Pymaceutical Visualization

Type *Markdown* and LaTeX: α^2

In [1]:
```
# Dependencies and Setup
import matplotlib.pyplot as plt
from matplotlib.pyplot import figure
import pandas as pd
import numpy as np
from collections import Counter
import scipy.stats as st
from scipy.stats import linregress

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

In [2]:
```
# 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 dataset
merged_data = pd.merge(mouse_metadata, study_results, how='outer', on="Mous
# Display the data table for preview
pd.set_option("display.max_rows", None, "display.max_columns", None)
display(merged_data)
```

	Mouse ID	Drug Regimen	Sex	Age_months	Weight (g)	Timepoint	Tumor Volume (mm3)	Metastatic Sites
0	k403	Ramicane	Male	21	16	0	45.000000	0
1	k403	Ramicane	Male	21	16	5	38.825898	0
2	k403	Ramicane	Male	21	16	10	35.014271	1
3	k403	Ramicane	Male	21	16	15	34.223992	1
4	k403	Ramicane	Male	21	16	20	32.997729	1
5	k403	Ramicane	Male	21	16	25	33.464577	1
6	k403	Ramicane	Male	21	16	30	31.099498	1
7	k403	Ramicane	Male	21	16	35	26.546993	1
8	k403	Ramicane	Male	21	16	40	24.365505	1
9	k403	Ramicane	Male	21	16	45	22.050126	1

Merging tables using Mouse ID as a primary key allows all data to be displayed on 1 table

In [3]:
```
# How many mice are in this study?
total_mice = len(pd.unique(merged_data['Mouse ID']))
display(total_mice)
```

```
249
```

In [4]:
```
# Eliminate any duplicates to clean data
duplicate_mice = merged_data.loc[merged_data.duplicated(subset = ['Mouse ID
```

In [5]:
```
# Display duplicate mouse ID.
dupe_mouse_df = pd.DataFrame(duplicate_mice)
dupe_mouse_df
```

Out[5]:

	0
0	g989

This duplicate mouse was found by searching for multiple pairs of mouse ID's and timepoints, which could only exist in the case of a duplicated result.

In [6]:
```
# Create a clean DataFrame by dropping the duplicate mouse by its ID.
cleaned_df = merged_data[merged_data['Mouse ID'].isin(duplicate_mice)==Fals
display(cleaned_df)
```

	Mouse ID	Drug Regimen	Sex	Age_months	Weight (g)	Timepoint	Tumor Volume (mm3)	Metastatic Sites
0	k403	Ramicane	Male	21	16	0	45.000000	0
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8	k403	Ramicane	Male	21	16	40	24.365505	1
9	k403	Ramicane	Male	21	16	45	22.050126	1

In [7]:
```
# Checking the number of mice in the clean DataFrame.
cleaned_mouse_count = len(pd.unique(cleaned_df['Mouse ID']))
print(cleaned_mouse_count)
```

```
248
```

Summary Statistics

In [8]:
```
# Generate a summary statistics table of mean, median, variance, standard d
# Use groupby and summary statistical methods to calculate the following pr
# mean, median, variance, standard deviation, and SEM of the tumor volume.
volume_mean = cleaned_df.groupby('Drug Regimen').mean()['Tumor Volume (mm3)
volume_median = cleaned_df.groupby('Drug Regimen').median()['Tumor Volume (
volume_variance = cleaned_df.groupby('Drug Regimen').var()['Tumor Volume (m
volume_std = cleaned_df.groupby('Drug Regimen').std()['Tumor Volume (mm3)']
volume_sem = cleaned_df.groupby('Drug Regimen').sem()['Tumor Volume (mm3)']
