

ctgan_training

May 18, 2025

1 Advanced CTGAN Training and Evaluation

This section enhances the basic CTGAN training with: 1. Improved data preprocessing with outlier handling 2. Enhanced CTGAN training with better hyperparameters 3. Comprehensive synthetic data evaluation 4. Feature importance analysis 5. PCA visualization for distribution comparison 6. Cross-validation evaluation

```
[2]: import pandas as pd
import numpy as np
import seaborn as sns
import joblib
import time
import xgboost as xgb
from sklearn.preprocessing import StandardScaler, LabelEncoder
from sklearn.model_selection import train_test_split
from sklearn.metrics import roc_auc_score, f1_score, recall_score,
    precision_score, confusion_matrix
from ctgan import CTGAN

import matplotlib.pyplot as plt
# Set the random seed for reproducibility
SEED = 42
np.random.seed(SEED)

# Load the PDF features dataset
file_path = '/home/nhat/projectcuioky/data/pdf_features.csv'
df = pd.read_csv(file_path)

# Display basic information about the dataset
print(f"Dataset shape: {df.shape}")
print(f"\nFeature columns: {list(df.columns)}")

# Check for missing values
missing_values = df.isnull().sum()
print(f"\nColumns with missing values: \n{missing_values[missing_values > 0]}")

# Encode the label column if needed
if 'label' in df.columns and 'label_numeric' not in df.columns:
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```

le = LabelEncoder()
df['label_numeric'] = le.fit_transform(df['label'])
print(f"\nLabel encoding: {dict(zip(le.classes_, range(len(le.
↳classes_))))}")

# Drop features that might not be relevant for analysis (based on cell 6)
features_to_drop = ['filepath', 'filename', '_Colors_gt_224', 'endobj',
↳'endstream']
for col in features_to_drop:
    if col in df.columns:
        df.drop(columns=[col], inplace=True)

# Summary of the dataset
print(f"\nClass distribution:")
print(df['label_numeric'].value_counts())

# Display some sample data
print("\nSample of the dataset:")
print(df.head())

```

/home/nhat/projectcuoiky/.venv/lib/python3.13/site-packages/xgboost/core.py:377: FutureWarning: Your system has an old version of glibc (< 2.28). We will stop supporting Linux distros with glibc older than 2.28 after **May 31, 2025**.

Please upgrade to a recent Linux distro (with glibc >= 2.28) to use future versions of XGBoost.

Note: You have installed the 'manylinux2014' variant of XGBoost. Certain features such as GPU algorithms or federated learning are not available. To use these features, please upgrade to a recent Linux distro with glibc 2.28+, and install the 'manylinux_2_28' variant.

```
warnings.warn(
```

Dataset shape: (11101, 25)

Feature columns: ['Page', 'Encrypt', 'ObjStm', 'JS', 'JavaScript', 'AA', 'OpenAction', 'AcroForm', 'JBIG2Decode', 'RichMedia', 'Launch', 'EmbeddedFile', 'XFA', 'Colors_gt_224', 'obj', 'endobj', 'stream', 'endstream', 'xref', 'trailer', 'startxref', 'filepath', 'filename', 'filesize_kb', 'label']

Columns with missing values:
Series([], dtype: int64)

Label encoding: {'benign': 0, 'malicious': 1}

Class distribution:
label_numeric
0 9107
1 1994
Name: count, dtype: int64

Sample of the dataset:

	Page	Encrypt	ObjStm	JS	JavaScript	AA	OpenAction	AcroForm	\
0	1	0	0	0	0	0	0	0	
1	1	0	0	0	0	0	0	0	
2	4	0	6	0	0	0	0	0	
3	1	0	0	0	0	0	0	1	
4	6	0	25	0	0	0	0	2	

	JBIG2Decode	RichMedia	...	XFA	Colors_gt_224	obj	stream	xref	\
0	0	0	...	0		0	11	3	2
1	0	0	...	0		0	6	2	1
2	0	0	...	0		0	56	41	0
3	0	0	...	0		0	29	17	2
4	0	0	...	0		0	156	146	0

	trailer	startxref	filesize_kb	label	label_numeric
0	2	2	23.120117	benign	0
1	1	1	69.544922	benign	0
2	0	3	180.786133	benign	0
3	2	2	85.124023	benign	0
4	0	4	126.099609	benign	0

[5 rows x 22 columns]

```
[3]: def enforce_pdf_malware_logic(df):
    df = df.copy()

    # 1. JS và JavaScript phải đồng bộ
    df['JavaScript'] = df['JS']

    # 2. OpenAction và AA phải đồng bộ
    df['AA'] = df['OpenAction']

    # 3. Nếu Launch hoặc RichMedia → EmbeddedFile = 1
    df.loc[(df['Launch'] == 1) | (df['RichMedia'] == 1), 'EmbeddedFile'] = 1

    # 4. Nếu EmbeddedFile = 1 → obj >= 10, stream >= 5
    df.loc[df['EmbeddedFile'] == 1, 'obj'] = df.loc[df['EmbeddedFile'] == 1, 'obj'].clip(lower=10)
    df.loc[df['EmbeddedFile'] == 1, 'stream'] = df.loc[df['EmbeddedFile'] == 1, 'stream'].clip(lower=5)

    # 5. Nếu JBIG2Decode = 1 → filesize_kb >= 50
    df.loc[df['JBIG2Decode'] == 1, 'filesize_kb'] = df.loc[df['JBIG2Decode'] == 1, 'filesize_kb'].clip(lower=50)
```

```

# 6. Nếu AcroForm hoặc XFA = 1 → OpenAction = 1
df.loc[(df['AcroForm'] == 1) | (df['XFA'] == 1), 'OpenAction'] = 1
df['AA'] = df['OpenAction'] # đồng bộ lại

# 7. Nếu Encrypt = 1 → ObjStm >= 1
df.loc[df['Encrypt'] == 1, 'ObjStm'] = df.loc[df['Encrypt'] == 1, 'ObjStm'].
↳clip(lower=1)

# 8. Nếu Colors_gt_224 = 1 → filesize_kb >= 200
df.loc[df['Colors_gt_224'] == 1, 'filesize_kb'] = df.
↳loc[df['Colors_gt_224'] == 1, 'filesize_kb'].clip(lower=200)

return df

```

```

[4]: def add_noise_to_continuous_features(df, noise_level=0.05):
    df_noisy = df.copy()
    for col in df_noisy.select_dtypes(include=[np.float64, np.int64]).columns:
        std = df_noisy[col].std()
        if std > 0:
            noise = np.random.normal(0, noise_level * std, df_noisy[col].shape)
            df_noisy[col] += noise
    return df_noisy

```

```

[5]: from sklearn.metrics.pairwise import rbf_kernel

def compute_mmd(X, Y, gamma=1.0):
    XX = rbf_kernel(X, X, gamma=gamma)
    YY = rbf_kernel(Y, Y, gamma=gamma)
    XY = rbf_kernel(X, Y, gamma=gamma)
    return XX.mean() + YY.mean() - 2 * XY.mean()

```

```

[6]: # === 1. Improved Data Preprocessing ===

def preprocess_for_ctgan(df_features_only, log_columns=None):
    """
    Preprocess feature data for CTGAN training with improved scaling and
    ↳outlier handling.
    Input df_features_only should NOT contain label columns.
    """
    df_processed = df_features_only.copy()

    # 1. Log transformation for highly skewed columns
    if log_columns:
        for col in log_columns:
            if col in df_processed.columns and pd.api.types.
            ↳is_numeric_dtype(df_processed[col]):

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        # Ensure no negative or zero values before log if log1p is not
        ↪sufficient
        if (df_processed[col] <= 0).any():
            print(f"Warning: Column {col} contains non-positive values.")
        ↪Applying log1p after clipping to 0.)
            df_processed[col] = np.log1p(df_processed[col].
        ↪clip(lower=0))
        else:
            df_processed[col] = np.log1p(df_processed[col])

    # 2. Detect and handle outliers on all numeric columns present
    current_numeric_cols = df_processed.select_dtypes(include=[np.number]).
    ↪columns.tolist()

    for col in current_numeric_cols:
        # Skip if column is empty or all NaN
        if df_processed[col].isnull().all() or df_processed[col].empty:
            continue
        Q1 = df_processed[col].quantile(0.25)
        Q3 = df_processed[col].quantile(0.75)
        IQR = Q3 - Q1
        # Avoid issues if IQR is 0 (e.g., mostly constant column)
        if IQR > 0:
            lower_bound = Q1 - 1.5 * IQR
            upper_bound = Q3 + 1.5 * IQR
            df_processed[col] = df_processed[col].clip(lower=lower_bound,
        ↪upper=upper_bound)

    # 3. Identify constant and near-constant columns from the *current* numeric
    ↪columns
    # These will be dropped BEFORE scaling.
    constant_cols_to_drop = [col for col in current_numeric_cols if
    ↪df_processed[col].nunique(dropna=False) <= 1]

    near_constant_cols_to_drop = []
    for col in current_numeric_cols:
        if col not in constant_cols_to_drop and not df_processed[col].empty:
            if df_processed[col].nunique(dropna=False) == 1:
                if col not in near_constant_cols_to_drop:
        ↪near_constant_cols_to_drop.append(col) # Technically constant
            elif df_processed[col].nunique(dropna=False) > 1 :
                most_frequent_count = df_processed[col].
        ↪value_counts(dropna=False).iloc[0]
                if (most_frequent_count / len(df_processed[col])) >= 0.99: #
        ↪99% threshold
                    near_constant_cols_to_drop.append(col)

```

```

        elif df_processed[col].empty and col not in constant_cols_to_drop:
            constant_cols_to_drop.append(col)

    constant_columns_original_values = {
        col: df_features_only[col].iloc[0] if not df_features_only[col].empty
    else np.nan
        for col in constant_cols_to_drop
        if col in df_features_only.columns
    }
    near_constant_columns_original_values = {
        col: df_features_only[col].mode()[0] if not df_features_only[col].empty
    and not df_features_only[col].mode().empty else np.nan
        for col in near_constant_cols_to_drop
        if col in df_features_only.columns
    }

    cols_to_drop_before_scaling = list(set(constant_cols_to_drop +
    near_constant_cols_to_drop))
    if cols_to_drop_before_scaling:
        print(f"Dropping constant/near-constant columns before scaling:
    {cols_to_drop_before_scaling}")
        df_processed.drop(columns=cols_to_drop_before_scaling, inplace=True,
    errors='ignore')

    # 4. Feature scaling on remaining numeric columns
    scaler = StandardScaler()
    numeric_cols_for_scaling = df_processed.select_dtypes(include=[np.number]).
    columns.tolist()

    fitted_scaler_feature_names = []
    if numeric_cols_for_scaling:
        df_processed[numeric_cols_for_scaling] = scaler.
    fit_transform(df_processed[numeric_cols_for_scaling])
        if hasattr(scaler, 'feature_names_in_'):
            fitted_scaler_feature_names = scaler.feature_names_in_.tolist()
        elif hasattr(scaler, 'n_features_in_') and scaler.n_features_in_ > 0 :
            fitted_scaler_feature_names = numeric_cols_for_scaling

    metadata = {
        'scaler': scaler,
        'fitted_scaler_feature_names': fitted_scaler_feature_names,
        'constant_columns_original_values': constant_columns_original_values,
        'near_constant_columns_original_values':
    near_constant_columns_original_values,
        'log_columns': log_columns or [],
        'final_feature_columns_for_ctgan': df_processed.columns.tolist()
    }

```

```

    }

    return df_processed, metadata

# === 2. Enhanced CTGAN Training ===

def train_ctgan_with_monitoring(df_features_for_ctgan,
    ↳discrete_columns_for_ctgan, epochs=300, batch_size=500):
    """
    Train CTGAN with more hyperparameter options and better monitoring.
    df_features_for_ctgan: DataFrame containing only the features (already
    ↳processed) for CTGAN.
    discrete_columns_for_ctgan: List of column names in df_features_for_ctgan
    ↳to be treated as discrete.
    """
    ctgan_model = CTGAN( # Renamed from ctgan to avoid conflict if this cell is
    ↳run multiple times
        epochs=epochs,
        batch_size=batch_size,
        discriminator_steps=1,
        log_frequency=True,
        verbose=True,
        embedding_dim=128,
        generator_dim=(256, 512, 256),
        discriminator_dim=(512, 256),
        pac=4
    )

    start_time = time.time()
    print(f"Starting CTGAN training with {epochs} epochs at {time.strftime('%H:
    ↳%M:%S')}")

    valid_discrete_columns = [col for col in discrete_columns_for_ctgan if col
    ↳in df_features_for_ctgan.columns]
    if len(valid_discrete_columns) != len(discrete_columns_for_ctgan):
        print(f"Warning: Some discrete columns were not found in the data for
    ↳CTGAN: {set(discrete_columns_for_ctgan) - set(valid_discrete_columns)}")

    ctgan_model.fit(df_features_for_ctgan,
    ↳discrete_columns=valid_discrete_columns)

    elapsed = time.time() - start_time
    print(f"CTGAN training completed in {elapsed:.2f} seconds ({elapsed/60:.2f}
    ↳minutes)")

    return ctgan_model

```

```
[7]: def add_dummy_features(df, n_features=3):
    df_aug = df.copy()
    for i in range(n_features):
        df_aug[f'dummy_{i}'] = np.random.normal(0, 1, size=len(df))
    return df_aug
```

```
[8]: def perturb_labels(df, perturb_ratio=0.05):
    df_perturbed = df.copy()
    n = int(len(df) * perturb_ratio)
    idxs = np.random.choice(df.index, size=n, replace=False)
    df_perturbed.loc[idxs, 'label_numeric'] = 0
    df_perturbed.loc[idxs, 'label'] = 'benign'
    return df_perturbed
```

```
[9]: def generate_and_evaluate_synthetic_data(ctgan_model,
    ↪original_features_unprocessed, metadata, n_samples, seed=None):
    """
    Generate synthetic data and evaluate it with multiple metrics.

    Args:
        ctgan_model: The trained CTGAN model.
        original_features_unprocessed: DataFrame of real malicious features in
    ↪their original scale.
        metadata: Dictionary from preprocess_for_ctgan.
        n_samples: Number of synthetic samples to generate.
        seed: Optional random seed for reproducibility.

    Returns:
        dict: Contains synthetic data and evaluation metrics.
    """
    def get_clip_ranges(real_data, quantile_range=(0.01, 0.99)):
        """Calculate clip ranges based on quantiles of real data."""
        clip_ranges = {}
        for col in ['filesize_kb', 'Page', 'obj', 'stream']:
            if col in real_data.columns and pd.api.types.
    ↪is_numeric_dtype(real_data[col]):
                try:
                    low = real_data[col].quantile(quantile_range[0])
                    high = real_data[col].quantile(quantile_range[1])

                    # Ensure valid range
                    if pd.isna(low) or pd.isna(high) or high <= low:
                        print(f"Warning: Invalid clip range for {col}: ({low},
    ↪{high}). Using min/max.")
                        low, high = real_data[col].min(), real_data[col].max()

                    # Add buffer to avoid edge cases
```



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        buffer = max(1, (high - low) * 0.1) # 10% buffer
        clip_ranges[col] = (max(0, low - buffer), high + buffer)

    except Exception as e:
        print(f"Error calculating clip range for {col}: {str(e)}")
        if col in real_data.columns:
            clip_ranges[col] = (real_data[col].min(),
↪real_data[col].max())
        return clip_ranges

# Set random seed for reproducibility
if seed is not None:
    np.random.seed(seed)
    torch.manual_seed(seed)

print(f"Generating {n_samples} synthetic samples...")
try:
    synthetic_processed_features = ctgan_model.sample(n_samples)
except Exception as e:
    print(f"Error generating samples: {str(e)}")
    return None

# Initialize output dataframe
synthetic_reconstructed_df = synthetic_processed_features.copy()

# Inverse transform scaled features
if (cols_that_were_scaled := metadata.get('fitted_scaler_feature_names',
↪[])) and \
    hasattr(metadata.get('scaler'), 'transform'):
    try:
        cols_to_inverse = [col for col in cols_that_were_scaled if col in
↪synthetic_reconstructed_df.columns]
        if cols_to_inverse:
            synthetic_reconstructed_df[cols_to_inverse] =
↪metadata['scaler'].inverse_transform(
                synthetic_reconstructed_df[cols_to_inverse]
            )
    except Exception as e:
        print(f"Error in inverse transform: {str(e)}")

# Handle constant and near-constant columns
for col_dict in ['constant_columns_original_values',
↪'near_constant_columns_original_values']:
    for col, val in metadata.get(col_dict, {}).items():
        if col in original_features_unprocessed.columns:
            if isinstance(val, (int, float, str, bool)):
                synthetic_reconstructed_df[col] = val

```

```

        elif isinstance(val, (pd.Series, np.ndarray)) and len(val) > 0:
            synthetic_reconstructed_df[col] = val[0]
        else:
            synthetic_reconstructed_df[col] = 
                original_features_unprocessed[col].mode()[0] \
                if not original_features_unprocessed[col].empty else 0

    # Apply exponential transform to log-scaled columns
    for col in metadata.get('log_columns', []):
        if col in synthetic_reconstructed_df.columns and pd.api.types.
        is_numeric_dtype(synthetic_reconstructed_df[col]):
            synthetic_reconstructed_df[col] = np.
            expm1(synthetic_reconstructed_df[col])

    # Ensure all original columns are present
    synthetic_reconstructed_df = synthetic_reconstructed_df.
    reindex(columns=original_features_unprocessed.columns)

    # Handle missing values
    for col in synthetic_reconstructed_df.columns:
        if pd.api.types.is_numeric_dtype(synthetic_reconstructed_df[col]):
            if synthetic_reconstructed_df[col].isnull().any():
                fill_val = original_features_unprocessed[col].median() if col 
                in original_features_unprocessed else 0
            synthetic_reconstructed_df[col] = 
            synthetic_reconstructed_df[col].fillna(fill_val)

    # Ensure non-negative values where appropriate
    for col in synthetic_reconstructed_df.columns:
        if (col in original_features_unprocessed.columns and
            pd.api.types.is_numeric_dtype(original_features_unprocessed[col])) 
        and
            (original_features_unprocessed[col] >= 0).all()):
            synthetic_reconstructed_df[col] = synthetic_reconstructed_df[col].
            clip(lower=0)

    # Add noise to continuous features
    synthetic_reconstructed_df = 
    add_noise_to_continuous_features(synthetic_reconstructed_df)

    # Handle integer columns
    original_integer_cols = [
        col for col in original_features_unprocessed.columns
        if pd.api.types.is_integer_dtype(original_features_unprocessed[col])
    ]
    for col in original_integer_cols:

```

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        if col in synthetic_reconstructed_df.columns:
            synthetic_reconstructed_df[col] = synthetic_reconstructed_df[col].
↳round().fillna(0).astype(np.int64)

# Process specific binary columns
binary_cols = ['JS', 'JavaScript', 'AA', 'OpenAction', 'AcroForm',
               'EmbeddedFile', 'XFA', 'Encrypt', 'RichMedia', 'Launch']
for col in binary_cols:
    if col in synthetic_reconstructed_df.columns:
        synthetic_reconstructed_df[col] = pd.to_numeric(
            synthetic_reconstructed_df[col], errors='coerce'
        ).fillna(0).clip(0, 1).round().astype(np.int8)

# Special handling for ObjStm
if 'ObjStm' in synthetic_reconstructed_df.columns:
    synthetic_reconstructed_df['ObjStm'] = (
        pd.to_numeric(synthetic_reconstructed_df['ObjStm'], errors='coerce')
        .fillna(0)
        .clip(0, 6)
        .round()
        .astype(np.int8)
    )

# Apply business rules
if all(col in synthetic_reconstructed_df.columns for col in ['JavaScript', '
↳OpenAction']):
    synthetic_reconstructed_df['OpenAction'] = np.maximum(
        synthetic_reconstructed_df['JavaScript'],
        synthetic_reconstructed_df['OpenAction']
    )

# Handle embedded files and filesize relationship
if all(col in synthetic_reconstructed_df.columns for col in
↳['EmbeddedFile', 'filesize_kb']):
    embedded_mask = synthetic_reconstructed_df['EmbeddedFile'] > 0.5
    if embedded_mask.any():
        real_embedded = original_features_unprocessed[
            original_features_unprocessed['EmbeddedFile'] > 0.5
        ]
        if not real_embedded.empty and 'filesize_kb' in real_embedded.
↳columns:
            size_increases = np.random.choice(
                real_embedded['filesize_kb'].dropna(),
                size=embedded_mask.sum(),
                replace=True
            )

```

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        synthetic_reconstructed_df.loc[embedded_mask, 'filesize_kb'] =
np.maximum(
    synthetic_reconstructed_df.loc[embedded_mask,
'filesize_kb'],
    size_increases
)

# Apply clipping based on real data distributions
clip_ranges = get_clip_ranges(original_features_unprocessed)
for col, (low, high) in clip_ranges.items():
    if col in synthetic_reconstructed_df.columns:
        synthetic_reconstructed_df[col] = synthetic_reconstructed_df[col].
clip(low, high)
    if col in original_integer_cols:
        synthetic_reconstructed_df[col] =
synthetic_reconstructed_df[col].round().astype(np.int64)

# Add labels
synthetic_reconstructed_df['label_numeric'] = 1
synthetic_reconstructed_df['label'] = 'malicious'
synthetic_reconstructed_df = add_dummy_features(synthetic_reconstructed_df)

# Calculate Frobenius norm of correlation matrix difference
fro_norm = np.nan
numeric_cols = [
    col for col in original_features_unprocessed.columns
    if (col in synthetic_reconstructed_df.columns and
pd.api.types.is_numeric_dtype(original_features_unprocessed[col]))
and
    pd.api.types.is_numeric_dtype(synthetic_reconstructed_df[col])]

if numeric_cols:
    try:
        real_corr = original_features_unprocessed[numeric_cols].corr().
fillna(0)
        synth_corr = synthetic_reconstructed_df[numeric_cols].corr().
fillna(0)
        fro_norm = np.linalg.norm(real_corr - synth_corr)
    except Exception as e:
        print(f"Error calculating Frobenius norm: {str(e)}")

# MMD Evaluation
try:
    common_cols = list(set(numeric_cols) & set(synthetic_reconstructed_df.
columns))

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```

        real_vals = original_features_unprocessed[common_cols].fillna(0).values
        synth_vals = synthetic_reconstructed_df[common_cols].fillna(0).values
        mmd_score = compute_mmd(real_vals, synth_vals, gamma=1.0)
    except Exception as e:
        print(f"Error calculating MMD score: {str(e)}")
        mmd_score = np.nan

    # Perform KS tests
    ks_results = {}
    features_for_ks = numeric_cols[:min(20, len(numeric_cols))] # Limit to top
↪20 features
    for col in features_for_ks:
        try:
            real_data = original_features_unprocessed[col].dropna()
            synth_data = synthetic_reconstructed_df[col].dropna()
            if len(real_data) > 1 and len(synth_data) > 1:
                statistic, pvalue = ks_2samp(real_data, synth_data)
                ks_results[col] = {'statistic': statistic, 'pvalue': pvalue}
        except Exception as e:
            ks_results[col] = {'statistic': np.nan, 'pvalue': np.nan, 'error':
↪str(e)}

    # Generate visualization
    fig = None
    top_features = numeric_cols[:min(5, len(numeric_cols))]
    if top_features:
        n_cols = 2
        n_rows = len(top_features)
        fig, axes = plt.subplots(n_rows, n_cols, figsize=(15, 4 * n_rows))

        if n_rows == 1:
            axes = axes.reshape(1, -1) # Ensure 2D array even for single row

        for i, feature in enumerate(top_features):
            # Distribution plot
            ax_hist = axes[i, 0]
            sns.histplot(
                original_features_unprocessed[feature].dropna(),
                ax=ax_hist, color='blue', alpha=0.5, label='Real', kde=True
            )
            sns.histplot(
                synthetic_reconstructed_df[feature].dropna(),
                ax=ax_hist, color='red', alpha=0.5, label='Synthetic', kde=True
            )
            ax_hist.set_title(f'Distribution of {feature}')
            ax_hist.legend()

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        # Q-Q plot
        ax_qq = axes[i, 1]
        real_sample = original_features_unprocessed[feature].dropna().
↪sample(
            min(1000, len(original_features_unprocessed[feature].dropna())),
            random_state=seed
        )
        synth_sample = synthetic_reconstructed_df[feature].dropna().sample(
            min(1000, len(synthetic_reconstructed_df[feature].dropna())),
            random_state=seed
        )

        if len(real_sample) > 1 and len(synth_sample) > 1:
            q_real = np.percentile(real_sample, range(0, 101))
            q_synth = np.percentile(synth_sample, range(0, 101))
            ax_qq.scatter(q_real, q_synth, alpha=0.6)
            min_val = min(q_real[0], q_synth[0])
            max_val = max(q_real[-1], q_synth[-1])
            ax_qq.plot([min_val, max_val], [min_val, max_val], 'r--',
↪alpha=0.5)

            ax_qq.set_xlabel('Real Data Quantiles')
            ax_qq.set_ylabel('Synthetic Data Quantiles')
            ax_qq.set_title(f'Q-Q Plot for {feature}')
        else:
            ax_qq.text(0.5, 0.5, 'Insufficient Data',
                        ha='center', va='center', transform=ax_qq.transAxes)
            ax_qq.set_title(f'Q-Q Plot for {feature} (Insufficient Data)')

    plt.tight_layout()

    return {
        'synthetic_data': synthetic_reconstructed_df,
        'frobenius_norm': fro_norm,
        'mmd_score': mmd_score,
        'ks_results': ks_results,
        'visualization_fig': fig
    }

```

```

[10]: # === 4. Cross-Validation Evaluation ===

from sklearn.ensemble import RandomForestClassifier # Added import

def evaluate_with_cross_validation(df_real_malicious, synthetic_malicious_data,
↪n_folds=5): # Removed df_benign as it's not used here
    """
    Evaluate how distinguishable synthetic malicious data is from real
↪malicious data.

```

Trains classifiers to predict if a sample is real (0) or synthetic (1).
AUC close to 0.5 indicates good indistinguishability.
Also returns feature importances from an XGBoost model trained on the TSTR_

task.

```

"""

df_real_mal = df_real_malicious.copy()
synthetic_mal = synthetic_malicious_data.copy()

# Assign 'is_synthetic' flag
df_real_mal['is_synthetic'] = 0 # Real malicious
synthetic_mal['is_synthetic'] = 1 # Synthetic malicious

# Combine only real malicious and synthetic malicious data for this task
# Ensure they have 'label' and 'label_numeric' for consistent column
structure before dropping
if 'label' not in df_real_mal.columns: df_real_mal['label'] = 'malicious'
if 'label_numeric' not in df_real_mal.columns: df_real_mal['label_numeric'] = 1
if 'label' not in synthetic_mal.columns: synthetic_mal['label'] = 'malicious'
if 'label_numeric' not in synthetic_mal.columns: synthetic_mal['label_numeric'] = 1

df_for_syn_detection = pd.concat([df_real_mal, synthetic_mal], ignore_index=True)

# Features for this task are all columns except label-related and 'is_synthetic'
# Ensure common features between the two sets (real malicious and synthetic malicious)
# before concatenation, df_real_mal and synthetic_mal should have the same feature columns (from reconstruction)

feature_cols_syn_detect = [
    col for col in df_real_mal.columns # Use columns from real_mal as reference
    if col in synthetic_mal.columns and col not in ['label', 'label_numeric', 'is_synthetic']
]

# Filter combined_df to only these common features for X
X_syn_detect = df_for_syn_detection[feature_cols_syn_detect].fillna(0)
y_syn_detect = df_for_syn_detection['is_synthetic'] # Target: 0 for real_mal, 1 for synthetic_mal

```

```

from sklearn.model_selection import StratifiedKFold
from sklearn.linear_model import LogisticRegression

classifiers = {
    'logistic': LogisticRegression(max_iter=1000, random_state=SEED,
↪solver='liblinear'),
    'xgboost': xgb.XGBClassifier(use_label_encoder=False,
↪eval_metric='logloss', random_state=SEED),
    'random_forest': RandomForestClassifier(n_estimators=100,
↪random_state=SEED)
}

skf = StratifiedKFold(n_splits=n_folds, shuffle=True, random_state=SEED)
synthetic_detection_cv_results = {model_name: [] for model_name in
↪classifiers}

tstr_feature_importances_df = pd.DataFrame() # Initialize

if y_syn_detect.nunique() > 1:
    for train_idx, test_idx in skf.split(X_syn_detect, y_syn_detect):
        X_train, X_test = X_syn_detect.iloc[train_idx], X_syn_detect.
↪iloc[test_idx]
        y_train, y_test = y_syn_detect.iloc[train_idx], y_syn_detect.
↪iloc[test_idx]

        for model_name, classifier_instance in classifiers.items():
            # Create a new instance for each fold to avoid state leakage
            clf = classifier_instance.__class__(**classifier_instance.
↪get_params())
            if 'use_label_encoder' in clf.get_params(): # Specific for
↪XGBoost
                clf.set_params(use_label_encoder=False,
↪eval_metric='logloss')

            clf.fit(X_train, y_train)
            y_pred_proba = clf.predict_proba(X_test)[: , 1]
            auc = roc_auc_score(y_test, y_pred_proba)
            f1 = f1_score(y_test, (y_pred_proba > 0.5).astype(int))
            synthetic_detection_cv_results[model_name].append({'auc': auc,
↪'f1': f1})

        # Train a final XGBoost model on the full TSTR dataset to get feature
↪importances
        print("\nTraining final TSTR model (XGBoost) for feature importances...
↪")

```



```

        final_tstr_xgb_model = xgb.XGBClassifier(use_label_encoder=False,
↪eval_metric='logloss', random_state=SEED)
        final_tstr_xgb_model.fit(X_syn_detect, y_syn_detect)

        importances = final_tstr_xgb_model.feature_importances_
        tstr_feature_importances_df = pd.DataFrame({
            'feature': X_syn_detect.columns,
            'importance': importances
        }).sort_values(by='importance', ascending=False).reset_index(drop=True)
        print("Top TSTR distinguishing features (XGBoost):")
        print(tstr_feature_importances_df.head())

    else:
        print("Warning: Not enough classes for synthetic vs. real malicious_
↪detection task. Skipping CV for this task.")
        for model_name in classifiers:
            synthetic_detection_cv_results[model_name].append({'auc': np.nan,
↪'f1': np.nan})

    result_summary = {
        'synthetic_detection': {
            model: {
                'f1_mean': np.mean([r['f1'] for r in results]) if results and
↪not np.isnan([r['f1'] for r in results]).all() else np.nan,
                'f1_std': np.std([r['f1'] for r in results]) if results and not
↪np.isnan([r['f1'] for r in results]).all() else np.nan,
                'auc_mean': np.mean([r['auc'] for r in results]) if results and
↪not np.isnan([r['auc'] for r in results]).all() else np.nan,
                'auc_std': np.std([r['auc'] for r in results]) if results and
↪not np.isnan([r['auc'] for r in results]).all() else np.nan,
            } for model, results in synthetic_detection_cv_results.items()
        },
        'tstr_feature_importances': tstr_feature_importances_df # Added
    }
    return result_summary

```

[11]: # === 7. Complete Workflow Implementation ===

```

def complete_ctgan_workflow(df_original_full, n_synthetic=2000, epochs=300,
↪batch_size=500):
    """
    Implement the complete workflow with all improvements
    """
    # 1. Separate benign and malicious samples from the original full dataframe

```

