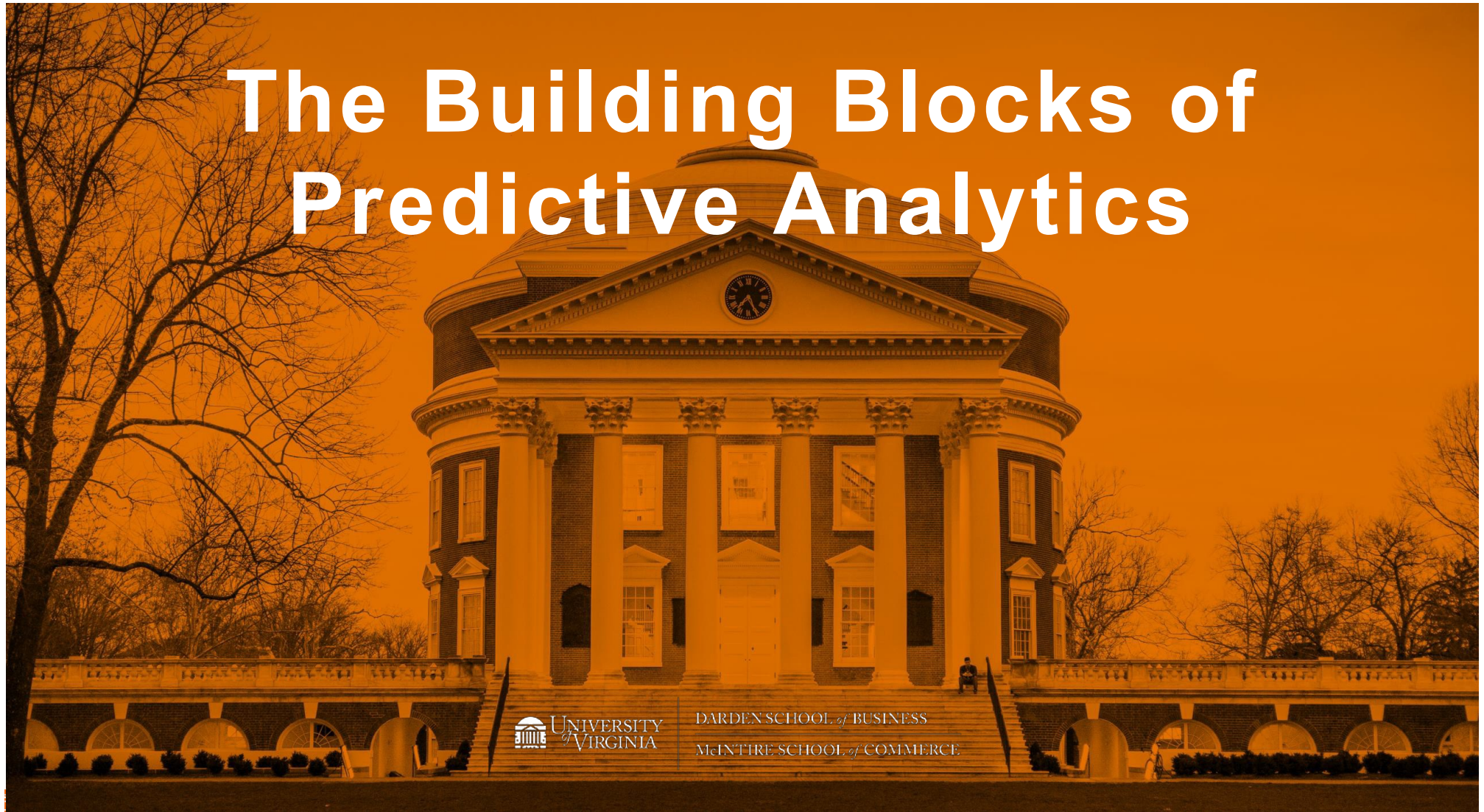


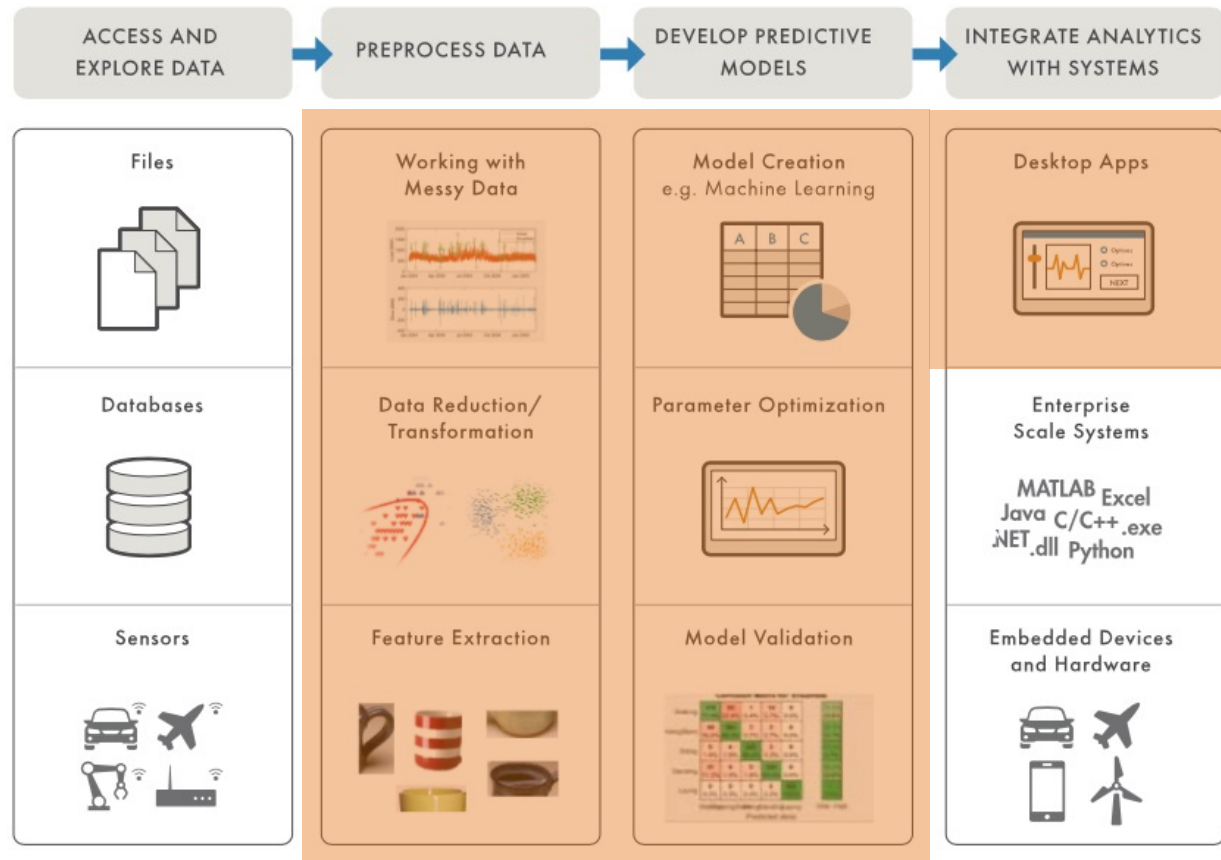
# The Building Blocks of Predictive Analytics



UNIVERSITY  
of VIRGINIA

DARDEN SCHOOL of BUSINESS  
McINTIRE SCHOOL of COMMERCE

# Predictive Analytics Workflow

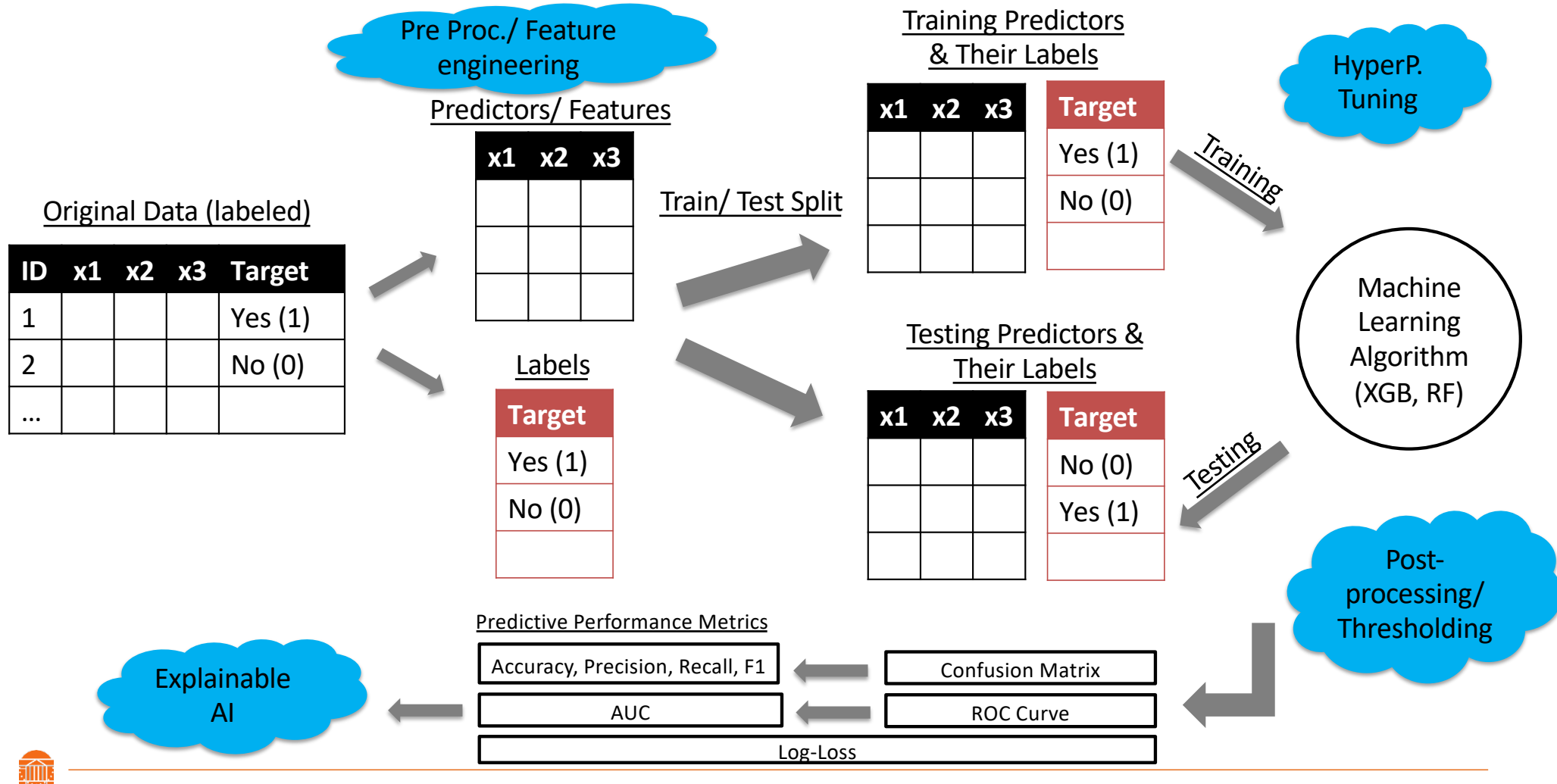


# Develop Predictive Models

## Machine learning models cheat sheet

Supervised learning	Unsupervised learning	Semi-supervised learning	Reinforcement learning
<p>Data scientists provide input, output and feedback to build model (as the definition)</p> <p><b>EXAMPLE ALGORITHMS:</b></p> <p><b>Linear regressions</b></p> <ul style="list-style-type: none"><li>■ sales forecasting</li><li>■ risk assessment</li></ul> <p><b>Support vector machines</b></p> <ul style="list-style-type: none"><li>■ image classification</li><li>■ financial performance comparison</li></ul> <p><b>Decision tree</b></p> <ul style="list-style-type: none"><li>■ predictive analytics</li><li>■ pricing</li></ul>	<p>Use deep learning to arrive at conclusions and patterns through unlabeled training data.</p> <p><b>EXAMPLE ALGORITHMS:</b></p> <p><b>Apriori</b></p> <ul style="list-style-type: none"><li>■ sales functions</li><li>■ word associations</li><li>■ searcher</li></ul> <p><b>K-means clustering</b></p> <ul style="list-style-type: none"><li>■ performance monitoring</li><li>■ searcher intent</li></ul>	<p>Builds a model through a mix of labeled and unlabeled data, a set of categories, suggestions and exemplar labels.</p> <p><b>EXAMPLE ALGORITHMS:</b></p> <p><b>Generative adversarial networks</b></p> <ul style="list-style-type: none"><li>■ audio and video manipulation</li><li>■ data creation</li></ul> <p><b>Self-trained Naïve Bayes classifier</b></p> <ul style="list-style-type: none"><li>■ natural language processing</li></ul>	<p>Self-interpreting but based on a system of rewards and punishments learned through trial and error, seeking maximum reward.</p> <p><b>EXAMPLE ALGORITHMS:</b></p> <p><b>Q-learning</b></p> <ul style="list-style-type: none"><li>■ policy creation</li><li>■ consumption reduction</li></ul> <p><b>Model-based value estimation</b></p> <ul style="list-style-type: none"><li>■ linear tasks</li><li>■ estimating parameters</li></ul>

# How to Develop a Classifier?



## EVALUATING MODELS

# PREDICTION SCORES AND CONFIDENCE

Observation	Actual Training Label/Class	Predicted Label/Class	Classification Type	Prediction Score Model A	Prediction Score Model B
1	Yes	Yes	TP	0.9	1.0
2	No	No	TN	0.2	0.1
3	Yes	Yes	TP	0.8	0.9
4	Yes	No	FN	0.1	0.4
5	Yes	Yes	TP	0.7	0.8
6	Yes	No	FN	0.3	0.4
7	No	No	TN	0.4	0.3
8	No	No	TN	0.3	0.2
9	No	No	TN	0.4	0.3
10	No	Yes	FP	0.6	0.5



## EVALUATION METRICS

# PRECISION AND RECALL

Predicted Class	Actual Class			
		Class = Yes	Class = No	Precision
	Class = Yes	3	1	$\frac{3}{4}$ 75%
	Class = No	2	4	$\frac{4}{6}$ 66.7%
Recall		$\frac{3}{5}$ 60%	$\frac{4}{5}$ 80%	





# ROC CURVE



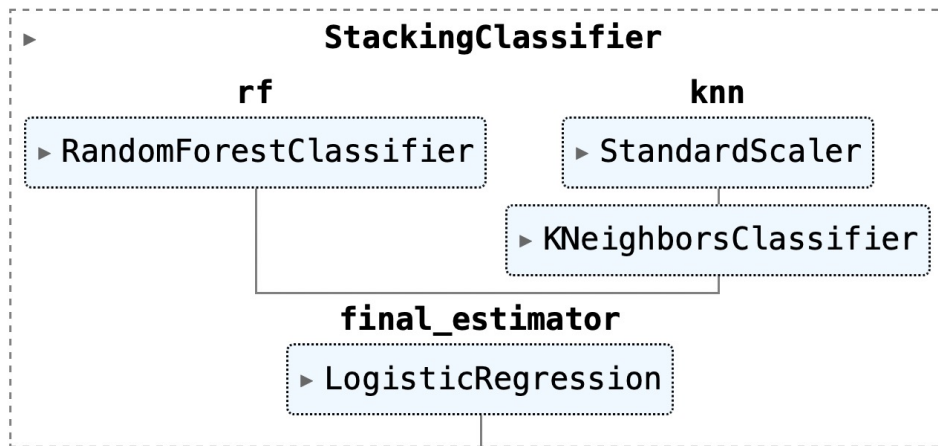
# Advanced Concepts in Classification

- 1- Stacking classifiers
- 2- Voting classifiers
- 3- Hyperparameter optimization





# Stacking Classifiers



```
%%time
estimators = [
    ('rf', RandomForestClassifier(n_estimators=50,
                                random_state=42)),
    ('knn', make_pipeline(StandardScaler(),
                           KNeighborsClassifier(n_neighbors=5)))]

clf = StackingClassifier(
    estimators = estimators,
    final_estimator = LogisticRegression(),
    n_jobs = -1, verbose=True
)

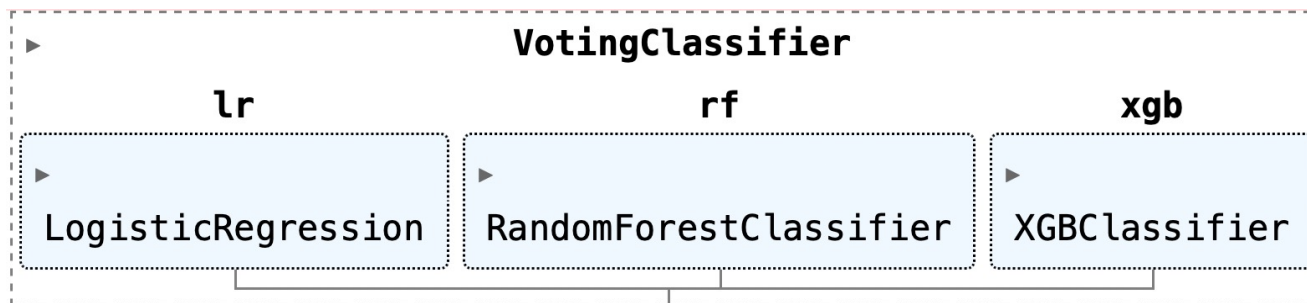
clf.fit(trainData, trainLabels)
```

# Voting Classifiers

```
clf1 = LogisticRegression(random_state=1)
clf2 = RandomForestClassifier(n_estimators=50, random_state=1)
clf3 = XGBClassifier(random_state=1)

vclf = VotingClassifier(estimators=[
    ('lr', clf1), ('rf', clf2), ('xgb', clf3)],
    voting='soft')

vclf.fit(trainData, trainLabels)
```



# Hyperparameter Optimization

```
!pip install hyperopt
```

...

```
# import packages for hyperparameters tuning  
from hyperopt import import STATUS_OK, Trials, fmin, hp, tpe
```

```
space={ 'max_depth': hp.quniform("max_depth", 3, 18, 1),  
        'gamma': hp.uniform ('gamma', 1,9),  
        'reg_alpha' : hp.quniform('reg_alpha', 40,180,1),  
        'reg_lambda' : hp.uniform('reg_lambda', 0,1),  
        'colsample_bytree' : hp.uniform('colsample_bytree', 0.5,1),  
        'min_child_weight' : hp.quniform('min_child_weight', 0, 10, 1),  
        'n_estimators': hp.quniform('n_estimators', 100, 200, 20),  
        'eta': hp.uniform('eta', 0.1,0.9),  
        'seed': 0,  
        'random_state': 1  
}
```



# Hyperparameter Optimization- “hyperopt” Package

Step 1: Define a space for the hyperparameters.

Step 2: Create the objective function.

Step 3: Run trials.

Step 4: Export and use the best hyperparameter values in a new model.



# Hyperopt

Step 1: Define a space for the hyperparameters.

```
space={ 'max_depth': hp.quniform("max_depth", 3, 18, 1),
        'gamma': hp.uniform('gamma', 1,9),
        'reg_alpha' : hp.quniform('reg_alpha', 40,180,1),
        'reg_lambda' : hp.uniform('reg_lambda', 0,1),
        'colsample_bytree' : hp.uniform('colsample_bytree', 0.5,1),
        'min_child_weight' : hp.quniform('min_child_weight', 0, 10, 1),
        'n_estimators': hp.quniform('n_estimators', 100, 200, 20),
        'eta': hp.uniform('eta', 0.1,0.9),
        'seed': 0,
        'random_state': 1
    }
```

# Hyperopt

Step 2: Create the objective function.

```
def objective(space):
    clf=XGBClassifier(
        random_state = space['random_state'],
        eta = space['eta'],
        n_estimators = int(space['n_estimators']),
        max_depth = int(space['max_depth']),
        gamma = space['gamma'],
        reg_alpha = int(space['reg_alpha']),
        min_child_weight=int(space['min_child_weight']),
        colsample_bytree=int(space['colsample_bytree']))

    evaluation = [( trainData, trainLabels), ( testData, testLabels)]

    clf.fit(trainData, trainLabels,
            eval_set=evaluation, eval_metric="auc",
            early_stopping_rounds=10,verbose=False)

    pred = clf.predict(testData)
    accuracy = roc_auc_score(testLabels, pred>0.5)
    print ("SCORE:", accuracy)
    return {'loss': -accuracy, 'status': STATUS_OK }
```



# Hyperopt

## Step 3: Run trials.

```
trials = Trials()

best_hyperparams = fmin(fn = objective,
                        space = space,
                        algo = tpe.suggest,
                        max_evals = 100,
                        trials = trials)
```

## Step 4: Export values and build a new model.

```
best_hyperparams = {
    'colsample_bytree': 0.8182902035285777,
    'eta': 0.7974676615890914,
    'gamma': 7.870558816361137,
    'max_depth': 13, # Should be int
    'min_child_weight': 4, # Should be int
    'n_estimators': 180, # Should be int
    'reg_alpha': 48.0,
    'reg_lambda': 0.8050195284705558}
```

```
best_xgb = XGBClassifier(**best_hyperparams, random_state=1)
best_xgb.fit(trainData, trainLabels)
```

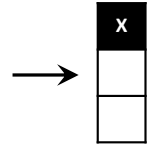




# Supervised Learning Cheat Sheet



ID	X	Y



Y

Process	Method	Code
Feat. Select	<a href="#">Boruta</a>	BorutaPy(...)
	<a href="#">sklearn.feature_selection</a>	RFE(...)
Imputation	<a href="#">sklearn.impute</a>	IterativeImputer(...)
Cat. Vars./ Scale Vars.	<a href="#">category_encoders</a>	BaseNEncoder(...)
	<a href="#">sklearn.preprocessing</a>	OneHotEncoder(...) StandardScaler(...)
All Feat. Eng.	<a href="#">feature-engine</a>	MeanMedianImputer(...) OutlierTrimmer(...) MathematicalCombination(...) DropCorrelatedFeatures(...) DecisionTreeDiscretiser(...)

Process	Method	Code
Encoding	<a href="#">sklearn.preprocessing</a>	LabelEncoder(...)

Process	Method	Code
Split	<a href="#">sklearn.model_selection</a>	train_test_split(...)

trainData/ Labels

X	Y

Process	Method	Code
Select Algo.	<a href="#">mljar-supervised</a>	AutoML(...)
	<a href="#">pycaret</a>	compare_models(...)

Process	Method	Code
Hyper Param. Tuning	<a href="#">hyperopt</a>	fmin(...)
	<a href="#">sklearn.model_selection</a>	GridSearchCV(...)
		RandomizedSearchCV(...)

Process	Method	Code
Final Tuned Algo.	<a href="#">xgboost</a>	XGBClassifier(...)
	<a href="#">catboost</a>	CatBoostClassifier(...)
	<a href="#">lightgbm</a>	LGBMClassifier(...)

testData/ Labels

X	Y



Process	Method	Code
Model Eval.	<a href="#">sklearn.metrics</a>	roc_auc_score() log_loss() confusion_matrix()
Interpret/ Explain	<a href="#">statsmodels</a>	sm.Logit(y, X).fit()
	<a href="#">shap</a>	shap.summary_plot(...) shap.plots.scatter(...) shap.force_plot(...) shap.plots.waterfall(...)
	<a href="#">lime</a>	explainer.explain_instance(...)
	<a href="#">imodels</a>	HSTreeClassifierCV(...)
	<a href="#">explainerdashboard</a>	ClassifierExplainer(clf, testData, testLabels)



# PhishCasting Competition (Leaderboard & Lessons Learned)

- 1- What algorithm did you use?
- 2- Did you do any feature engineering?
- 3- Explain your hyperparameter tuning approach.
- 4- Did you balance (resample) the training data?
- 5- Any best practices you would like to share?



