Random Forest Classifier: Baseline

Table of Contents

Section I: Environment Setup and Configuration

In this section, we begin by importing all the essential Python libraries commonly used for data analysis, visualization, and preprocessing.

- **Pandas** and **NumPy** provide robust functionality for handling structured data and efficient numerical computations.
- **Matplotlib** and **Seaborn** are used for visualizations, enabling us to better understand trends, patterns, and distributions within the dataset.

Following this, we load all the **notebook-specific configurations** from an external YAML file. This configuration file stores paths for different dataset splits (training, validation, and testing) in **raw**, **engineered**, and **processed** forms, both for input features (`X`) and corresponding labels (`y`).

By structuring the data loading process via a configuration file, we ensure flexibility and easier reproducibility across experiments.

In [16]:
```
# Importing all of the necessary libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
```

In [17]:
```
# Loading the notebook cofigurations
import yaml
with open("../notebook_config.yaml", "rb") as f:
    config = yaml.safe_load(f)
    X_train_eng, X_val_eng, X_test_eng = config['paths']["X_train_eng"], config[
    y_train_eng, y_val_eng, y_test_eng = config['paths']["y_train_eng"], config[

    X_train_raw, X_val_raw, X_test_raw = config['paths']["X_train_raw"], config[
```

```
    y_train_raw, y_val_raw, y_test_raw = config['paths']["y_train_raw"], config[

    X_train, X_val, X_test = config['paths']["X_train"], config['paths']["X_val"
    y_train, y_val, y_test = config['paths']["y_train"], config['paths']["y_val"
```

Section II: Data Loading

In this section, we load the different dataset splits into memory. The Wisconsin Breast Cancer dataset has been preprocessed and stored in three different forms:

1. **Engineered Features (`*_eng`)**
    - These contain features that have undergone transformations such as scaling, feature engineering, or other preprocessing steps to enhance model performance.
2. **Raw Features (`*_raw`)**
    - The unmodified dataset, preserved in its original state to allow for baseline comparisons and exploratory analysis without preprocessing bias.
3. **Main Split (`X_train` , `X_val` , `X_test`)**
    - A curated version of the dataset intended as the primary set for model training, validation, and testing. This split reflects the actual datasets that will be used across modeling experiments.

All labels (`y`) are loaded alongside their corresponding features and immediately converted into **Series objects** (via `.squeeze()`) for easier handling in downstream tasks. By separating raw, engineered, and main splits, we can compare model performance across different preprocessing strategies in a consistent and reproducible manner.

In [18]:
```
# Load engineered features and labels
X_train_eng = pd.read_csv(X_train_eng)
X_val_eng = pd.read_csv(X_val_eng)
X_test_eng = pd.read_csv(X_test_eng)
y_train_eng = pd.read_csv(y_train_eng).squeeze()
y_val_eng = pd.read_csv(y_val_eng).squeeze()
y_test_eng = pd.read_csv(y_test_eng).squeeze()

# Load raw features and labels
X_train_raw = pd.read_csv(X_train_raw)
X_val_raw = pd.read_csv(X_val_raw)
X_test_raw = pd.read_csv(X_test_raw)
y_train_raw = pd.read_csv(y_train_raw).squeeze()
y_val_raw = pd.read_csv(y_val_raw).squeeze()
y_test_raw = pd.read_csv(y_test_raw).squeeze()

# Load the main split as well
X_train = pd.read_csv(X_train)
X_val = pd.read_csv(X_val)
X_test = pd.read_csv(X_test)
y_train = pd.read_csv(y_train).squeeze()
y_val = pd.read_csv(y_val).squeeze()
y_test = pd.read_csv(y_test).squeeze()
```

Section III: Baseline Model and Learning Curves

To establish a solid baseline for classification performance on the Wisconsin Breast Cancer dataset, we begin by **initializing a Random Forest model** using Scikit-Learn's `RandomForestClassifier`. The hyperparameters are carefully chosen to mitigate overfitting, with constraints on tree depth, minimum samples per split and leaf, and balanced class weighting to address potential class imbalance in malignant versus benign labels.

Next, we implement a reusable function to **plot learning curves**, allowing for a visual assessment of how model generalization behaves as the size of the training set increases. The function displays both mean scores and standard deviations for training and validation sets, supporting customizable scoring metrics—here primarily recall for the malignancy class—to align with medical application priorities.

Finally, we adopt **StratifiedKFold cross-validation** to maintain robust class distribution across splits and plot learning curves for both **engineered and raw features**. This comparative approach highlights the impact of feature engineering on overfitting and generalization, guiding further model optimization or preprocessing efforts.

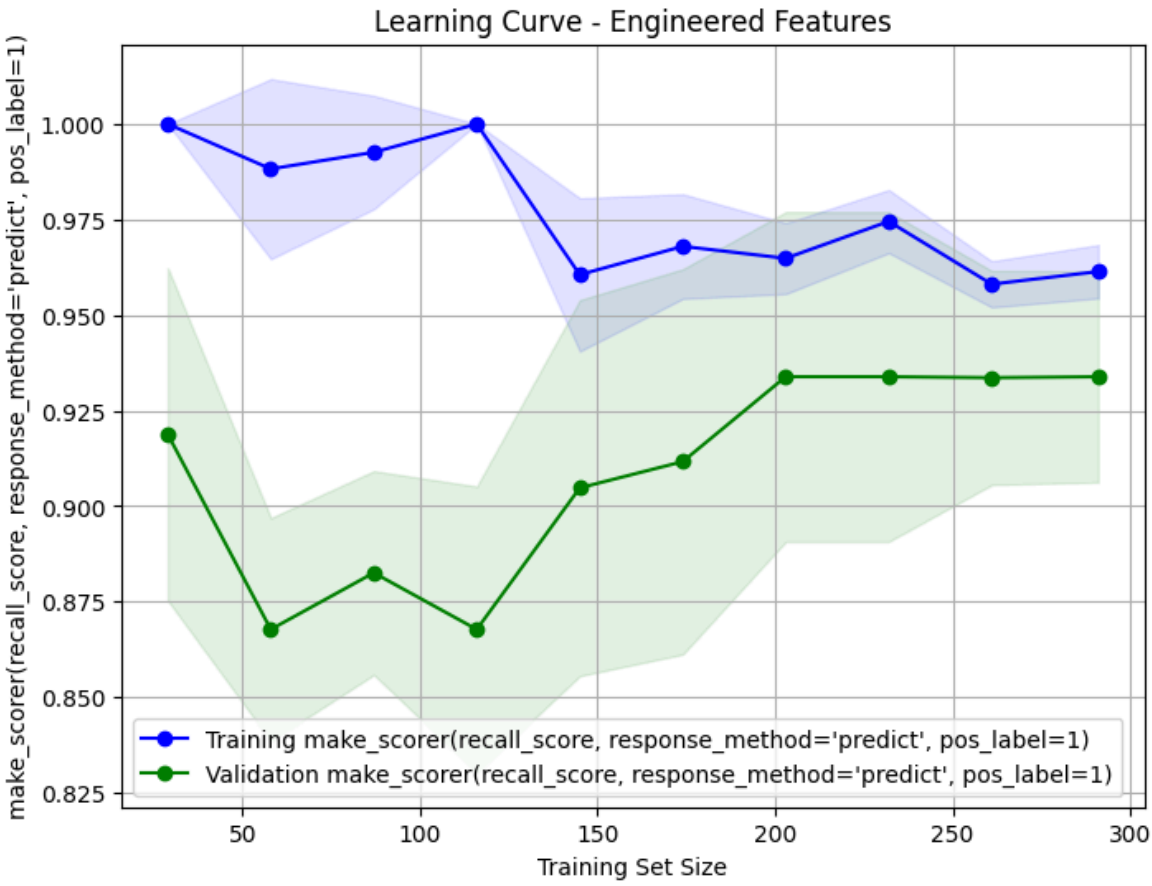
In [19]:
```
# Initializing a Random Forest Model
from sklearn.ensemble import RandomForestClassifier

# Initializing the model
rf_v1_eng = RandomForestClassifier(
    n_estimators=100,
    max_depth=3,
    random_state=42,
    class_weight='balanced',
    n_jobs=-1,
```

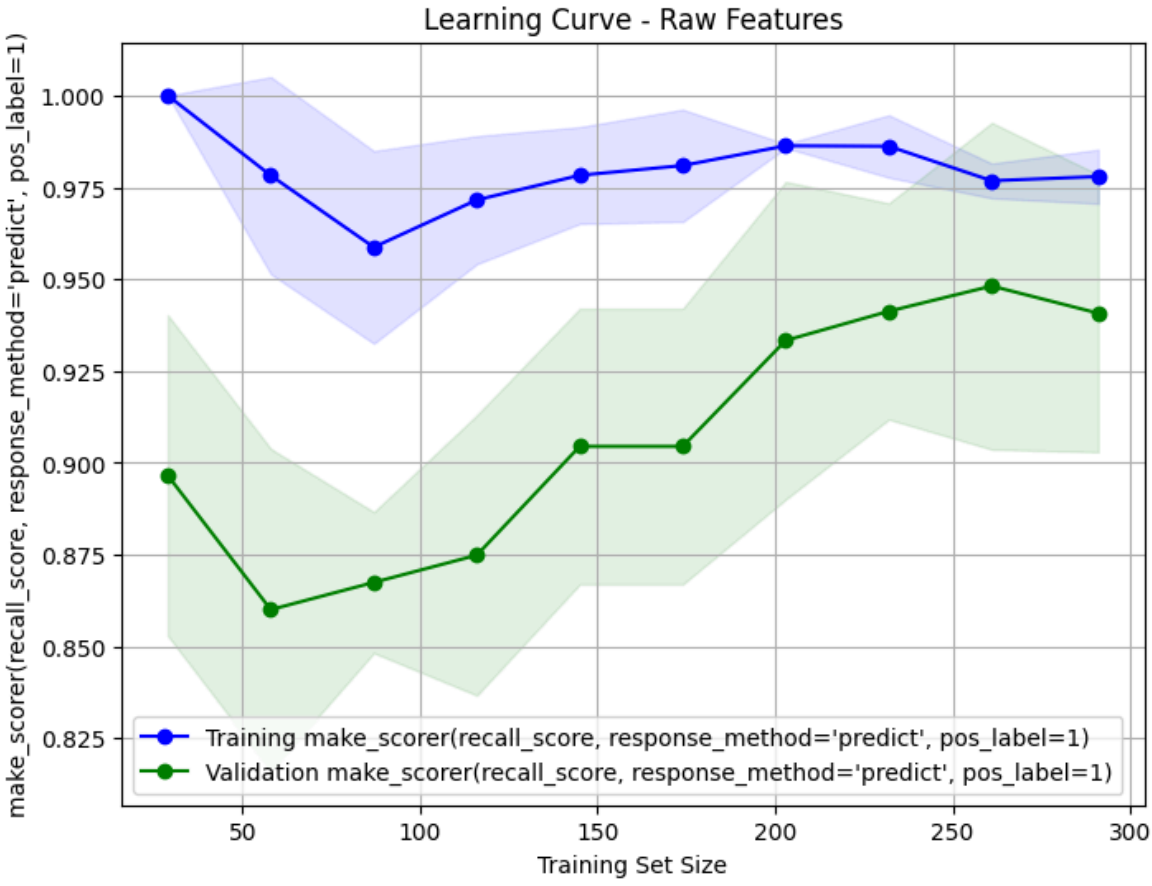
```
    min_samples_split=12,
    min_samples_leaf=10,
    max_features='sqrt'
)

rf_v1_raw = RandomForestClassifier(
    n_estimators=100,
    max_depth=3,
    random_state=42,
    class_weight='balanced',
    n_jobs=-1,
    min_samples_split=12,
    min_samples_leaf=10,
    max_features='sqrt'
)
```

In [20]:
```
# Code for plotting the learning curve
from sklearn.model_selection import learning_curve

def plot_learning_curve(model, X_train, y_train, title, cv=5, scoring='accuracy'
    train_sizes, train_scores, val_scores = learning_curve(
        model, X_train, y_train, cv=cv, scoring=scoring,
        train_sizes=np.linspace(0.1, 1.0, 10), n_jobs=-1, random_state=42)

    train_mean = np.mean(train_scores, axis=1)
    train_std = np.std(train_scores, axis=1)
    val_mean = np.mean(val_scores, axis=1)
    val_std = np.std(val_scores, axis=1)

    plt.figure(figsize=(8,6))
    plt.plot(train_sizes, train_mean, 'o-', color='blue', label=f'Training {scor
    plt.fill_between(train_sizes, train_mean - train_std, train_mean + train_std
    plt.plot(train_sizes, val_mean, 'o-', color='green', label=f'Validation {sco
    plt.fill_between(train_sizes, val_mean - val_std, val_mean + val_std, alpha=

    plt.title(title)
    plt.xlabel('Training Set Size')
    plt.ylabel(f'{scoring}')
    plt.legend()
    plt.grid(True)
    plt.show()

# Custom Scorer for the Recall of the malignancy class
from sklearn.metrics import make_scorer, recall_score, precision_score, f1_score
recall_malignant = make_scorer(recall_score, pos_label=1)
```

In [21]:
```
# Plotting the learning curves
from sklearn.model_selection import StratifiedKFold

# Create StratifiedKFold instance
stratified_cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=42)
# Plot on engineered features
plot_learning_curve(
    rf_v1_eng, X_train_eng, y_train_eng,
    'Learning Curve - Engineered Features',
    cv=stratified_cv, scoring=recall_malignant
)
# Plot on raw features
plot_learning_curve(
```

```
    rf_v1_raw, X_train_raw, y_train_raw,
    'Learning Curve - Raw Features',
    cv=stratified_cv, scoring=recall_malignant
)
```





Section IV: Cross-Validation and Hyperparameter Optimization

In this section, we implement robust **cross-validation** to estimate the real-world performance of our Random Forest classifier using multiple metrics tailored to the detection of malignant cases: recall, precision, and F1-score. By evaluating both the engineered and raw feature sets, we gain unbiased insight into how each preprocessing variant generalizes across stratified folds. Summary statistics from five-fold cross-validation highlight the trade-offs between recall, precision, and combined F1-score on both input types, ensuring that our models do not simply memorize the training data but achieve reliable predictive accuracy for cancer detection.

We further perform an extensive **hyperparameter tuning** using `RandomizedSearchCV` across a carefully designed parameter grid, applying stratified cross-validation and optimizing for malignant recall. The best hyperparameters are selected from 50 randomized configurations for each feature set, resulting in tuned models optimized for medical relevance. This process helps validate the stability and performance of our baseline approach, while ensuring reproducibility and high recall for critical classes.

The resulting best parameters and cross-validation scores provide actionable benchmarks and guide further experimentation or model refinement.

In [22]:
```
# Cross Validation for robust, unbiased estimates of your model's real-world per
from sklearn.model_selection import cross_validate

# Some more scoring tailored towards malignant cases
precision_malignant = make_scorer(precision_score, pos_label=1)
f1_malignant = make_scorer(f1_score, pos_label=1)
scoring = {
    'recall_malignant': recall_malignant,
    'precision_malignant': precision_malignant,
    'f1_malignant': f1_malignant
}
# Cross-validation with multiple scoring metrics on Engineered features
cv_results_eng = cross_validate(
    rf_v1_eng, X_train_eng, y_train_eng,
    cv=stratified_cv, scoring=scoring, n_jobs=-1,
    return_train_score=False
)

# Cross-validation with multiple scoring metrics on Raw features
cv_results_raw = cross_validate(
    rf_v1_eng, X_train_raw, y_train_raw,
    cv=stratified_cv, scoring=scoring, n_jobs=-1,
    return_train_score=False
)

# Print results summary for Engineered Features
for metric in scoring.keys():
    scores = cv_results_eng[f'test_{metric}']
    print(f"Engineered Features - {metric}: {scores.mean():.3f} ± {scores.std():

# Print results summary for Raw Features
for metric in scoring.keys():
```

```
    scores = cv_results_raw[f'test_{metric}']
    print(f"Raw Features - {metric}: {scores.mean():.3f} ± {scores.std():.3f}")
```

```
Engineered Features - recall_malignant: 0.934 ± 0.028
Engineered Features - precision_malignant: 0.915 ± 0.048
Engineered Features - f1_malignant: 0.924 ± 0.035
Raw Features - recall_malignant: 0.948 ± 0.044
Raw Features - precision_malignant: 0.890 ± 0.073
Raw Features - f1_malignant: 0.916 ± 0.041
```

In [23]:

```
from sklearn.model_selection import RandomizedSearchCV

# Define malignant and benign recall scorers
recall_malignant = make_scorer(recall_score, pos_label=1)
recall_benign = make_scorer(recall_score, pos_label=0)

scoring = {
    'recall_malignant': recall_malignant,
    'recall_benign': recall_benign
}

# Define hyperparameter distribution
param_dist = {
    'n_estimators': [100, 150, 200, 250],
    'max_depth': [3, 4, 5, 6, None],
    'min_samples_split': [2, 4, 8, 12],
    'min_samples_leaf': [1, 4, 8, 12],
    'max_features': ['sqrt', 'log2', 0.5, None],
    'class_weight': ['balanced', 'balanced_subsample', None]
}

# Initialize base model
rf_eng = RandomForestClassifier(random_state=42, n_jobs=-1)
rf_raw = RandomForestClassifier(random_state=42, n_jobs=-1)

# Hyperparameter tuning for Engineered Features
random_search_eng = RandomizedSearchCV(
    estimator=rf_eng,
    param_distributions=param_dist,
    n_iter=50,
    scoring=scoring,
    refit='recall_malignant',  # Select best model using malignant recall
    cv=stratified_cv,
    n_jobs=-1,
    verbose=2,
    random_state=42
)

random_search_eng.fit(X_train_eng, y_train_eng)
print("Best Parameters (Engineered):", random_search_eng.best_params_)

# Hyperparameter tuning for Raw Features
random_search_raw = RandomizedSearchCV(
    estimator=rf_raw,
    param_distributions=param_dist,
    n_iter=50,
    scoring=scoring,
    refit='recall_malignant',
    cv=stratified_cv,
    n_jobs=-1,
```

```
    verbose=2,
    random_state=42
)

random_search_raw.fit(X_train_raw, y_train_raw)
print("Best Parameters (Raw):", random_search_raw.best_params_)

# Access best estimators after tuning
best_rf_eng = random_search_eng.best_estimator_
best_rf_raw = random_search_raw.best_estimator_

# Access cv results if needed
results_eng = random_search_eng.cv_results_
results_raw = random_search_raw.cv_results_
```

```
Fitting 5 folds for each of 50 candidates, totalling 250 fits
Best Parameters (Engineered): {'n_estimators': 100, 'min_samples_split': 2, 'min_
samples_leaf': 8, 'max_features': 'log2', 'max_depth': None, 'class_weight': 'bal
anced_subsample'}
Fitting 5 folds for each of 50 candidates, totalling 250 fits
Best Parameters (Raw): {'n_estimators': 200, 'min_samples_split': 8, 'min_samples
_leaf': 8, 'max_features': None, 'max_depth': 5, 'class_weight': 'balanced'}
```

Section V: Model Evaluation with Classification Reports

After hyperparameter tuning and model selection, we evaluate the final Random Forest classifiers on both validation and test splits for engineered and raw feature sets.

Using Scikit-Learn's `classification_report`, we generate comprehensive summaries of key classification metrics—precision, recall, F1-score, and support—for each target class: **Benign** and **Malignant**. These reports provide detailed insights into model performance beyond overall accuracy, highlighting strengths and weaknesses in identifying the critical malignant cases.

Presenting reports on both validation and test sets helps confirm that performance generalizes well and that the models have not overfit the training data. This step is crucial for reliable assessment before any deployment or further experimentation.

In [24]:
```
# Classification report on the Validation Splits
from sklearn.metrics import classification_report

# Predict on validation set with best estimator from engineered feature pool
y_val_pred_eng = best_rf_eng.predict(X_val_eng)
print("Classification Report - Engineered Features Validation Set")
print(classification_report(y_val_eng, y_val_pred_eng, target_names=['Benign', '

# Predict on test set with best estimator from engineered feature pool
y_test_pred_eng = best_rf_eng.predict(X_test_eng)
print("Classification Report - Engineered Features Test Set")
print(classification_report(y_test_eng, y_test_pred_eng, target_names=['Benign',
```

```
Classification Report - Engineered Features Validation Set
              precision    recall  f1-score   support

      Benign       0.97      0.98      0.97        57
   Malignant       0.97      0.94      0.96        34

    accuracy                           0.97        91
   macro avg       0.97      0.96      0.96        91
weighted avg       0.97      0.97      0.97        91

Classification Report - Engineered Features Test Set
              precision    recall  f1-score   support

      Benign       0.97      0.97      0.97        72
   Malignant       0.95      0.95      0.95        42

    accuracy                           0.96       114
   macro avg       0.96      0.96      0.96       114
weighted avg       0.96      0.96      0.96       114
```

In [25]:
```
# Predict on validation set with best estimator from raw feature pool
y_val_pred_raw = best_rf_raw.predict(X_val_raw)
print("Classification Report - Raw Features Validation Set")
print(classification_report(y_val_raw, y_val_pred_raw, target_names=['Benign', '

# Predict on test set with best estimator from raw feature pool
y_test_pred_raw = best_rf_raw.predict(X_test_raw)
print("Classification Report - Raw Features Test Set")
print(classification_report(y_test_raw, y_test_pred_raw, target_names=['Benign',
```

```
Classification Report - Raw Features Validation Set
              precision    recall  f1-score   support

      Benign       0.96      0.96      0.96        57
   Malignant       0.94      0.94      0.94        34

    accuracy                           0.96        91
   macro avg       0.95      0.95      0.95        91
weighted avg       0.96      0.96      0.96        91

Classification Report - Raw Features Test Set
              precision    recall  f1-score   support

      Benign       0.96      0.99      0.97        72
   Malignant       0.97      0.93      0.95        42

    accuracy                           0.96       114
   macro avg       0.97      0.96      0.96       114
weighted avg       0.97      0.96      0.96       114
```

Section VI: Feature Importance Analysis Using Permutation Importance

We replaced the previous SHAP-based feature interpretation with **Permutation Importance**, a robust and model-agnostic method.

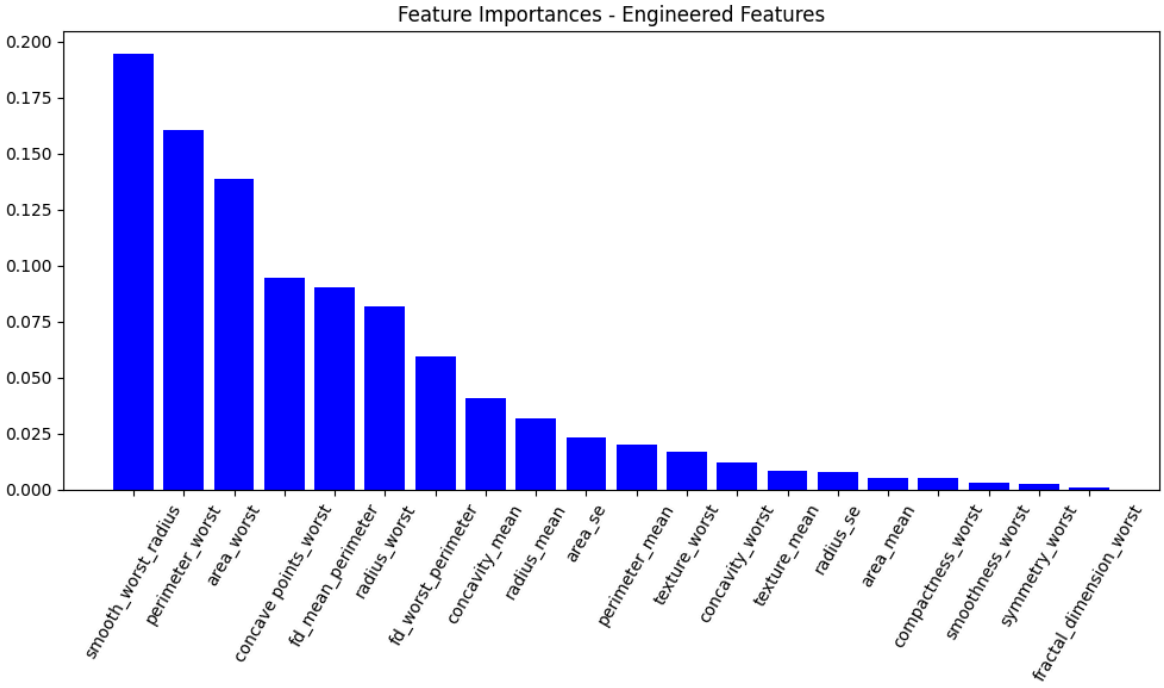
- **Permutation Importance** measures how much the model's accuracy decreases when a single feature's values are randomly shuffled, breaking its connection with the target.
- Features causing a larger drop in accuracy are deemed more important for the model's predictions.
- This method works reliably for any model type, including Random Forests, and avoids the compatibility issues encountered with SHAP.

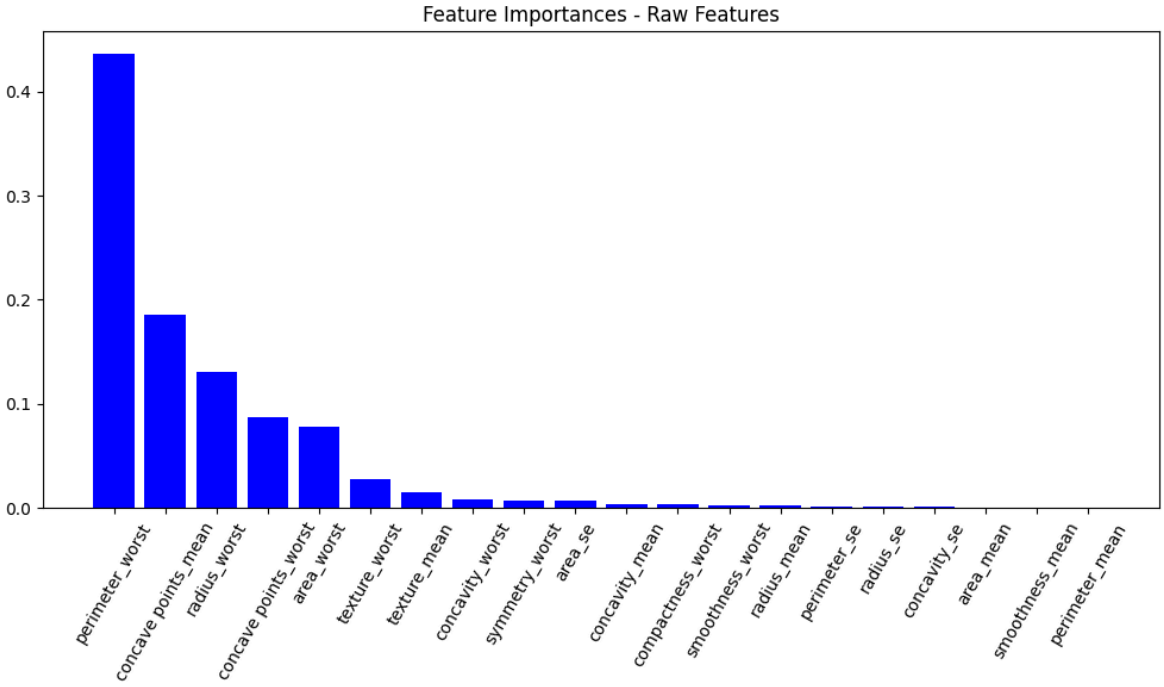
Implementation Overview

- We calculate permutation importances on the validation sets for both engineered and raw feature pools.
- The importance scores are averaged over multiple shuffles (`n_repeats=10`) to ensure stability.
- Visualizations display the mean importance values with error bars indicating variability.
- We select features whose importance exceeds a threshold, capturing the most impactful attributes.
- Finally, we combine unique important features from both feature sets, prioritizing higher importance if duplicates appear.

This approach ensures that feature selection is directly driven by the model's observed predictive impact, guiding us toward a more meaningful and refined feature pool for subsequent modeling.

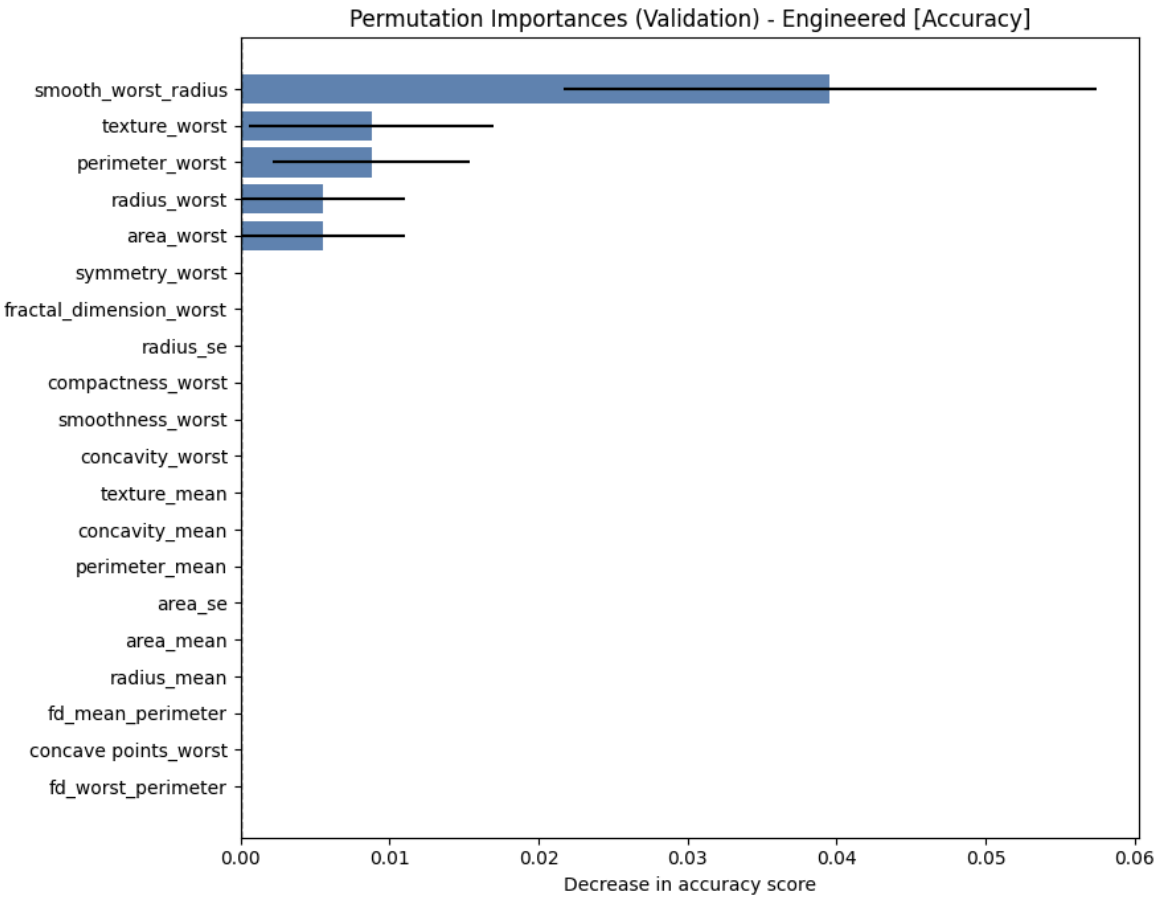
In [26]:
```
# Plotting the feature Importances
def plot_feature_importances(model, feature_names, title):
    importances = model.feature_importances_
    indices = importances.argsort()[::-1]
    plt.figure(figsize=(10,6))
    plt.title(title)
    plt.bar(range(len(importances)), importances[indices], color='b', align='cen
    plt.xticks(range(len(importances)), [feature_names[i] for i in indices], rot
    plt.tight_layout()
    plt.show()

# For engineered features
plot_feature_importances(best_rf_eng, X_val_eng.columns, "Feature Importances -

# For raw features
plot_feature_importances(best_rf_raw, X_val_raw.columns, "Feature Importances -
```

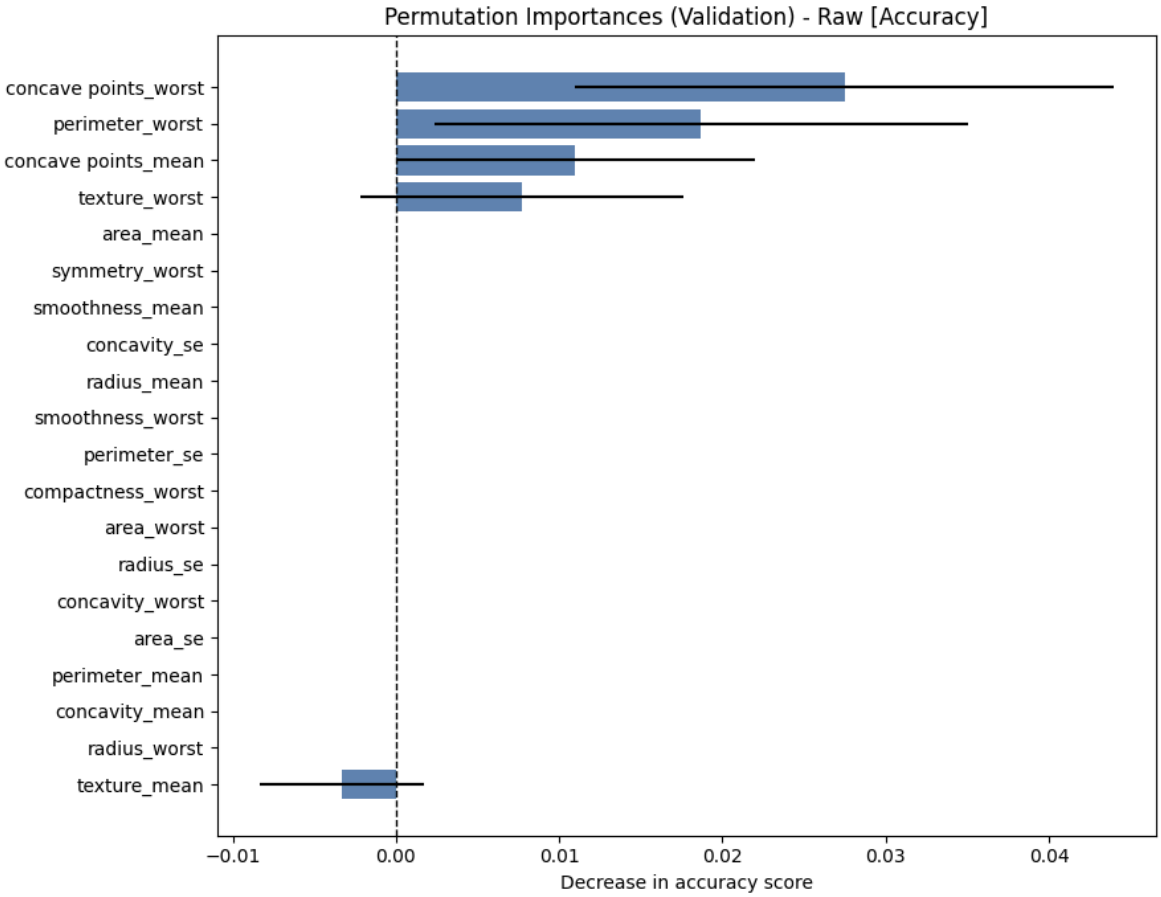




In [27]:
```
from sklearn.inspection import permutation_importance

def plot_perm_importances_hbar(importances_result, feature_names, title="Permuta
    # Extract means/stds and order by mean importance
    imp_mean = importances_result.importances_mean
    imp_std  = importances_result.importances_std
    order = np.argsort(imp_mean)  # ascending for barh

    # Build plot
    plt.figure(figsize=(9, max(6, 0.35*len(feature_names))))
    plt.barh(np.array(feature_names)[order], imp_mean[order], xerr=imp_std[order
             color="#4e79a7", alpha=0.9)
    plt.axvline(0.0, color="k", linestyle="--", linewidth=1)
    plt.title(title)
    plt.xlabel("Decrease in accuracy score")
    plt.tight_layout()
    plt.show()
```

```
# Engineered features on validation data
perm_importance_eng = permutation_importance(
    best_rf_eng, X_val_eng, y_val_eng,
    scoring="accuracy",
    n_repeats=10,
    random_state=42,
    n_jobs=-1
)

# Raw features on validation data
perm_importance_raw = permutation_importance(
    best_rf_raw, X_val_raw, y_val_raw,
    scoring="accuracy",
    n_repeats=10,
    random_state=42,
    n_jobs=-1
)

# Plots (same style as NN)
plot_perm_importances_hbar(perm_importance_eng, X_val_eng.columns, "Permutation
plot_perm_importances_hbar(perm_importance_raw, X_val_raw.columns, "Permutation
```





In [28]:
```
def select_features_above_threshold_perm(perm_result, feature_names, threshold):
    importances = perm_result.importances_mean
    selected = [(feature, imp) for feature, imp in zip(feature_names, importance
    # Sort in descending order of importance
    selected_sorted = sorted(selected, key=lambda x: x[1], reverse=True)
    return selected_sorted

# Select important engineered features using a threshold
selected_eng = select_features_above_threshold_perm(perm_importance_eng, X_val_e
print("Selected Engineered Features:", [f[0] for f in selected_eng])

# Select important raw features using a threshold
selected_raw = select_features_above_threshold_perm(perm_importance_raw, X_val_r
print("Selected Raw Features:", [f[0] for f in selected_raw])

# Combine unique features from both sets, keeping max importance when duplicated
combined_dict = {}
for feature, importance in selected_eng + selected_raw:
    if feature in combined_dict:
        combined_dict[feature] = max(combined_dict[feature], importance)
    else:
        combined_dict[feature] = importance

# Sort combined features by importance descending
combined_sorted = sorted(combined_dict.items(), key=lambda x: x[1], reverse=True
combined_features = [f[0] for f in combined_sorted]

print("Combined Unique Features:", len(combined_features))
print("Combined Feature Set:", combined_features)
```

```
Selected Engineered Features: ['smooth_worst_radius', 'texture_worst', 'perimeter
_worst', 'radius_worst', 'area_worst']
Selected Raw Features: ['concave points_worst', 'perimeter_worst', 'concave point
s_mean', 'texture_worst']
Combined Unique Features: 7
Combined Feature Set: ['smooth_worst_radius', 'concave points_worst', 'perimeter_
worst', 'concave points_mean', 'texture_worst', 'radius_worst', 'area_worst']
```

Section VII: Model Training and Evaluation on Combined Selected Features

In this final section, we leverage the curated combined feature set selected from previous importance and permutation importances to train a new Random Forest classifier. This streamlined feature space aims to retain the most predictive attributes while reducing model complexity and improving interpretability.

We again perform **hyperparameter tuning using RandomizedSearchCV** with a focused parameter grid tailored to this reduced feature set, optimizing for malignant recall as the primary metric. This ensures the model prioritizes detecting malignant cases effectively while maintaining balance across classes.

After fitting the best model, we evaluate it on validation and test splits using detailed classification reports. The results demonstrate strong performance with balanced precision, recall, and F1-scores, confirming that the combined feature approach yields a robust and efficient classifier suitable for downstream applications.

In [29]:
```
X_train_combined = X_train[combined_features]
X_val_combined = X_val[combined_features]
X_test_combined = X_test[combined_features]
y_train_combined = y_train
y_val_combined = y_val
y_test_combined = y_test
```

In [30]:
```
rf_combined = RandomForestClassifier(random_state=42, n_jobs=-1)

recall_malignant = make_scorer(recall_score, pos_label=1)
recall_benign = make_scorer(recall_score, pos_label=0)

scoring = {
    'recall_malignant': recall_malignant,
    'recall_benign': recall_benign
}

# Define hyperparameter distribution to search
param_dist = {
    'n_estimators': [100, 150, 200, 250],
    'max_depth': [3, 5, 7, None],
    'min_samples_split': [2, 4, 8],
    'min_samples_leaf': [1, 2, 4],
    'max_features': ['sqrt', 'log2', None],
    'class_weight': ['balanced', 'balanced_subsample', None]
}

random_search = RandomizedSearchCV(
    estimator=rf_combined,
```

```
    param_distributions=param_dist,
    n_iter=50,
    scoring=scoring,
    refit='recall_malignant',
    cv=stratified_cv,
    n_jobs=-1,
    verbose=2,
    random_state=42
)
# Fit on combined training data
random_search.fit(X_train_combined, y_train_combined)

# Best params and estimator
print("Best Hyperparameters:", random_search.best_params_)
best_rf_combined = random_search.best_estimator_

# Validate on validation set
y_val_pred = best_rf_combined.predict(X_val_combined)
print("Validation Classification Report:\n", classification_report(y_val_combine

# Test performance
y_test_pred = best_rf_combined.predict(X_test_combined)
print("Test Classification Report:\n", classification_report(y_test_combined, y_
```

```
Fitting 5 folds for each of 50 candidates, totalling 250 fits
Best Hyperparameters: {'n_estimators': 150, 'min_samples_split': 8, 'min_samples_
leaf': 2, 'max_features': 'log2', 'max_depth': None, 'class_weight': 'balanced'}
Validation Classification Report:
              precision    recall  f1-score   support

           0       0.97      0.98      0.97        57
           1       0.97      0.94      0.96        34

    accuracy                           0.97        91
   macro avg       0.97      0.96      0.96        91
weighted avg       0.97      0.97      0.97        91

Test Classification Report:
              precision    recall  f1-score   support

           0       0.97      1.00      0.99        72
           1       1.00      0.95      0.98        42

    accuracy                           0.98       114
   macro avg       0.99      0.98      0.98       114
weighted avg       0.98      0.98      0.98       114
```