Non-Linear Regression Analysis

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Introduction

This report presents the analysis of a given dataset, following non-linear regression modeling techniques. We explore three possible models for the data generation process, estimate model parameters via least squares, determine the best fit, and validate assumptions.

1. Least Square Estimators

Parameter	Model 1 Estimate	Model 2 Estimate	Model 3 Estimate
α_0	0.0263	2.2440	NA
α_1	3.7749	1.2230	NA
α_2	4.5377	NA	NA
β_0	NA	0.2762	8.3342
β_1	0.1072	-0.1382	7.4091
β_2	1.5322	NA	5.3294
β_3	NA	NA	2.2203
β_4	NA	NA	1.9307

Table 1: Comparison of Parameter Estimates for Each Model

1 2. Method and Initial Guesses

The models considered are as follows:

- **Model 1:** $y(t) = \alpha_0 + \alpha_1 e^{\beta_1 t} + \alpha_2 e^{\beta_2 t} + \epsilon(t)$
  - For this non-linear model, we used the **Gauss-Newton Method** to iteratively estimate the parameters by linearizing around current estimates and minimizing the sum of squared residuals. I have used small values (0.1) for the exponential terms and unit values for other non exponential parameters.
- **Model 2:** $y(t) = \frac{\alpha_0 + \alpha_1 t}{\beta_0 + \beta_1 t} + \epsilon(t)$
  - This model was estimated using **Gradient Descent**, where we optimized the parameters by following the gradient of the cost function to reach the minimum sum of squared errors. We have used unit value for each parameter in this model. This initial guess offers uniform parameter values, ideal for gradient-based optimization methods without assuming specific parameter ranges.
- **Model 3:** $y(t) = \beta_0 + \beta_1 t + \beta_2 t^2 + \beta_3 t^3 + \beta_4 t^4 + \epsilon(t)$
  - For this polynomial model, we have used the direct approach of the estimator for polynomial regression taught in class, i.e., $\boldsymbol{\beta} = (\mathbf{X^T X})^{-1} \mathbf{X^T Y}$. In this model no initial guesses were needed.

3. Model Selection Criteria

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Criteria	Model 1	Model 2	Model 3
Residual Sum of Squares (RSS)	0.3793	1.0143	0.3605

Table 2: Comparison of Model Selection Criteria

We will choose Model 3 as it provides the minimum RSS (0.3605) compared to Model 1 (0.3793) and Model 2 (1.0143).

4. Variance Estimation σ^2

The estimated variance for the residuals is shown below:

Model	Estimated σ^2
Model 1	0.0041
Model 2	0.0135
Model 3	0.0039

Table 3: Estimated Variance σ^2 for Each Model

5. Confidence Intervals for Parameters

Parameter	Model 1 CI	Model 2 CI	Model 3 CI
α_0	(-2696.1374, 2696.1969)	(-1715.5703, 1720.0583)	NA
α_1	(-2665.2783, 2672.8210)	(-935.0489, 937.4950)	NA
α_2	(-22.6054, 31.6809)	NA	NA
β_0	NA	(-105.4381, 105.9904)	(8.2572, 8.4112)
β_1	(-83.9087, 84.1234)	(-53.0300, 52.7537)	(6.3716, 8.4465)
β_2	(-0.7578, 3.8221)	NA	(1.2034, 9.4554)
β_3	NA	NA	(-3.8799, 8.3206)
β_4	NA	NA	(-1.0567, 4.9181)

Table 4: 95% Confidence Intervals for Parameter Estimates

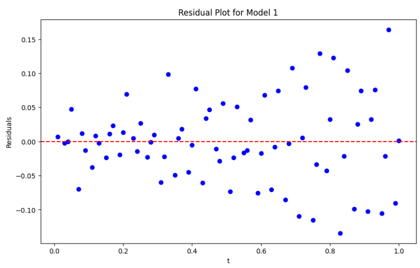
7. Normality Test Results

Model	Normality Test p-value
Model 1	0.6023
Model 2	0.0173
Model 3	0.6590

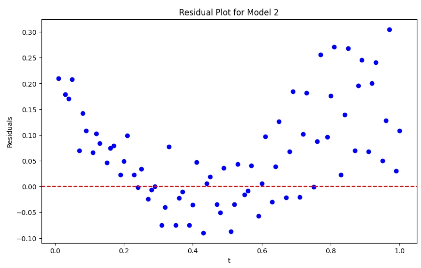
Table 5: Normality Test Results for Residuals

The normality test results indicate that Models 1 and 3 have residuals consistent with normality (p-values 0.6023 and 0.6590, respectively), while Model 2's residuals significantly deviate from normality.

