

1. Import Libraries

```
In [1]: import pandas as pd
import numpy as np
from pathlib import Path
import time
import re

import matplotlib.pyplot as plt

from sklearn.ensemble import RandomForestClassifier
from sklearn.model_selection import train_test_split, StratifiedKFold, GridSearchCV, StratifiedKFold, GridSearchCV
from sklearn.preprocessing import LabelEncoder, label_binarize, MinMaxScaler, label_binarize
from sklearn.calibration import calibration_curve
from sklearn.metrics import (
    cohen_kappa_score,
    matthews_corrcoef,
    make_scorer,
    f1_score,
    accuracy_score,
    balanced_accuracy_score,
    classification_report,
    confusion_matrix,
    precision_recall_curve,
    average_precision_score,
    brier_score_loss,
    roc_auc_score,
    roc_curve,
    log_loss,
    auc
)

from xgboost import XGBClassifier

from IPython.display import display
```

```
In [2]: # CPU core usage for VM troubleshooting
import os
print(os.cpu_count())
```

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2. Data Preprocessing

2.1. Data Loading

This cell scans the dataset folder for input CSV files (excluding previously generated combined outputs), reads each file into a DataFrame, concatenates them into one merged dataset, saves the merged CSV to disk, and loads it into `df` for cleaning and modeling.

```
In [3]: # Directory containing the dataset CSV files
data_dir = Path("/datasets")

# Grab all csv files in directory
csv_files = sorted(
    f for f in data_dir.glob("*.csv")
    if f.name != "CICIDS2017_combined.csv" # Skip these output files to avoid re-reading & merging them
    if f.name != "CICIDS2017_combined_clean.csv"
)
print(f"Found {len(csv_files)} CSV files\n") # Log how many input files were discovered

dfs = [] # Holds each per-file DataFrame before concatenation
for f in csv_files:
    print("Reading:", f.name) # Log which file is being read
    df = pd.read_csv(f, low_memory=False) # To not infer dtypes in chunks
    dfs.append(df) # Store the DataFrame for later concatenation

combined = pd.concat(dfs, ignore_index=True, sort=False) # Create a new index and keep original column order
print("\nCombined shape:", combined.shape) # Log rows and columns of the final merged DataFrame

out_path = data_dir / "CICIDS2017_combined.csv" # Output file path for the merged dataset
combined.to_csv(out_path, index=False) # To not write the DataFrame index as an extra column in the CSV
print("\nSaved to:", out_path) # Display where the combined CSV was written

# Load the combined CSV dataset into a DataFrame
df = pd.read_csv("/datasets/CICIDS2017_combined.csv", low_memory=False)
print("\nLoaded merged dataset into DataFrame")
```

Found 8 CSV files

Reading: Friday-WorkingHours-Afternoon-DDos.pcap_ISCX.csv
Reading: Friday-WorkingHours-Afternoon-PortScan.pcap_ISCX.csv
Reading: Friday-WorkingHours-Morning.pcap_ISCX.csv
Reading: Monday-WorkingHours.pcap_ISCX.csv
Reading: Thursday-WorkingHours-Afternoon-Infiltration.pcap_ISCX.csv
Reading: Thursday-WorkingHours-Morning-WebAttacks.pcap_ISCX.csv
Reading: Tuesday-WorkingHours.pcap_ISCX.csv
Reading: Wednesday-workingHours.pcap_ISCX.csv

Combined shape: (2830743, 79)

Saved to: /datasets/CICIDS2017_combined.csv

Loaded merged dataset into DataFrame

2.2. Data Preprocessing

2.2.1 BEFORE Clean-up

This cell runs a pre-cleaning quality check on the merged dataset, flagging header whitespace/collisions, string-based infinity tokens, NaN/Inf issues in rate features (and whether they come from Flow Duration = 0), duplicate rows, constant/all-zero columns, mixed dtypes, label formatting inconsistencies, and identifier-like columns that may cause leakage.

```
In [4]: def _safe_df(rows, columns, sort_by=None, ascending=False):
# To build a stable DataFrame (always same columns; safe if empty; optional sort)
# If rows is empty, return an empty DataFrame with `columns`
if not rows:
    return pd.DataFrame(columns=columns)
d = pd.DataFrame(rows)
# Ensures all `columns` exist (missing are filled with NaN)
for c in columns:
    if c not in d.columns:
        d[c] = np.nan
d = d[columns]
# sort by sort_by if present
if sort_by is not None and sort_by in d.columns:
    d = d.sort_values(sort_by, ascending=ascending)
return d.reset_index(drop=True)

def qc_merged_report(df: pd.DataFrame, label_col: str | None = None, show_top: int = 25) -> dict:
# To build a QC report, scan merged dataset for common data issues and return summary tables
out = {}

# ----- 1 - Column name cleanup (whitespace + collisions)
raw_cols = df.columns.astype(str).tolist() # Original column headers as strings
stripped_cols = [c.strip() for c in raw_cols] # Same headers after removing outer spaces
whitespace_cols = [c for c in raw_cols if c != c.strip()] # Headers that actually change when stripped
dup_after_strip_mask = pd.Series(stripped_cols).duplicated(keep=False) # Which stripped names repeat
dup_after_strip_originals = sorted(set( # Original headers involved in collisions
    pd.Series(raw_cols)[dup_after_strip_mask].tolist()
))
out["whitespace_cols"] = _safe_df( # Output table for original vs stripped
    [{ "original": c, "stripped": c.strip() } for c in whitespace_cols],
    columns=["original", "stripped"],
    sort_by="original",
    ascending=True
)
out["duplicate_names_after_strip"] = dup_after_strip_originals # Output headers that would clash after strip()
col_map = {c: c.strip() for c in df.columns.astype(str)} # Mapping by original header to stripped header
# Inverted mapping by normalized name to originals
inv_map = {}
for orig, stripped in col_map.items():
    inv_map.setdefault(stripped.lower(), []).append(orig) # Normalize case to match headers

# ----- 2 - "Inf" tokens in text columns
obj_cols = df.select_dtypes(include=["object"]).columns # Only scan object/text columns
tokens = {"infinity", "inf", "+inf", "-inf"} # String forms treated as Infinity
# Store columns that contain these tokens
hits = []
for c in obj_cols:
    s = df[c].astype(str).str.strip().str.lower() # Normalize text (string + trim + Lowercase)
    mask = s.isin(tokens) # Rows where the value is an inf-token
    if mask.any(): # Only report columns with at least one hit
        hits.append({
            "column": c, # Which column has the issue
            "count_token_inf": int(mask.sum()), # How many inf-tokens appear
            "examples": df.loc[mask, c].head(5).tolist() # A few sample values for debugging
        })
out["string_inf_cols"] = _safe_df( # Output as a clean, sortable table
    hits, ["column", "count_token_inf", "examples"],
    sort_by="count_token_inf", ascending=False # Show worst columns first
)
```

```

# ----- 3 - Rate features: NaN/Inf + divide-by-zero check
rate_targets = ["flow bytes/s", "flow packets/s"] # The rate columns containing Infs when manually checked
rate_rows = []
for target in rate_targets:
    for col in inv_map.get(target, []): # Handle case/whitespace variants via inv_map
        num = pd.to_numeric(df[col], errors="coerce") # Force numeric by bad values to NaN
        n_total = len(df)
        n_nan = int(num.isna().sum()) # Count NaNs after conversion
        n_inf = int(np.isinf(num).sum()) # Count infinite values
        rate_rows.append({ # Store per-column summary
            "column": col,
            "n_nan": n_nan,
            "pct_nan": round(100 * n_nan / max(n_total, 1), 4),
            "n_inf": n_inf,
            "pct_inf": round(100 * n_inf / max(n_total, 1), 4),
        })
    if target not in inv_map: # If the expected feature is missing
        rate_rows.append({"column": f"(missing) {target}", "n_nan": None, "pct_nan": None, "n_inf": None, "pct_inf": None})
out["rate_feature_issues"] = _safe_df( # Output table of NaN/Inf rates per feature
    rate_rows, ["column", "n_nan", "pct_nan", "n_inf", "pct_inf"],
    sort_by="column", ascending=True
)
# Check if bad rates are caused by Flow Duration == 0
dur_col = (inv_map.get("flow duration") or [None])[0]
if dur_col:
    dur_zero = (pd.to_numeric(df[dur_col], errors="coerce") == 0) # Rows where duration is zero
    corr_rows = []
    for target in rate_targets:
        for col in inv_map.get(target, []):
            num = pd.to_numeric(df[col], errors="coerce")
            bad = num.isna() | np.isinf(num) # "bad" = NaN or Inf
            corr_rows.append({
                "duration_col_used": dur_col, # Which duration column were used
                "rate_col": col, # Which rate column were tested
                "bad_rate_rows": int(bad.sum()), # Total bad rows in this rate feature
                "bad_when_dur_zero": int((bad & dur_zero).sum()), # Bad rows specifically when duration==0
                "pct_bad_with_dur_zero": round(100 * (bad & dur_zero).sum() / max(bad.sum(), 1), 4),
            })
    out["rate_vs_duration_zero"] = _safe_df( # Output how strongly duration==0 explains bad rates
        corr_rows,
        ["duration_col_used", "rate_col", "bad_rate_rows", "bad_when_dur_zero", "pct_bad_with_dur_zero"],
        sort_by="bad_rate_rows", ascending=False
    )
else:
    out["rate_vs_duration_zero"] = pd.DataFrame([{"note": "No Flow Duration column found."}])

# ----- 4 - Duplicate rows
n_dupes = int(df.duplicated().sum())
out["duplicates_summary"] = { # Output amount of duplicate rows
    "rows": int(len(df)),
    "duplicate_rows": n_dupes,
    "pct_duplicates": round(100 * n_dupes / max(len(df), 1), 6)
}

# ----- 5 - Constant / all-zero features (no variance to no ML signal)
rows = []
for c in df.columns:
    nunq = int(df[c].nunique(dropna=False)) # Uniques incl. NaN, treating NaN as a value
    if nunq == 1: # Fully constant column
        rows.append({"column": c, "n_unique": 1, "value": df[c].iloc[0]})
    elif pd.api.types.is_numeric_dtype(df[c]) and (df[c].fillna(0) == 0).all():
        rows.append({"column": c, "n_unique": nunq, "value": "all_zero_or_nan"}) # Effectively constant
out["constant_cols"] = _safe_df( # Output as a clean table
    rows, ["column", "n_unique", "value"],
    sort_by="column", ascending=True
)

# ----- 6 - Text columns that are mostly numeric
rows = []
for c in obj_cols:
    num = pd.to_numeric(df[c], errors="coerce") # Convert failures into NaN
    pct_num = 100 * float(num.notna().mean()) # % values that look numeric
    if pct_num >= 90: # Threshold to treat as numeric column
        examples = ( # Show a few values that failed conversion
            df.loc[num.isna(), c].astype(str).str.strip()
            .replace({"nan": np.nan}).dropna().head(10).tolist()
        )
        rows.append({"column": c, "pct_numeric": round(pct_num, 3), "bad_examples": examples})
out["object_numeric_suspects"] = _safe_df( # Output which object cols should be numeric
    rows, ["column", "pct_numeric", "bad_examples"],
    sort_by="pct_numeric", ascending=False
)

# ----- 7 - Label inconsistencies (same class written in different ways)
if label_col is None: # Detect 'Label' column
    label_col = next((c for c in df.columns.astype(str) if c.strip().lower() == "label"), None)
if label_col in df.columns: # Only run if label column exists

```

```

raw = df[label_col].astype(str) # Original Labels as-is
norm = raw.str.strip().str.lower() # Normalized Labels (trim + Lowercase)
# Count how many times each (raw, normalized) pair appears
variants = pd.DataFrame({"raw": raw, "norm": norm}).value_counts().reset_index(name="count")
# Group by normalized label to see which raw spellings map to the same class
by_norm = (variants.groupby("norm", dropna=False)
            .apply(lambda g: g.sort_values("count", ascending=False)[["raw", "count"]]
            .head(show_top).to_dict("records"))
            .reset_index(name="raw_variants"))
out["label_col_used"] = label_col # Output which column was used
out["label_inconsistencies"] = by_norm[by_norm["raw_variants"].apply(len).gt(1)].reset_index(drop=True)
out["label_counts_normalized"] = norm.value_counts().head(50).to_frame("count") # Top classes
else:
    out["label_col_used"] = None
    out["label_inconsistencies"] = pd.DataFrame([{"note": "No label column found."}])
    out["label_counts_normalized"] = pd.DataFrame()

# ----- 8 - Identifier / Leakage-like columns
id_like = { # Common ID fields to flag
    "flow id", "timestamp",
    "src ip", "dst ip", "source ip", "destination ip",
    "src port", "dst port", "source port", "destination port",
    "protocol"
}
# Find any columns whose normalized name matches an ID-like field
found = [orig for norm, originals in inv_map.items() if norm in id_like for orig in originals]
out["identifier_cols_found"] = sorted(set(found)) # Output unique list with original column names

# ----- 9 - Dtype summary
out["dtype_summary"] = df.dtypes.astype(str).value_counts().to_frame("n_columns")
return out

# Run QC and display outputs
qc = qc_merged_report(df)

print("---- 1 - Columns with leading/trailing whitespace")
print(qc["whitespace_cols"].head(200))
print("\n---- 1b - Potential collisions after stripping (original names involved)")
print(qc["duplicate_names_after_strip"])

print("\n---- 2 - 'Infinity/inf' tokens found in OBJECT columns")
print(qc["string_inf_cols"].head(50)) # will be empty (no crash) if none found

print("\n---- 3 - Rate feature NaN/Inf issues (Flow Bytes/s, Flow Packets/s)")
print(qc["rate_feature_issues"])
print("\n---- 3b - Bad rate values vs Flow Duration == 0 (if Flow Duration exists)")
print(qc["rate_vs_duration_zero"].head(50))

print("\n---- 4 - Duplicate rows summary")
print(qc["duplicates_summary"])

print("\n---- 5 - Constant / all-zero columns")
print(qc["constant_cols"].head(100))

print("\n---- 6 - Object columns that are mostly numeric (dtype issues)")
print(qc["object_numeric_suspects"].head(50))

print("\n---- 7 - Label inconsistencies (raw variants mapping to same normalized label)")
print("Label column used:", qc["label_col_used"])
print(qc["label_inconsistencies"].head(50))
print("\n---- 7b - Normalized label counts (top 50)")
print(qc["label_counts_normalized"].head(50))

print("\n---- 8 - Identifier-like columns found (possible leakage)")
print(qc["identifier_cols_found"])

print("\n---- 9 - Dtype summary")
print(qc["dtype_summary"])

```

---- 1 - Columns with leading/trailing whitespace

	original	stripped
0	ACK Flag Count	ACK Flag Count
1	Active Max	Active Max
2	Active Min	Active Min
3	Active Std	Active Std
4	Average Packet Size	Average Packet Size
..
60	Total Fwd Packets	Total Fwd Packets
61	Total Length of Bwd Packets	Total Length of Bwd Packets
62	URG Flag Count	URG Flag Count
63	act_data_pkt_fwd	act_data_pkt_fwd
64	min_seg_size_forward	min_seg_size_forward

[65 rows x 2 columns]

---- 1b - Potential collisions after stripping (original names involved)

[]

---- 2 - 'Infinity/inf' tokens found in OBJECT columns

Empty DataFrame

Columns: [column, count_token_inf, examples]

Index: []

---- 3 - Rate feature NaN/Inf issues (Flow Bytes/s, Flow Packets/s)

	column	n_nan	pct_nan	n_inf	pct_inf
0	Flow Packets/s	0	0.000	2867	0.1013
1	Flow Bytes/s	1358	0.048	1509	0.0533

---- 3b - Bad rate values vs Flow Duration == 0 (if Flow Duration exists)

	duration_col_used	rate_col	bad_rate_rows	bad_when_dur_zero \
0	Flow Duration	Flow Bytes/s	2867	2867
1	Flow Duration	Flow Packets/s	2867	2867

	pct_bad_with_dur_zero
0	100.0
1	100.0

---- 4 - Duplicate rows summary

{'rows': 2830743, 'duplicate_rows': 308381, 'pct_duplicates': 10.893995}

---- 5 - Constant / all-zero columns

	column	n_unique	value
0	Bwd Avg Bytes/Bulk	1	0
1	Bwd Avg Packets/Bulk	1	0
2	Bwd PSH Flags	1	0
3	Bwd URG Flags	1	0
4	Fwd Avg Bulk Rate	1	0
5	Fwd Avg Packets/Bulk	1	0
6	Bwd Avg Bulk Rate	1	0
7	Fwd Avg Bytes/Bulk	1	0

---- 6 - Object columns that are mostly numeric (dtype issues)

Empty DataFrame

Columns: [column, pct_numeric, bad_examples]

Index: []

---- 7 - Label inconsistencies (raw variants mapping to same normalized label)

Label column used: Label

Empty DataFrame

Columns: [norm, raw_variants]

Index: []

---- 7b - Normalized label counts (top 50)

	count
Label	
benign	2273097
dos hulk	231073
portscan	158930
ddos	128027
dos goldeneye	10293
ftp-patator	7938
ssh-patator	5897
dos slowloris	5796
dos slowhttptest	5499
bot	1966
web attack 💎 brute force	1507
web attack 💎 xss	652
infiltration	36
web attack 💎 sql injection	21
heartbleed	11

---- 8 - Identifier-like columns found (possible leakage)

[' Destination Port']

---- 9 - Dtype summary

n_columns

int64	54
float64	24
object	1

/tmp/ipykernel_8902/549497848.py:154: FutureWarning: DataFrameGroupBy.apply operated on the grouping columns. This behavior is deprecated, and in a future version of pandas the grouping columns will be excluded from the operation. Either pass `include_groups=False` to exclude the groupings or explicitly select the grouping columns after groupby to silence this warning.
.apply(lambda g: g.sort_values("count", ascending=False)[["raw", "count"]])

2.2.2 AFTER Clean-up

This cell reports the dataset quality after cleaning by summarising the final shape, confirming duplicates and constant/all-zero columns were removed, verifying Flow Bytes/s and Flow Packets/s no longer contain invalid values (e.g. Flow Duration = 0), and checking that label values are consistently formatted before saving and reloading the cleaned dataset.

```
In [5]: def find_col(df, name: str):
        # Robust column lookup, ignore whitespace and case, return the real header or None
        target = name.strip().lower()
        return next((c for c in df.columns if str(c).strip().lower() == target), None)

def constant_or_zero_cols(df):
    # Find 'no-signal' columns, constant (1 unique incl NaN) OR numeric all 0/NaN
    cols = []
    for c in df.columns:
        if df[c].nunique(dropna=False) == 1: # Fully constant
            cols.append(c)
        elif pd.api.types.is_numeric_dtype(df[c]) and (df[c].fillna(0) == 0).all():
            cols.append(c) # Effectively constant (all 0/NaN)
    return sorted(set(cols))

def report_key_stats(df, title=""):
    # Quick before/after QC snapshot (shape, dupes, no-signal cols, rate sanity, Label preview)
    print(f"\n{'-'*60}\n{title}\n{'-'*60}")
    dup = int(df.duplicated().sum())
    print("Shape:", df.shape, "| Duplicate rows:", dup, f"({100*dup/max(len(df),1):.4f}%)")
    const_cols = constant_or_zero_cols(df) # Columns safe to drop
    print("Constant/all-zero cols:", len(const_cols),
          (f"| ex: {const_cols[:10]}" if const_cols else ""))
    # Fix rate features when duration==0 (avoid NaN/Inf from divide-by-zero)
    dur = find_col(df, "Flow Duration")
    fb = find_col(df, "Flow Bytes/s")
    fp = find_col(df, "Flow Packets/s")
    if dur and (fb or fp):
        dur_zero = (pd.to_numeric(df[dur], errors="coerce") == 0)
        for col in [fb, fp]:
            if not col:
                continue
            x = pd.to_numeric(df[col], errors="coerce")
            bad = x.isna() | np.isinf(x)
            print(f"{col}: bad={int(bad.sum())}  bad&dur0={int((bad & dur_zero).sum())}")
    else:
        print("Rate check skipped (missing duration and/or rate columns).")
    # Label preview in normalized counts to spot casing/whitespace variants
    lab = find_col(df, "Label")
    if lab:
        print("Label column:", repr(lab))
        print(df[lab].astype(str).str.strip().str.lower().value_counts().head(12))
    else:
        print("No Label column found.")
    return const_cols

# ---- BEFORE Report
_ = report_key_stats(df, "BEFORE CLEANING")

# ---- CLEANING PIPELINE
df = df.copy()

df.columns = df.columns.astype(str).str.strip() # 1. Trim header whitespace
df = df.drop_duplicates().reset_index(drop=True) # 2. Remove duplicate rows
df = df.drop(columns=constant_or_zero_cols(df), errors="ignore") # 3. Drop no-signal features

# 4. Fix rate features when duration==0 (avoid NaN/Inf from divide-by-zero)
FIX_RATE_MODE = "set_zero"
dur = find_col(df, "Flow Duration")
fb = find_col(df, "Flow Bytes/s")
fp = find_col(df, "Flow Packets/s")
if dur and (fb or fp):
    dur_zero = (pd.to_numeric(df[dur], errors="coerce") == 0) # Duration==0 rows
    for col in [fb, fp]:
        if not col:
            continue
        x = pd.to_numeric(df[col], errors="coerce").replace([np.inf, -np.inf], np.nan) # Unify bad values
        bad = x.isna() # After replace bad == NaN
        if FIX_RATE_MODE == "set_zero":
            x.loc[dur_zero & bad] = 0.0 # Set bad rates to 0 when duration==0
            df[col] = x
        elif FIX_RATE_MODE == "drop_rows":
            df = df.loc[~(dur_zero & bad)].reset_index(drop=True) # Drop those rows entirely
```

```

        else:
            raise ValueError("FIX_RATE_MODE must be 'set_zero' or 'drop_rows'")

# 5. Label cleanup and standardization
lab = find_col(df, "Label")
if lab:
    df[lab] = (df[lab].astype(str).str.strip() # Trim whitespace
               .str.replace("❖", "-", regex=False) # Fix encoding artifact
               .str.replace(r"\s+", " ", regex=True)) # Collapse repeated spaces
    label_map = { # Normalize common Label variants
        "web attack - brute force": "Web Attack - Brute Force",
        "web attack - xss": "Web Attack - XSS",
        "web attack - sql injection": "Web Attack - SQL Injection",
        "benign": "BENIGN",
        "ddos": "DDoS",
        "bot": "Bot",
        "portscan": "PortScan",
        "infiltration": "Infiltration",
        "heartbleed": "Heartbleed",
        "dos hulk": "DoS Hulk",
        "dos slowloris": "DoS Slowloris",
        "dos slowhttptest": "DoS SlowHTTPTest",
        "dos goldeneye": "DoS GoldenEye",
    }
    df[lab] = df[lab].apply(lambda s: label_map.get(s.lower(), s)) # Apply mapping safely

# ---- AFTER Report
_ = report_key_stats(df, "AFTER CLEANING")
print("Total NaN cells:", int(df.isna().sum().sum())) # Quick sanity check

# Save and reload
path = "/datasets/CICIDS2017_combined_clean.csv"
df.to_csv(path, index=False); print("Saved:", path)
df = pd.read_csv(path, low_memory=False); print("Reloaded:", path)
```

BEFORE CLEANING

Shape: (2830743, 79) | Duplicate rows: 308381 (10.8940%)
Constant/all-zero cols: 8 | ex: [' Bwd Avg Bytes/Bulk', ' Bwd Avg Packets/Bulk', ' Bwd PSH Flags', ' Bwd URG Flags', ' Fwd Avg Bulk Rate', ' Fwd Avg Packets/Bulk', 'Bwd Avg Bulk Rate', 'Fwd Avg Bytes/Bulk']
Flow Bytes/s: bad=2867 bad&dur0=2867
Flow Packets/s: bad=2867 bad&dur0=2867
Label column: ' Label'
Label
benign 2273097
dos hulk 231073
portscan 158930
ddos 128027
dos goldeneye 10293
ftp-patator 7938
ssh-patator 5897
dos slowloris 5796
dos slowhttptest 5499
bot 1966
web attack ❖ brute force 1507
web attack ❖ xss 652
Name: count, dtype: int64

AFTER CLEANING

Shape: (2522362, 71) | Duplicate rows: 0 (0.0000%)
Constant/all-zero cols: 0
Flow Bytes/s: bad=0 bad&dur0=0
Flow Packets/s: bad=0 bad&dur0=0
Label column: 'Label'
Label
benign 2096484
dos hulk 172849
ddos 128016
portscan 90819
dos goldeneye 10286
ftp-patator 5933
dos slowloris 5385
dos slowhttptest 5228
ssh-patator 3219
bot 1953
web attack - brute force 1470
web attack - xss 652
Name: count, dtype: int64
Total NaN cells: 0
Saved: /datasets/CICIDS2017_combined_clean.csv
Reloaded: /datasets/CICIDS2017_combined_clean.csv

2.3. Feature Engineering

This cell coerces key columns to numeric, fixes negative/zero-duration artifacts and rate infinities, creates additional engineered traffic features (volume, ratios, timing variability, flags, port categories, log transforms), then performs a final cleanup pass to replace any remaining inf/NaN in engineered columns so the dataset is fully numeric and model-ready.

In [6]:

```
# ---- 1 - Ensure key columns are numeric
for col in [
    "Flow Duration", "Flow Bytes/s", "Flow Packets/s",
    "Total Fwd Packets", "Total Backward Packets",
    "Total Length of Fwd Packets", "Total Length of Bwd Packets",
    "Flow IAT Std", "Flow IAT Mean",
    "Fwd IAT Std", "Fwd IAT Mean",
    "Bwd IAT Std", "Bwd IAT Mean",
    "Active Mean", "Idle Mean",
    "SYN Flag Count", "RST Flag Count", "ACK Flag Count",
    "Destination Port"
]:
    if col in df.columns:
        df[col] = pd.to_numeric(df[col], errors="coerce")

# ---- 2 - Fix negative Flow Duration before Log transforms
df["Flow Duration"] = df["Flow Duration"].fillna(0).clip(lower=0)

# ---- 3 - Fix rates when Flow Duration == 0
dur_zero = df["Flow Duration"].eq(0)
for rate_col in ["Flow Bytes/s", "Flow Packets/s"]:
    if rate_col in df.columns:
        x = df[rate_col].replace([np.inf, -np.inf], np.nan)
        # If duration==0 and rate is missing/inf, set it to 0
        x.loc[dur_zero & x.isna()] = 0.0
        df[rate_col] = x.fillna(0) # Keep fully numeric

# ---- 4 - Feature engineering
eps = 1e-6 # small constant to avoid divide-by-zero

df["total_packets"] = df["Total Fwd Packets"].fillna(0) + df["Total Backward Packets"].fillna(0)
df["total_bytes"] = df["Total Length of Fwd Packets"].fillna(0) + df["Total Length of Bwd Packets"].fillna(0)

# Directional ratios
df["fwd_bwd_pkt_ratio"] = (df["Total Fwd Packets"].fillna(0) + 1) / (df["Total Backward Packets"].fillna(0) + 1) # Added 1 to avoid divide-by-zero and to keep scale stable
df["fwd_bwd_byte_ratio"] = (df["Total Length of Fwd Packets"].fillna(0) + 1) / (df["Total Length of Bwd Packets"].fillna(0) + 1)

# Size-per-packet features
df["bytes_per_packet"] = df["total_bytes"] / (df["total_packets"] + 1)
df["fwd_bytes_per_packet"] = df["Total Length of Fwd Packets"].fillna(0) / (df["Total Fwd Packets"].fillna(0) + 1)
df["bwd_bytes_per_packet"] = df["Total Length of Bwd Packets"].fillna(0) / (df["Total Backward Packets"].fillna(0) + 1)

# Variability features
df["flow_iat_cv"] = df["Flow IAT Std"].fillna(0) / (df["Flow IAT Mean"].fillna(0) + eps)
df["fwd_iat_cv"] = df["Fwd IAT Std"].fillna(0) / (df["Fwd IAT Mean"].fillna(0) + eps)
df["bwd_iat_cv"] = df["Bwd IAT Std"].fillna(0) / (df["Bwd IAT Mean"].fillna(0) + eps)

# Activity vs idle
df["active_fraction"] = df["Active Mean"].fillna(0) / (df["Active Mean"].fillna(0) + df["Idle Mean"].fillna(0) + 1)

# Flag counts normalized by flow size
df["syn_per_packet"] = df["SYN Flag Count"].fillna(0) / (df["total_packets"] + 1)
df["rst_per_packet"] = df["RST Flag Count"].fillna(0) / (df["total_packets"] + 1)
df["ack_per_packet"] = df["ACK Flag Count"].fillna(0) / (df["total_packets"] + 1)
df["syn_ack_imbalance"] = (df["SYN Flag Count"].fillna(0) - df["ACK Flag Count"].fillna(0)) / (df["total_packets"] + 1)

# Port categorisation
ports = df["Destination Port"].fillna(-1) # Fill NaNs with -1 so that port-range comparisons behave predictably
df["port_well_known"] = (ports.between(0, 1023)).astype(int)
df["port_registered"] = (ports.between(1024, 49151)).astype(int)
df["port_dynamic"] = (ports >= 49152).astype(int)

# Log transforms
df["log_flow_duration"] = np.log1p(df["Flow Duration"])
df["log_total_bytes"] = np.log1p(df["total_bytes"].clip(lower=0))
df["log_total_packets"] = np.log1p(df["total_packets"].clip(lower=0))
df["log_flow_bytes_per_s"] = np.log1p(df["Flow Bytes/s"].clip(lower=0))
df["log_flow_packets_per_s"] = np.log1p(df["Flow Packets/s"].clip(lower=0))

# ---- 5 - Final safety pass by removing inf/nan in feature engineered columns
engineered_cols = [
    "total_packets", "total_bytes",
    "fwd_bwd_pkt_ratio", "fwd_bwd_byte_ratio",
    "bytes_per_packet", "fwd_bytes_per_packet", "bwd_bytes_per_packet",
    "flow_iat_cv", "fwd_iat_cv", "bwd_iat_cv", "active_fraction",
    "syn_per_packet", "rst_per_packet", "ack_per_packet", "syn_ack_imbalance",
    "port_well_known", "port_registered", "port_dynamic",
    "log_flow_duration", "log_total_bytes", "log_total_packets",
    "log_flow_bytes_per_s", "log_flow_packets_per_s"
]
df[engineered_cols] = (
    df[engineered_cols]
    .replace([np.inf, -np.inf], np.nan)
```



```
        .fillna(0)
    )

print("Inf in engineered cols:", np.isinf(df[engineered_cols].to_numpy()).sum())
print("NaN in engineered cols:", np.isnan(df[engineered_cols].to_numpy()).sum())
```

