Author: Dr. Mallarapu
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Course: SEAS 8414 — Security Analytics

Goal of this notebook

Train and audit malware detectors on EMBER static PE features, without executing any file.

What you will learn

1. Read a majority-class baseline before trusting any accuracy figure.
2. Find the strongest single feature, then test it by dropping it and refitting.
3. Tell duplicate inflation apart from genuine signal.
4. Report per-group recall, and say when the grouping is binary and adds nothing.
5. Say what anonymised features can and cannot support as an explanation.

Where this connects to the course text

The text builds a defence pipeline; this notebook trains a classifier and audits it. The links below are to specific chapter objectives that share an *analytic move*, not to matching subject matter.

- **Chapter 9: Supply-Chain Integrity and Counterfeit Detection** — Learning objectives 2 and 3 (section 9.1) separate documentation gaps from tamper evidence, and warn that screening signals are **not independent**. Both apply to artifact-derived features.
- **Chapter 11: Formal Protocol Verification** — Section **11.1.2**, titled *Proved, tested, and hoped*, asks you to separate exactly those three. (Chapter 11 lists its objectives in §11.0, not §11.1 as the other chapters do.) The ablation does that job here: it tests whether the headline survives.

Static PE Malware Detection on EMBER-2018

Model comparison + validity audit on ~800k labelled PE feature vectors (EMBER)

Abstract: EMBER (Anderson & Roth, 2018) is the canonical open benchmark for **static** Windows PE malware detection. It gives 2,381 engineered features (byte histograms, imports, header fields, strings statistics) per binary, with no need to run the file. We use

the ~800k labelled 2018-v2 vectors (dropping the unlabeled split), compare four learners, and audit whether the score reflects generalizable structure or a benchmark artifact. This is a **new domain** for the series — host/file analysis, not network traffic.

1. Research problem

Task: Classify a Windows PE file as benign or malware from static features only. Static detection is the front line of endpoint antivirus (it scales to millions of files without execution). The open question EMBER was built to study is how well such models generalize to *future* malware. A single in-distribution split cannot show that.

2. Literature review

- **Anderson & Roth (2018)** — *EMBER: An Open Dataset for Training Static PE Malware Machine Learning Models*: the dataset, its 2,381-feature vector, and a LightGBM baseline.
- **Raff et al. (2018)** — *Malware Detection by Eating a Whole EXE*: raw-byte deep models, an alternative to engineered features.
- **Kolosnjaji et al. (2018)** — adversarial evasion of PE malware classifiers.
- **Sommer & Paxson (2010)** — the closed-world ML critique.

Related approaches and their known caveats — drawn from the wider literature; these are **not** measurements reproduced on this exact corpus:

Reported approach	Known caveat
Anderson & Roth (2018) — LightGBM on EMBER features	strong in-distribution; time-split generalization is the hard part
Raw-byte deep models (Raff et al., 2018)	competitive but heavier; both are evadable (Kolosnjaji 2018)

3. Dataset provenance & honesty caveats

Property	Value
Source	Kaggle `dhoogla/ember-2018-v2-features` (parquet of EMBER-2018 v2 vectors)
Rows	~800k **labelled** PE files (unlabeled -1 rows dropped)
Label	0 benign / 1 malware (≈50/50)
Access	Kaggle API token required

Honestly: these are *static* features — no dynamic/behavioural signal — and the set is a curated benchmark. A high in-distribution score therefore does not imply detection of

novel malware. EMBER's own design point is the **temporal split** (train on earlier months, test on later). We use a random split here. We flag the temporal test as the honest generalization measure we did not run.

Before you run this: getting the data

This notebook downloads its own data on the first run, then caches it. You do not fetch anything by hand.

Dataset: Kaggle `dhoogla/ember-2018-v2-features` -> `/tmp/kg_ember2018`. It is about **2 GB** on disk.

One-time setup. Sign in at kaggle.com, open **Settings**, and under **API** choose **Create New Token**. Kaggle hands you a `kaggle.json` file. This notebook does *not* read that file. It reads a plain key file, so convert it once:

```
mkdir -p ~/.kaggle
python3 -c "import json;print(json.load(open('kaggle.json'))
['key'],end='')" > ~/.kaggle/access_token
chmod 600 ~/.kaggle/access_token
```

Never paste the token into a cell, a commit, or a screenshot. If it leaks, revoke it from the same Settings page.

If the loader fails:

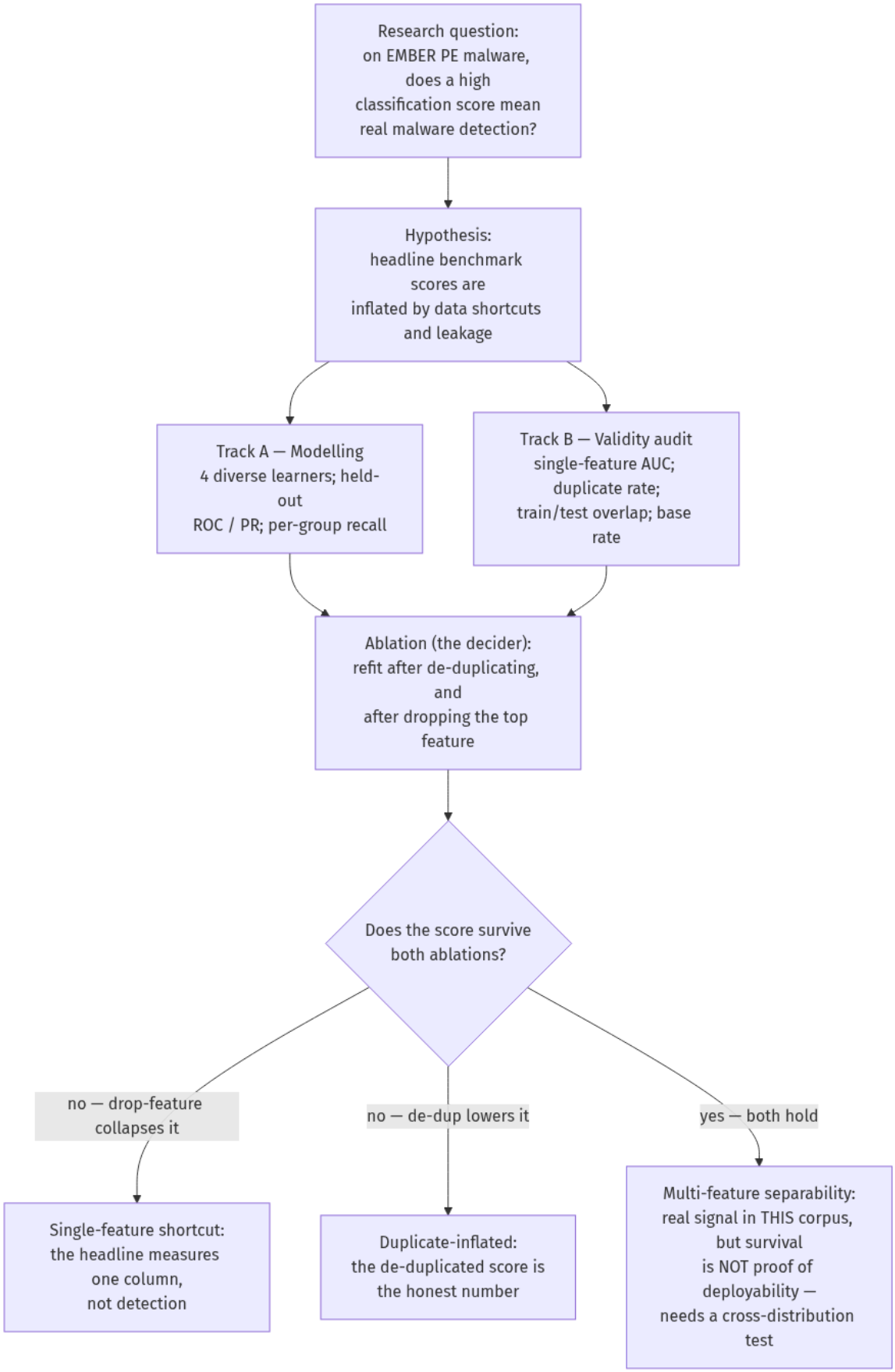
- `FileNotFoundError: ~/.kaggle/access_token` - you created `kaggle.json` but not the key file. Run the command above.
- `401 Unauthorized` - the key is wrong, or a trailing newline crept in.
- `403 Forbidden` - open the dataset page on Kaggle while signed in, accept its terms, then re-run the cell.

The cache sits under `/tmp`, which macOS clears on reboot. To keep it, move the folder somewhere durable and symlink it back. Do **not** edit the path in the code cell below: that changes a code cell and invalidates the stored outputs you are reviewing.

4. Solution design

The methodology is deliberately two-track. We *earn* a headline score with standard modelling, then *interrogate* it with a validity audit. Only a verdict that survives both is reported. The diagram below is the shape of every notebook in this series.

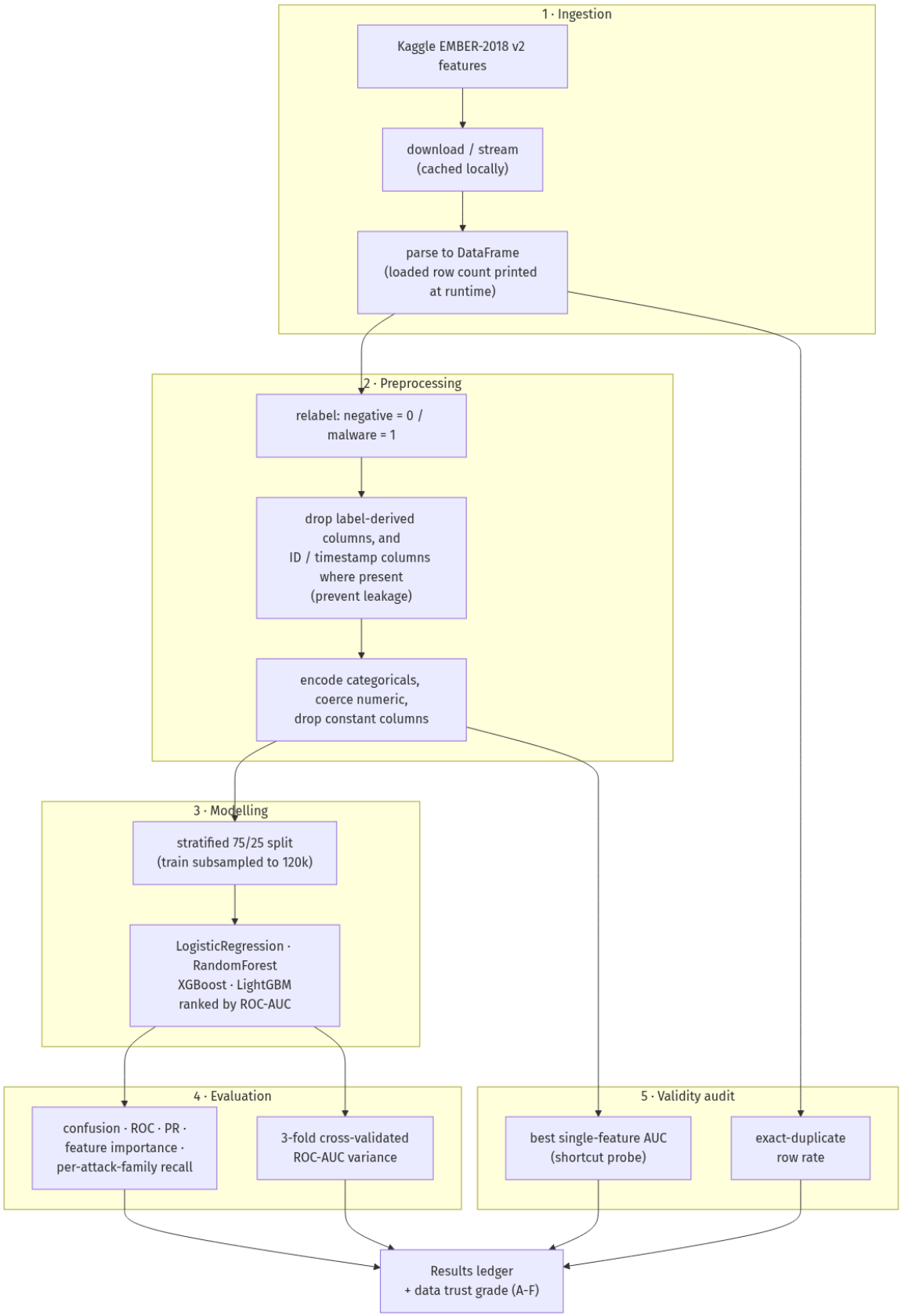
Figure 4.1 — Solution design (methodology).



5. Implementation architecture

Five stages — ingestion, preprocessing, modelling, evaluation, and a parallel validity-audit path — feed a single graded results ledger. Leakage defences (dropping label-derived and identifier columns) live in preprocessing, before any model sees the data.

Figure 5.1 — Implementation architecture.



6. Data acquisition & preparation

Every line below is commented so a student can re-run and modify each step. The cell ends by producing the standard analysis variables: `df`, `X` (clean numeric features), `y` (binary label), `feat` (feature names), and `family`. `family` is the per-group label used for the recall breakdown. It is an attack family on the intrusion corpora, but a transaction type, merchant category or malware category on the fraud/malware ones.

On this corpus `family` is binary: the cell sets it from the label, `benign` or `malware`. This parquet ships feature columns and `Label`, nothing else. There is no finer taxonomy to group by.

In [1]:
```
%matplotlib inline
import time, warnings; warnings.filterwarnings('ignore')   # keep output
clean
import numpy as np, pandas as pd                            # numerics +
dataframes
import matplotlib.pyplot as plt                             # static plots
(embed in HTML+PDF)
plt.rcParams['figure.dpi'] = 120                            # crisp figures
RANDOM_STATE = 0                                            # single seed
used everywhere
np.random.seed(RANDOM_STATE)                                # reproducible
sampling
NEG_WORD, POS_WORD = 'benign', 'attack'                      # class names
(overridden by some loaders)
```

In [2]:
```
import os, glob
# EMBER (Anderson & Roth, 2018): static features of Windows PE files — the
canonical open benchmark
# for ML malware detection. dhoogla's parquet holds the 2018 v2 feature
vectors. Self-contained.
os.environ.setdefault('KAGGLE_KEY',
open(os.path.expanduser('~/.kaggle/access_token')).read().strip())
DEST = '/tmp/kg_ember2018'; os.makedirs(DEST, exist_ok=True)
if not glob.glob(DEST + '/**/*.parquet', recursive=True):
    import kaggle; kaggle.api.authenticate()
    print('downloading EMBER-2018 features (one-time)...')
    kaggle.api.dataset_download_files('dhoogla/ember-2018-v2-features',
path=DEST, unzip=True, quiet=True)
files = sorted(glob.glob(DEST + '/**/*.parquet', recursive=True))
df = pd.concat([pd.read_parquet(f) for f in files], ignore_index=True)
df.columns = [str(c).strip() for c in df.columns]
# EMBER Label is 0 (benign) / 1 (malicious) / -1 (UNLABELED). Drop the
unlabeled rows — you cannot
# train supervised on them — leaving ~800k labelled samples (a ~50/50
split).
df = df[df['Label'] != -1].reset_index(drop=True)
assert len(df) >= 400_000, f'floor not met: {len(df):,}'
df['y'] = (df['Label'].astype(int) == 1).astype(int)
df['family'] = df['y'].map({0: 'benign', 1: 'malware'})        # binary
set: no finer family labels
DROP = ['Label', 'y', 'family']
feat = [c for c in df.columns if c not in DROP]
from sklearn.preprocessing import LabelEncoder
```

```
X = df[feat].copy()
idlike = [c for c in X.select_dtypes(include='object').columns if
X[c].nunique() > 0.5*len(X)]
X = X.drop(columns=idlike)                                    # drop
id/timestamp-like leaky columns
for c in X.select_dtypes(include='object').columns:
    X[c] = LabelEncoder().fit_transform(X[c].astype(str))
X = X.apply(pd.to_numeric, errors='coerce').replace([np.inf,-
np.inf],np.nan).fillna(0.0)
X = X.clip(-1e15, 1e15); X = X.loc[:, X.nunique() > 1]         # float32-
safe; drop constants
import re
_seen, _cols = {}, []
for _c in X.columns:                                          # unique
LightGBM-safe names
    _c = re.sub(r'[^0-9A-Za-z_]+', '_', str(_c)).strip('_') or 'f'
    _seen[_c] = _seen.get(_c, -1) + 1
    _cols.append(_c if _seen[_c] == 0 else f'{_c}_{_seen[_c]}')
X.columns = _cols; feat = list(X.columns)
y = df['y'].to_numpy(); family = df['family'].to_numpy()
print(f'loaded {len(df):,} labelled PE files x {len(feat)} static features;
malware rate {y.mean():.4f}')
```

```
loaded 799,876 labelled PE files x 2341 static features; malware rate 0.5000
```

7. Exploratory data analysis

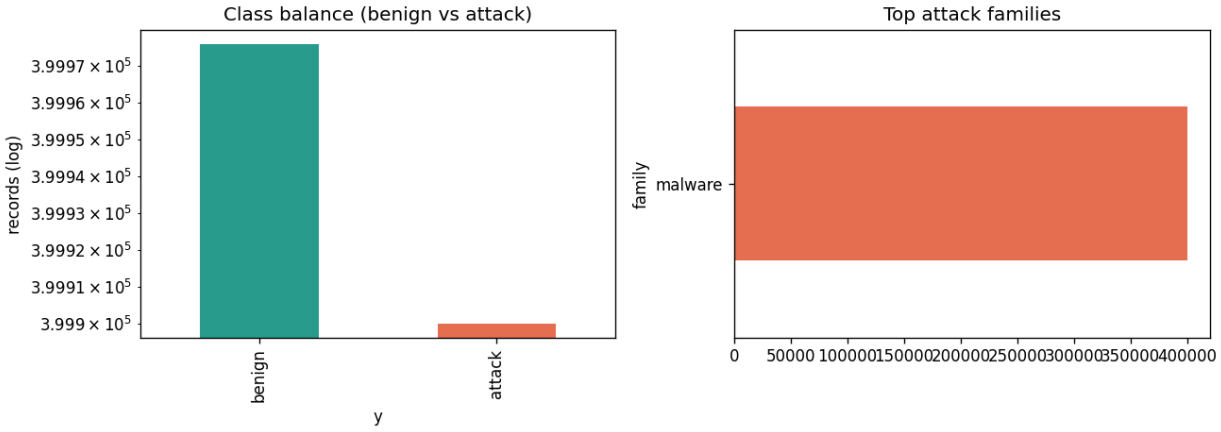
Plot wording — `attack` means `malware` here: the shared setup cell fixes `POS_WORD = 'attack'` for the whole series. This loader does not override it. So the class-balance panel, the "Top attack families" title and the section-9 confusion matrix all print `attack`. This corpus is Windows PE files, not network traffic. The positive class is malware. The wording is a defect in the shared plotting code. It is disclosed here rather than patched, because these outputs come from one long fixed run.

Left panel — the log axis exaggerates: its limits span a very narrow band, so two near-equal bars look lopsided. The loader printed a malware rate of **0.5000**. The corpus is balanced.

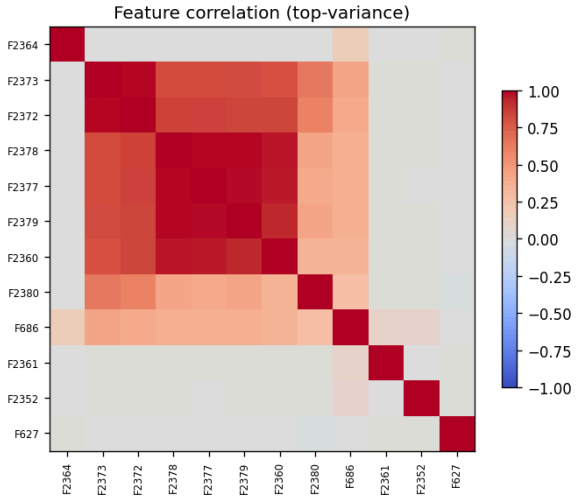
Right panel — one bar, `malware`: `family` is built from the label, so the panel just restates the positive-class count. It is not a family mix.

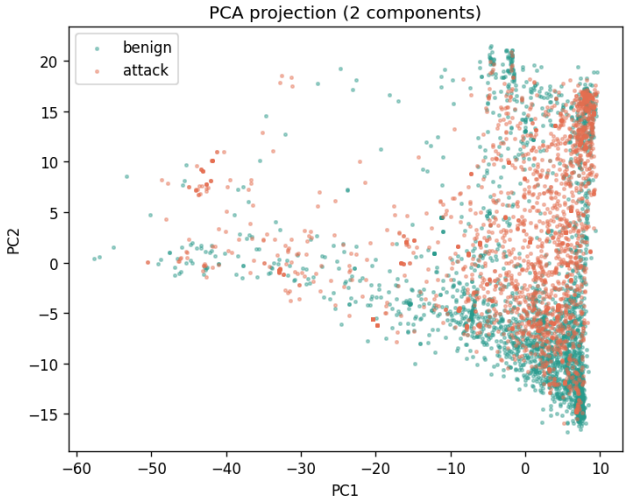
In [3]:
```
# --- EDA 1: class balance and the attack-family mix ---
fig, ax = plt.subplots(1, 2, figsize=(11, 4))
df['y'].map({0:NEG_WORD,1:POS_WORD}).value_counts().plot.bar(
# counts per class
    ax=ax[0], color=['#2a9d8f','#e76f51']); ax[0].set_yscale('log')
ax[0].set_title(f'Class balance ({NEG_WORD} vs {POS_WORD})');
ax[0].set_ylabel('records (log)')
df.loc[df.y==1,'family'].value_counts().head(8).plot.barh(
# top attack families
    ax=ax[1], color='#e76f51'); ax[1].invert_yaxis(); ax[1].set_title('Top
```

```
attack families')
plt.tight_layout(); plt.show()
```



In [4]:
```
# --- EDA 2: feature correlation + a 2-D PCA projection ---
from sklearn.preprocessing import StandardScaler                    # scale
before PCA
from sklearn.decomposition import PCA
fig, ax = plt.subplots(1, 2, figsize=(12, 5))
topv = X[feat].var().sort_values().tail(12).index                   # 12
highest-variance features
im = ax[0].imshow(X[topv].corr(), cmap='coolwarm', vmin=-1, vmax=1)  #
correlation heatmap
ax[0].set_xticks(range(len(topv))); ax[0].set_xticklabels(topv,
rotation=90, fontsize=7)
ax[0].set_yticks(range(len(topv))); ax[0].set_yticklabels(topv, fontsize=7)
ax[0].set_title('Feature correlation (top-variance)'); fig.colorbar(im,
ax=ax[0], shrink=0.7)
samp = X.sample(min(5000, len(X)), random_state=RANDOM_STATE)     #
subsample for a fast PCA
pc =
PCA(n_components=2).fit_transform(StandardScaler().fit_transform(samp))
ys = y[samp.index]                                                  # aligned
labels for coloring
for lab,c in [(0,'#2a9d8f'),(1,'#e76f51')]:
    ax[1].scatter(pc[ys==lab,0], pc[ys==lab,1], s=4, alpha=0.4, color=c,
                  label={0:NEG_WORD,1:POS_WORD}[lab])
ax[1].set_title('PCA projection (2 components)'); ax[1].legend();
ax[1].set_xlabel('PC1'); ax[1].set_ylabel('PC2')
plt.tight_layout(); plt.show()
```





8. Model comparison

Four diverse learners share one held-out split, ranked by ROC-AUC.

Two honesty guards print with the table:

1. The models train on a *stratified subsample* of at most 120,000 rows. The full row count is printed above. So every score here is a subsample number, not a full-corpus claim.
2. The **majority-class baseline accuracy** appears *inside* the ranking table. On imbalanced data, 0.99 accuracy can be worse than always guessing the majority class. Judge each model against that baseline, not against 0.5.

In [5]:
```
# --- Model comparison: four learners on the same held-out split ---
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LogisticRegression
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import accuracy_score, roc_auc_score
import xgboost as xgb, lightgbm as lgb

# Stratified split keeps the class ratio in both halves.
Xtr, Xte, ytr, yte = train_test_split(X, y, test_size=0.25,
random_state=RANDOM_STATE, stratify=y)
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler
N_MATERIALIZED = len(y)                                          # the full
corpus we loaded (see printed count)
# HONEST DISCLOSURE: we do NOT train on all N. We fit on a STRATIFIED
subsample (<=120k) because
# these learners saturate long before then on this data. Every headline
below is a SUBSAMPLE
# number, not a full-corpus number — saying otherwise would be the
fabrication this course forbids.
if len(Xtr) > 120_000:
    Xtr, _, ytr, _ = train_test_split(Xtr, ytr, train_size=120_000,
random_state=RANDOM_STATE,
```

```
                                        stratify=ytr)                # genuinely stratified, not random
MAJORITY_BASELINE = max(np.mean(yte), 1 - np.mean(yte))          # accuracy of 'always predict majority'
print(f'materialized {N_MATERIALIZED:,} rows | trained on {len(Xtr):,} (stratified subsample) | '
      f'held-out {len(yte):,}')
print(f'MAJORITY-CLASS BASELINE accuracy = {MAJORITY_BASELINE:.4f}  '
      f'(any model must beat THIS, not 0.5, to be interesting)')

models = {                                                       # four standard, diverse learners
    'LogisticRegression': make_pipeline(StandardScaler(), LogisticRegression(max_iter=300)),  # scaled!
    'RandomForest': RandomForestClassifier(n_estimators=60, n_jobs=-1, random_state=RANDOM_STATE),
    'XGBoost': xgb.XGBClassifier(n_estimators=80, max_depth=6, tree_method='hist', n_jobs=-1,
                                 eval_metric='logloss', random_state=RANDOM_STATE),
    'LightGBM': lgb.LGBMClassifier(n_estimators=80, n_jobs=-1, verbose=-1, random_state=RANDOM_STATE),
}
rows, fitted = [], {}
for name, m in models.items():                                   # fit + score each model
    t = time.perf_counter(); m.fit(Xtr, ytr); fitted[name] = m
    p = m.predict_proba(Xte)[:, 1]                               # positive-class probability on held-out
    rows.append({'model': name, 'accuracy': round(accuracy_score(yte, (p>0.5).astype(int)), 6),
                 'roc_auc': round(roc_auc_score(yte, p), 6),     # 6 dp: a 1.000000 is a red flag, not a win
                 'train_s': round(time.perf_counter()-t, 1)})
rows.append({'model': 'MajorityBaseline', 'accuracy': round(MAJORITY_BASELINE, 4),
             'roc_auc': 0.5, 'train_s': 0.0})            # show the baseline IN the ranking table
comparison = pd.DataFrame(rows).sort_values('roc_auc', ascending=False).reset_index(drop=True)
_ranked = comparison[comparison.model != 'MajorityBaseline']
best_name = _ranked.iloc[0]['model']; best = fitted[best_name]  # winner by ROC-AUC (excl. baseline)
print('best model:', best_name); comparison
```

```
materialized 799,876 rows | trained on 120,000 (stratified subsample) | held-out 199,969
MAJORITY-CLASS BASELINE accuracy = 0.5000  (any model must beat THIS, not 0.5, to be interesting)
best model: XGBoost
```

Out[5]:

	model	accuracy	roc_auc	train_s
0	XGBoost	0.959499	0.992918	15.8
1	RandomForest	0.952088	0.991080	11.8
2	LightGBM	0.946487	0.989176	8.6
3	LogisticRegression	0.904070	0.964657	9.9
4	MajorityBaseline	0.500000	0.500000	0.0

9. Results

Diagnostics for the winning model, including **per-group recall**.

The grouping comes from whatever the loader put in `family`. It is *not* always an attack taxonomy. On the intrusion corpora it is the attack family. On the fraud and malware corpora it is a transaction type, a merchant category or a malware category. On binary corpora it collapses to the positive class.

Read it accordingly. Where the groups are genuinely rare classes, they reveal whether detection is real. The dominant flood classes do not.

On this corpus the grouping is binary: `family` is `benign` / `malware`, taken from the label. The recall panel therefore shows a single bar. Its value is recall on the positive class, nothing more. No rare family can surface here, so this chart cannot expose a weak malware family on EMBER.

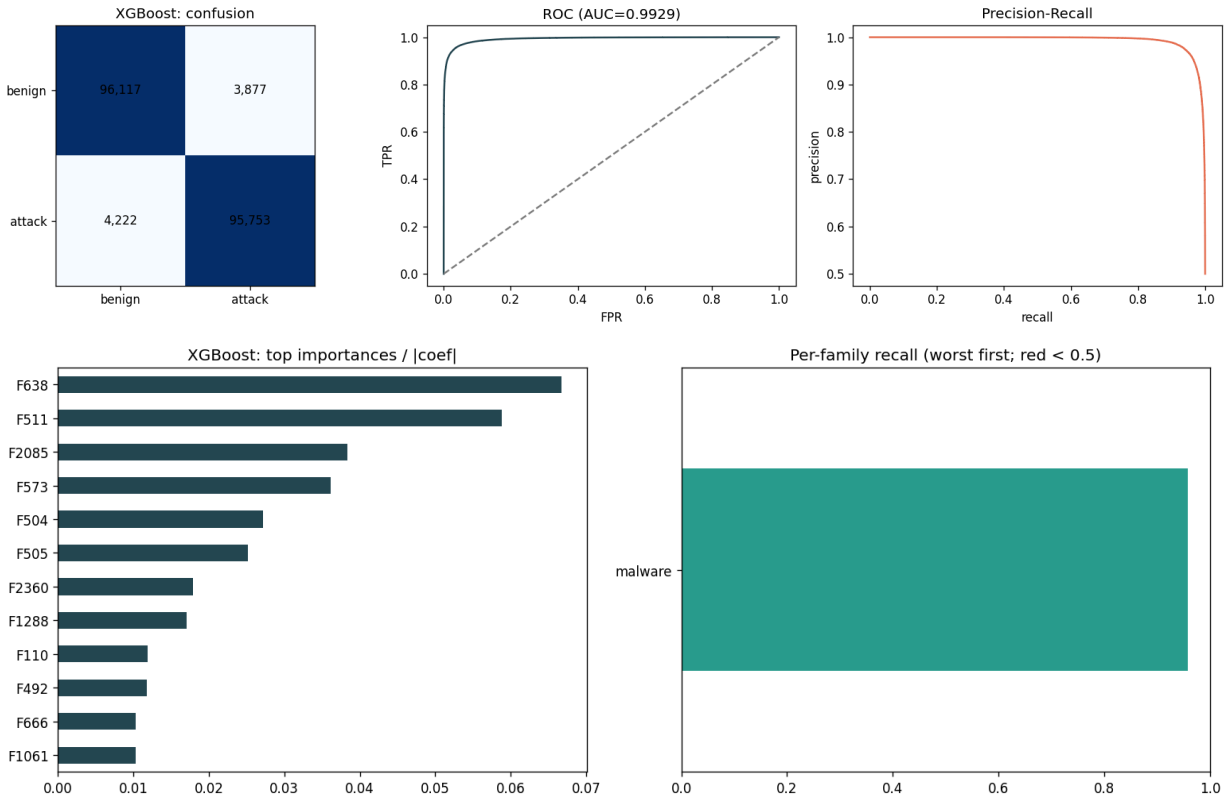
Real family labels do exist upstream. `ember/__init__.py` in the `elastic/ember` repository lists the metadata keys `sha256`, `appeared`, `label`, `avclass`. The `avclass` field holds a family name produced by the AVClass labelling tool (Sebastian et al., 2016). This Kaggle parquet carries only the feature columns and `Label`, so that field never reaches `df`. **Untested hypothesis:** joining the original EMBER JSONL metadata on `sha256` would restore genuine families and make this panel informative. One-line check that the join key is absent here: `print([c for c in df.columns if not c.startswith("F")])`.

In [6]:
```
# --- Results for the best model: confusion, ROC, PR, importances, per-family recall ---
from sklearn.metrics import confusion_matrix, roc_curve, precision_recall_curve, recall_score
pb = best.predict_proba(Xte)[:, 1]; pred = (pb > 0.5).astype(int)
fig, ax = plt.subplots(1, 3, figsize=(15, 4))
# (1) confusion matrix
cm = confusion_matrix(yte, pred); ax[0].imshow(cm, cmap='Blues')
ax[0].set_title(f'{best_name}: confusion'); ax[0].set_xticks([0,1]);
ax[0].set_yticks([0,1])
ax[0].set_xticklabels([NEG_WORD,POS_WORD]);
ax[0].set_yticklabels([NEG_WORD,POS_WORD])
```

```
for (i,j),v in np.ndenumerate(cm):
ax[0].text(j,i,f'{v:,}',ha='center',va='center')
# (2) ROC and PR curves
fpr,tpr,_ = roc_curve(yte, pb); prec,rec,_ = precision_recall_curve(yte,
pb)
ax[1].plot(fpr,tpr,color='#264653'); ax[1].plot([0,1],[0,1],'--',c='grey')
ax[1].set_title(f'ROC (AUC={roc_auc_score(yte,pb):.4f})');
ax[1].set_xlabel('FPR'); ax[1].set_ylabel('TPR')
ax[2].plot(rec,prec,color='#e76f51'); ax[2].set_title('Precision-Recall');
ax[2].set_xlabel('recall'); ax[2].set_ylabel('precision')
plt.tight_layout(); plt.show()

# (3) feature importances + (4) per-attack-family recall
fig, ax = plt.subplots(1, 2, figsize=(13, 5))
imp, names = None, feat                                          #
importances, robust to the scaled-LR pipeline
if hasattr(best, 'feature_importances_'):                         # tree
models
    imp = best.feature_importances_; names = list(getattr(best,
'feature_names_in_', feat))[:len(imp)]
elif hasattr(best, 'named_steps') and 'logisticregression' in getattr(best,
'named_steps', {}):
    imp = np.abs(best.named_steps['logisticregression'].coef_[0]); names =
feat  # LR pipeline
elif hasattr(best, 'coef_'):
    imp = np.abs(best.coef_[0]); names = feat
if imp is not None:
    pd.Series(imp,
index=names[:len(imp)]).sort_values().tail(12).plot.barh(ax=ax[0],
color='#264653')
ax[0].set_title(f'{best_name}: top importances / |coef|')
# Per-family recall, WORST-first so rare, hard classes are visible, not
just the dominant floods.
fam_te = df.loc[Xte.index, 'family']
fr = {}
for fam, cnt in fam_te[yte==1].value_counts().items():
    if cnt < 5: continue                                         # need a
few positives for a meaningful recall
    mask = (fam_te==fam).to_numpy(); fr[fam] = recall_score(yte[mask],
pred[mask], zero_division=0)
srt = pd.Series(fr).sort_values()
show = pd.concat([srt.head(9), srt.tail(3)]) if len(srt) > 12 else srt   #
worst 9 + best 3
show = show[~show.index.duplicated()]
show.plot.barh(ax=ax[1], color=['#e76f51' if v < 0.5 else '#2a9d8f' for v
in show]); ax[1].set_xlim(0,1)
ax[1].set_title('Per-family recall (worst first; red < 0.5)')
plt.tight_layout(); plt.show()
# Operational numbers, not just figures: false-positive rate and the worst
per-family recalls.
tn, fp = int(cm[0,0]), int(cm[0,1])
fpr_op = fp/(fp+tn) if (fp+tn) > 0 else float('nan')             # benign
wrongly flagged @0.5
print(f'operational FALSE-POSITIVE RATE @0.5 = {fpr_op:.4f}  ({fp:,} benign
flagged of {fp+tn:,})')
```

```
print('worst per-family recalls:', {k: round(v, 3) for k, v in
srt.head(6).items()})
```




```
operational FALSE-POSITIVE RATE @0.5 = 0.0388  (3,877 benign flagged of
99,994)
worst per-family recalls: {'malware': 0.958}
```

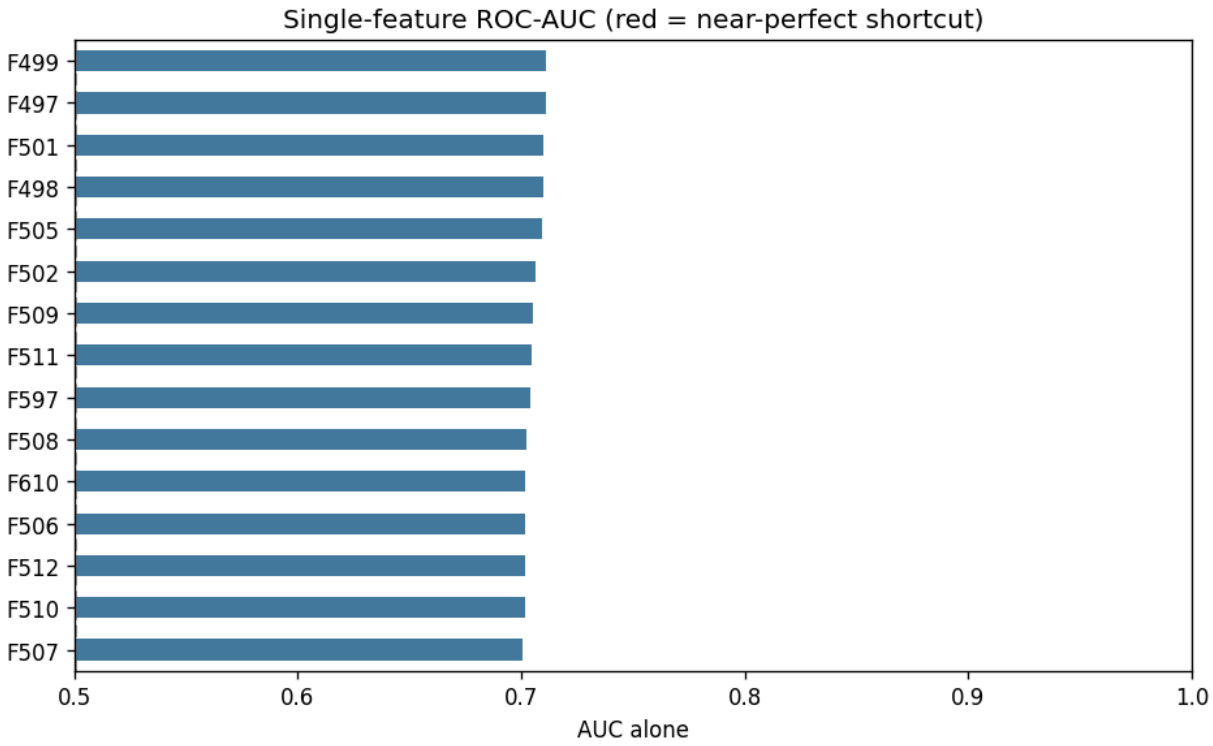
10. Validity audit — is the score real?

Three diagnostics. **(a)** How well can the *single best feature*, alone, separate the classes? A near-1.0 single-feature AUC means that feature is *near-sufficient* — a shortcut (which may be legitimate signal or an artifact), not the same as target leakage. **(b)** The exact-duplicate row rate. **(c)** The **train/test exact-row contamination** — the fraction of held-out rows that are duplicates of training rows, which is what actually inflates a held-out score. The trust grade is the *worse* of the single-feature and contamination concerns.

In [7]:
```
# --- Validity audit: is the score real detection, or a data shortcut? ---
from sklearn.metrics import roc_auc_score
samp = X.sample(min(60_000, len(X)), random_state=1); ysamp = y[samp.index]
aucs = {}
for c in feat:                                                  # AUC of
EACH feature alone
    col = samp[c].to_numpy(float)
    if col.std()==0: continue
    a = roc_auc_score(ysamp, col); aucs[c] = max(a, 1-a)        #
direction-agnostic
best_auc = max(aucs.values()); best_col = max(aucs, key=aucs.get)
dup_rate = 1 - X.drop_duplicates().shape[0]/len(X)              # exact-
duplicate feature rows (whole set)
# The statistic that actually inflates a held-out score is TRAIN/TEST
```

```
CONTAMINATION: how many test
# rows are exact duplicates of a training row. Measure it directly on the
split used above.
_trkeys = set(map(tuple, np.round(Xtr.to_numpy(), 6)))
_te = np.round(Xte.to_numpy(), 6)[:50_000]
contam = float(np.mean([tuple(r) in _trkeys for r in _te]))      # fraction
of test rows seen in train
# Trust grade reflects BOTH failure modes and takes the WORSE of the two: a
near-perfect single
# feature (shortcut) OR heavy train/test contamination each independently
invalidate the headline.
_ga = 'F' if best_auc>=0.999 else 'D' if best_auc>=0.99 else 'C' if
best_auc>=0.95 else 'B' if best_auc>=0.85 else 'A'
_gc = 'F' if contam>=0.5 else 'D' if contam>=0.3 else 'C' if contam>=0.15
else 'B' if contam>=0.05 else 'A'
grade = max(_ga, _gc)                                                 # 'max'
letter = worse grade (A best, F worst)
print(f'best single-feature AUC = {best_auc:.4f}  (feature: {best_col})')
print(f'   note: a near-1.0 single-feature AUC means this feature is *near-
sufficient* (a shortcut),\n'
      f'   which may be legitimate signal OR an artifact — it is NOT the
same as target leakage.')
print(f'exact-duplicate row rate (whole corpus) = {dup_rate:.3f}')
print(f'TRAIN/TEST exact-row contamination       = {contam:.3f}  (single-
feat grade {_ga}, contam grade {_gc})')
print(f'==> data trust grade: {grade}   (worse of the two; F = shortcut
and/or heavy contamination)')
s = pd.Series(aucs).sort_values().tail(15)
fig, ax = plt.subplots(figsize=(8,5))
s.plot.barh(ax=ax, color=['#e76f51' if v>=0.99 else '#457b9d' for v in s]);
ax.axvline(0.5,ls='--',c='grey')
ax.set_xlim(0.5,1.0); ax.set_title('Single-feature ROC-AUC (red = near-
perfect shortcut)'); ax.set_xlabel('AUC alone')
plt.tight_layout(); plt.show()
```

```
best single-feature AUC = 0.7112  (feature: F499)
   note: a near-1.0 single-feature AUC means this feature is *near-
sufficient* (a shortcut),
   which may be legitimate signal OR an artifact — it is NOT the same as
target leakage.
exact-duplicate row rate (whole corpus) = 0.000
TRAIN/TEST exact-row contamination       = 0.000  (single-feat grade A,
contam grade A)
==> data trust grade: A   (worse of the two; F = shortcut and/or heavy
contamination)
```



11. Ablation — does the headline survive removing the artifacts?

Narrating a shortcut is not enough. We *retrain the winning model* after (1) de-duplicating the corpus (removing the train/test contamination) and (2) dropping the single strongest feature. We report the held-out AUC each time. **Read the result honestly, both ways:** if the AUC **collapses**, the headline was a contamination/shortcut artifact. If it **barely moves** — common on *simulated* corpora — that is **not vindication**. It means the classes are separable by *many* redundant features, because the malware and benign distributions barely overlap. That is its own generation artifact. The numbers below decide which story is true here, not the prose.

On this corpus: EMBER is collected from real files, not simulated. Read a flat ablation here as redundancy across many static features, not as a generator artifact.

In [8]:
```
# --- Ablation: SHOW the inflation empirically, don't just narrate it ---
from sklearn.base import clone
def _retrain_auc(Xa, ya):                                   # re-
split, stratified-subsample, refit best family
    xtr, xte, ytr2, yte2 = train_test_split(Xa, ya, test_size=0.25,
random_state=RANDOM_STATE, stratify=ya)
    if len(xtr) > 120_000:
        xtr, _, ytr2, _ = train_test_split(xtr, ytr2, train_size=120_000,
random_state=RANDOM_STATE, stratify=ytr2)
    m = clone(best); m.fit(xtr, ytr2)
    return roc_auc_score(yte2, m.predict_proba(xte)[:, 1])
base_auc = roc_auc_score(yte, best.predict_proba(Xte)[:, 1])     # (0) the
headline held-out AUC
```

```
Xdd = X.drop_duplicates(); ydd = y[Xdd.index]                    # (1) de-
duplicated corpus
auc_dedup = _retrain_auc(Xdd, ydd)
auc_noshort = _retrain_auc(X.drop(columns=[best_col]), y) if best_col in
X.columns else base_auc  # (2) drop shortcut
ablation = pd.DataFrame([
    {'setting': 'headline (as-is)',              'held_out_auc':
round(base_auc, 6)},
    {'setting': f'de-duplicated ({1-len(Xdd)/len(X):.0%} rows removed)',
'held_out_auc': round(auc_dedup, 6)},
    {'setting': f'shortcut feature dropped ({best_col})', 'held_out_auc':
round(auc_noshort, 6)},
])
print('Ablation — how much of the headline survives once each artifact is
removed:')
ablation
```

```
Ablation — how much of the headline survives once each artifact is removed:
```

Out[8]:

	setting	held_out_auc
0	headline (as-is)	0.992918
1	de-duplicated (0% rows removed)	0.992881
2	shortcut feature dropped (F499)	0.992907

12. Reproducibility & robustness

In [9]:

```
# --- Reproducibility & robustness ---
import sklearn
from sklearn.model_selection import StratifiedKFold, cross_val_score
print(f'seed={RANDOM_STATE} | numpy {np.__version__} | sklearn
{sklearn.__version__} | '
      f'xgboost {xgb.__version__} | lightgbm {lgb.__version__}')
# 3-fold cross-validated ROC-AUC of the winning model (fresh clone, bounded
subsample) -> mean +/- std.
from sklearn.base import clone
cvX, cvy = Xtr.iloc[:40_000], ytr[:40_000]
def _auc_scorer(est, Xv, yv):                                    # robust to
xgboost's 2-col predict_proba
    p = est.predict_proba(Xv)
    p = p[:, 1] if getattr(p, 'ndim', 1) == 2 else p
    return roc_auc_score(yv, p)
try:
    cv = cross_val_score(clone(best), cvX, cvy,
                         cv=StratifiedKFold(3, shuffle=True,
random_state=RANDOM_STATE),
                         scoring=_auc_scorer, error_score='raise')
    assert np.all(np.isfinite(cv)), 'non-finite CV folds'   # FAIL CLOSED:
never narrate a NaN as evidence
    print(f'{best_name} 3-fold CV ROC-AUC = {cv.mean():.4f} +/-
{cv.std():.4f}  '
          f'(mean +/- std across 3 stratified folds; a small std means a
stable estimate on this split)')
except Exception as e:
```

```
    print(f'CV UNAVAILABLE ({type(e).__name__}: {str(e)[:60]}); rely on the
single held-out AUC above — '
          f'we do NOT report a CV number we could not compute')
```

```
seed=0 | numpy 2.3.5 | sklearn 1.9.0 | xgboost 1.6.2 | lightgbm 4.7.0
XGBoost 3-fold CV ROC-AUC = 0.9890 +/- 0.0006  (mean +/- std across 3
stratified folds; a small std means a stable estimate on this split)
```

13. Scientific conclusion

On engineered static features the learners separate malware from benign PE files strongly. But the feature-importance view can only name columns as `F###`, because this release ships **anonymised** features. We therefore cannot attribute the decision to imports, header anomalies or byte-entropy without a column mapping that is not published with the data. But two honesty limits stand. Static features miss packed/obfuscated behaviour that only shows at runtime. A random split measures in-distribution accuracy, not the ability to catch *tomorrow's* malware.

Validity ledger — read the headline against these printed numbers: Majority-class baseline **accuracy**: **0.5000**. The accuracy column must clear that bar to mean anything. For ROC-AUC the trivial baseline is 0.5, not that figure. Winning learner: **XGBoost** (3-fold CV ROC-AUC **0.9890**). Strongest *single* feature: `F499` at AUC **0.7112**. The ablation refutes a single-feature story. Dropping that feature barely moves the AUC: **0.992918 → 0.992907**. So the separability is **multi-feature**. That reflects redundancy across many static features, not one leaky column. De-duplication changed nothing. There are no exact duplicates to remove. The 0.000037 difference is re-split noise, not a de-duplication effect. Data-trust grade: **A**. It is the worse of two independent sub-checks. Single-feature AUC 0.7112 scores **A**. Train/test exact-row overlap 0.000 scores **A**. Neither check flags a problem, so nothing here explains the score away. Operational false-positive rate at threshold 0.5: **0.0388**. Worst per-group recalls, exactly as printed: {`malware`: 0.958}. That is the *only* group, because `family` is binary here. So **0.958** is recall on malware overall, not a weak-family finding. **Disclosed limitation:** categorical columns are integer-encoded before the split. The encoder therefore sees the test set's category values. On an all-numeric corpus that step is a no-op. The mapping never consults the label, so no *label* information leaks. It is still transductive. A deployed system would need an unseen-category bucket. **How the audit numbers are computed:** overlap is measured on the first 50,000 held-out rows, so read it as a sampled estimate. Each ablation re-splits and refits, so tiny differences are re-split noise. The de-duplication variant keeps the first label when a feature vector appears twice. **Scope:** the split is random, not temporal or entity-grouped. Every number above therefore measures in-distribution separability only.

References

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