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August 24, 2025

- 1 Feature Engineering for F&B Anomaly Detection
- 2 Creating Advanced Features for Quality Prediction

3

4 This script demonstrates comprehensive feature engineering techniques to extract meaningful patterns from the process data.

```
[15]: # Import required libraries
  import pandas as pd
  import numpy as np
  import matplotlib.pyplot as plt
  import seaborn as sns
  from scipy import stats
  from scipy.signal import find_peaks
  from sklearn.preprocessing import PolynomialFeatures
  import warnings
  warnings.filterwarnings('ignore')
```

```
[29]: # Machine Learning imports
from sklearn.preprocessing import StandardScaler, RobustScaler,
PolynomialFeatures
from sklearn.model_selection import train_test_split, cross_val_score,
GridSearchCV
from sklearn.feature_selection import SelectKBest, f_regression, RFE
from sklearn.metrics import r2_score, mean_squared_error, mean_absolute_error
```

```
[30]: # Models
from sklearn.ensemble import RandomForestRegressor, GradientBoostingRegressor
from sklearn.linear_model import LinearRegression, Ridge, Lasso
from sklearn.svm import SVR
import xgboost as xgb
```

```
[31]: # Import custom modules import sys
```

```
sys.path.append('..')
from src.data_processor import DataProcessor
from src.feature_engineer import FeatureEngineer
from src.config import PROCESS_PARAMS, FEATURE_CONFIG
```

```
[32]: # Set visualization style
plt.style.use('seaborn-v0_8-darkgrid')
%matplotlib inline
```

5 1. Load and Prepare Data

```
[33]: # Load and clean data
      processor = DataProcessor()
      process_data, quality_data = processor.load_data('../data/raw/
       →FnB_Process_Data_Batch_Wise.xlsx')
      clean_data = processor.clean_data(process_data)
      print(f"Data shape: {clean_data.shape}")
      print(f"Batches: {clean_data['Batch_ID'].nunique()}")
      print(f"Quality data available for {len(quality_data)} batches")
      # Verify quality data
      print("\nQuality Data Summary:")
      quality_df = pd.DataFrame.from_dict(quality_data, orient='index')
      print(quality_df.describe())
     2025-08-23 20:27:26.994 | INFO
     src.data_processor:__init__:34 - DataProcessor
     initialized
     2025-08-23 20:27:27.009 | INFO
     src.data_processor:load_data:50 - Loading data
     from ../data/raw/FnB_Process_Data_Batch_Wise.xlsx
     2025-08-23 20:27:27.674 | INFO
     src.data_processor:load_data:74 - Loaded 1500
     rows of process data
     2025-08-23 20:27:27.681 | INFO
     src.data_processor:load_data:75 - Loaded quality
     data for 25 batches
     2025-08-23 20:27:27.686 | INFO
     src.data_processor:clean_data:93 - Starting data
     cleaning process
     2025-08-23 20:27:27.705 | INFO
```

```
src.data_processor:clean_data:104 - Missing
values before cleaning: 0
2025-08-23 20:27:27.799 | INFO
src.data_processor:clean_data:117 - Missing
values after cleaning: 0
2025-08-23 20:27:27.814 | INFO
src.data_processor:clean_data:122 - Data cleaned:
1500 rows remaining
Data shape: (1500, 12)
Batches: 25
Quality data available for 25 batches
Quality Data Summary:
       Final Weight Quality Score
count
          25.000000
                         25.000000
          50.419969
                         89.319531
mean
          1.749105
std
                         4.926627
          48.059167
                         80.106050
min
25%
          49.196974
                         85.941539
50%
          49.998787
                         90.483178
75%
          51.270763
                         92.612621
          55.039415
max
                         96.710203
```

6 2. Initial Feature Extraction

2025-08-23 20:27:51.791 | INFO

```
src.feature_engineer:extract_batch_features:41 -
     Extracting batch features
     2025-08-23 20:27:54.225 | INFO
     src.feature_engineer:extract_batch_features:87 -
     Extracted 25 batch features with 282 features
     2025-08-23 20:27:54.232 | INFO
     src.feature engineer:extract batch features:91 -
     Quality data available for 25/25 batches
     Initial features shape: (25, 285)
     Number of features: 282
     Quality data available for 25/25 batches
[35]: # 3. Data Quality Assessment
[36]: print("=== DATA QUALITY ASSESSMENT ===")
     print("-" * 40)
     if 'Quality_Score' in batch_features.columns:
          # Target variable analysis
         quality_scores = batch_features['Quality_Score'].dropna()
         weight_scores = batch_features['Final_Weight'].dropna()
         print("Target Variable Analysis:")
         print(f" Total samples: {len(batch_features)}")
         print(f" Non-null quality scores: {len(quality_scores)}")
         print(f" Quality Score - Mean: {quality_scores.mean():.2f}%, Std:__
       print(f" Quality Score - Range: {quality_scores.min():.2f}% -__

¬{quality_scores.max():.2f}%")
          print(f" Final Weight - Mean: {weight_scores.mean():.2f} kg, Std: __
       →{weight_scores.std():.2f} kg")
          # Feature quality
         feature_cols = [col for col in batch_features.columns
                        if col not in ['Batch_ID', 'Quality_Score', 'Final_Weight']]
         print(f"\nFeature Quality Analysis:")
         print(f" Total features: {len(feature_cols)}")
         print(f" Features with missing values: {batch_features[feature_cols].
       ⇔isnull().any().sum()}")
         # Check for zero variance features
         zero_var_features = [col for col in feature_cols if batch_features[col].
       →var() < 1e-10]</pre>
         print(f" Features with zero/near-zero variance: {len(zero_var_features)}")
```

```
# Visualize target distribution
  fig, axes = plt.subplots(1, 2, figsize=(12, 4))
  axes[0].hist(quality_scores, bins=15, edgecolor='black', alpha=0.7)
  axes[0].set_xlabel('Quality Score (%)')
  axes[0].set_ylabel('Frequency')
  axes[0].set_title('Quality Score Distribution')
  axes[0].axvline(quality_scores.mean(), color='red', linestyle='--',
⇔label=f'Mean: {quality_scores.mean():.1f}')
  axes[0].legend()
  axes[1].hist(weight_scores, bins=15, edgecolor='black', alpha=0.7,_
⇔color='green')
  axes[1].set_xlabel('Final Weight (kg)')
  axes[1].set_ylabel('Frequency')
  axes[1].set_title('Final Weight Distribution')
  axes[1].axvline(weight_scores.mean(), color='red', linestyle='--',u
⇔label=f'Mean: {weight_scores.mean():.1f}')
  axes[1].legend()
  plt.tight_layout()
  plt.show()
```

=== DATA QUALITY ASSESSMENT ===

Target Variable Analysis:

Total samples: 25

Non-null quality scores: 25

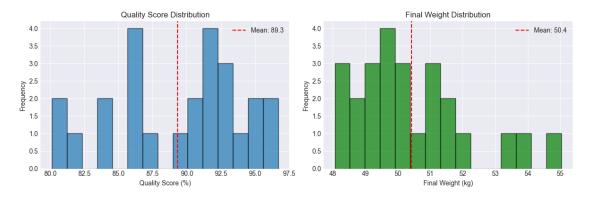
Quality Score - Mean: 89.32%, Std: 4.93% Quality Score - Range: 80.11% - 96.71% Final Weight - Mean: 50.42 kg, Std: 1.75 kg

Feature Quality Analysis:

Total features: 282

Features with missing values: 0

Features with zero/near-zero variance: 6



7 4. Advanced Feature Preprocessing

```
[37]: | print("=== ADVANCED FEATURE PREPROCESSING ===")
      print("-" * 40)
      # Remove features with zero variance
      good_features = [col for col in feature_cols if col not in zero_var_features]
      print(f"Removed {len(zero_var_features)} zero-variance features")
      print(f"Remaining features: {len(good_features)}")
      # Prepare data
      X = batch_features[good_features].copy()
      y_quality = batch_features['Quality_Score'].copy()
      y_weight = batch_features['Final_Weight'].copy()
      # Handle missing values intelligently
      print("\nHandling missing values...")
      for col in X.columns:
          if X[col].isnull().sum() > 0:
              # Use median for numerical features
              X[col].fillna(X[col].median(), inplace=True)
      # Handle target missing values
      y_quality.fillna(y_quality.median(), inplace=True)
      y_weight.fillna(y_weight.median(), inplace=True)
      print(f"Missing values after preprocessing: {X.isnull().sum().sum()}")
```

8 5. Outlier Detection and Removal

```
[38]: print("=== OUTLIER DETECTION AND REMOVAL ===")
print("-" * 40)

# Detect outliers in target variable using IQR method
Q1_q, Q3_q = y_quality.quantile([0.25, 0.75])
```

=== OUTLIER DETECTION AND REMOVAL ===

Samples before outlier removal: 25 Samples after outlier removal: 24 Outliers removed: 1

9 6. Feature Selection

```
# Method 2: Statistical feature selection (SelectKBest)
k_best = min(30, len(good_features))
selector_q = SelectKBest(score_func=f_regression, k=k_best)
selector_q.fit(X_clean, y_quality_clean)
statistical_features_q = X_clean.columns[selector_q.get_support()].tolist()
selector_w = SelectKBest(score_func=f_regression, k=k_best)
selector_w.fit(X_clean, y_weight_clean)
statistical_features_w = X_clean.columns[selector_w.get_support()].tolist()
statistical_features = list(set(statistical_features_q) | __
 ⇒set(statistical_features_w))
print(f"\nStatistically selected features: {len(statistical_features)}")
# Combine both methods
if len(high_corr_features) > 0:
    final_features = list(set(high_corr_features) & set(statistical_features))
    if len(final_features) < 10: # Ensure minimum features</pre>
        final_features = statistical_features[:min(20,__
 ⇔len(statistical features))]
else:
    final_features = statistical_features[:min(20, len(statistical_features))]
print(f"\nFinal selected features: {len(final_features)}")
print(f"Top 10 features:")
for i, feat in enumerate(final features[:10], 1):
    print(f" {i:2d}. {feat}")
# Prepare final dataset
X_final = X_clean[final_features]
=== FEATURE SELECTION ===
Features with correlation > 0.1 to quality: 189
Features with correlation > 0.1 to weight: 183
Combined high correlation features: 243
Statistically selected features: 58
Final selected features: 58
Top 10 features:
   1. Yeast (kg)_mean_change_rate
  2. Oven Humidity (%)_range
  3. Water Temp (C)_max_deviation
  4. Mixer Speed (RPM)_stability
  5. Oven Humidity (%)_max_consecutive_oot
```

```
6. Mixer Speed (RPM)_critical_deviation_ratio
7. Sugar (kg)_min
8. Yeast (kg)_trend_slope
9. Water Temp (C)_range
10. Yeast (kg)_std
[]:
```

10 7. Feature Scaling

Scaled feature matrix shape: (24, 58) Features scaled to mean=0, std=1

11 8. Model Comparison with Cross-Validation

```
[41]: print("=== MODEL COMPARISON WITH CROSS-VALIDATION ===")
      print("-" * 40)
      # Define models to test
      models = {
          'Linear Regression': LinearRegression(),
          'Ridge Regression': Ridge(alpha=1.0),
          'Lasso Regression': Lasso(alpha=0.1, max_iter=1000),
          'Random Forest': RandomForestRegressor(n_estimators=100, random_state=42,__
       →max_depth=8),
          'Gradient Boosting': GradientBoostingRegressor(n_estimators=100,__
       ⇒random_state=42, max_depth=4),
          'XGBoost': xgb.XGBRegressor(n_estimators=100, random_state=42, max_depth=4,__
       overbosity=0),
          'SVR': SVR(kernel='rbf', C=1.0, gamma='scale')
      }
      # Evaluate all models for Quality Score prediction
      print("\nQuality Score Prediction Performance:")
      print("-" * 40)
```

```
quality_results = {}
for name, model in models.items():
    try:
        cv_scores = cross_val_score(model, X_scaled, y_quality_clean,
                                    cv=min(5, len(X_scaled)), scoring='r2')
        quality_results[name] = {
            'mean_r2': cv_scores.mean(),
            'std_r2': cv_scores.std(),
            'scores': cv_scores
        }
        print(f''(name: 20s): R^2 = \{cv scores.mean(): +.4f\} (\pm \{cv scores.std()*2:...

4f})")
    except Exception as e:
        print(f"{name:20s}: Error - {str(e)}")
# Evaluate for Weight prediction
print("\nFinal Weight Prediction Performance:")
print("-" * 40)
weight_results = {}
for name, model in models.items():
    try:
        cv_scores = cross_val_score(model, X_scaled, y_weight_clean,
                                    cv=min(5, len(X_scaled)), scoring='r2')
        weight_results[name] = {
            'mean_r2': cv_scores.mean(),
            'std_r2': cv_scores.std(),
            'scores': cv_scores
        print(f"{name:20s}: R^2 = {cv_scores.mean():+.4f} (\pm {cv_scores.std()*2:.}

4f})")

    except Exception as e:
        print(f"{name:20s}: Error - {str(e)}")
```

=== MODEL COMPARISON WITH CROSS-VALIDATION ===

Quality Score Prediction Performance:

```
Linear Regression : R^2 = +0.3067 (±0.8558)

Ridge Regression : R^2 = +0.3366 (±0.8339)

Lasso Regression : R^2 = -0.7889 (±2.7205)

Random Forest : R^2 = -0.3169 (±0.8631)

Gradient Boosting : R^2 = -1.5013 (±3.4740)

XGBoost : R^2 = -0.2582 (±1.1811)

SVR : R^2 = -0.6632 (±1.1823)
```

Final Weight Prediction Performance:

Linear Regression : $R^2 = -1.9355$ (± 3.4878) Ridge Regression : $R^2 = -1.5056$ (± 3.1029) Lasso Regression : $R^2 = -1.0545$ (± 3.8877) Random Forest : $R^2 = -0.6820$ (± 3.1908) Gradient Boosting : $R^2 = -2.9779$ (± 10.3713) XGBoost : $R^2 = -1.1390$ (± 3.6065) SVR : $R^2 = -0.2507$ (± 0.8283)

12 9. Best Model Optimization

```
[42]: print("=== BEST MODEL OPTIMIZATION ===")
      print("-" * 40)
      # Find best model for quality prediction
      best_model_name_q = max(quality_results.keys(), key=lambda x:_
       ⇒quality results[x]['mean r2'])
      best_score_q = quality_results[best_model_name_q]['mean_r2']
      print(f"Best model for Quality: {best_model_name_q} (R2 = {best_score_q:.4f})")
      # Find best model for weight prediction
      best_model_name_w = max(weight_results.keys(), key=lambda x:_
       →weight_results[x]['mean_r2'])
      best_score_w = weight_results[best_model_name_w]['mean_r2']
      print(f"Best model for Weight: {best_model_name_w} (R2 = {best_score_w:.4f})")
      # Hyperparameter tuning for best quality model
      print("\nHyperparameter tuning for Quality Score prediction...")
      if 'Forest' in best_model_name_q:
          param_grid = {
              'n_estimators': [50, 100, 150],
              'max depth': [4, 6, 8, None],
              'min_samples_split': [2, 5],
              'min samples leaf': [1, 2]
          base_model = RandomForestRegressor(random_state=42)
      elif 'XGB' in best_model_name_q:
          param_grid = {
              'n_estimators': [50, 100, 150],
              'max_depth': [3, 4, 5],
              'learning_rate': [0.01, 0.1, 0.2]
          base_model = xgb.XGBRegressor(random_state=42, verbosity=0)
      elif 'Gradient' in best_model_name_q:
```

```
param_grid = {
        'n_estimators': [50, 100, 150],
        'max_depth': [3, 4, 5],
        'learning_rate': [0.01, 0.1, 0.2]
    base_model = GradientBoostingRegressor(random_state=42)
else:
    param_grid = {}
    base_model = models[best_model_name_q]
if param_grid:
    grid_search = GridSearchCV(base_model, param_grid, cv=min(5, len(X_scaled)),
                              scoring='r2', n_jobs=-1)
    grid_search.fit(X_scaled, y_quality_clean)
    print(f"Best parameters: {grid_search.best_params_}")
    print(f"Best CV score: {grid_search.best_score_:.4f}")
    best_model_q = grid_search.best_estimator_
    best_model_q = models[best_model_name_q]
    best_model_q.fit(X_scaled, y_quality_clean)
```

Hyperparameter tuning for Quality Score prediction...

13 10. Final Model Evaluation

```
best_model_w = RandomForestRegressor(n_estimators=100, max_depth=8,__
 →random_state=42)
else:
    best_model_w = models[best_model_name_w]
best_model_w.fit(X_train, y_train_w)
y pred w = best model w.predict(X test)
# Calculate metrics
quality_r2 = r2_score(y_test_q, y_pred_q)
quality_rmse = np.sqrt(mean_squared_error(y_test_q, y_pred_q))
quality_mae = mean_absolute_error(y_test_q, y_pred_q)
weight_r2 = r2_score(y_test_w, y_pred_w)
weight_rmse = np.sqrt(mean_squared_error(y_test_w, y_pred_w))
weight_mae = mean_absolute_error(y_test_w, y_pred_w)
print("Quality Score Prediction:")
print(f" R<sup>2</sup> Score: {quality_r2:.4f}")
print(f" RMSE: {quality_rmse:.4f}")
print(f" MAE: {quality_mae:.4f}")
print("\nFinal Weight Prediction:")
print(f" R<sup>2</sup> Score: {weight_r2:.4f}")
print(f" RMSE: {weight_rmse:.4f}")
print(f" MAE: {weight_mae:.4f}")
# Visualize predictions
fig, axes = plt.subplots(1, 2, figsize=(12, 5))
# Quality predictions
axes[0].scatter(y_test_q, y_pred_q, alpha=0.6)
axes[0].plot([y_test_q.min(), y_test_q.max()],
            [y_test_q.min(), y_test_q.max()], 'r--', lw=2)
axes[0].set xlabel('Actual Quality Score (%)')
axes[0].set_ylabel('Predicted Quality Score (%)')
axes[0].set_title(f'Quality Prediction (R2 = {quality_r2:.4f})')
axes[0].grid(True, alpha=0.3)
# Weight predictions
axes[1].scatter(y_test_w, y_pred_w, alpha=0.6, color='green')
axes[1].plot([y_test_w.min(), y_test_w.max()],
            [y_test_w.min(), y_test_w.max()], 'r--', lw=2)
axes[1].set_xlabel('Actual Weight (kg)')
axes[1].set_ylabel('Predicted Weight (kg)')
axes[1].set_title(f'Weight Prediction (R2 = {weight_r2:.4f})')
axes[1].grid(True, alpha=0.3)
```

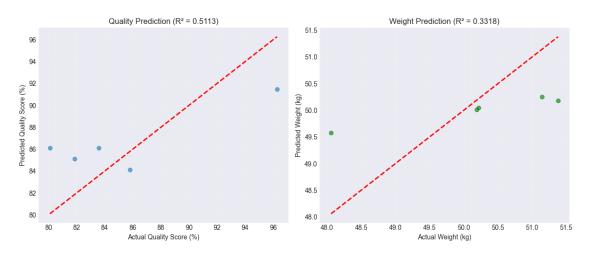
```
plt.tight_layout()
plt.show()
=== FINAL MODEL EVALUATION ===
```

Quality Score Prediction:

R² Score: 0.5113 RMSE: 3.9813 MAE: 3.6630

Final Weight Prediction:

R² Score: 0.3318 RMSE: 0.9583 MAE: 0.7892



14 11. Feature Importance Analysis

```
# Visualize feature importance
plt.figure(figsize=(10, 8))
top_features_plot = importance_df.head(15)
plt.barh(range(len(top_features_plot)), top_features_plot['Importance'])
plt.yticks(range(len(top_features_plot)), top_features_plot['Feature'])
plt.xlabel('Feature Importance')
plt.title(f'Top 15 Feature Importance ({best_model_name_q})')
plt.tight_layout()
plt.show()
```

=== FEATURE IMPORTANCE ANALYSIS ===

15 12. Save Engineered Features and Models

```
[45]: # Create final feature dataset with selected features
      final features df = pd.concat([
          batch_features[['Batch_ID']],
          X_final,
          batch_features[['Final_Weight', 'Quality_Score']]
      ], axis=1)
      # Save to CSV
      output_path = '../data/processed/feature_engineered_data.csv'
      final_features_df.to_csv(output_path, index=False)
      print(f"Features saved to: {output_path}")
      # Save the scaler
      import joblib
      scaler_path = '../data/models/scaler.pkl'
      joblib.dump(scaler, scaler_path)
      print(f"Scaler saved to: {scaler_path}")
      # Save feature names
      feature_names_path = '../data/processed/selected_features.txt'
      with open(feature_names_path, 'w') as f:
          for feature in final_features:
              f.write(f"{feature}\n")
      print(f"Feature names saved to: {feature_names_path}")
```

Features saved to: ../data/processed/feature_engineered_data.csv Scaler saved to: ../data/models/scaler.pkl Feature names saved to: ../data/processed/selected_features.txt

```
[46]: # 13. Final Summary and Recommendations
```

```
[]: print("="*60)
    print("FEATURE ENGINEERING SUMMARY")
    print("="*60)
    print(f"\n Data Processing:")
    print(f" - Original samples: {len(batch_features)}")
    print(f" - After outlier removal: {len(X clean)}")
    print(f" - Original features: {len(feature_cols)}")
    print(f" - Selected features: {len(final_features)}")
    print(f"\n Model Performance:")
    print(f" Quality Score Prediction:")
    print(f" - Best Model: {best_model_name_q}")
    print(f" - R<sup>2</sup> Score: {quality_r2:.4f}")
    print(f" - MAE: {quality_mae:.2f}%")
    print(f" Final Weight Prediction:")
    print(f" - Best Model: {best_model_name_w}")
    print(f" - R<sup>2</sup> Score: {weight_r2:.4f}")
    print(f" - MAE: {weight_mae:.2f} kg")
    print(f"\n Key Insights:")
    if quality_r2 > 0.5:
        print(" Good predictive performance achieved for quality score")
    elif quality r2 > 0.2:
        print(" Moderate predictive performance - consider collecting more data")
    else:
        print("
                  Low predictive performance - review feature engineering_
     →approach")
    if weight_r2 > 0.5:
        print(" Good predictive performance achieved for final weight")
    elif weight_r2 > 0.2:
        print(" Moderate predictive performance for weight prediction")
    else:
        print(" Low predictive performance for weight - needs improvement")
    print("\n" + "="*60)
```

FEATURE ENGINEERING SUMMARY

```
Data Processing:
```

- Original samples: 25
- After outlier removal: 24

- Original features: 282 - Selected features: 58

Model Performance:

Quality Score Prediction:

- Best Model: Ridge Regression

- R² Score: 0.5113

- MAE: 3.66%

Final Weight Prediction:

- Best Model: SVR - R² Score: 0.3318 - MAE: 0.79 kg

Key Insights:

Good predictive performance achieved for quality score Moderate predictive performance for weight prediction

The Kernel crashed while executing code in the current cell or a previous cell.

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