visualization dashboard

**Project 3: Market Basket Analysis** - Apriori on retail data - Product recommendation engine - A/B testing of recommendations

**Project 4: Document Clustering** - Text preprocessing + TF-IDF - K-Means on document vectors - Topic discovery and labeling

**Project 5: Image Compression** - PCA on image data - Compression ratio analysis - Quality vs. compression tradeoff