# Amazon SageMaker Autopilot Candidate Definition Notebook

This notebook was automatically generated by the AutoML job **automl-fraudcase-03-00-14-16**. This notebook allows you to customize the candidate definitions and execute the SageMaker Autopilot workflow.

The dataset has **29** columns and the column named **Class** is used as the target column. This is being treated as a **BinaryClassification** problem. The dataset also has **2** classes. This notebook will build a **BinaryClassification** (https://en.wikipedia.org/wiki/Binary\_classification) model that **maximizes** the "F1" quality metric of the trained models. The "F1" metric applies for binary classification with a positive and negative class. It mixes between precision and recall, and is recommended in cases where there are more negative examples compared to positive examples.

As part of the AutoML job, the input dataset has been randomly split into two pieces, one for **training** and one for **validation**. This notebook helps you inspect and modify the data transformation approaches proposed by Amazon SageMaker Autopilot. You can interactively train the data transformation models and use them to transform the data. Finally, you can execute a multiple algorithm hyperparameter optimization (multi-algo HPO) job that helps you find the best model for your dataset by jointly optimizing the data transformations and machine learning algorithms.

Available Knobs Look for sections like this for recommended settings that you can change.

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# Sagemaker Setup

Before you launch the SageMaker Autopilot jobs, we'll setup the environment for Amazon SageMaker

- Check environment & dependencies.
- Create a few helper objects/function to organize input/output data and SageMaker sessions.

#### **Minimal Environment Requirements**

- Jupyter: Tested on JupyterLab 1.0.6, jupyter\_core 4.5.0 and IPython 6.4.0
- Kernel: conda python3
- · Dependencies required
  - sagemaker-python-sdk>=2.40.0
    - Use !pip install sagemaker==2.40.0 to download this dependency.
    - Kernel may need to be restarted after download.
- Expected Execution Role/permission
  - S3 access to the bucket that stores the notebook.

## **Downloading Generated Modules**

Download the generated data transformation modules and an SageMaker Autopilot helper module used by this notebook. Those artifacts will be downloaded to **automI-fraudcase-03-00-14-16-artifacts** folder.

```
In []: M !mkdir -p automl-fraudcase-03-00-14-16-artifacts
!aws s3 sync s3://sagemaker-us-east-1-629589781736/cc_fraud/output/automl-fra
!aws s3 sync s3://sagemaker-us-east-1-629589781736/cc_fraud/output/automl-fra
import sys
sys.path.append("automl-fraudcase-03-00-14-16-artifacts")
```

# SageMaker Autopilot Job and Amazon Simple Storage Service (Amazon S3) Configuration

The following configuration has been derived from the SageMaker Autopilot job. These items configure where this notebook will look for generated candidates, and where input and output data is stored on Amazon S3.

```
In [ ]:
         ▶ | from sagemaker automl import uid, AutoMLLocalRunConfig
            # Where the preprocessed data from the existing AutoML job is stored
            BASE AUTOML JOB NAME = 'automl-fraudcase-03-00-14-16'
            BASE AUTOML JOB CONFIG = {
                'automl_job_name': BASE_AUTOML_JOB_NAME,
                'automl_output_s3_base_path': 's3://sagemaker-us-east-1-629589781736/cc_f
                'data transformer image repo version': '2.5-1-cpu-py3',
                'algo_image_repo_versions': {'xgboost': '1.3-1-cpu-py3', 'linear-learner'
                'algo_inference_image_repo_versions': {'xgboost': '1.3-1-cpu-py3', 'linea
            }
            # Path conventions of the output data storage path from the local AutoML job
            LOCAL AUTOML JOB NAME = 'automl-fra-notebook-run-{}'.format(uid())
            LOCAL AUTOML JOB CONFIG = {
                'local_automl_job_name': LOCAL_AUTOML_JOB_NAME,
                'local_automl_job_output_s3_base_path': 's3://sagemaker-us-east-1-6295897
                'data_processing_model_dir': 'data-processor-models',
                'data_processing_transformed_output_dir': 'transformed-data',
                'multi algo tuning output dir': 'multi-algo-tuning'
            }
            AUTOML LOCAL RUN CONFIG = AutoMLLocalRunConfig(
                role='arn:aws:iam::629589781736:role/service-role/AmazonSageMaker-Executi
                base automl job config=BASE AUTOML JOB CONFIG,
                local automl job config=LOCAL AUTOML JOB CONFIG,
                security config={'EnableInterContainerTrafficEncryption': False, 'VpcConf
            AUTOML LOCAL RUN CONFIG.display()
```

# **Candidate Pipelines**

The AutoMLLocalRunner keeps track of selected candidates and automates many of the steps needed to execute feature engineering and tuning steps.

#### **Generated Candidates**

The SageMaker Autopilot Job has analyzed the dataset and has generated **4** machine learning pipeline(s) that use **3** algorithm(s). Each pipeline contains a set of feature transformers and an algorithm.

# **Available Knobs**

- 1. The resource configuration: instance type & count
- 2. Select candidate pipeline definitions by cells

3. The linked data transformation script can be reviewed and updated. Please refer to the README.md (./automl-fraudcase-03-00-14-16-artifacts/generated\_module/README.md) for detailed customization instructions.

#### dpp0-xgboost (automl-fraudcase-03-00-14-16-

<u>artifacts/generated\_module/candidate\_data\_processors/dpp0.py)</u>: This data transformation strategy first transforms 'numeric' features using <u>RobustImputer (converts missing values to nan)</u> (<a href="https://github.com/aws/sagemaker-scikit-learn-">https://github.com/aws/sagemaker-scikit-learn-</a>

<u>extension/blob/master/src/sagemaker\_sklearn\_extension/impute/base.py)</u>. It merges all the generated features and applies <u>RobustStandardScaler (https://github.com/aws/sagemaker-scikit-learn-extension/blob/master/src/sagemaker\_sklearn\_extension/preprocessing/data.py)</u>. The transformed data will be used to tune a *xgboost* model. Here is the definition:

```
In [ ]:
            automl_interactive_runner.select_candidate({
                 "data_transformer": {
                     "name": "dpp0",
                     "training resource config": {
                         "instance type": "ml.m5.4xlarge",
                         "instance count": 1,
                         "volume size in gb":
                     "transform_resource_config": {
                         "instance type": "ml.m5.4xlarge",
                         "instance_count": 1,
                     },
                     "transforms label": True,
                     "transformed_data_format": "text/csv",
                     "sparse encoding": False
                },
                 "algorithm": {
                     "name": "xgboost",
                     "training resource config": {
                         "instance_type": "ml.m5.4xlarge",
                         "instance count": 1,
                    },
                }
            })
```

#### dpp1-xgboost (automl-fraudcase-03-00-14-16-

<u>artifacts/generated\_module/candidate\_data\_processors/dpp1.py)</u>: This data transformation strategy first transforms 'numeric' features using <u>RobustImputer</u>

(https://github.com/aws/sagemaker-scikit-learn-

extension/blob/master/src/sagemaker\_sklearn\_extension/impute/base.py). It merges all the generated features and applies RobustPCA (https://github.com/aws/sagemaker-scikit-learn-extension/blob/master/src/sagemaker\_sklearn\_extension/decomposition/robust\_pca.py) followed by RobustStandardScaler (https://github.com/aws/sagemaker-scikit-learn-extension/blob/master/src/sagemaker\_sklearn\_extension/preprocessing/data.py). The transformed data will be used to tune a xgboost model. Here is the definition:

```
In [ ]:
         ▶ automl interactive runner.select candidate({
                "data transformer": {
                    "name": "dpp1",
                    "training resource config": {
                        "instance type": "ml.m5.4xlarge",
                        "instance count": 1,
                        "volume size in gb":
                    },
                    "transform resource config": {
                        "instance type": "ml.m5.4xlarge",
                        "instance count": 1,
                    "transforms label": True,
                    "transformed data format": "text/csv",
                    "sparse encoding": False
               "name": "xgboost",
                    "training_resource_config": {
                        "instance type": "ml.m5.4xlarge",
                        "instance count": 1,
                    },
                }
            })
```

dpp2-linear-learner (automl-fraudcase-03-00-14-16-artifacts/generated\_module/candidate\_data\_processors/dpp2.py): This data transformation strategy first transforms 'numeric' features using combined RobustImputer and RobustImsingIndicator (https://github.com/aws/sagemaker-scikit-learn-extension/blob/master/src/sagemaker\_sklearn\_extension/impute/base.py) followed by QuantileExtremeValuesTransformer (https://github.com/aws/sagemaker-scikit-learn-extension/blob/master/src/sagemaker\_sklearn\_extension/preprocessing/base.py). It merges all the generated features and applies RobustPCA (https://github.com/aws/sagemaker-scikit-learn-extension/blob/master/src/sagemaker\_sklearn\_extension/decomposition/robust\_pca.py) followed by RobustStandardScaler (https://github.com/aws/sagemaker-scikit-learn-extension/blob/master/src/sagemaker\_sklearn\_extension/preprocessing/data.py). The transformed data will be used to tune a linear-learner model. Here is the definition:

```
In [ ]:
         ▶ automl interactive runner.select candidate({
                "data transformer": {
                    "name": "dpp2",
                    "training resource config": {
                        "instance type": "ml.m5.4xlarge",
                        "instance_count": 1,
                        "volume size in gb":
                    },
                    "transform resource config": {
                        "instance_type": "ml.m5.4xlarge",
                        "instance_count": 1,
                    "transforms label": True,
                    "transformed_data_format": "application/x-recordio-protobuf",
                    "sparse encoding": False
               "name": "linear-learner",
                    "training_resource_config": {
                        "instance type": "ml.m5.4xlarge",
                        "instance count": 1,
                    },
                }
            })
```

#### dpp3-mlp (automl-fraudcase-03-00-14-16-

<u>artifacts/generated\_module/candidate\_data\_processors/dpp3.py)</u>: This data transformation strategy transforms 'numeric' features using <u>RobustImputer (https://github.com/aws/sagemaker\_scikit-learn-extension/blob/master/src/sagemaker\_sklearn\_extension/impute/base.py)</u> followed by <u>RobustStandardScaler (https://github.com/aws/sagemaker-scikit-learn-extension/blob/master/src/sagemaker\_sklearn\_extension/preprocessing/data.py)</u>. The transformed data will be used to tune a *mlp* model. Here is the definition:

```
In [ ]:
         ▶ automl interactive runner.select candidate({
                "data transformer": {
                    "name": "dpp3",
                    "training resource config": {
                        "instance type": "ml.m5.4xlarge",
                        "instance_count": 1,
                        "volume size in gb":
                    },
                    "transform resource config": {
                        "instance_type": "ml.m5.4xlarge",
                        "instance count": 1,
                    "transforms_label": True,
                    "transformed_data_format": "text/csv",
                    "sparse encoding": False
                "name": "mlp",
                    "training_resource_config": {
                        "instance_type": "ml.m5.4xlarge",
                        "instance count": 1,
                    "candidate specific static hyperparameters": {
                        "num categorical features": '0',
                    }
                }
            })
```

#### **Selected Candidates**

You have selected the following candidates (please run the cell below and click on the feature transformer links for details):

The feature engineering pipeline consists of two SageMaker jobs:

- Generated trainable data transformer Python modules like <u>dpp0.py</u> (<u>automl-fraudcase-03-00-14-16-artifacts/generated\_module/candidate\_data\_processors/dpp0.py</u>), which has been downloaded to the local file system
- 2. A training job to train the data transformers
- 3. A **batch transform** job to apply the trained transformation to the dataset to generate the algorithm compatible data

The transformers and its training pipeline are built using open sourced <u>sagemaker-scikit-learn-container</u> (https://github.com/aws/sagemaker-scikit-learn-container) and <u>sagemaker-scikit-learn-extension</u> (https://github.com/aws/sagemaker-scikit-learn-extension).

# **Executing the Candidate Pipelines**

Each candidate pipeline consists of two steps, feature transformation and algorithm training. For efficiency first execute the feature transformation step which will generate a featurized dataset on S3 for each pipeline.

After each featurized dataset is prepared, execute a multi-algorithm tuning job that will run tuning jobs in parallel for each pipeline. This tuning job will execute training jobs to find the best set of hyper-parameters for each pipeline, as well as finding the overall best performing pipeline.

#### **Run Data Transformation Steps**

Now you are ready to start execution all data transformation steps. The cell below may take some time to finish, feel free to go grab a cup of coffee. To expedite the process you can set the number of parallel\_jobs to be up to 10. Please check the account limits to increase the limits before increasing the number of jobs to run in parallel.

In [ ]: | automl\_interactive\_runner.fit\_data\_transformers(parallel\_jobs=2)

### **Multi Algorithm Hyperparameter Tuning**

Now that the algorithm compatible transformed datasets are ready, you can start the multialgorithm model tuning job to find the best predictive model. The following algorithm training job configuration for each algorithm is auto-generated by the AutoML Job as part of the recommendation.



- 1. Hyperparameter ranges
- 2. Objective metrics
- 3. Recommended static algorithm hyperparameters.

Please refers to <u>Xgboost tuning (https://docs.aws.amazon.com/sagemaker/latest/dg/xgboost-tuning.html)</u> and <u>Linear learner tuning</u> (https://docs.aws.amazon.com/sagemaker/latest/dg/linear-learner-tuning.html) for detailed

explanations of the parameters.

The AutoML recommendation job has recommended the following hyperparameters, objectives and accuracy metrics for the algorithm and problem type:

```
In [ ]:
         ► ALGORITHM OBJECTIVE METRICS = {
                 'xgboost': 'validation:f1_binary',
                'linear-learner': 'validation:binary f beta',
                 'mlp': 'validation:binary f beta',
            }
            STATIC HYPERPARAMETERS = {
                 'xgboost': {
                     'objective': 'binary:logistic',
                     'eval_metric': 'accuracy,f1_binary,auc',
                     'scale pos weight': 577.2893401015228,
                     'save_model_on_termination': 'true',
                },
                 'linear-learner': {
                     'predictor type': 'binary classifier',
                     'ml_application': 'linear_learner',
                     'loss function': 'SoftmaxCrossEntropyLoss',
                    'reporting_metrics': 'binary_classification_accuracy,binary_f_beta,ro
                     'positive_example_weight_mult': 577.2893401015228,
                     'eval metric': 'binary f beta',
                },
                 'mlp': {
                     'problem type': 'binary classification',
                     'positive_example_weight_mult': 577.2893401015228,
                     'ml application': 'mlp',
                     'use_batchnorm': 'true',
                     'activation': 'relu',
                     'warmup_epochs': 10,
                     'reporting_metrics': 'accuracy,binary_f_1,roc_auc',
                     'eval_metric': 'binary_f_1',
                },
            }
```

The following tunable hyperparameters search ranges are recommended for the Multi-Algo tuning job:

```
In [ ]:
         | from sagemaker.parameter import CategoricalParameter, ContinuousParameter, Ir
            ALGORITHM TUNABLE HYPERPARAMETER RANGES = {
                'xgboost': {
                    'num round': IntegerParameter(64, 1024, scaling type='Logarithmic'),
                    'max_depth': IntegerParameter(2, 8, scaling_type='Logarithmic'),
                    'eta': ContinuousParameter(1e-3, 1.0, scaling type='Logarithmic'),
                    'gamma': ContinuousParameter(1e-6, 64.0, scaling type='Logarithmic'),
                    'min child weight': ContinuousParameter(1e-6, 32.0, scaling type='Log
                    'subsample': ContinuousParameter(0.5, 1.0, scaling_type='Linear'),
                    'colsample bytree': ContinuousParameter(0.3, 1.0, scaling type='Linea
                    'lambda': ContinuousParameter(1e-6, 2.0, scaling_type='Logarithmic'),
                    'alpha': ContinuousParameter(1e-6, 2.0, scaling_type='Logarithmic'),
                },
                 'linear-learner': {
                    'mini_batch_size': IntegerParameter(128, 512, scaling_type='Linear'),
                    'wd': ContinuousParameter(1e-12, 1e-2, scaling type='Logarithmic'),
                    'learning_rate': ContinuousParameter(1e-6, 1e-2, scaling_type='Logari
                },
                'mlp': {
                    'mini batch size': IntegerParameter(128, 512, scaling type='Linear'),
                    'learning_rate': ContinuousParameter(1e-6, 1e-2, scaling_type='Logari
                    'weight decay': ContinuousParameter(1e-12, 1e-2, scaling type='Logari
                    'dropout_prob': ContinuousParameter(0.25, 0.5, scaling_type='Linear')
                    'embedding size factor': ContinuousParameter(0.65, 0.95, scaling type
                    'network_type': CategoricalParameter(['feedforward', 'widedeep']),
                    'layers': CategoricalParameter(['256', '50, 25', '100, 50', '200, 100
                },
            }
```

#### **Prepare Multi-Algorithm Tuner Input**

To use the multi-algorithm HPO tuner, prepare some inputs and parameters. Prepare a dictionary whose key is the name of the trained pipeline candidates and the values are respectively:

- 1. Estimators for the recommended algorithm
- 2. Hyperparameters search ranges
- 3. Objective metrics

Below you prepare the inputs data to the multi-algo tuner:

#### **Create Multi-Algorithm Tuner**

With the recommended Hyperparameter ranges and the transformed dataset, create a multialgorithm model tuning job that coordinates hyper parameter optimizations across the different possible algorithms and feature processing strategies.

#### **Available Knobs**

- Tuner strategy: <u>Bayesian</u> (<a href="https://en.wikipedia.org/wiki/Hyperparameter\_optimization#Bayesian\_optimization">https://en.wikipedia.org/wiki/Hyperparameter\_optimization#Bayesian\_optimization</a>), Random Search
  - (https://en.wikipedia.org/wiki/Hyperparameter optimization#Random search)
- 2. Objective type: Minimize, Maximize, see optimization (https://en.wikipedia.org/wiki/Mathematical\_optimization)
- 3. Max Job size: the max number of training jobs HPO would be launching to run experiments. Note the default value is **250** which is the default of the managed flow.
- 4. Parallelism. Number of jobs that will be executed in parallel. Higher value will expedite the tuning process. Please check the account limits to increase the limits before increasing the number of jobs to run in parallel
- 5. Please use a different tuning job name if you re-run this cell after applied customizations.

#### **Run Multi-Algorithm Tuning**

Now you are ready to start running the **Multi-Algo Tuning** job. After the job is finished, store the tuning job name which you use to select models in the next section. The tuning process will take some time, please track the progress in the Amazon SageMaker Hyperparameter tuning jobs console.

```
In []: M from IPython.display import display, Markdown

# Run tuning
tuner.fit(inputs=multi_algo_tuning_inputs, include_cls_metadata=None)
tuning_job_name = tuner.latest_tuning_job.name

display(
    Markdown(f"Tuning Job {tuning_job_name} started, please track the progres

# Wait for tuning job to finish
tuner.wait()
```

# **Model Selection and Deployment**

This section guides you through the model selection process. Afterward, you construct an inference pipeline on Amazon SageMaker to host the best candidate.

Because you executed the feature transformation and algorithm training in two separate steps, you now need to manually link each trained model with the feature transformer that it is associated with. When running a regular Amazon SageMaker Autopilot job, this will automatically be done for you.

#### **Tuning Job Result Overview**

The performance of each candidate pipeline can be viewed as a Pandas dataframe. For more interactive usage please refers to <a href="mailto:model-tuning-monitor">model tuning monitor</a> (<a href="https://docs.aws.amazon.com/sagemaker/latest/dg/automatic-model-tuning-monitor.html">https://docs.aws.amazon.com/sagemaker/latest/dg/automatic-model-tuning-monitor.html</a>).

The best training job can be selected as below:

**▽ Tips:** You could select alternative job by using the value from `TrainingJobName` column above and assign to `best\_training\_job` below

#### **Linking Best Training Job with Feature Pipelines**

Finally, deploy the best training job to Amazon SageMaker along with its companion feature engineering models. At the end of the section, you get an endpoint that's ready to serve online inference or start batch transform jobs!

Deploy a <u>PipelineModel (https://sagemaker.readthedocs.io/en/stable/pipeline.html)</u> that has multiple containers of the following:

- Data Transformation Container: a container built from the model we selected and trained during the data transformer sections
- 2. Algorithm Container: a container built from the trained model we selected above from the best HPO training job.
- 3. Inverse Label Transformer Container: a container that converts numerical intermediate prediction value back to non-numerical label value.

Get both best data transformation model and algorithm model from best training job and create an pipeline model:

```
In [ ]:
         ▶ from sagemaker.estimator import Estimator
            from sagemaker import PipelineModel
            from sagemaker automl import select inference output
            # Get a data transformation model from chosen candidate
            best_candidate = automl_interactive_runner.choose_candidate(df_tuning_job_and
            best data transformer model = best candidate.get data transformer model(role=
            # Our first data transformation container will always return recordio-protobu
            best_data_transformer_model.env["SAGEMAKER_DEFAULT_INVOCATIONS_ACCEPT"] = 'ap
            # Add environment variable for sparse encoding
            if best_candidate.data_transformer_step.sparse_encoding:
                best_data_transformer_model.env["AUTOML_SPARSE_ENCODE_RECORDIO_PROTOBUF"]
            # Get a algo model from chosen training job of the candidate
            algo_estimator = Estimator.attach(best_training_job)
            best algo model = algo estimator.create model(**best candidate.algo step.get
            # Final pipeline model is composed of data transformation models and algo mod
            # inverse label transform model if we need to transform the intermediates bac
            model containers = [best data transformer model, best algo model]
            if best candidate.transforms label:
                model containers.append(best candidate.get data transformer model(
                    transform mode="inverse-label-transform",
                    role=SAGEMAKER ROLE,
                    sagemaker session=SAGEMAKER SESSION))
            # This model can emit response ['predicted label', 'probability', 'labels',
            # of the response content, pass the keys to `output key` keyword argument in
            model containers = select inference output("BinaryClassification", model cont
            pipeline model = PipelineModel(
                name="AutoML-{}".format(AUTOML_LOCAL_RUN_CONFIG.local_automl_job_name),
                role=SAGEMAKER ROLE,
                models=model containers,
                vpc config=AUTOML LOCAL RUN CONFIG.vpc config)
```

# **Deploying Best Pipeline**

# **Available Knobs**

- 1. You can customize the initial instance count and instance type used to deploy this model.
- 2. Endpoint name can be changed to avoid conflict with existing endpoints.

Finally, deploy the model to SageMaker to make it functional.

Congratulations! Now you could visit the sagemaker <u>endpoint console page (https://us-east-1.console.aws.amazon.com/sagemaker/home?region=us-east-1#/endpoints)</u> to find the deployed endpoint (it'll take a few minutes to be in service).

#### To rerun this notebook, delete or change the name of your endpoint!

If you rerun this notebook, you'll run into an error on the last step because the endpoint already exists. You can either delete the endpoint from the endpoint console page or you can change the endpoint name in the previous code block.