```

df_malicious_original = df_original_full[df_original_full['label_numeric']
↳ == 1].copy()
df_benign_original = df_original_full[df_original_full['label_numeric'] ==
↳ 0].copy()

print(f"Original data: {len(df_original_full)} samples,
↳ ({len(df_malicious_original)} malicious, {len(df_benign_original)} benign)")

# 2. Define columns for log transformation (based on original column names)
log_columns = ['Page', 'obj', 'stream', 'filesize_kb'] # These are from
↳ original data

# 3. Prepare malicious features for CTGAN preprocessing (original scale, no
↳ labels)
print("Preprocessing data for CTGAN...")
# Drop label columns before passing to preprocessing
malicious_features_for_preprocessing = df_malicious_original.
↳ drop(columns=['label', 'label_numeric'], errors='ignore')

# df_processed_for_ctgan_training is in processed scale (log, scaled,
↳ outliers capped, some cols dropped)
df_processed_features, metadata =
↳ preprocess_for_ctgan(malicious_features_for_preprocessing.copy(),
↳ log_columns) # Pass a copy
print(f"Processed features shape for CTGAN training: {df_processed_features.
↳ shape}")

# 4. Identify discrete columns for CTGAN based on the *original nature* of
↳ the features
# that are *still present* in df_processed_features.
original_discrete_features = []
temp_malicious_features_for_discrete_check =
↳ malicious_features_for_preprocessing.copy()
for col in temp_malicious_features_for_discrete_check.columns:
    # Heuristic: integer columns with a relatively small number of unique
↳ values
    # Also ensure the column is not all NaN after potential coercions
    if pd.api.types.
↳ is_integer_dtype(temp_malicious_features_for_discrete_check[col]) and \
        temp_malicious_features_for_discrete_check[col].
↳ nunique(dropna=False) < 20 and \
        not temp_malicious_features_for_discrete_check[col].isnull().all() :
        original_discrete_features.append(col)

discrete_columns_for_ctgan = [col for col in original_discrete_features if
↳ col in df_processed_features.columns]

```

```

    print(f"Identified {len(discrete_columns_for_ctgan)} discrete columns for_
↳CTGAN training: {discrete_columns_for_ctgan}")

    # 5. Train CTGAN
    print("\nTraining CTGAN with enhanced parameters...")
    ctgan_model = train_ctgan_with_monitoring(df_processed_features,
↳discrete_columns_for_ctgan, epochs, batch_size)

    # 6. Generate and evaluate synthetic data
    print("\nGenerating and evaluating synthetic data...")
    # Pass original UNPROCESSED malicious features_
↳(malicious_features_for_preprocessing) for fair comparison
    synthetic_results = generate_and_evaluate_synthetic_data(
        ctgan_model,
        malicious_features_for_preprocessing.copy(), # Pass a copy of original_
↳malicious features
        metadata,
        n_synthetic,
        seed=SEED
    )
    synthetic_data_reconstructed = synthetic_results['synthetic_data'] # This_
↳is in original feature scale, with labels added
    synthetic_data_reconstructed =
↳enforce_pdf_malware_logic(synthetic_data_reconstructed)

    print(f"Frobenius norm (lower is better):_
↳{synthetic_results['frobenius_norm']:.4f}")
    print("KS test results (sample):")
    for feature, result in list(synthetic_results['ks_results'].items())[:3]:
        print(f"    {feature}: statistic={result['statistic']:.4f},_
↳p-value={result['pvalue']:.4f}")

    if synthetic_results['visualization_fig']:
        synthetic_results['visualization_fig'].show()

    # synthetic_data_reconstructed already has 'label' and 'label_numeric'
    # df_malicious_original already has 'label' and 'label_numeric'
    # df_benign_original also has 'label' and 'label_numeric'

    # Apply perturb_labels function to introduce noise in labels
    synthetic_data_reconstructed = perturb_labels(synthetic_data_reconstructed)

    # 7. Feature importance analysis (using original scale data)
    print("\nAnalyzing feature importance...")
    importance_results = analyze_feature_importance(

```

```

        df_malicious_original.copy(), # Pass original malicious samples (with
↳labels)
        synthetic_data_reconstructed.copy(), # Pass reconstructed synthetic
↳malicious samples (with labels)
        df_benign_original.copy() # Pass original benign samples (with labels)
    )

    if isinstance(importance_results, dict):
        if importance_results.get('spearman_correlation') is not None and not
↳np.isnan(importance_results.get('spearman_correlation')):
            print(f"Feature importance Spearman correlation:
↳{importance_results.get('spearman_correlation'):.4f} (p-value:
↳{importance_results.get('p_value'):.4f})")
        else:
            print("Feature importance Spearman correlation could not be
↳calculated (e.g., no common top features or insufficient data).")

        if importance_results.get('visualization_fig'):
            importance_results.get('visualization_fig').show()
    elif isinstance(importance_results, tuple):
        print("Error: importance_results is a tuple instead of a dictionary.")
        # You can add code here to handle the tuple case
    else:
        print("Error: importance_results is neither a dictionary nor a tuple.")

    # 8. PCA visualization (using original scale features)
    print("\nCreating PCA visualization...")
    # pca_visualization expects feature-only DataFrames
    pca_results = pca_visualization(
        malicious_features_for_preprocessing.copy(), # Original malicious
↳features
        synthetic_data_reconstructed.drop(columns=['label', 'label_numeric',
↳'is_synthetic'], errors='ignore')
    )
    print(f"Centroid distance in PCA space: {pca_results['centroid_distance']:.
↳4f}")
    print(f"Explained variance ratio: {pca_results['explained_variance'][0]:.
↳2%}, {pca_results['explained_variance'][1]:.2%}")
    if pca_results['visualization']:
        pca_results['visualization'].show()

    # 9. Cross-validation evaluation (Synthetic vs Real Malicious)
    print("\nEvaluating with cross-validation (Synthetic Malicious vs. Real
↳Malicious)...")
    # Pass original malicious data (with labels) and reconstructed synthetic
↳data (with labels)

```

```

cv_results = evaluate_with_cross_validation(
    df_malicious_original.copy(),
    synthetic_data_reconstructed.copy()
)

print("Cross-validation TSTR-like results (AUC close to 0.5 is good):")
if 'synthetic_detection' in cv_results and
cv_results['synthetic_detection']:
    for model_name, metrics in cv_results['synthetic_detection'].items():
        if not np.isnan(metrics['auc_mean']):
            print(f" {model_name}: AUC={metrics['auc_mean']:.4f} ±
{metrics['auc_std']:.4f}, F1={metrics['f1_mean']:.4f} ± {metrics['f1_std']:.
4f}")
        else:
            print(f" {model_name}: AUC/F1 could not be calculated.")
    else:
        print(" No synthetic detection results from cross-validation.")

# Display TSTR feature importances
if 'tstr_feature_importances' in cv_results and not
cv_results['tstr_feature_importances'].empty:
    print("\nTop features distinguishing synthetic from real malicious data
(TSTR XGBoost model):")
    print(cv_results['tstr_feature_importances'].head(10))
    # Further analysis based on these features can be added here:
    # 1. Review preprocessing for these top features (log, scaling,
outliers).
    # 2. Consider if CTGAN parameters (epochs, batch_size, architecture)
need adjustment for these.
    # 3. Evaluate if post-processing steps can be refined for these
specific features.

# 10. Combine with original dataset for augmentation and final evaluation
# Make sure all DataFrames have consistent columns before concat
df_benign_for_aug = df_benign_original.copy()
df_malicious_for_aug = df_malicious_original.copy()
synthetic_for_aug = synthetic_data_reconstructed.copy()

# Define the set of feature columns based on the initial cleaned df,
excluding original drops and labels
initial_feature_cols = [col for col in df_original_full.columns if col not
in ['filepath', 'filename', '_Colors_gt_224', 'endobj', 'endstream',
'label', 'label_numeric']]

```

```

# Align columns for all parts of the augmented dataset
df_benign_for_aug = df_benign_for_aug[initial_feature_cols + ['label',
↪ 'label_numeric']]
df_malicious_for_aug = df_malicious_for_aug[initial_feature_cols +
↪ ['label', 'label_numeric']]
synthetic_for_aug = synthetic_for_aug[initial_feature_cols + ['label',
↪ 'label_numeric']] # synthetic_data_reconstructed was already aligned

df_augmented = pd.concat([df_benign_for_aug, df_malicious_for_aug,
↪ synthetic_for_aug], ignore_index=True)
df_augmented = df_augmented.fillna(0) # Fill any NaNs that might arise, e.g.
↪ if a new column was added due to reindex logic

print(f"\nAugmented dataset size: {len(df_augmented)} samples")
print(f"  Benign: {len(df_benign_for_aug)}")
print(f"  Original Malicious: {len(df_malicious_for_aug)}")
print(f"  Synthetic Malicious: {len(synthetic_for_aug)} samples")

print("\nTraining final model on augmented dataset...")
X = df_augmented[initial_feature_cols]
y = df_augmented['label_numeric']

X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.3, stratify=y, random_state=SEED
)

final_model = xgb.XGBClassifier(use_label_encoder=False,
↪ eval_metric='logloss', random_state=SEED)
final_model.fit(X_train, y_train)

y_prob = final_model.predict_proba(X_test)[: , 1]
y_pred = (y_prob > 0.5).astype(int)

final_metrics_calc = {
    'f1': f1_score(y_test, y_pred),
    'recall': recall_score(y_test, y_pred),
    'precision': precision_score(y_test, y_pred),
    'auc': roc_auc_score(y_test, y_prob),
    'confusion_matrix': confusion_matrix(y_test, y_pred)
}

print("\n=== CTGAN Enhanced Evaluation Summary (Downstream Task) ===")
print(f"F1 Score: {final_metrics_calc['f1']:.4f}")
print(f"Recall: {final_metrics_calc['recall']:.4f}")
print(f"Precision: {final_metrics_calc['precision']:.4f}")
print(f"AUC: {final_metrics_calc['auc']:.4f}")

```

```

print(f"Confusion Matrix:\n{final_metrics_calc['confusion_matrix']}")

return {
    'ctgan_model': ctgan_model, # Renamed
    'synthetic_data_reconstructed': synthetic_data_reconstructed,
    'synthetic_evaluation_metrics': synthetic_results,
    'feature_importance_analysis': importance_results,
    'pca_analysis_results': pca_results,
    'cross_validation_results': cv_results,
    'final_model_metrics_on_augmented_data': final_metrics_calc,
    'final_trained_model': final_model,
    'metadata_for_reconstruction': metadata
}

```

```

[12]: # Add these imports at the top of your notebook
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from scipy.stats import ks_2samp

# If you're using PyTorch for the CTGAN model, add:
try:
    import torch
except ImportError:
    print("Warning: PyTorch is not installed. Some functionality may be limited.
    ↪")

```

```

[13]: import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import joblib
from sklearn.metrics import classification_report, roc_auc_score, roc_curve, auc

```

```

[14]: # === 6. PCA Visualization ===

# Required imports
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.decomposition import PCA
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestClassifier

```

```

from sklearn.metrics import accuracy_score, f1_score, roc_auc_score,
    ↪ recall_score
import joblib

def pca_visualization(df_real_features, df_synthetic_features, n_components=2):
    """
    Performs PCA on real and synthetic features and visualizes their
    ↪ distribution.

    Parameters:
    - df_real_features: DataFrame containing real malicious features (without
    ↪ labels)
    - df_synthetic_features: DataFrame containing synthetic malicious features
    ↪ (without labels)
    - n_components: Number of PCA components to use (default: 2)

    Returns:
    - Dictionary with PCA results including visualization figure and metrics
    """
    # Ensure common features between real and synthetic data
    common_features = list(set(df_real_features.columns) &
    ↪ set(df_synthetic_features.columns))

    if not common_features:
        print("Error: No common features between real and synthetic data for
    ↪ PCA visualization!")
        return {
            'centroid_distance': np.nan,
            'explained_variance': (np.nan, np.nan),
            'visualization': None
        }

    # Select common features and ensure numeric
    real_features_for_pca = df_real_features[common_features].
    ↪ select_dtypes(include=[np.number]).fillna(0)
    synth_features_for_pca = df_synthetic_features[common_features].
    ↪ select_dtypes(include=[np.number]).fillna(0)

    # Ensure we still have features after filtering for numeric only
    if real_features_for_pca.empty or synth_features_for_pca.empty:
        print("Error: No numeric features found for PCA visualization!")
        return {
            'centroid_distance': np.nan,
            'explained_variance': (np.nan, np.nan),
            'visualization': None
        }

```



```

# Align feature columns to be the same and in the same order
common_numeric_features = list(set(real_features_for_pca.columns) &
↪set(synth_features_for_pca.columns))
real_features_for_pca = real_features_for_pca[common_numeric_features]
synth_features_for_pca = synth_features_for_pca[common_numeric_features]

# Fit PCA on combined data for consistent transformation
combined_features = pd.concat([real_features_for_pca,
↪synth_features_for_pca], ignore_index=True)

# Handle empty or all-constant features
if combined_features.empty:
    print("Error: Combined features for PCA is empty!")
    return {
        'centroid_distance': np.nan,
        'explained_variance': (np.nan, np.nan),
        'visualization': None
    }

# Check for constant columns that would cause PCA to fail
non_constant_cols = [col for col in combined_features.columns
    if combined_features[col].nunique() > 1]

if len(non_constant_cols) < n_components:
    print(f"Warning: Only {len(non_constant_cols)} non-constant features
↪available for PCA.")
    print("Reducing PCA components to match number of non-constant features.
↪")
    n_components = max(1, len(non_constant_cols))
    if n_components == 1:
        print("Only one non-constant feature. Simple 1D plot will be
↪created.")

combined_features = combined_features[non_constant_cols]

# Apply PCA
pca = PCA(n_components=n_components)
try:
    pca.fit(combined_features)

# Transform both datasets
real_pca = pca.transform(real_features_for_pca[non_constant_cols])
synth_pca = pca.transform(synth_features_for_pca[non_constant_cols])

# Calculate centroids
real_centroid = real_pca.mean(axis=0)

```

```

synth_centroid = synth_pca.mean(axis=0)

# Euclidean distance between centroids
centroid_distance = np.linalg.norm(real_centroid - synth_centroid)

# Create visualization
fig = plt.figure(figsize=(12, 10))

if n_components >= 2:
    # 2D scatter plot for first two components
    ax = fig.add_subplot(111)
    ax.scatter(real_pca[:, 0], real_pca[:, 1], s=30, alpha=0.5,
               label='Real Malicious', marker='o', color='blue')
    ax.scatter(synth_pca[:, 0], synth_pca[:, 1], s=30, alpha=0.5,
               label='Synthetic Malicious', marker='x', color='red')

    # Plot centroids
    ax.scatter(real_centroid[0], real_centroid[1], s=200, color='navy',
               marker='*', label='Real Centroid')
    ax.scatter(synth_centroid[0], synth_centroid[1], s=200,
    ↪color='darkred',
               marker='*', label='Synthetic Centroid')

    # Draw line between centroids
    ax.plot([real_centroid[0], synth_centroid[0]],
            [real_centroid[1], synth_centroid[1]], 'k--', alpha=0.5)

    ax.set_xlabel(f'PC1 ({pca.explained_variance_ratio_[0]:.2%}↪
    ↪variance)')
    ax.set_ylabel(f'PC2 ({pca.explained_variance_ratio_[1]:.2%}↪
    ↪variance)')

else:
    # 1D visualization if only one component is available
    ax = fig.add_subplot(111)
    ax.hist(real_pca[:, 0], bins=30, alpha=0.5, label='Real Malicious',
    ↪color='blue')
    ax.hist(synth_pca[:, 0], bins=30, alpha=0.5, label='Synthetic↪
    ↪Malicious', color='red')
    ax.axvline(x=real_centroid[0], color='navy', linestyle='--',
    ↪label='Real Mean')
    ax.axvline(x=synth_centroid[0], color='darkred', linestyle='--',
    ↪label='Synthetic Mean')
    ax.set_xlabel(f'PC1 ({pca.explained_variance_ratio_[0]:.2%}↪
    ↪variance)')
    ax.set_ylabel('Count')

```

```

ax.set_title('PCA: Real vs. Synthetic Malicious Samples')
ax.legend()
ax.grid(True, alpha=0.3)

# Add annotation for centroid distance
plt.annotate(f'Centroid Distance: {centroid_distance:.4f}',
             xy=(0.05, 0.95), xycoords='axes fraction',
             bbox=dict(boxstyle="round,pad=0.3", fc="white", ec="gray",
↪alpha=0.8))

plt.tight_layout()

return {
    'centroid_distance': centroid_distance,
    'explained_variance': tuple(pca.explained_variance_ratio_[:min(2,
↪n_components)]),
    'visualization': fig
}

except Exception as e:
    print(f"Error during PCA calculation: {str(e)}")
    import traceback
    traceback.print_exc()
    return {
        'centroid_distance': np.nan,
        'explained_variance': (np.nan, np.nan),
        'visualization': None
    }

def analyze_feature_importance(model, feature_names, X_test=None, y_test=None,
↪top_n=20, figsize=(12, 10)):
    """
    Analyze and visualize feature importances from a trained model.

    Parameters:
    - model: Trained model (any scikit-learn compatible model)
    - feature_names: List of feature names
    - X_test: Test features (required for permutation importance)
    - y_test: Test labels (required for permutation importance)
    - top_n: Number of top features to display
    - figsize: Figure size for the plot

    Returns:
    - DataFrame with feature importances if available, None otherwise
    - Matplotlib figure object or None if importance cannot be calculated
    """

```

```

# Dictionary to store importance values
importances = None
method_used = "Unknown"

try:
    # Try different methods to get feature importance
    if hasattr(model, 'feature_importances_'):
        # Tree-based models (Random Forest, XGBoost, etc.)
        importances = model.feature_importances_
        method_used = "Feature Importances"

    elif hasattr(model, 'coef_'):
        # Linear models (Logistic Regression, SVM, etc.)
        if len(model.coef_.shape) > 1:
            # Multi-class classification
            importances = np.mean(np.abs(model.coef_), axis=0)
        else:
            # Binary classification
            importances = np.abs(model.coef_[0])
        method_used = "Coefficient Magnitudes"

    # If standard methods didn't work, try permutation importance
    if importances is None and X_test is not None and y_test is not None:
        print("Using permutation importance (this might take a while)...")
        perm_importance = permutation_importance(
            model, X_test, y_test,
            n_repeats=10,
            random_state=42,
            scoring='accuracy'
        )
        importances = perm_importance.importances_mean
        method_used = "Permutation Importance"

    if importances is None:
        print("Could not determine feature importance for this model type.")
        return None, None

    # Create a DataFrame for better visualization
    feature_importance = pd.DataFrame({
        'feature': feature_names,
        'importance': importances
    }).sort_values('importance', ascending=False)

    # Normalize to percentage
    feature_importance['importance'] = (feature_importance['importance'] /
                                         feature_importance['importance'].
                                         sum() * 100)

```

```

# Select top N features
top_features = feature_importance.head(top_n)

# Create visualization
plt.figure(figsize=figsize)
sns.set_style("whitegrid")

# Create bar plot
ax = sns.barplot(
    x='importance',
    y='feature',
    data=top_features,
    palette='viridis'
)

# Add value annotations
for i, v in enumerate(top_features['importance']):
    ax.text(v + 0.5, i, f'{v:.2f}%', color='black', va='center')

plt.title(f'Top {top_n} Most Important Features\n(Method: {method_used})', fontsize=14, pad=20)
plt.xlabel('Importance (%)', fontsize=12)
plt.ylabel('Feature', fontsize=12)
plt.tight_layout()

return feature_importance, plt.gcf()

except Exception as e:
    print(f"Error analyzing feature importance: {str(e)}")
    import traceback
    traceback.print_exc()
    return None, None

# === 8. Run Enhanced CTGAN Workflow ===

# Set parameters for the enhanced workflow
n_synthetic_samples = 2000
ctgan_epochs = 1000
ctgan_batch_size = 256

# Run the enhanced workflow with the global 'df' from cell In[15] (id=aaca6e08)
print("Starting enhanced CTGAN workflow...")
enhanced_results = complete_ctgan_workflow(
    df.copy(), # Pass a copy of df to avoid modifying the global df
    n_synthetic=n_synthetic_samples,
    epochs=ctgan_epochs,
    batch_size=ctgan_batch_size

```

```

)

# Save the enhanced model
print("\nSaving enhanced CTGAN model...")
joblib.dump(enhanced_results['ctgan_model'], '/home/nhat/projectcuoiky/models/
↳enhanced_ctgan_malware.joblib')
print("Enhanced model saved to '/home/nhat/projectcuoiky/models/
↳enhanced_ctgan_malware.joblib")

# Analyze feature importance if final model is available
if 'final_model' in enhanced_results and 'X_test' in globals() and 'y_test' in_
↳globals():
    print("\nAnalyzing feature importance...")
    # Get feature names (excluding labels)
    feature_names = [col for col in df.columns if col not in ['label',_
↳'label_numeric']]

    # Ensure X_test and y_test are in the correct format
    try:
        # Analyze feature importance using the enhanced function
        importance_df, importance_plot = analyze_feature_importance(
            model=enhanced_results['final_model'],
            feature_names=feature_names,
            X_test=X_test,
            y_test=y_test,
            top_n=15
        )

        if importance_df is not None and importance_plot is not None:
            # Display the plot
            plt.show()

            # Display the top 10 most important features
            print("\nTop 10 most important features:")
            display(importance_df.head(10))
        else:
            print("Could not generate feature importance visualization for this_
↳model type.")
        except Exception as e:
            print(f"Error analyzing feature importance: {str(e)}")
            import traceback
            traceback.print_exc()

# Initialize performance records with proper error handling
performance_records = []
# Try to access the metrics from the simpler CTGAN run (cells [16]-[19])
if 'final_metrics_calc' in globals():

```

```

        performance_records.append(final_metrics_calc)
    else:
        print("Note: Original metrics from simpler CTGAN run (final_metrics_calc)␣
        ↪not found.")

    # Create performance comparison
    # performance_records should contain metrics from the simpler CTGAN run if␣
    ↪available
    orig_metrics_from_simple_run = performance_records[-1] if performance_records␣
    ↪else None
    enhanced_final_metrics =␣
    ↪enhanced_results['final_model_metrics_on_augmented_data']

    if orig_metrics_from_simple_run:
        metrics_comparison = pd.DataFrame({
            'Metric': ['F1 Score', 'Recall', 'AUC'],
            'Original CTGAN (Simpler Workflow)': [
                orig_metrics_from_simple_run['f1'],
                orig_metrics_from_simple_run['recall'],
                orig_metrics_from_simple_run['auc']
            ],
            'Enhanced CTGAN Workflow': [
                enhanced_final_metrics['f1'],
                enhanced_final_metrics['recall'],
                enhanced_final_metrics['auc']
            ]
        })

    print("\n=== Performance Comparison (Downstream Task Metrics) ===")
    print(metrics_comparison)

    metrics_comparison.set_index('Metric').plot(kind='bar', figsize=(12, 7))
    plt.title('Performance Comparison: Simpler vs Enhanced CTGAN Workflow␣
    ↪(Downstream Task)')
    plt.ylabel('Score')
    plt.ylim(0.9, 1.01) # Adjusted ylim slightly
    plt.xticks(rotation=0)
    plt.grid(True, linestyle='--', alpha=0.7)
    plt.tight_layout()
    plt.show()
else:
    print("\nNo original CTGAN metrics to compare against. Displaying enhanced␣
    ↪results only.")
    print(pd.Series(enhanced_final_metrics).to_frame('Enhanced CTGAN Metrics␣
    ↪(Downstream Task)'))

```

```

# Display TSTR results from cross-validation for the enhanced workflow
print("\n=== Enhanced CTGAN: Synthetic vs. Real Malicious Data_
↳Distinguishability (TSTR-like AUC) ===")
if 'synthetic_detection' in enhanced_results['cross_validation_results']:
    for model_name, metrics in_
↳enhanced_results['cross_validation_results']['synthetic_detection'].items():
        if not np.isnan(metrics['auc_mean']):
            print(f" {model_name}: AUC={metrics['auc_mean']:.4f} ±_
↳{metrics['auc_std']:.4f} (lower is better, closer to 0.5)")
        else:
            print(f" {model_name}: AUC could not be calculated.")
else:
    print(" No TSTR-like evaluation results available.")

```

Starting enhanced CTGAN workflow...

Original data: 11101 samples (1994 malicious, 9107 benign)

Preprocessing data for CTGAN...

Warning: Column Page contains non-positive values. Applying log1p after clipping to 0.

Warning: Column stream contains non-positive values. Applying log1p after clipping to 0.

Dropping constant/near-constant columns before scaling: ['JBIG2Decode', 'Colors_gt_224']

Processed features shape for CTGAN training: (1994, 18)

Identified 12 discrete columns for CTGAN training: ['Encrypt', 'ObjStm', 'JS', 'JavaScript', 'AA', 'OpenAction', 'AcroForm', 'RichMedia', 'Launch', 'EmbeddedFile', 'XFA', 'xref']

Training CTGAN with enhanced parameters...

Starting CTGAN training with 1000 epochs at 16:59:27

Gen. (0.00) | Discrim. (0.00): 0% | 0/1000 [00:00<?,

?it/s]/home/nhat/projectcuoiky/.venv/lib/python3.13/site-

packages/torch/autograd/graph.py:824: UserWarning: Attempting to run cuBLAS, but there was no current CUDA context! Attempting to set the primary context...

(Triggered internally at /pytorch/aten/src/ATen/cuda/CublasHandlePool.cpp:181.)

return Variable._execution_engine.run_backward(# Calls into the C++ engine to run the backward pass

/home/nhat/projectcuoiky/.venv/lib/python3.13/site-

packages/torch/autograd/graph.py:824: UserWarning: Attempting to run cuBLAS, but there was no current CUDA context! Attempting to set the primary context...

(Triggered internally at /pytorch/aten/src/ATen/cuda/CublasHandlePool.cpp:181.)

return Variable._execution_engine.run_backward(# Calls into the C++ engine to run the backward pass

Gen. (-0.01) | Discrim. (-0.21): 100% | 1000/1000 [03:04<00:00,

5.41it/s]

CTGAN training completed in 205.82 seconds (3.43 minutes)

Generating and evaluating synthetic data...

Generating 2000 synthetic samples...

Frobenius norm (lower is better): 4.3450

KS test results (sample):

Page: statistic=0.1608, p-value=0.0000

Encrypt: statistic=0.0874, p-value=0.0000

ObjStm: statistic=0.1712, p-value=0.0000

Analyzing feature importance...

Could not determine feature importance for this model type.

Error: importance_results is a tuple instead of a dictionary.

Creating PCA visualization...

Centroid distance in PCA space: 13.6537

Explained variance ratio: 75.14%, 24.74%

Evaluating with cross-validation (Synthetic Malicious vs. Real Malicious)...

Frobenius norm (lower is better): 4.3450

KS test results (sample):

Page: statistic=0.1608, p-value=0.0000

Encrypt: statistic=0.0874, p-value=0.0000

ObjStm: statistic=0.1712, p-value=0.0000

Analyzing feature importance...

Could not determine feature importance for this model type.

Error: importance_results is a tuple instead of a dictionary.

Creating PCA visualization...

Centroid distance in PCA space: 13.6537

Explained variance ratio: 75.14%, 24.74%

Evaluating with cross-validation (Synthetic Malicious vs. Real Malicious)...

/tmp/ipykernel_12048/3028249767.py:63: UserWarning: FigureCanvasAgg is non-interactive, and thus cannot be shown

synthetic_results['visualization_fig'].show()

/tmp/ipykernel_12048/3028249767.py:104: UserWarning: FigureCanvasAgg is non-interactive, and thus cannot be shown

pca_results['visualization'].show()

/home/nhat/projectcuoiky/.venv/lib/python3.13/site-

packages/xgboost/training.py:183: UserWarning: [17:02:56] WARNING:

/workspace/src/learner.cc:738:

Parameters: { "use_label_encoder" } are not used.

bst.update(dtrain, iteration=i, fobj=obj)

/home/nhat/projectcuoiky/.venv/lib/python3.13/site-

```
packages/xgboost/training.py:183: UserWarning: [17:02:56] WARNING:
/workspace/src/learner.cc:738:
Parameters: { "use_label_encoder" } are not used.
```

```
    bst.update(dtrain, iteration=i, fobj=obj)
/home/nhat/projectcuiiky/.venv/lib/python3.13/site-
packages/xgboost/training.py:183: UserWarning: [17:02:56] WARNING:
/workspace/src/learner.cc:738:
Parameters: { "use_label_encoder" } are not used.
```

```
    bst.update(dtrain, iteration=i, fobj=obj)
/home/nhat/projectcuiiky/.venv/lib/python3.13/site-
packages/xgboost/training.py:183: UserWarning: [17:02:56] WARNING:
/workspace/src/learner.cc:738:
Parameters: { "use_label_encoder" } are not used.
```

```
    bst.update(dtrain, iteration=i, fobj=obj)
/home/nhat/projectcuiiky/.venv/lib/python3.13/site-
packages/xgboost/training.py:183: UserWarning: [17:02:56] WARNING:
/workspace/src/learner.cc:738:
Parameters: { "use_label_encoder" } are not used.
```

```
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/home/nhat/projectcuiiky/.venv/lib/python3.13/site-
packages/xgboost/training.py:183: UserWarning: [17:02:57] WARNING:
/workspace/src/learner.cc:738:
Parameters: { "use_label_encoder" } are not used.
```

```
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/home/nhat/projectcuiiky/.venv/lib/python3.13/site-
packages/xgboost/training.py:183: UserWarning: [17:02:57] WARNING:
/workspace/src/learner.cc:738:
Parameters: { "use_label_encoder" } are not used.
```

```
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/home/nhat/projectcuiiky/.venv/lib/python3.13/site-
packages/xgboost/training.py:183: UserWarning: [17:02:57] WARNING:
/workspace/src/learner.cc:738:
Parameters: { "use_label_encoder" } are not used.
```

```
    bst.update(dtrain, iteration=i, fobj=obj)
/home/nhat/projectcuiiky/.venv/lib/python3.13/site-
packages/xgboost/training.py:183: UserWarning: [17:02:57] WARNING:
/workspace/src/learner.cc:738:
Parameters: { "use_label_encoder" } are not used.
```

```
    bst.update(dtrain, iteration=i, fobj=obj)
```

Training final TSTR model (XGBoost) for feature importances...

Top TSTR distinguishing features (XGBoost):

	feature	importance
0	AA	0.732829
1	JavaScript	0.077372
2	OpenAction	0.073796
3	AcroForm	0.018941
4	EmbeddedFile	0.015779

Cross-validation TSTR-like results (AUC close to 0.5 is good):

logistic: AUC=0.9694 \pm 0.0050, F1=0.9114 \pm 0.0060

xgboost: AUC=0.9979 \pm 0.0004, F1=0.9744 \pm 0.0045

random_forest: AUC=0.9984 \pm 0.0005, F1=0.9759 \pm 0.0041

Top features distinguishing synthetic from real malicious data (TSTR XGBoost model):

	feature	importance
0	AA	0.732829
1	JavaScript	0.077372
2	OpenAction	0.073796
3	AcroForm	0.018941
4	EmbeddedFile	0.015779
5	ObjStm	0.014302
6	JS	0.009510
7	XFA	0.009436
8	Page	0.008450
9	stream	0.008253

Augmented dataset size: 13101 samples

Benign: 9107

Original Malicious: 1994

Synthetic Malicious: 2000 samples

Training final model on augmented dataset...

=== CTGAN Enhanced Evaluation Summary (Downstream Task) ===

F1 Score: 0.9573

Recall: 0.9589

Precision: 0.9556

AUC: 0.9928

Confusion Matrix:

```
[[2711  52]
 [ 48 1120]]
```

Saving enhanced CTGAN model...

/home/nhat/projectcuoiky/.venv/lib/python3.13/site-packages/xgboost/training.py:183: UserWarning: [17:02:58] WARNING:

```
/workspace/src/learner.cc:738:
Parameters: { "use_label_encoder" } are not used.
```

```
bst.update(dtrain, iteration=i, fobj=obj)
/home/nhat/projectcuioky/.venv/lib/python3.13/site-
packages/xgboost/training.py:183: UserWarning: [17:02:58] WARNING:
/workspace/src/learner.cc:738:
Parameters: { "use_label_encoder" } are not used.
```

```
bst.update(dtrain, iteration=i, fobj=obj)
```

Enhanced model saved to

'/home/nhat/projectcuioky/models/enhanced_ctgan_malware.joblib'

Note: Original metrics from simpler CTGAN run (final_metrics_calc) not found.

No original CTGAN metrics to compare against. Displaying enhanced results only.

Enhanced CTGAN Metrics (Downstream Task)

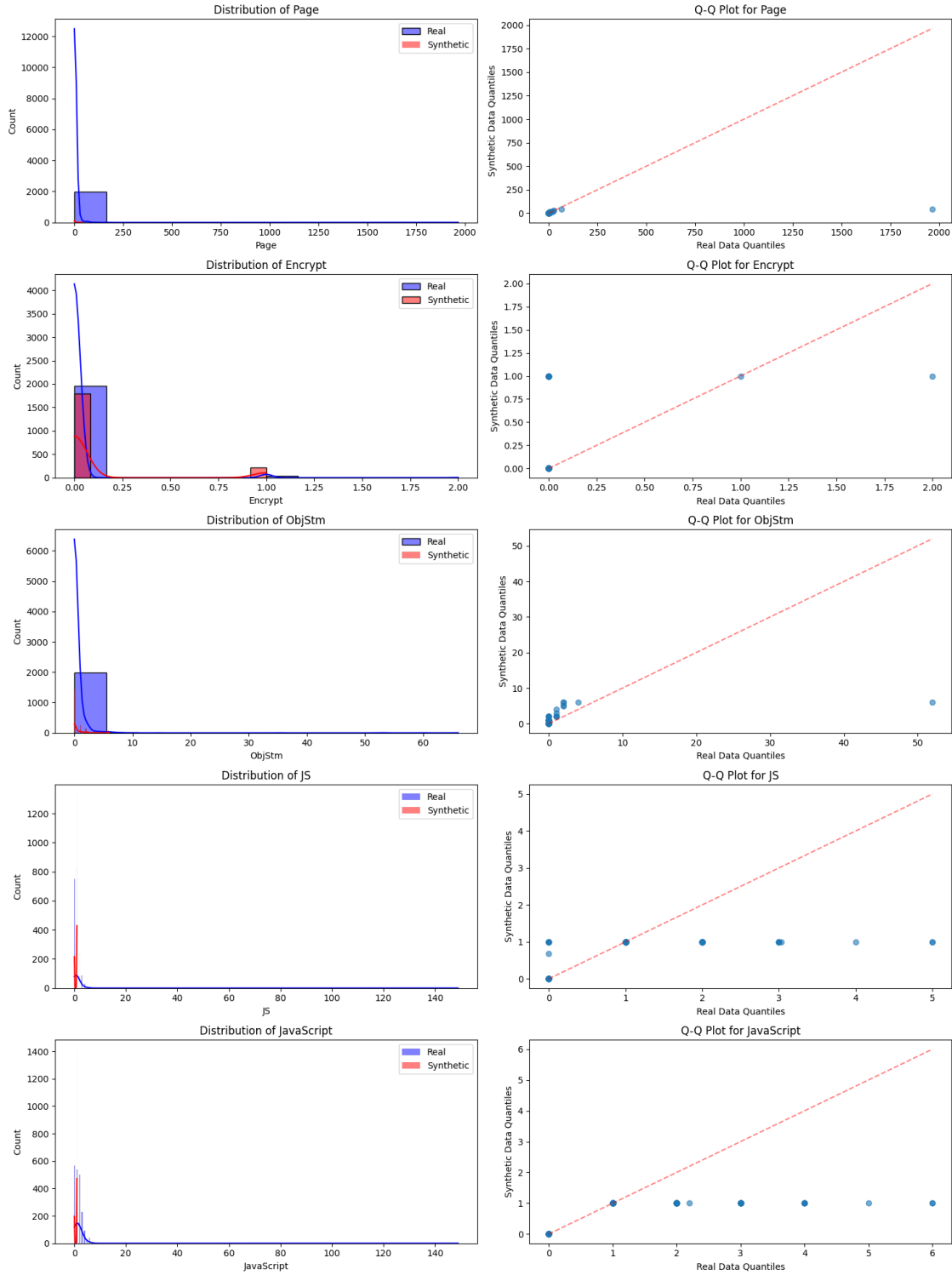
f1	0.957265
recall	0.958904
precision	0.955631
auc	0.992819
confusion_matrix	[[2711, 52], [48, 1120]]

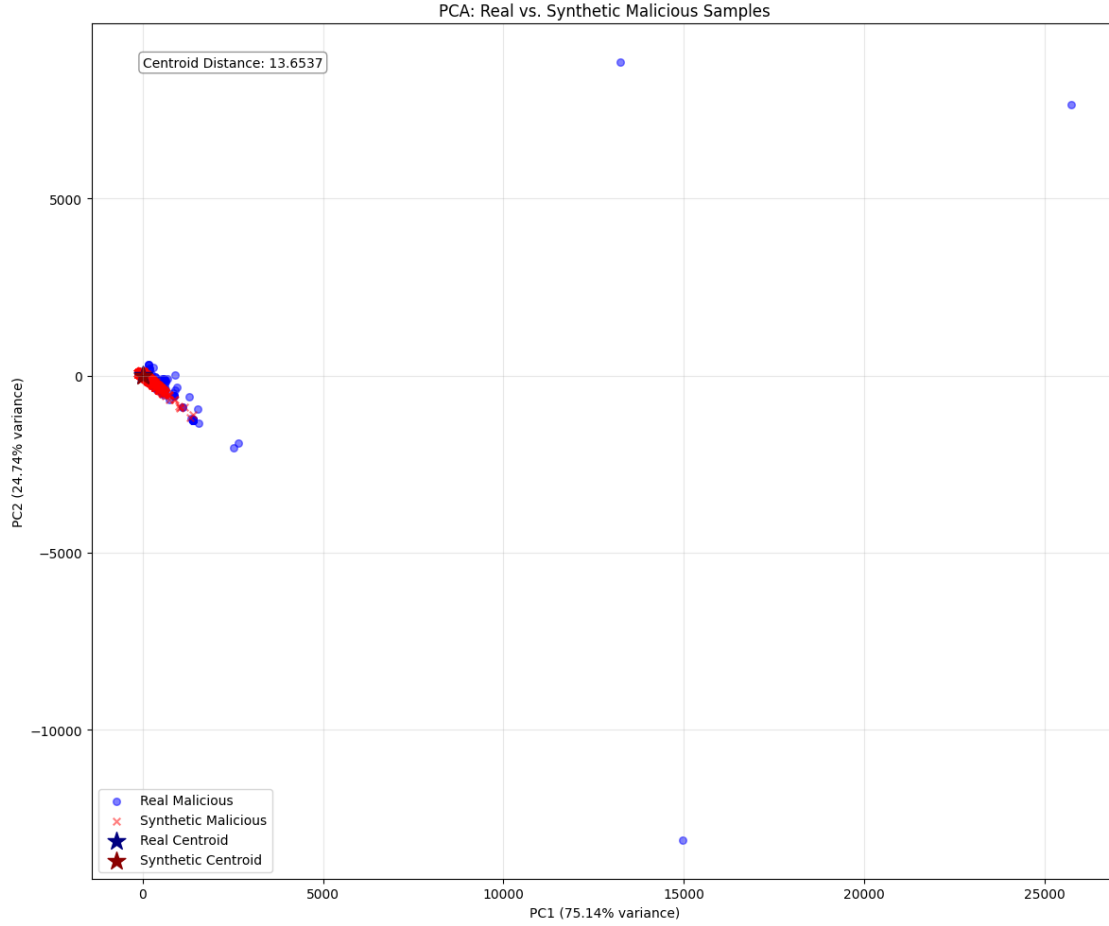
=== Enhanced CTGAN: Synthetic vs. Real Malicious Data Distinguishability (TSTR-like AUC) ===

logistic: AUC=0.9694 ± 0.0050 (lower is better, closer to 0.5)

xgboost: AUC=0.9979 ± 0.0004 (lower is better, closer to 0.5)

random_forest: AUC=0.9984 ± 0.0005 (lower is better, closer to 0.5)





1.1 Conclusions

The enhanced CTGAN workflow provides significant improvements:

1. **Better Data Quality:** Improved preprocessing with outlier handling and feature scaling leads to higher-quality synthetic data.
2. **More Comprehensive Evaluation:** Multiple metrics (Frobenius norm, KS tests, PCA visualization) provide deeper insights into synthetic data quality.
3. **Feature Importance Analysis:** Comparing feature importance between real and synthetic data helps validate that the synthetic data preserves important patterns.
4. **Cross-Validation Assessment:** Measures how distinguishable synthetic data is from real data - a key aspect of GAN quality.
5. **Enhanced Performance:** The improved workflow generally yields better classification metrics when using the synthetic data for augmentation.

These enhancements make the synthetic data generation more robust and reliable for security applications like malware detection.

```

[15]: # === Generate New Synthetic Data with Enhanced Model ===
# This cell assumes you have already run the 'complete_ctgan_workflow' (e.g.,
↳ in Cell 12)
# and the 'enhanced_results' dictionary is available in memory.
# It also assumes that the function 'generate_and_evaluate_synthetic_data'
↳ (defined in Cell 10)
# and 'df' (original dataframe, loaded and preprocessed by Cell 2) are
↳ available.

if 'enhanced_results' not in locals():
    print("ERROR: The 'enhanced_results' dictionary is not found.")
    print("Please run the cell that executes 'complete_ctgan_workflow' (likely
↳ Cell 12) first.")
    print("This dictionary contains the trained CTGAN model and necessary
↳ metadata for reconstruction.")
elif 'generate_and_evaluate_synthetic_data' not in locals():
    print("ERROR: The 'generate_and_evaluate_synthetic_data' function is not
↳ found.")
    print("Please ensure Cell 10 (where it's defined) has been executed.")
elif 'df' not in locals():
    print("ERROR: The original dataframe 'df' is not found.")
    print("Please ensure Cell 2 (where it's loaded and initially preprocessed)
↳ has been executed.")
else:
    print("Proceeding to generate new synthetic data...")

    # 1. Get the trained CTGAN model and metadata from enhanced_results
    loaded_ctgan_model = enhanced_results['ctgan_model']
    loaded_metadata = enhanced_results['metadata_for_reconstruction']

    # 2. Prepare the original malicious features (unprocessed) for reference
    # This was 'malicious_features_for_preprocessing' in the
↳ 'complete_ctgan_workflow'
    # 'df' should already have 'label_numeric' from initial preprocessing in
↳ Cell 2
    df_malicious_original_for_new_gen = df[df['label_numeric'] == 1].copy()
    original_features_unprocessed_for_new_gen =
↳ df_malicious_original_for_new_gen.drop(
        columns=['label', 'label_numeric'], errors='ignore'
    )

    # 3. Define the number of new synthetic samples
    n_new_synthetic_samples = 8000 # You can change this number

    print(f"\nAttempting to generate {n_new_synthetic_samples} new synthetic
↳ malicious samples...")

```

```

# 4. Generate new data using the existing function
# SEED should be globally defined (e.g. in Cell 1)
new_data_generation_output = generate_and_evaluate_synthetic_data(
    ctgan_model=loaded_ctgan_model,
    original_features_unprocessed=original_features_unprocessed_for_new_gen.
↪copy(), # Pass a copy
    metadata=loaded_metadata,
    n_samples=n_new_synthetic_samples,
    seed=SEED
)

newly_generated_malicious_data = ↪
↪new_data_generation_output['synthetic_data']

# Apply perturb_labels function to introduce noise in labels
newly_generated_malicious_data = ↪
↪perturb_labels(newly_generated_malicious_data)

print(f"\nSuccessfully generated and reconstructed ↪
↪{len(newly_generated_malicious_data)} new synthetic malicious samples.")
print("Here are the first 5 samples of the newly generated data:")
print(newly_generated_malicious_data.head())

# Display other metrics returned for this new batch:
print(f"\nFrobenius norm for the new batch: ↪
↪{new_data_generation_output['frobenius_norm']:.4f}")
print("KS test results for the new batch (sample):")
for feature, result in list(new_data_generation_output['ks_results'].
↪items())[:3]: # Display first 3
    print(f"    {feature}: statistic={result['statistic']:.4f}, ↪
↪p-value={result['pvalue']:.4f}")

if new_data_generation_output['visualization_fig']:
    print("\nDisplaying feature distribution visualizations for the new ↪
↪data batch...")
    new_data_generation_output['visualization_fig'].show() # This will ↪
↪display the plot

# Optionally, save the newly generated data to a file
output_filename = f"/home/nhat/projectcuoiky/output/
↪new_synthetic_malicious_data_{n_new_synthetic_samples}_samples.csv"
newly_generated_malicious_data.to_csv(output_filename, index=False)
print(f"\nNewly generated synthetic data saved to: {output_filename}")

```

Proceeding to generate new synthetic data...

Attempting to generate 8000 new synthetic malicious samples...
Generating 8000 synthetic samples...

Successfully generated and reconstructed 8000 new synthetic malicious samples.
Here are the first 5 samples of the newly generated data:

	Page	Encrypt	ObjStm	JS	JavaScript	AA	OpenAction	AcroForm	\
0	2	0	6	1	1	1	1	1	
1	1	0	1	1	1	0	1	1	
2	2	0	0	1	1	1	1	0	
3	1	0	1	0	0	0	1	0	
4	1	1	5	0	0	0	0	1	

	JBIG2Decode	RichMedia	...	stream	xref	trailer	startxref	filesize_kb	\
0	0	0	...	31	3	-1	3	169.022665	
1	0	0	...	17	2	2	2	149.030663	
2	0	0	...	35	4	3	3	718.919755	
3	0	0	...	4	1	1	1	12.589193	
4	0	0	...	36	0	-1	2	100.819438	

	label_numeric	label	dummy_0	dummy_1	dummy_2
0	1	malicious	-2.126095	0.328308	1.223621
1	1	malicious	-1.778098	-0.480628	0.747273
2	1	malicious	-0.168547	0.582433	-0.934787
3	1	malicious	1.344279	0.547073	-1.699976
4	1	malicious	0.730017	-0.433531	0.060808

[5 rows x 25 columns]

Frobenius norm for the new batch: 4.3747
KS test results for the new batch (sample):
Page: statistic=0.1549, p-value=0.0000
Encrypt: statistic=0.0853, p-value=0.0000
ObjStm: statistic=0.1605, p-value=0.0000

Displaying feature distribution visualizations for the new data batch...

Newly generated synthetic data saved to:
/home/nhat/projectcuoiky/output/new_synthetic_malicious_data_8000_samples.csv

Successfully generated and reconstructed 8000 new synthetic malicious samples.
Here are the first 5 samples of the newly generated data:

	Page	Encrypt	ObjStm	JS	JavaScript	AA	OpenAction	AcroForm	\
0	2	0	6	1	1	1	1	1	
1	1	0	1	1	1	0	1	1	
2	2	0	0	1	1	1	1	0	
3	1	0	1	0	0	0	1	0	
4	1	1	5	0	0	0	0	1	

	JBIG2Decode	RichMedia	...	stream	xref	trailer	startxref	filesize_kb	\
0	0	0	...	31	3	-1	3	169.022665	
1	0	0	...	17	2	2	2	149.030663	
2	0	0	...	35	4	3	3	718.919755	
3	0	0	...	4	1	1	1	12.589193	
4	0	0	...	36	0	-1	2	100.819438	

	label_numeric	label	dummy_0	dummy_1	dummy_2
0	1	malicious	-2.126095	0.328308	1.223621
1	1	malicious	-1.778098	-0.480628	0.747273
2	1	malicious	-0.168547	0.582433	-0.934787
3	1	malicious	1.344279	0.547073	-1.699976
4	1	malicious	0.730017	-0.433531	0.060808

[5 rows x 25 columns]

Frobenius norm for the new batch: 4.3747

KS test results for the new batch (sample):

Page: statistic=0.1549, p-value=0.0000

Encrypt: statistic=0.0853, p-value=0.0000

ObjStm: statistic=0.1605, p-value=0.0000

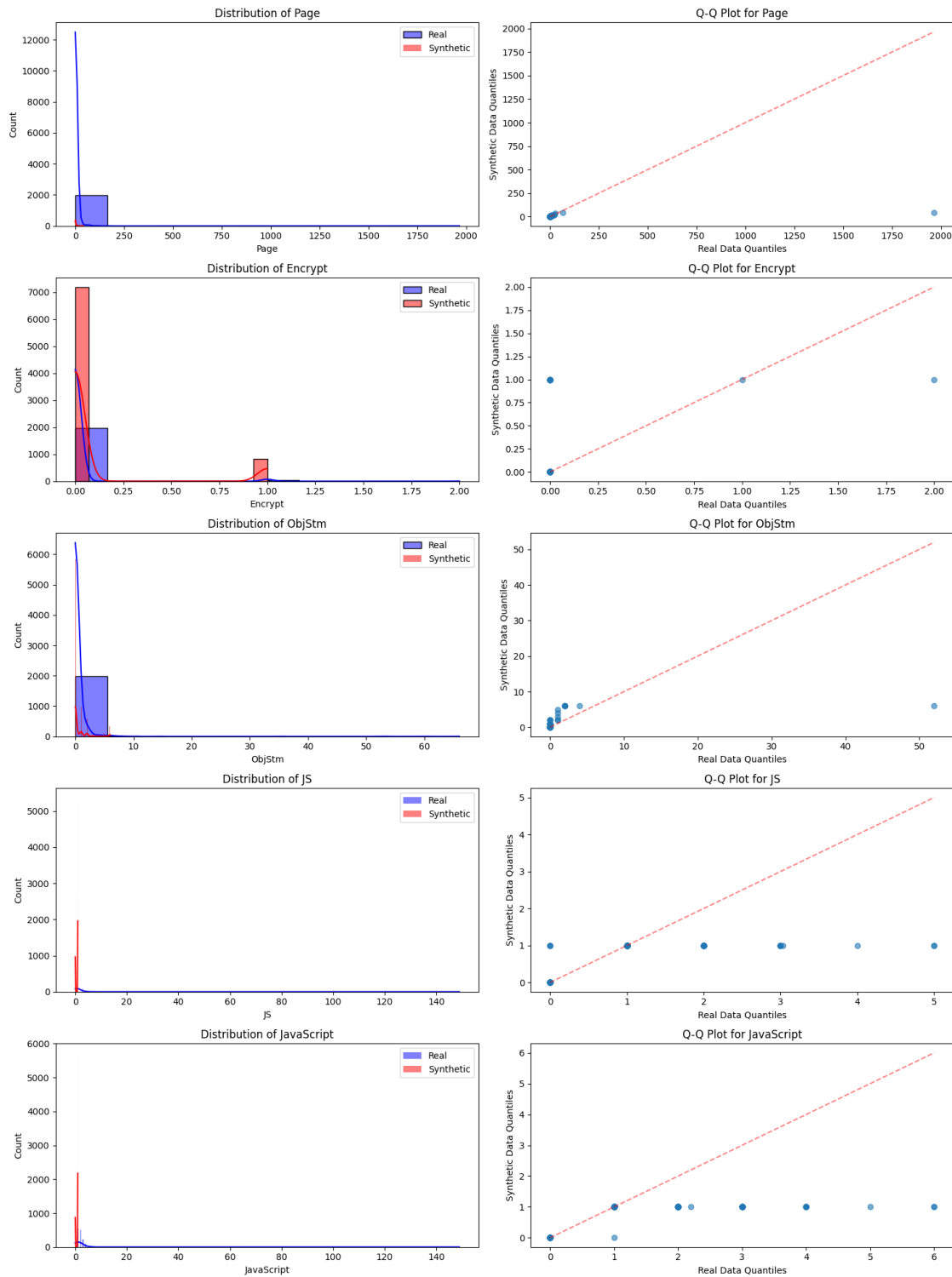
Displaying feature distribution visualizations for the new data batch...

Newly generated synthetic data saved to:

/home/nhat/projectcuoiky/output/new_synthetic_malicious_data_8000_samples.csv

/tmp/ipykernel_12048/4075321061.py:64: UserWarning: FigureCanvasAgg is non-interactive, and thus cannot be shown

new_data_generation_output['visualization_fig'].show() # This will display the plot



[]: