1. Imports and Project Environment

- I have turned this Notebook file into a multipurpose project report because combining the Markdown and Python output was very convenient.
- Some functions that I have written are inside the `/project/util.py` file to reduce visual clutter.

In [3]:
```
from project.util import *
```

In [4]:
```
%watermark -v -p sklearn,pandas,numpy,matplotlib,seaborn
```

```
Python implementation: CPython
Python version       : 3.13.7
IPython version      : 9.6.0

sklearn   : 1.7.2
pandas    : 2.3.3
numpy     : 2.3.4
matplotlib: 3.10.7
seaborn   : 0.13.2
```

2. Data Preparation

- Reading the raw data in CSV format and renaming the columns
- Extracting labels (Diagnosis) from the features and mapping classes as "Malignant -> 1" and "Benign -> 0"
- Normalizing features using MinMaxScaler

In [5]:
```
# Column names taken from the "Variables Table" part of the dataset source
col_names = ['ID', 'Diagnosis',
             'radius1', 'texture1', 'perimeter1', 'area1', 'smoothness1', 'compactness1',
             'concavity1', 'concave_points1', 'symmetry1', 'fractal_dimension1',
             'radius2', 'texture2', 'perimeter2', 'area2', 'smoothness2', 'compactness2',
             'concavity2', 'concave_points2', 'symmetry2', 'fractal_dimension2',
             'radius3', 'texture3', 'perimeter3', 'area3', 'smoothness3', 'compactness3',
             'concavity3', 'concave_points3', 'symmetry3', 'fractal_dimension3']

data_df = pd.read_csv('data/wdbc.data', sep=',', names=col_names)
display_pruned_df(data_df)
```

Out[5]:

	ID	Diagnosis	radius1	texture1	...	concave_points3	symmetry3	fractal_dimension3
0	842302	M	17.99	10.38	...	0.2654	0.4601	0.1189
1	842517	M	20.57	17.77	...	0.186	0.275	0.08902
...	...	...	...	...	...	...	...	...
567	927241	M	20.6	29.33	...	0.265	0.4087	0.124
568	92751	B	7.76	24.54	...	0.0	0.2871	0.07039

569 rows x 32 columns

In [6]:
```
features = data_df.drop(['ID'], axis=1)
labels = features.pop('Diagnosis').map({'B': 0, 'M': 1})
```

In [7]:
```
scaler = MinMaxScaler()
features = pd.DataFrame(scaler.fit_transform(features), columns=col_names[2:])
display_pruned_df(features)
```

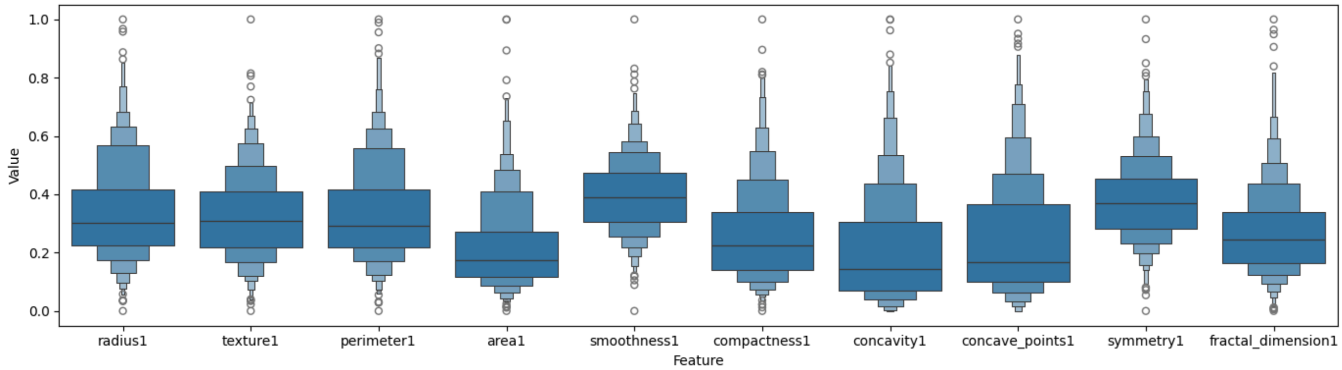
Out[7]:

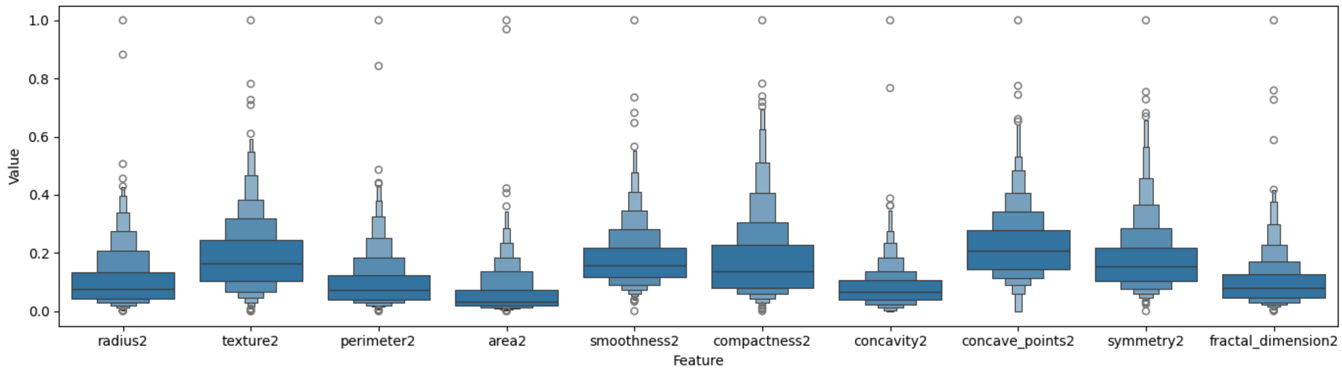
	radius1	texture1	perimeter1	area1	...	concave_points3	symmetry3	fractal_dimension3
0	0.521037	0.022658	0.545989	0.363733	...	0.912027	0.598462	0.418864
1	0.643144	0.272574	0.615783	0.501591	...	0.639175	0.23359	0.222878
...	...	...	...	...	...	...	...	...
567	0.644564	0.66351	0.665538	0.475716	...	0.910653	0.497142	0.452315
568	0.036869	0.501522	0.02854	0.015907	...	0.0	0.257441	0.100682

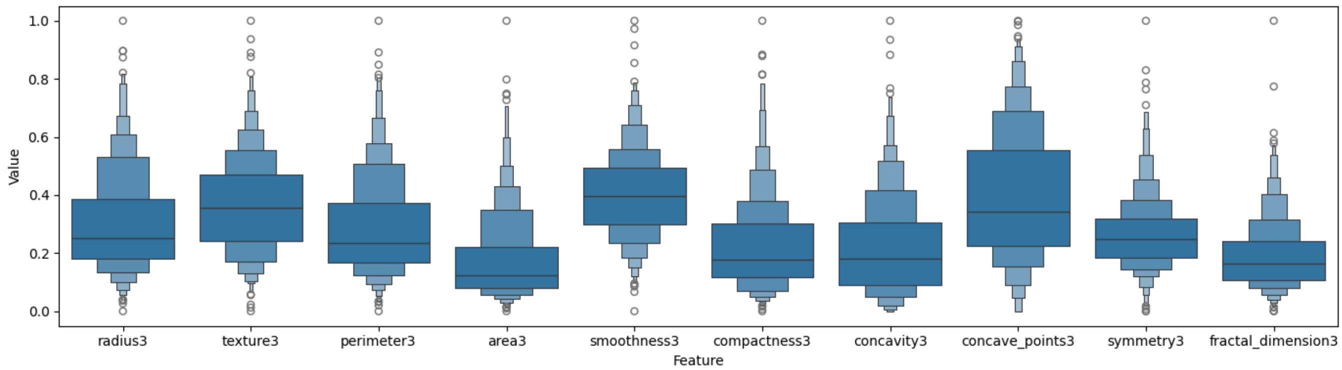
569 rows x 30 columns

3. Distribution of Features

In [8]:
```python
for i in range(3):
    f, ax = plt.subplots(figsize=(14, 4))
    subset = features.iloc[:, i*10:(i+1)*10].melt(var_name='Feature', value_name='Value')
    sns.boxenplot(data=subset, x='Feature', y='Value', ax=ax)
    plt.tight_layout()
    plt.show()
```







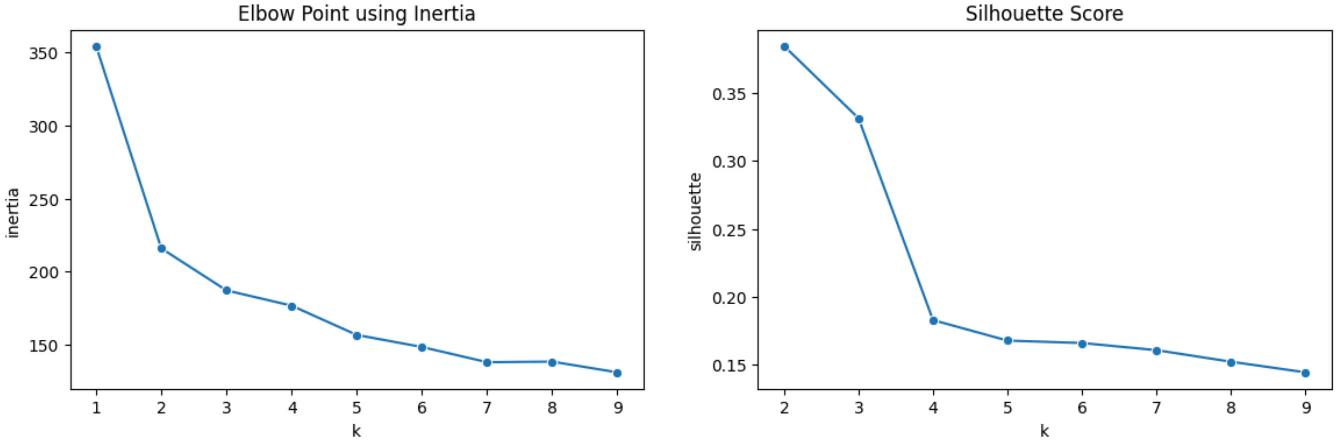
4. Determining the Number of Clusters

- The elbow point can be selected as `k=2`, since the change in inertia becomes less significant after that point.
- While determining the number of clusters, higher silhouette score is desired. So, `k=2` is once again the best choice.

- Therefore, we can safely assume that the number of clusters is 2.

In [9]:
```
f, (ax1, ax2) = plt.subplots(1, 2, figsize=(14, 4))

plot_elbow_method_with_k(ax1, features, k_start=1, k_end=9)
plot_silhouette_score_with_k(ax2, features, k_start=2, k_end=9)
```



5. Clustering and Evaluation

5.1. K-Means

- `k=2` was found as the number of clusters in the previous section, so we use it here as the parameter **n_clusters=2**.
- Using Adjusted Rand Index (ARI) as the evaluation metric (which ranges between 0 and 1) gives a decent result.

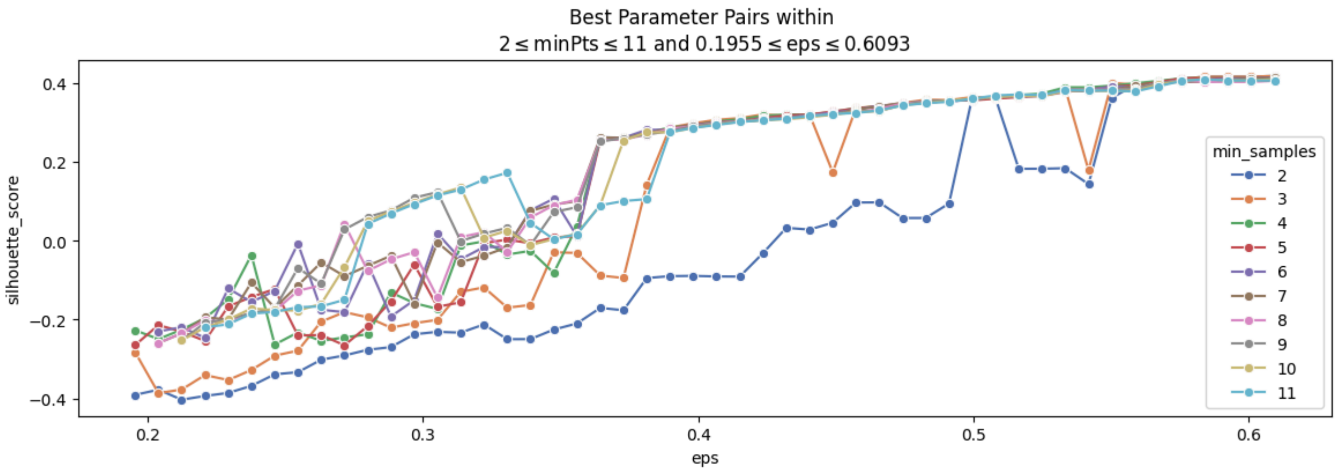
In [10]:
```
k_means = KMeans(n_clusters=2, random_state=0).fit(features)
k_means_ari_score = adjusted_rand_score(labels, k_means.labels_)
print(f'+ K-Means ARI Score: {k_means_ari_score:.6f}')
```

```
+ K-Means ARI Score: 0.730175
```

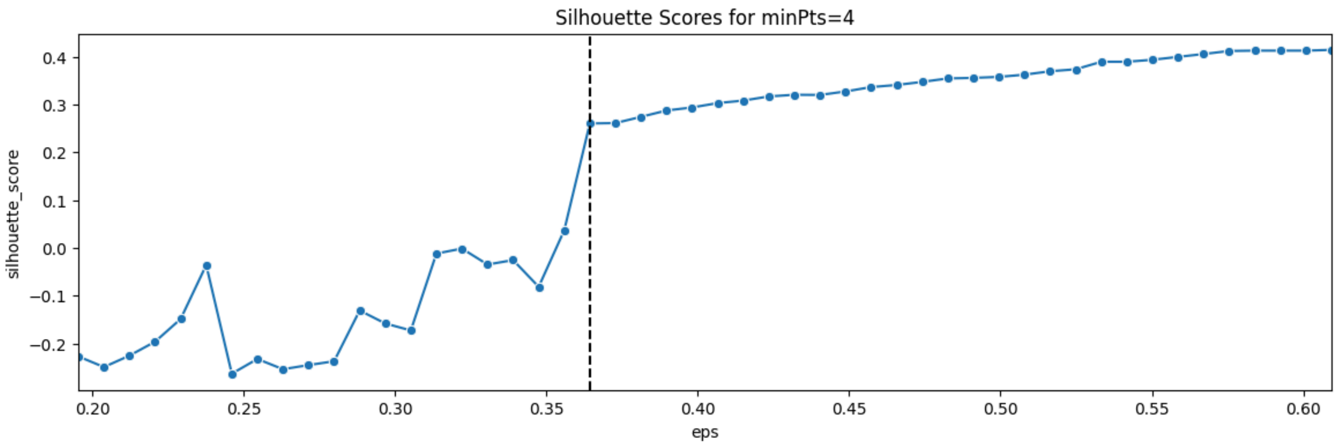
5.2. DBSCAN

- First, I have used the range `2 <= minPts <= 11` to find the optimal eps ranges using 10th and 95th percentile distances of Nearest Neighbor pairs.
- When evaluated with the Silhouette Score metric, the scores for `minPts=[2,3]` seems ill-behaved even after the potential knee-point. Therefore, I have decided to use `minPts=4` going forward.
- Furthermore, evaluating the DBSCAN labels against the ground truth using ARI metric yields a significantly worse score compared to the K-Means algorithm.

In [11]:
```
dbscan_params_df = find_optimal_dbscan_params(features, min_samples_range=(2, 11))
```



In [12]:
```python
min_samples = 4
eps = find_optimal_eps(dbscan_params_df, min_samples=min_samples, min_eps=0.34)
```



In [13]:
```python
dbscan = DBSCAN(min_samples=min_samples, eps=eps)
dbscan_labels = dbscan.fit_predict(features)
dbscan_ari_score = adjusted_rand_score(labels, dbscan_labels)
print(f'+ DBSCAN ARI Score: {dbscan_ari_score:.4f}')
```

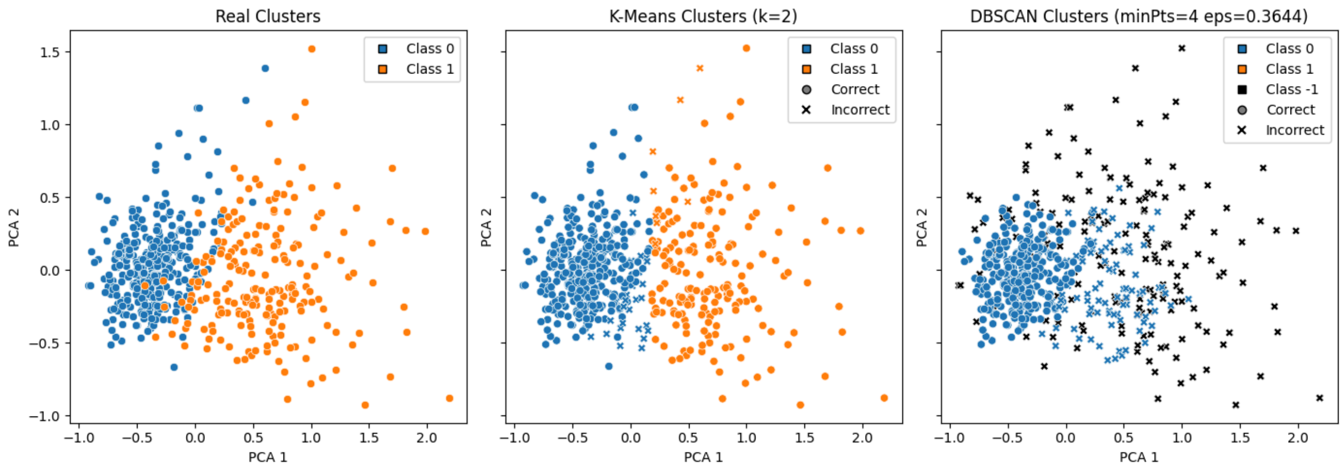
```
+ DBSCAN ARI Score: 0.2115
```

6. Visualisation on 2D Space

- To visualise the clusters on 2D, I have used PCA to get the two best components that represent the 30-dimensional space.

In [14]:
```python
f, (ax1, ax2, ax3) = plt.subplots(1, 3, sharey=True, figsize=(14, 5))

plot_on_pca(ax1, features, labels, title='Real Clusters')
plot_on_pca(ax2, features, labels, k_means.labels_, title='K-Means Clusters (k=2)')
plot_on_pca(ax3, features, labels, dbscan_labels, title=f'DBSCAN Clusters (minPts={min_samples} eps={eps
plt.tight_layout()
```



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