# Lab 1 — Interpretable by Design Models

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This lab covers three **interpretable-by-design** classifiers and how to extract meaningful explanations from each:

| Model | Interpretability type |
|---|---|
| **Decision Tree** | Global (tree structure, feature importance, depth trade-off) + Local (decision path) |
| **Logistic Regression** | Global (coefficients, odds ratios, correlation matrix) |
| **K-Nearest Neighbors** | Local (example-based, neighbor inspection + visualisation) |

**Guide:**

- ⚙️ Preprocessing recap
- 🌳 Decision Tree
- 📈 Logistic Regression
- 👥 KNN

## ⚙️ Preprocessing Recap (~10 min)

We are using the **Diabetes prediction dataset** and the same pipeline from Lab 0. Rather than stepping through every operation again, this section is structured as a **quick recap** — each cell highlights one key concept with a reminder of *why* it matters.

> 💡 The goal here is to consolidate what you learned in Lab 0, not to learn new things! By the end of this section you should be able to answer: *what would go wrong if you skipped each step?*

### ⚙️ Step 1 — Imports & Load

```
from google.colab import drive
drive.mount('/content/drive')
```

```
Mounted at /content/drive
```

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import OrdinalEncoder, OneHotEncoder, MinMaxScaler
from sklearn.metrics import classification_report, confusion_matrix, ConfusionMatrixDisplay
from sklearn import tree

# ── Load the dataset ──────────────────────────────────────────────
# Uncomment the line that matches your environment:
df = pd.read_csv('/content/drive/MyDrive/XAI 2026/diabetes.csv')  # Google Drive
# df = pd.read_csv('diabetes.csv')                                  # Local / GitHub

df.columns = [c.lower().replace('-', '_') for c in df.columns]
if 'class' in df.columns:
    df.rename(columns={'class': 'diabetes'}, inplace=True)
df['diabetes'] = (df['diabetes'].astype(str).str.strip().str.lower()
                  .map({'tested_positive': 1, 'tested_negative': 0,
                        '1': 1, '0': 0, 'positive': 1, 'negative': 0})
                  .astype(int))

print(f"Loaded {len(df)} rows  |  Columns: {df.columns.tolist()}")
df.head()
```

```
Loaded 100000 rows  |  Columns: ['gender', 'age', 'hypertension', 'heart_disease', 'smoking_history', 'bmi', 'hba
```

| | gender | age | hypertension | heart_disease | smoking_history | bmi | hba1c_level | blood_glucose_level | diabetes |
|---|---|---|---|---|---|---|---|---|---|
| **0** | Female | 80.0 | 0 | 1 | never | 25.19 | 6.6 | 140 | 0 |
| **1** | Female | 54.0 | 0 | 0 | No Info | 27.32 | 6.6 | 80 | 0 |
| **2** | Male | 28.0 | 0 | 0 | never | 27.32 | 5.7 | 158 | 0 |
| **3** | Female | 36.0 | 0 | 0 | current | 23.45 | 5.0 | 155 | 0 |
| **4** | Male | 76.0 | 1 | 1 | current | 20.14 | 4.8 | 155 | 0 |

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## Step 2 — Check Class Balance & Duplicates

> 🔑 **Key reminder:** an imbalanced dataset means **accuracy is a misleading metric**. If 91% of patients are non-diabetic, a model that always predicts "no diabetes" gets 91% accuracy — and is completely useless. Always check balance *before* splitting so you can choose `stratify=` and the right evaluation metric.

```
print("Class distribution:")
print(df['diabetes'].value_counts())
print(f"\nImbalance ratio: {df['diabetes'].value_counts()[0] / df['diabetes'].value_counts()[1]:.1f}:1")

# Duplicates
n_dupes = df.duplicated(keep=False).sum()
print(f"\nDuplicate rows: {n_dupes}")
df.drop_duplicates(inplace=True)
print(f"Rows after dedup: {len(df)}")
```

```
Class distribution:
diabetes
0    91500
1     8500
Name: count, dtype: int64

Imbalance ratio: 10.8:1

Duplicate rows: 6939
Rows after dedup: 96146
```

## Step 3 — Stratified Train/Test Split

> 🔑 **Key reminder:** split *before* any transformation. Fitting scalers or encoders on the full dataset lets test-set statistics leak into your preprocessing, making your evaluation overly optimistic — this is called **data leakage**. `stratify=` preserves the class ratio in both subsets.

```
df_train, df_test = train_test_split(
    df, test_size=0.2, shuffle=True, random_state=42, stratify=df['diabetes'])

print(f"Train: {len(df_train)} rows  |  Test: {len(df_test)} rows")
print(f"\nTrain class balance:\n{df_train['diabetes'].value_counts()}")
print(f"\nTest class balance:\n{df_test['diabetes'].value_counts()}")
```

```
Train: 76916 rows  |  Test: 19230 rows

Train class balance:
diabetes
0    70130
1     6786
Name: count, dtype: int64

Test class balance:
diabetes
0    17534
1     1696
Name: count, dtype: int64
```

## Step 4 — Feature Engineering & Encoding

> 🔑 **Key reminder:** ML models need numbers. Categorical features must be encoded, but the *type* of encoding matters:
>
> - **Ordinal Encoder** — when categories have a natural order (e.g. Child < Young < Adult < Senior)
> - **One-Hot Encoder** — when categories have no order (e.g. gender) Using the wrong encoder imposes false numeric relationships the model will exploit.

```
# ── Discretize age into 4 ordered bins ──────────────────────────────
age_bins   = [0, 14, 24, 50, 100]
age_labels = ['Child (0–14]', 'Young (14–24]', 'Adults (24–50]', 'Senior (50+]']
for d in [df_train, df_test]:
    d['age_disc'] = pd.cut(d['age'], bins=age_bins, labels=age_labels)
    d.drop(columns=['age'], inplace=True)

# ── Merge sparse smoking categories ─────────────────────────────────
# 'former' and 'not current' mean the same thing — combining them avoids sparse encoding
for d in [df_train, df_test]:
```

```
    d.loc[d['smoking_history'] == 'former', 'smoking_history'] = 'not current'

# ── Remove rare 'Other' gender rows (too few to encode reliably) ──────────────
df_train = df_train[df_train['gender'] != 'Other'].copy()
df_test  = df_test[df_test['gender']  != 'Other'].copy()

# ── Ordinal encode: smoking_history and age_disc (both have natural order) ────
smoking_order = ["never", "not current", "No Info", "current", "ever"]
ord_enc = OrdinalEncoder(categories=[smoking_order, age_labels])
ord_enc.fit(df_train[['smoking_history', 'age_disc']])   # fit on train only!
for d in [df_train, df_test]:
    d[['smoking_history', 'age_disc']] = ord_enc.transform(d[['smoking_history', 'age_disc']])

# ── One-hot encode: gender (no natural order) ─────────────────────────────────
ohe = OneHotEncoder(handle_unknown='ignore', sparse_output=False, drop='first')
ohe.fit(df_train[['gender']])                            # fit on train only!
for d in [df_train, df_test]:
    ohe_cols = pd.DataFrame(ohe.transform(d[['gender']]),
                            columns=ohe.get_feature_names_out(), index=d.index)
    d.drop(columns=['gender'], inplace=True)
    for col in ohe_cols.columns:
        d[col] = ohe_cols[col]

print("Encoding done. Columns:", df_train.columns.tolist())
df_train.head(3)
```

```
Encoding done. Columns: ['hypertension', 'heart_disease', 'smoking_history', 'bmi', 'hba1c_level', 'blood_glucose
```

| | hypertension | heart_disease | smoking_history | bmi | hba1c_level | blood_glucose_level | diabetes | age_disc | ge |
|---|---|---|---|---|---|---|---|---|---|
| **79000** | 0 | 0 | 2.0 | 23.87 | 5.7 | 126 | 0 | 2.0 | |
| **32011** | 0 | 0 | 1.0 | 33.03 | 4.0 | 126 | 0 | 3.0 | |
| **95559** | 0 | 0 | 2.0 | 27.32 | 6.6 | 126 | 0 | 2.0 | |

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## ⚙️ Step 5 — Scaling & Final Split

> 🔑 **Key reminder:** scaling is essential for distance-based models (KNN) and gradient-based models (Logistic Regression), which are sensitive to feature magnitude. Decision trees are *scale-invariant* — they only care about split thresholds, not absolute values. We scale anyway so all three models share the same `X_train` / `X_test`.

```
scale_cols = ['bmi', 'hba1c_level', 'blood_glucose_level', 'age_disc', 'smoking_history']

scaler = MinMaxScaler()
df_train[scale_cols] = scaler.fit_transform(df_train[scale_cols])  # fit on train only!
df_test[scale_cols]  = scaler.transform(df_test[scale_cols])

# ── Extract X / y ─────────────────────────────────────────────────────────────
y_train = df_train['diabetes'];  X_train = df_train.drop('diabetes', axis=1)
y_test  = df_test['diabetes'];   X_test  = df_test.drop('diabetes',  axis=1)
feature_names = X_train.columns.tolist()

print(f"X_train: {X_train.shape}  |  X_test: {X_test.shape}")
print(f"Features: {feature_names}")
```

```
X_train: (76902, 8)  |  X_test: (19226, 8)
Features: ['hypertension', 'heart_disease', 'smoking_history', 'bmi', 'hba1c_level', 'blood_glucose_level', 'age_
```

> ✅ **Preprocessing complete.** The three rules to always remember:
>
> 1. Split *before* fitting any transformer
> 2. Fit transformers on training data only, then `.transform()` both sets
> 3. Choose your encoding based on whether categories have a natural order

---

## Exercise 1 — Decision Tree 🌳

Decision trees are **interpretable by design**: the tree structure *is* the explanation — no separate explanation method needed.

They give a **transparent** and **intuitive** representation of the decision-making process followed by the model. This transparency allows domain experts to easily understand and validate the model's predictions.

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**Global interpretability** — inspecting the whole tree. . The measures for the global interpretability are:

- **Depth** → shallower = simpler, more interpretable
- **Node count / splits** → proxy for complexity. A larger tree with more nodes and splits may capture intricate patterns in the data but could also lead to overtting and decreased interpretability
- **Feature importances** → which features drive most decisions (via Gini impurity reduction)

**Local interpretability** — local path for a single prediction.Then, as mesures for the local interpretability there is:

- **Length of the decision path** → the exact sequence of rules that routed this instance to its leaf

### Your tasks

1. Fit a `DecisionTreeClassifier`.

> - Visualize the decision tree obtained. Are you able to interpret the decision
> - Try again with `max_depth=4` and compare the two trees. Which one is the most interpretable?

2. Analyze **Global Interpretability**: Continue visualizing the obtained decision tree with `max_depth=4` .

> - Which attributes are the **most discriminating**? Plot the feature importances and then analyze the values.
> - Calculate the size of the decision tree in terms of the number of nodes, subdivisions, and depth. How these metrics affect the interpretability of the decision tree globally?

3. Analyze **Local Interpretability**: Consider the instances *100, 150 and 200* of the train dataset.

> - What are the individual paths? What are the instances allocated in the paths?
>
>> - For each of the previous instances, calculate the **length** of each path from the root node to the leaf node to which the instance belongs. How the length of these paths contributes to the interpretability of the decision tree locally?

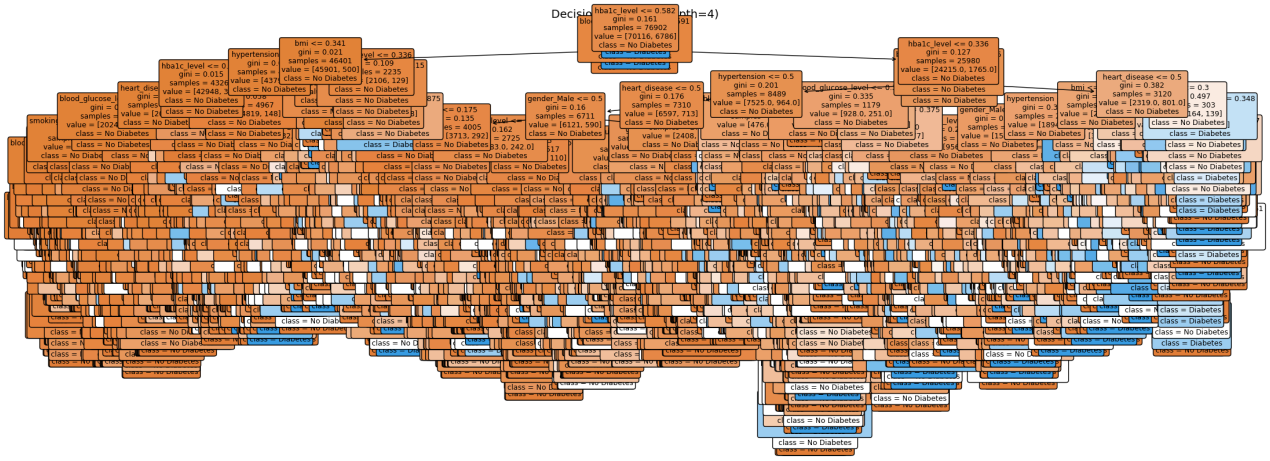
## 1.1 — Fit & Visualise

```
# ── 1.1 Depth vs Accuracy ──────────────────────────────────────
depths = range(1, 10)
train_accs, test_accs = [], []

for d in depths:
    dt = tree.DecisionTreeClassifier(max_depth=d, random_state=42)
    dt.fit(X_train, y_train)
    train_accs.append(dt.score(X_train, y_train))
    test_accs.append(dt.score(X_test, y_test))

fig, ax = plt.subplots(figsize=(8, 4))
ax.plot(depths, train_accs, 'o-', label='Train accuracy')
ax.plot(depths, test_accs,  's-', label='Test accuracy')
ax.axvline(4, color='red', linestyle='--', label='Depth = 4 (interpretable)')
ax.set_xlabel('Max Depth')
ax.set_ylabel('Accuracy')
ax.set_title('Decision Tree: Depth vs. Accuracy')
ax.legend()
ax.grid(True, alpha=0.3)
plt.tight_layout()
plt.savefig('dt_depth_accuracy.png', dpi=120)
plt.close()
print("Saved: dt_depth_accuracy.png")

best_test_depth = depths[np.argmax(test_accs)]
print(f"Best depth by test accuracy: {best_test_depth}")
#print(f"Test accuracy at depth=4: {test_accs[3]:.4f}")
print(f"Test accuracy at best depth ({best_test_depth}): {max(test_accs):.4f}")
```

```
Saved: dt_depth_accuracy.png
Best depth by test accuracy: 2
Test accuracy at best depth (2): 0.9716
```

```
#### START CODE HERE ####
# define the model
model = tree.DecisionTreeClassifier()
# fit the model
model.fit(X_train, y_train)
# extract the feature names
feature_names = X_train.columns
```

```
# This is the code to plot the decision tree dt
plt.figure(figsize=(22, 8))
tree.plot_tree(model, feature_names=feature_names,
               class_names=['No Diabetes', 'Diabetes'],
               filled=True, rounded=True, fontsize=9)
plt.title("Decision Tree (max_depth=4)", fontsize=14)
plt.tight_layout()
plt.show()

### OR you can plot directly with tree.plot_tree(model, feature_names=feature_names)

#### END CODE HERE ####
```



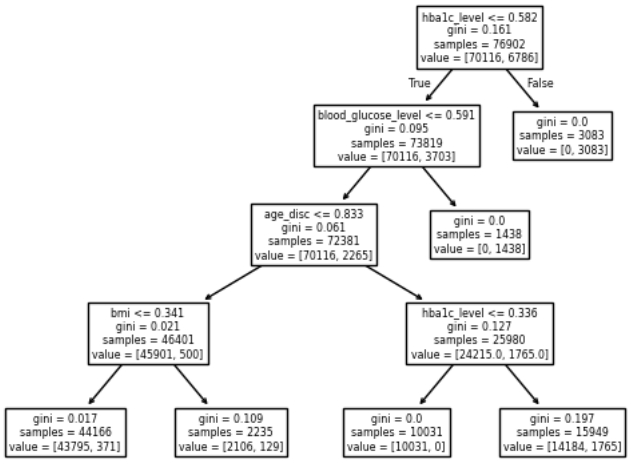
```
# Decision Tree Predict
y_pred = model.predict(X_test)
print('Model accuracy: ', model.score(X_test, y_test)*100)
```

```
Model accuracy:  95.07957973577447
```

## 1.2 — Max Depth 4

```
#### START CODE HERE -- Decision Tree max_depth=4 ####
# define the model with max_depth = 4
model = tree.DecisionTreeClassifier(max_depth=4)
# fit the model
model.fit(X_train, y_train)
# extract the feature names
feature_names = X_train.columns
tree.plot_tree(model, feature_names=feature_names)
#### END CODE HERE ####
```

```
[Text(0.75, 0.9, 'hba1c_level <= 0.582\ngini = 0.161\nsamples = 76902\nvalue = [70116, 6786]'),
 Text(0.625, 0.7, 'blood_glucose_level <= 0.591\ngini = 0.095\nsamples = 73819\nvalue = [70116, 3703]'),
 Text(0.6875, 0.8, 'True  '),
 Text(0.5, 0.5, 'age_disc <= 0.833\ngini = 0.061\nsamples = 72381\nvalue = [70116, 2265]'),
 Text(0.25, 0.3, 'bmi <= 0.341\ngini = 0.021\nsamples = 46401\nvalue = [45901, 500]'),
 Text(0.125, 0.1, 'gini = 0.017\nsamples = 44166\nvalue = [43795, 371]'),
 Text(0.375, 0.1, 'gini = 0.109\nsamples = 2235\nvalue = [2106, 129]'),
 Text(0.75, 0.3, 'hba1c_level <= 0.336\ngini = 0.127\nsamples = 25980\nvalue = [24215.0, 1765.0]'),
 Text(0.625, 0.1, 'gini = 0.0\nsamples = 10031\nvalue = [10031, 0]'),
 Text(0.875, 0.1, 'gini = 0.197\nsamples = 15949\nvalue = [14184, 1765]'),
 Text(0.75, 0.5, 'gini = 0.0\nsamples = 1438\nvalue = [0, 1438]'),
 Text(0.875, 0.7, 'gini = 0.0\nsamples = 3083\nvalue = [0, 3083]'),
 Text(0.8125, 0.8, '  False')]
```

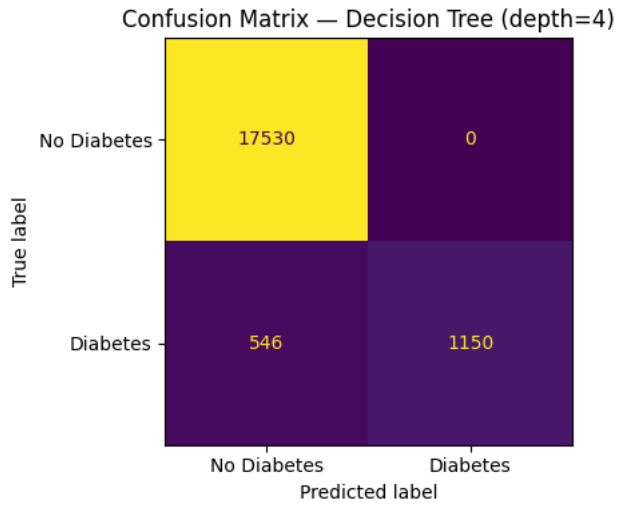



```
# Decision Tree Predict
y_pred = model.predict(X_test)
print('Model accuracy: ', model.score(X_test, y_test)*100)
```

```
Model accuracy:  97.16009570373453
```

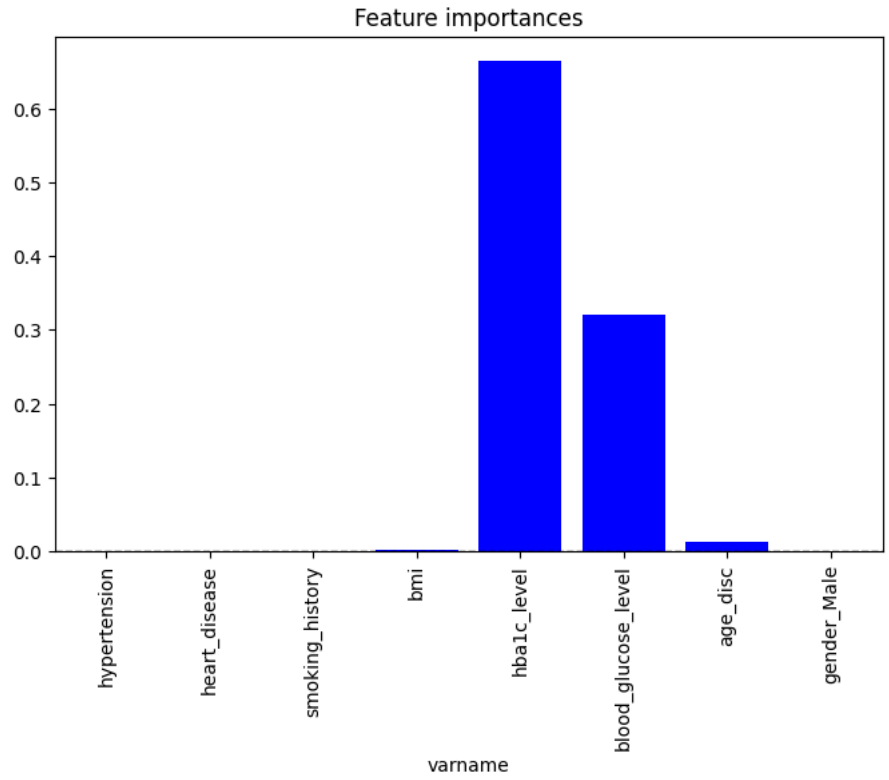
```
print("\n--- Classification Report (DT, depth=4) ---")
print(classification_report(y_test, y_pred, target_names=['No Diabetes', 'Diabetes']))

cm = confusion_matrix(y_test, y_pred)
disp = ConfusionMatrixDisplay(confusion_matrix=cm, display_labels=['No Diabetes','Diabetes'])
fig, ax = plt.subplots(figsize=(5, 4))
disp.plot(ax=ax, colorbar=False)
ax.set_title('Confusion Matrix — Decision Tree (depth=4)')
plt.tight_layout()
```

```
--- Classification Report (DT, depth=4) ---
              precision    recall  f1-score   support

 No Diabetes       0.97      1.00      0.98     17530
    Diabetes       1.00      0.68      0.81      1696

    accuracy                           0.97     19226
   macro avg       0.98      0.84      0.90     19226
weighted avg       0.97      0.97      0.97     19226
```



## 1.3 — Global Interpretability

```
#### START CODE HERE -- Decision Tree Global Interpretability ####

#Plot the feature importances and PLOT
importance = model.feature_importances_

#Plot the weights
coef_df = pd.DataFrame({'coef': importance,
                        'varname': X_train.columns
                       })

coef_df.plot(y='coef', x='varname', kind='bar', color='none', legend=False, figsize=(8,5))
plt.bar(coef_df['varname'], coef_df['coef'], color='blue')
plt.axhline(y=0, linestyle='--', color='black', linewidth=1)
#plt.title("Coefficients of Logistic Regression")
plt.title("Feature importances")
plt.show()

#### END CODE HERE ####
```




```
# Feature importances
importances = model.feature_importances_

# Display feature importances
feature_importance_df = pd.DataFrame({'Feature': feature_names, 'Importance': importances})
feature_importance_df = feature_importance_df.sort_values(by='Importance', ascending=False)
print(feature_importance_df)
```

```
              Feature  Importance
4          hba1c_level    0.665046
5  blood_glucose_level    0.320518
6             age_disc    0.013182
3                  bmi    0.001253
2      smoking_history    0.000000
1        heart_disease    0.000000
0         hypertension    0.000000
7          gender_Male    0.000000
```

```
# Compute the number of nodes
num_nodes = model.tree_.node_count
print(num_nodes)
```

```
11
```

```
# Compute the number of splits
num_splits = num_nodes - 1  # Total number of splits is one less than the number of nodes
```

```
print(num_splits)
```

```
10
```

```
#Compute the depth
depth = model.tree_.max_depth
print(depth)
```

```
4
```

## 1.4 — Local Interpretability: Decision Paths

```
#### START CODE HERE -- Decision Tree Local Interpretability ####
print("\n--- Local Interpretability: Decision Paths ---")
instance_indices = [100, 150, 200]
node_indicator = model.decision_path(X_train)
leaf_id = model.apply(X_train)
threshold = model.tree_.threshold
feature_idx = model.tree_.feature

for sample_id in instance_indices:
    node_ids = node_indicator[sample_id].indices
    pred = model.predict(X_train.iloc[[sample_id]])[0]
    actual = y_train.iloc[sample_id]
    print(f"\n{'-'*55}")
    print(f"Instance {sample_id} | Predicted: {'Diabetes' if pred==1 else 'No Diabetes'} | Actual: {'Diabetes' i
    print(f"Path length: {len(node_ids)} nodes")
    for node_id in node_ids[:-1]:
        feat = feature_names[feature_idx[node_id]]
        thresh = threshold[node_id]
        val = X_train.iloc[sample_id, feature_idx[node_id]]
        direction = "<=" if val <= thresh else ">"
        print(f"  Node {node_id}: {feat} = {val:.3f}  {direction}  {thresh:.3f}")
    print(f"  → Leaf {leaf_id[sample_id]}: class = {'Diabetes' if pred==1 else 'No Diabetes'}")
#### END CODE HERE ####
```

```
--- Local Interpretability: Decision Paths ---

-------------------------------------------------------
Instance 100 | Predicted: Diabetes | Actual: Diabetes
Path length: 2 nodes
  Node 0: hba1c_level = 0.855  >  0.582
  → Leaf 10: class = Diabetes

-------------------------------------------------------
Instance 150 | Predicted: No Diabetes | Actual: No Diabetes
Path length: 5 nodes
  Node 0: hba1c_level = 0.491  <=  0.582
  Node 1: blood_glucose_level = 0.295  <=  0.591
  Node 2: age_disc = 1.000  >  0.833
  Node 6: hba1c_level = 0.491  >  0.336
  → Leaf 8: class = No Diabetes

-------------------------------------------------------
Instance 200 | Predicted: No Diabetes | Actual: No Diabetes
Path length: 5 nodes
  Node 0: hba1c_level = 0.491  <=  0.582
  Node 1: blood_glucose_level = 0.091  <=  0.591
  Node 2: age_disc = 0.000  <=  0.833
  Node 3: bmi = 0.138  <=  0.341
  → Leaf 4: class = No Diabetes
```

> **Reflection:** Look at the path lengths for your three instances. A shorter path means fewer rules were needed — usually a more "clear-cut" case. Do instances with shorter paths have more extreme feature values (very high blood glucose, very high HbA1c)?

---

# Exercise 2 — Logistic Regression 📈

Logistic Regression is interpretable through its **coefficients** and derived **odds ratios**. Unlike Linear regression, the interpretation of logistic regression weights varies since the outcome in logistic regression is a probability confined within the range of 0 to 1. These weights undergo transformation through the logistic function, influencing the probability non-linearly.

- **Coefficient > 0** → feature increases the log-odds of the positive class (diabetes)
- **Coefficient < 0** → feature decreases the log-odds
- **Odds ratio = exp(coef)** → multiplicative change in odds for a 1-unit increase in the feature

- OR > 1 ⟶ increases odds of diabetes
- OR < 1 ⟶ decreases odds of diabetes
- OR = 1 ⟶ no effect

### Your tasks

1. Fit a **Logistic Regression** model on the same dataset as before.
2. Compute the Correlation Matrix.
3. Evaluate the model using Precision, Recall and F1-score metrics.
4. Analyze **Interpretability**:

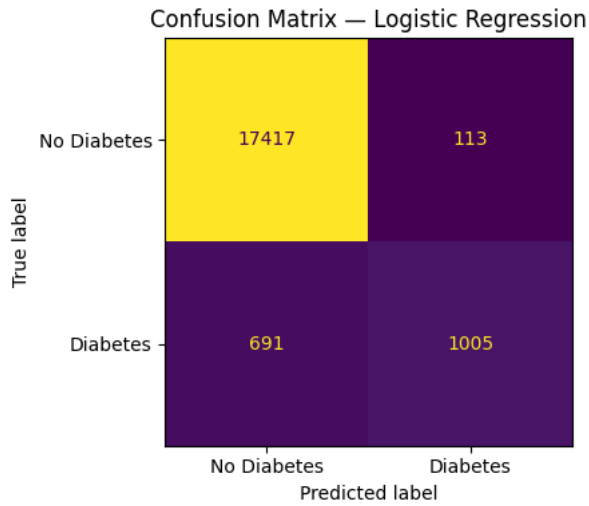
> - Visualize the estimated **weights** and **odds ratios** obtained from logistic regression for each feature.
> - Put them into a tabular form and interpret the logistic regression model for different types of features. Specifically, analyze the ***bmi*** feature and ***gender_Male*** and ***gender_Female*** features.

## 2.1 — Fit & Evaluate

```
from sklearn.linear_model import LogisticRegression

#### START CODE HERE ####
lr = LogisticRegression(max_iter=1000, C=0.1, random_state=42, solver='lbfgs')
lr.fit(X_train, y_train)
y_pred_lr = lr.predict(X_test)
#### END CODE HERE ####
```

```
print("\n--- Classification Report (Logistic Regression) ---")
print(classification_report(y_test, y_pred_lr, target_names=['No Diabetes', 'Diabetes']))

cm_lr = confusion_matrix(y_test, y_pred_lr)
disp_lr = ConfusionMatrixDisplay(confusion_matrix=cm_lr, display_labels=['No Diabetes','Diabetes'])
fig, ax = plt.subplots(figsize=(5, 4))
disp_lr.plot(ax=ax, colorbar=False)
ax.set_title('Confusion Matrix — Logistic Regression')
plt.tight_layout()
```

```
--- Classification Report (Logistic Regression) ---
              precision    recall  f1-score   support

 No Diabetes       0.96      0.99      0.98     17530
    Diabetes       0.90      0.59      0.71      1696

    accuracy                           0.96     19226
   macro avg       0.93      0.79      0.85     19226
weighted avg       0.96      0.96      0.95     19226
```

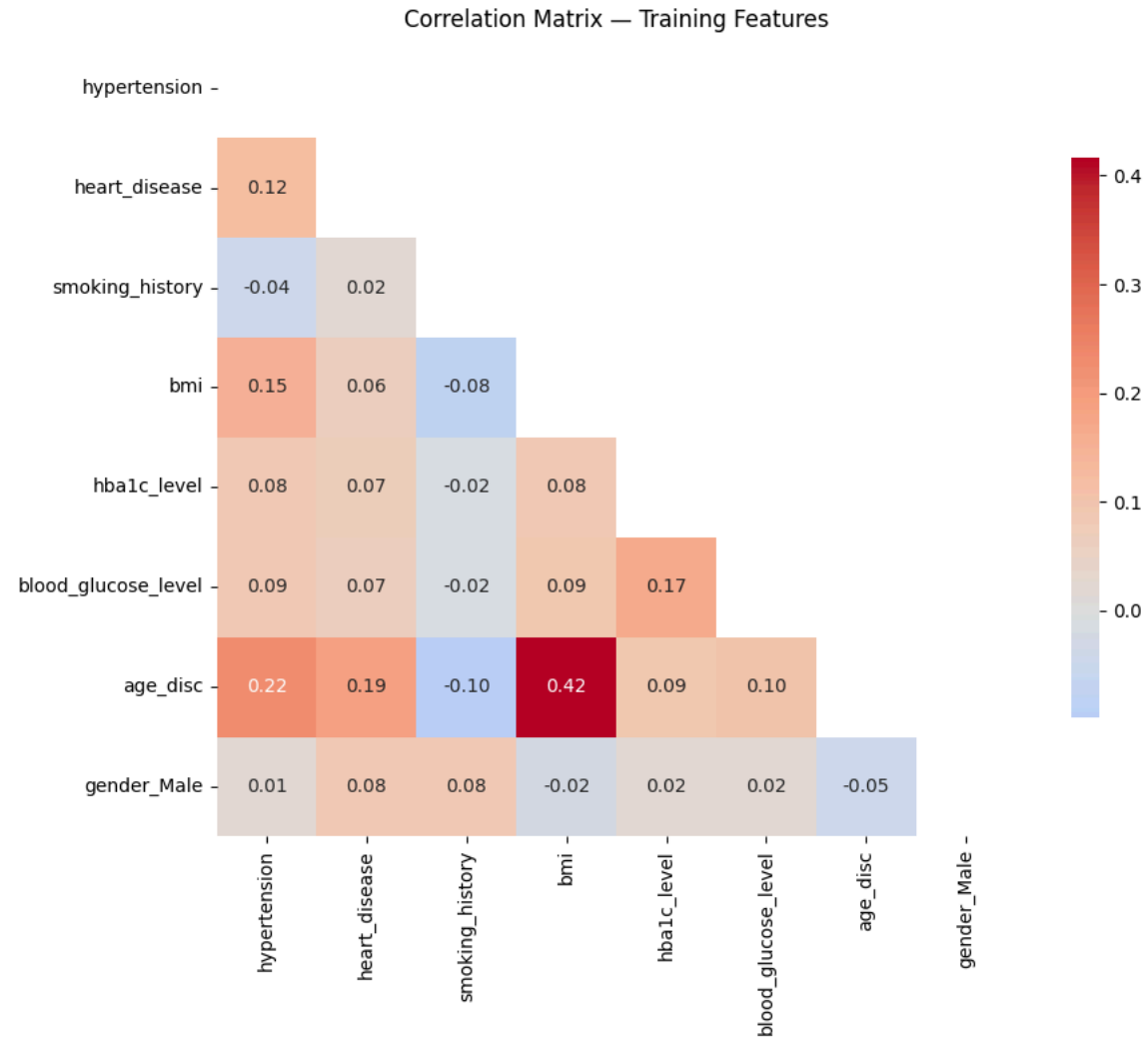



## 2.2 — Correlation Matrix

> 🔑 Before interpreting coefficients, always check for **multicollinearity** — when two features are highly correlated, the model distributes their shared explanatory power between them arbitrarily. This makes individual coefficients unreliable

as explanations, even if the model's predictions are fine.

```
#### START CODE HERE ####
fig, ax = plt.subplots(figsize=(10, 8))
corr = X_train.corr()
mask = np.triu(np.ones_like(corr, dtype=bool))
sns.heatmap(corr, mask=mask, annot=True, fmt='.2f', cmap='coolwarm',
            center=0, square=True, ax=ax, cbar_kws={'shrink': 0.7})
ax.set_title('Correlation Matrix — Training Features')
plt.tight_layout()
#### END CODE HERE ####
```

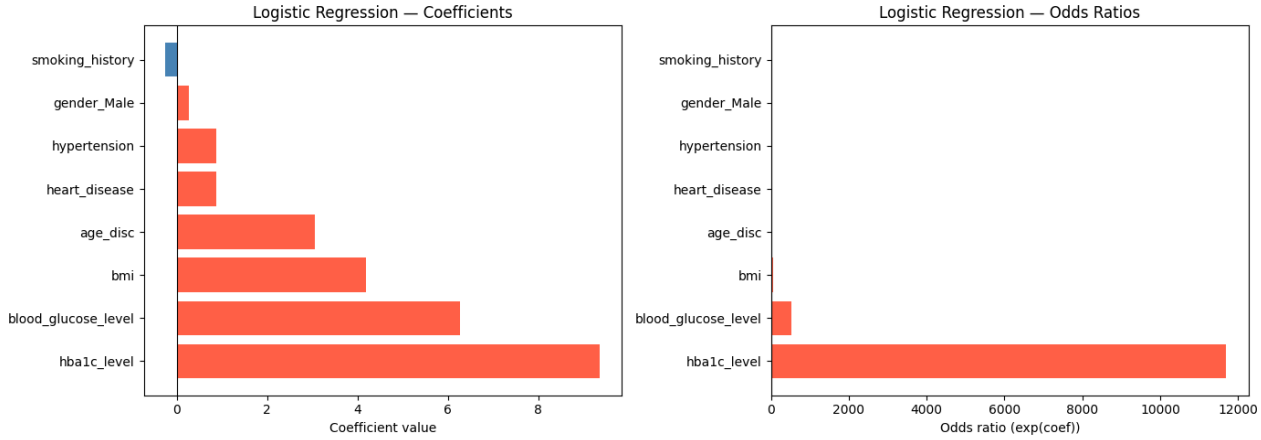



## 2.3 — Coefficients Weights & Odds Ratios

```
#### START CODE HERE ####
coef = lr.coef_[0]
odds_ratios = np.exp(coef)

coef_df = pd.DataFrame({
    'Feature': feature_names,
    'Coefficient': coef,
    'Odds Ratio': odds_ratios
}).sort_values('Coefficient', ascending=False)

print("\n--- Coefficients & Odds Ratios ---")
print(coef_df.to_string(index=False))

fig, axes = plt.subplots(1, 2, figsize=(14, 5))

# Coefficients
colors = ['tomato' if c > 0 else 'steelblue' for c in coef_df['Coefficient']]
axes[0].barh(coef_df['Feature'], coef_df['Coefficient'], color=colors)
axes[0].axvline(0, color='black', linewidth=0.8)
axes[0].set_title('Logistic Regression — Coefficients')
axes[0].set_xlabel('Coefficient value')

# Odds Ratios
```

```
or_colors = ['tomato' if o > 1 else 'steelblue' for o in coef_df['Odds Ratio']]
axes[1].barh(coef_df['Feature'], coef_df['Odds Ratio'], color=or_colors)
axes[1].axvline(1, color='black', linewidth=0.8)
axes[1].set_title('Logistic Regression — Odds Ratios')
axes[1].set_xlabel('Odds ratio (exp(coef))')

plt.tight_layout()
#### END CODE HERE ####
```

```
--- Coefficients & Odds Ratios ---
            Feature  Coefficient   Odds Ratio
        hba1c_level     9.366304 11687.838205
blood_glucose_level     6.266600   526.683543
                bmi     4.191100    66.095423
           age_disc     3.049509    21.104970
      heart_disease     0.879548     2.409810
       hypertension     0.862074     2.368066
        gender_Male     0.262965     1.300782
    smoking_history    -0.253393     0.776163
```




```
# Interpretation
bmi_row = coef_df[coef_df['Feature'] == 'bmi']
male_row = coef_df[coef_df['Feature'] == 'gender_Male'] if 'gender_Male' in coef_df['Feature'].values else None
female_row = coef_df[coef_df['Feature'] == 'gender_Female'] if 'gender_Female' in coef_df['Feature'].values else

print("\n--- Feature Interpretations ---")
if not bmi_row.empty:
    b = bmi_row.iloc[0]
    print(f"BMI: coef={b['Coefficient']:.4f}, OR={b['Odds Ratio']:.4f}")
    print(f"  → A 1-unit increase in scaled BMI multiplies diabetes odds by {b['Odds Ratio']:.2f}x")
for name, row in [('gender_Male', male_row), ('gender_Female', female_row)]:
    if row is not None and not row.empty:
        r = row.iloc[0]
        direction = "increases" if r['Odds Ratio'] > 1 else "decreases"
        print(f"{name}: coef={r['Coefficient']:.4f}, OR={r['Odds Ratio']:.4f}")
        print(f"  → Being {name.split('_')[1]} {direction} the odds of diabetes by factor {r['Odds Ratio']:.2f}"
```

```
--- Feature Interpretations ---
BMI: coef=4.1911, OR=66.0954
  → A 1-unit increase in scaled BMI multiplies diabetes odds by 66.10x
gender_Male: coef=0.2630, OR=1.3008
  → Being Male increases the odds of diabetes by factor 1.30
```

## Exercise 3 — K-Nearest Neighbors 👥

KNN is an **instance-based learner**: there are no learned weights or tree structures to inspect. In KNN, the prediction for a new data point is determined by the **majority class** (for classification) or the **mean** of the closest k neighbors' values (for regression) among the training data points, where *k* is a user-defined parameter.

Finding *k* can be tricky and you typically use techniques like cross-validation, **grid search**, or random search.

The interpretation and explanation of KNN does not follow procedures similar to the ones above. This because the KNN is an **instance-based learning algorithm** and so the interpretability comes entirely from **looking at the neighbors** used to make a prediction:

> *"This patient is predicted diabetic because their **6 most similar** patients in the training set were all diabetic."*

Hence, to explain a prediction in KNN:

1. Retrieve the *k neighbors* that were used for the prediction.
2. Analyze the k neighbors.

Hence, this is **purely local** interpretability — each prediction gets its own explanation given by its closest example.

### Your tasks

1. Find the best `k` parameter iterating over a range (1, 15) using a GridSearchCV.

   - Use the **best k** already found and fit a **KNN** on the same dataset as before.
   - Evaluate the KNN calculating the **mean accuracy** over test dataset.

2. Analyze **Interpretability** explaining 3 instances:

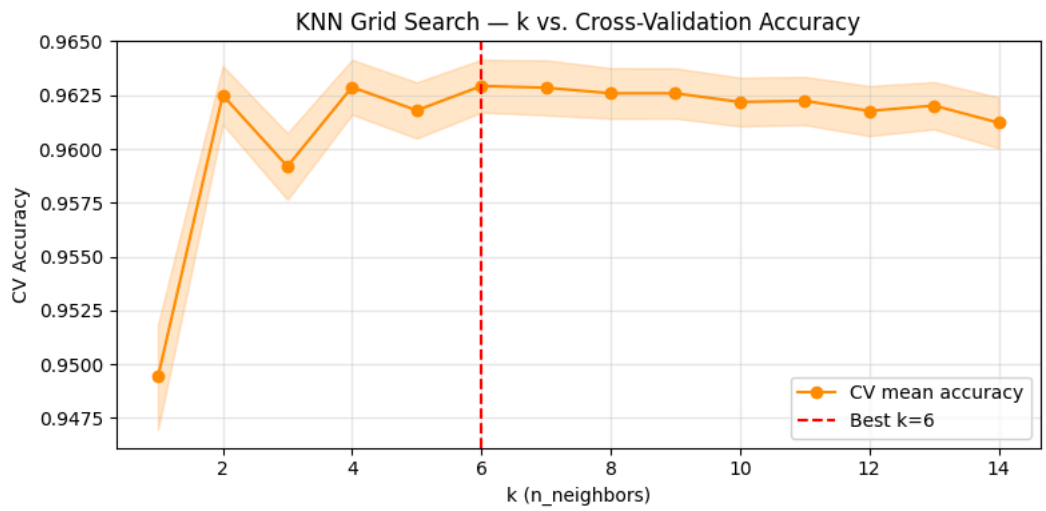
   - Consider the instances 100, 150 and 200 of the train dataset.
   - **Check** the **predicted target** for each instance.
   - **Retrieve** the relative k-nearest neighbors.
   - To **explain** the **predicted target** check the predicted targets for each of the k-nearest neighbors.

## 3.1 — Grid Search for Best K

```
from sklearn.neighbors import KNeighborsClassifier
from sklearn.model_selection import GridSearchCV

#### START CODE HERE ####
param_grid = {'n_neighbors': list(range(1, 15))}
knn_cv = GridSearchCV(KNeighborsClassifier(), param_grid,
                      cv=5, scoring='accuracy', n_jobs=-1)
knn_cv.fit(X_train, y_train)

best_k = knn_cv.best_params_['n_neighbors']
cv_results = pd.DataFrame(knn_cv.cv_results_)
print(f"Best k = {best_k}  (CV accuracy = {knn_cv.best_score_:.4f})")
#### END CODE HERE ####
```

```
Best k = 6  (CV accuracy = 0.9629)
```

```
# Plot CV scores
fig, ax = plt.subplots(figsize=(8, 4))
ax.plot(range(1, 15), cv_results['mean_test_score'], 'o-', color='darkorange', label='CV mean accuracy')
ax.fill_between(range(1, 15),
                cv_results['mean_test_score'] - cv_results['std_test_score'],
                cv_results['mean_test_score'] + cv_results['std_test_score'],
                alpha=0.2, color='darkorange')
ax.axvline(best_k, color='red', linestyle='--', label=f'Best k={best_k}')
ax.set_xlabel('k (n_neighbors)')
ax.set_ylabel('CV Accuracy')
ax.set_title('KNN Grid Search — k vs. Cross-Validation Accuracy')
ax.legend()
ax.grid(True, alpha=0.3)
plt.tight_layout()
```



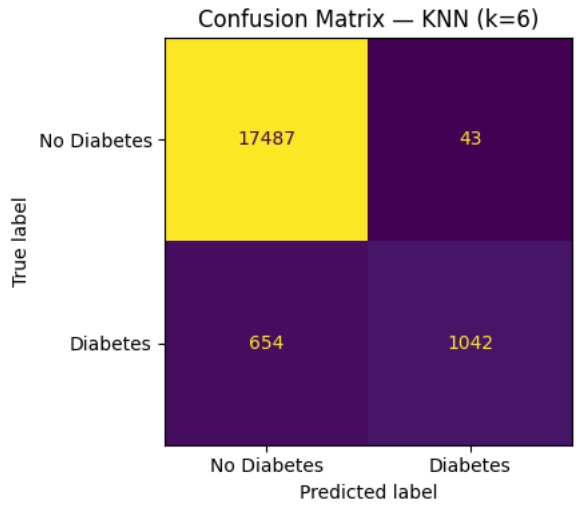
```
# Fit final KNN with best k
knn = KNeighborsClassifier(n_neighbors=best_k)
knn.fit(X_train, y_train)
```

```
KNeighborsClassifier
KNeighborsClassifier(n_neighbors=6)
```

## 3.2 — Mean Accuracy over test dataset

```
#### START CODE HERE ####
test_accuracy = knn.score(X_test, y_test)
print(f"\nKNN (k={best_k}) — Mean accuracy on test set: {test_accuracy:.4f}")

y_pred_knn = knn.predict(X_test)
print("\n--- Classification Report (KNN) ---")
print(classification_report(y_test, y_pred_knn, target_names=['No Diabetes', 'Diabetes']))

cm_knn = confusion_matrix(y_test, y_pred_knn)
disp_knn = ConfusionMatrixDisplay(confusion_matrix=cm_knn, display_labels=['No Diabetes','Diabetes'])
fig, ax = plt.subplots(figsize=(5, 4))
disp_knn.plot(ax=ax, colorbar=False)
ax.set_title(f'Confusion Matrix — KNN (k={best_k})')
plt.tight_layout()
#### END CODE HERE ####
```

```
KNN (k=6) — Mean accuracy on test set: 0.9637

--- Classification Report (KNN) ---
              precision    recall  f1-score   support

 No Diabetes       0.96      1.00      0.98     17530
    Diabetes       0.96      0.61      0.75      1696

    accuracy                           0.96     19226
   macro avg       0.96      0.81      0.86     19226
weighted avg       0.96      0.96      0.96     19226
```



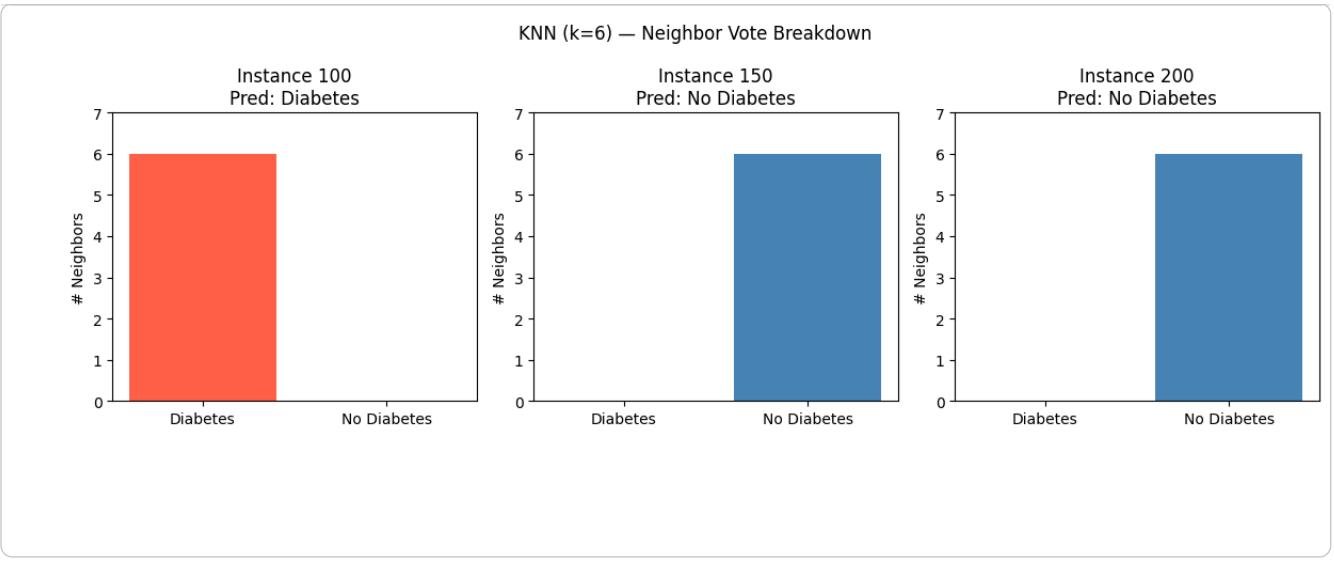

## 3.3 — Explain 3 instances

```
#### START CODE HERE
print("\n--- Local Interpretability: Neighbor Inspection ---")

X_train_arr = X_train.values
y_train_arr = y_train.values

for sample_id in [100, 150, 200]:
    instance = X_train.iloc[[sample_id]]
    predicted = knn.predict(instance)[0]
    actual    = y_train.iloc[sample_id]

    distances, neighbor_indices = knn.kneighbors(instance)
    neighbor_labels = y_train_arr[neighbor_indices[0]]
    n_diabetic = neighbor_labels.sum()
    n_non      = best_k - n_diabetic
```

```
    print(f"\n{'—'*55}")
    print(f"Instance {sample_id}")
    print(f"  Predicted : {'Diabetes' if predicted==1 else 'No Diabetes'}")
    print(f"  Actual    : {'Diabetes' if actual==1 else 'No Diabetes'}")
    print(f"  k={best_k} neighbors → {int(n_diabetic)} Diabetes | {int(n_non)} No Diabetes")
    print(f"  Confidence: {max(n_diabetic, n_non)/best_k*100:.0f}% majority vote")

    neighbor_df = X_train.iloc[neighbor_indices[0]].copy()
    neighbor_df['diabetes'] = neighbor_labels
    neighbor_df['distance'] = distances[0]
    print(f"\n  Neighbors (key features):")
    display_cols = ['blood_glucose_level', 'hba1c_level', 'bmi', 'diabetes', 'distance']
    display_cols = [c for c in display_cols if c in neighbor_df.columns]
    print(neighbor_df[display_cols].to_string())####

#### END CODE HERE ####
```

```
--- Local Interpretability: Neighbor Inspection ---

————————————————————————————————————————————————————
Instance 100
  Predicted : Diabetes
  Actual    : Diabetes
  k=6 neighbors → 6 Diabetes | 0 No Diabetes
  Confidence: 100% majority vote

  Neighbors (key features):
       blood_glucose_level  hba1c_level       bmi  diabetes  distance
96371             0.272727     0.854545  0.312170         1  0.000000
90797             0.295455     0.854545  0.356414         1  0.049740
51696             0.227273     0.854545  0.339631         1  0.053106
48413             0.340909     0.854545  0.287877         1  0.072380
70050             0.359091     0.854545  0.370262         1  0.104083
74568             0.209091     0.854545  0.229668         1  0.104193

————————————————————————————————————————————————————
Instance 150
  Predicted : No Diabetes
  Actual    : No Diabetes
  k=6 neighbors → 0 Diabetes | 6 No Diabetes
  Confidence: 100% majority vote

  Neighbors (key features):
       blood_glucose_level  hba1c_level       bmi  diabetes  distance
3969              0.295455     0.490909  0.210421         0  0.000000
93181             0.295455     0.490909  0.211008         0  0.000587
232               0.295455     0.490909  0.203145         0  0.007276
67989             0.295455     0.490909  0.203145         0  0.007276
76634             0.295455     0.490909  0.203145         0  0.007276
46041             0.295455     0.490909  0.203145         0  0.007276

————————————————————————————————————————————————————
Instance 200
  Predicted : No Diabetes
  Actual    : No Diabetes
  k=6 neighbors → 0 Diabetes | 6 No Diabetes
  Confidence: 100% majority vote

  Neighbors (key features):
       blood_glucose_level  hba1c_level       bmi  diabetes  distance
74316             0.090909     0.490909  0.137777         0  0.000000
59850             0.090909     0.490909  0.132731         0  0.005046
69390             0.090909     0.490909  0.151273         0  0.013496
36152             0.090909     0.472727  0.148339         0  0.021027
46371             0.090909     0.472727  0.159840         0  0.028590
33003             0.090909     0.472727  0.114423         0  0.029597
```

```
fig, axes = plt.subplots(1, 3, figsize=(12, 4))
for ax, sample_id in zip(axes, [100, 150, 200]):
    instance = X_train.iloc[[sample_id]]
    predicted = knn.predict(instance)[0]
    _, neighbor_indices = knn.kneighbors(instance)
    neighbor_labels = y_train_arr[neighbor_indices[0]]
    n_d = int(neighbor_labels.sum())
    n_n = best_k - n_d
    ax.bar(['Diabetes', 'No Diabetes'], [n_d, n_n],
           color=['tomato', 'steelblue'])
    ax.set_title(f"Instance {sample_id}\nPred: {'Diabetes' if predicted==1 else 'No Diabetes'}")
    ax.set_ylabel('# Neighbors')
    ax.set_ylim(0, best_k + 1)
plt.suptitle(f'KNN (k={best_k}) — Neighbor Vote Breakdown', fontsize=12)
plt.tight_layout()
```




## 🔍 Reflection Questions

1. **Decision Tree:** The depth–accuracy plot shows that depth=4 costs some performance. Is that trade-off justified for a medical application like diabetes prediction — and *who* needs to read this model (clinician? regulator? patient)?
2. **Logistic Regression:** `blood_glucose_level` and `HbA1c_level` are likely correlated. If both have large positive coefficients,