Real Data Example: The study uses alcohol solubility data from Romanelli et al. The dependent variable is ln(Sol)exp (natural log of solubility in water). The dataset contains 44 observations of aliphatic alcohols. There are 6 independent variables: **Log P (octanol-water partition coefficient) - measures hydrophobicity, P (polarizability), SAG (solvent-accessible surface-bounded molecular volume), Mass (M), RM (molar refractivity), V (volume)**

In [1]:
```python
import numpy as np
import pandas as pd
from scipy.stats import chi2
import matplotlib.pyplot as plt
```

In [2]:
```python
df = pd.read_csv('C:/Users/91959/Desktop/CODE'
                 '/Robust-Penalized-Empirical-Likelihood-Estimation-Method-for-Linear-Regression/Data/Alcohol.csv')

X = df.drop(['Alcohol', 'ln (Sol)exp'], axis=1)
y = df['ln (Sol)exp']
```

In [3]:
```python
# 1. Dataset Description
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 44 entries, 0 to 43
Data columns (total 8 columns):
 #   Column       Non-Null Count  Dtype  
---  ------       --------------  -----  
 0   Alcohol      44 non-null     object 
 1   SAG          44 non-null     float64
 2   V            44 non-null     float64
 3   Log P        44 non-null     float64
 4   P            44 non-null     float64
 5   RM           44 non-null     float64
 6   Mass         44 non-null     float64
 7   ln (Sol)exp  44 non-null     float64
dtypes: float64(7), object(1)
memory usage: 2.9+ KB
```

In [4]:
```python
# 2. Basic Statistical Summary
df.describe()
```

Out[4]:

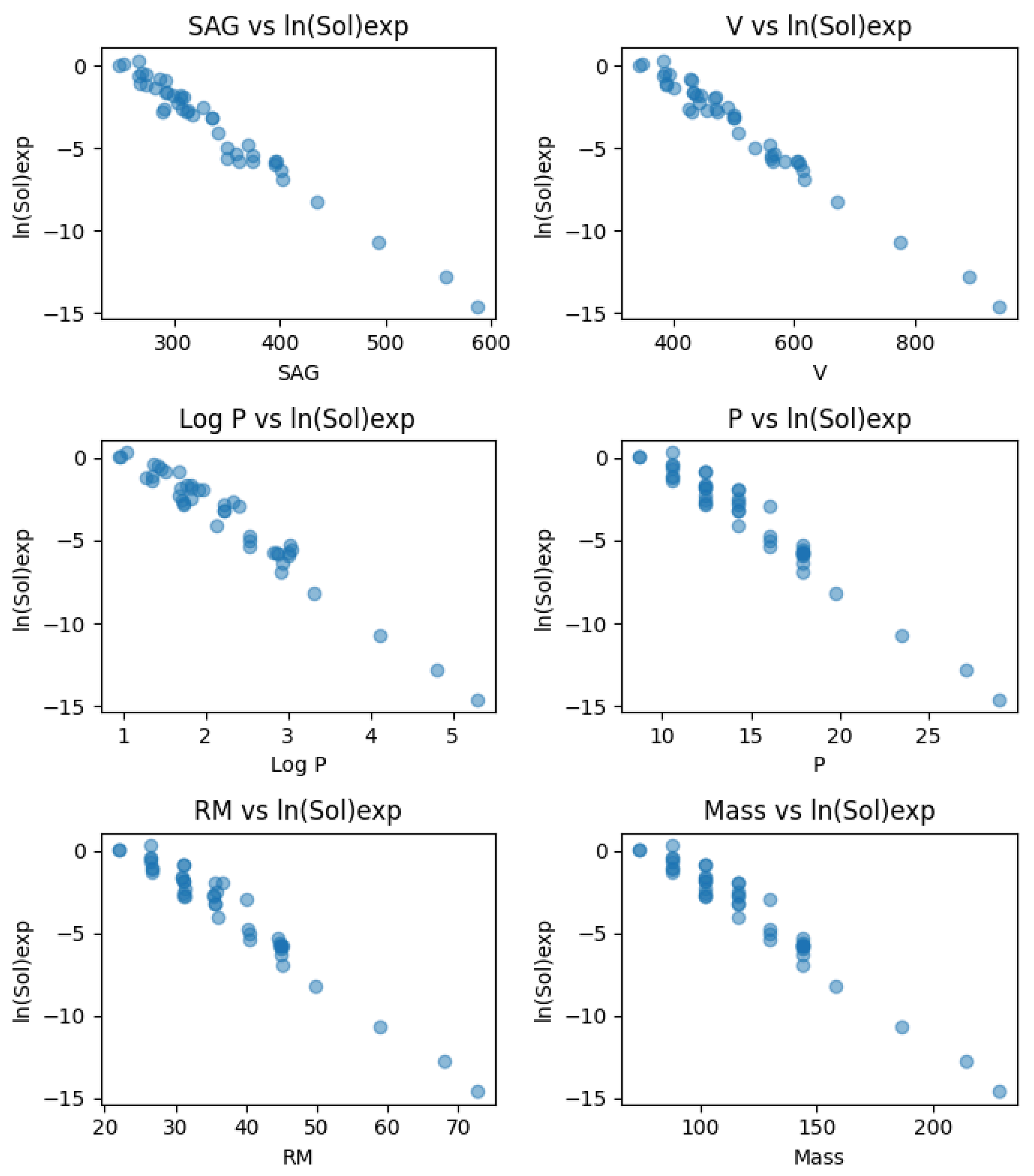
	SAG	V	Log P	P	RM	Mass	ln (Sol)exp
count	44.000000	44.000000	44.000000	44.000000	44.000000	44.000000	44.000000
mean	337.788864	509.640455	2.254318	14.883409	37.327727	120.985909	-3.710564
std	74.011456	128.593538	0.940693	4.316224	10.847843	32.992404	3.284330
min	247.550000	344.910000	0.940000	8.750000	21.950000	74.120000	-14.614020
25%	290.382500	429.655000	1.677500	12.420000	31.065000	102.180000	-5.615712
50%	312.345000	471.965000	2.050000	14.260000	35.635000	116.200000	-2.752595
75%	371.282500	565.057500	2.865000	17.930000	44.787500	144.260000	-1.543848
max	587.000000	938.540000	5.300000	28.940000	72.750000	228.420000	0.338610

In [5]:
```python
# 3. Correlation Analysis
correlation_matrix = df.drop('Alcohol', axis=1).corr()
correlation_matrix
```

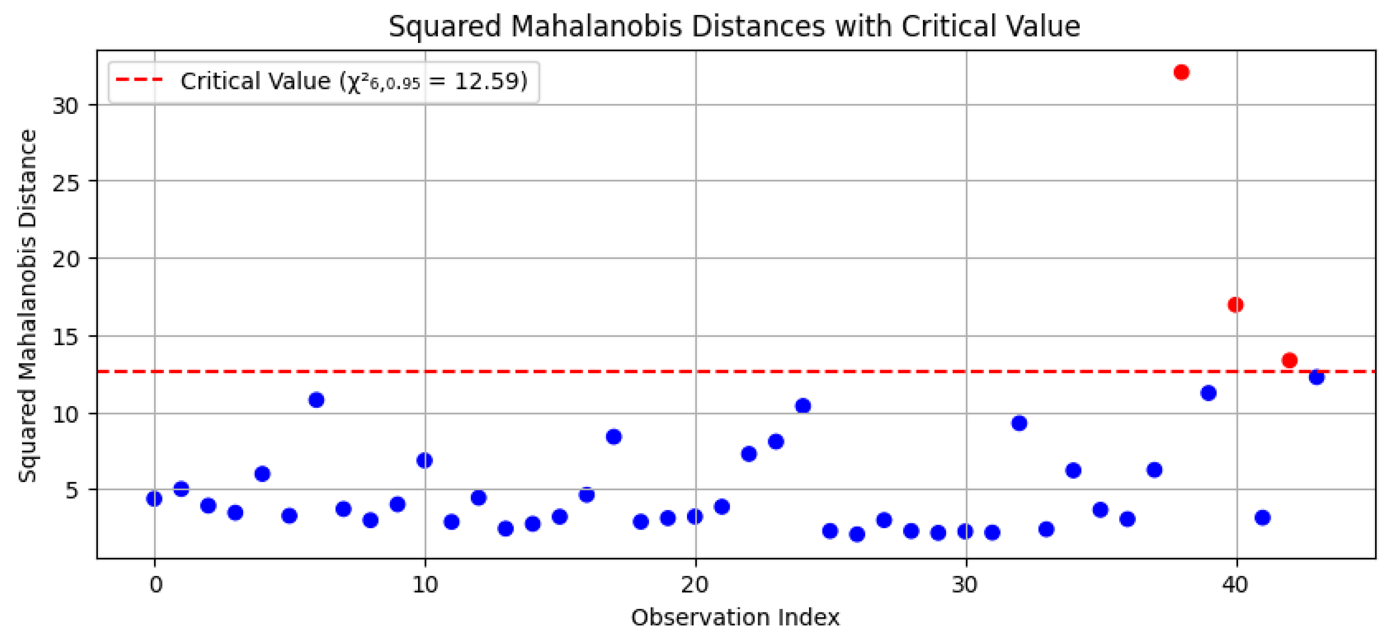
Out[5]:

	SAG	V	Log P	P	RM	Mass	ln (Sol)exp
SAG	1.000000	0.997048	0.973976	0.978384	0.980033	0.978402	-0.986840
V	0.997048	1.000000	0.986253	0.991123	0.992075	0.991134	-0.988882
Log P	0.973976	0.986253	1.000000	0.993428	0.992425	0.993425	-0.980229
P	0.978384	0.991123	0.993428	1.000000	0.999810	1.000000	-0.978261
RM	0.980033	0.992075	0.992425	0.999810	1.000000	0.999811	-0.979391
Mass	0.978402	0.991134	0.993425	1.000000	0.999811	1.000000	-0.978286
ln (Sol)exp	-0.986840	-0.988882	-0.980229	-0.978261	-0.979391	-0.978286	1.000000

In [6]:
```python
# 4. Feature distributions and their relationships with target

fig, axes = plt.subplots(3, 2, figsize=(7, 8))
axes = axes.ravel()

for idx, column in enumerate(X.columns):
    # Scatter plot against target
    axes[idx].scatter(X[column], y, alpha=0.5)
    axes[idx].set_xlabel(column)
    axes[idx].set_ylabel('ln(Sol)exp')
    axes[idx].set_title(f'{column} vs ln(Sol)exp')

plt.tight_layout()
plt.show()
```



In [7]:
```python
# 5. Calculating Mahalanobis Distance for outlier detection

# Calculate mean vector and covariance matrix
mean_vector = np.mean(X, axis=0)
covariance_matrix = np.cov(X.T)

# Calculate inverse of covariance matrix
inv_covariance_matrix = np.linalg.inv(covariance_matrix)

# Calculate Mahalanobis distance for each point
mahalanobis_distances = []
n = len(X)
p = X.shape[1]  # number of variables

for i in range(n):
    x_i = X.iloc[i, :]
    diff = x_i - mean_vector
    md = np.sqrt(diff.dot(inv_covariance_matrix).dot(diff))
    mahalanobis_distances.append(md)

# Calculate squared distances
md_squared = np.array(mahalanobis_distances) ** 2

# Calculate critical value
critical_value = chi2.ppf(0.95, p)  # 95% confidence level with p degrees of freedom

# Identify outliers
outliers = pd.DataFrame({
    'Alcohol': df['Alcohol'],
    'MD_squared': md_squared,
    'is_outlier': md_squared > critical_value
})

# Plot the results
plt.figure(figsize=(10, 4))
plt.scatter(range(len(outliers)), outliers['MD_squared'],
        c=['red' if x else 'blue' for x in outliers['is_outlier']])
plt.axhline(y=critical_value, color='r', linestyle='--',
        label=f'Critical Value (χ²₆,₀.₉₅ = {critical_value:.2f})')
plt.xlabel('Observation Index')
plt.ylabel('Squared Mahalanobis Distance')
plt.title('Squared Mahalanobis Distances with Critical Value')
plt.legend()
plt.grid(True)
plt.show()

# Print outlier details
print("\nDetected Outliers (MD² > χ²₆,₀.₉₅):")
print(outliers[outliers['is_outlier']][['Alcohol', 'MD_squared']].sort_values('MD_squared', ascending=False))

# Print summary statistics
print(f"\nTotal number of observations: {len(outliers)}")
print(f"Number of outliers detected: {sum(outliers['is_outlier'])}")
print(f"Percentage of outliers: {(sum(outliers['is_outlier'])/len(outliers))*100:.1f}%")
```




```
Detected Outliers (MD² > χ²₆,₀.₉₅):
                Alcohol  MD_squared
38      3-Ethyl-3-pentanol   32.027452
40  2,2-Diethyl-1-pentanol   16.932877
42         1-Tetradecanol   13.352777
```

```
Total number of observations: 44
Number of outliers detected: 3
Percentage of outliers: 6.8%
```