# Assemble the resulting series into a single summary dataframe.
summary_df = pd.DataFrame({'Mean Tumor Volume (mm3)': volume_mean,
                           'Median Tumor Volume (mm3)': volume_median,
                           'Variance in Tumor Volume (mm3)': volume_variance
                           'Standard Dev. of Tumor Volume (mm3)': volume_std
                           'SEM of Tumor Volume (mm3)': volume_sem})
display(summary_df)
```

Drug Regimen	Mean Tumor Volume (mm3)	Median Tumor Volume (mm3)	Variance in Tumor Volume (mm3)	Standard Dev. of Tumor Volume (mm3)	SEM of Tumor Volume (mm3)
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

In [9]:
```
# Generate a summary statistics table of mean, median, variance, standard d
# Using the aggregation method, produce the same summary statistics in a si
agg_summary = cleaned_df.groupby('Drug Regimen').agg({'Tumor Volume (mm3)':
agg_summary.head(10)
```

Out[9]:

	Tumor Volume (mm3)				
	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
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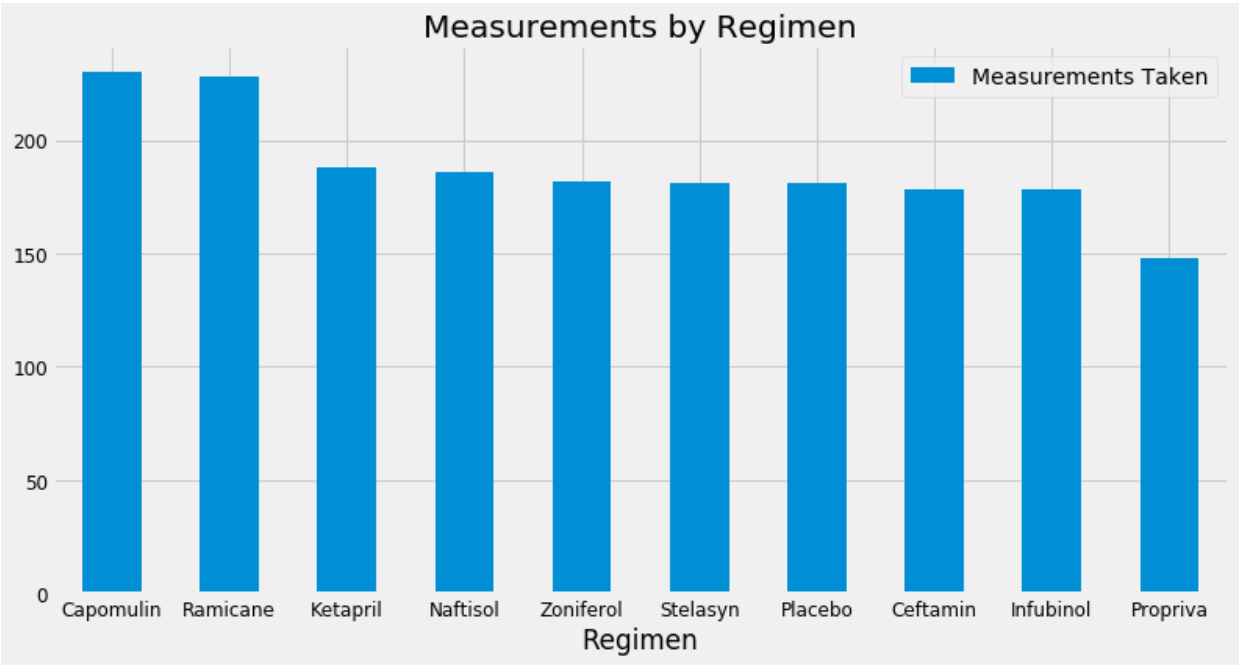
Zoniferol	53.236507	51.818479	48.533355	6.966589	0.516398

Bar and Pie Charts

In [10]:
```
# Generate a bar plot showing the total number of measurements taken on eac
barchartdf = pd.DataFrame(cleaned_df['Drug Regimen'].value_counts().reset_i
                          .rename(columns={"index": "Regimen", "Drug Regime
                                  .set_index("Regimen")
                         )
plt.style.use('fivethirtyeight')
