pymaceuticals

May 31, 2024

0.1 # Pymaceuticals Inc.

0.2 Analyzing the Linear Regression of Capomulin Drug Regimen

0.3 ### Data Analysis by Thay Chansy

0.3.1 Summary

The results suggest a strong positive linear relationship between the independent and dependent variables, with a very high p-value indicating a statistically significant association. A lower Standard Error at 1.0249 suggests a relatively tight fit of the regression model.
The R-squared value of 0.9034 confirms that the linear model explains a significant portion of the variance in the data and indicates a very strong positive linear relationship between x_values and y_values.. A P-value of 0.9999999999999923 is extremely high, indicating that the observed positive association is almost certainly not due to chance.

x-value: Weight (g)

y-value: Avg Tumor Volume (mm3)

Slope (m): 0.8947726097340611

Y-intercept (b): 22.764229983591935

Standard error of the estimate (SE): 1.0249929158261613

R-squared: 0.9034966277438602

P-value: 0.9999999999999923

Linear Equation: y = 0.8947726097340611(X) + 22.764229983591935

[1]:
```python
# Dependencies and Setup
import matplotlib.pyplot as plt
import pandas as pd
from scipy import stats
from scipy.stats import sem
from scipy.stats import linregress
import numpy as np
from scipy.stats import pearsonr

# Study data files
mouse_metadata_path = "data/Mouse_metadata.csv"
study_results_path = "data/Study_results.csv"
```

```
# Read the mouse data and the study results
mouse_metadata = pd.read_csv(mouse_metadata_path)
study_results = pd.read_csv(study_results_path)

# Combine the data into a single DataFrame
mouse_study_combined_df = pd.merge(study_results, mouse_metadata, on='Mouse ID')

# Display the data table for preview
mouse_study_combined_df.head()
```

[1]:

```
  Mouse ID  Timepoint  Tumor Volume (mm3)  Metastatic Sites Drug Regimen  \
0     b128          0           45.000000                 0    Capomulin
1     b128          5           45.651331                 0    Capomulin
2     b128         10           43.270852                 0    Capomulin
3     b128         15           43.784893                 0    Capomulin
4     b128         20           42.731552                 0    Capomulin

      Sex  Age_months  Weight (g)
0  Female           9          22
1  Female           9          22
2  Female           9          22
3  Female           9          22
4  Female           9          22
```

[2]:

```
# Checking the number of mice.
total_mice = mouse_study_combined_df['Mouse ID'].nunique()

#display results
total_mice
```

[2]: 249

[3]:

```
# Our data should be uniquely identified by Mouse ID and Timepoint
# Get the duplicate mice by ID number that shows up for Mouse ID and Timepoint.
duplicate_mice_id = mouse_study_combined_df.loc[mouse_study_combined_df.
 ↪duplicated(subset=['Mouse ID', 'Timepoint',]),'Mouse ID'].unique()

# display results
duplicate_mice_id
```

[3]: array(['g989'], dtype=object)

[4]:

```
# Optional: Get all the data for the duplicate mouse ID.

# Identify duplicate mouse IDs (considering both 'Mouse ID' and 'Timepoint' for␣
 ↪duplicates)
```

```
duplicate_mice_id_df = mouse_study_combined_df.loc[mouse_study_combined_df.
 ↪duplicated(subset=['Mouse ID', 'Timepoint']), 'Mouse ID'].unique()

# Filter the DataFrame to get all data for those IDs
duplicate_mice_data_df = mouse_study_combined_df[mouse_study_combined_df['Mouse␣
 ↪ID'].isin(duplicate_mice_id_df)]

# display results
duplicate_mice_data_df
```

[4]:

```
    Mouse ID  Timepoint  Tumor Volume (mm3)  Metastatic Sites Drug Regimen  \
860     g989          0           45.000000                 0     Propriva
861     g989          0           45.000000                 0     Propriva
862     g989          5           48.786801                 0     Propriva
863     g989          5           47.570392                 0     Propriva
864     g989         10           51.745156                 0     Propriva
865     g989         10           49.880528                 0     Propriva
866     g989         15           51.325852                 1     Propriva
867     g989         15           53.442020                 0     Propriva
868     g989         20           55.326122                 1     Propriva
869     g989         20           54.657650                 1     Propriva
870     g989         25           56.045564                 1     Propriva
871     g989         30           59.082294                 1     Propriva
872     g989         35           62.570880                 2     Propriva

        Sex  Age_months  Weight (g)
860  Female          21          26
861  Female          21          26
862  Female          21          26
863  Female          21          26
864  Female          21          26
865  Female          21          26
866  Female          21          26
867  Female          21          26
868  Female          21          26
869  Female          21          26
870  Female          21          26
871  Female          21          26
872  Female          21          26
```

[5]:

```
# Create a clean DataFrame by dropping the duplicate mouse by its ID.
mouse_study_clean_df = mouse_study_combined_df[mouse_study_combined_df["Mouse␣
 ↪ID"].isin(duplicate_mice_id_df)==False]

# Display results
mouse_study_clean_df.head()
```

[5]:

```
  Mouse ID  Timepoint  Tumor Volume (mm3)  Metastatic Sites Drug Regimen  \
0     b128          0           45.000000                 0    Capomulin
1     b128          5           45.651331                 0    Capomulin
2     b128         10           43.270852                 0    Capomulin
3     b128         15           43.784893                 0    Capomulin
4     b128         20           42.731552                 0    Capomulin

      Sex  Age_months  Weight (g)
0  Female           9          22
1  Female           9          22
2  Female           9          22
3  Female           9          22
4  Female           9          22
```

[6]:

```
# Checking the number of mice in the clean DataFrame.
total_mice_clean = mouse_study_clean_df['Mouse ID'].nunique()

# Display results
total_mice_clean
```

[6]: 248

0.4 Summary Statistics

[7]:

```
# Generate a summary statistics table of mean, median, variance, standard␣
↪deviation, and SEM of the tumor volume for each regimen

# Use groupby and summary statistical methods to calculate the following␣
↪properties of each drug regimen:
# mean, median, variance, standard deviation, and SEM of the tumor volume.
# Assemble the resulting series into a single summary DataFrame.
drug_regimen_mean = mouse_study_clean_df.groupby('Drug Regimen')["Tumor Volume␣
↪(mm3)"].mean()
drug_regimen_median = mouse_study_clean_df.groupby('Drug Regimen')["Tumor␣
↪Volume (mm3)"].median()
drug_regimen_variance = mouse_study_clean_df.groupby('Drug Regimen')["Tumor␣
↪Volume (mm3)"].var()
drug_regimen_std = mouse_study_clean_df.groupby('Drug Regimen')["Tumor Volume␣
↪(mm3)"].std()
drug_regimen_sem = mouse_study_clean_df.groupby('Drug Regimen')["Tumor Volume␣
↪(mm3)"].sem()

# Assemble the resulting series into a single summary dataframe.
summary_table_df = pd.DataFrame({
    "Mean Tumor Volume": drug_regimen_mean,
     "Median Tumor Volume": drug_regimen_median,
     "Tumor Volume Variance": drug_regimen_variance,
```

```
    "Tumor Volume Std. Dev.": drug_regimen_std,
    "Tumor Volume Std. Err.": drug_regimen_sem})

# Display Dataframe
summary_table_df
```

[7]:

```
              Mean Tumor Volume  Median Tumor Volume  Tumor Volume Variance  \
Drug Regimen
Capomulin             40.675741            41.557809              24.947764
Ceftamin              52.591172            51.776157              39.290177
Infubinol             52.884795            51.820584              43.128684
Ketapril              55.235638            53.698743              68.553577
Naftisol              54.331565            52.509285              66.173479
Placebo               54.033581            52.288934              61.168083
Propriva              52.320930            50.446266              43.852013
Ramicane              40.216745            40.673236              23.486704
Stelasyn              54.233149            52.431737              59.450562
Zoniferol             53.236507            51.818479              48.533355

              Tumor Volume Std. Dev.  Tumor Volume Std. Err.
Drug Regimen
Capomulin                   4.994774                0.329346
Ceftamin                    6.268188                0.469821
Infubinol                   6.567243                0.492236
Ketapril                    8.279709                0.603860
Naftisol                    8.134708                0.596466
Placebo                     7.821003                0.581331
Propriva                    6.622085                0.544332
Ramicane                    4.846308                0.320955
Stelasyn                    7.710419                0.573111
Zoniferol                   6.966589                0.516398
```

[8]:

```
# A more advanced method to generate a summary statistics table of mean,␣
↪median, variance, standard deviation,
# and SEM of the tumor volume for each regimen (only one method is required in␣
↪the solution)
single_group_by = mouse_study_clean_df.groupby('Drug Regimen')

# Using the aggregation method, produce the same summary statistics in a single␣
↪line
summary_table_single_line = single_group_by['Tumor Volume (mm3)'].
↪agg(['mean','median','var','std','sem'])

# Display Dataframe
summary_table_single_line
```

[8]:

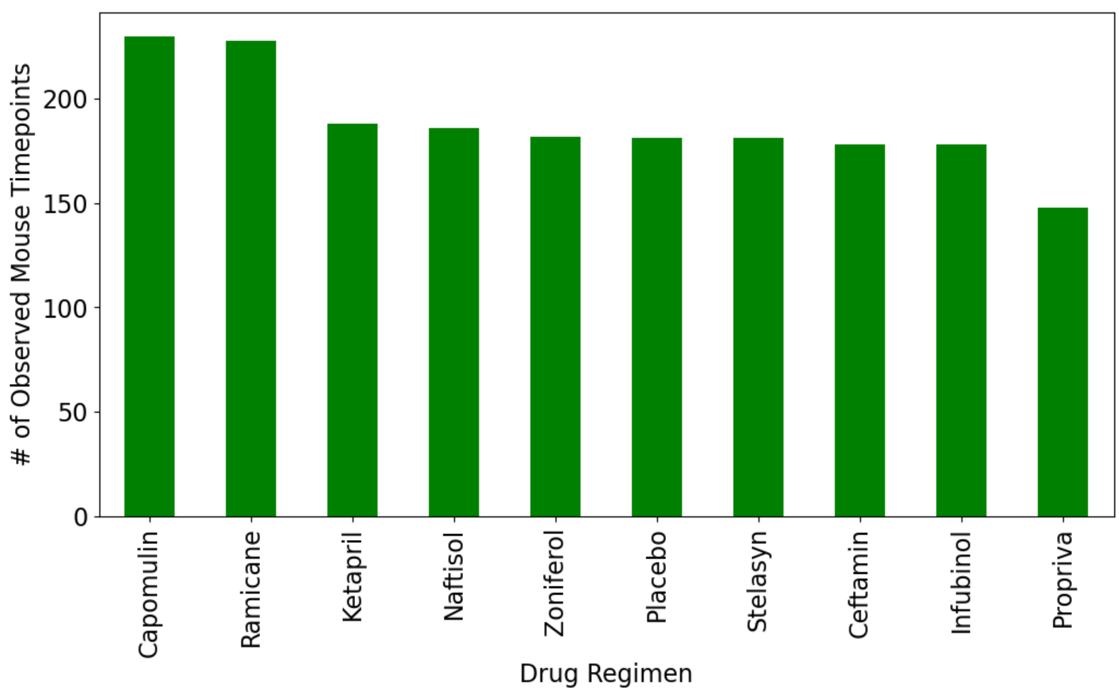
	mean	median	var	std	sem
Drug Regimen					
Capomulin	40.675741	41.557809	24.947764	4.994774	0.329346
Ceftamin	52.591172	51.776157	39.290177	6.268188	0.469821
Infubinol	52.884795	51.820584	43.128684	6.567243	0.492236
Ketapril	55.235638	53.698743	68.553577	8.279709	0.603860
Naftisol	54.331565	52.509285	66.173479	8.134708	0.596466
Placebo	54.033581	52.288934	61.168083	7.821003	0.581331
Propriva	52.320930	50.446266	43.852013	6.622085	0.544332
Ramicane	40.216745	40.673236	23.486704	4.846308	0.320955
Stelasyn	54.233149	52.431737	59.450562	7.710419	0.573111
Zoniferol	53.236507	51.818479	48.533355	6.966589	0.516398

0.5 Bar and Pie Charts

[9]:

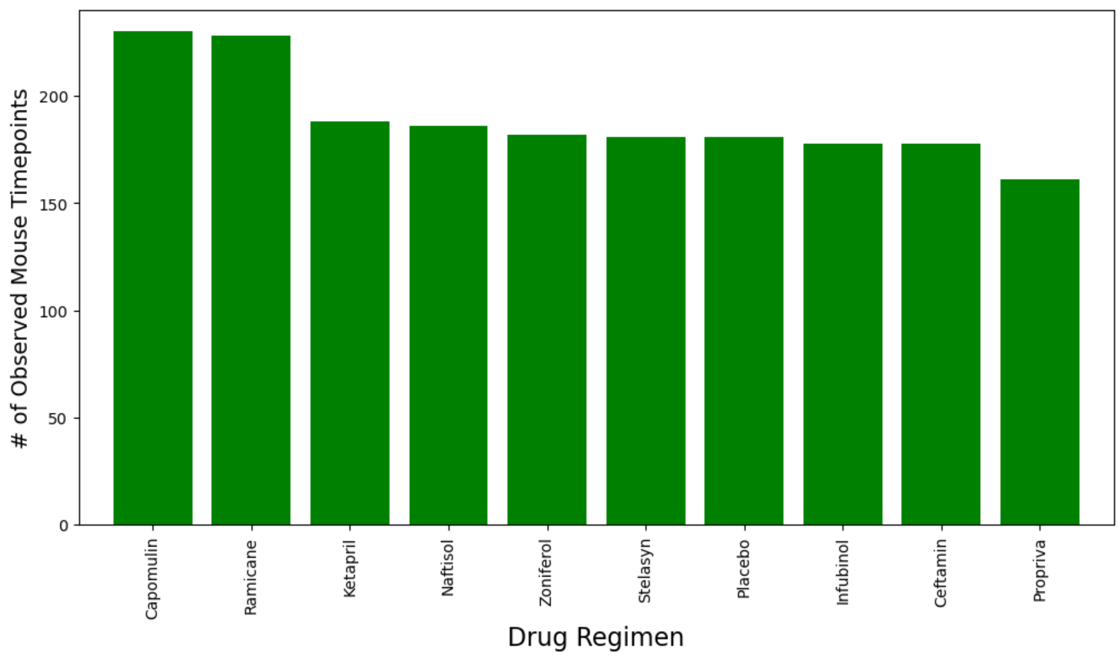
```
# Generate a bar plot showing the total number of rows (Mouse ID/Timepoints)␣
↪for each drug regimen using Pandas.
bar_timepoints_drugs = mouse_study_clean_df.groupby(["Drug Regimen"])["Mouse␣
↪ID"].count().sort_values(ascending=False)

bar_plot_pandas = bar_timepoints_drugs.plot.bar(rot=90, fontsize=16,␣
↪figsize=(12,6), color='green')

plt.xlabel("Drug Regimen", fontsize=16)
plt.ylabel("# of Observed Mouse Timepoints", fontsize=16)
```

[9]: Text(0, 0.5, '# of Observed Mouse Timepoints')

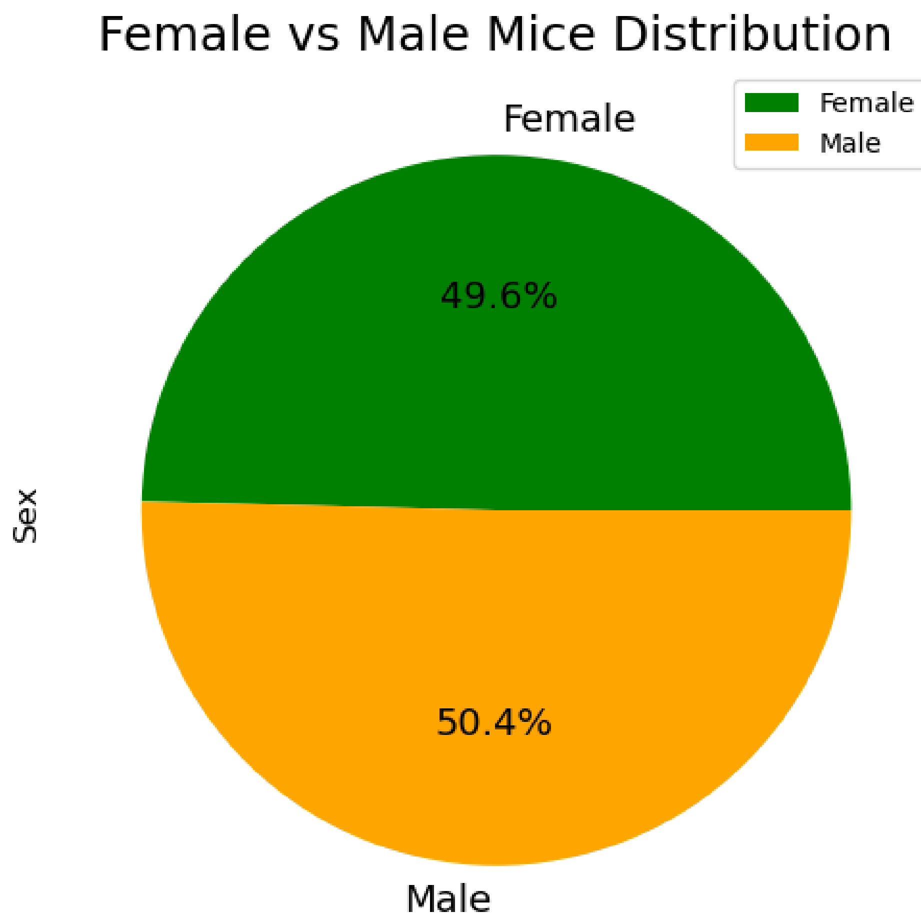


[10]:
```
# Generate a bar plot showing the total number of rows (Mouse ID/Timepoints)␣
↪for each drug regimen using pyplot.

# Create an array for timepoints
timepoints_list =(mouse_study_combined_df.groupby(["Drug␣
↪Regimen"])["Timepoint"].count()).sort_values(ascending=False)
timepoints_list

# Bar pyplot
x_axis = np.arange(len(bar_timepoints_drugs))
fig1, ax1 = plt.subplots(figsize=(12, 6))
plt.bar(x_axis,timepoints_list, color='green')
tick_locations = [value for value in x_axis]

plt.xticks(tick_locations, ['Capomulin', 'Ramicane', 'Ketapril', 'Naftisol',␣
↪'Zoniferol', 'Stelasyn',
                            'Placebo', 'Infubinol', 'Ceftamin', 'Propriva'], ␣
↪rotation='vertical')
plt.xlim(-0.75, len(x_axis)-0.25)
plt.ylim(0, max(timepoints_list)+10)

plt.xlabel("Drug Regimen",fontsize = 16)
plt.ylabel("# of Observed Mouse Timepoints",fontsize = 14)

# Dispoay Timepoint List
timepoints_list
```

[10]:
```
Drug Regimen
Capomulin    230
Ramicane     228
Ketapril     188
Naftisol     186
Zoniferol    182
Placebo      181
Stelasyn     181
Ceftamin     178
Infubinol    178
Propriva     161
Name: Timepoint, dtype: int64
```

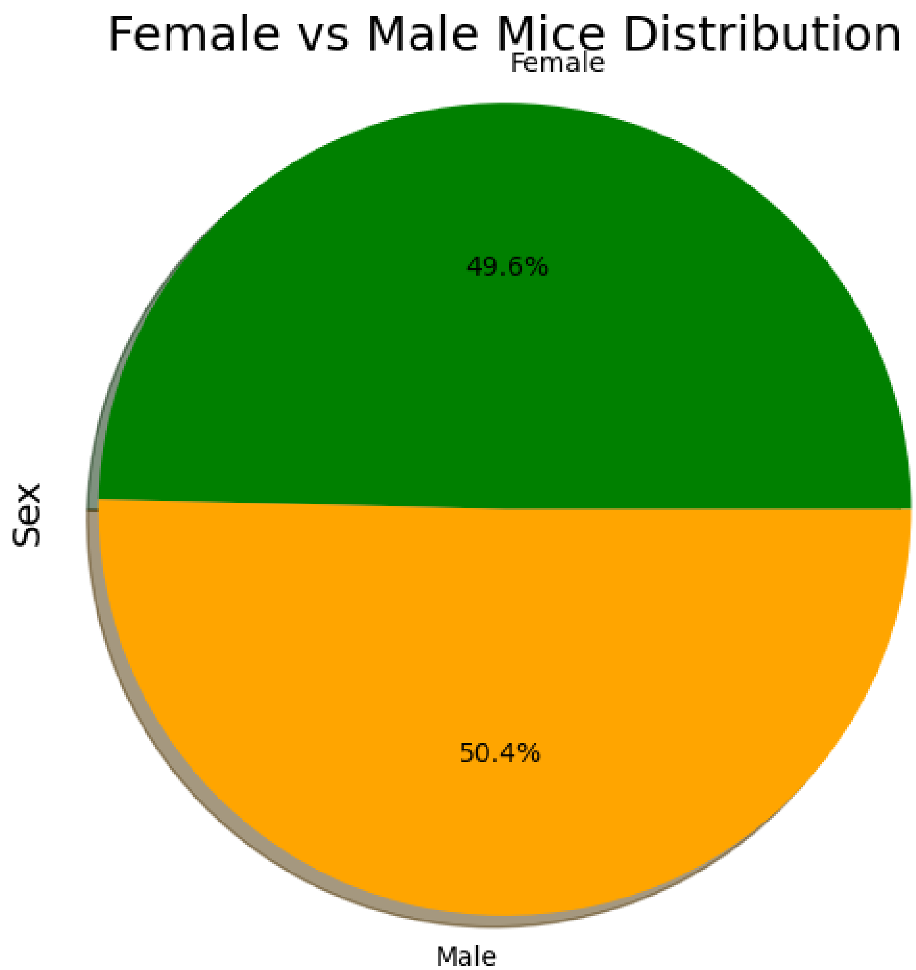


[11]:
```
# Generate a pie plot showing the distribution of female versus male mice using␣
↪Pandas
groupedby_gender = mouse_study_clean_df.groupby(["Mouse ID", "Sex"])
groupedby_gender_df = pd.DataFrame(groupedby_gender.size())

mice_gender = pd.DataFrame(groupedby_gender_df.groupby(["Sex"]).count())
mice_gender.columns = ["Total Count"]

colors = ['green','orange']
m_f_pie_chart_pandas = mice_gender.plot.pie(y="Total Count",
                                            title= "Female vs Males Mice␣
↪Distribution",
                                            fontsize= 14,
                                            figsize=(6,6),autopct="%1.1f%%",
                                            colors= colors)
plt.title('Female vs Male Mice Distribution',fontsize = 18)
plt.ylabel('Sex',fontsize = 12)
plt.show()
```



[12]:

```
# Generate a pie plot showing the distribution of female versus male mice using␣
↪pyplot
labels = ["Female","Male"]

total_count_gender = [123,125]

fig1, ax1 = plt.subplots(figsize=(6, 6))
plt.pie(total_count_gender,labels=labels, autopct="%1.1f%%",
        colors= colors, shadow= True)
plt.title("Female vs Male Mice Distribution",fontsize = 18)
plt.ylabel("Sex", fontsize = 14)
plt.axis("equal")
plt.show()
```



0.6 Quartiles, Outliers and Boxplots

[13]:
```
# Calculate the final tumor volume of each mouse across four of the treatment␣
↪regimens:

# Capomulin, Ramicane, Infubinol, and Ceftamin

# Start by getting the last (greatest) timepoint for each mouse
last_timepoint_df = pd.DataFrame(mouse_study_clean_df.groupby('Mouse␣
↪ID')['Timepoint'].max().sort_values()).reset_index().
↪rename(columns={"Timepoint": "max_Timepoint"})

# Merge this group df with the original DataFrame to get the tumor volume at␣
↪the last timepoint
final_timepoint_df = pd.merge(mouse_study_clean_df, last_timepoint_df,␣
↪on='Mouse ID')
```

```
# Display results
final_timepoint_df
```

[13]:

```
     Mouse ID  Timepoint  Tumor Volume (mm3)  Metastatic Sites Drug Regimen  \
0        b128          0           45.000000                 0    Capomulin
1        b128          5           45.651331                 0    Capomulin
2        b128         10           43.270852                 0    Capomulin
3        b128         15           43.784893                 0    Capomulin
4        b128         20           42.731552                 0    Capomulin
…         …        …                 …                …         …
1875     m601         25           33.118756                 1    Capomulin
1876     m601         30           31.758275                 1    Capomulin
1877     m601         35           30.834357                 1    Capomulin
1878     m601         40           31.378045                 1    Capomulin
1879     m601         45           28.430964                 1    Capomulin

         Sex  Age_months  Weight (g)  max_Timepoint
0     Female           9          22             45
1     Female           9          22             45
2     Female           9          22             45
3     Female           9          22             45
4     Female           9          22             45
…       …           …          …            …
1875    Male          22          17             45
1876    Male          22          17             45
1877    Male          22          17             45
1878    Male          22          17             45
1879    Male          22          17             45

[1880 rows x 9 columns]
```

[14]:

```
# Put treatments into a list for for loop (and later for plot labels)
drug_treatments_list = final_timepoint_df['Drug Regimen'].unique().tolist()

# Create empty list to fill with tumor vol data (for plotting)
tumor_volume_values = []

# Calculate the IQR and quantitatively determine if there are any potential␣
↪outliers.
for treatment in drug_treatments_list:
  subset = final_timepoint_df[final_timepoint_df['Drug Regimen'] == treatment]
  q1 = subset['Tumor Volume (mm3)'].quantile(0.25)
  q3 = subset['Tumor Volume (mm3)'].quantile(0.75)
  iqr = q3 - q1
  lower_bound = q1 - 1.5 * iqr
  upper_bound = q3 + 1.5 * iqr
```

```
    outliers = subset[(subset['Tumor Volume (mm3)'] < lower_bound) |␣
↪(subset['Tumor Volume (mm3)'] > upper_bound)]

    # Print the treatment and the number of outliers
    print(f"Treatment: {treatment}")
    print(f"IQR: {iqr}")
    print(f"Number of outliers: {len(outliers)}")
    print(f"Lower Bound: {(lower_bound)}")
    print(f"Upper Bound: {(upper_bound)}")
    print("=======================================")

    # Add tumor volume values to the list for plotting
    tumor_volume_values.append(subset['Tumor Volume (mm3)'].values)
```

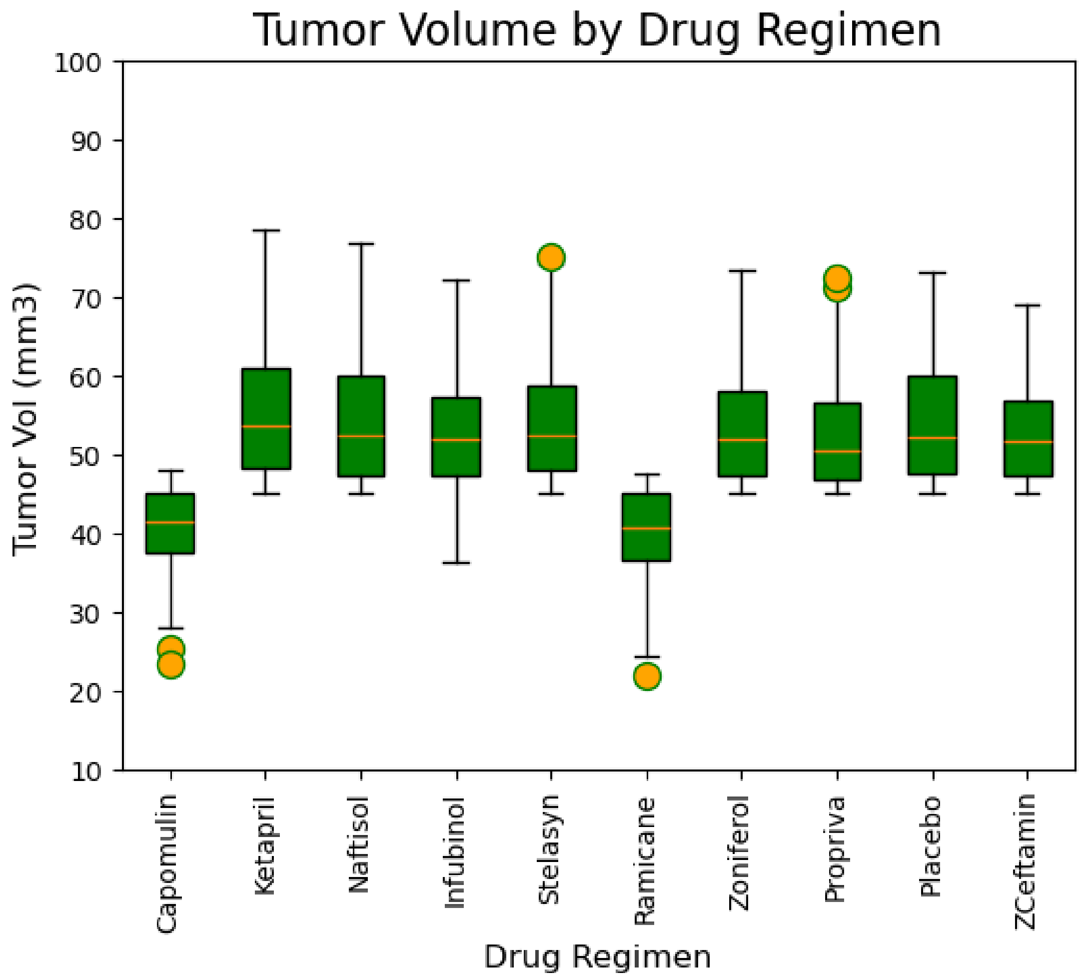
```
Treatment: Capomulin
IQR: 7.314067135000002
Number of outliers: 2
Lower Bound: 26.714832162499995
Upper Bound: 55.9711007025
=======================================
Treatment: Ketapril
IQR: 12.637963814999999
Number of outliers: 0
Lower Bound: 29.27604157
Upper Bound: 79.82789683
=======================================
Treatment: Naftisol
IQR: 12.677160092499996
Number of outliers: 0
Lower Bound: 28.270133771250006
Upper Bound: 78.97877414124999
=======================================
Treatment: Infubinol
IQR: 10.002090667500006
Number of outliers: 0
Lower Bound: 32.309217298749985
Upper Bound: 72.31757996875001
=======================================
Treatment: Stelasyn
IQR: 10.67215848
Number of outliers: 1
Lower Bound: 32.038901100000004
Upper Bound: 74.72753502
=======================================
Treatment: Ramicane
IQR: 8.325365415
Number of outliers: 1
Lower Bound: 24.1865864625
```

```
Upper Bound: 57.488048122500004
========================================
Treatment: Zoniferol
IQR: 10.616382797500002
Number of outliers: 0
Lower Bound: 31.413301711249996
Upper Bound: 73.87883290125001
========================================
Treatment: Propriva
IQR: 9.597257012500002
Number of outliers: 2
Lower Bound: 32.49844293375
Upper Bound: 70.88747098375
========================================
Treatment: Placebo
IQR: 12.457881529999995
Number of outliers: 0
Lower Bound: 28.77223060500001
Upper Bound: 78.60375672499998
========================================
Treatment: Ceftamin
IQR: 9.593010457500007
Number of outliers: 0
Lower Bound: 32.81891142624998
Upper Bound: 71.19095325625001
========================================
```

[15]:

```
# Generate a box plot that shows the distrubution of the tumor volume for each␣
↪treatment group

# Show outliers on boxplot for visibility
outlier_design = dict(marker="o", markerfacecolor="orange", markersize=10,␣
↪markeredgecolor="green")

# Create Boxplot
plt.boxplot(tumor_volume_values, widths=0.5, patch_artist=True,␣
↪boxprops=dict(facecolor="green"), flierprops=outlier_design)
plt.title('Tumor Volume by Drug Regimen', fontsize= 16)
plt.xlabel('Drug Regimen', fontsize=12)
plt.ylabel('Tumor Vol (mm3)', fontsize=12)

plt.xticks([1,2,3,4,5,6,7,8,9,10], ['Capomulin', 'Ketapril', 'Naftisol',␣
↪'Infubinol',
                            'Stelasyn', 'Ramicane', 'Zoniferol', 'Propriva',
                            'Placebo', 'ZCeftamin'], rotation='vertical')
#plt.xlim(-0.95, len(x_axis)+2)
plt.ylim(10, 100)
```

```
plt.show()
```

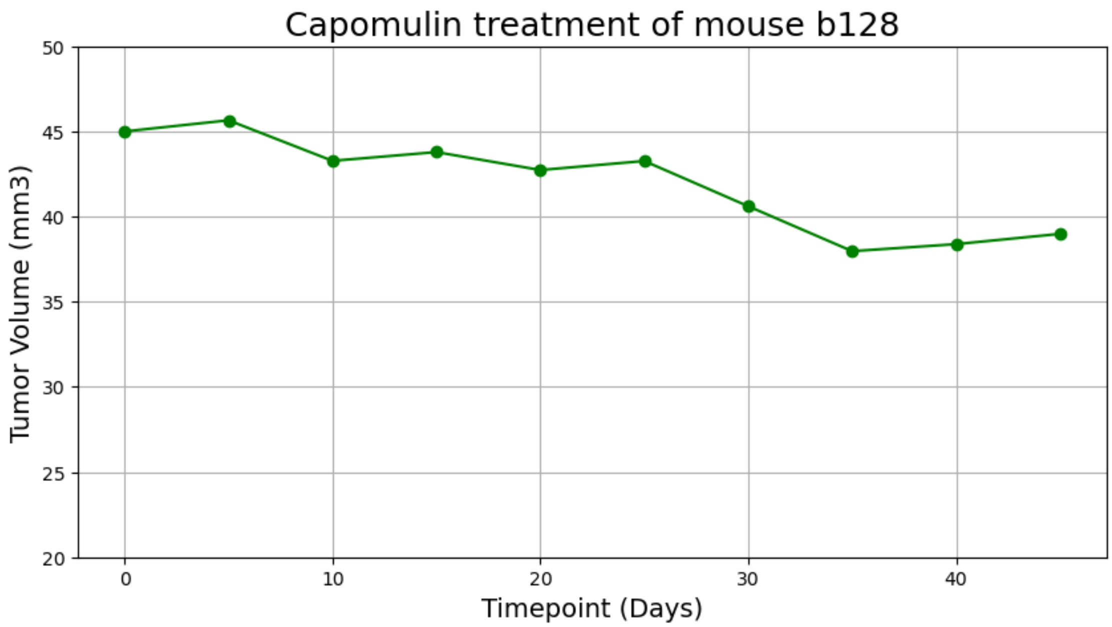


0.7 Line and Scatter Plots

[16]:
```
# Generate a line plot of tumor volume vs. time point for a single mouse␣
↪treated with Capomulin
capomulin_df = mouse_study_combined_df.loc[mouse_study_combined_df["Drug␣
↪Regimen"] == "Capomulin",:]

cap_line_df = capomulin_df.loc[capomulin_df["Mouse ID"]== "b128",:]

cap_timepoint_x_axis = cap_line_df["Timepoint"]
cap_tumorsize_y_axis = cap_line_df["Tumor Volume (mm3)"]

fig1, axl = plt.subplots(figsize=(10,5))
```

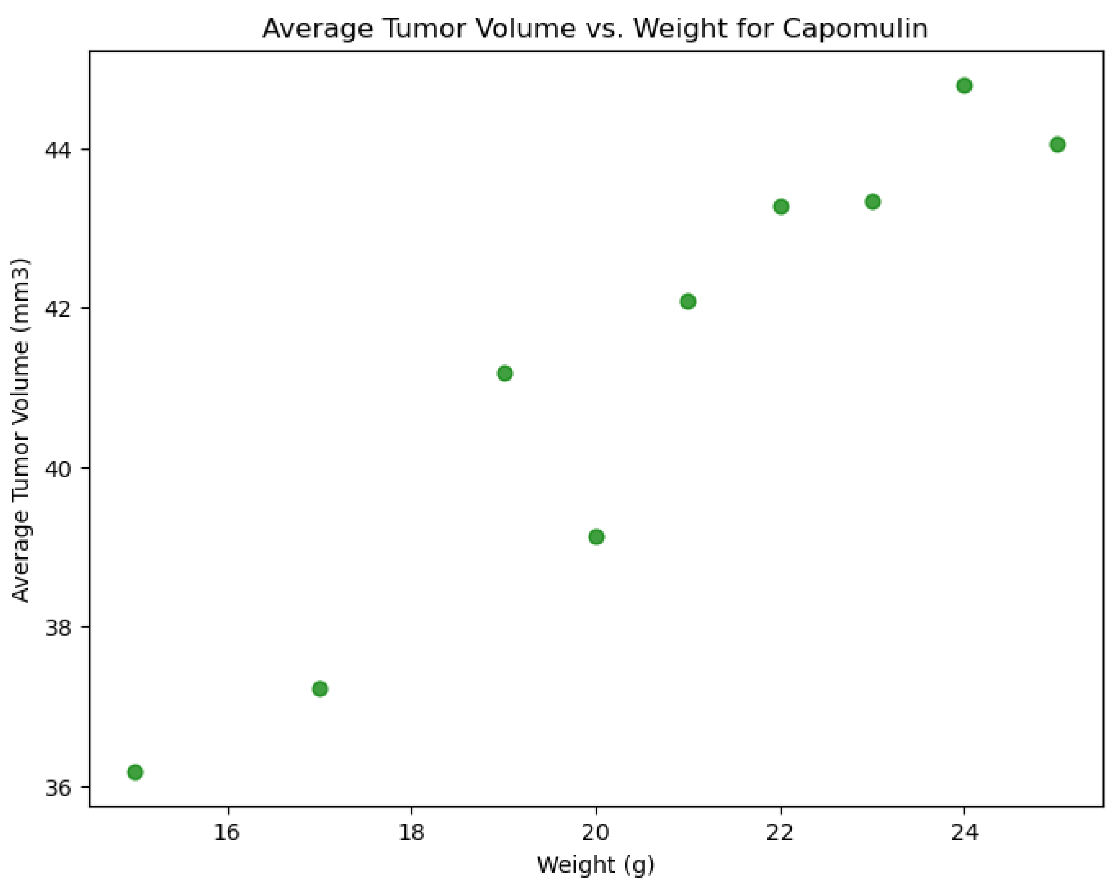
```
plt.plot(cap_timepoint_x_axis, cap_tumorsize_y_axis,
        marker="o", color="green")
plt.title("Capomulin treatment of mouse b128", fontsize= 18)
plt.xlabel("Timepoint (Days)", fontsize= 14)
plt.ylabel("Tumor Volume (mm3)", fontsize= 14)
plt.grid(True)
plt.ylim(20, 50)
```

[16]: (20.0, 50.0)



[17]:
```
# Generate a scatter plot of mouse weight vs. the average observed tumor volume␣
↪for the entire Capomulin regimen

# Calculate average tumor volume per weight group
avg_wgt_tum_vol_cap = capomulin_df.groupby('Weight (g)')['Tumor Volume (mm3)'].
↪mean()

# Create the scatter plot
# Set figure size
plt.figure(figsize=(8, 6))

# Customize plot
plt.scatter(avg_wgt_tum_vol_cap.index, avg_wgt_tum_vol_cap.values, s=40,␣
↪c='green', alpha=0.75)

# Add labels and title
```

```
plt.xlabel('Weight (g)')
plt.ylabel('Average Tumor Volume (mm3)')
plt.title('Average Tumor Volume vs. Weight for Capomulin')

# Display the plot
plt.show()

avg_wgt_tum_df = pd.DataFrame(avg_wgt_tum_vol_cap)

# Dispay Dataframe
avg_wgt_tum_df

# Rese the index of the dataframe
new_index_avg_wgt_df = avg_wgt_tum_df.reset_index()

# Display new index dataframe
new_index_avg_wgt_df
```

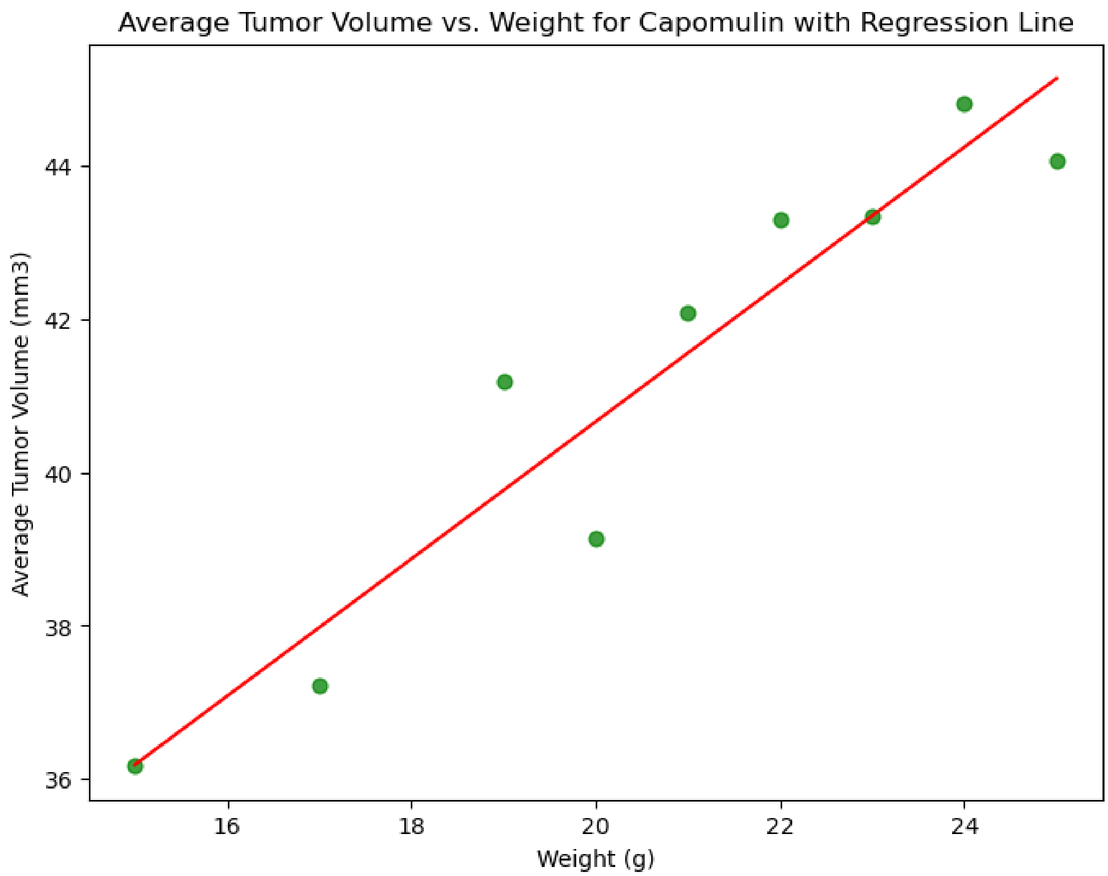


[17]:
```
   Weight (g)  Tumor Volume (mm3)
0          15           36.182040
1          17           37.214133
2          19           41.182391
3          20           39.141053
4          21           42.088700
5          22           43.288490
6          23           43.341051
7          24           44.805810
8          25           44.062109
```

0.8 Correlation and Regression

[18]:
```python
# Calculate the correlation coefficient and a linear regression model
# for mouse weight and average observed tumor volume for the entire Capomulin␣
↪regimen

# Calculate the linear regression line
m, b = np.polyfit(avg_wgt_tum_vol_cap.index, avg_wgt_tum_vol_cap.values, 1)

# Create the scatter plot
plt.figure(figsize=(8, 6))

# Customize plot
plt.scatter(avg_wgt_tum_vol_cap.index, avg_wgt_tum_vol_cap.values, s=40,␣
↪c='green', alpha=0.75)
plt.plot(avg_wgt_tum_vol_cap.index, m * avg_wgt_tum_vol_cap.index + b,␣
↪color='red')

# Add labels and title
plt.xlabel('Weight (g)')
plt.ylabel('Average Tumor Volume (mm3)')
plt.title('Average Tumor Volume vs. Weight for Capomulin with Regression Line')

# Display the plot
plt.show()

# Calculate residuals
residuals = new_index_avg_wgt_df['Tumor Volume (mm3)'] - (m *␣
↪new_index_avg_wgt_df['Weight (g)'] + b)

# Calculate standard error of the estimate (SSE)
sse = np.sum(residuals**2)

# Calculate degrees of freedom
df_freedom = len(new_index_avg_wgt_df) - 2  # 2 for slope and intercept
```

```
# Calculate mean squared error (MSE)
mse = sse / df_freedom

# Calculate standard error of the estimate (SE)
se = np.sqrt(mse)

# Calculate r-squared
r_squared = 1 - (sse / np.sum((new_index_avg_wgt_df['Tumor Volume (mm3)'] -␣
 ↪new_index_avg_wgt_df['Tumor Volume (mm3)'].mean())**2))

# Calculate p-value
from scipy import stats
t_stat, p_value = stats.ttest_rel(new_index_avg_wgt_df['Tumor Volume (mm3)'],␣
 ↪(m * new_index_avg_wgt_df['Weight (g)'] + b))

# Print results
print(f"Slope (m): {m}")
print(f"Y-intercept (b): {b}")
print(f"Standard error of the estimate (SE): {se}")
print(f"R-squared: {r_squared}")
print(f"P-value: {p_value}")
print(f"Linear Equation: y = {m}(X) + {b}")
```




```
Slope (m): 0.8947726097340611
Y-intercept (b): 22.764229983591935
Standard error of the estimate (SE): 1.0249929158261613
R-squared: 0.9034966277438602
P-value: 0.9999999999999923
Linear Equation: y = 0.8947726097340611(X) + 22.764229983591935
```