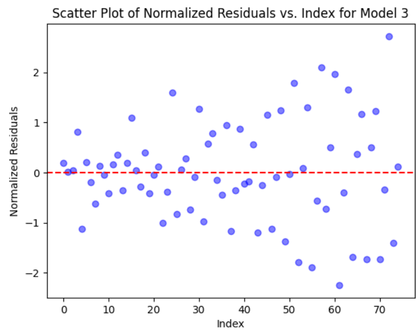
6. Residual Analysis



(a) Image 1



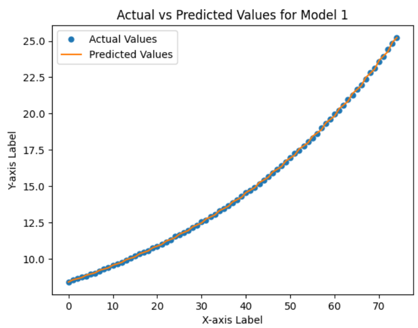
(b) Image 2



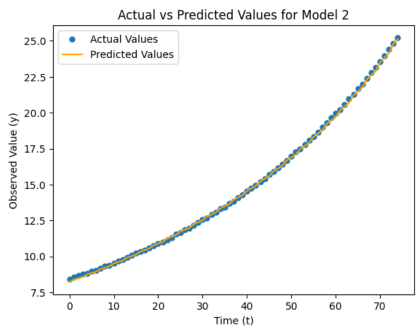
(c) Image 3

Figure 1: Three images side by side

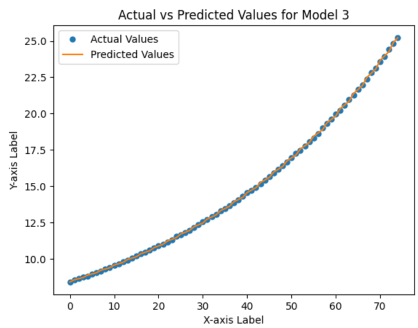
8. Plots



(a) Image 1



(b) Image 2



(c) Image 3

Figure 2: Three images side by side

Conclusion

Based on normality test and model adequacy, Model 3 is the best, followed by Model 1. Model 2 performs worst, showing significant deviation from normality.

Appendix A: Code

A Code for Model 1

```
import numpy as np
from scipy.stats import norm
from scipy.optimize import least_squares
import statsmodels.api as sm
from scipy import stats
import matplotlib.pyplot as plt
from numpy.linalg import cond
# Define the model function (same as before)
def model(t, alpha0, alpha1, beta1, alpha2, beta2):
    return alpha0 + alpha1 * np.exp(beta1 * t) + alpha2 * np.exp(beta2 * t)
# Define the residuals function (same as before)
def residuals(params, t, y):
    alpha0, alpha1, beta1, alpha2, beta2 = params
    return y - model(t, alpha0, alpha1, beta1, alpha2, beta2)
t_data = X
y_data = y
# Initial guess for parameters
initial_guess = [1.0, 1.0, -0.1, 1.0, -0.1]
#1.Calculating the LSE
result = least_squares(residuals, initial_guess, args=(t_data, y_data), method='lm')
alpha0_opt, alpha1_opt, beta1_opt, alpha2_opt, beta2_opt = result.x
print(f"Optimized Parameters:")
print(f"  alpha0 = {alpha0_opt:.4f}")
print(f"  alpha1 = {alpha1_opt:.4f}")
print(f"  beta1  = {beta1_opt:.4f}")
print(f"  alpha2 = {alpha2_opt:.4f}")
print(f"  beta2  = {beta2_opt:.4f}")
#4.Calculating variance
residuals_squared = residuals(result.x, t_data, y_data) ** 2
sigma2 = np.sum(residuals_squared) / (len(t_data) - len(result.x))
print(f"Estimated sigma^2: {sigma2}")
#5.Calculating Fischer Information Matrix for Confidence Interval
J = result.jac
cov_matrix = np.linalg.pinv(J.T @ J) * sigma2
param_std_devs = np.sqrt(np.diag(cov_matrix))
z_score = norm.ppf(0.975)
param_estimates = result.x
confidence_intervals = []
for i in range(len(param_estimates)):
    lower_bound = param_estimates[i] - z_score * param_std_devs[i]
    upper_bound = param_estimates[i] + z_score * param_std_devs[i]
    confidence_intervals.append((lower_bound, upper_bound))
print("95% Confidence intervals for parameters:")
for i, (lower, upper) in enumerate(confidence_intervals):
    print(f"Parameter{i}",lower,upper)
#6.Plot the residuals
y_pred = model(t_data, *result.x)
residuals_vals = residuals(result.x, t_data, y_data)
plt.figure(figsize=(10, 6))
plt.scatter(t_data, residuals_vals, color='blue')
plt.axhline(0, color='red', linestyle='--')
plt.xlabel("t")
plt.ylabel("Residuals")
plt.title("Residual Plot for Model 2")
plt.show()
#7. Normality of residuals
stat, p_value = stats.shapiro(residuals_vals)
print(f"P Value:{p_value}")
plt.figure(figsize=(10, 6))
```

```
plt.hist(residuals_vals, bins=20, color='lightblue', edgecolor='black')
plt.xlabel('Residuals')
plt.ylabel('Frequency')
plt.title('Histogram of Residuals')
plt.show()
#8.Final Plot
plt.plot(y, linestyle='None', marker='o', markersize=5, label='Actual Values')  # 'o' for
↪ circular markers
plt.plot(y_pred, label='Predicted Values')  # Solid line for predictions
plt.xlabel("X-axis Label")  # Add labels as needed
plt.ylabel("Y-axis Label")
plt.title("Actual vs Predicted Values")
plt.legend()
plt.show()
```