barchart1= barchartdf.plot.bar(figsize=(12, 6), rot=(0), fontsize=12, title
display(barchart1)
display(barchartdf)
```

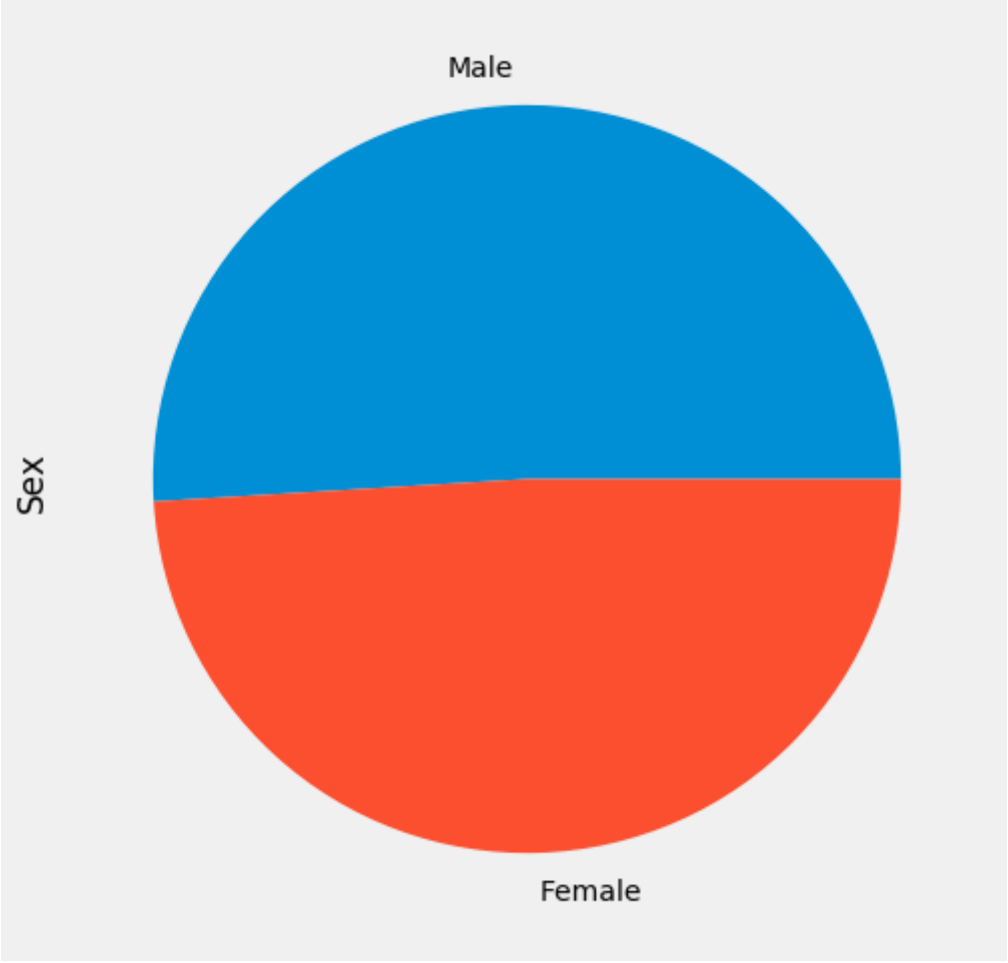
```
<matplotlib.axes._subplots.AxesSubplot at 0x7fe7424f78d0>
```

Regimen	Measurements Taken
Capomulin	230
Ramicane	228
Ketapril	188
Naftisol	186
Zoniferol	182
Stelasyn	181
Placebo	181
Ceftamin	178
Infubinol	178
Propriva	148

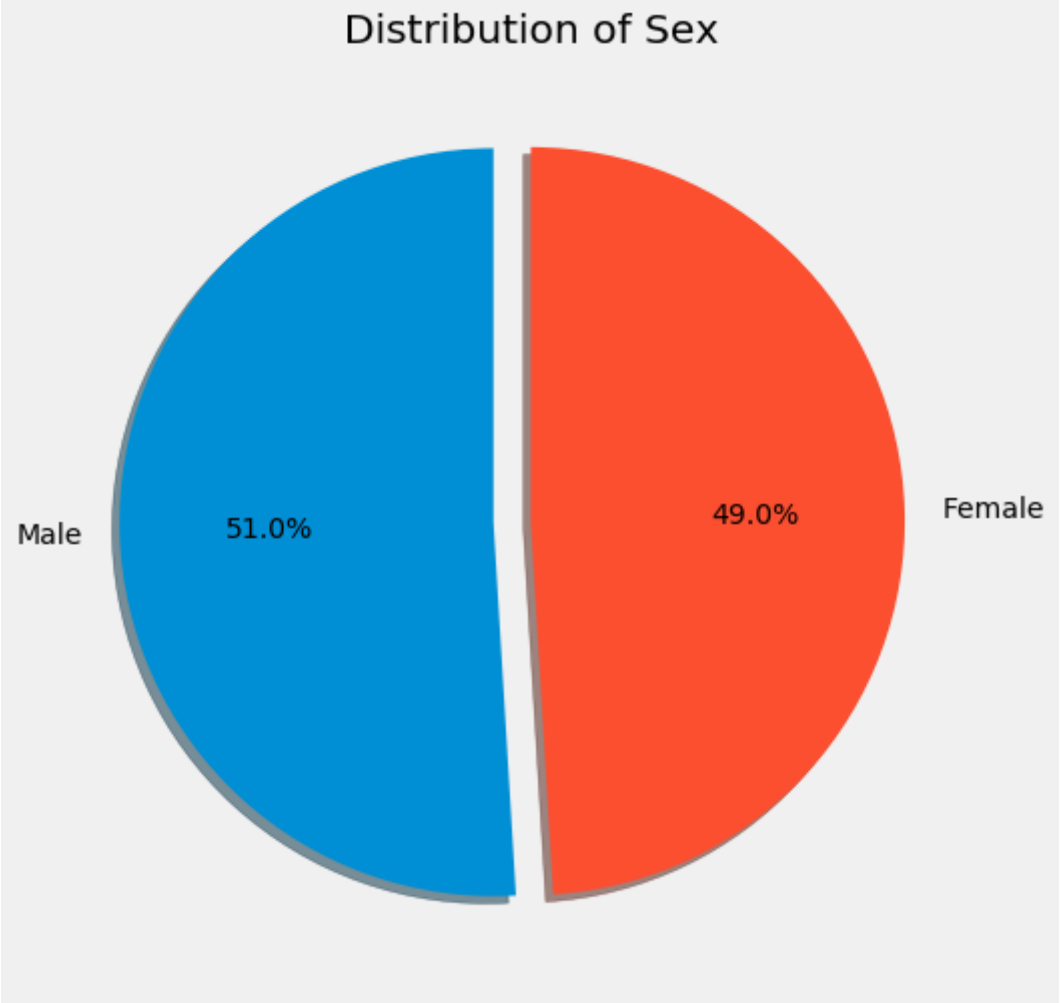


Most medications are within ~10 measurements of 180, while three have a significant difference. Capomulin and Ramicane are measured near 230 times, while Propriva is measured 148 times.

In [11]:
```
# Generate a pie plot showing the distribution of female versus male mice u
piechart = cleaned_df['Sex'].value_counts().plot(figsize=(8,8), kind='pie')
```



In [44]:
```
# Generate a pie plot showing the distribution of female versus male mice u
male = cleaned_df.Sex.value_counts().Male
female = cleaned_df.Sex.value_counts().Female
# fig1, ax1 = plt.subplots()
sex_data = [male, female]
mylabels='Male', 'Female'
explode = (0.1, 0)
figure(figsize=(8,8))

plt.pie(sex_data, labels=mylabels,autopct='%1.1f%%', explode=explode,
        shadow=True, startangle=90)
ax1.axis('equal')
plt.title('Distribution of Sex')
plt.show()
```



Quartiles, Outliers and Boxplots

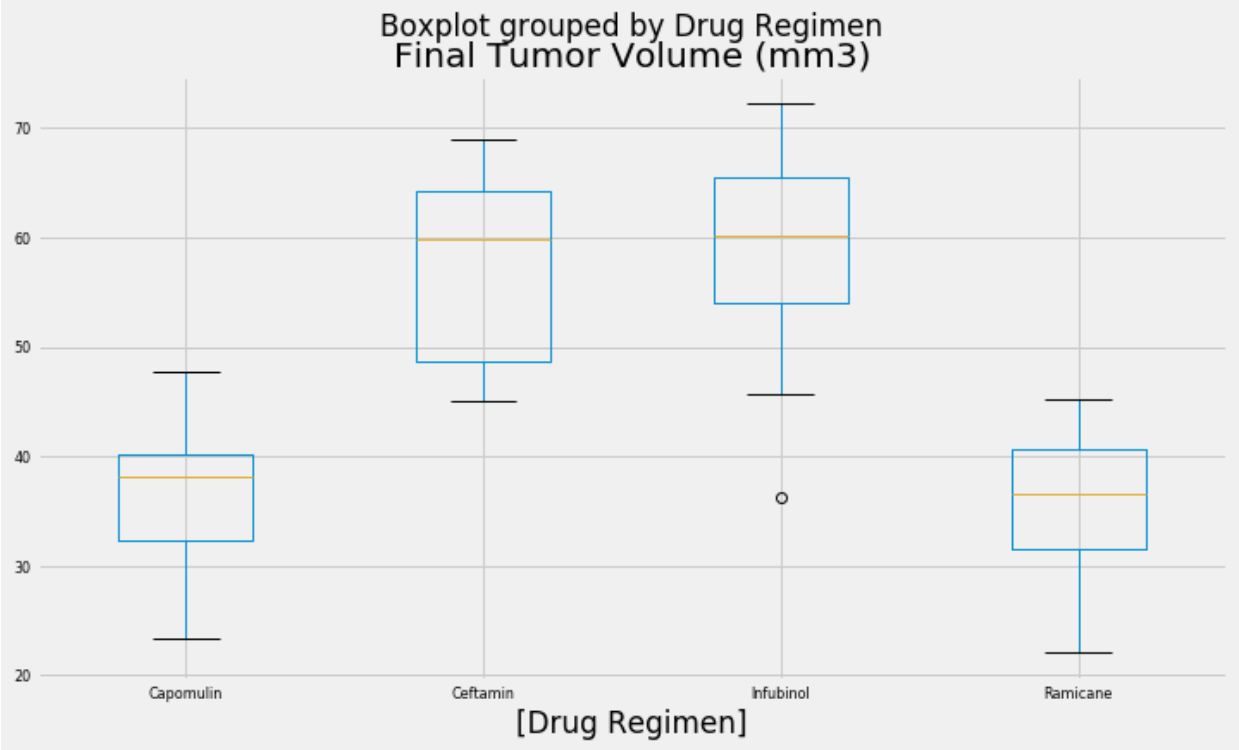
In [13]:
```
# Calculate the final tumor volume of each mouse across four of the treatme
# Capomulin, Ramicane, Infubinol, and Ceftamin
# Start by getting the last (greatest) timepoint for each mouse
max_timepoint = cleaned_df.groupby('Mouse ID').max()['Timepoint']
timepoints_df = pd.DataFrame(max_timepoint)
timepoint_merge = pd.merge(timepoints_df, cleaned_df, on=('Mouse ID','Timep
#use list of the desired medications to create df of final tumor volumes
regimens = ['Capomulin', 'Ramicane', 'Infubinol', 'Ceftamin']
filtered_timepoints = timepoint_merge.loc[timepoint_merge['Drug Regimen'].i
filtered_timepoints = filtered_timepoints.rename(columns={"Timepoint": "Fin
# Merge this group df with the original dataframe to get the tumor volume a
display(filtered_timepoints)
```

	Mouse ID	Final Timepoint	Drug Regimen	Sex	Age_months	Weight (g)	Final Tumor Volume (mm3)	Metastatic Sites
0	a203	45	Infubinol	Female	20	23	67.973419	2
1	a251	45	Infubinol	Female	21	25	65.525743	1
3	a275	45	Ceftamin	Female	20	28	62.999356	3
6	a411	45	Ramicane	Male	3	22	38.407618	1
7	a444	45	Ramicane	Female	10	25	43.047543	0
10	a520	45	Ramicane	Male	13	21	38.810366	1
11	a577	30	Infubinol	Female	6	25	57.031862	2
12	a644	45	Ramicane	Female	7	17	32.978522	1
13	a685	45	Infubinol	Male	8	30	66.083066	3
19	b128	45	Capomulin	Female	9	22	38.982878	2

Generate a box plot of the final tumor volume of each mouse across four regimens of interest

In [69]:
```
filtered_timepoints.boxplot(column = ['Final Tumor Volume (mm3)'],
                                        by=['Drug Regimen'], fontsize=8, f
display(volume_plot)
```

```
<matplotlib.axes._subplots.AxesSubplot at 0x7fe742695b70>
```



Line and Scatter Plots

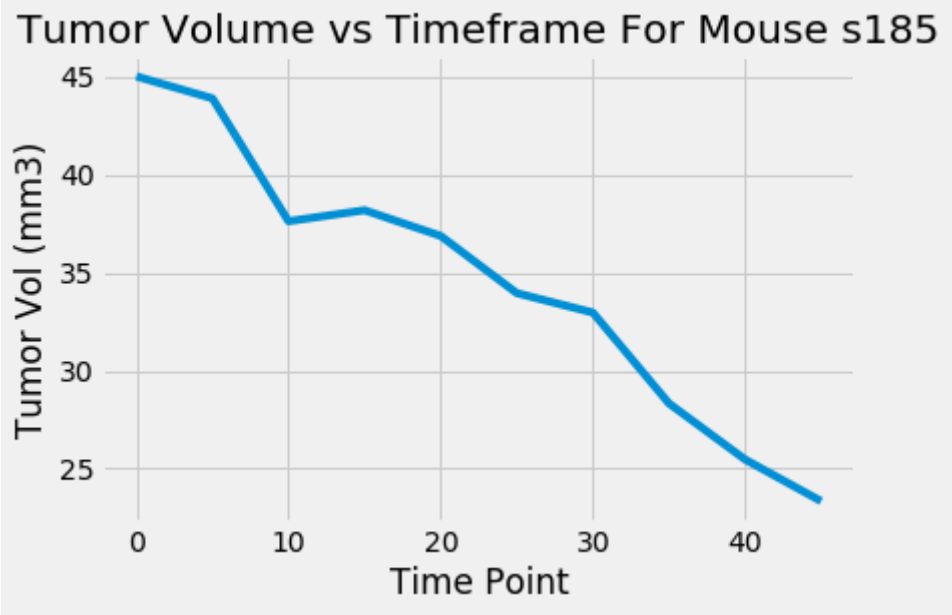
In [15]:
```
# Put treatments into a list for for loop (and later for plot labels)

# Create empty list to fill with tumor vol data (for plotting)

tumor_vol0 = []
tumor_vol1 = []
tumor_vol2 = []
tumor_vol3 = []

# Calculate the IQR and quantitatively determine if there are any potential
# Locate the rows which contain mice on each drug and get the tumor volume
tumor_vol0 = filtered_timepoints.loc[filtered_timepoints['Drug Regimen']==re
tumor_vol1 = filtered_timepoints.loc[filtered_timepoints['Drug Regimen']==re
tumor_vol2 = filtered_timepoints.loc[filtered_timepoints['Drug Regimen']==re
tumor_vol3 = filtered_timepoints.loc[filtered_timepoints['Drug Regimen']==re

cap_vol = tumor_vol0.tolist()
ram_vol = tumor_vol1.tolist()
inf_vol = tumor_vol2.tolist()
cef_vol = tumor_vol3.tolist()

boxplot_df = pd.DataFrame({"Capomulin:":cap_vol,
                           "Ramicane:":ram_vol,
                           "Infubinol:":inf_vol,
                           "Ceftamin:": cef_vol})
#calculating quantiles of final tumor volumes
Q01 = np.quantile(cap_vol, 0.25)
Q03 = np.quantile(cap_vol, 0.75)
IQR0 = Q03 - Q01
outlier01 = Q01-(IQR0*1.5)
outlier02 = Q03+(IQR0*1.5)
#formatting for neat print statements
outlier01_formatted = "{:.3f}".format(outlier01)
outlier02_formatted = "{:.3f}".format(outlier02)
#process for Ramicane
Q11 = np.quantile(ram_vol, 0.25)
Q13 = np.quantile(ram_vol, 0.75)
IQR1 = Q13 - Q11
outlier11 = Q11-(IQR1*1.5)
outlier12 = Q13+(IQR1*1.5)
outlier11_formatted = "{:.3f}".format(outlier11)
outlier12_formatted = "{:.3f}".format(outlier12)
#process for infubinol
Q21 = np.quantile(inf_vol, 0.25)
Q23 = np.quantile(inf_vol, 0.75)
IQR2 = Q23 - Q21
outlier21 = Q21-(IQR2*1.5)
outlier22 = Q23+(IQR2*1.5)
outlier21_formatted = "{:.3f}".format(outlier21)
outlier22_formatted = "{:.3f}".format(outlier22)
#process for ceftamin
Q31 = np.quantile(cef_vol, 0.25)
Q33 = np.quantile(cef_vol, 0.75)
IQR3 = Q33 - Q31
outlier31 = Q31-(IQR3*1.5)
outlier32 = Q33+(IQR3*1.5)
```

```
outlier31_formatted = "{:.3f}".format(outlier31)
outlier32_formatted = "{:.3f}".format(outlier32)
    # Determine outliers using upper and lower bounds
cap_outliers = []
ram_outliers = []
inf_outliers = []
cef_outliers = []
#append outliers to list based on being above/below +/- 1.5 x IQR
for x in cap_vol:
    if x < int(outlier01) or x > int(outlier02):
        cap_outliers.append(x)
for y in (ram_vol):
    if y < int(outlier11) or y > int(outlier12):
        ram_outliers.append(y)
for i in inf_vol:
    if i < int(outlier21) or i > int(outlier22):
        inf_outliers.append(i)
for z in (cef_vol):
    if z < int(outlier31) or z > int(outlier32):
        cef_outliers.append(z)
#print outlier bounds and outlier count
print("For Capomulin, outliers in final tumor volume are below " + str(outli
print("For Ramicane, outliers in final tumor volume are below " + str(outlie
print("For Infubinol, outliers in final tumor volume are below " + str(outli
print("For Ceftamin, outliers in final tumor volume are below " + str(outlie
```

```
For Capomulin, outliers in final tumor volume are below 20.705 (mm3) and
above 51.832 (mm3). There are 0 in the set.
For Ramicane, outliers in final tumor volume are below 17.913 (mm3) and a
bove 54.307 (mm3). There are 0 in the set.
For Infubinol, outliers in final tumor volume are below 36.833 (mm3) and
above 82.741 (mm3). There are 0 in the set.
For Ceftamin, outliers in final tumor volume are below 25.355 (mm3) and a
bove 87.666 (mm3). There are 0 in the set.
```

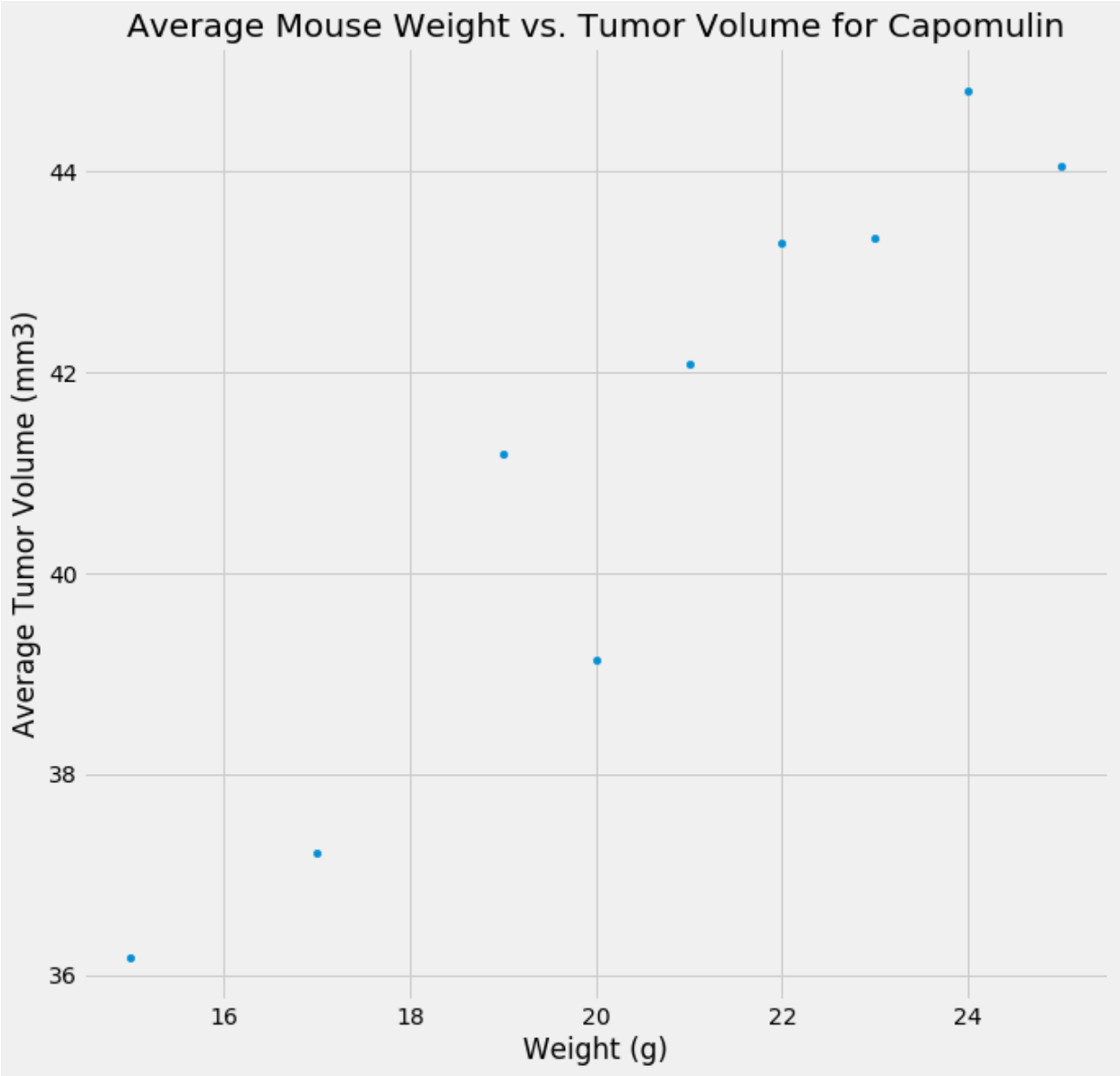
In [16]:
```
# Generate a line plot of tumor volume vs. time point for a mouse treated w
#generate a df containing only capomulin info
capo = ['Capomulin']
capo_df = cleaned_df.loc[cleaned_df['Drug Regimen'].isin(capo)]
#use an id from a mouse that went all the way to the highest timepoint(45)
capo_id = ['s185']
single_capo_df = capo_df.loc[cleaned_df['Mouse ID'].isin(capo_id)]
#display(single_capo_df)
#use matplotlib
fig=plt.figure()
ax=plt.axes()
plt.title("Tumor Volume vs Timeframe For Mouse s185")
plt.xlabel("Time Point")
plt.ylabel("Tumor Vol (mm3)")
plt.plot(single_capo_df['Timepoint'], single_capo_df['Tumor Volume (mm3)'])
```

Out[16]:
```
[<matplotlib.lines.Line2D at 0x7fe742d356d8>]
```



In [17]:
```
# Generate a scatter plot of average tumor volume vs. mouse weight for the
avg_vol = capo_df.groupby('Weight (g)').mean()['Tumor Volume (mm3)']
avg_vol_df = pd.merge(avg_vol, capo_df, on=('Weight (g)','Tumor Volume (mm3
avg_vol_df = avg_vol_df[['Weight (g)','Tumor Volume (mm3)']]
avg_tumor_vol = avg_vol_df.plot(kind="scatter", x='Weight (g)', y='Tumor Vo
                                figsize=(10,10), title="Average Mouse Weight vs
plt.ylabel('Average Tumor Volume (mm3)')
plt.xlabel='Mouse Weight (g)'
display(avg_tumor_vol)
```

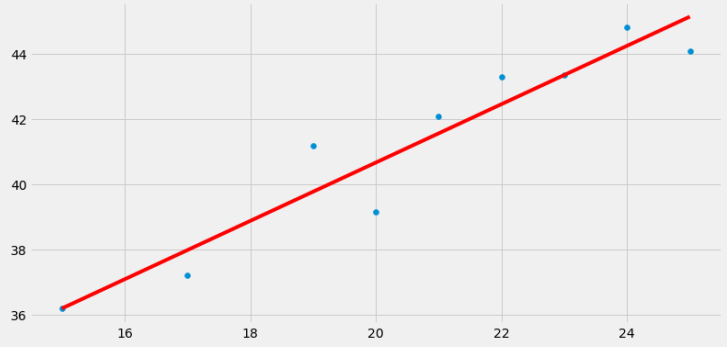
```
<matplotlib.axes._subplots.AxesSubplot at 0x7fe742d67a90>
```



Correlation and Regression

In [18]:
```
# Calculate the correlation coefficient and linear regression model
# for mouse weight and average tumor volume for the Capomulin regimen
```

In [76]:
```
x_values = avg_vol_df['Weight (g)']
y_values = avg_vol_df['Tumor Volume (mm3)']
(slope, intercept, rvalue, pvalue, stderr) = linregress(x_values, y_values)
regress_values = x_values * slope + intercept
line_eq = "y = " + str(round(slope,2)) + "x + " + str(round(intercept,2))
plt.figure(figsize=(12,6))
plt.scatter(x_values,y_values)
plt.plot(x_values,regress_values,"r-")
plt.annotate(line_eq,(6,10),fontsize=7,color="red")
plt.ylabel=('Average Tumor Volume')
plt.xlabel=('Mouse Weight (g)')
correlation = y_values.corr(x_values)
plt.show()
print("The correlation coefficient is " + str(correlation) +".")
```




```
The correlation coefficient is 0.9505243961855271.
```

In [ ]: