

# 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 0.999999999999923 is extremely high, indicating that the observed positive association is almost certainly not due to chance. Lastly, the drug regimen of Capomulin has shown to significantly reduce tumor volume (mm3) on average compared to the other drug regimen trials.

$x\_value$ : 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: 0.999999999999923

Linear Equation:  $y = 0.8947726097340611(X) + 22.764229983591935$

```
[1]: # 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
Propriova          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
Propriova          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

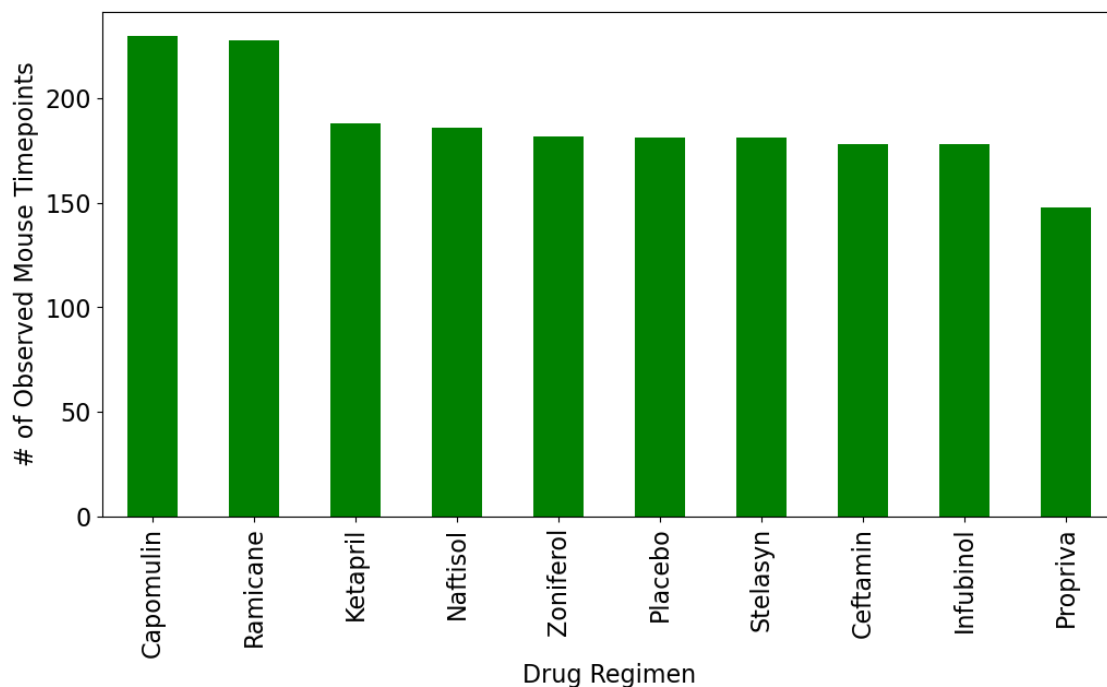
## 0.5 Bar and Pie Charts

```
[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

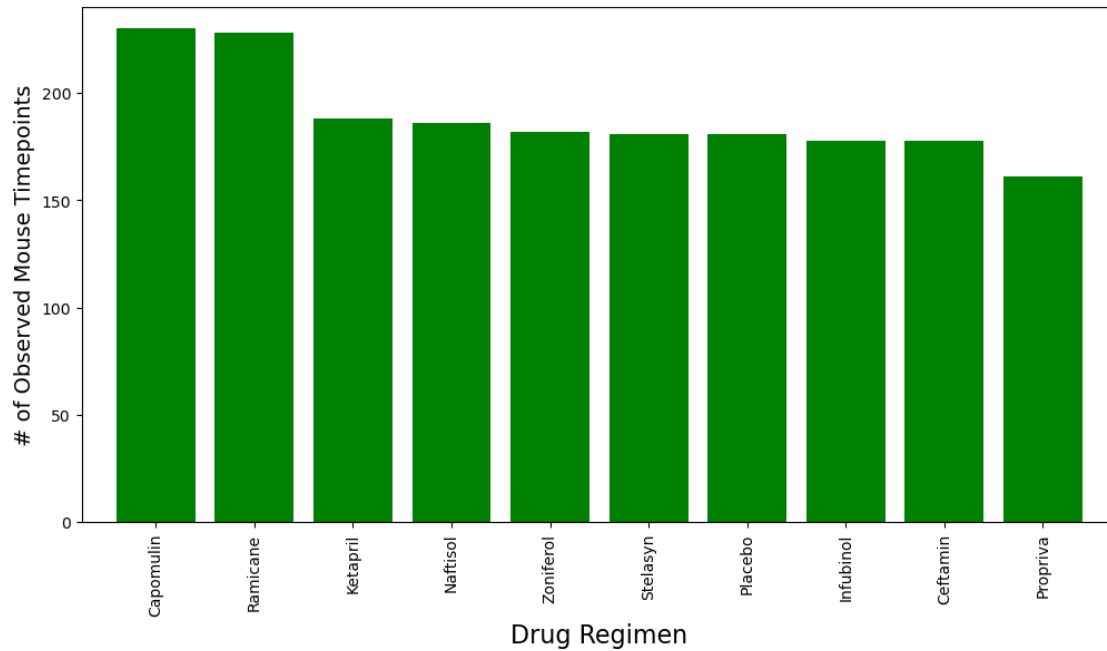
      # Bar pyplot
      x_axis = np.arange(len(bar_timepoints_drugs))
      fig1, ax1 = plt.subplots(figsize=(12, 6))
      plt.bar(x_axis,timepoints_list, color='green')
      tick_locations = [value for value in x_axis]

      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)

      # Display 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
```



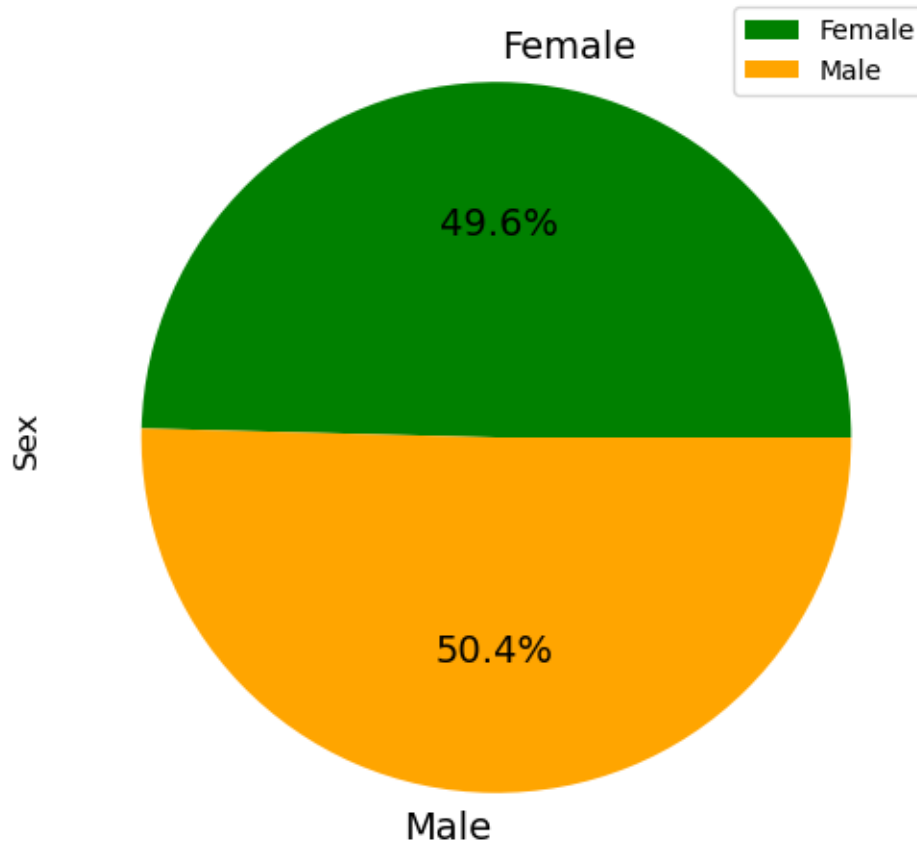
```
[11]: # Generate a pie plot showing the distribution of female versus male mice using
↳Pandas
groupedby_gender = mouse_study_clean_df.groupby(["Mouse ID", "Sex"])
groupedby_gender_df = pd.DataFrame(groupedby_gender.size())

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()
```



## Female vs Male Mice Distribution

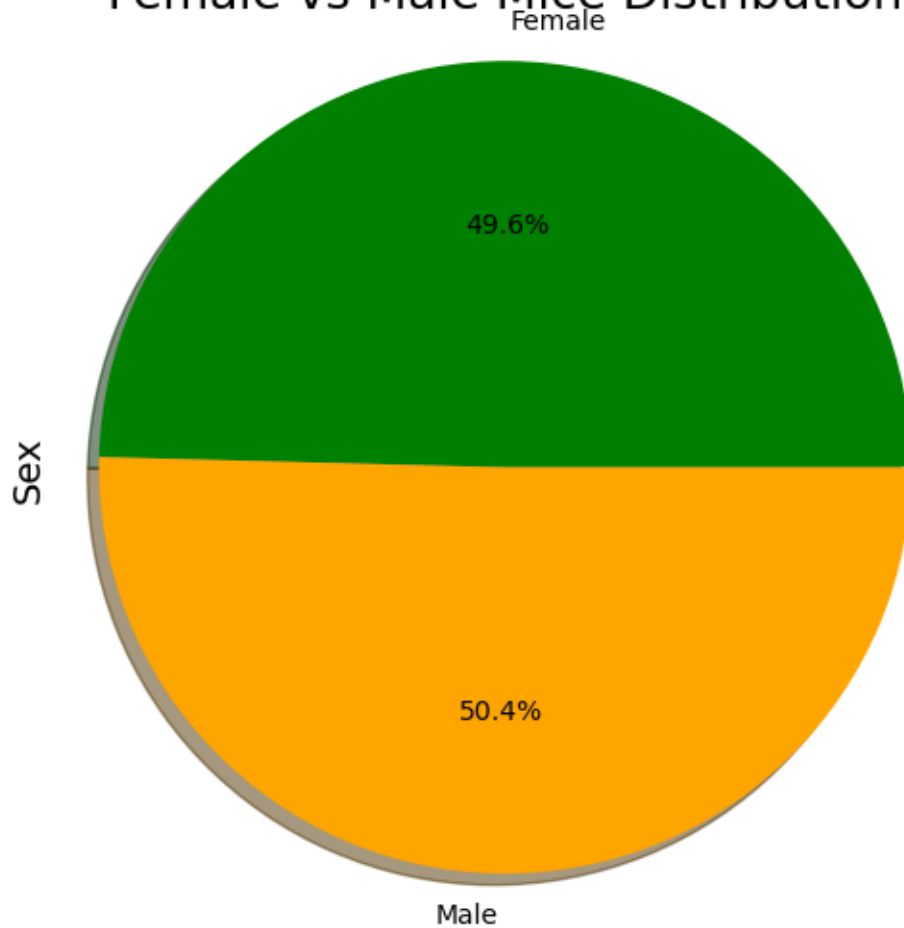


```
[12]: # Generate a pie plot showing the distribution of female versus male mice using
      ↪ pyplot
      labels = ["Female","Male"]

      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()
```

## Female vs Male Mice Distribution



### 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 = ["Capomulin", "Ramican", "Infubinol", "Ceftamin"]

# 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: Ramicane
IQR: 8.325365415
Number of outliers: 1
Lower Bound: 24.1865864625
Upper Bound: 57.488048122500004
=====
Treatment: Infubinol
IQR: 10.002090667500006
Number of outliers: 0
Lower Bound: 32.309217298749985
Upper Bound: 72.31757996875001
=====
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")

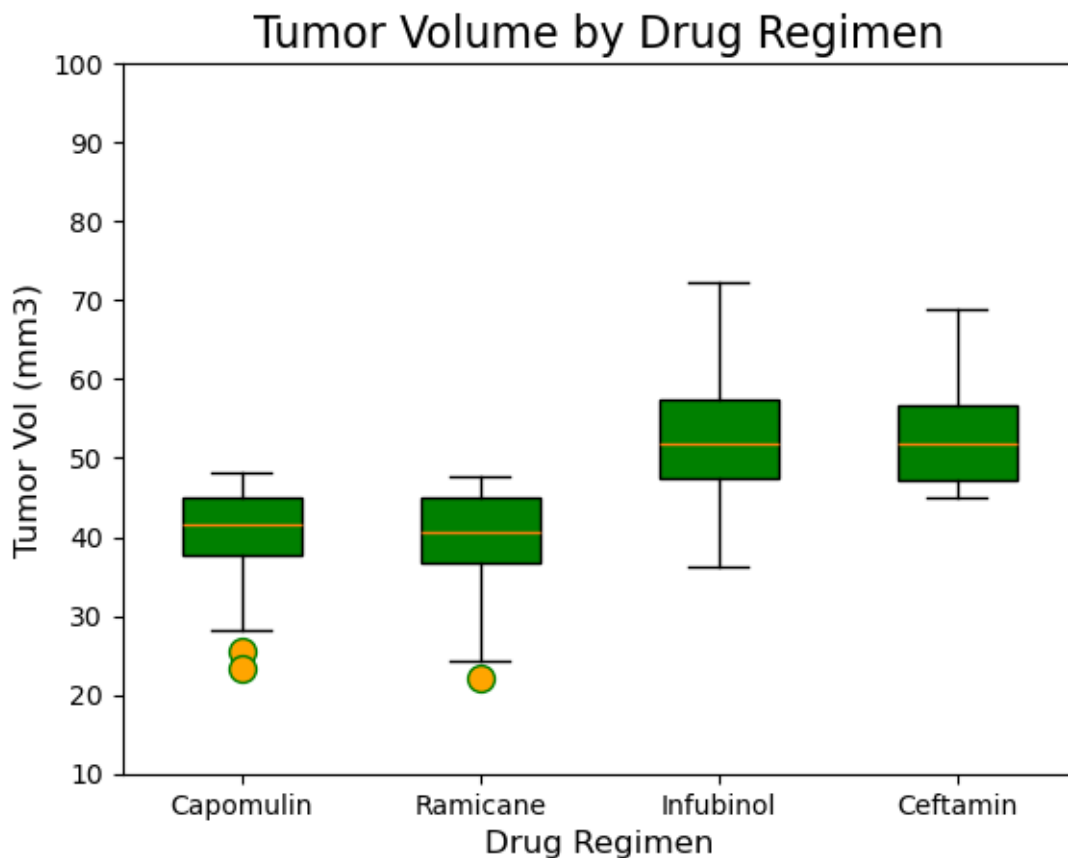
# Create Boxplot

```

```
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], ['Capomulin', 'Ramican', 'Infubinol', 'Ceftamin'])
#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",:]
```

```

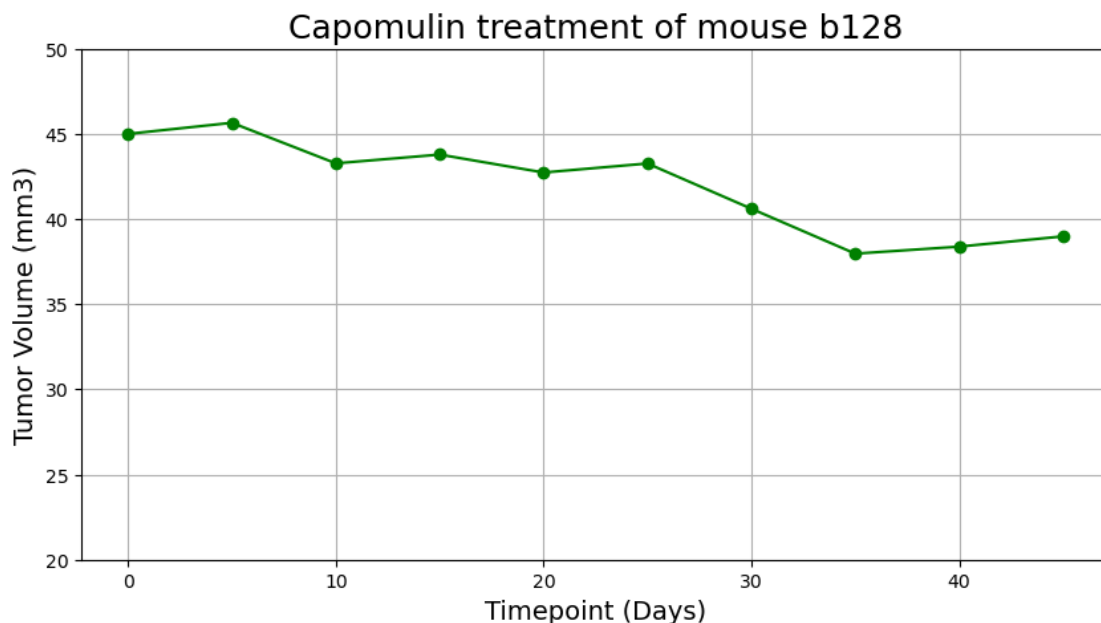
cap_line_df = capomulin_df.loc[capomulin_df["Mouse ID"]== "b128",:]

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

fig1, ax1 = 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()

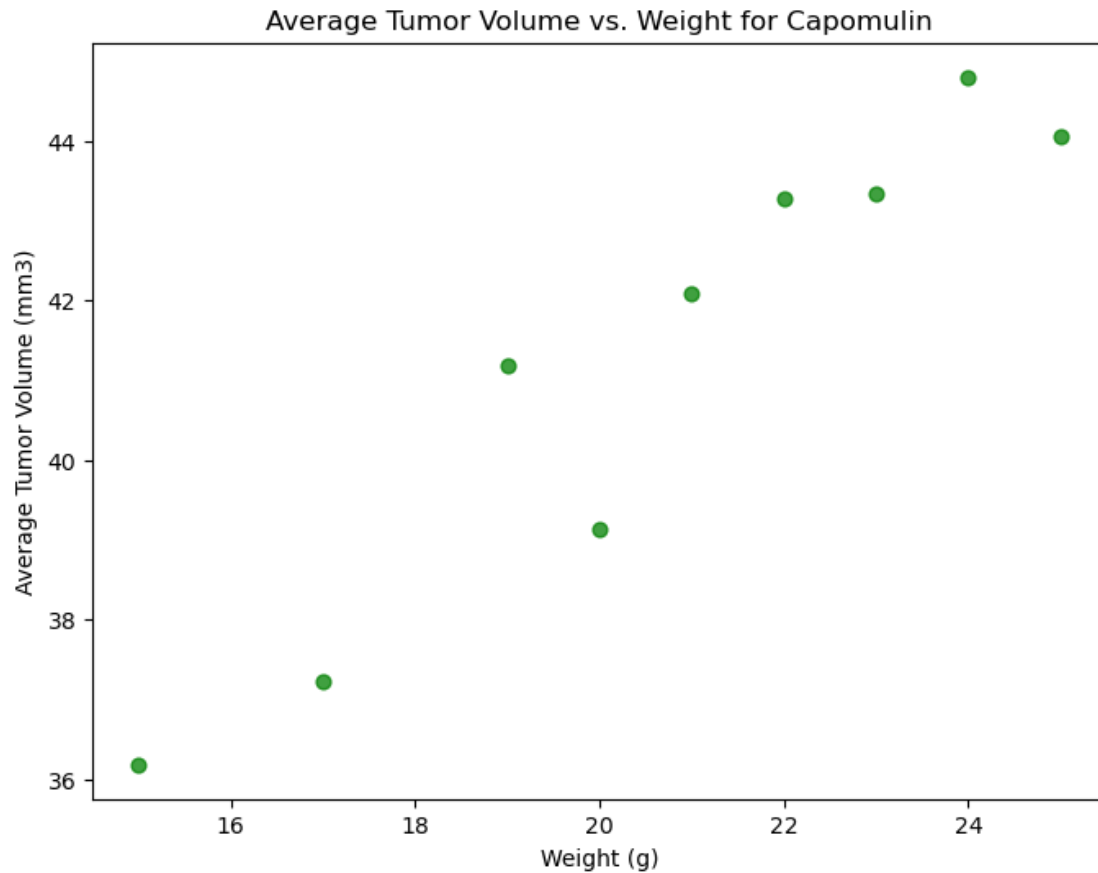
avg_wgt_tum_df = pd.DataFrame(avg_wgt_tum_vol_cap)

# Display Dataframe
avg_wgt_tum_df

# Reset 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]: # 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)

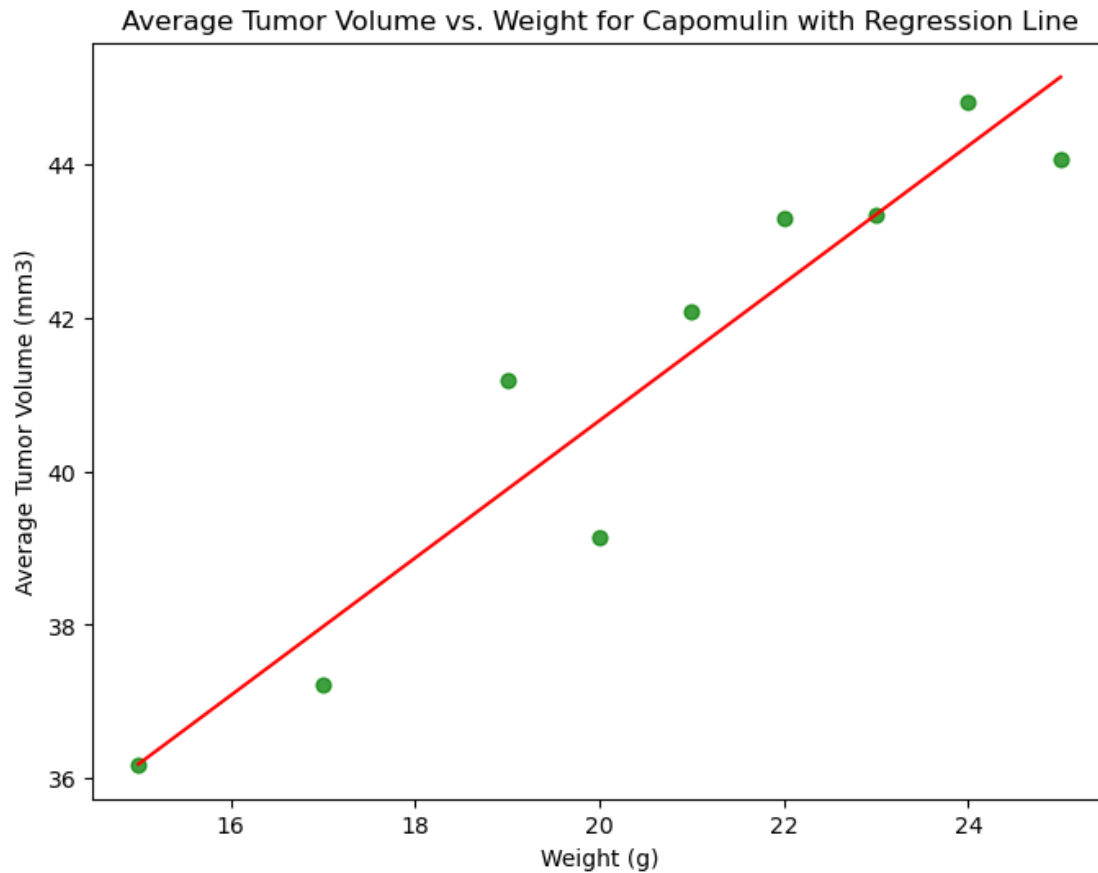
# Calculate r-squared
r_squared = 1 - (sse / np.sum((new_index_avg_wgt_df['Tumor Volume (mm3)'] -
            ↪new_index_avg_wgt_df['Tumor Volume (mm3)'].mean())**2))

# 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:  $y = 0.8947726097340611(X) + 22.764229983591935$