

Oblig2 - Lars Christer Molteberg

```
In [41]: # Imports
import pandas as pd
from sklearn.preprocessing import StandardScaler
import matplotlib.pyplot as plt
import numpy as np
from sklearn.impute import SimpleImputer
from sklearn.model_selection import train_test_split, cross_val_score, StratifiedKFold
from sklearn.tree import DecisionTreeClassifier
from sklearn.svm import SVC
from sklearn.pipeline import make_pipeline
from sklearn.metrics import accuracy_score, roc_curve, auc, fbeta_score, classification_report
import seaborn as sns
```

Exercise 1 - Data Preparation

1.1 - Load the dataset, inspect feature names and target distribution. Comment on dataset imbalance.

```
In [42]: df = pd.read_csv('data.csv')
# Finn ut hva som menes med Feature names og target distribution, boka maybe

# Feature names
print("Feature names:", list(df.columns))

# Target distribution
print(df['diagnosis'].value_counts())
print("\nFraction:\n", df['diagnosis'].value_counts(normalize=True))
```

```
Feature names: ['id', 'diagnosis', 'radius_mean', 'texture_mean', 'perimeter_mean',
 'area_mean', 'smoothness_mean', 'compactness_mean', 'concavity_mean', 'concave points_mean', 'symmetry_mean', 'fractal_dimension_mean', 'radius_se', 'texture_se',
 'perimeter_se', 'area_se', 'smoothness_se', 'compactness_se', 'concavity_se', 'concave points_se', 'symmetry_se', 'fractal_dimension_se', 'radius_worst', 'texture_worst', 'perimeter_worst', 'area_worst', 'smoothness_worst', 'compactness_worst', 'concavity_worst', 'concave points_worst', 'symmetry_worst', 'fractal_dimension_worst']
diagnosis
B      357
M      212
Name: count, dtype: int64
```

```
Fraction:
diagnosis
B      0.627417
M      0.372583
Name: proportion, dtype: float64
```

The dataset is a bit unbalanced, as it does have more benign than malicious data, but I think the amount of malicious data is enough. If I am unlucky the random splits might turn out with too few malicious but it should be enough.

1.2 - Analyze all features with and without standardization (i.e., zero mean and unit variance). Plot the feature analysis with and without standardization and decide which version is more suitable.

```
In [43]: # Drop id and diagnosis to get features, these are not numerical
X = df.drop(columns=["id", "diagnosis"], errors="ignore")

# Standardize features
scaler = StandardScaler()
X_scaled = pd.DataFrame(scaler.fit_transform(X), columns=X.columns, index=X.index)

# Describe statistics before and after
print("No Standardization\n", X.describe().T[['mean', 'std']])
print("\nStandardization:\n", X_scaled.describe().T[['mean', 'std']])

# Plot boxplots for all features
plt.figure(figsize=(14,6))

plt.subplot(1,2,1)
X.boxplot()
plt.title("Features without standardization")
plt.xticks(rotation=90)

plt.subplot(1,2,2)
X_scaled.boxplot()
plt.title("Features with standardization")
plt.xticks(rotation=90)

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

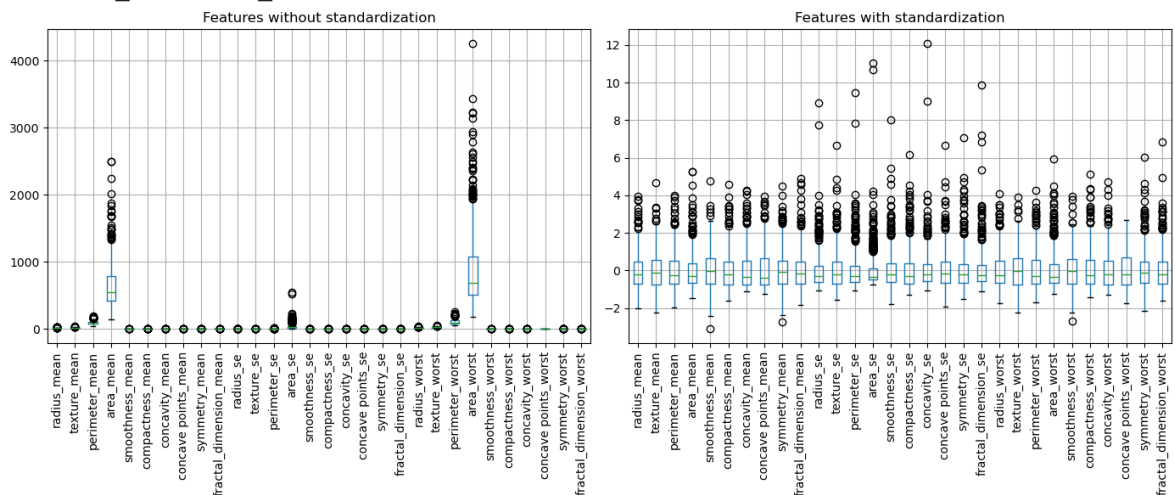
No Standardization

	mean	std
radius_mean	14.127292	3.524049
texture_mean	19.289649	4.301036
perimeter_mean	91.969033	24.298981
area_mean	654.889104	351.914129
smoothness_mean	0.096360	0.014064
compactness_mean	0.104341	0.052813
concavity_mean	0.088799	0.079720
concave points_mean	0.048919	0.038803
symmetry_mean	0.181162	0.027414
fractal_dimension_mean	0.062798	0.007060
radius_se	0.405172	0.277313
texture_se	1.216853	0.551648
perimeter_se	2.866059	2.021855
area_se	40.337079	45.491006
smoothness_se	0.007041	0.003003
compactness_se	0.025478	0.017908
concavity_se	0.031894	0.030186
concave points_se	0.011796	0.006170
symmetry_se	0.020542	0.008266
fractal_dimension_se	0.003795	0.002646
radius_worst	16.269190	4.833242
texture_worst	25.677223	6.146258
perimeter_worst	107.261213	33.602542
area_worst	880.583128	569.356993
smoothness_worst	0.132369	0.022832
compactness_worst	0.254265	0.157336
concavity_worst	0.272188	0.208624
concave points_worst	0.114606	0.065732
symmetry_worst	0.290076	0.061867
fractal_dimension_worst	0.083946	0.018061

Standardization:

	mean	std
radius_mean	-1.373633e-16	1.00088
texture_mean	6.868164e-17	1.00088
perimeter_mean	-1.248757e-16	1.00088
area_mean	-2.185325e-16	1.00088
smoothness_mean	-8.366672e-16	1.00088
compactness_mean	1.873136e-16	1.00088
concavity_mean	4.995028e-17	1.00088
concave points_mean	-4.995028e-17	1.00088
symmetry_mean	1.748260e-16	1.00088
fractal_dimension_mean	4.745277e-16	1.00088
radius_se	2.372638e-16	1.00088
texture_se	-1.123881e-16	1.00088
perimeter_se	-1.123881e-16	1.00088
area_se	-1.311195e-16	1.00088
smoothness_se	-1.529727e-16	1.00088
compactness_se	1.748260e-16	1.00088
concavity_se	1.623384e-16	1.00088
concave points_se	0.000000e+00	1.00088
symmetry_se	8.741299e-17	1.00088
fractal_dimension_se	-6.243785e-18	1.00088
radius_worst	-8.241796e-16	1.00088
texture_worst	1.248757e-17	1.00088
perimeter_worst	-3.746271e-16	1.00088
area_worst	0.000000e+00	1.00088
smoothness_worst	-2.372638e-16	1.00088

compactness_worst	-3.371644e-16	1.00088
concavity_worst	7.492542e-17	1.00088
concave points_worst	2.247763e-16	1.00088
symmetry_worst	2.622390e-16	1.00088
fractal_dimension_worst	-5.744282e-16	1.00088



Looking at the plots it seems like it is best to use the standardized one, as the left plot shows that there are huge differences in scaling, where some values are in the thousands, and others are barely over zero. Using the standardized one means the scales are more comparable and therefore not having some values dominate the models. And the aesthetics of the right boxplot looks right to use.

1.3 - Comment on importance of three way split with respect to hyperparameter search and robustness of any learned model.

The three way split is important in regards to hyperparameters as we don't use the test set to cheat the hyperparameters to fit the test set. For robustness it's good because it keeps the test set separate from the hyperparameter search, and thus we don't risk fitting the hyperparameters to the test data, but rather use the test data to see how the hyperparameters work on new data.

Exercise 2 - Decision Trees

Splits

DO NOT TOUCH

(After closer reconsideration, it turns out the random state makes sure the splits are the same, this was made to make sure it was the same, woops. Keeping this now so I don't have to split anymore I guess.)

```
In [44]: # Features and target
X = df.drop(columns=["id", "diagnosis"], errors="ignore")
y = df["diagnosis"].map({"M": 1, "B": 0})

# Split into 60% train, 20% val, 20% test
```

```

X_train, X_temp, y_train, y_temp = train_test_split(
    X, y, test_size=0.4, stratify=y, random_state=42
)
X_val, X_test, y_val, y_test = train_test_split(
    X_temp, y_temp, test_size=0.5, stratify=y_temp, random_state=42
)

print("Train:", X_train.shape)
print("Validation:", X_val.shape)
print("Test:", X_test.shape)

```

Train: (341, 30)
 Validation: (114, 30)
 Test: (114, 30)

2.1 - Train a Decision Tree classifier using default parameters. Evaluate it on validation sets from original splits (report accuracy mean and std).

```

In [45]: # Only training set
# Modell with default parameters
clf = DecisionTreeClassifier(random_state=42)

# 5-fold cross-validation on training set
cv_scores = cross_val_score(clf, X_train, y_train, cv=5, scoring="accuracy")

print("Cross Validation Accuracy mean:", np.mean(cv_scores))
print("Cross Validation Accuracy std: ", np.std(cv_scores))

decison_tree_train_result = cv_scores

```

Cross Validation Accuracy mean: 0.9238704177323104
 Cross Validation Accuracy std: 0.040627367474774134

```

In [46]: # Validation set
clf.fit(X_train, y_train)
val_score = clf.score(X_val, y_val)
print("Validation Accuracy:", val_score)

```

Validation Accuracy: 0.9385964912280702

Validation set better accuracy than cross validation mean

2.2 - From the trained model, comment on feature importance values and identify the top 3 features from your model.

```

In [47]: # Get important features from the trained model, all features, and sorting them
importances = clf.feature_importances_
feature_names = X.columns
feature_importances = pd.Series(importances, index=feature_names).sort_values(ascending=False)
print("Feature importances:\n", feature_importances)

```

```

Feature importances:
  perimeter_worst      0.704881
concave points_worst  0.136016
texture_worst         0.038957
smoothness_worst     0.032706
fractal_dimension_se  0.028150
area_se              0.019922
symmetry_mean        0.010456
radius_mean          0.009410
radius_worst         0.009410
area_worst           0.008365
smoothness_se        0.001726
area_mean            0.000000
perimeter_mean       0.000000
texture_mean         0.000000
perimeter_se         0.000000
texture_se           0.000000
radius_se            0.000000
fractal_dimension_mean 0.000000
concavity_mean       0.000000
concave points_mean  0.000000
smoothness_mean      0.000000
compactness_mean     0.000000
symmetry_se          0.000000
compactness_se       0.000000
concavity_se         0.000000
concave points_se    0.000000
compactness_worst    0.000000
concavity_worst      0.000000
symmetry_worst       0.000000
fractal_dimension_worst 0.000000
dtype: float64

```

The model places high importance perimeter_worst, a little important on concave points_worst. It also places absolutely no importance at all on about 20 features. To me, this feels a little weird but perimeter_worst might just be a good classifier between malicious and benign. It might also be a case of overfitting when it relies that much on one value.

2.3 - Vary the max depth parameter (e.g., depth 2-10). Use validation accuracy (mean \pm std from cross-validation on the training set) to choose the best depth. Provide performance for each chosen depth (at-least 5 to be reported) and discuss the aspects of overfitting vs. underfitting.

```

In [48]: # Varying max depth from 2 to 10
depths = range(2, 11)

for d in depths:
    clf = DecisionTreeClassifier(max_depth=d, random_state=42)
    cv_scores = cross_val_score(clf, X_train, y_train, cv=5, scoring="accuracy")
    print(f"Max Depth: {d}, CV Accuracy mean: {np.mean(cv_scores):.4f}, std: {np

```

Max Depth: 2, CV Accuracy mean: 0.9298, std: 0.0309
 Max Depth: 3, CV Accuracy mean: 0.9355, std: 0.0236
 Max Depth: 4, CV Accuracy mean: 0.9326, std: 0.0343
 Max Depth: 5, CV Accuracy mean: 0.9298, std: 0.0309
 Max Depth: 6, CV Accuracy mean: 0.9298, std: 0.0395
 Max Depth: 7, CV Accuracy mean: 0.9239, std: 0.0280
 Max Depth: 8, CV Accuracy mean: 0.9239, std: 0.0406
 Max Depth: 9, CV Accuracy mean: 0.9239, std: 0.0406
 Max Depth: 10, CV Accuracy mean: 0.9239, std: 0.0406

The accuracy is about the same, although Depth=3 does have the highest mean as well as the lowest std. The variance does increase whilst mean starts to decrease from max depth 6 and onwards, except for std on 7, this might be a sign of overfitting. The accuracy and std is worse on max depth 2 than 3, this could be some underfitting. The first CV training was also worse than depth 2

```
In [49]: # Max depth 3 on validation set
clf = DecisionTreeClassifier(max_depth=3, random_state=42)
clf.fit(X_train, y_train)
val_score_dt = clf.score(X_val, y_val)
print("Validation Accuracy with max depth 3:", val_score_dt)

best_decision_tree_results = {
    "max_depth": 3,
    "val_acc": val_score_dt
}
```

Validation Accuracy with max depth 3: 0.9385964912280702

Max depth 3 does get higher accuracy

2.4 - Repeat previous exercise with different min samples leaf values. Which setting generalizes best according to the validation set?

```
In [50]: # For Loops for min_samples_leaf from 1 to 20, both mean, std, and validation ac
leaf_sizes = range(1, 21)
for leaf_size in leaf_sizes:
    clf = DecisionTreeClassifier(min_samples_leaf=leaf_size, random_state=42)
    clf.fit(X_train, y_train)
    cv_scores = cross_val_score(clf, X_train, y_train, cv=5, scoring="accuracy")
    print(f"Cross Validation Accuracy mean with min_samples_leaf {leaf_size}:")
    print(f"Cross Validation Accuracy std with min_samples_leaf {leaf_size}:")
    val_score = clf.score(X_val, y_val)
    print(f"Validation Accuracy with min_samples_leaf {leaf_size}:")
```

Cross Validation Accuracy mean with min_samples_leaf	1: 0.92387 mean
Cross Validation Accuracy std with min_samples_leaf	1: 0.04063 std
Validation Accuracy with min_samples_leaf	1: 0.9386 val
Cross Validation Accuracy mean with min_samples_leaf	2: 0.93261 mean
Cross Validation Accuracy std with min_samples_leaf	2: 0.03151 std
Validation Accuracy with min_samples_leaf	2: 0.9386 val
Cross Validation Accuracy mean with min_samples_leaf	3: 0.93261 mean
Cross Validation Accuracy std with min_samples_leaf	3: 0.02709 std
Validation Accuracy with min_samples_leaf	3: 0.92105 val
Cross Validation Accuracy mean with min_samples_leaf	4: 0.92664 mean
Cross Validation Accuracy std with min_samples_leaf	4: 0.02471 std
Validation Accuracy with min_samples_leaf	4: 0.92105 val
Cross Validation Accuracy mean with min_samples_leaf	5: 0.92084 mean
Cross Validation Accuracy std with min_samples_leaf	5: 0.02381 std
Validation Accuracy with min_samples_leaf	5: 0.91228 val
Cross Validation Accuracy mean with min_samples_leaf	6: 0.91799 mean
Cross Validation Accuracy std with min_samples_leaf	6: 0.02989 std
Validation Accuracy with min_samples_leaf	6: 0.91228 val
Cross Validation Accuracy mean with min_samples_leaf	7: 0.91211 mean
Cross Validation Accuracy std with min_samples_leaf	7: 0.02755 std
Validation Accuracy with min_samples_leaf	7: 0.92982 val
Cross Validation Accuracy mean with min_samples_leaf	8: 0.92093 mean
Cross Validation Accuracy std with min_samples_leaf	8: 0.02514 std
Validation Accuracy with min_samples_leaf	8: 0.92982 val
Cross Validation Accuracy mean with min_samples_leaf	9: 0.92387 mean
Cross Validation Accuracy std with min_samples_leaf	9: 0.02953 std
Validation Accuracy with min_samples_leaf	9: 0.92982 val
Cross Validation Accuracy mean with min_samples_leaf	10: 0.92387 mean
Cross Validation Accuracy std with min_samples_leaf	10: 0.02953 std
Validation Accuracy with min_samples_leaf	10: 0.92982 val
Cross Validation Accuracy mean with min_samples_leaf	11: 0.92387 mean
Cross Validation Accuracy std with min_samples_leaf	11: 0.02803 std
Validation Accuracy with min_samples_leaf	11: 0.92982 val
Cross Validation Accuracy mean with min_samples_leaf	12: 0.92093 mean
Cross Validation Accuracy std with min_samples_leaf	12: 0.02986 std
Validation Accuracy with min_samples_leaf	12: 0.92982 val
Cross Validation Accuracy mean with min_samples_leaf	13: 0.91211 mean
Cross Validation Accuracy std with min_samples_leaf	13: 0.02421 std
Validation Accuracy with min_samples_leaf	13: 0.92982 val
Cross Validation Accuracy mean with min_samples_leaf	14: 0.90921 mean
Cross Validation Accuracy std with min_samples_leaf	14: 0.02797 std
Validation Accuracy with min_samples_leaf	14: 0.92982 val
Cross Validation Accuracy mean with min_samples_leaf	15: 0.90627 mean
Cross Validation Accuracy std with min_samples_leaf	15: 0.02831 std
Validation Accuracy with min_samples_leaf	15: 0.92982 val

Cross Validation Accuracy mean with min_samples_leaf	16: 0.90332 mean
Cross Validation Accuracy std with min_samples_leaf	16: 0.02835 std
Validation Accuracy with min_samples_leaf	16: 0.92982 val
Cross Validation Accuracy mean with min_samples_leaf	17: 0.90332 mean
Cross Validation Accuracy std with min_samples_leaf	17: 0.02835 std
Validation Accuracy with min_samples_leaf	17: 0.92982 val
Cross Validation Accuracy mean with min_samples_leaf	18: 0.89744 mean
Cross Validation Accuracy std with min_samples_leaf	18: 0.03188 std
Validation Accuracy with min_samples_leaf	18: 0.92982 val
Cross Validation Accuracy mean with min_samples_leaf	19: 0.89744 mean
Cross Validation Accuracy std with min_samples_leaf	19: 0.03188 std
Validation Accuracy with min_samples_leaf	19: 0.9386 val
Cross Validation Accuracy mean with min_samples_leaf	20: 0.89744 mean
Cross Validation Accuracy std with min_samples_leaf	20: 0.03188 std
Validation Accuracy with min_samples_leaf	20: 0.9386 val

For min_samples_leaf 1, 2, 19, 20 gave the same accuracy on the validation set. Low number of leaf samples might have high variance and therefore overfit, whilst the the (longer,deeper?) tree might have to high bias and underfit. Also interesting is the mean from the training splits keep getting worse the more min samples gets added.

These min samples gives the same result as the best max depth setting.

As a summary, decision tree gives the same validation accuracy regardless of settings, be it max depth or min sample leaves or default settings.

Exercise 3: Support Vector MACHines (SVM)

3.1 - Train a linear SVM (kernel="linear") and evaluate on validation sets (use the original 5 splits that was created in previous exercise). Report accuracy mean, std and plot the ROC for each split.

```
In [51]: # Trains a linear SVM (kernel="linear") and evaluate on validation sets (use the
svm_clf = make_pipeline(StandardScaler(), SVC(kernel="linear", random_state=42,
cv_scores_svm_linear = cross_val_score(svm_clf, X_train, y_train, cv=5, scoring=

print("SVM Cross Validation Accuracy mean:", np.round(np.mean(cv_scores_svm_line
print("SVM Cross Validation Accuracy std:", np.round(np.std(cv_scores_svm_linear

skf = StratifiedKFold(n_splits=5, shuffle=False)
plt.figure(figsize=(8,6))
for i, (tr_idx, va_idx) in enumerate(skf.split(X_train, y_train), start=1):
    X_tr, X_va = X_train.iloc[tr_idx], X_train.iloc[va_idx]
    y_tr, y_va = y_train.iloc[tr_idx], y_train.iloc[va_idx]
    svm_clf.fit(X_tr, y_tr)
    y_proba = svm_clf.predict_proba(X_va)[: , 1]
    fpr, tpr, _ = roc_curve(y_va, y_proba)
```

```

roc_auc = auc(fpr, tpr)
plt.plot(fpr, tpr, label=f'Fold {i} (AUC = {roc_auc:.2f})')

plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('ROC Curve for SVM Classifier')
plt.legend()
plt.show()

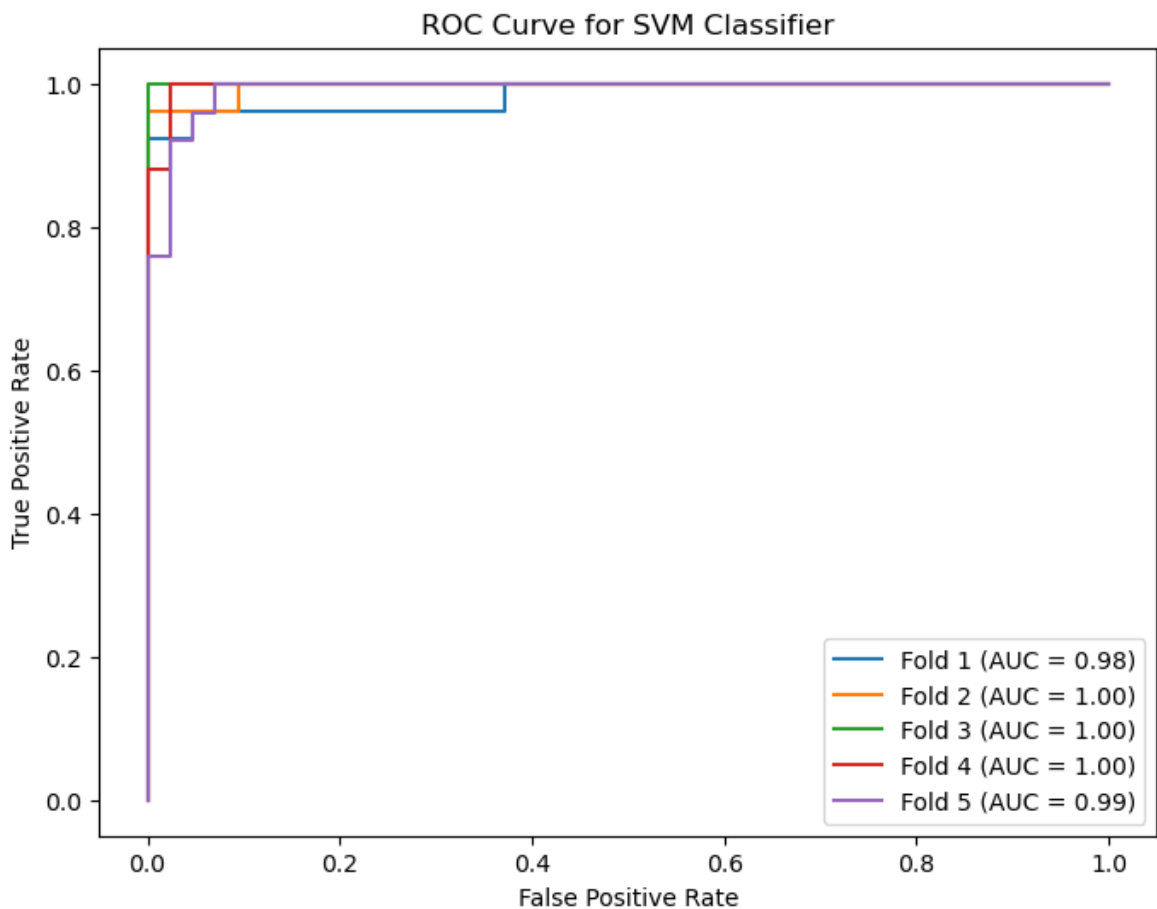
svm_clf.fit(X_train, y_train)
val_score_svm_linear = svm_clf.score(X_val, y_val)
print("SVM kernel=linear Validation Accuracy:", np.round(val_score_svm_linear, 5))

# Best results for linear is this one, so values saved for comparison

```

SVM Cross Validation Accuracy mean: 0.96483 mean

SVM Cross Validation Accuracy std: 0.01492 std



SVM kernel=linear Validation Accuracy: 0.96491 val

ROC shows how good the model separates by class. False positive rate - how many benign being classified as malignant here, false as true True positive rate - Malignant being classified as malignant, true as true

3.2 - Train an Radial Basis Function (RBF) kernel SVM.
Compare its performance to the linear kernel using validation accuracy. Plot ROC for these models.

```

In [52]: # Train same splits on RBF model
svm_rbf_clf = make_pipeline(StandardScaler(), SVC(kernel="rbf", gamma="scale", r
rbf_cv = cross_val_score(svm_rbf_clf, X_train, y_train, cv=5, scoring="accuracy")

```

```

print("RBF SVM Cross Validation Accuracy mean:", np.round(np.mean(rbf_cv), 5), "
print("RBF SVM Cross Validation Accuracy std:", np.round(np.std(rbf_cv), 5), "st

# ROC on validation set
y_proba_rbf = svm_rbf_clf.fit(X_train, y_train).predict_proba(X_val)[: , 1]
fpr_rbf, tpr_rbf, _ = roc_curve(y_val, y_proba_rbf)
roc_auc_rbf = auc(fpr_rbf, tpr_rbf)

plt.figure(figsize=(8,6))
plt.plot(fpr_rbf, tpr_rbf, label=f'RBF SVM (AUC = {roc_auc_rbf:.2f})')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('ROC Curve for RBF SVM Classifier')
plt.legend()
plt.show()

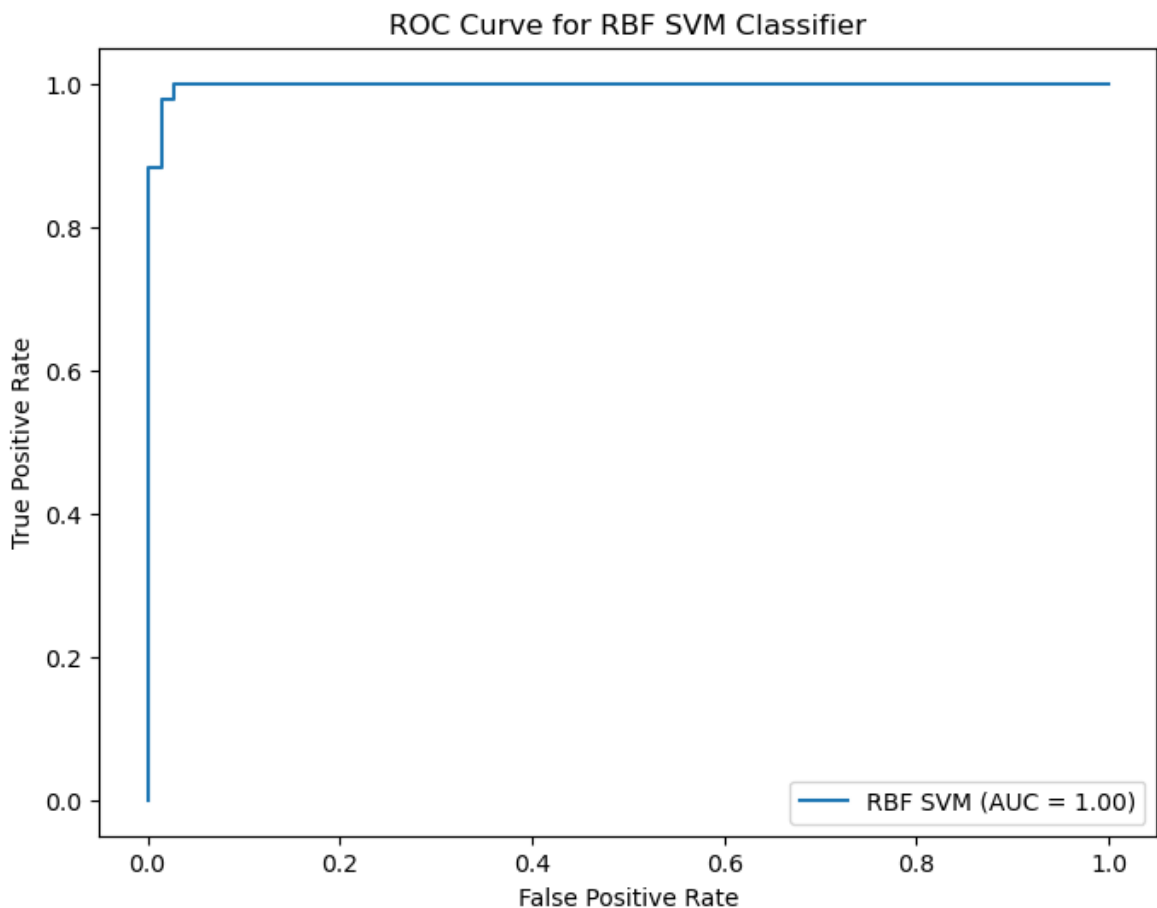
# Saving best fold results for comparison
best_rbf_fold_idx = int(np.argmax(rbf_cv))
best_rbf_fold_score = rbf_cv[best_rbf_fold_idx]

rbf_results_trainingset = {
    "cv_scores": rbf_cv,
    "cv_mean": rbf_cv.mean(),
    "cv_std": rbf_cv.std(),
    "best_fold": best_rbf_fold_idx + 1,
    "best_fold_acc": best_rbf_fold_score,
    "roc_auc": roc_auc_rbf
}

# Pointy curves cause few data??

```

RBF SVM Cross Validation Accuracy mean: 0.96475 mean
RBF SVM Cross Validation Accuracy std: 0.01506 std



Comparing the validation accuracy between these two models we get:

- SVM kernel=linear Validation Accuracy: 0.96491
- RBF SVM Cross Validation Accuracy mean: 0.96475

Currently the SVM with linear kernel is 0.0002 ahead, or 0.02%, which is basically no difference in this dataset, considering the size of the set

3.3 - Experiment with different values of C (regularization strength). Use the validation set to select the best C. Report results as a plot of accuracy vs. C

```
In [53]: Cs = [0.001, 0.01, 0.1, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 15, 50, 100, 500, 1000]

# Pipelines for linear and RBF
def make_lin(C): return make_pipeline(StandardScaler(), SVC(kernel="linear", C=C))
def make_rbf(C): return make_pipeline(StandardScaler(), SVC(kernel="rbf", C=C))

lin_val_acc = []
rbf_val_acc = []

# Train on training set, evaluate on validation set for each C
for C in Cs:
    lin = make_lin(C)
    rbf = make_rbf(C)

    lin.fit(X_train, y_train)
    rbf.fit(X_train, y_train)

    lin_val_acc.append(lin.score(X_val, y_val))
    rbf_val_acc.append(rbf.score(X_val, y_val))

# Plot accuracy vs C for both models
plt.figure(figsize=(7,5))
plt.plot(Cs, lin_val_acc, marker='o', label='Linear SVM')
plt.plot(Cs, rbf_val_acc, marker='o', label='RBF SVM')
plt.xscale('log')
plt.xlabel('C (log-scale)')
plt.ylabel('Validation accuracy')
plt.title('Validation accuracy vs. C (Linear vs. RBF SVM)')
plt.legend()
plt.grid(True, which='both', linestyle='--', alpha=0.5)
plt.show()

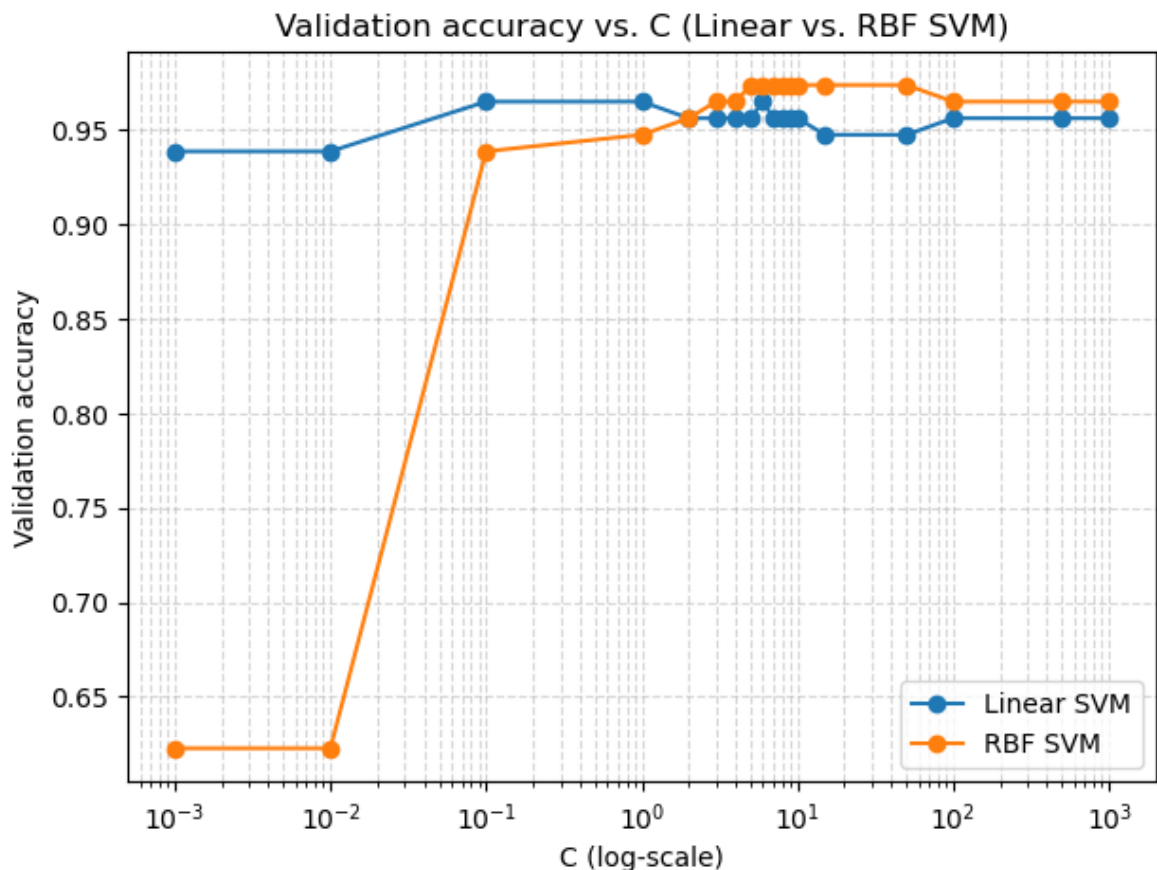
# Best C and accuracy for both models
best_lin_idx = int(np.argmax(lin_val_acc))
best_rbf_idx = int(np.argmax(rbf_val_acc))

print(f"Best Linear SVM: C={Cs[best_lin_idx]} | Val acc={lin_val_acc[best_lin_idx]}")
print(f"Best RBF SVM: C={Cs[best_rbf_idx]} | Val acc={rbf_val_acc[best_rbf_idx]}")

# Save for comparisons
best_rbf_idx = int(np.argmax(rbf_val_acc))

best_rbf_results = {
    "C": Cs[best_rbf_idx],
    "val_acc": rbf_val_acc[best_rbf_idx]}
```

```
}
```



Best Linear SVM: C=0.1 | Val acc=0.9649

Best RBF SVM: C=5 | Val acc=0.9737

C strength is how much the SVM tries to separate classes. Low C means it allows more mistakes during training and can give better generalization, also might underfit. High C is more strict when classifying during training, also risks overfitting.

3.4 - Experiment with different γ values for the RBF kernel. Discuss the effect on bias-variance trade-off for all experimented values. Select the best γ using the validation set and report the performance on validation set.

```
In [54]: C_fixed = 5 # C from previous experiment

# Gamma values to test
gammas = [0.001, 0.003, 0.006, 0.009, 0.01, 0.02, 0.03, 0.1, 0.3, 1, 3, 10]

val_accs = []
for g in gammas:
    rbf = make_pipeline(StandardScaler(),
                        SVC(kernel="rbf", C=C_fixed, gamma=g, probability=True),
    rbf.fit(X_train, y_train)
    val_accs.append(rbf.score(X_val, y_val))

# Select best gamma
best_idx = int(np.argmax(val_accs))
best_gamma = gammas[best_idx]
best_val_acc = val_accs[best_idx]
```

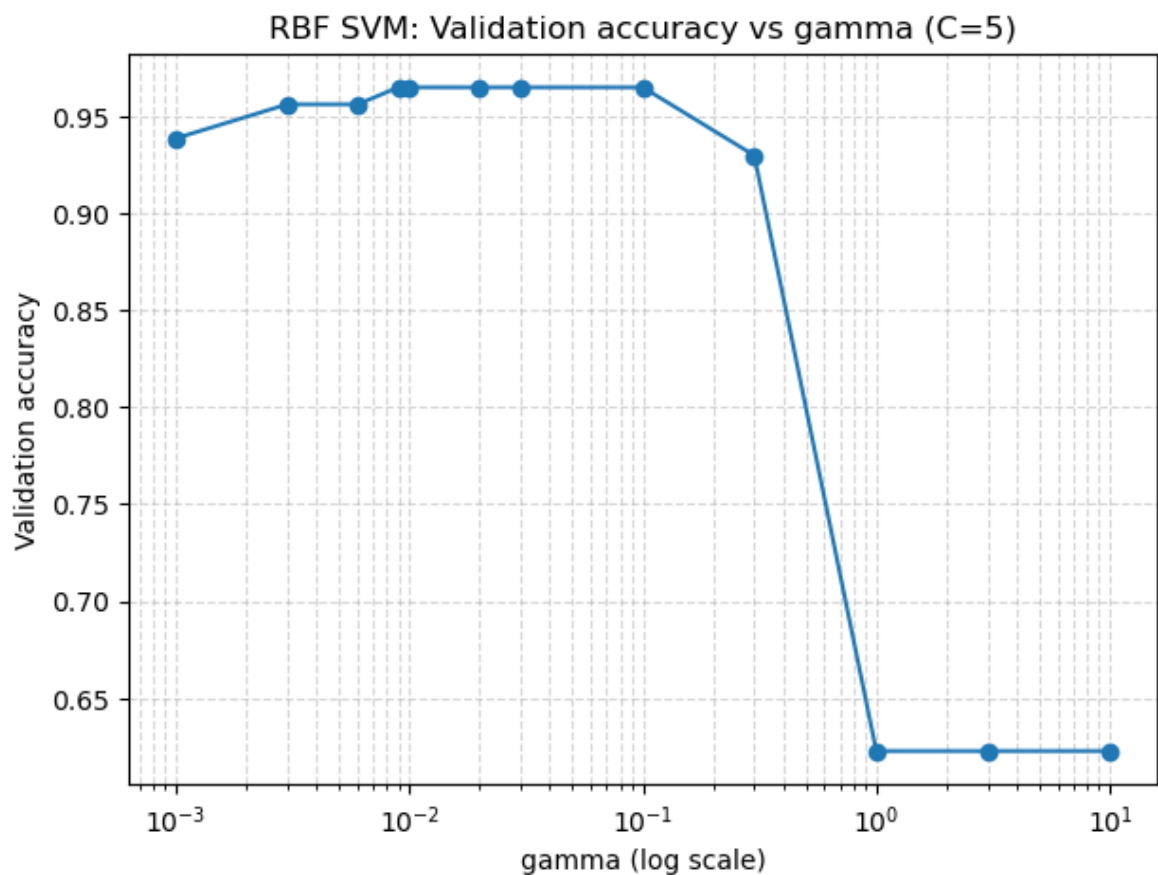
```

print("Gammas:", gammas)
print("Validation accuracies:", [round(a, 4) for a in val_accs])
print(f"Best gamma: {best_gamma} | Validation accuracy: {best_val_acc:.4f}")

plt.figure(figsize=(7,5))
plt.plot(gammas, val_accs, marker='o')
plt.xscale('log')
plt.xlabel('gamma (log scale)')
plt.ylabel('Validation accuracy')
plt.title(f'RBF SVM: Validation accuracy vs gamma (C={C_fixed})')
plt.grid(True, which='both', linestyle='--', alpha=0.5)
plt.show()

```

Gammas: [0.001, 0.003, 0.006, 0.009, 0.01, 0.02, 0.03, 0.1, 0.3, 1, 3, 10]
 Validation accuracies: [0.9386, 0.9561, 0.9561, 0.9649, 0.9649, 0.9649, 0.9649, 0.9649, 0.9298, 0.6228, 0.6228, 0.6228]
 Best gamma: 0.009 | Validation accuracy: 0.9649



Exercise - 4: Model Comparison

4.1 - Compare Decision Tree and SVM results from the training set (cross-validation mean \pm std) and validation set. Plot the performance comparison plots (e.g., scatter plots, ROC curves). Which model generalizes better?

```

In [55]: # Training result decision tree
decision_tree_train_result
# Best decision tree results for comparison
best_decision_tree_results

# Linear SVM results for comparison

```

```

np.mean(cv_scores_svm_linear)
np.std(cv_scores_svm_linear)
val_score_svm_linear

# Best RBF training set results for comparison
rbf_results_trainingset
# RBF SVM results for comparison
best_rbf_results

```

Out[55]: {'C': 5, 'val_acc': 0.9736842105263158}

```

In [56]: # Summary table for all models, easy reading
results = pd.DataFrame({
    "Model": ["Decision Tree", "SVM (Linear)", "SVM (RBF)"],
    "CV Mean": [
        np.mean(decison_tree_train_result),
        np.mean(cv_scores_svm_linear),
        rbf_results_trainingset["cv_mean"]
    ],
    "CV Std": [
        np.std(decison_tree_train_result),
        np.std(cv_scores_svm_linear),
        rbf_results_trainingset["cv_std"]
    ],
    "Validation Accuracy": [
        best_decision_tree_results["val_acc"],
        val_score_svm_linear,
        best_rbf_results["val_acc"]
    ]
})

print(results)

```

	Model	CV Mean	CV Std	Validation Accuracy
0	Decision Tree	0.923870	0.040627	0.938596
1	SVM (Linear)	0.964834	0.014924	0.964912
2	SVM (RBF)	0.964749	0.015056	0.973684

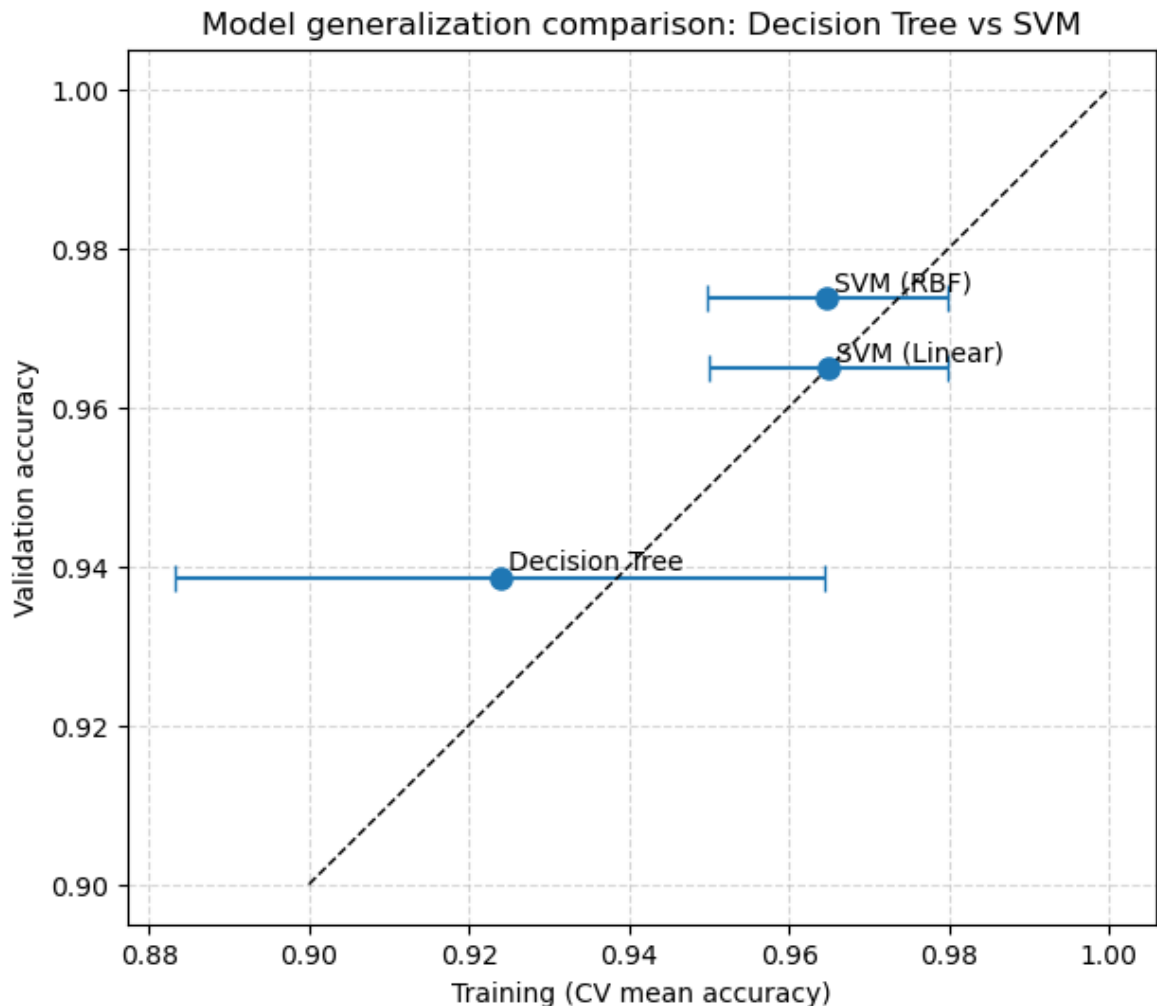
```

In [57]: plt.figure(figsize=(7,6))
plt.errorbar(results["CV Mean"], results["Validation Accuracy"],
             xerr=results["CV Std"], fmt='o', capsize=5, markersize=8)

for i, row in results.iterrows():
    plt.text(row["CV Mean"]+0.001, row["Validation Accuracy"]+0.001,
            row["Model"], fontsize=10)

# Perfect generalization line
plt.plot([0.9, 1.0], [0.9, 1.0], 'k--', lw=1)
plt.xlabel("Training (CV mean accuracy)")
plt.ylabel("Validation accuracy")
plt.title("Model generalization comparison: Decision Tree vs SVM")
plt.grid(True, linestyle="--", alpha=0.5)
plt.show()

```



The decision tree has a bit lower accuracy for both validation and training than the SVM variants. The decision tree also has higher variance and these characteristics tell me that the decision tree is worse for this task than the SVM variants. To my understanding the SVM RBF variant has a slight tendency to overfits as the point is above the diagonal. The SVM linear variant is bang on the line but the validation accuracy is a bit lower. Both their variance is about the same. Even though the RBF kernel is not directly on the diagonal, it is close enough to say it is robust enough and generalizes best because of the increased accuracy.

4.2 - Discuss the trade-off between usability and accuracy for this dataset. Which model would you recommend for a medical decision-support system, and why? (Hint - Make use of F_β score analysis)

```
In [58]: # Predictions for each model
y_pred_dt = clf.predict(X_val)           # Decision Tree
y_pred_svm = svm_clf.predict(X_val)      # Linear SVM
y_pred_rbf = svm_rbf_clf.predict(X_val)  # RBF SVM

# F0.5 (β=0.5), F1 (β=1), F2 (β=2) and F3 (β=3) scores
for name, y_pred in [
    ("Decision Tree", y_pred_dt),
    ("SVM (Linear)", y_pred_svm),
    ("SVM (RBF)", y_pred_rbf)]
```



```
]:
    f0_5 = fbeta_score(y_val, y_pred, beta=0.5)
    f1 = fbeta_score(y_val, y_pred, beta=1)
    f2 = fbeta_score(y_val, y_pred, beta=2)
    f3 = fbeta_score(y_val, y_pred, beta=3)
    print(f"{name:15s} | F0.5 = {f0_5:.4f} | F1 = {f1:.4f} | F2 = {f2:.4f} | F3 = {f3:.4f}")
```

Decision Tree	F0.5 = 0.9242	F1 = 0.9176	F2 = 0.9112	F3 = 0.9091
SVM (Linear)	F0.5 = 0.9799	F1 = 0.9512	F2 = 0.9242	F3 = 0.9155
SVM (RBF)	F0.5 = 0.9686	F1 = 0.9250	F2 = 0.8852	F3 = 0.8726

Considering this data is from detecting breast cancer, accuracy is very important so we can get all cases and also not misclassify. F1 shows how balanced the model is, between precision and recall. F2 emphasises recall more, meaning its better at picking up false negative, i.e diagnosing someone with cancer as not having it, which is very dangerous. Since the linear scores better for both metric, this seems like the obvious choice.

4.3 - Use GridSearchCV with the training set to tune hyperparameters for both Decision Trees and SVMs. Confirm your final choice with the validation set. Summarize the best settings and provide relevant performance plots

```
In [59]: cv5 = StratifiedKFold(n_splits=5, shuffle=False)
# Decision Tree with GridSearchCV
dt = DecisionTreeClassifier(random_state=42)
dt_grid = {
    "max_depth": [None, 2, 3, 4, 5, 6, 8, 10],
    "min_samples_leaf": [1, 2, 5, 10, 20],
    "min_samples_split": [2, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 20],
    "criterion": ["gini", "entropy"],
}

dt_gs = GridSearchCV(dt, dt_grid, scoring="accuracy", cv=cv5, n_jobs=-1, refit=True)
dt_gs.fit(X_train, y_train)

# Full table of CV results (sorted)
dt_res = pd.DataFrame(dt_gs.cv_results_)
dt_res = dt_res[["params", "mean_test_score", "std_test_score", "rank_test_score"]]
dt_res = dt_res.sort_values(["rank_test_score", "std_test_score"]).reset_index(drop=True)
print("\n=== Decision Tree - all CV results ===")
print(dt_res)

# Best summary + validation
dt_cv_mean = dt_gs.best_score_
dt_cv_std = dt_gs.cv_results_["std_test_score"][dt_gs.best_index_]
dt_val_acc = accuracy_score(y_val, dt_gs.predict(X_val))
print("\n=== Decision Tree - best ===")
print("Best params:", dt_gs.best_params_)
print(f"CV accuracy (mean ± std): {dt_cv_mean:.4f} ± {dt_cv_std:.4f}")
print(f"Validation accuracy: {dt_val_acc:.4f}")

dt_best = {"best_params": dt_gs.best_params_, "cv_mean": dt_cv_mean, "cv_std": dt_cv_std, "val_acc": dt_val_acc}
```

=== Decision Tree - all CV results ===

	params	mean_test_score \
0	{'criterion': 'gini', 'max_depth': 3, 'min_sam...	0.938491
1	{'criterion': 'gini', 'max_depth': 3, 'min_sam...	0.938491
2	{'criterion': 'gini', 'max_depth': 3, 'min_sam...	0.938491
3	{'criterion': 'gini', 'max_depth': 3, 'min_sam...	0.938491
4	{'criterion': 'gini', 'max_depth': 3, 'min_sam...	0.938491
..
955	{'criterion': 'gini', 'max_depth': 10, 'min_sa...	0.897442
956	{'criterion': 'gini', 'max_depth': 10, 'min_sa...	0.897442
957	{'criterion': 'gini', 'max_depth': 10, 'min_sa...	0.897442
958	{'criterion': 'gini', 'max_depth': 10, 'min_sa...	0.897442
959	{'criterion': 'gini', 'max_depth': 10, 'min_sa...	0.897442

	std_test_score	rank_test_score
0	0.021304	1
1	0.021304	1
2	0.021304	1
3	0.021304	1
4	0.021304	1
..
955	0.031876	865
956	0.031876	865
957	0.031876	865
958	0.031876	865
959	0.031876	865

[960 rows x 4 columns]

=== Decision Tree - best ===

Best params: {'criterion': 'gini', 'max_depth': 3, 'min_samples_leaf': 1, 'min_samples_split': 6}

CV accuracy (mean ± std): 0.9385 ± 0.0213

Validation accuracy: 0.9386

```
In [60]: # SVM with linear kernel and GridSearchCV
svm_lin = make_pipeline(StandardScaler(), SVC(kernel="linear", probability=True,
svm_lin_grid = {"svc_C": [0.001, 0.01, 0.1, 0.5, 0.6, 0.7, 0.8, 0.9, 1, 1.1, 2,

svm_lin_gs = GridSearchCV(svm_lin, svm_lin_grid, scoring="accuracy", cv=cv5, n_j
svm_lin_gs.fit(X_train, y_train)

# Full table of CV results (sorted)
svm_lin_res = pd.DataFrame(svm_lin_gs.cv_results_)
svm_lin_res = svm_lin_res[["params", "mean_test_score", "std_test_score", "rank_
svm_lin_res = svm_lin_res.sort_values(["rank_test_score", "std_test_score"]).res
print("\n=== SVM (Linear) - all CV results ===")
print(svm_lin_res)

# Best summary + validation
lin_cv_mean = svm_lin_gs.best_score_
lin_cv_std = svm_lin_gs.cv_results_["std_test_score"][svm_lin_gs.best_index_]
lin_val_acc = accuracy_score(y_val, svm_lin_gs.predict(X_val))
print("\n=== SVM (Linear) - best ===")
print("Best params:", svm_lin_gs.best_params_)
print(f"CV accuracy (mean ± std): {lin_cv_mean:.4f} ± {lin_cv_std:.4f}")
print(f"Validation accuracy: {lin_val_acc:.4f}")

svm_lin_best = {"best_params": svm_lin_gs.best_params_, "cv_mean": lin_cv_mean,
```

```

=== SVM (Linear) - all CV results ===

```

	params	mean_test_score	std_test_score	rank_test_score
0	{'svc__C': 0.7}	0.967775	0.017064	1
1	{'svc__C': 0.8}	0.967775	0.017064	1
2	{'svc__C': 0.9}	0.967775	0.017064	1
3	{'svc__C': 0.6}	0.964834	0.014924	4
4	{'svc__C': 1}	0.964834	0.014924	4
5	{'svc__C': 1.1}	0.964834	0.014924	4
6	{'svc__C': 2}	0.964791	0.023916	7
7	{'svc__C': 5}	0.964791	0.023916	7
8	{'svc__C': 0.5}	0.961893	0.014949	9
9	{'svc__C': 3}	0.961893	0.023864	9
10	{'svc__C': 0.01}	0.961850	0.007310	11
11	{'svc__C': 0.1}	0.958951	0.010974	12
12	{'svc__C': 7}	0.958909	0.025341	13
13	{'svc__C': 100}	0.953026	0.028569	14
14	{'svc__C': 10}	0.953026	0.036541	14
15	{'svc__C': 0.001}	0.932609	0.021775	16

```

=== SVM (Linear) - best ===
Best params: {'svc__C': 0.7}
CV accuracy (mean ± std): 0.9678 ± 0.0171
Validation accuracy:      0.9649

```

```

In [61]: # SVM with RBF kernel and GridSearchCV
svm_rbf = make_pipeline(StandardScaler(), SVC(kernel="rbf", probability=True, ra
svm_rbf_grid = {
    "svc__C":      [0.001, 0.01, 0.1, 1, 3, 5, 6, 7, 8, 10, 100],
    "svc__gamma": ["scale", 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1, 3, 10],
}

svm_rbf_gs = GridSearchCV(svm_rbf, svm_rbf_grid, scoring="accuracy", cv=cv5, n_j
svm_rbf_gs.fit(X_train, y_train)

# Full table of CV results (sorted)
svm_rbf_res = pd.DataFrame(svm_rbf_gs.cv_results_)
svm_rbf_res = svm_rbf_res[["params", "mean_test_score", "std_test_score", "rank_
svm_rbf_res = svm_rbf_res.sort_values(["rank_test_score", "std_test_score"]).res
print("\n=== SVM (RBF) - all CV results ===")
print(svm_rbf_res)

# Best summary + validation
rbf_cv_mean = svm_rbf_gs.best_score_
rbf_cv_std  = svm_rbf_gs.cv_results_["std_test_score"][svm_rbf_gs.best_index_]
rbf_val_acc = accuracy_score(y_val, svm_rbf_gs.predict(X_val))
print("\n=== SVM (RBF) - best ===")
print("Best params:", svm_rbf_gs.best_params_)
print(f"CV accuracy (mean ± std): {rbf_cv_mean:.4f} ± {rbf_cv_std:.4f}")
print(f"Validation accuracy:      {rbf_val_acc:.4f}")

svm_rbf_best = {"best_params": svm_rbf_gs.best_params_, "cv_mean": rbf_cv_mean,

```

```

=== SVM (RBF) - all CV results ===

```

	params	mean_test_score	std_test_score \
0	{'svc__C': 7, 'svc__gamma': 0.01}	0.976556	0.007136
1	{'svc__C': 8, 'svc__gamma': 0.01}	0.976556	0.007136
2	{'svc__C': 5, 'svc__gamma': 0.03}	0.976513	0.011797
3	{'svc__C': 5, 'svc__gamma': 0.01}	0.973615	0.005842
4	{'svc__C': 6, 'svc__gamma': 0.01}	0.973615	0.005842
..
105	{'svc__C': 8, 'svc__gamma': 10}	0.627579	0.006104
106	{'svc__C': 10, 'svc__gamma': 3}	0.627579	0.006104
107	{'svc__C': 10, 'svc__gamma': 10}	0.627579	0.006104
108	{'svc__C': 100, 'svc__gamma': 3}	0.627579	0.006104
109	{'svc__C': 100, 'svc__gamma': 10}	0.627579	0.006104

	rank_test_score
0	1
1	1
2	3
3	4
4	4
..	...
105	71
106	71
107	71
108	71
109	71

[110 rows x 4 columns]

```

=== SVM (RBF) - best ===
Best params: {'svc__C': 7, 'svc__gamma': 0.01}
CV accuracy (mean ± std): 0.9766 ± 0.0071
Validation accuracy: 0.9649

```

```

In [62]: #Summary of all CV
models = {
    "Decision Tree": dt_gs.best_estimator_,
    "SVM (Linear)": svm_lin_gs.best_estimator_,
    "SVM (RBF)": svm_rbf_gs.best_estimator_
}

# For plotting
rows = []
for name, gs in [
    ("Decision Tree", dt_gs),
    ("SVM (Linear)", svm_lin_gs),
    ("SVM (RBF)", svm_rbf_gs),
]:
    mean = gs.best_score_
    std = gs.cv_results_["std_test_score"][gs.best_index_]
    val_acc = accuracy_score(y_val, gs.predict(X_val))
    rows.append({"Model": name, "CV Mean": mean, "CV Std": std, "Val Acc": val_a

perf = pd.DataFrame(rows)
print("\n=== Summary of Best Models ===")
print(perf)

```

```

=== Summary of Best Models ===
      Model    CV Mean    CV Std    Val Acc
0  Decision Tree  0.938491  0.021304  0.938596
1    SVM (Linear)  0.967775  0.017064  0.964912
2      SVM (RBF)  0.976556  0.007136  0.964912

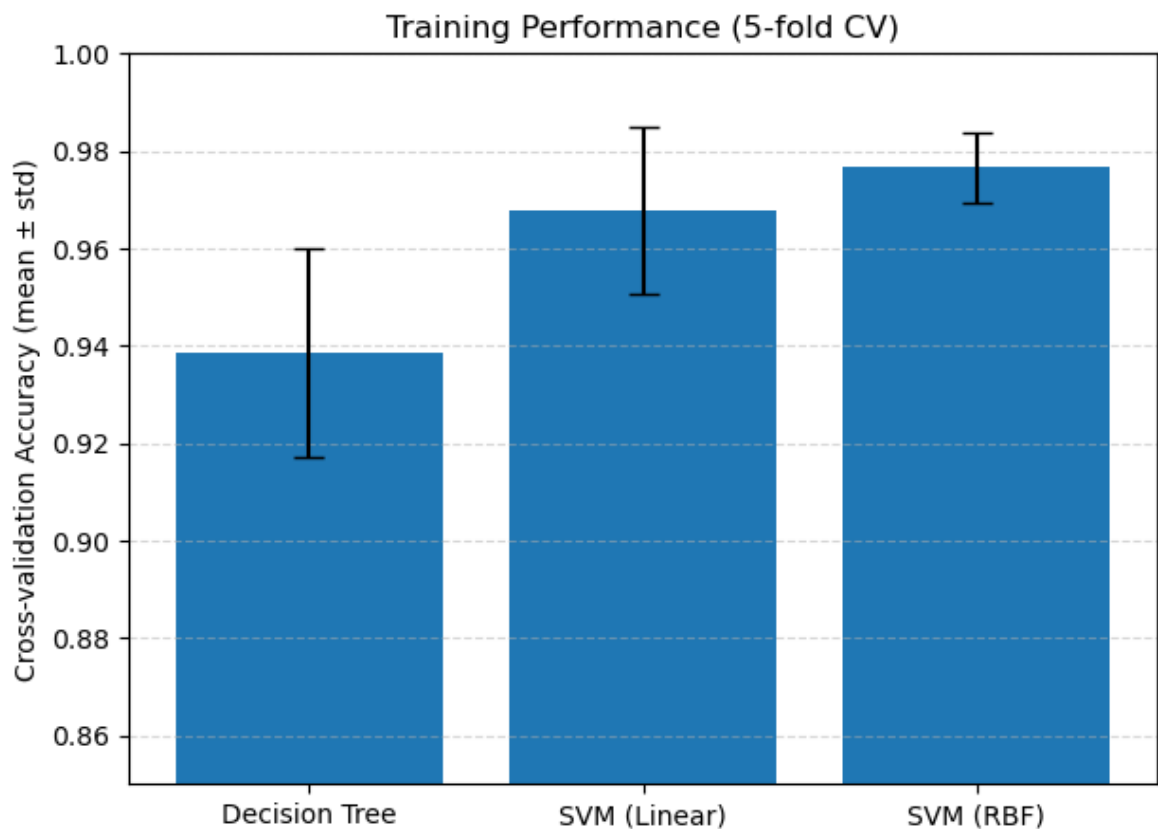
```

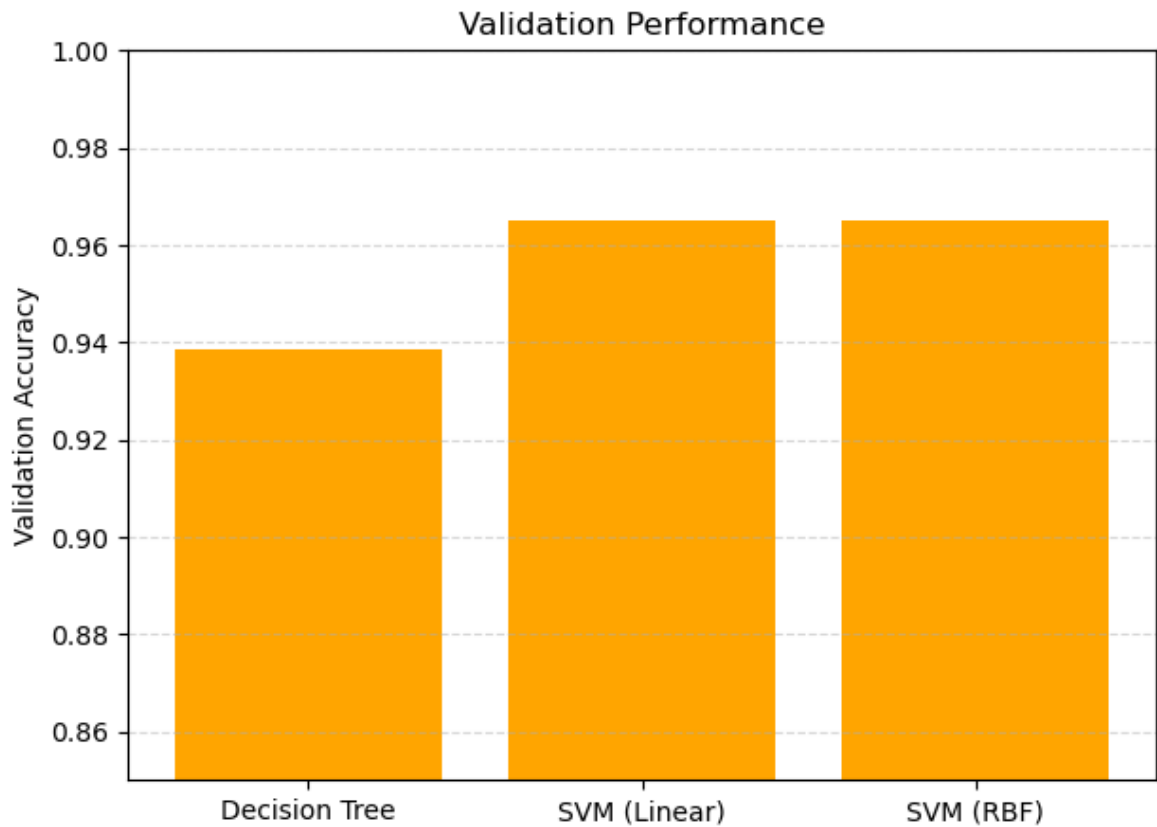
```

In [63]: # Plotting training performance
plt.figure(figsize=(7,5))
plt.bar(perf["Model"], perf["CV Mean"], yerr=perf["CV Std"], capsize=6)
plt.ylabel("Cross-validation Accuracy (mean  $\pm$  std)")
plt.title("Training Performance (5-fold CV)")
plt.ylim(0.85, 1.0)
plt.grid(axis='y', linestyle='--', alpha=0.5)
plt.show()

# Plotting validation performance
plt.figure(figsize=(7,5))
plt.bar(perf["Model"], perf["Val Acc"], color='orange')
plt.ylabel("Validation Accuracy")
plt.title("Validation Performance")
plt.ylim(0.85, 1.0)
plt.grid(axis='y', linestyle='--', alpha=0.5)
plt.show()

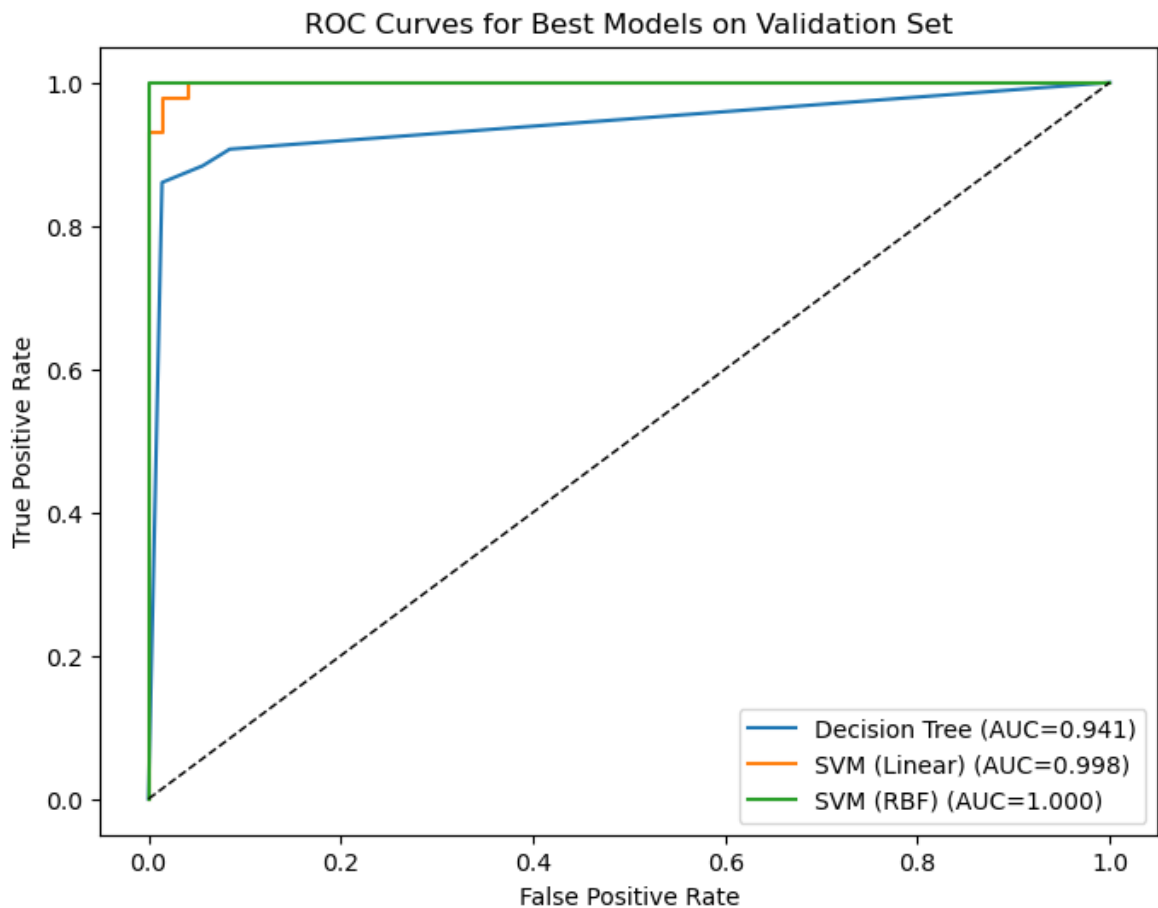
```





Looking at these two plots, you can see that the RBF SVM overfit a small amount to the training set, whilst the linear perform about the same which means in generalizes a little better.

```
In [64]: # ROC curves for best models on validation set
plt.figure(figsize=(8,6))
for name, model in models.items():
    y_proba = model.predict_proba(X_val)[: , 1]
    fpr, tpr, _ = roc_curve(y_val, y_proba)
    auc_val = auc(fpr, tpr)
    plt.plot(fpr, tpr, label=f"{name} (AUC={auc_val:.3f})")
plt.plot([0,1], [0,1], 'k--', lw=1)
plt.xlabel("False Positive Rate")
plt.ylabel("True Positive Rate")
plt.title("ROC Curves for Best Models on Validation Set")
plt.legend()
plt.show()
```



Exercise 4.4 - Compare the final test set accuracy of the best Decision Tree and best SVM. Which model performs better in practice?

```
In [65]: # Best models
best_dt   = dt_gs.best_estimator_
best_lin  = svm_lin_gs.best_estimator_
best_rbf  = svm_rbf_gs.best_estimator_

# Final evaluation on test set
models = {
    "Decision Tree": best_dt,
    "SVM (Linear)": best_lin,
    "SVM (RBF)": best_rbf
}

print("\n=== Final Test Set Performance ===")
for name, model in models.items():
    y_pred = model.predict(X_test)
    acc = accuracy_score(y_test, y_pred)
    print(f"{name}: Test Accuracy = {acc:.4f}")
```

```
=== Final Test Set Performance ===
Decision Tree: Test Accuracy = 0.9386
SVM (Linear): Test Accuracy = 0.9561
SVM (RBF): Test Accuracy = 0.9912
```

```
In [66]: from sklearn.metrics import roc_curve, auc, ConfusionMatrixDisplay
import matplotlib.pyplot as plt

# Best models already defined
```

```

models = {
    "Decision Tree": dt_gs.best_estimator_,
    "SVM (Linear)": svm_lin_gs.best_estimator_,
    "SVM (RBF)": svm_rbf_gs.best_estimator_,
}

# Test set accuracy for each model
test_accs = {name: accuracy_score(y_test, mdl.predict(X_test))
              for name, mdl in models.items()}

print({k: round(v, 4) for k, v in test_accs.items()})

# bar chart
plt.figure(figsize=(6,4))
plt.bar(test_accs.keys(), test_accs.values())
plt.ylabel("Accuracy")
plt.title("Test Set Accuracy Comparison")
plt.ylim(0.9, 1.0)
plt.grid(axis="y", linestyle="--", alpha=0.5)
plt.show()

# 2. ROC curves
plt.figure(figsize=(7,5))
for name, model in models.items():
    y_proba = model.predict_proba(X_test)[: , 1]
    fpr, tpr, _ = roc_curve(y_test, y_proba)
    roc_auc = auc(fpr, tpr)
    plt.plot(fpr, tpr, label=f"{name} (AUC={roc_auc:.3f})")

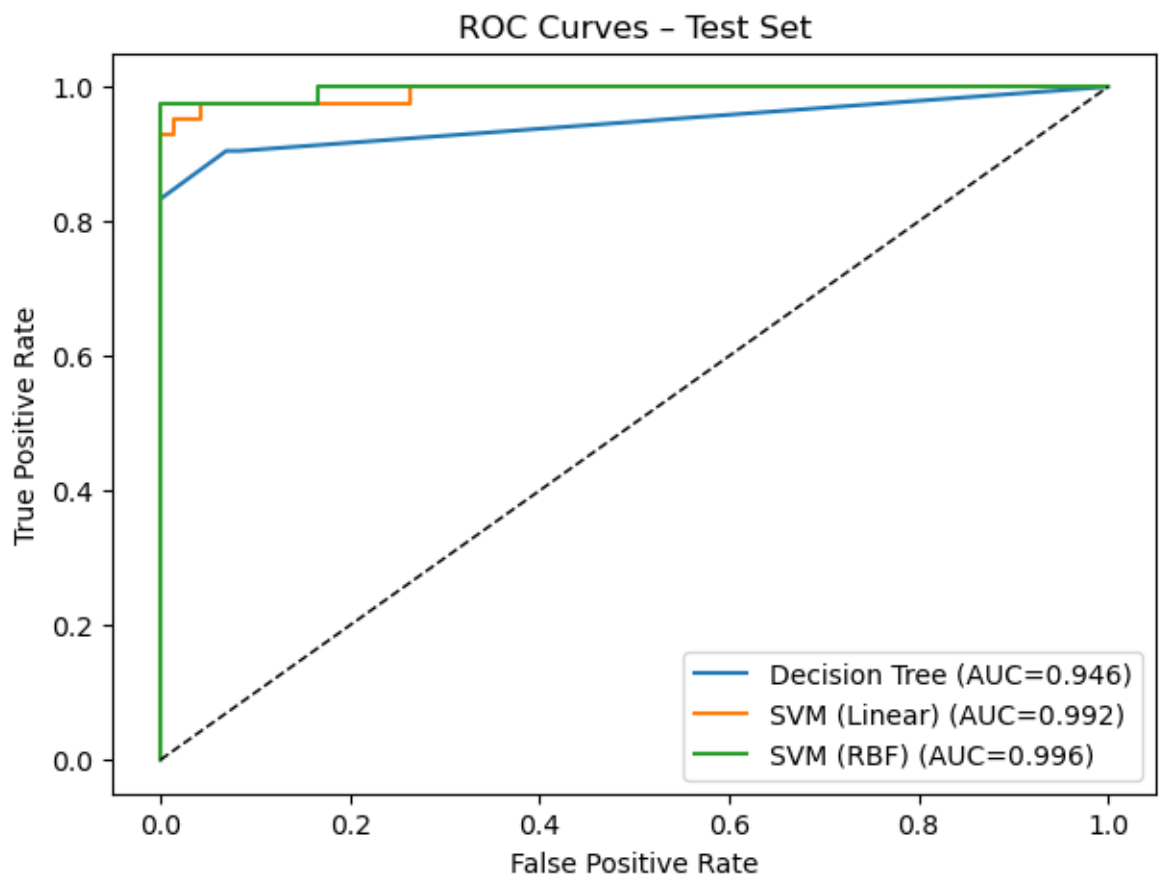
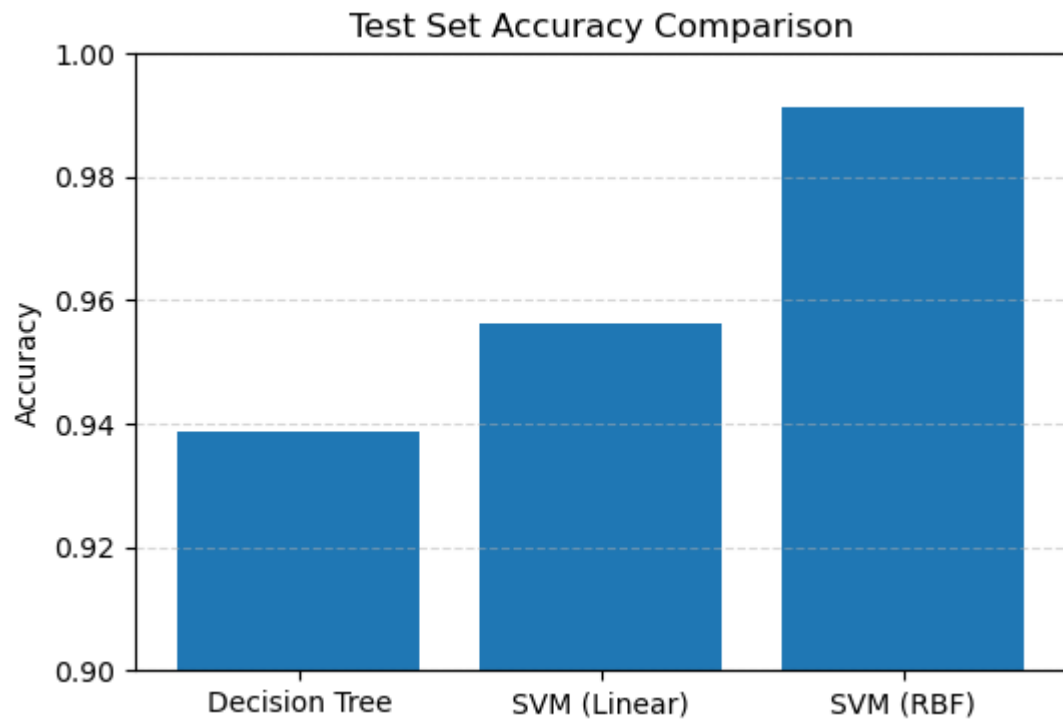
plt.plot([0,1],[0,1], 'k--', lw=1)
plt.xlabel("False Positive Rate")
plt.ylabel("True Positive Rate")
plt.title("ROC Curves - Test Set")
plt.legend()
plt.show()

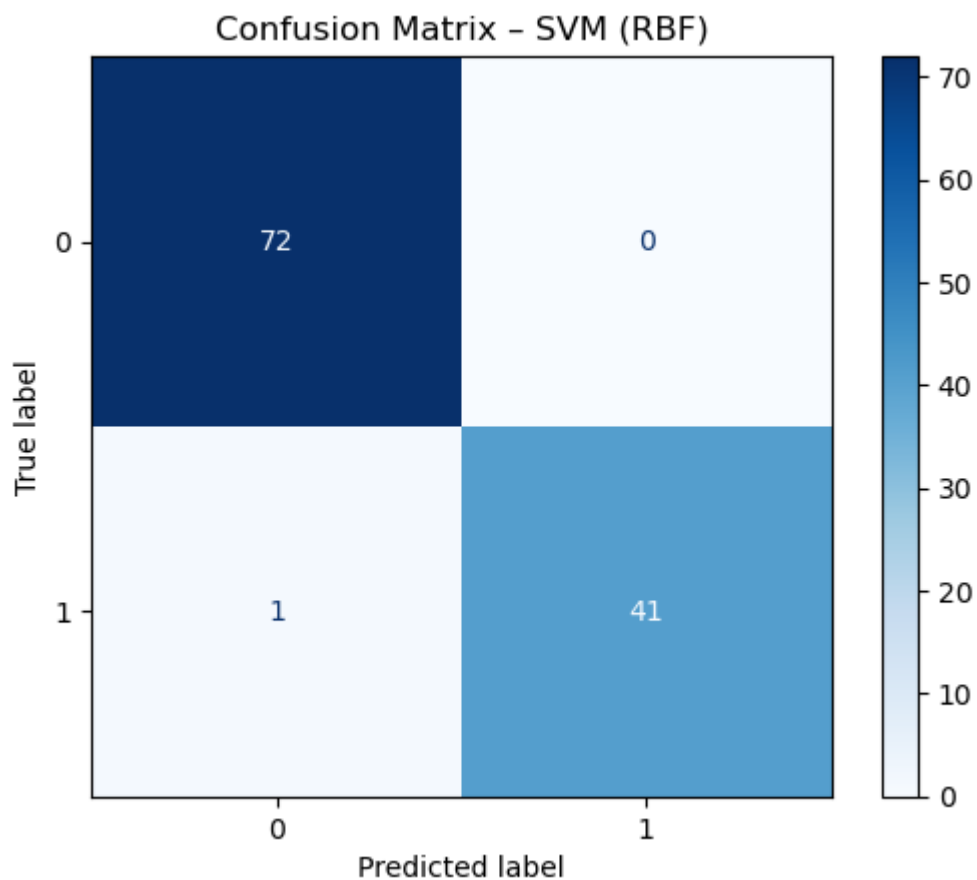
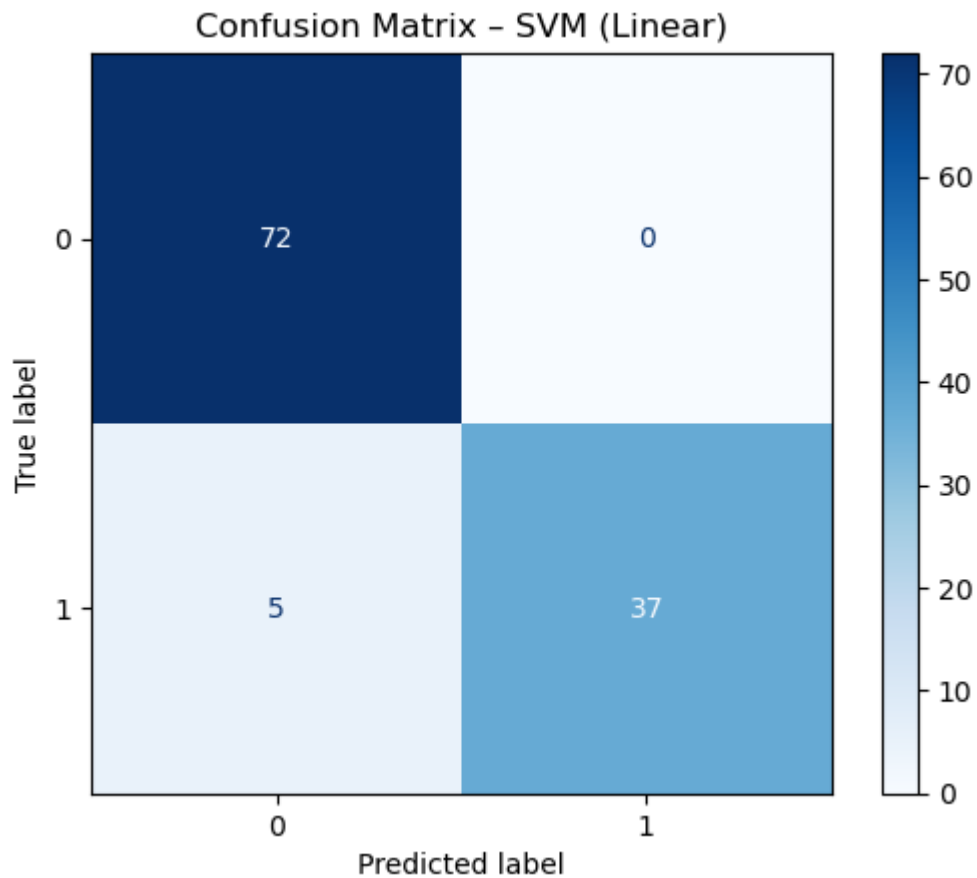
# Confusion matrix for best model (SVM Linear)
linear_best_model_matrix=svm_lin_gs.best_estimator_
ConfusionMatrixDisplay.from_estimator(linear_best_model_matrix, X_test, y_test,
plt.title("Confusion Matrix - SVM (Linear)")
plt.show()

# Confusion matrix for best model (RBF)
best_model = svm_rbf_gs.best_estimator_
ConfusionMatrixDisplay.from_estimator(best_model, X_test, y_test, cmap="Blues")
plt.title("Confusion Matrix - SVM (RBF)")
plt.show()

```

```
{'Decision Tree': 0.9386, 'SVM (Linear)': 0.9561, 'SVM (RBF)': 0.9912}
```



Looking at the plots you can see the RBF model performing best. The confusion matrix shows only one mis-classification, however it is a bad one. In practice, this means taht the model sees a malignant case as begin, which is very dangerous for the patient receiving this diagnosis. The accuracy of the RBF model is good, other than the mis of one case.

4.5 - The Breast Cancer Wisconsin dataset has 30 continuous features, many of which are correlated and not linearly separable. Explain why a linear SVM might fail to capture complex patterns in this dataset. How does using an RBF kernel help in this case? Discuss your answer in terms of the dataset's feature space and the geometry of the decision boundary.

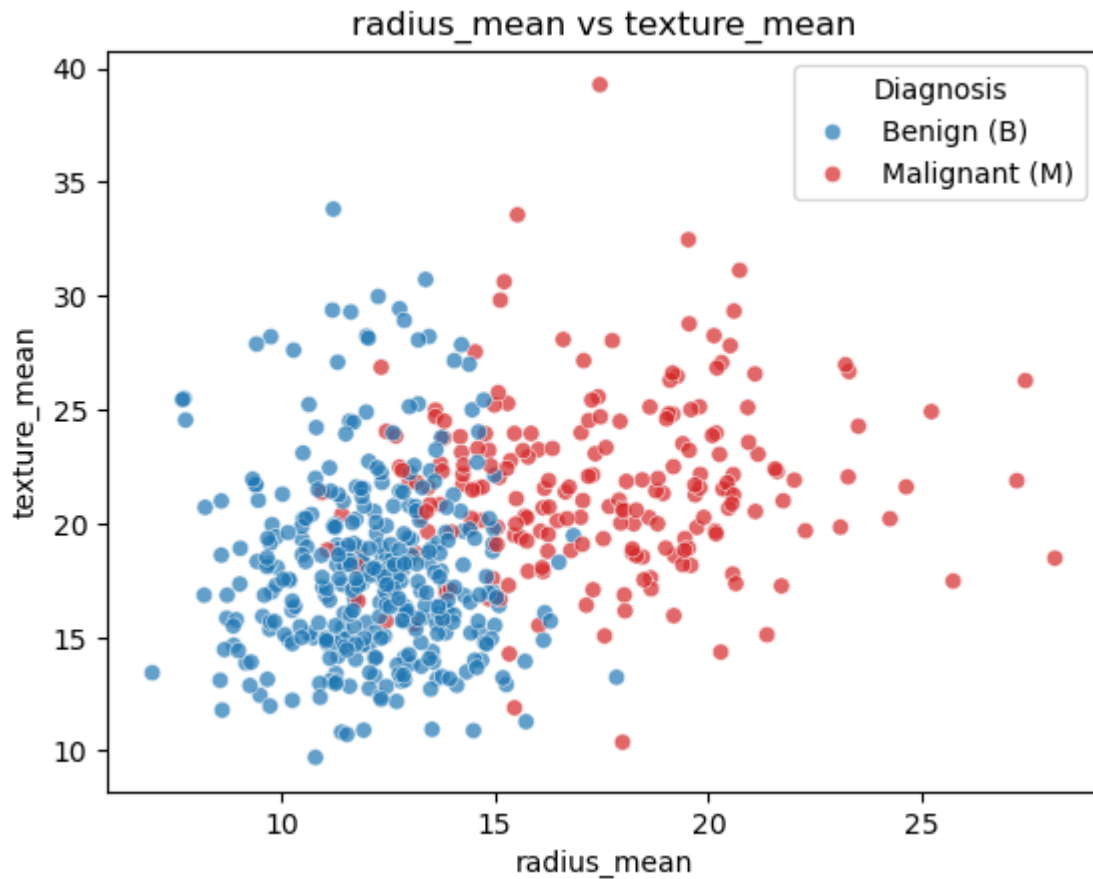
Linear SVM assumes possibility to separate linearly

```
In [67]: # Scatter plot of two features colored by diagnosis, radius_mean and texture_mean
feat1, feat2 = "radius_mean", "texture_mean"

# Plot
ax = sns.scatterplot(
    data=df,
    x=feat1, y=feat2,
    hue="diagnosis",
    hue_order=["B", "M"],
    palette=["tab:blue", "tab:red"],
    alpha=0.7
)

# Customize Legend
handles, labels = ax.get_legend_handles_labels()
label_map = {"B": "Benign (B)", "M": "Malignant (M)"}
labels = [label_map.get(l, l) for l in labels]
ax.legend(handles=handles, labels=labels, title="Diagnosis", loc="best")

plt.title(f"{feat1} vs {feat2}")
plt.show()
```

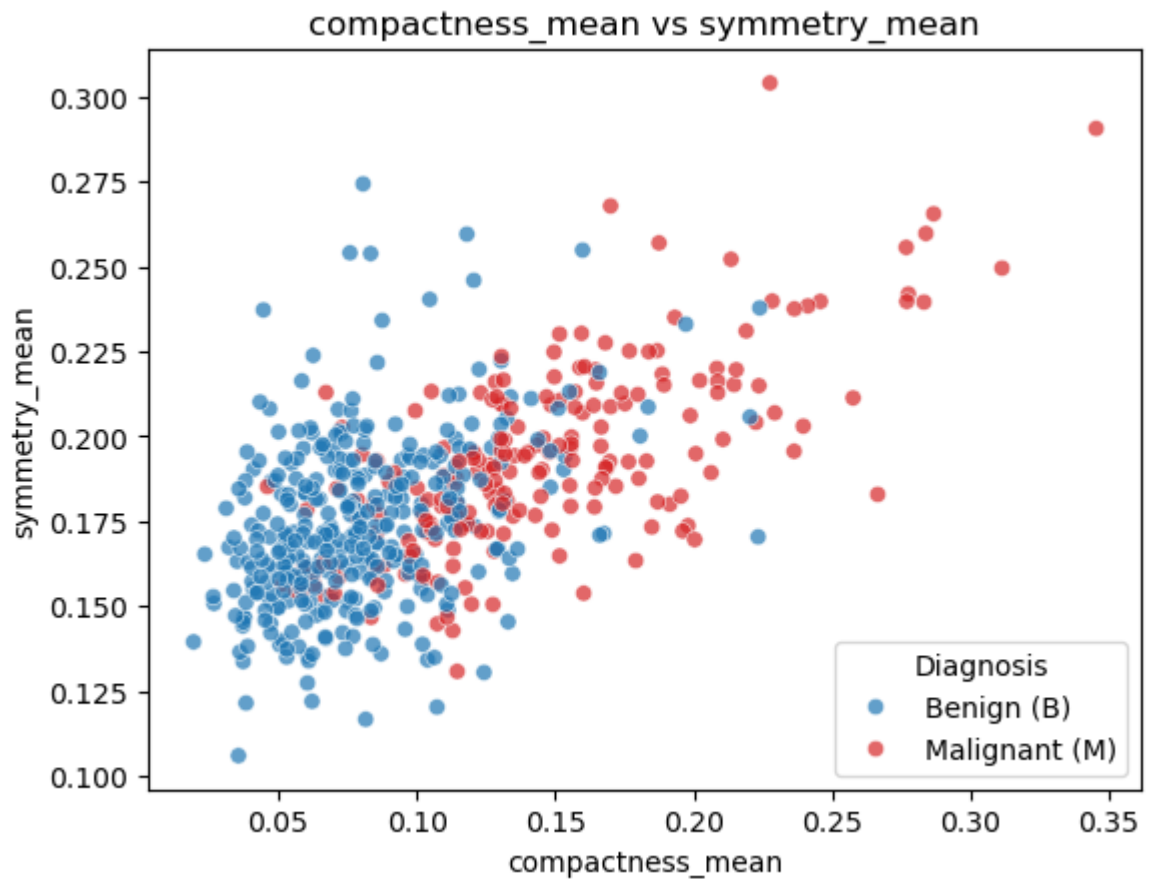


```
In [68]: # Scatter plot of two features colored by diagnosis, compactness_mean and symmet.
feat1, feat2 = "compactness_mean", "symmetry_mean"

# plot
ax = sns.scatterplot(
    data=df,
    x=feat1, y=feat2,
    hue="diagnosis",
    hue_order=["B", "M"],
    palette=["tab:blue", "tab:red"],
    alpha=0.7
)

# Customize Legend
handles, labels = ax.get_legend_handles_labels()
label_map = {"B": "Benign (B)", "M": "Malignant (M)"}
labels = [label_map.get(l, l) for l in labels]
ax.legend(handles=handles, labels=labels, title="Diagnosis", loc="best")

plt.title(f"{feat1} vs {feat2}")
plt.show()
```



Since linear SVM requires the classes to be separable with a straight line, and looking at the two plots above, you can see that these features, and others, are close to impossible to separate linearly. Many of the features are not linearly independent of each other. For example, `perimeter_worst`, `perimeter_mean` and `perimeter_se` have a dependency on each other. Every feature in the data set has 3 different categories, the same way as `perimeter` has.

Using a technique called similarity features, which measures how much each instance resembles a particular landmark, in combination with the RBF kernel can help make features linearly separable. The simplest way to select landmark positions is doing it for every instance in the dataset. This is computationally heavy and creates many dimensions, but also increases the chances of getting a linearly separable training set. The hyperparameter `gamma` helps create a bell curve, and tuning this correctly for the RBF kernel creates a decision boundary which the data set can fit in.