exploration

November 21, 2025

1 Comparação de Modelos (Exploration)

Notebook para comparar diferentes classificadores no pipeline de Predictive RCA, mantendo boas práticas: divisão estratificada, pré-processamento único, random seed fixo e avaliação consistente em validação e teste.

Notas de boas práticas

- Manter o mesmo pré-processamento e splits para todos os modelos (evita vazamento e garante comparabilidade).
- Fixar `random_state` para reprodutibilidade.
- Avaliar em validação e teste com a mesma métrica principal (AUC-ROC) e threshold padrão 0.5 para classificação.
- Inspecionar relatórios por classe para checar precisão/recall e usar gráficos (ROC, matriz de confusão) para entender a resposta de cada algoritmo.

[15]:
```
import sys
import os

sys.path.append(os.path.abspath(".."))
```

[16]:
```
from pathlib import Path
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.metrics import (
    ConfusionMatrixDisplay,
    classification_report,
    confusion_matrix,
    roc_auc_score,
    roc_curve,
)

from src.config.settings import CONFIG
from src.preprocessing.build_features import build_case_features
from src.preprocessing.split import stratified_case_split
from src.preprocessing.preprocess import (
    build_preprocessor,
    fit_preprocessor_and_transform,
)
```

```python
from src.models.lightgbm_model import LightGBMModel
from src.models.random_forest import RandomForestModel
from src.models.logistic_regression import LogisticRegressionModel
from src.models.xgboost_model import XGBoostModel

pd.options.display.float_format = lambda v: f"{v:.4f}"
plt.style.use("ggplot")
```

[17]:
```python
# Carregar e preparar dataset em nível de caso
log_path = Path("../data/raw/event_log_sintetico_2000_cases.csv")
sla_hours = CONFIG.SLA_HOURS

df_events = pd.read_csv(log_path)
if "timestamp" in df_events.columns:
    df_events["timestamp"] = pd.to_datetime(df_events["timestamp"])

df_cases = build_case_features(df_events, sla_hours=sla_hours)
df_cases.head()
```

[17]:
```
   case_id  throughput_hours  num_events  num_unique_activities  rework_count  \
0        1           46.3033           4                      4             0
1        2           69.1386           5                      5             0
2        3            8.9614           6                      5             1
3        4           41.3628           7                      5             2
4        5           26.1333           6                      6             0

   start_activity end_activity start_resource  mean_cost  sla_violated
0  Receber Pedido    Finalizar            Ana    87.5350             1
1  Receber Pedido    Finalizar           João    72.2880             1
2  Receber Pedido    Finalizar          Pedro    79.4467             0
3  Receber Pedido    Finalizar           João    75.1771             1
4  Receber Pedido    Finalizar         Marina    79.8367             1
```

[18]:
```python
# Split estratificado e pré-processamento único para todos os modelos
splits, numeric_features, categorical_features = stratified_case_split(
    df_cases,
    target_col="sla_violated",
    id_col="case_id",
    random_state=CONFIG.RANDOM_STATE,
)

preprocessor = build_preprocessor(numeric_features, categorical_features)
artifacts, X_train_pre, X_val_pre, X_test_pre = fit_preprocessor_and_transform(
    preprocessor, splits, numeric_features, categorical_features
)

y_train = splits.y_train.to_numpy()
```

```
y_val = splits.y_val.to_numpy()
y_test = splits.y_test.to_numpy()

numeric_features, categorical_features
```

[18]:
```
(['throughput_hours',
  'num_events',
  'num_unique_activities',
  'rework_count',
  'mean_cost'],
 ['start_activity', 'end_activity', 'start_resource'])
```

[19]:
```
from typing import Any, Dict, List, Tuple


def summarize_split(y_true, y_proba, threshold: float = 0.5):
    y_pred = (y_proba >= threshold).astype(int)
    report_dict = classification_report(
        y_true, y_pred, output_dict=True, zero_division=0
    )
    return {
        "auc": roc_auc_score(y_true, y_proba),
        "precision": report_dict["1"]["precision"],
        "recall": report_dict["1"]["recall"],
        "f1": report_dict["1"]["f1-score"],
        "support": int(report_dict["1"]["support"]),
        "report_text": classification_report(y_true, y_pred, zero_division=0),
        "confusion": confusion_matrix(y_true, y_pred),
        "pred": y_pred,
        "proba": y_proba,
    }


def train_and_eval(
    model_class, params: Dict[str, Any] | None = None, name: str | None = None
):
    params = params or {}
    model = model_class(**params)
    model.train(X_train_pre, y_train)

    val = summarize_split(y_val, model.predict_proba(X_val_pre)[:, 1])
    test = summarize_split(y_test, model.predict_proba(X_test_pre)[:, 1])

    return {
        "model": name or model_class.__name__,
        "val_auc": val["auc"],
        "test_auc": test["auc"],
        "val_precision": val["precision"],
        "test_precision": test["precision"],
        "val_recall": val["recall"],
        "test_recall": test["recall"],
        "val_f1": val["f1"],
        "test_f1": test["f1"],
        "val_report": val["report_text"],
        "test_report": test["report_text"],
        "val_confusion": val["confusion"],
        "test_confusion": test["confusion"],
        "val_pred": val["pred"],
        "test_pred": test["pred"],
        "val_proba": val["proba"],
        "test_proba": test["proba"],
    }


experiments: List[Tuple[str, Any, Dict[str, Any]]] = [
    (
        "LightGBM",
        LightGBMModel,
        {
            "objective": "binary",
            "n_estimators": 300,
            "learning_rate": 0.05,
            "num_leaves": 64,
            "max_depth": -1,
            "feature_fraction": 0.8,
            "random_state": CONFIG.RANDOM_STATE,
            "n_jobs": -1,
        },
    ),
    (
        "RandomForest",
        RandomForestModel,
        {
            "n_estimators": 400,
            "max_depth": 12,
            "min_samples_leaf": 2,
            "random_state": CONFIG.RANDOM_STATE,
            "n_jobs": -1,
        },
    ),
    (
        "LogisticRegression",
        LogisticRegressionModel,
        {
            "max_iter": 1000,
            "class_weight": "balanced",
            "n_jobs": -1,
        },
    ),
    (
        "XGBoost",
        XGBoostModel,
        {
            "n_estimators": 300,
            "learning_rate": 0.05,
            "max_depth": 6,
            "subsample": 0.8,
            "colsample_bytree": 0.8,
            "random_state": CONFIG.RANDOM_STATE,
            "n_jobs": -1,
        },
    ),
]
```

```
[20]: results = []
for name, cls, params in experiments:
    res = train_and_eval(cls, params, name=name)
    results.append(res)

metrics_df = (
    pd.DataFrame(results)[
        [
            "model",
            "val_auc",
            "test_auc",
            "val_precision",
            "test_precision",
            "val_recall",
            "test_recall",
            "val_f1",
            "test_f1",
        ]
    ]
    .sort_values("val_auc", ascending=False)
    .reset_index(drop=True)
)
metrics_df
```

```
[LightGBM] [Warning] feature_fraction is set=0.8, colsample_bytree=1.0 will be
ignored. Current value: feature_fraction=0.8
[LightGBM] [Warning] feature_fraction is set=0.8, colsample_bytree=1.0 will be
ignored. Current value: feature_fraction=0.8
```

```
[LightGBM] [Info] Number of positive: 964, number of negative: 236
[LightGBM] [Info] Auto-choosing col-wise multi-threading, the overhead of
testing was 0.000176 seconds.
You can set `force_col_wise=true` to remove the overhead.
[LightGBM] [Info] Total Bins 537
[LightGBM] [Info] Number of data points in the train set: 1200, number of used
features: 10
[LightGBM] [Info] [binary:BoostFromScore]: pavg=0.803333 -> initscore=1.407259
[LightGBM] [Info] Start training from score 1.407259
[LightGBM] [Warning] No further splits with positive gain, best gain: -inf
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[LightGBM] [Warning] No further splits with positive gain, best gain: -inf
[LightGBM] [Warning] No further splits with positive gain, best gain: -inf
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[LightGBM] [Warning] No further splits with positive gain, best gain: -inf
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[LightGBM] [Warning] No further splits with positive gain, best gain: -inf
[LightGBM] [Warning] No further splits with positive gain, best gain: -inf
[LightGBM] [Warning] No further splits with positive gain, best gain: -inf
[LightGBM] [Warning] feature_fraction is set=0.8, colsample_bytree=1.0 will be
ignored. Current value: feature_fraction=0.8
[LightGBM] [Warning] feature_fraction is set=0.8, colsample_bytree=1.0 will be
ignored. Current value: feature_fraction=0.8
```
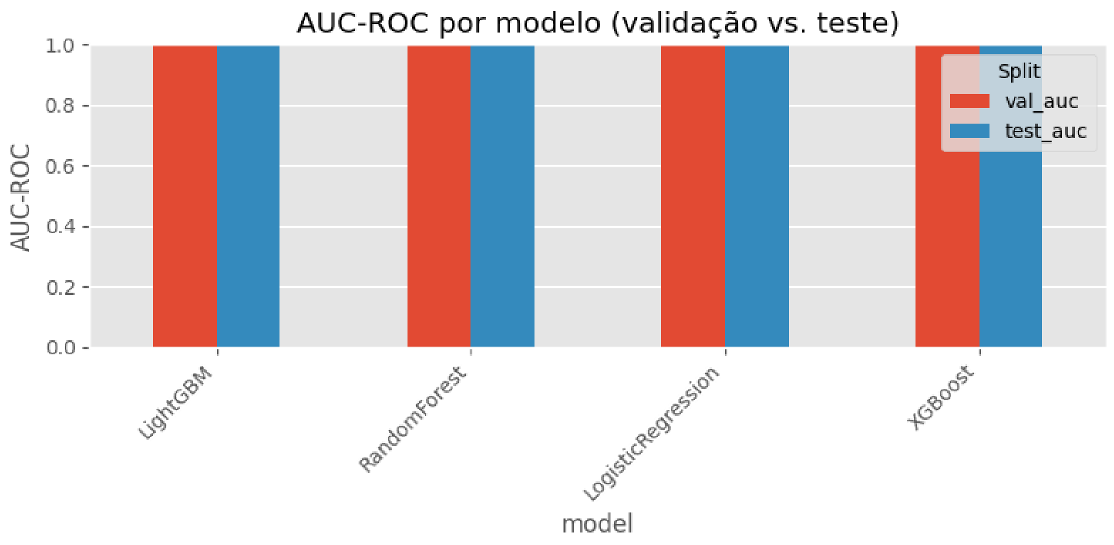

```
/Users/pedroeckel/.local/share/virtualenvs/predictive-
rca-9dRCaVbd/lib/python3.13/site-packages/sklearn/utils/validation.py:2749:
UserWarning: X does not have valid feature names, but LGBMClassifier was fitted
with feature names
  warnings.warn(
/Users/pedroeckel/.local/share/virtualenvs/predictive-
rca-9dRCaVbd/lib/python3.13/site-packages/sklearn/utils/validation.py:2749:
UserWarning: X does not have valid feature names, but LGBMClassifier was fitted
with feature names
  warnings.warn(
/Users/pedroeckel/.local/share/virtualenvs/predictive-
rca-9dRCaVbd/lib/python3.13/site-packages/xgboost/training.py:199: UserWarning:
[01:30:14] WARNING: /Users/runner/work/xgboost/xgboost/src/learner.cc:790:
Parameters: { "use_label_encoder" } are not used.

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

[20]:

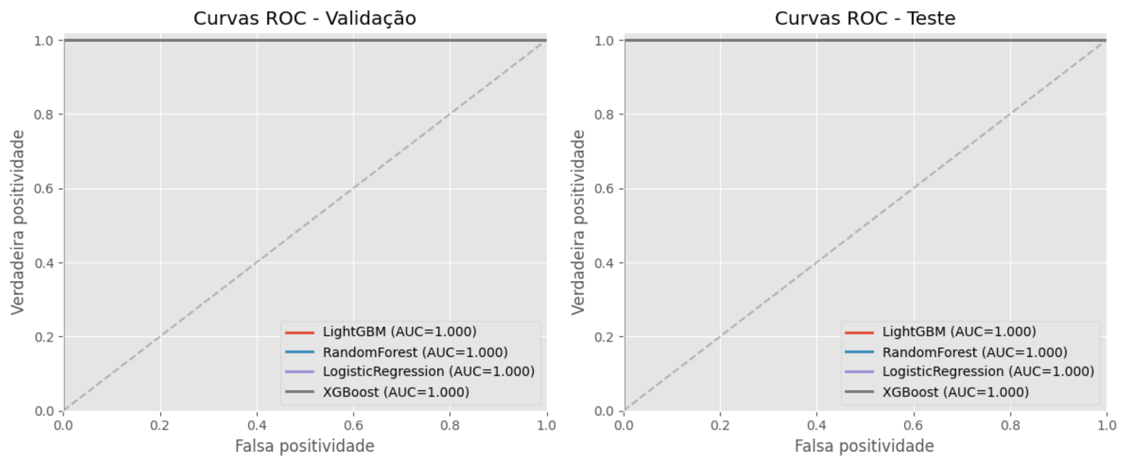
```
                 model  val_auc  test_auc  val_precision  test_precision  \
0             LightGBM   1.0000    1.0000         1.0000          1.0000
1         RandomForest   1.0000    1.0000         1.0000          1.0000
2   LogisticRegression   1.0000    1.0000         1.0000          1.0000
3              XGBoost   1.0000    1.0000         1.0000          1.0000
```

```
   val_recall  test_recall  val_f1  test_f1
0      1.0000       0.9969  1.0000   0.9984
1      1.0000       1.0000  1.0000   1.0000
2      0.9969       0.9907  0.9984   0.9953
3      1.0000       1.0000  1.0000   1.0000
```

[21]:
```python
ax = metrics_df.set_index("model")[["val_auc", "test_auc"]].plot.bar(
    figsize=(8, 4), ylim=(0, 1)
)
ax.set_ylabel("AUC-ROC")
ax.set_title("AUC-ROC por modelo (validação vs. teste)")
ax.legend(title="Split")
plt.xticks(rotation=45, ha="right")
plt.tight_layout()
plt.show()
```

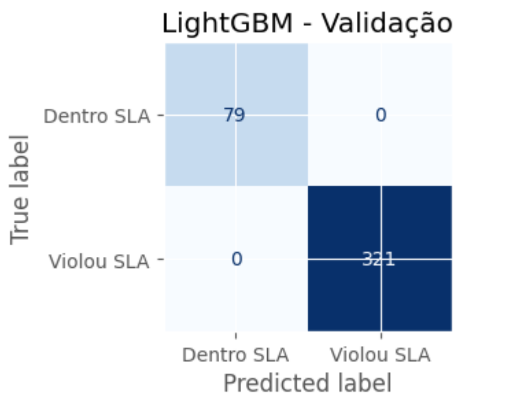


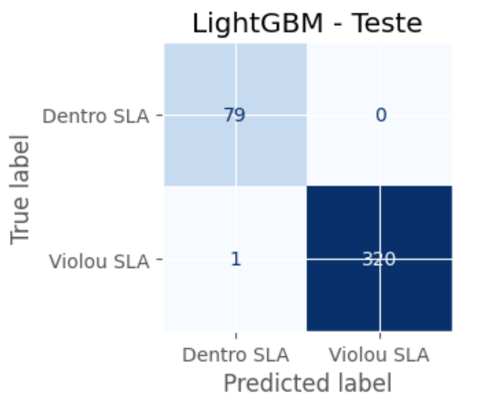
[22]:
```python
fig, axes = plt.subplots(1, 2, figsize=(12, 5))
for res in results:
    fpr_val, tpr_val, _ = roc_curve(y_val, res["val_proba"])
    fpr_test, tpr_test, _ = roc_curve(y_test, res["test_proba"])
    axes[0].plot(
        fpr_val,
        tpr_val,
        lw=2,
        label=f"{res['model']} (AUC={res['val_auc']:.3f})",
    )
    axes[1].plot(
        fpr_test,
        tpr_test,
        lw=2,
        label=f"{res['model']} (AUC={res['test_auc']:.3f})",
    )

for ax, title in zip(axes, ["Validação", "Teste"]):
    ax.plot([0, 1], [0, 1], color="gray", linestyle="--", alpha=0.5)
    ax.set_xlim(0, 1)
    ax.set_ylim(0, 1.02)
    ax.set_title(f"Curvas ROC - {title}")
    ax.set_xlabel("Falsa positividade")
    ax.set_ylabel("Verdadeira positividade")
    ax.legend()

plt.tight_layout()
plt.show()
```

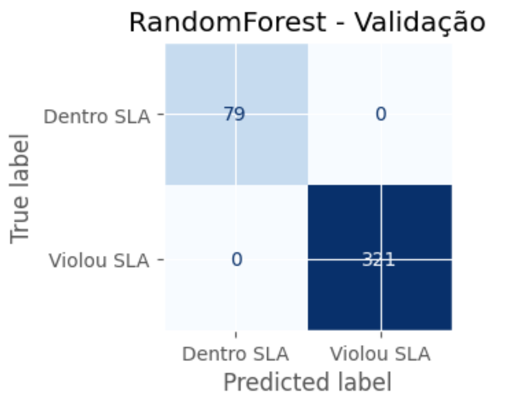


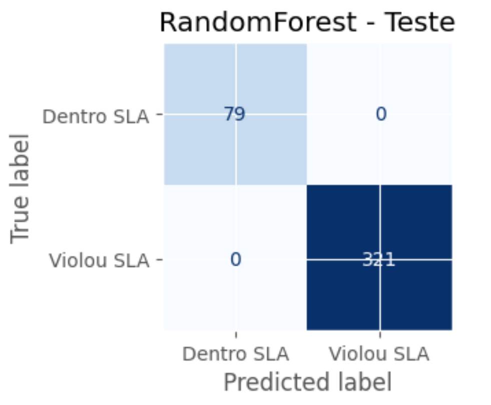
[23]:
```
fig, axes = plt.subplots(len(results), 2, figsize=(10, 3 * len(results)))
axes = axes if len(results) > 1 else [axes]
for i, res in enumerate(results):
    row_axes = axes[i]
    for ax, (split_label, cm) in zip(
        row_axes,
        [("Validação", res["val_confusion"]), ("Teste", res["test_confusion"])],
    ):
        disp = ConfusionMatrixDisplay(cm, display_labels=["Dentro SLA", "Violou␣
 ↪SLA"])
        disp.plot(ax=ax, colorbar=False, cmap="Blues")
        ax.set_title(f"{res['model']} - {split_label}")
```

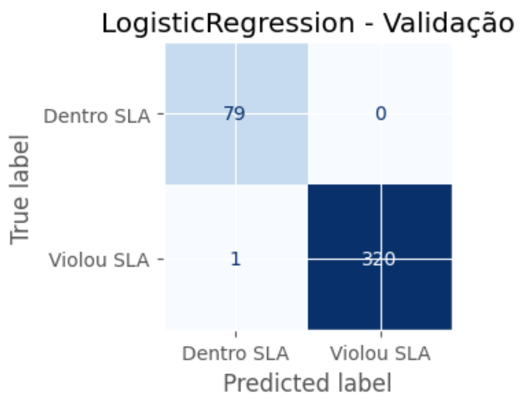
```
plt.tight_layout()
plt.show()
```

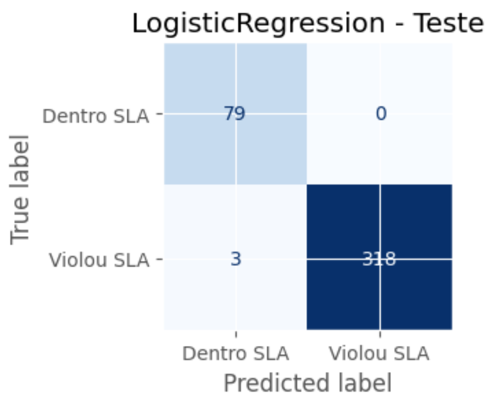

LightGBM - Validação
True label
Dentro SLA
Violou SLA
79
0
0
321
Dentro SLA
Violou SLA
Predicted label

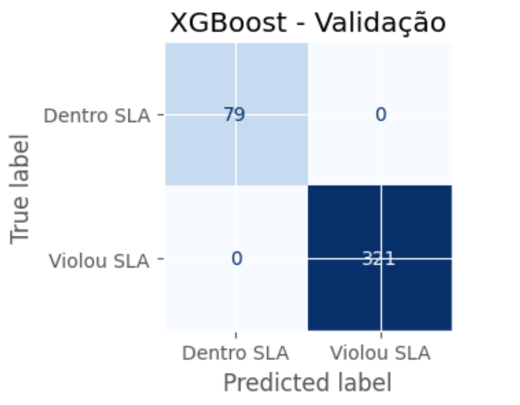

LightGBM - Teste
True label
Dentro SLA
Violou SLA
79
0
1
320
Dentro SLA
Violou SLA
Predicted label

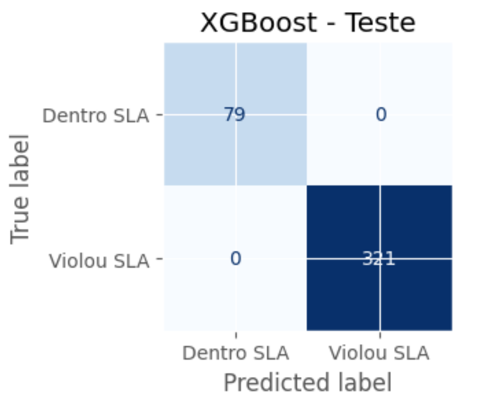

RandomForest - Validação
True label
Dentro SLA
Violou SLA
79
0
0
321
Dentro SLA
Violou SLA
Predicted label


RandomForest - Teste
True label
Dentro SLA
Violou SLA
79
0
0
321
Dentro SLA
Violou SLA
Predicted label


LogisticRegression - Validação
True label
Dentro SLA
Violou SLA
79
0
1
320
Dentro SLA
Violou SLA
Predicted label


LogisticRegression - Teste
True label
Dentro SLA
Violou SLA
79
0
3
318
Dentro SLA
Violou SLA
Predicted label


XGBoost - Validação
True label
Dentro SLA
Violou SLA
79
0
0
321
Dentro SLA
Violou SLA
Predicted label


XGBoost - Teste
True label
Dentro SLA
Violou SLA
79
0
0
321
Dentro SLA
Violou SLA
Predicted label

```
[24]: class_map = {"0": "Dentro do SLA", "1": "Violou SLA"}
report_rows = []
for res in results:
    for split_label, y_true, y_pred in [
        ("Validação", y_val, res["val_pred"]),
        ("Teste", y_test, res["test_pred"]),
    ]:
        report_dict = classification_report(
            y_true, y_pred, output_dict=True, zero_division=0
        )
        for cls in ("0", "1"):
            stats = report_dict[cls]
            report_rows.append(
                {
                    "modelo": res["model"],
                    "split": split_label,
                    "classe": class_map[cls],
                    "precisao": stats["precision"],
                    "recall": stats["recall"],
                    "f1": stats["f1-score"],
                    "suporte": int(stats["support"]),
                }
            )

per_class_reports = pd.DataFrame(report_rows)
per_class_reports
```

```
[24]:                 modelo      split         classe  precisao  recall     f1  \
0             LightGBM  Validação  Dentro do SLA    1.0000  1.0000 1.0000
1             LightGBM  Validação     Violou SLA    1.0000  1.0000 1.0000
2             LightGBM      Teste  Dentro do SLA    0.9875  1.0000 0.9937
3             LightGBM      Teste     Violou SLA    1.0000  0.9969 0.9984
4         RandomForest  Validação  Dentro do SLA    1.0000  1.0000 1.0000
5         RandomForest  Validação     Violou SLA    1.0000  1.0000 1.0000
6         RandomForest      Teste  Dentro do SLA    1.0000  1.0000 1.0000
7         RandomForest      Teste     Violou SLA    1.0000  1.0000 1.0000
8   LogisticRegression  Validação  Dentro do SLA    0.9875  1.0000 0.9937
9   LogisticRegression  Validação     Violou SLA    1.0000  0.9969 0.9984
10  LogisticRegression      Teste  Dentro do SLA    0.9634  1.0000 0.9814
11  LogisticRegression      Teste     Violou SLA    1.0000  0.9907 0.9953
12             XGBoost  Validação  Dentro do SLA    1.0000  1.0000 1.0000
13             XGBoost  Validação     Violou SLA    1.0000  1.0000 1.0000
14             XGBoost      Teste  Dentro do SLA    1.0000  1.0000 1.0000
15             XGBoost      Teste     Violou SLA    1.0000  1.0000 1.0000

    suporte
0        79
```

```
1       321
2        79
3       321
4        79
5       321
6        79
7       321
8        79
9       321
10       79
11      321
12       79
13      321
14       79
15      321
```

[25]:
```python
reports_text = {
    res["model"]: {"validacao": res["val_report"], "teste": res["test_report"]}
    for res in results
}
reports_text
```

[25]:
```
{'LightGBM': {'validacao': '              precision    recall  f1-score
support\n\n           0       1.00      1.00      1.00        79\n           1
1.00      1.00      1.00       321\n\n    accuracy
1.00       400\n   macro avg       1.00      1.00      1.00       400\nweighted
avg       1.00      1.00      1.00       400\n',
  'teste': '              precision    recall  f1-score   support\n\n
0       0.99      1.00      0.99        79\n           1       1.00      1.00
1.00       321\n\n    accuracy                           1.00       400\n
macro avg       0.99      1.00      1.00       400\nweighted avg       1.00
1.00      1.00       400\n'},
 'RandomForest': {'validacao': '              precision    recall  f1-score
support\n\n           0       1.00      1.00      1.00        79\n           1
1.00      1.00      1.00       321\n\n    accuracy
1.00       400\n   macro avg       1.00      1.00      1.00       400\nweighted
avg       1.00      1.00      1.00       400\n',
  'teste': '              precision    recall  f1-score   support\n\n
0       1.00      1.00      1.00        79\n           1       1.00      1.00
1.00       321\n\n    accuracy                           1.00       400\n
macro avg       1.00      1.00      1.00       400\nweighted avg       1.00
1.00      1.00       400\n'},
 'LogisticRegression': {'validacao': '              precision    recall
f1-score   support\n\n           0       0.99      1.00      0.99        79\n
1       1.00      1.00      1.00       321\n\n    accuracy
1.00       400\n   macro avg       0.99      1.00      1.00       400\nweighted
avg       1.00      1.00      1.00       400\n',
  'teste': '              precision    recall  f1-score   support\n\n
0       0.96      1.00      0.98        79\n           1       1.00      0.99
1.00       321\n\n    accuracy                           0.99       400\n
macro avg       0.98      1.00      0.99       400\nweighted avg       0.99
0.99      0.99       400\n'},
 'XGBoost': {'validacao': '              precision    recall  f1-score
support\n\n           0       1.00      1.00      1.00        79\n           1
1.00      1.00      1.00       321\n\n    accuracy
1.00       400\n   macro avg       1.00      1.00      1.00       400\nweighted
avg       1.00      1.00      1.00       400\n',
  'teste': '              precision    recall  f1-score   support\n\n
0       1.00      1.00      1.00        79\n           1       1.00      1.00
1.00       321\n\n    accuracy                           1.00       400\n
macro avg       1.00      1.00      1.00       400\nweighted avg       1.00
1.00      1.00       400\n'}}
```