Inf in engineered cols: 0
NaN in engineered cols: 0

2.4. Train-Test Split

This cell separates features and labels, encodes the multiclass target, performs a stratified 75/25 train-test split, applies Min–Max scaling fitted on the training set only, checks class coverage/distribution in both splits, and computes capped class-balanced sample weights from the training set for use during model training.

```
In [7]: # Prepare feature matrix X and multiclass target y for 75/25 stratified hold-out split
RANDOM_STATE = 42
TARGET_COL = "Label"

# ---- 1 - Split features (X) and target labels (y_raw)
X = df.drop(columns=[TARGET_COL]).copy() # ALL input features, excluding the target column
y_raw = df[TARGET_COL].astype(str).copy() # Raw label values as strings, kept separate from X

# ---- 2 - Encode string labels into integer class IDs (0 to n_classes-1)
le = LabelEncoder() # Learn the mapping from each unique label string to an integer ID
y = le.fit_transform(y_raw) # Convert y_raw into numeric class IDs for modeling
class_names = le.classes_ # Unique label names in the encoder, ordered by assigned class ID
n_classes = len(class_names) # Total number of classes
print("Number of classes:", n_classes)
print("Top label counts:\n", y_raw.value_counts().head(10))

# ---- 3 - Train/test split (75/25), stratified to preserve class proportions
TEST_SIZE = 0.25
X_train, X_test, y_train, y_test = train_test_split(
    X, y,
    test_size=TEST_SIZE,
    stratify=y, # Preserve class distribution
    shuffle=True, # Not time-series data
    random_state=RANDOM_STATE
)
print("\nSplit summary:")
print(f"  Training set: {X_train.shape[0]} rows ({(1-TEST_SIZE)*100:.0f}%), {X_train.shape[1]} features")
print(f"  Test set:      {X_test.shape[0]} rows ({TEST_SIZE*100:.0f}%), {X_test.shape[1]} features")

# ---- 3b - Min-Max scale features (fit on TRAIN only to avoid Leakage)
scaler = MinMaxScaler()
X_train_raw = X_train.copy() # Keep unscaled copies
X_test_raw = X_test.copy()
X_train_mm = pd.DataFrame(scaler.fit_transform(X_train), columns=X_train.columns, index=X_train.index)
X_test_mm = pd.DataFrame(scaler.transform(X_test), columns=X_test.columns, index=X_test.index)
# Use scaled features for modeling
X_train_model = X_train_mm
X_test_model = X_test_mm

# ---- 4 - Sanity check on train/test class distributions and missing classes
train_counts = np.bincount(y_train, minlength=n_classes)
test_counts = np.bincount(y_test, minlength=n_classes)
train_dist = train_counts / len(y_train)
test_dist = test_counts / len(y_test)

print("\nClass distribution check (top 10 classes):")
for i in np.argsort(-train_dist)[:10]:
    print(f"  {class_names[i]:25s} train={train_dist[i]:.4%} test={test_dist[i]:.4%}")

# Ensure every class appears in both splits for small classes
missing_in_train = [class_names[i] for i in range(n_classes) if train_counts[i] == 0]
missing_in_test = [class_names[i] for i in range(n_classes) if test_counts[i] == 0]
print("\nClasses missing in TRAIN:", missing_in_train)
print("Classes missing in TEST:", missing_in_test)

print("\nRarest classes (bottom 5 by TRAIN count):")
for i in np.argsort(train_counts)[:5]:
    print(f"  {class_names[i]:25s} train_count={train_counts[i]:6d} test_count={test_counts[i]:6d}")

tiny_threshold = 20
tiny_classes = [class_names[i] for i in range(n_classes) if train_counts[i] < tiny_threshold]
print(f"\nClasses with < {tiny_threshold} training samples:", tiny_classes)

# ---- 5 - Class-balanced sample weights from TRAIN only
class_weights = (len(y_train) / (n_classes * np.maximum(train_counts, 1)))

sample_weight_train = class_weights[y_train] # Assign each training sample the weight of its class

# Capping extreme weights so that rare classes like Heartbleed don't dominate training
MAX_W = 1000
sample_weight_train = np.clip(sample_weight_train, 0, MAX_W)

print("\nClass weight examples (first 10 classes):")
```

```
for i in range(min(10, n_classes)):
    print(f"  {class_names[i]:25s} count={train_counts[i]:7d}  weight={class_weights[i]:.4f}")

print("\nSample-weight range after capping:",
      "min =", float(sample_weight_train.min()),
      "max =", float(sample_weight_train.max()))
```

Number of classes: 15
Top label counts:
Label
BENIGN 2096484
DoS Hulk 172849
DDoS 128016
PortScan 90819
DoS GoldenEye 10286
FTP-Patator 5933
DoS Slowloris 5385
DoS SlowHTTPTest 5228
SSH-Patator 3219
Bot 1953
Name: count, dtype: int64

Split summary:
Training set: 1891771 rows (75%), 93 features
Test set: 630591 rows (25%), 93 features

Class distribution check (top 10 classes):
BENIGN train=83.1159% test=83.1158%
DoS Hulk train=6.8527% test=6.8526%
DDoS train=5.0752% test=5.0752%
PortScan train=3.6005% test=3.6006%
DoS GoldenEye train=0.4078% test=0.4079%
FTP-Patator train=0.2352% test=0.2352%
DoS Slowloris train=0.2135% test=0.2135%
DoS SlowHTTPTest train=0.2073% test=0.2073%
SSH-Patator train=0.1276% test=0.1277%
Bot train=0.0774% test=0.0774%

Classes missing in TRAIN: []
Classes missing in TEST: []

Rarest classes (bottom 5 by TRAIN count):
Heartbleed train_count= 8 test_count= 3
Web Attack - SQL Injection train_count= 16 test_count= 5
Infiltration train_count= 27 test_count= 9
Web Attack - XSS train_count= 489 test_count= 163
Web Attack - Brute Force train_count= 1102 test_count= 368

Classes with < 20 training samples: ['Heartbleed', 'Web Attack - SQL Injection']

Class weight examples (first 10 classes):
BENIGN count=1572363 weight=0.0802
Bot count= 1465 weight=86.0874
DDoS count= 96012 weight=1.3136
DoS GoldenEye count= 7714 weight=16.3492
DoS Hulk count= 129637 weight=0.9729
DoS SlowHTTPTest count= 3921 weight=32.1648
DoS Slowloris count= 4039 weight=31.2251
FTP-Patator count= 4450 weight=28.3411
Heartbleed count= 8 weight=15764.7583
Infiltration count= 27 weight=4671.0395

Sample-weight range after capping: min = 0.08020925617472979 max = 1000.0

3. Model Training

3.1. Training Helpers

This cell sanitizes and de-duplicates feature names, coerces any object/string columns to numeric, replaces any Inf values with NaN, and reports remaining missing-value counts so the train/test matrices are safe and consistent before fitting XGBoost.

```
In [8]: def sanitize_feature_names(cols):
        # Make feature names XGBoost-friendly and unique
        cols = [str(c).strip() for c in cols] # Normalize whitespace
        cols = [re.sub(r"[^\w]+", "_", c) for c in cols] # Replace unsafe chars with "_"
        # Track duplicates
        seen = {}
        out = []
        for c in cols:
            if c not in seen:
                seen[c] = 0
                out.append(c) # Keep first occurrence
            else:
                seen[c] += 1
                out.append(f"{c}__{seen[c]}") # Suffix duplicates
```

```
    return out

def xgb_preflight(X_train, X_test):
    # Make X matrices XGBoost-safe and consistent
    X_train = X_train.copy() # Protect the original DataFrames with copy
    X_test = X_test.copy()

    # ---- 1 - Sanitize column names and keep train/test aligned
    new_cols = sanitize_feature_names(X_train.columns) # Safe and unique feature names
    X_train.columns = new_cols # Apply to train
    X_test.columns = new_cols # Apply same names to test

    # ---- 2 - Coerce object/string feature columns to numeric
    obj_cols = X_train.select_dtypes(include=["object", "string"]).columns.tolist() # Non-numeric cols
    if obj_cols:
        print("Object feature columns detected (coercing to numeric):", obj_cols) # Visibility
        for c in obj_cols:
            X_train[c] = pd.to_numeric(X_train[c], errors="coerce") # Bad parses become NaN
            X_test[c] = pd.to_numeric(X_test[c], errors="coerce")

    # ---- 3 - Count Inf values per split without building huge arrays
    num_cols = X_train.select_dtypes(include=[np.number]).columns # Numeric-only columns
    inf_train = sum(np.isinf(X_train[c].to_numpy()).sum() for c in num_cols) # Total Inf in train
    inf_test = sum(np.isinf(X_test[c].to_numpy()).sum() for c in num_cols) # Total Inf in test

    if inf_train or inf_test:
        print(f"Found Inf values. Replacing with NaN (train={inf_train}, test={inf_test})") # Summary
        X_train = X_train.replace([np.inf, -np.inf], np.nan) # Clean train
        X_test = X_test.replace([np.inf, -np.inf], np.nan) # Clean test

    nan_train = int(X_train.isna().sum().sum()) # Total missing cells in train
    nan_test = int(X_test.isna().sum().sum()) # Total missing cells in test
    print(f"Preflight OK | features={X_train.shape[1]} | NaN cells train={nan_train}, test={nan_test}") # Quick QC
    return X_train, X_test

X_train_model, X_test_model = xgb_preflight(X_train_model.copy(), X_test_model.copy()) # Clean names and values for XGBoost
```

Preflight OK | features=93 | NaN cells train=0, test=0

3.2. XGBoost Training (All Features)

This cell trains an XGBoost multiclass classifier on the full feature set using fixed hyperparameters (based on Faysal et al.'s paper), optionally applying class-balancing sample weights, and reports the training runtime before moving to the evaluation step.

```
In [9]: # XGBoost training with all features, based on Faysal et al.'s settings, no tuning
xgb_all_paper = XGBClassifier(
    objective="multi:softprob",
    num_class=n_classes,
    eval_metric="mlogloss",
    tree_method="hist",
    n_estimators=500,
    max_depth=6,
    learning_rate=0.1,
    subsample=1.0,
    colsample_bytree=1.0,
    random_state=RANDOM_STATE,
    n_jobs=-1
)

t0 = time.time() # Start timer
xgb_all_paper.fit(
    X_train_model, y_train,
    sample_weight=(sample_weight_train if "sample_weight_train" in globals() else None)
)
print("XGB (all features) fit time (sec):", round(time.time() - t0, 2))
print("XGBoost trained. Proceed to the evaluation section.")
```

XGB (all features) fit time (sec): 266.01
XGBoost trained. Proceed to the evaluation section.

3.3. Random Forest + XGBoost Training (RF-selected Features) with TOP_K sweep

This cell runs a validation sweep over several TOP_K values to choose how many RF-ranked features to keep (selecting the K that maximizes validation Macro-F1), then retrains RF on the full training set to select the final feature subset, trains XGBoost on those selected features, and saves the resulting model and reduced train/test matrices for the evaluation section.

```
In [10]: # ---- 1 - Configuration
RF_TREES = 300
TOPK_LIST = [20, 40, 60, 80] # Candidate K values
RUN_TOPK_SWEEP = True # Toggle validation sweep
VAL_SIZE = 0.20 # Validation share from training
EPS = 1e-12 # Small constant

# XGBoost training with all features, based on Faysal et al.'s settings, no tuning
XGB_PARAMS = dict(
    objective="multi:softprob",
```

```

num_class=n_classes,
eval_metric="mlogloss",
tree_method="hist",
n_estimators=500,
max_depth=6,
learning_rate=0.1,
subsample=1.0,
colsample_bytree=1.0,
random_state=RANDOM_STATE,
n_jobs=-1
)

# ---- 2 - Helpers
def _get_sample_weights():
    if "sample_weight_train" in globals() and sample_weight_train is not None:
        return np.asarray(sample_weight_train) # Training weights
    return None

def _get_benign_index(class_names, benign_label="BENIGN"):
    class_names = np.asarray(class_names) # Ensure array
    if benign_label in class_names:
        return int(np.where(class_names == benign_label)[0][0]) # BENIGN class id
    return None

def rf_select_topk_features(X_train_df, y_train_arr, top_k, rf_trees, random_state, sample_weight=None):
    # Fit RF on train only and return top K feature names
    rf = RandomForestClassifier(
        n_estimators=rf_trees,
        random_state=random_state,
        n_jobs=-1
    )
    rf.fit(X_train_df, y_train_arr, sample_weight=sample_weight) # Fit selector
    importances = pd.Series(rf.feature_importances_, index=X_train_df.columns).sort_values(ascending=False)
    top_features = importances.index[:top_k].tolist() # Select top K
    return top_features, importances

def train_xgb_on_selected(X_train_sel, y_train_arr, xgb_params, sample_weight=None):
    # Train XGBoost on selected features
    model = XGBClassifier(**xgb_params) # Build model
    model.fit(X_train_sel, y_train_arr, sample_weight=sample_weight) # Fit model
    return model

def evaluate_multiclass_and_operational(y_true, y_pred, benign_idx=None):
    # Metrics for multiclass and BENIGN vs ATTACK when available
    acc = accuracy_score(y_true, y_pred)
    macro_f1 = f1_score(y_true, y_pred, average="macro")
    weighted_f1 = f1_score(y_true, y_pred, average="weighted")
    bal_acc = balanced_accuracy_score(y_true, y_pred)
    kappa = cohen_kappa_score(y_true, y_pred)
    mcc = matthews_corrcoef(y_true, y_pred)
    out = dict(
        Accuracy=acc,
        Macro_F1=macro_f1,
        Weighted_F1=weighted_f1,
        Balanced_Acc=bal_acc,
        Kappa=kappa,
        MCC=mcc
    )
    if benign_idx is not None:
        y_true_attack = (np.asarray(y_true) != benign_idx).astype(int) # 1 attack, 0 benign
        y_pred_attack = (np.asarray(y_pred) != benign_idx).astype(int) # 1 attack, 0 benign
        tn, fp, fn, tp = confusion_matrix(y_true_attack, y_pred_attack).ravel() # Binary counts
        tpr = tp / (tp + fn + EPS) # Recall for attack
        fpr = fp / (fp + tn + EPS) # False alarm rate
        precision = tp / (tp + fp + EPS) # Precision for attack
        specificity = tn / (tn + fp + EPS) # True negative rate
        ts = tp / (tp + fn + fp + EPS) # Threat score
        out.update(dict(
            TP=tp, FP=fp, TN=tn, FN=fn,
            TPR=tpr, FPR=fpr,
            Precision=precision,
            Specificity=specificity,
            ThreatScore=ts
        ))
    else:
        out.update(dict(
            TP=np.nan, FP=np.nan, TN=np.nan, FN=np.nan,
            TPR=np.nan, FPR=np.nan,
            Precision=np.nan,
            Specificity=np.nan,
            ThreatScore=np.nan
        ))
    return out

# ---- 3 - Normalize inputs
if not isinstance(X_train_model, pd.DataFrame):
    X_train_model = pd.DataFrame(X_train_model) # Keep feature names

```

```

if not isinstance(X_test_model, pd.DataFrame):
    X_test_model = pd.DataFrame(X_test_model) # Keep feature names

y_train_arr = y_train.to_numpy() if hasattr(y_train, "to_numpy") else np.asarray(y_train) # y as array
y_test_arr = y_test.to_numpy() if hasattr(y_test, "to_numpy") else np.asarray(y_test) # y as array

class_names_arr = np.asarray(class_names) # Class labels
sw_train = _get_sample_weights() # Optional weights
benign_idx = _get_benign_index(class_names_arr, benign_label="BENIGN") # Benign ID

print("Train shape:", X_train_model.shape, "| Test shape:", X_test_model.shape)
print("n_classes:", n_classes, "| BENIGN idx:", benign_idx)
print("Using sample weights:", sw_train is not None)

# ---- 4 - Validation split for TOP_K selection
if RUN_TOPK_SWEEP:
    idx_all = np.arange(len(y_train_arr)) # Row indices
    idx_tr, idx_val = train_test_split(
        idx_all,
        test_size=VAL_SIZE,
        random_state=RANDOM_STATE,
        stratify=y_train_arr # Preserve class mix
    )
    X_tr = X_train_model.iloc[idx_tr] # Training subset
    y_tr = y_train_arr[idx_tr]
    X_val = X_train_model.iloc[idx_val] # Validation subset
    y_val = y_train_arr[idx_val]
    # If using weights, recompute from y_tr only
    if sw_train is not None:
        tr_counts = np.bincount(y_tr, minlength=n_classes)
        tr_class_w = (len(y_tr) / (n_classes * np.maximum(tr_counts, 1)))
        sw_tr = np.clip(tr_class_w[y_tr], 0, 1000)
    else:
        sw_tr = None

    print(f"\nValidation split for TOP_K selection: X_tr={X_tr.shape}, X_val={X_val.shape}")

# ---- 5 - TOP_K sweep on validation only
rows = []
topk_to_features = {}

for TOP_K in TOPK_LIST:
    print(f"\n--- TOP_K = {TOP_K} (validation) ---")
    t0 = time.time() # RF timer
    top_features, importances = rf_select_topk_features(
        X_train_df=X_tr,
        y_train_arr=y_tr,
        top_k=TOP_K,
        rf_trees=RF_TREES,
        random_state=RANDOM_STATE,
        sample_weight=sw_tr
    )
    rf_time = time.time() - t0 # RF time
    # Reduce X_tr / X_val
    X_tr_sel = X_tr.loc[:, top_features].copy() # Selected train features
    X_val_sel = X_val.loc[:, top_features].copy() # Selected val features
    t0 = time.time() # XGB timer
    model = train_xgb_on_selected(
        X_train_sel=X_tr_sel, # XGB fit data
        y_train_arr=y_tr,
        xgb_params=XGB_PARAMS,
        sample_weight=sw_tr
    )
    xgb_time = time.time() - t0 # XGB time
    y_pred_val = model.predict(X_val_sel) # Validation predictions
    # Evaluate on validation
    metrics = evaluate_multiclass_and_operational(
        y_true=y_val,
        y_pred=y_pred_val,
        benign_idx=benign_idx
    )
    metrics.update({
        "TOP_K": TOP_K,
        "RF_fit_sec": rf_time,
        "XGB_fit_sec": xgb_time
    })
    rows.append(metrics) # Store results
    topk_to_features[TOP_K] = top_features # Store feature list
df_topk_val = pd.DataFrame(rows) # Results table
df_topk_val_sorted = df_topk_val.sort_values("Macro_F1", ascending=False).reset_index(drop=True) # Rank by Macro F1

print("\nTOP_K sweep results on VALIDATION (sorted by Macro_F1)")
display(df_topk_val_sorted)

BEST_TOP_K = int(df_topk_val_sorted.loc[0, "TOP_K"])
print("\nChosen BEST_TOP_K by validation Macro_F1:", BEST_TOP_K)
else:

```



```

    raise RuntimeError('RUN_TOPK_SWEEP is disabled. Enable it to select BEST_TOP_K via validation.')
```

```

# ---- 6 - Train final model on full training with BEST_TOP_K
print(f"\nTraining FINAL RF to XGB on FULL training set (BEST_TOP_K={BEST_TOP_K})...")

# Fit RF on full training set (still no Leakage)
t0 = time.time()
top_features_full, importances_full = rf_select_topk_features(
    X_train_df=X_train_model,
    y_train_arr=y_train_arr,
    top_k=BEST_TOP_K,
    rf_trees=RF_TREES,
    random_state=RANDOM_STATE,
    sample_weight=sw_train
)
print("Final RF fit+rank time (sec):", round(time.time() - t0, 2))

# Reduce full train/test to selected features
X_train_best = X_train_model.loc[:, top_features_full].copy()
X_test_best = X_test_model.loc[:, top_features_full].copy()

# Train final XGB on selected features
xgb_final = XGBClassifier(**XGB_PARAMS)
t0 = time.time()
xgb_final.fit(X_train_best, y_train_arr, sample_weight=sw_train)
print("Final XGB fit time (sec):", round(time.time() - t0, 2))

# Test predictions
y_pred_best = xgb_final.predict(X_test_best)
y_proba_best = xgb_final.predict_proba(X_test_best)

print("\nRF to XGB FINAL model trained. Test predictions ready for evaluation.")

# ---- 7 - Aliases for evaluation section
# Evaluation cell expects xgb_sel, X_test_sel, y_pred_sel, y_proba_sel and optional TOP_K and top_features
RF_XGB_BEST_TOP_K = int(BEST_TOP_K) # Chosen K
rf_xgb_bestk_features = list(top_features_full) # Selected features
rf_xgb_bestk_model = xgb_final # Trained model
X_train_rf_xgb_bestk = X_train_best # Selected train matrix
X_test_rf_xgb_bestk = X_test_best # Selected test matrix

print(f"\nSaved RF to XGB BEST_TOP_K artifacts (RF_XGB_BEST_TOP_K={RF_XGB_BEST_TOP_K}).")
print("RF + XGBoost trained. Proceed to the evaluation section.")
```

Train shape: (1891771, 93) | Test shape: (630591, 93)
n_classes: 15 | BENIGN idx: 0
Using sample weights: True

Validation split for TOP_K selection: X_tr=(1513416, 93), X_val=(378355, 93)

--- TOP_K = 20 (validation) ---

--- TOP_K = 40 (validation) ---

--- TOP_K = 60 (validation) ---

--- TOP_K = 80 (validation) ---

TOP_K sweep results on VALIDATION (sorted by Macro_F1)

	Accuracy	Macro_F1	Weighted_F1	Balanced_Acc	Kappa	MCC	TP	FP	TN	FN	TPR	FPR	Precision	Specificity	ThreatScore	TOP_K	RF_fit_sec	XGB_fit_sec
0	0.998644	0.890777	0.998676	0.887574	0.995501	0.995506	63872	375	314098	10	0.999843	0.001192	0.994163	0.998808	0.994008	80	95.470211	191.378726
1	0.998628	0.876366	0.998662	0.886565	0.995448	0.995453	63871	375	314098	11	0.999828	0.001192	0.994163	0.998808	0.993993	60	95.795172	169.608823
2	0.998274	0.858515	0.998380	0.887196	0.994277	0.994286	63868	490	313983	14	0.999781	0.001558	0.992386	0.998442	0.992171	40	98.628180	144.793568
3	0.998285	0.825860	0.998383	0.864227	0.994312	0.994321	63866	486	313987	16	0.999750	0.001545	0.992448	0.998455	0.992201	20	100.193316	123.273914

Chosen BEST_TOP_K by validation Macro_F1: 80

Training FINAL RF to XGB on FULL training set (BEST_TOP_K=80)...
Final RF fit+rank time (sec): 125.44
Final XGB fit time (sec): 239.83

RF to XGB FINAL model trained. Test predictions ready for evaluation.

Saved RF to XGB BEST_TOP_K artifacts (RF_XGB_BEST_TOP_K=80).
RF + XGBoost trained. Proceed to the evaluation section.

4. Model Evaluation

4.1. Evaluation Helpers

This cell defines reusable evaluation utilities that compute a set of multiclass and operational BENIGN-vs-ATTACK metrics from model predictions (including TP/FP/TN/FN, sensitivity/specificity/threat score, F1/balanced accuracy, and ROC-AUC/PR when probabilities are available) and optionally plot ROC/PR and calibration curves for both the binary operational view and selected one-vs-rest classes.

```
In [11]: EPS = 1e-12 # Tiny constant

def _ovr_from_confusion(cm: np.ndarray):
    # Compute per-class Ovr TP/FP/TN/FN from a multiclass confusion matrix
    total = cm.sum() # Total samples
    tp = np.diag(cm) # True positives
    fn = cm.sum(axis=1) - tp # False negatives
    fp = cm.sum(axis=0) - tp # False positives
    tn = total - (tp + fn + fp) # True negatives
    return tp, fp, tn, fn

def _safe_multiclass_auc_ovr(y_true, y_proba, n_classes):
    # Compute multiclass Ovr ROC-AUC macro/weighted robustly (skips classes missing in y_true)
    y_true = np.asarray(y_true) # Ensure array
    present = np.unique(y_true) # Classes present
    if len(present) < 2:
        return np.nan, np.nan # AUC undefined
    classes = np.arange(n_classes) # Class IDs
    y_bin = label_binarize(y_true, classes=classes) # Labels
    # Compute per-class AUC where both positives and negatives exist
    aucs = []
    weights = []
    for i in range(n_classes):
        y_i = y_bin[:, i] # Binary labels for class i
        if y_i.max() == y_i.min():
            continue # Skip all-0 or all-1
        auc_i = roc_auc_score(y_i, y_proba[:, i]) # Class AUC
        aucs.append(auc_i)
        weights.append(y_i.sum()) # Number of positives
    if len(aucs) == 0:
        return np.nan, np.nan # Nothing valid
    macro = float(np.mean(aucs)) # Macro average
    w = np.asarray(weights, dtype=float)
    weighted = float(np.sum(w * np.asarray(aucs)) / (np.sum(w) + EPS)) # Weighted average
    return macro, weighted

def evaluate_model(
    name: str,
    X_test,
    y_true,
    y_pred,
    y_proba=None,
    class_names=None,
    benign_label: str = "BENIGN",
    selected_labels=None,
    show_plots: bool = True,
    digits: int = 4
):
    # Unified evaluation that matches Faysal et al.'s metrics + keeps TP/FP/TN/FN
    y_true = np.asarray(y_true)
    y_pred = np.asarray(y_pred)
    if class_names is None:
        # fallback: numeric class names
        class_names = np.array([str(i) for i in range(len(np.unique(y_true)))])
    else:
        class_names = np.asarray(class_names)
    n_classes = len(class_names) # Number of classes

    print(f"\n----- {name} -----")

    # ---- 1 - Core metrics
    acc = accuracy_score(y_true, y_pred) # Accuracy
    macro_f1 = f1_score(y_true, y_pred, average="macro", zero_division=0) # Macro F1
    weighted_f1 = f1_score(y_true, y_pred, average="weighted", zero_division=0) # Weighted F1
    bal_acc = balanced_accuracy_score(y_true, y_pred) # Balanced accuracy
    print("Accuracy:", round(acc, 6))
    print("Macro F1:", round(macro_f1, 6))
    print("Weighted F1:", round(weighted_f1, 6))
    print("Balanced Accuracy:", round(bal_acc, 6))

    # ---- 2 - Faysal et al.'s agreement/correlation metrics
    kappa = cohen_kappa_score(y_true, y_pred) # Agreement
    mcc = matthews_corrcoef(y_true, y_pred) # Correlation
    print("Cohen's Kappa:", round(float(kappa), 6))
    print("Matthews Corrcoef (MCC):", round(float(mcc), 6))

    # ---- 3 - Probabilistic metrics (multiclass)
    multiclass_logloss = np.nan
    attack_logloss = np.nan
    attack_brier = np.nan

    # ---- 4 - Report + Confusion
    print("\nClassification report:")
```

```

try:
    # Per-class precision and recall
    print(classification_report(y_true, y_pred, labels=np.arange(n_classes), target_names=class_names, digits=digits, zero_division=0))
except Exception:
    # Fallback report
    print(classification_report(y_true, y_pred, labels=np.arange(n_classes), digits=digits, zero_division=0))
cm = confusion_matrix(y_true, y_pred, labels=np.arange(n_classes))
print("Confusion matrix shape:", cm.shape)

# ---- 5 - OvR TP/FP/TN/FN per class + Sens/Spec/TS
tp, fp, tn, fn = _ovr_from_confusion(cm) # OVR Counts
sens = tp / (tp + fn + EPS) # Recall
spec = tn / (tn + fp + EPS) # Specificity
ts = tp / (tp + fn + fp + EPS) # Threat Score
support = cm.sum(axis=1).astype(float) # Samples per class
weights = support / (support.sum() + EPS) # Class weights
print("\n---- Sensitivity / Specifity / Threat Score (OvR Aggregates) ----")
print("Macro Sensitivity:", round(float(np.mean(sens)), 6))
print("Weighted Sensitivity:", round(float(np.sum(weights * sens)), 6))
print("Macro Specificity:", round(float(np.mean(spec)), 6))
print("Weighted Specificity:", round(float(np.sum(weights * spec)), 6))
print("Macro Threat Score (TS/CSI):", round(float(np.mean(ts)), 6))
print("Weighted Threat Score:", round(float(np.sum(weights * ts)), 6))
per_class_df = pd.DataFrame({
    "Class": class_names,
    "Support": support.astype(int),
    "TP": tp.astype(int),
    "FP": fp.astype(int),
    "TN": tn.astype(int),
    "FN": fn.astype(int),
    "Sensitivity_recall": sens,
    "Specificity": spec,
    "Threat_score_CSI": ts
}).sort_values("Support", ascending=False)
print("\n---- Per-class OvR breakdown (includes TP/FP/TN/FN) ----")
print(per_class_df.to_string(index=False, float_format=lambda x: f"{x:.6f}"))

# ---- 6 - AUC/PR (requires probabilities)
if y_proba is not None:
    y_proba = np.asarray(y_proba)
    # Multiclass Log Loss
    try:
        multiclass_logloss = log_loss(y_true, y_proba, labels=np.arange(n_classes))
    except Exception:
        multiclass_logloss = np.nan
    print("Log Loss (Multiclass):", round(float(multiclass_logloss), 6) if np.isfinite(multiclass_logloss) else "nan")
    macro_auc, weighted_auc = _safe_multiclass_auc_ovr(y_true, y_proba, n_classes)
    print("\n---- ROC-AUC (Multiclass OvR) ----")
    print("OvR Macro AUC:", round(float(macro_auc), 6) if np.isfinite(macro_auc) else "nan")
    print("OvR Weighted AUC:", round(float(weighted_auc), 6) if np.isfinite(weighted_auc) else "nan")
    # BENIGN vs ATTACK
    if benign_label in class_names:
        benign_idx = int(np.where(class_names == benign_label)[0][0])
        y_true_attack = (y_true != benign_idx).astype(int) # Attack flag
        p_attack = 1.0 - y_proba[:, benign_idx] # Attack probability
        # Probabilistic quality of attack alerts (calibration-sensitive)
        try:
            attack_logloss = log_loss(
                y_true_attack,
                np.column_stack([1.0 - p_attack, p_attack]),
                labels=[0, 1]
            )
        except Exception:
            attack_logloss = np.nan
        try:
            attack_brier = brier_score_loss(y_true_attack, p_attack) # Calibration error
        except Exception:
            attack_brier = np.nan
        print("Log Loss (Attack probability):", round(float(attack_logloss), 6) if np.isfinite(attack_logloss) else "nan")
        print("Brier Score (Attack probability):", round(float(attack_brier), 6) if np.isfinite(attack_brier) else "nan")
        if len(np.unique(y_true_attack)) > 1:
            auc_attack = roc_auc_score(y_true_attack, p_attack)
        else:
            auc_attack = np.nan

    print("\n---- Operational BENIGN vs ATTACK ----")
    print("Attack ROC-AUC:", round(float(auc_attack), 6) if np.isfinite(auc_attack) else "nan")
    y_pred_attack = (y_pred != benign_idx).astype(int)
    tn_b, fp_b, fn_b, tp_b = confusion_matrix(y_true_attack, y_pred_attack).ravel()
    tpr_point = tp_b / (tp_b + fn_b + EPS)
    fpr_point = fp_b / (fp_b + tn_b + EPS)
    precision_point = tp_b / (tp_b + fp_b + EPS)
    specificity_point = tn_b / (tn_b + fp_b + EPS)
    threat_score_point = tp_b / (tp_b + fn_b + fp_b + EPS)
    print(f"TP (attacks detected): {tp_b}")
    print(f"FP (false alarms): {fp_b}")
    print(f"TN (benign passed): {tn_b}")

```

```

print(f"FN (missed attacks):    {fn_b}")
print(f"Detection Rate (TPR/Recall): {tpr_point:.6f}")
print(f"Specificity (TNR):          {specificity_point:.6f}")
print(f"False Alarm Rate (FPR):      {fpr_point:.6f}")
print(f"Alert Precision:             {precision_point:.6f}")
print(f"Threat Score (TS/CSI):      {threat_score_point:.6f}")
# ROC curve + PR curve for operational binary
if show_plots and len(np.unique(y_true_attack)) > 1:
    fpr, tpr, _ = roc_curve(y_true_attack, p_attack)
    roc_auc_val = auc(fpr, tpr)
    plt.figure()
    plt.plot(fpr, tpr, label=f"ROC (AUC = {roc_auc_val:.4f})")
    plt.plot([0, 1], [0, 1], linestyle="--", label="Chance")
    plt.xlabel("False Positive Rate (FPR)")
    plt.ylabel("True Positive Rate (TPR / Recall)")
    plt.title(f"ROC Curve - {name} (BENIGN vs ATTACK)")
    plt.legend(loc="lower right")
    plt.tight_layout()
    plt.show()

    ap_attack = average_precision_score(y_true_attack, p_attack)
    prec, rec, _ = precision_recall_curve(y_true_attack, p_attack)
    plt.figure()
    plt.plot(rec, prec, label=f"PR (AP = {ap_attack:.4f})")
    plt.xlabel("Recall (TPR)")
    plt.ylabel("Precision")
    plt.title(f"Precision-Recall - {name} (BENIGN vs ATTACK)")
    plt.legend(loc="lower left")
    plt.tight_layout()
    plt.show()

    # Reliability curve / calibration (Attack probability)
    frac_pos, mean_pred = calibration_curve(y_true_attack, p_attack, n_bins=10, strategy="uniform")
    plt.figure()
    plt.plot(mean_pred, frac_pos, marker="o", label="Reliability") # Calibration curve
    plt.plot([0, 1], [0, 1], linestyle="--", label="Perfectly calibrated") # Ideal line
    plt.xlabel("Mean predicted probability (attack)")
    plt.ylabel("Fraction of positives (attack)")
    plt.title(f"Reliability Curve - {name} (BENIGN vs ATTACK)")
    plt.legend(loc="lower right")
    plt.tight_layout()
    plt.show()
    print("Average Precision (Attack):", round(float(ap_attack), 6))

else:
    print("\nBENIGN label not found; skipping BENIGN vs ATTACK operational metrics.")

# Per-class ROC/PR curves for selected labels
if selected_labels:
    selected_labels = [lab for lab in selected_labels if lab in class_names]
    if len(selected_labels) > 0:
        y_bin = label_binarize(y_true, classes=np.arange(n_classes))
        if show_plots:
            plt.figure()
            for lab in selected_labels:
                i = int(np.where(class_names == lab)[0][0])
                if y_bin[:, i].max() == y_bin[:, i].min():
                    continue
                fpr_i, tpr_i, _ = roc_curve(y_bin[:, i], y_proba[:, i])
                auc_i = auc(fpr_i, tpr_i)
                plt.plot(fpr_i, tpr_i, label=f"{lab} (AUC={auc_i:.4f})")
            plt.plot([0, 1], [0, 1], linestyle="--", label="Chance")
            plt.xlabel("False Positive Rate (FPR)")
            plt.ylabel("True Positive Rate (TPR / Recall)")
            plt.title(f"ROC Curves - One-vs-Rest ({name})")
            plt.legend(loc="lower right")
            plt.tight_layout()
            plt.show()

            plt.figure()
            for lab in selected_labels:
                i = int(np.where(class_names == lab)[0][0])
                if y_bin[:, i].max() == y_bin[:, i].min():
                    continue
                prec_i, rec_i, _ = precision_recall_curve(y_bin[:, i], y_proba[:, i])
                ap_i = average_precision_score(y_bin[:, i], y_proba[:, i])
                plt.plot(rec_i, prec_i, label=f"{lab} (AP={ap_i:.4f})")
            plt.xlabel("Recall")
            plt.ylabel("Precision")
            plt.title(f"Precision-Recall Curves - One-vs-Rest ({name})")
            plt.legend(loc="lower left")
            plt.tight_layout()
            plt.show()

        else:
            print("\nNo selected labels found for per-class ROC/PR plotting.")
    else:
        print("\nProbabilities not provided; skipping AUC/ROC/PR metrics.")

```

```
summary = {
    "model": name,
    "accuracy": float(acc),
    "macro_f1": float(macro_f1),
    "weighted_f1": float(weighted_f1),
    "balanced_accuracy": float(bal_acc),
    "kappa": float(kappa),
    "mcc": float(mcc),
    "multiclass_logloss": float(multiclass_logloss) if np.isfinite(multiclass_logloss) else np.nan,
    "attack_logloss": float(attack_logloss) if np.isfinite(attack_logloss) else np.nan,
    "attack_brier": float(attack_brier) if np.isfinite(attack_brier) else np.nan,
    "macro_sensitivity": float(np.mean(sens)),
    "weighted_sensitivity": float(np.sum(weights * sens)),
    "macro_specificity": float(np.mean(spec)),
    "weighted_specificity": float(np.sum(weights * spec)),
    "macro_threat_score": float(np.mean(ts)),
    "weighted_threat_score": float(np.sum(weights * ts)),
}

return summary, per_class_df

# Default Labels for optional per-class ROC/PR plots
SELECTED_LABELS = ["DDoS", "DoS Hulk", "PortScan", "Bot", "Web Attack - XSS"]
```

4.2. XGBoost Evaluation

This cell evaluates the trained all-features XGBoost model on the test set by generating class predictions and probabilities, then generating the full metric summary (F1, balanced accuracy, AUC, confusion matrix) via the `evaluate_model` helper.

```
In [12]: # Evaluation of XGBoost (All Features)
SHOW_PLOTS_XGB_ALL = True # Toggle plots

if "xgb_all_paper" not in globals():
    print("xgb_all_paper not found. Run the training cell first.")
else:
    y_pred_xgb_all_paper_eval = xgb_all_paper.predict(X_test_model)
    y_proba_xgb_all_paper_eval = xgb_all_paper.predict_proba(X_test_model)
    summary_xgb_all_paper, per_class_xgb_all_paper = evaluate_model(
        name="XGBoost (All Features)",
        X_test=X_test_model,
        y_true=y_test,
        y_pred=y_pred_xgb_all_paper_eval,
        y_proba=y_proba_xgb_all_paper_eval,
        class_names=class_names,
        benign_label="BENIGN",
        selected_labels=SELECTED_LABELS,
        show_plots=SHOW_PLOTS_XGB_ALL
    )
```


----- XGBoost (All Features) -----
Accuracy: 0.998655
Macro F1: 0.913488
Weighted F1: 0.998692
Balanced Accuracy: 0.942018
Cohen's Kappa: 0.995537
Matthews Corrccoef (MCC): 0.995541

Classification report:

	precision	recall	f1-score	support
BENIGN	1.0000	0.9989	0.9994	524121
Bot	0.6827	0.9918	0.8087	488
DDoS	0.9997	1.0000	0.9998	32004
DoS GoldenEye	0.9862	0.9988	0.9925	2572
DoS Hulk	0.9978	0.9992	0.9985	43212
DoS SlowHTTPTest	0.9819	0.9946	0.9882	1307
DoS Slowloris	0.9940	0.9926	0.9933	1346
FTP-Patator	0.9993	0.9993	0.9993	1483
Heartbleed	1.0000	1.0000	1.0000	3
Infiltration	0.9000	1.0000	0.9474	9
PortScan	0.9899	0.9991	0.9945	22705
SSH-Patator	1.0000	0.9975	0.9988	805
Web Attack - Brute Force	0.7256	0.7473	0.7363	368
Web Attack - SQL Injection	0.7143	1.0000	0.8333	5
Web Attack - XSS	0.4136	0.4110	0.4123	163
accuracy			0.9987	630591
macro avg	0.8923	0.9420	0.9135	630591
weighted avg	0.9988	0.9987	0.9987	630591

Confusion matrix shape: (15, 15)

---- Sensitivity / Specificity / Threat Score (OvR Aggregates) ----
Macro Sensitivity: 0.942018
Weighted Sensitivity: 0.998655
Macro Specificity: 0.999901
Weighted Specificity: 0.999864
Macro Threat Score (TS/CSI): 0.870976
Weighted Threat Score: 0.997613

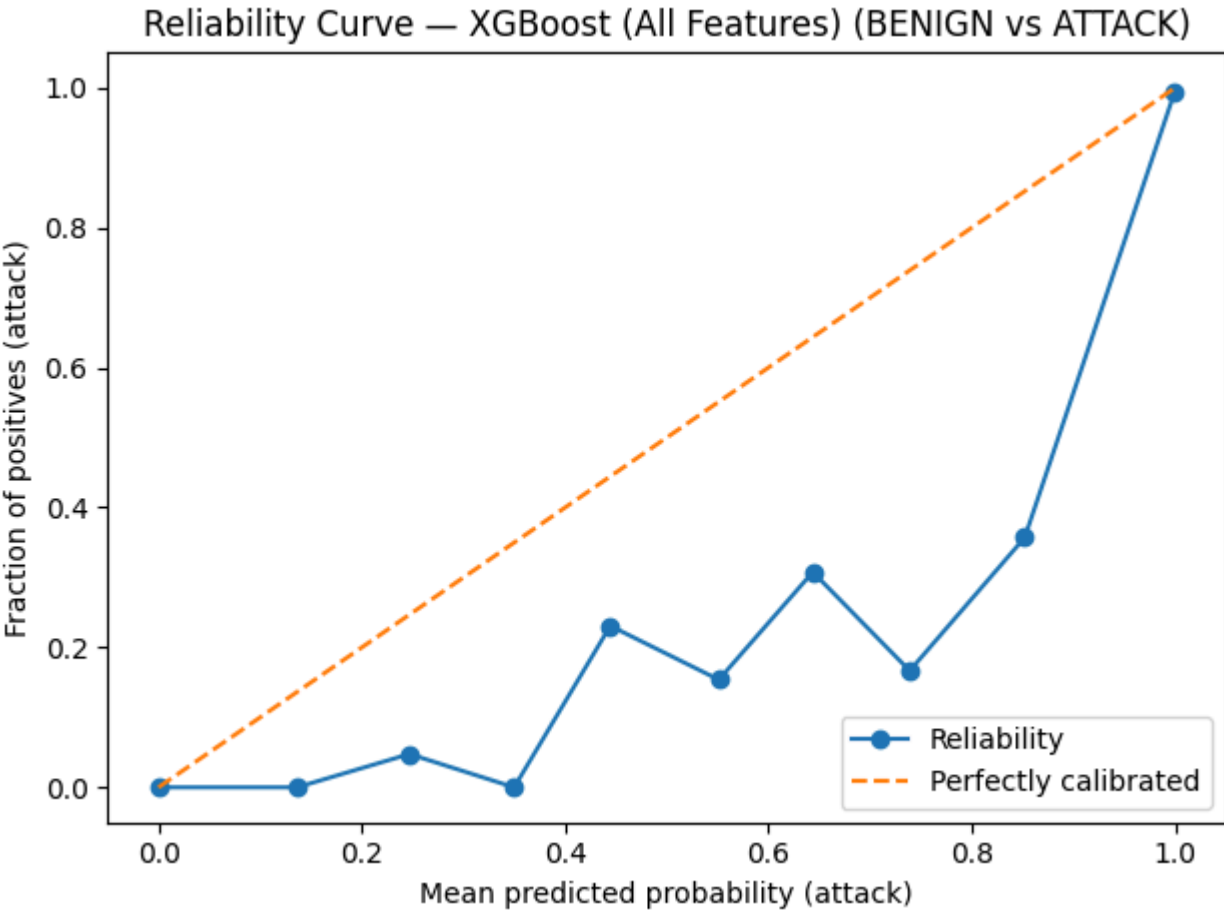
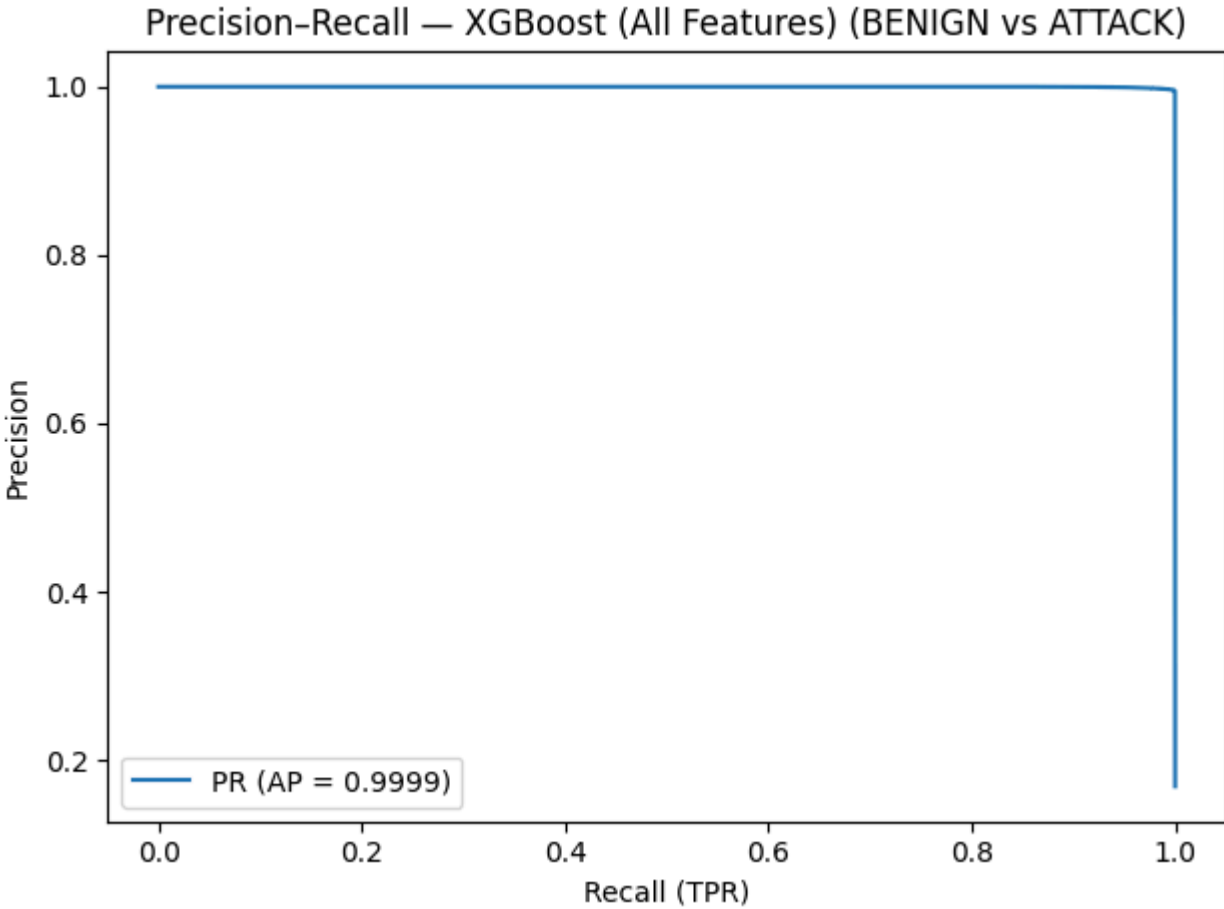
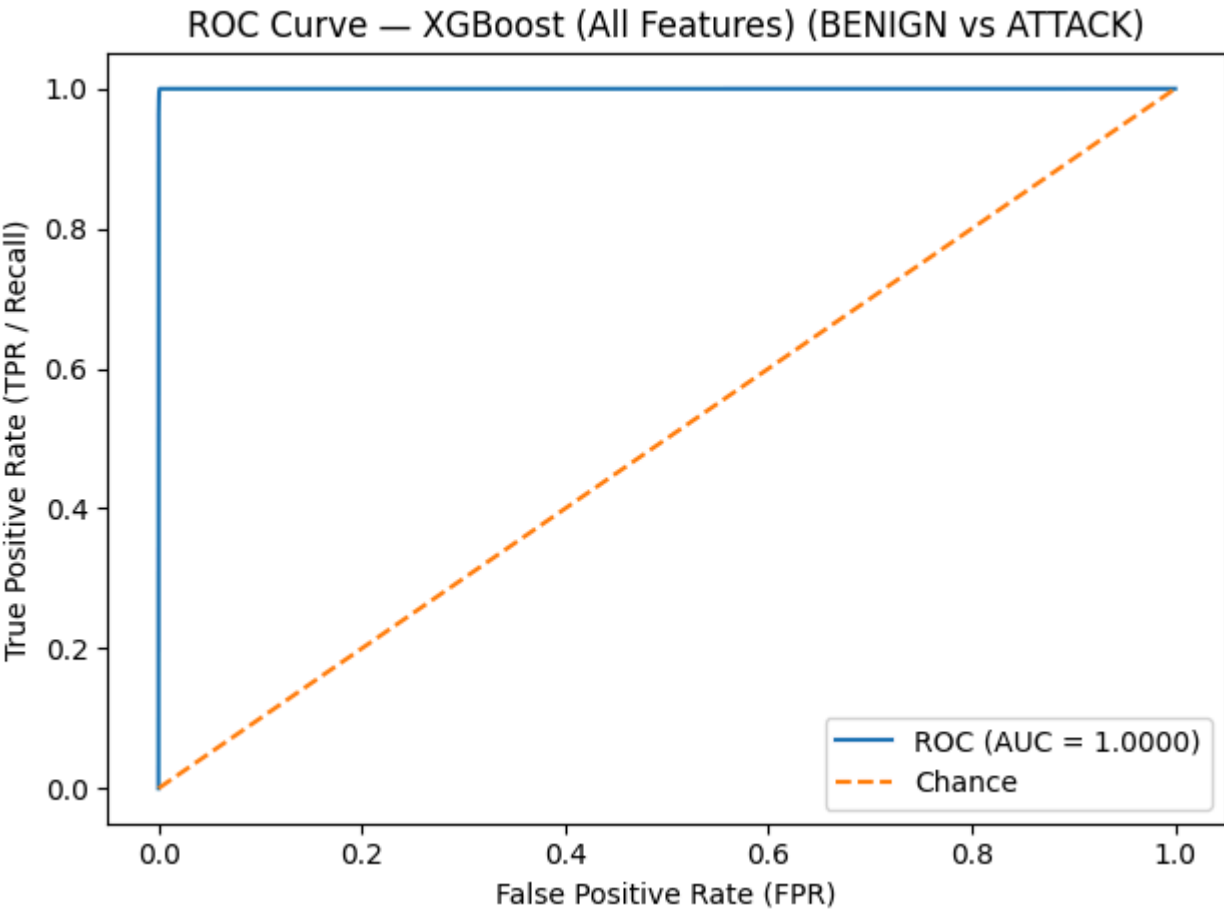
---- Per-class OvR breakdown (includes TP/FP/TN/FN) ----

Class	Support	TP	FP	TN	FN	Sensitivity_recall	Specificity	Threat_score_CSI
BENIGN	524121	523542	14	106456	579	0.998895	0.999869	0.998869
DoS Hulk	43212	43179	96	587283	33	0.999236	0.999837	0.997021
DDoS	32004	32004	10	598577	0	1.000000	0.999983	0.999688
PortScan	22705	22685	232	607654	20	0.999119	0.999618	0.989013
DoS GoldenEye	2572	2569	36	627983	3	0.998834	0.999943	0.985046
FTP-Patator	1483	1482	1	629107	1	0.999326	0.999998	0.998652
DoS Slowloris	1346	1336	8	629237	10	0.992571	0.999987	0.986706
DoS SlowHTTPTest	1307	1300	24	629260	7	0.994644	0.999962	0.976709
SSH-Patator	805	803	0	629786	2	0.997516	1.000000	0.997516
Bot	488	484	225	629878	4	0.991803	0.999643	0.678822
Web Attack - Brute Force	368	275	104	630119	93	0.747283	0.999835	0.582627
Web Attack - XSS	163	67	95	630333	96	0.411043	0.999849	0.259690
Infiltration	9	9	1	630581	0	1.000000	0.999998	0.900000
Web Attack - SQL Injection	5	5	2	630584	0	1.000000	0.999997	0.714286
Heartbleed	3	3	0	630588	0	1.000000	1.000000	1.000000

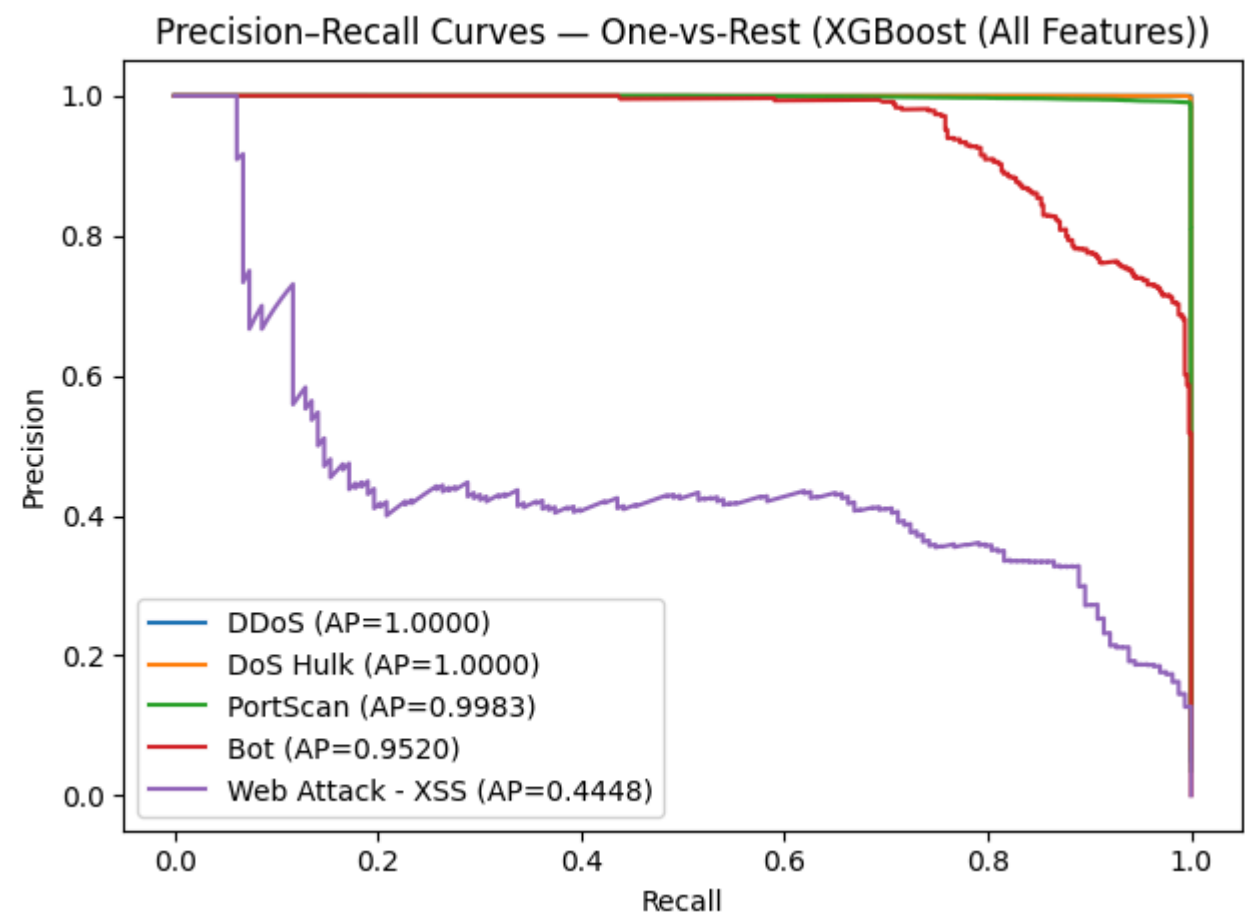
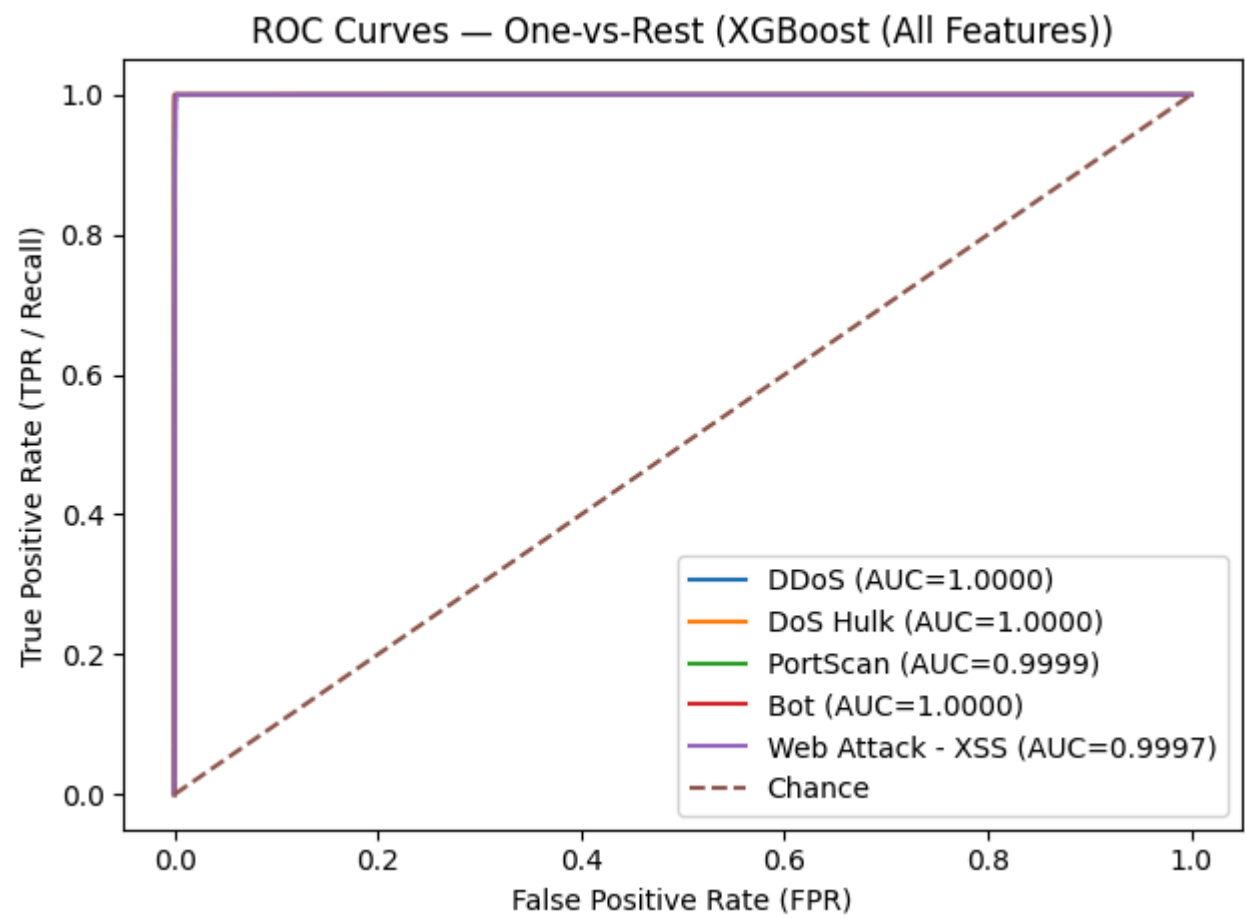
Log Loss (Multiclass): 0.006491

---- ROC-AUC (Multiclass OvR) ----
OvR Macro AUC: 0.999958
OvR Weighted AUC: 0.999977
Log Loss (Attack probability): 0.005225
Brier Score (Attack probability): 0.000902

---- Operational BENIGN vs ATTACK ----
Attack ROC-AUC: 0.999976
TP (attacks detected): 106456
FP (false alarms): 579
TN (benign passed): 523542
FN (missed attacks): 14
Detection Rate (TPR/Recall): 0.999869
Specificity (TNR): 0.998895
False Alarm Rate (FPR): 0.001105
Alert Precision: 0.994591
Threat Score (TS/CSI): 0.994460



Average Precision (Attack): 0.999878



4.3. Random Forest + XGBoost Evaluation

This cell evaluates the trained RF-selected-features XGBoost model (using the best TOP_K from the sweep) on the test set, computing predictions and probabilities, then generating the full metric summary (F1, balanced accuracy, AUC, confusion matrix) via the `evaluate_model` helper.

```
In [13]: # Evaluation of Random Forest to XGBoost (RF-selected Features + BEST_TOP_K from sweep)
SHOW_PLOTS_RF_XGB = True # Toggle plots

if "rf_xgb_bestk_model" not in globals():
    print("rf_xgb_bestk_model not found. Run the training cell first.")
elif "X_test_rf_xgb_bestk" not in globals():
    print("X_test_rf_xgb_bestk not found. Run the training cell first.")
else:
    y_pred_rf_xgb_bestk_eval = rf_xgb_bestk_model.predict(X_test_rf_xgb_bestk)
    y_proba_rf_xgb_bestk_eval = rf_xgb_bestk_model.predict_proba(X_test_rf_xgb_bestk)
    summary_rf_xgb_bestk, per_class_rf_xgb_bestk = evaluate_model(
        name=f"RF to XGBoost (Selected Features) - BEST_TOP_K={RF_XGB_BEST_TOP_K}",
        X_test=X_test_rf_xgb_bestk,
        y_true=y_test,
        y_pred=y_pred_rf_xgb_bestk_eval,
        y_proba=y_proba_rf_xgb_bestk_eval,
        class_names=class_names,
        benign_label="BENIGN",
        selected_labels=SELECTED_LABELS,
        show_plots=SHOW_PLOTS_RF_XGB
    )
```

----- RF to XGBoost (Selected Features) – BEST_TOP_K=80 -----

Accuracy: 0.99856
Macro F1: 0.914594
Weighted F1: 0.998601
Balanced Accuracy: 0.94361
Cohen's Kappa: 0.995222
Matthews Corrcoeff (MCC): 0.995228

Classification report:

	precision	recall	f1-score	support
BENIGN	1.0000	0.9988	0.9994	524121
Bot	0.6831	0.9939	0.8097	488
DDoS	0.9997	1.0000	0.9998	32004
DoS GoldenEye	0.9854	0.9988	0.9921	2572
DoS Hulk	0.9965	0.9992	0.9979	43212
DoS SlowHTTPTest	0.9826	0.9954	0.9890	1307
DoS Slowloris	0.9918	0.9926	0.9922	1346
FTP-Patator	0.9993	0.9993	0.9993	1483
Heartbleed	1.0000	1.0000	1.0000	3
Infiltration	0.9000	1.0000	0.9474	9
PortScan	0.9899	0.9991	0.9945	22705
SSH-Patator	0.9988	0.9975	0.9981	805
Web Attack - Brute Force	0.7417	0.7255	0.7335	368
Web Attack - SQL Injection	0.7143	1.0000	0.8333	5
Web Attack - XSS	0.4134	0.4540	0.4327	163
accuracy			0.9986	630591
macro avg	0.8931	0.9436	0.9146	630591
weighted avg	0.9987	0.9986	0.9986	630591

Confusion matrix shape: (15, 15)

---- Sensitivity / Specificity / Threat Score (OvR Aggregates) ----

Macro Sensitivity: 0.94361
Weighted Sensitivity: 0.99856
Macro Specificity: 0.999895
Weighted Specificity: 0.999858
Macro Threat Score (TS/CSI): 0.87166
Weighted Threat Score: 0.997425

---- Per-class OvR breakdown (includes TP/FP/TN/FN) ----

Class	Support	TP	FP	TN	FN	Sensitivity_recall	Specificity	Threat_score_CSI
BENIGN	524121	523482	14	106456	639	0.998781	0.999869	0.998754
DoS Hulk	43212	43178	151	587228	34	0.999213	0.999743	0.995734
DDoS	32004	32004	11	598576	0	1.000000	0.999982	0.999656
PortScan	22705	22685	232	607654	20	0.999119	0.999618	0.989013
DoS GoldenEye	2572	2569	38	627981	3	0.998834	0.999939	0.984291
FTP-Patator	1483	1482	1	629107	1	0.999326	0.999998	0.998652
DoS Slowloris	1346	1336	11	629234	10	0.992571	0.999983	0.984525
DoS SlowHTTPTest	1307	1301	23	629261	6	0.995409	0.999963	0.978195
SSH-Patator	805	803	1	629785	2	0.997516	0.999998	0.996278
Bot	488	485	225	629878	3	0.993852	0.999643	0.680224
Web Attack - Brute Force	368	267	93	630130	101	0.725543	0.999852	0.579176
Web Attack - XSS	163	74	105	630323	89	0.453988	0.999833	0.276119
Infiltration	9	9	1	630581	0	1.000000	0.999998	0.900000
Web Attack - SQL Injection	5	5	2	630584	0	1.000000	0.999997	0.714286
Heartbleed	3	3	0	630588	0	1.000000	1.000000	1.000000

Log Loss (Multiclass): 0.006665

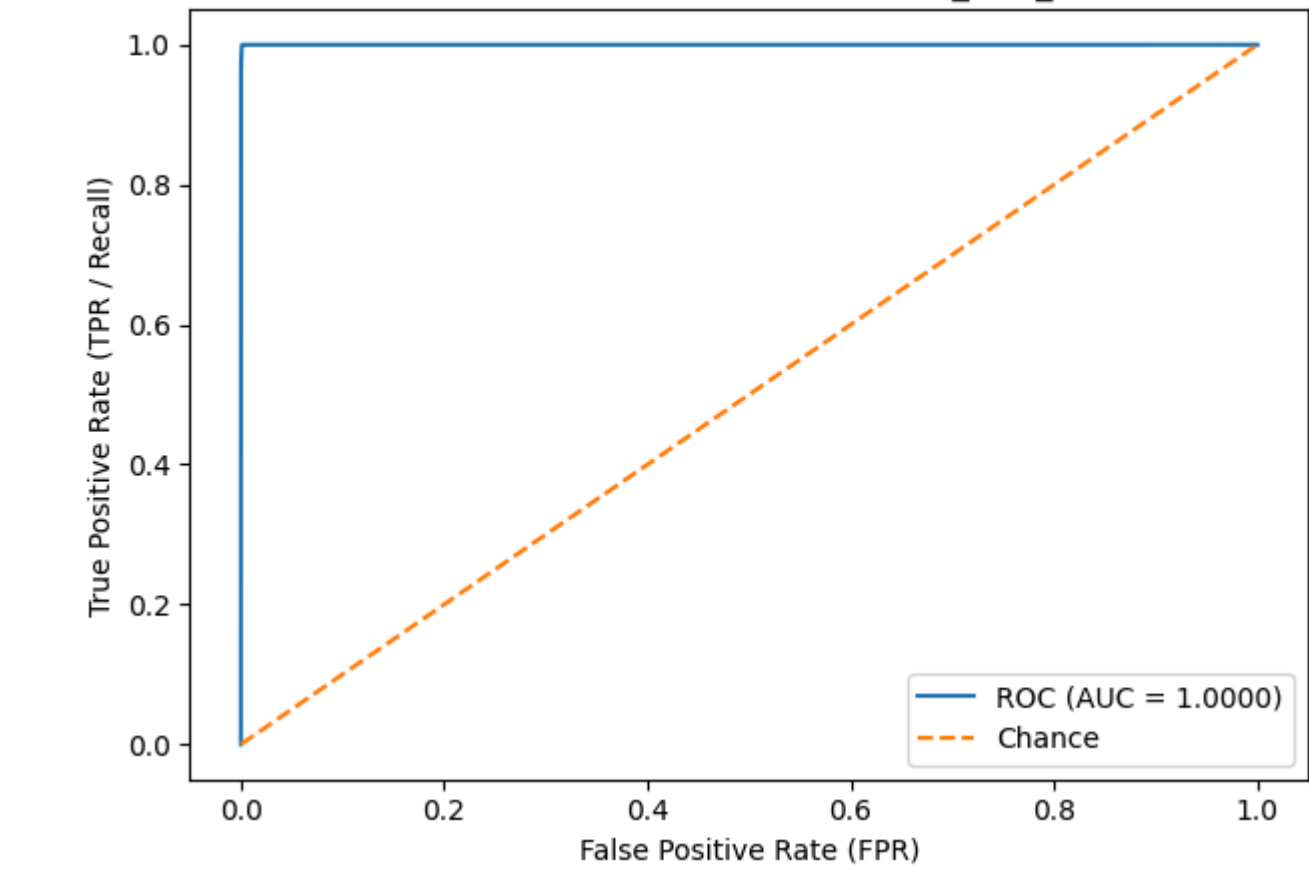
---- ROC-AUC (Multiclass OvR) ----

OvR Macro AUC: 0.999958
OvR Weighted AUC: 0.999977
Log Loss (Attack probability): 0.005379
Brier Score (Attack probability): 0.000968

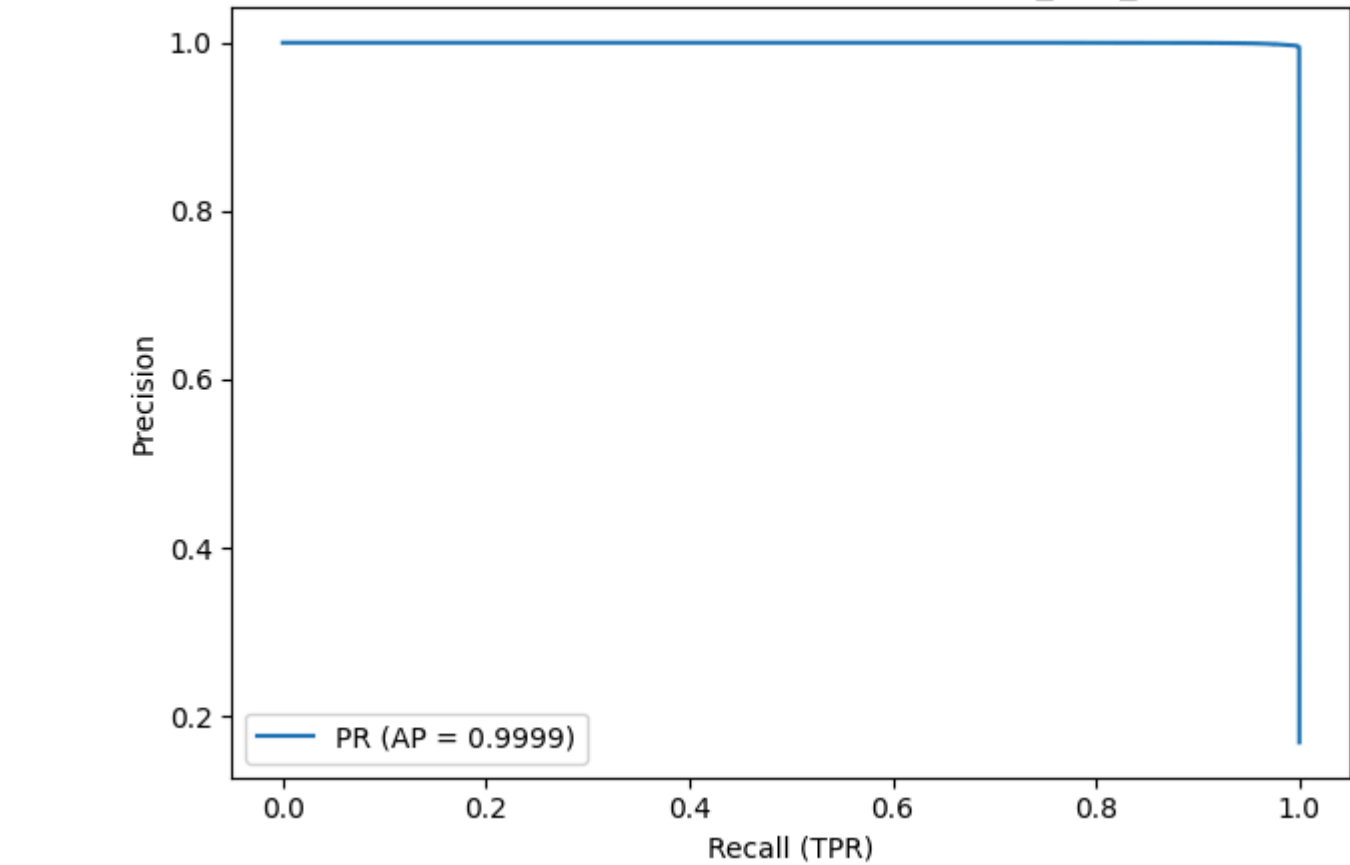
---- Operational BENIGN vs ATTACK ----

Attack ROC-AUC: 0.999976
TP (attacks detected): 106456
FP (false alarms): 639
TN (benign passed): 523482
FN (missed attacks): 14
Detection Rate (TPR/Recall): 0.999869
Specificity (TNR): 0.998781
False Alarm Rate (FPR): 0.001219
Alert Precision: 0.994033
Threat Score (TS/CSI): 0.993903

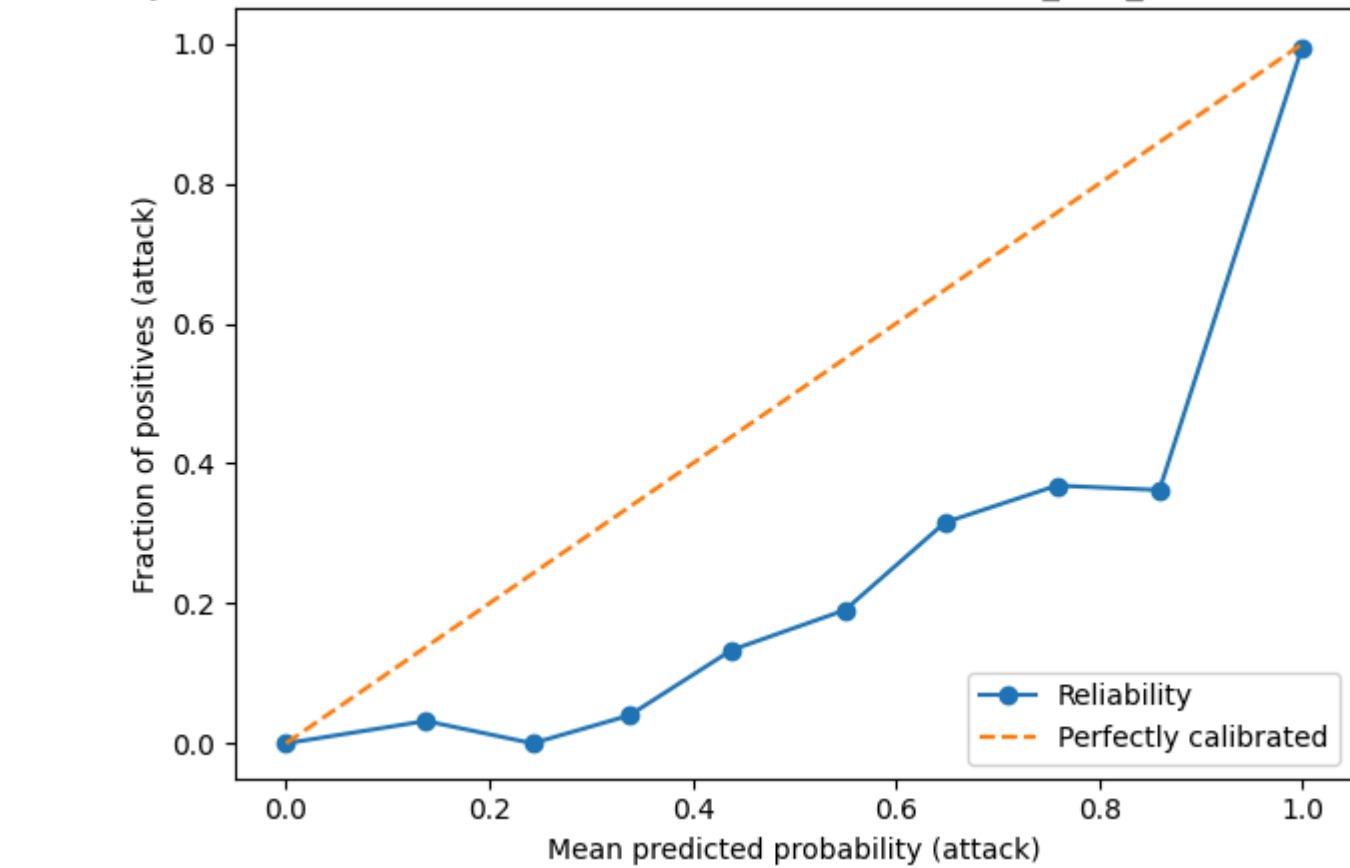
ROC Curve — RF to XGBoost (Selected Features) — BEST_TOP_K=80 (BENIGN vs ATTACK)



Precision-Recall — RF to XGBoost (Selected Features) — BEST_TOP_K=80 (BENIGN vs ATTACK)

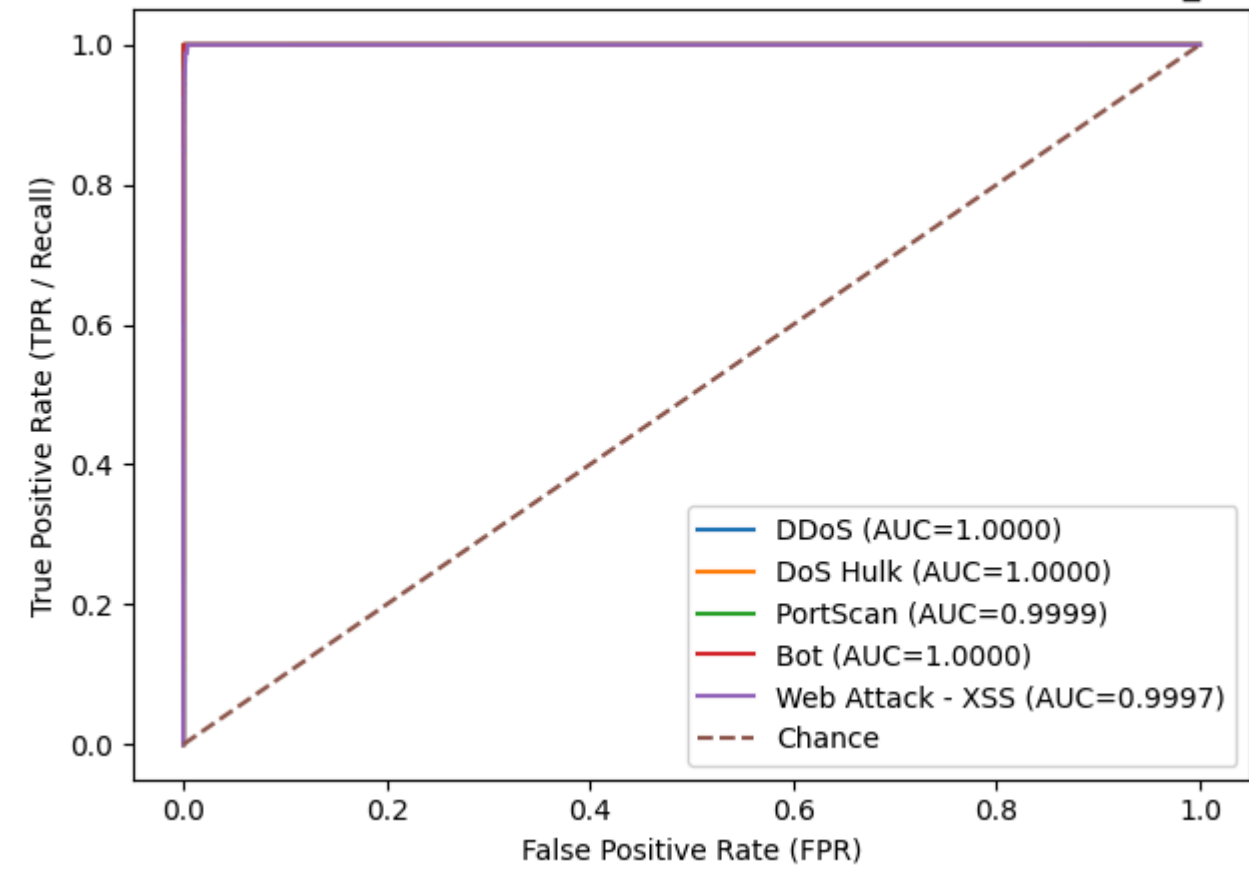


Reliability Curve — RF to XGBoost (Selected Features) — BEST_TOP_K=80 (BENIGN vs ATTACK)

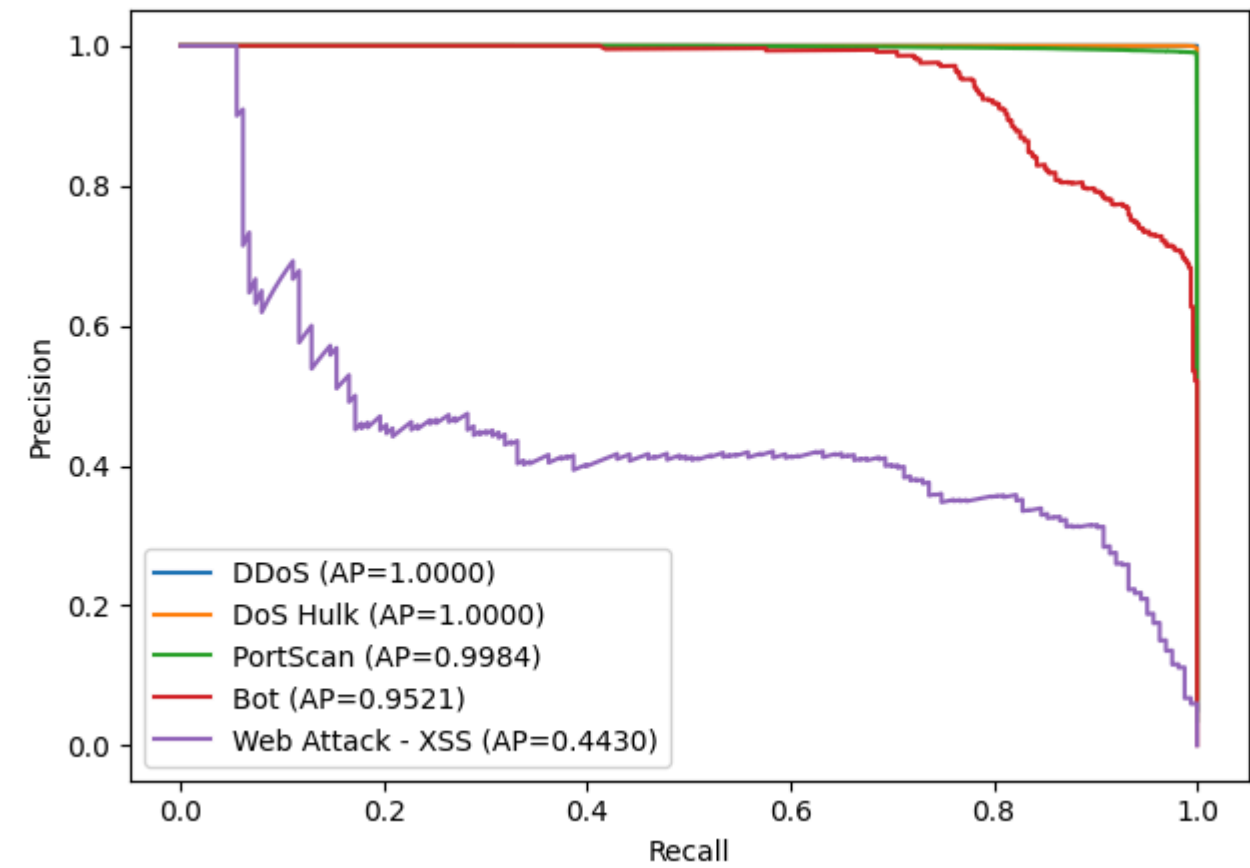


Average Precision (Attack): 0.999879

ROC Curves — One-vs-Rest (RF to XGBoost (Selected Features) — BEST_TOP_K=80)



Precision-Recall Curves — One-vs-Rest (RF to XGBoost (Selected Features) — BEST_TOP_K=80)



4.4. Comparison Summary

This cell builds a side-by-side table comparing the evaluation summaries for the two models (XGBoost on all features vs RF-selected features + XGBoost). It checks that both summary dictionaries exist, then displays their key metrics in a single dataframe for easy comparison.

In [14]:

```
needed = ["summary_xgb_all_paper", "summary_rf_xgb_bestk"]
missing = [v for v in needed if v not in globals()]

if missing:
    print("Missing summaries:", missing)
    print("Run the model evaluation cells first (XGB all-features evaluation and RF + XGB evaluation)")
else:
    summary_df = pd.DataFrame([summary_xgb_all_paper, summary_rf_xgb_bestk]).set_index("model")
    print("\n--- Summary Comparison Table ---")
    display(summary_df)
```

Summary Comparison Table ----

	accuracy	macro_f1	weighted_f1	balanced_accuracy	kappa	mcc	multiclass_logloss	attack_logloss	attack_brier	macro_sensitivity	weighted_sensitivity	macro_specificity	weighted_specificity	macro_threat_score	weighted_threat_score
model															
XGBoost (All Features)	0.998655	0.913488	0.998692	0.942018	0.995537	0.995541	0.006491	0.005225	0.000902	0.942018	0.998655	0.999901	0.999864	0.870976	0.997613
RF to XGBoost (Selected Features) — BEST_TOP_K=80	0.998560	0.914594	0.998601	0.943610	0.995222	0.995228	0.006665	0.005379	0.000968	0.943610	0.998560	0.999895	0.999858	0.871660	0.997425

4.5. Split Ratio Sensitivity Check (75/25 vs 70/30 vs 67/33)

This cell reruns the RF feature selection + XGBoost training pipeline under multiple train/test ratios (75/25, 70/30, 67/33) to check whether performance is stable across different splits. It reports core multiclass metrics plus operational BENIGN-vs-ATTACK rates (TP/FP/TN/FN, TPR/FPR, AUC/AP), and flags if any classes are missing in train or test due to class imbalance.

In [15]:

```
# Configuration
MAX_W = 1000 # Weight cap
EPS = 1e-12 # Tiny constant

# Use BEST_TOP_K found by the RF to XGB sweep
if "RF_XGB_BEST_TOP_K" not in globals():
    raise NameError("RF_XGB_BEST_TOP_K not found. Run the training cell first.")
TOP_K = int(RF_XGB_BEST_TOP_K)
print("Using TOP_K from sweep:", TOP_K)

SPLITS = [
    ("75/25", 0.25),
    ("70/30", 0.30),
    ("67/33", 0.33)
]

def safe_multiclass_auc_ovr(y_true, y_proba, n_classes):
    # Macro/weighted OvR AUC strong for missing classes
    y_true = np.asarray(y_true)
    present = np.unique(y_true)
    if len(present) < 2:
        return np.nan, np.nan
    classes = np.arange(n_classes)
    y_bin = label_binarize(y_true, classes=classes)
    aucs = []
    weights = []
    for i in range(n_classes):
        y_i = y_bin[:, i]
        # Need both positives and negatives
        if np.all(y_i == 0) or np.all(y_i == 1):
            continue
        aucs.append(roc_auc_score(y_i, y_proba[:, i]))
        weights.append(y_i.sum())
    if len(aucs) == 0:
        return np.nan, np.nan
    aucs = np.asarray(aucs)
    weights = np.asarray(weights, dtype=float)
    return float(np.mean(aucs)), float(np.average(aucs, weights=weights))

def summary_from_preds(y_true, y_pred, y_proba, class_names):
    n_classes = len(class_names)
    acc = accuracy_score(y_true, y_pred)
    macro_f1 = f1_score(y_true, y_pred, average="macro", zero_division=0)
    weighted_f1 = f1_score(y_true, y_pred, average="weighted", zero_division=0)
    bal_acc = balanced_accuracy_score(y_true, y_pred)
    kappa = cohen_kappa_score(y_true, y_pred)
    mcc = matthews_corrcoef(y_true, y_pred)
    cm = confusion_matrix(y_true, y_pred, labels=np.arange(n_classes))
    total = cm.sum()
    tp = np.diag(cm)
    fn = cm.sum(axis=1) - tp
    fp = cm.sum(axis=0) - tp
    tn = total - (tp + fn + fp)
    sens = tp / (tp + fn + EPS)
    spec = tn / (tn + fp + EPS)
    ts = tp / (tp + fn + fp + EPS) # Threat Score / CSI
    support = cm.sum(axis=1).astype(float)
    w = support / (support.sum() + EPS)
    auc_macro, auc_weighted = (np.nan, np.nan)
    if y_proba is not None:
        auc_macro, auc_weighted = safe_multiclass_auc_ovr(y_true, y_proba, n_classes)
    out = {
        "Accuracy": acc,
        "Macro F1": macro_f1,
        "Weighted F1": weighted_f1,
        "Balanced Acc": bal_acc,
        "Kappa": kappa,
        "MCC": mcc,
        "Macro Sensitivity": float(np.mean(sens)),
        "Weighted Sensitivity": float(np.sum(w * sens)),
        "Macro Specificity": float(np.mean(spec)),
        "Weighted Specificity": float(np.sum(w * spec)),
        "Macro Threat Score": float(np.mean(ts)),
        "Weighted Threat Score": float(np.sum(w * ts)),
        "OvR AUC (macro)": auc_macro,
        "OvR AUC (weighted)": auc_weighted,
    }
    # Operational BENIGN vs ATTACK metrics
    if "BENIGN" in class_names and y_proba is not None:
        benign_idx = int(np.where(class_names == "BENIGN")[0][0])
        y_attack = (y_true != benign_idx).astype(int)
        p_attack = 1.0 - y_proba[:, benign_idx]
        # argmax TP/FP/TN/FN at operational point
```

```

y_pred_attack = (y_pred != benign_idx).astype(int)
tn_b, fp_b, fn_b, tp_b = confusion_matrix(y_attack, y_pred_attack).ravel()
out.update({
    "Attack TP": int(tp_b),
    "Attack FP": int(fp_b),
    "Attack TN": int(tn_b),
    "Attack FN": int(fn_b),
    "Attack TPR": float(tp_b / (tp_b + fn_b + EPS)),
    "Attack FPR": float(fp_b / (fp_b + tn_b + EPS)),
    "Attack Precision": float(tp_b / (tp_b + fp_b + EPS)),
    "Attack Specificity": float(tn_b / (tn_b + fp_b + EPS)),
    "Attack Threat Score": float(tp_b / (tp_b + fn_b + fp_b + EPS)),
    "Attack ROC-AUC": float(roc_auc_score(y_attack, p_attack)) if len(np.unique(y_attack)) > 1 else np.nan,
    "Attack AP": float(average_precision_score(y_attack, p_attack)) if len(np.unique(y_attack)) > 1 else np.nan,
})
return out

def run_rf_xgb_paper(test_size):
    # Split
    X_tr, X_te, y_tr, y_te = train_test_split(
        X, y,
        test_size=test_size,
        stratify=y,
        shuffle=True,
        random_state=RANDOM_STATE
    )
    # Scale (fit on train only)
    scaler = MinMaxScaler()
    X_tr = pd.DataFrame(scaler.fit_transform(X_tr), columns=X.columns, index=X_tr.index)
    X_te = pd.DataFrame(scaler.transform(X_te), columns=X.columns, index=X_te.index)
    # Sample weights (same as your split cell)
    train_counts = np.bincount(y_tr, minlength=n_classes)
    class_weights = (len(y_tr) / (n_classes * np.maximum(train_counts, 1)))
    sw_tr = np.clip(class_weights[y_tr], 0, MAX_W)
    # RF for feature importances
    rf = RandomForestClassifier(
        n_estimators=RF_TREES,
        random_state=RANDOM_STATE,
        n_jobs=-1,
        class_weight=None
    )
    rf.fit(X_tr, y_tr, sample_weight=sw_tr)
    importances = pd.Series(rf.feature_importances_, index=X_tr.columns).sort_values(ascending=False)
    top_features = importances.index[:TOP_K].tolist()
    X_tr_sel = X_tr.loc[:, top_features]
    X_te_sel = X_te.loc[:, top_features]
    # XGB model
    xgb = XGBClassifier(
        objective="multi:softprob",
        num_class=n_classes,
        eval_metric="mlogloss",
        tree_method="hist",
        n_estimators=500,
        max_depth=6,
        learning_rate=0.1,
        subsample=1.0,
        colsample_bytree=1.0,
        random_state=RANDOM_STATE,
        n_jobs=-1
    )
    xgb.fit(X_tr_sel, y_tr, sample_weight=sw_tr)
    y_pred = xgb.predict(X_te_sel)
    y_proba = xgb.predict_proba(X_te_sel)
    missing_train = int(np.sum(np.bincount(y_tr, minlength=n_classes) == 0))
    missing_test = int(np.sum(np.bincount(y_te, minlength=n_classes) == 0))
    return y_te, y_pred, y_proba, missing_train, missing_test

rows = []
for split_name, test_size in SPLITS:
    t0 = time.time()
    y_te, y_pred, y_proba, miss_tr, miss_te = run_rf_xgb_paper(test_size=test_size)
    metrics = summary_from_preds(y_te, y_pred, y_proba, class_names=np.asarray(class_names))
    metrics["Split"] = split_name
    metrics["Missing classes in train"] = miss_tr
    metrics["Missing classes in test"] = miss_te
    metrics["Runtime (sec)"] = round(time.time() - t0, 2)
    rows.append(metrics)
split_df = pd.DataFrame(rows).set_index("Split")

preferred_order = [
    "Accuracy", "Macro F1", "Balanced Acc", "Kappa", "MCC",
    "Macro Sensitivity", "Macro Specificity", "Macro Threat Score",
    "Weighted Sensitivity", "Weighted Specificity", "Weighted Threat Score",
    "OvR AUC (macro)", "OvR AUC (weighted)",
    "Missing classes in train", "Missing classes in test", "Runtime (sec)"
]

ordered_cols = [c for c in preferred_order if c in split_df.columns] + [c for c in split_df.columns if c not in preferred_order]

```

```
split_df = split_df[ordered_cols] # Re-order columns

print("\n---- Split Ratio Sensitivity (RF-to-XGB) ----")
display(split_df) # Show results
```

Using TOP_K from sweep: 80

---- Split Ratio Sensitivity (RF-to-XGB) ----

	Accuracy	Macro F1	Balanced Acc	Kappa	MCC	Macro Sensitivity	Macro Specificity	Macro Threat Score	Weighted Sensitivity	Weighted Specificity	...	Attack FP	Attack TN	Attack FN	Attack TPR	Attack FPR	Attack Precision	Attack Specificity	Attack Threat Score	Attack ROC-AUC	Attack AP
Split																					
75/25	0.998560	0.914594	0.943610	0.995222	0.995228	0.943610	0.999895	0.871660	0.998560	0.999858	...	639	523482	14	0.999869	0.001219	0.994033	0.998781	0.993903	0.999976	0.999879
70/30	0.998560	0.914097	0.944959	0.995221	0.995226	0.944959	0.999895	0.870707	0.998560	0.999869	...	781	628164	15	0.999883	0.001242	0.993924	0.998758	0.993808	0.999974	0.999871
67/33	0.998549	0.921156	0.947045	0.995185	0.995191	0.947045	0.999894	0.880163	0.998549	0.999859	...	864	690976	18	0.999872	0.001249	0.993889	0.998751	0.993763	0.999973	0.999863

3 rows × 28 columns

4.6. Overfitting Check

This cell compares Macro-F1 on the training set vs the held-out test set for both models (XGBoost on all features and RF-selected-features + XGBoost). A much higher training score than test score can indicate overfitting, while similar scores suggest better generalisation. It also recomputes predictions each run to avoid using stale outputs.

```
In [16]: if "xgb_all_paper" in globals():
    train_pred = xgb_all_paper.predict(X_train_model) # Recompute pred to avoid stale outputs
    test_pred = xgb_all_paper.predict(X_test_model)
    print("XGBoost (All Features)")
    print("  Train Macro F1:", f1_score(y_train, train_pred, average="macro"))
    print("  Test  Macro F1:", f1_score(y_test, test_pred, average="macro"))
else:
    print("xgb_all_paper not found. Run training cell first.")

if "rf_xgb_bestk_model" in globals():
    train_pred = rf_xgb_bestk_model.predict(X_train_rf_xgb_bestk)
    test_pred = rf_xgb_bestk_model.predict(X_test_rf_xgb_bestk)
    print(f"\nRF + XGBoost (Selected Features) - BEST_TOP_K={RF_XGB_BEST_TOP_K}")
    print("  Train Macro F1:", f1_score(y_train, train_pred, average="macro"))
    print("  Test  Macro F1:", f1_score(y_test, test_pred, average="macro"))
else:
    print("rf_xgb_bestk_model not found. Run training cell first.")
```

XGBoost (All Features)
Train Macro F1: 0.984838816191811
Test Macro F1: 0.9134875602905458

RF + XGBoost (Selected Features) - BEST_TOP_K=80
Train Macro F1: 0.9847711388462018
Test Macro F1: 0.9145944829570607

In []: