Analysis 2: Food Dataset from the U.S. Department of Agriculture

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Linear Regression

Dataset Information

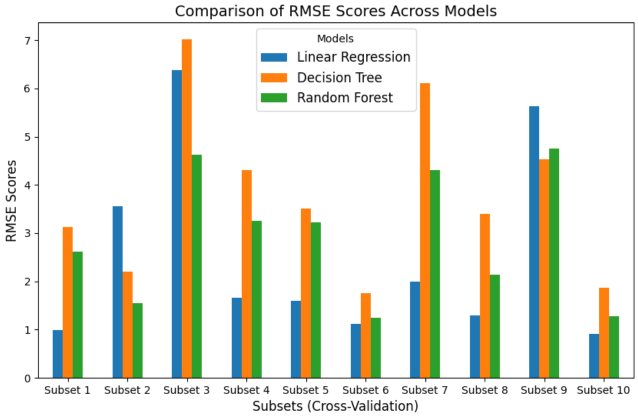
Dataset Information, Cleaning and Transformation

- SR Legacy Dataset: fdc.nal.usda.gov/download-datasets
- 7793 food items and 5 food nutrients – Carbohydrate (G) Energy (KCAL) Protein (G) Fat (G) Water (G) – were analyzed.
- Food items (rows) with missing nutrient values were removed from the dataset.
- Specific columns from the dataset – Food Names (e.g: "Bear, polar, meat, raw (Alaska Native)"), Food Categories (e.g: "American Indian/Alaska Native Foods"), Food Nutrient Amounts (e.g: "0.00 130.0 25.60 3.10 70.30"), and Nutrient Names ("Carbohydrate (G) Energy (KCAL) Protein (G) Fat (G) Water (G)") – were merged by shared id columns.
- The loaded dataset csv files were combined into a single dataframe for human readability.
- The resulting dataframe was saved in the file `food_dataset_reshaped.csv` inside the datasets folder `datasets/food_data_`2.
- All the missing values, if any, of the numerical nutrient columns were imputed with the mean of the respective nutrient column of the missing value.
- All the numerical nutrient columns were standardized through the transformation pipeline.

Linear Regression of the Protein Column

Root Mean Square Error (RMSE) values

The linear regression of the Protein Column of the Foundation Foods Database from the USDA was done by utilizing only a few major food nutrients – Carbohydrate, Energy, Fat, Water – as feature columns to predict the values of the label column – Protein.



Based on the RMSE values for each algorithm, we can evaluate the performance as follows:

	Linear Regression	Decision Tree	Random Forest
RMSE (Transformed Dataset)	2.8845	0.0008	0.7062
RMSE (Mean for subsets)	2.5108	3.8009	2.9790
RMSE (Standard deviation for subsets)	1.8943	1.5379	1.3743

Evaluation

RMSE (Transformed Dataset): The Decision Tree performs the best with a very low RMSE (0.0008), suggesting it's extremely overfitting to the dataset. This is unlikely to generalize well.

RMSE (Mean for subsets): The Linear Regression model has the lowest mean RMSE (2.5108), indicating better overall performance across subsets compared to the other models.

RMSE (Standard deviation for subsets): The Random Forest has the lowest standard deviation (1.3743), indicating the most stable performance across subsets, followed by the Decision Tree (1.5379), and the Linear Regression (1.8943).

Conclusion

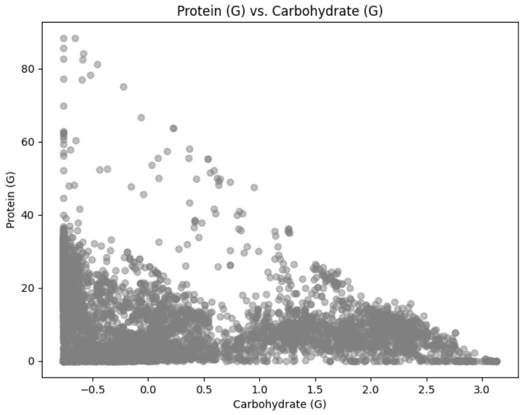
Best Overall Algorithm: Based on the mean and standard deviation of the RMSE values, the Random Forest model is likely the best-performing algorithm overall. It strikes a reasonable balance between good accuracy—its RMSE mean is relatively low—and stability, as it has the lowest standard deviation (the average deviation of RMSE values) among the algorithms.

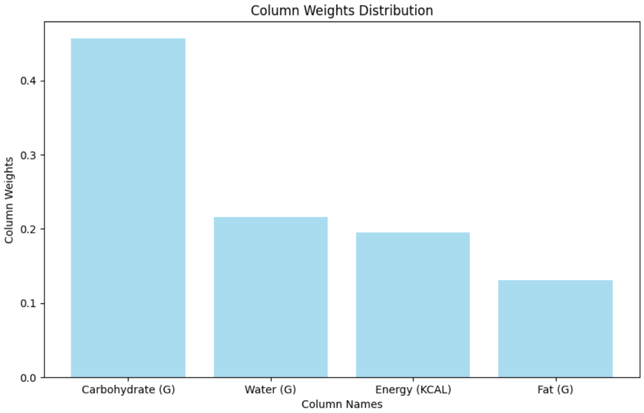
Overfitting Risk: The Decision Tree overfits on the transformed dataset and does not perform well across subsets, so it is not the best choice despite the low RMSE for the transformed dataset.

Thus, the Random Forest algorithm is the most reliable in terms of generalization and stability across subsets.

Linear Correlation and Column Weight

The carbohydrate column had the strongest negative linear correlation with the protein column and the highest column weight in predicting its values.



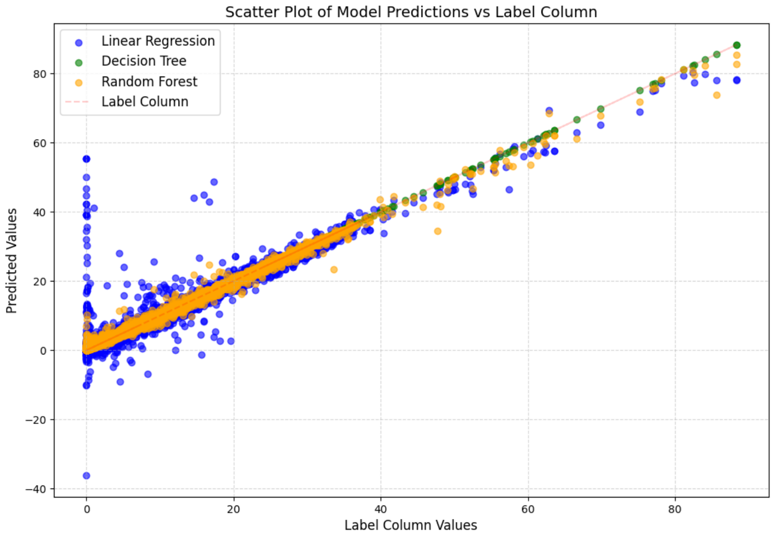


Prediction Columns

Some of the first protein values of the prediction columns made by the 3 algorithms –Linear Regression, Decision Tree, and Random Forest– and the label column with the true values:

```
Linear Regression,Decision Tree,Random Forest,Label Column
6.715908760633274,6.81,6.626399999999994,6.81
1.6468130378485188,0.99,1.299899999999999,0.99
3.5272559831981223,1.71,2.517100000000002,1.71
1.1876502536320412,0.52,0.5423000000000008,0.52
10.845169973353348,9.0,8.946900000000005,9.0
6.020795024133433,3.4,6.938999999999994,3.4
22.27595447156589,21.7,21.996600000000008,21.7
6.546676696946259,3.8,3.7119000000000035,3.8
18.81669569484038,20.1,20.060399999999973,20.1
24.042230735052414,25.6,25.382199999999962,25.6
```

And the next figure shows a graph between the predicted values of the prediction columns made by the algorithms and the original protein values of the label column:



Full Code

Listing 1: Linear Regression of the protein column from the Food Dataset of the USDA.

```
# Python STL
import os
import sys
import tarfile
import urllib.request
import shutil
import typing
import math

# Packages
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt

# Test Datasets
from sklearn.model_selection import train_test_split
from sklearn.model_selection import StratifiedShuffleSplit

# Tranformation Pipeline
from sklearn.impute import SimpleImputer
from sklearn.preprocessing import LabelEncoder
from sklearn.preprocessing import OneHotEncoder
from sklearn.preprocessing import LabelBinarizer
from sklearn.preprocessing import StandardScaler
from sklearn.base import BaseEstimator, TransformerMixin
from sklearn.pipeline import Pipeline
from sklearn.pipeline import FeatureUnion

# ML Algorithms
from sklearn.linear_model import LinearRegression
from sklearn.tree import DecisionTreeRegressor
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import cross_val_score
from sklearn.ensemble import RandomForestRegressor

# ML Models
```

```
import joblib
from sklearn.model_selection import GridSearchCV

# Modules




# Dataframe PD Display options
pd.set_option("display.max_columns", None)
pd.set_option("display.max_rows", None)
pd.set_option("display.max_colwidth", None)
pd.set_option("display.width", shutil.get_terminal_size().columns)
# Array NP Display Options
np.set_printoptions(threshold=np.inf)




# Paths
FILE_DIR = os.path.dirname(os.path.abspath(__file__))
PARENT_FILE_DIR = os.path.dirname(FILE_DIR)
PARENT_DIR = os.path.dirname(PARENT_FILE_DIR)
## Datasets
DATA_PATH = os.path.join(PARENT_DIR, "datasets")
FOOD_DATA_PATH = os.path.join(DATA_PATH, "food_data_2")
ZIP_FILE_PATH = os.path.join(FOOD_DATA_PATH, "food_data_files.zip")
EXTRACTED_PATH = os.path.join(FOOD_DATA_PATH, "food_data_files")
## Models
MODEL_DIR = os.path.join(PARENT_DIR, "models")
FOOD_MODEL_DIR = os.path.join(MODEL_DIR, "food_models_2")
## Images
IMAGES_DIR = os.path.join(PARENT_DIR, "img")
FOOD_IMAGES_DIR = os.path.join(IMAGES_DIR, "food_img_2")
GRAPHS_IMAGES_DIR = os.path.join(FOOD_IMAGES_DIR, "graphs")

directories = [DATA_PATH, FOOD_DATA_PATH, MODEL_DIR, FOOD_MODEL_DIR, IMAGES_DIR,
FOOD_IMAGES_DIR, GRAPHS_IMAGES_DIR]
for dir in directories:
    os.makedirs(dir, exist_ok=True)




# Download and Load the Dataset

def data_download(DATA_URL):

    urllib.request.urlretrieve(DATA_URL, ZIP_FILE_PATH)
    shutil.unpack_archive(ZIP_FILE_PATH, EXTRACTED_PATH)
    for root, dirs, files in os.walk(EXTRACTED_PATH, topdown=False):
        # Move files to extracted_path
        for file in files:
            src_file_path = os.path.join(root, file)
            dest_file_path = os.path.join(EXTRACTED_PATH, file)
            shutil.move(src_file_path, dest_file_path)
        # Remove empty directories
        if root != EXTRACTED_PATH:
            if not os.listdir(root):
                os.rmdir(root)

    print(f"\nDataset␣downloaded␣and␣extracted␣to:␣{EXTRACTED_PATH}.\n")

def data_load(DATA_URL):

    FOOD_PATH = os.path.join(EXTRACTED_PATH, "food.csv")
    FOOD_CATEGORY_PATH = os.path.join(EXTRACTED_PATH, "food_category.csv")
    FOOD_NUTRIENT_PATH = os.path.join(EXTRACTED_PATH, "food_nutrient.csv")
    NUTRIENT_PATH = os.path.join(EXTRACTED_PATH, "nutrient.csv")

    food_csv = pd.read_csv(FOOD_PATH)
    food_category_csv = pd.read_csv(FOOD_CATEGORY_PATH)
    food_nutrient_csv = pd.read_csv(FOOD_NUTRIENT_PATH, dtype={"footnote": "str"})
    nutrient_csv = pd.read_csv(NUTRIENT_PATH)

    print(f"Dataset␣loaded␣from␣the␣files␣inside:␣{EXTRACTED_PATH}.\n")
    return food_csv, food_category_csv, food_nutrient_csv, nutrient_csv




# Rename Columns
def rename_columns(df: pd.DataFrame, column_suffix_name: str) -> pd.DataFrame:

    if not isinstance(df, pd.DataFrame):
        raise TypeError("The␣input␣must␣be␣a␣pandas␣DataFrame.")

    return df.rename(columns={col: col + column_suffix_name for col in df.columns})




# Merge DataFrames
def merge_dataframes(df_left: pd.DataFrame, df_right: pd.DataFrame, key_left: str,
key_right: str, how: str = "left") -> pd.DataFrame:

    if not isinstance(df_left, pd.DataFrame) or not isinstance(df_right, pd.DataFrame):
        raise TypeError("Both␣inputs␣must␣be␣pandas␣DataFrames.")
    if key_left not in df_left.columns or key_right not in df_right.columns:
        raise ValueError(f"Specified␣keys␣’{key_left}’␣or␣’{key_right}’␣not␣found␣in␣
        the␣respective␣DataFrames.")

    return df_left.merge(df_right, left_on=key_left, right_on=key_right, how=how)




# Data Cleaning: Reshape Dataset
def reshape_dataset(food_dataset: pd.DataFrame, save_dataset: bool = False) -> pd.
DataFrame:

    # Get all unique nutrient names dynamically
    all_nutrients = food_dataset["name_nutrient"].unique()
    # print("All of the unique nutrient names inside food_dataset["name_nutrient"]
    column:\n", all_nutrients[:])

    # List of the relevant nutrients
    relevant_nutrients = [
        "Protein", "Carbohydrate,␣by␣difference", "Total␣lipid␣(fat)", "Energy",
        "Water", "Nitrogen"
    ]

    # Creates a subset of the dataset with rows containing only the relevant nutrients
    nutrients = food_dataset[food_dataset["name_nutrient"].isin(relevant_nutrients)].
    copy()

    # Combine name_nutrient ("Energy") and unit_name_nutrient ("KCAL") into a single
    column ("Energy (KCAL)")
    nutrients["name_unit_nutrient"] = nutrients["name_nutrient"] + "␣(" + nutrients["
    unit_name_nutrient"] + ")"

    # Rearranges rows into columns with values connected within the same row
    food_dataset_reshaped = nutrients.pivot_table(
        index=["description_food_category", "description_food"],
        columns="name_unit_nutrient",
        values="amount_food_nutrient",
        aggfunc="mean" # If there are 2 "columns" with equal names, it will take the
        mean of "values"
    ).reset_index()
    # print("Food Dataset reshaped:\n", food_dataset_reshaped.iloc[0:1])

    # Rename column names
    food_dataset_reshaped.columns.name = None
    food_dataset_reshaped.rename(
        columns={
            "description_food_category": "Category",
            "description_food": "Food",
            "Carbohydrate,␣by␣difference␣(G)": "Carbohydrate␣(G)",
            "Total␣lipid␣(fat)␣(G)": "Fat␣(G)"
        },
        inplace=True
    )
    # print("Food Dataset reshaped with renamed columns:\n", food_dataset_reshaped.iloc
    [0:1])

    # Delete columns and rows
    ## Delete specific columns
    food_dataset_reshaped = food_dataset_reshaped.drop(columns=["Energy␣(kJ)"])
    ## Delete columns where all values are missing
    food_dataset_reshaped = food_dataset_reshaped.dropna(axis=1, how="all")
    ## Delete rows where any relevant nutrient value is missing
    columns_to_check = list(food_dataset_reshaped.drop(columns={"Category", "Food"}))
    food_dataset_reshaped = food_dataset_reshaped.dropna(subset=columns_to_check)

    # Resets the index of rows to 0, 1, 2, 3, ...
    food_dataset_reshaped.reset_index(drop=True, inplace=True)

    # Convert the dataset to a CSV file
    if (save_dataset):
        food_dataset_reshaped_path = os.path.join(FOOD_DATA_PATH, "
        food_dataset_reshaped.csv")
        food_dataset_reshaped.to_csv(food_dataset_reshaped_path, index=False)
        print(f"\nFile␣converted␣to␣food_dataset_reshaped.csv␣and␣saved␣to␣{
        food_dataset_reshaped_path}.\n")

    return food_dataset_reshaped




# Transformation Pipeline
def transformation_pipeline(columns: list) -> Pipeline:

    # Selector: select the nutrients columns
    class CustomDataFrameSelector(BaseEstimator, TransformerMixin):

        def __init__(self, columns):
            self.columns = columns

        def fit(self, dataset, dataset_label = None):
            # self.columns = list(dataset.drop(columns=["Category", "Food", "Proteins (
            g)"]).columns)
            return self

        def transform(self, dataset, dataset_label = None):
            return dataset[self.columns]

    # Tranformation Pipeline
    full_pipeline = Pipeline([
        ("selector", CustomDataFrameSelector(columns)),  # Selects nutrient columns
        ("imputer", SimpleImputer(strategy="mean")),  # Handles missing values
        ("std_scaler", StandardScaler())  # Standardizes the columns
    ])

    return full_pipeline



# Standardized Columns
def standardization_column(dataset: pd.DataFrame, dataset_numerical_columns: list):

    print("Standardization␣of␣Columns␣(Mean␣=␣0,␣Standard␣Deviation␣=␣1):")
    for col in list(dataset_numerical_columns):
        print(f"Mean␣of␣{col}:␣", dataset[col].mean())
        print(f"Standard␣Deviation␣of␣{col}:␣", dataset[col].std(), "\n")




# Train Model
def train_models(
    dataset_transformed: np.ndarray,
    dataset_labels: pd.DataFrame,
    save_models: bool
):

    if (save_models == True):

        # Linear Regression
        lin_reg.fit(dataset_transformed, dataset_labels)
        lin_reg_path = os.path.join(FOOD_MODEL_DIR, "linear_regression_model.pkl")
        joblib.dump(lin_reg, lin_reg_path)
        dataset_predictions_lin = lin_reg.predict(dataset_transformed)
        lin_rmse = np.sqrt(mean_squared_error(dataset_labels, dataset_predictions_lin))
        lin_scores = cross_val_score(lin_reg, dataset_transformed, dataset_labels,
        scoring="neg_mean_squared_error", cv=10)
        lin_scores_rmse = np.sqrt(-lin_scores)

        # Decision Tree
        tree_reg.fit(dataset_transformed, dataset_labels)
        tree_reg_path = os.path.join(FOOD_MODEL_DIR, "decision_tree_model.pkl")
        joblib.dump(tree_reg, tree_reg_path)
        dataset_predictions_tree = tree_reg.predict(dataset_transformed)
        tree_rmse = np.sqrt(mean_squared_error(dataset_labels, dataset_predictions_tree
        ))
        tree_scores = cross_val_score(tree_reg, dataset_transformed, dataset_labels,
        scoring="neg_mean_squared_error", cv=10)
        tree_scores_rmse = np.sqrt(-tree_scores)

        # Random Forest
        forest_reg.fit(dataset_transformed, dataset_labels)
        forest_reg_path = os.path.join(FOOD_MODEL_DIR, "random_forest_model.pkl")
        joblib.dump(forest_reg, forest_reg_path)
        dataset_predictions_forest = forest_reg.predict(dataset_transformed)
        forest_rmse = np.sqrt(mean_squared_error(dataset_labels,
        dataset_predictions_forest))
        forest_scores = cross_val_score(forest_reg, dataset_transformed, dataset_labels
        , scoring="neg_mean_squared_error", cv=10)
        forest_scores_rmse = np.sqrt(-forest_scores)
    else:
        lin_reg_path = os.path.join(FOOD_MODEL_DIR, "linear_regression_model.pkl")
        tree_reg_path = os.path.join(FOOD_MODEL_DIR, "decision_tree_model.pkl")
        forest_reg_path = os.path.join(FOOD_MODEL_DIR, "random_forest_model.pkl")

        # Load pre-trained models
        lin_reg_loaded = joblib.load(lin_reg_path)
        tree_reg_loaded = joblib.load(tree_reg_path)
        forest_reg_loaded = joblib.load(forest_reg_path)

        dataset_predictions_lin = lin_reg_loaded.predict(dataset_transformed)
        dataset_predictions_tree = tree_reg_loaded.predict(dataset_transformed)
        dataset_predictions_forest = forest_reg_loaded.predict(dataset_transformed)

        lin_rmse = np.sqrt(mean_squared_error(dataset_labels, dataset_predictions_lin))
        lin_scores = cross_val_score(lin_reg_loaded, dataset_transformed,
        dataset_labels, scoring="neg_mean_squared_error", cv=10)
        lin_scores_rmse = np.sqrt(-lin_scores)

        tree_rmse = np.sqrt(mean_squared_error(dataset_labels, dataset_predictions_tree
        ))
        tree_scores = cross_val_score(tree_reg_loaded, dataset_transformed,
        dataset_labels, scoring="neg_mean_squared_error", cv=10)
        tree_scores_rmse = np.sqrt(-tree_scores)

        forest_rmse = np.sqrt(mean_squared_error(dataset_labels,
        dataset_predictions_forest))
        forest_scores = cross_val_score(forest_reg_loaded, dataset_transformed,
        dataset_labels, scoring="neg_mean_squared_error", cv=10)
        forest_scores_rmse = np.sqrt(-forest_scores)

    print("Linear␣Regression␣(RMSE␣of␣the␣transformed␣dataset):␣", lin_rmse)
    print("Linear␣Regression␣(RMSEs␣for␣10␣subsets):")
    print("RMSE␣for␣each␣subset:", lin_scores_rmse)
    print("Mean␣of␣the␣RMSEs:", lin_scores_rmse.mean())
    print("Standard␣deviation␣of␣the␣RMSEs:", lin_scores_rmse.std())
    print("\n")

    print("Decision␣Tree␣(RMSE␣of␣the␣transformed␣dataset):␣", tree_rmse)
    print("Decision␣Tree␣(RMSEs␣for␣10␣subsets):")
    print("RMSE␣for␣each␣subset:", tree_scores_rmse)
    print("Mean␣of␣the␣RMSEs:", tree_scores_rmse.mean())
    print("Standard␣deviation␣of␣the␣RMSEs:", tree_scores_rmse.std())
    print("\n")

    print("Random␣Forest␣(RMSE␣of␣the␣transformed␣dataset):␣", forest_rmse)
    print("Random␣Forest␣(RMSEs␣for␣10␣subsets):")
    print("RMSE␣for␣each␣subset:", forest_scores_rmse)
    print("Mean␣of␣the␣RMSEs:", forest_scores_rmse.mean())
    print("Standard␣deviation␣of␣the␣RMSEs:", forest_scores_rmse.std())
    print("\n")

    column_names = ["Linear␣Regression", "Decision␣Tree", "Random␣Forest"]
    RMSE_columns_arrays = np.column_stack([lin_scores_rmse, tree_scores_rmse,
    forest_scores_rmse])
    RMSE_columns = pd.DataFrame(RMSE_columns_arrays, columns=column_names)

    # Graph of RMSE Scores across subsets
    fig, ax = plt.subplots(figsize=(10, 6))
    RMSE_columns.plot(kind='bar', ax=ax)
    ax.set_title("Comparison␣of␣RMSE␣Scores␣Across␣Models", fontsize=14)
    ax.set_xlabel("Subsets␣(Cross-Validation)", fontsize=12)
    ax.set_ylabel("RMSE␣Scores", fontsize=12)
    ax.legend(title="Models", fontsize=12)
    plt.xticks(ticks=range(len(RMSE_columns)), labels=[f"Subset␣{i+1}" for i in range(
    len(RMSE_columns))], rotation=0)
    plt.savefig(os.path.join(GRAPHS_IMAGES_DIR, "RMSE_scores.png"))




# Prediction Columns
def prediction_columns(dataset_transformed: np.ndarray, dataset_labels: pd.DataFrame):

    lin_reg.fit(dataset_transformed, dataset_labels)
    tree_reg.fit(dataset_transformed, dataset_labels)
    forest_reg.fit(dataset_transformed, dataset_labels)

    dataset_predictions_lin = lin_reg.predict(dataset_transformed)
    dataset_predictions_tree = tree_reg.predict(dataset_transformed)
    dataset_predictions_forest = forest_reg.predict(dataset_transformed)
    column_names = ["Linear␣Regression", "Decision␣Tree", "Random␣Forest", "Label␣
    Column"]
    prediction_columns_arrays = np.column_stack([dataset_predictions_lin,
    dataset_predictions_tree, dataset_predictions_forest, dataset_labels])
    prediction_columns = pd.DataFrame(prediction_columns_arrays, columns=column_names)

    print("Prediction␣Columns:")
    print(prediction_columns.iloc[0:5])

    # Save the prediction columns dataframe as a csv file
    prediction_columns_path = os.path.join(FOOD_DATA_PATH, "prediction_columns.csv")
    prediction_columns.to_csv(prediction_columns_path, index=False)
    print(f"\nPrediction␣columns␣converted␣to␣prediction_columns.csv␣and␣saved␣to␣{
    prediction_columns_path}.\n")

    # Scatter plot: prediction columns vs label column
    plt.figure(figsize=(12,8))
    plt.scatter(prediction_columns["Label␣Column"], prediction_columns["Linear␣
    Regression"],color="blue",alpha=0.6,label="Linear␣Regression")
    plt.scatter(prediction_columns["Label␣Column"], prediction_columns["Decision␣Tree"
    ],color="green",alpha=0.6,label="Decision␣Tree")
    plt.scatter(prediction_columns["Label␣Column"], prediction_columns["Random␣Forest"
    ],color="orange",alpha=0.6,label="Random␣Forest")
    plt.plot(prediction_columns["Label␣Column"],prediction_columns["Label␣Column"],
    color="red",alpha=0.2,linestyle="--",label="Label␣Column")
    plt.title("Scatter␣Plot␣of␣Model␣Predictions␣vs␣Label␣Column", fontsize=14)
    plt.xlabel("Label␣Column␣Values", fontsize=12)
    plt.ylabel("Predicted␣Values", fontsize=12)
    plt.legend(fontsize=12)
    plt.grid(True, linestyle="--", alpha=0.5)
    plt.savefig(os.path.join(GRAPHS_IMAGES_DIR, "scatter_plot_prediction_columns.png"))




# Fine Tune Model
def fine_tune_model(
    dataset_transformed: np.ndarray,
    dataset_labels: pd.DataFrame,
    model: BaseEstimator,
    save_model: bool,
    model_name = "model",
) -> BaseEstimator:

    # Search for the best parameters for the model: minimum RMSE and best performance
    across the subsets
    param_grid = [
        {"n_estimators":[3,10,30], "max_features":[2,4,6,8]},
        {"bootstrap":[False], "n_estimators":[3,10], "max_features":[2,3,4]}
    ]
    grid_search = GridSearchCV(model, param_grid, cv=5, scoring="neg_mean_squared_error
    ")
    grid_search.fit(dataset_transformed, dataset_labels)

    best_parameters = grid_search.best_params_
    best_model = grid_search.best_estimator_
    best_model_predictions = best_model.predict(dataset_transformed)
    best_model_rmse = np.sqrt(mean_squared_error(dataset_labels, best_model_predictions
    ))

    cv_results = grid_search.cv_results_
    print("Mean␣of␣the␣RMSEs␣of␣the␣subsets␣for␣each␣parameter␣combination:")
    for mean_score, params in zip(cv_results["mean_test_score"], cv_results["params"]):
        print("Mean␣of␣the␣RMSEs:␣", np.sqrt(-mean_score), "for␣parameters:␣", params)

    print("Best␣parameters␣for␣the␣model:␣", best_parameters)
    print("Best␣model␣RMSE:␣", best_model_rmse)

    if (save_model):
        model_full_name = model_name + "_fine_tuned_model" + ".pkl"
        fine_tuned_model_path = os.path.join(FOOD_MODEL_DIR, model_full_name)
        joblib.dump(best_model, fine_tuned_model_path)
        print("\nFine-tuned␣model␣saved␣at:", fine_tuned_model_path, "\n")

    return best_model




# Column Weights
def column_weights(
    model: BaseEstimator,
    dataset_transformed: pd.DataFrame = None
):

    # Extract feature importance weights from the model
    column_weights = [float(weight) for weight in model.feature_importances_]

    # Get the column names of the transformed dataset
    columns = list(dataset_transformed.columns)

    # Pair and sort columns with their corresponding weights in descending order
    sorted_column_weights = sorted(zip(column_weights, columns), reverse=True)

    print("Column␣Weights:")
    print(sorted_column_weights, "\n")

    # Column Weights Graph
    weights, features = zip(*sorted_column_weights)
    plt.figure(figsize=(10, 6))
    plt.bar(features, weights, color=’skyblue’, alpha=0.7)
    plt.xticks(rotation=0)
    plt.xlabel(’Column␣Names’)
    plt.ylabel(’Column␣Weights’)
    plt.title(’Column␣Weights␣Distribution’)
    plt.savefig(os.path.join(GRAPHS_IMAGES_DIR, "column_weights.png"))




# Linear Correlation
def linear_correlation(dataset_numerical: pd.DataFrame, column_name: str, save_graphs:
bool):

    # Compute the correlation matrix
    corr_matrix = dataset_numerical.corr()
    linear_corr = corr_matrix[column_name].sort_values(ascending=False)

    # Plot scatter plots for each feature
    for col in dataset_numerical:
        if col == column_name:
            continue
        plt.figure(figsize=(8, 6))
        plt.scatter(dataset_numerical[col], dataset_numerical[column_name], alpha=0.5,
        c="gray")
        plt.title(f"{column_name}␣vs.␣{col}")
        plt.xlabel(col)
        plt.ylabel(column_name)
        plt.savefig(os.path.join(GRAPHS_IMAGES_DIR, f"linear_correlation_{column_name}_
        {col}.png"))

    return linear_corr




if __name__ == "__main__":

    # sys.exit("Sys.exit(): stops the code here.")

    # Download and Load the dataset files as DataFrames
    DATA_URL = "https://fdc.nal.usda.gov/fdc-datasets/
    FoodData_Central_sr_legacy_food_csv_2018-04.zip"
    data_download(DATA_URL)
    food_csv, food_category_csv, food_nutrient_csv, nutrient_csv = data_load(DATA_URL)

    # Add suffixes to column names to indicate their source
```

```
food_csv = rename_columns(food_csv, "_food")
food_category_csv = rename_columns(food_category_csv, "_food_category")
food_nutrient_csv = rename_columns(food_nutrient_csv, "_food_nutrient")
nutrient_csv = rename_columns(nutrient_csv, "_nutrient")

# Merge DataFrames to combine food, categories, and nutrient information
food_category_df = merge_dataframes(food_category_csv, food_csv, "id_food_category"
, "food_category_id_food")
food_nutrient_df = merge_dataframes(food_nutrient_csv, nutrient_csv, "
nutrient_id_food_nutrient", "id_nutrient")
food_merged_df = merge_dataframes(food_category_df, food_nutrient_df, "fdc_id_food"
, "fdc_id_food_nutrient")
print("Food␣Dataset␣merged␣dataframes:")
print(food_merged_df.iloc[0:10], "\n")

# Reshape the merged dataset: delete columns and create the ’Category’, ’Food’, and
 ’Nutrients’ columns
food_dataset_reshaped = reshape_dataset(food_dataset=food_merged_df, save_dataset=
True)
print(f"Food␣Dataset␣reshaped␣{food_dataset_reshaped.shape}:")
print(food_dataset_reshaped.iloc[0:10], "\n")

# ML Algorithms
lin_reg = LinearRegression()
tree_reg = DecisionTreeRegressor()
forest_reg = RandomForestRegressor()

# Split the dataset into label, nutrient, and textual columns
food_dataset = food_dataset_reshaped.drop(columns=["Protein␣(G)"])
food_dataset_labels = food_dataset_reshaped["Protein␣(G)"].copy()
food_dataset_nutrients = food_dataset.drop(columns=["Category", "Food"])
food_dataset_text = food_dataset.drop(columns=food_dataset_nutrients.columns)

print("Columns␣to␣be␣included␣in␣the␣transformation␣pipeline:")
print(list(food_dataset_nutrients.columns), "\n")

# Transformation Pipeline
full_pipeline = transformation_pipeline(list(food_dataset_nutrients.columns))
full_pipeline.fit(food_dataset_reshaped)
food_dataset_nutrients_transformed = full_pipeline.transform(food_dataset_reshaped)
# Merge the text, transformed nutrient columns, and labels into a single dataFrame
food_dataset_nutrients_transformed_df = pd.DataFrame(
food_dataset_nutrients_transformed, columns=food_dataset_nutrients.columns)
food_dataset_transformed = pd.concat([food_dataset_text,
food_dataset_nutrients_transformed_df, food_dataset_labels], axis=1)
# Check the standardization of the columns
print("Standardization␣of␣the␣nutrient␣columns␣made␣by␣the␣transformation␣pipeline
:\n")
```

```
standardization_column(food_dataset_transformed, list(food_dataset_nutrients.
columns))
# Display the food dataset transformed
print("Food␣Dataset␣after␣the␣transformation␣pipeline:")
print(food_dataset_transformed.iloc[0:1], "\n")




# Train the models: use the ML algorithms to create the prediction column and
measure their performance

# ML Algorithms
lin_reg = LinearRegression()
tree_reg = DecisionTreeRegressor()
forest_reg = RandomForestRegressor()

print("Root␣Mean␣Square␣Errors␣of␣the␣ML␣Algorithms\n")
train_models(
    dataset_transformed = food_dataset_nutrients_transformed,
    dataset_labels = food_dataset_labels,
    save_models = True
)

print("Prediction␣Columns␣created␣by␣the␣ML␣Algorithms\n")
prediction_columns(
        dataset_transformed = food_dataset_nutrients_transformed,
        dataset_labels = food_dataset_labels
    )

print("Results␣of␣the␣best␣model\n")
best_model = fine_tune_model(
    dataset_transformed = food_dataset_nutrients_transformed,
    dataset_labels = food_dataset_labels,
    model = forest_reg,
    save_model = True,
    model_name = "random_forest"
)

print("Column␣Weights␣created␣by␣the␣best␣model")
column_weights(
    model = best_model,
    dataset_transformed = food_dataset_transformed.drop(columns=["Category", "Food"
    , "Protein␣(G)"])
)

print("Linear␣Correlation␣between␣the␣nutrient␣columns␣and␣the␣label␣column")
linear_corr_protein = linear_correlation(
    dataset_numerical=food_dataset_transformed.drop(columns=["Category", "Food"]),
    column_name="Protein␣(G)",
    save_graphs=True
)
print(linear_corr_protein)
```

Appendix

Formulas

Mean

$$m = \frac{1}{n}\sum_{i=1}^{n} v_i$$

Variance

$$V = \frac{1}{n}\sum_{i=1}^{n}(v_i - m)^2$$

- Deviation from the mean: $v_i - mean$

Standard Deviation

$$SD = \sqrt{V}$$

Root Mean Square Error

$$RMSE(\boldsymbol{X}, h) = \sqrt{\frac{1}{m}\sum_{i=1}^{m}\left(h(x^{(i)}) - y^{(i)}\right)^2}$$

$$RMSE(\boldsymbol{Dataset}, MLAlgorithm) = \sqrt{\frac{1}{rows}\sum_{i=1}^{rows}\left(MLAlgorithm(predicted\,value^{(i)}) - label\,value^{(i)}\right)^2}$$

- Euclidean distance: straight line $d = \sqrt{\mathit{\Delta} x^2 + \mathit{\Delta} y^2}$
- The ML Algorithm takes into consideration all the column values of the dataset to form a column of predicted values.
- The RMSE measures the standard deviation of the predicted values from the label values.

Mean Absolute Error

$$MAE(\boldsymbol{X}, h) = \frac{1}{m} \sum_{i=1}^{m} \mid h(x^{(i)}) - y^{(i)} \mid$$

$$MAE(Dataset, MLAlgorithm) = \frac{1}{rows} \sum_{i=1}^{rows} \mid MLAlgorithm(predictedvalue^{(i)}) - labelvalue^{(i)} \mid$$

- Manhattan distance: grid $d = \mid \mathit{\Delta} x \mid + \mid \mathit{\Delta} y \mid$
- Both the RMSE and the MAE are ways to measure the distance between two vectors: the column of predicted values from the column of label values.
- The mean absolute error is preferred when the data has many outliers.

Difference between RMSE and Standard Deviation:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(y_{predicted}^{(i)} - y_{label}^{(i)} \right)^2}$$

$$STD = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(y_{predicted}^{(i)} - mean \right)^2}$$

RMSE (Root Mean Squared Error) measures the average magnitude (value) of the differences (errors) between the predicted values and the true values (labels). In other words, it's the average "distance" between the predicted values and the label values. It is the deviation from the label.

Standard Deviation measures the average distance of the differences between the predicted values from their own mean. It measures how spread out the values (in a dataset) are from the mean value. When applied to predictions, it measures how spread out the predicted values are from their own mean. It is the deviation from the mean.

Standardization of a Column

$$Column = V_0, V_1, V_2, V_3, ...V_n \rightarrow Column' = Z_0, Z_1, Z_2, Z_3, ...Z_n$$

$$Z_i = \frac{V_i - mean(Column)}{Standard\,Deviation(Column)}$$

$$Mean(Column') = \frac{1}{n}\sum_{i=1}^{n}(Z_i) \simeq 0$$

$$SD(Column') = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(Z_i - mean')^2} \simeq 1$$

Bibliography

[1] Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems

[2] Learning Deep Learning: Theory and Practice of Neural Networks, Computer Vision, Natural Language Processing, and Transformers Using Tensorflow

[3] Mathematics for Machine Learning