B Code for Model 2

```
import numpy as np
from scipy.stats import norm,shapiro
t_data = np.array(X)
y_data = np.array(y)
#Initial Guesses
alpha_0, alpha_1, beta_0, beta_1 = 1.0, 1.0, 1.0, 1.0
#1.Calculating LSE's using Gradient Descent
learning_rate = 1e-6
max_iters = 100000
tolerance = 1e-6
# Objective function (residual sum of squares)
def residual_sum_of_squares(alpha_0, alpha_1, beta_0, beta_1):
    prediction = (alpha_0 + alpha_1 * t_data) / (beta_0 + beta_1 * t_data)
    residuals = y_data - prediction
    return np.sum(residuals ** 2)
# Gradient calculation
def gradient(alpha_0, alpha_1, beta_0, beta_1):
    prediction = (alpha_0 + alpha_1 * t_data) / (beta_0 + beta_1 * t_data)
    residuals = y_data - prediction
    # Compute gradients
    grad_alpha_0 = -2 * np.sum(residuals / (beta_0 + beta_1 * t_data))
    grad_alpha_1 = -2 * np.sum(residuals * t_data / (beta_0 + beta_1 * t_data))
    grad_beta_0 = 2 * np.sum(residuals * prediction / (beta_0 + beta_1 * t_data))
    grad_beta_1 = 2 * np.sum(residuals * prediction * t_data / (beta_0 + beta_1 * t_data))
    return np.array([grad_alpha_0, grad_alpha_1, grad_beta_0, grad_beta_1])
# Gradient descent loop
for iteration in range(max_iters):
    # Calculate gradient
    grad = gradient(alpha_0, alpha_1, beta_0, beta_1)
    # Update parameters
    alpha_0 -= learning_rate * grad[0]
    alpha_1 -= learning_rate * grad[1]
    beta_0 -= learning_rate * grad[2]
    beta_1 -= learning_rate * grad[3]
    # Check for convergence
print(f"Estimated parameters: alpha_0 = {alpha_0}, alpha_1 = {alpha_1}, beta_0 = {beta_0}, beta_1
↪ = {beta_1}")
prediction = (alpha_0 + alpha_1 * t_data) / (beta_0 + beta_1 * t_data)
residuals = y_data - prediction
residuals_squared = residuals ** 2
sigma2 = np.sum(residuals_squared) / (len(t_data) - 4)  # degrees of freedom: 4 parameters
↪ estimated
print(f"Estimated sigma^2: {sigma2}")
#4.Calculating Confidence Interval using Fischer Information Matrix
def jacobian(alpha_0, alpha_1, beta_0, beta_1):
```

```
    prediction = (alpha_0 + alpha_1 * t_data) / (beta_0 + beta_1 * t_data)
    residuals = y_data - prediction
    J = np.zeros((len(t_data), 4))  # Jacobian matrix for each parameter
    J[:, 0] = -residuals / (beta_0 + beta_1 * t_data)
    J[:, 1] = -residuals * t_data / (beta_0 + beta_1 * t_data)
    J[:, 2] = 2 * residuals * prediction / (beta_0 + beta_1 * t_data)
    J[:, 3] = 2 * residuals * prediction * t_data / (beta_0 + beta_1 * t_data)
    return J
J=jacobian(alpha_0, alpha_1, beta_0, beta_1)
J_condition_number = np.linalg.cond(J)
print(f"Condition number of the Jacobian matrix: {J_condition_number}")
# Fisher Information Matrix (FIM) calculation
FIM = np.dot(J.T, J) / sigma2
regularization_term = 1e-6 * np.eye(FIM.shape[0])
FIM_regularized = FIM + regularization_term
cov_matrix = np.linalg.inv(FIM_regularized)
param_std_devs = np.sqrt(np.diag(cov_matrix))
params = np.array([alpha_0, alpha_1, beta_0, beta_1])
if np.any(np.isnan(param_std_devs)):
    print("Error: Standard deviations contain NaN values, indicating numerical instability.")
else:
    z_score = norm.ppf(0.975)
    confidence_intervals = [
        (param - z_score * std, param + z_score * std)
        for param, std in zip(params, param_std_devs)
    ]

    print("95% Confidence intervals for parameters:")
    for i, (lower, upper) in enumerate(confidence_intervals):
        print(f"Parameter {i}: ({lower:.4f}, {upper:.4f})")
# 6. Plot the Residuals
plt.figure(figsize=(10, 6))
plt.scatter(t_data, residuals, color='blue')
plt.axhline(0, color='red', linestyle='--')
plt.xlabel("t")
plt.ylabel("Residuals")
plt.title("Residual Plot")
plt.show()
# 7. Plot Histogram of Residuals
stat, p_value = shapiro(residuals)
print(f"P Value: {p_value}")
if p_value < 0.05:
    print("Residuals are not normally distributed.")
else:
    print("Residuals are normally distributed.")
plt.figure(figsize=(10, 6))
plt.hist(residuals, bins=20, color='lightblue', edgecolor='black')
plt.xlabel('Residuals')
plt.ylabel('Frequency')
plt.title('Histogram of Residuals')
plt.show()
# 8. Final Plot of Actual vs Predicted Values
plt.plot(y_data, linestyle='None', marker='o', markersize=5, label='Actual Values')
plt.plot(prediction, label='Predicted Values', color='orange')
plt.xlabel("Time (t)")
plt.ylabel("Observed Value (y)")
plt.title("Actual vs Predicted Values")
plt.legend()
plt.show()
```

C Code for Model 3

```
import numpy as np
import pandas as pd
import statsmodels.api as sm
from scipy import stats
import matplotlib.pyplot as plt
df = pd.read_csv("/content/data.csv")
X = df["t"]
y = df["y"]
X_matrix = np.column_stack((np.ones(len(X)), X, X**2, X**3, X**4))
#1.Calculating the LSE's
B_hat = np.linalg.inv(X_matrix.T @ X_matrix) @ X_matrix.T @ y
print(B_hat)
y_pred = X_matrix @ B_hat
#4 Calculating Variance
residuals = y - y_pred
n = len(y)
p = X_matrix.shape[1]
sigma2_hat = (residuals.T @ residuals) / (n - p)
print(f"Estimate of variance (sigma^2): {sigma2_hat}")
# 5.Calculating Confidence Interval using Fischer Information Matrix
mse = 0
for i in range(len(y)):
    mse+= (y_pred[i] - y[i])**2
mean_residuals = np.mean(residuals)
std_residuals = np.std(residuals)
fisher_info = (1 / sigma2_hat) * (X_matrix.T @ X_matrix)
covariance_matrix = np.linalg.inv(fisher_info)
std_errors = np.sqrt(np.diag(covariance_matrix))
t_critical = 1.96
lower_bounds = B_hat - t_critical * std_errors
upper_bounds = B_hat + t_critical * std_errors
print("Coefficients, Standard Errors and 95% Confidence Intervals:")
for i in range(len(B_hat)):
    print(f"Coefficient {i}: {B_hat[i]:.4f}")
    print(f"Standard Error {i}: {std_errors[i]:.4f}")
    print(f"95% Confidence Interval {i}: ({lower_bounds[i]:.4f}, {upper_bounds[i]:.4f})\n")
#6.Residuals Plot
normalized_residuals = (residuals - np.mean(residuals)) / np.std(residuals)
plt.scatter(range(len(normalized_residuals)), normalized_residuals, color='blue', alpha=0.5)
plt.axhline(y=0, color='red', linestyle='--')
plt.xlabel("Index")
plt.ylabel("Normalized Residuals")
plt.title("Scatter Plot of Normalized Residuals vs. Index")
plt.show()
#7.Normality Assumptions Check
stat, p_value = stats.shapiro(residuals)
print(f"P Value:{p_value}")
plt.hist(normalized_residuals, bins=15)  # Adjust the number of bins as needed
plt.xlabel("Normalized Residuals")
plt.ylabel("Frequency")
plt.title("Histogram of Normalized Residuals")
plt.show()
#8.Final Plot of predicted values vs actual values
plt.plot(y, linestyle='None', marker='o', markersize=5, label='Actual Values')  # 'o' for
↪ circular markers
plt.plot(y_pred, label='Predicted Values')  # Solid line for predictions
plt.xlabel("X-axis Label")  # Add labels as needed
plt.ylabel("Y-axis Label")
plt.title("Actual vs Predicted Values")
plt.legend()
plt.show()
```