

```
In [ ]: # Uncomment if necessary
```

```
In [1]: #!pip install -f http://h2o-release.s3.amazonaws.com/h2o/latest_stable_Py.html h2o
```

```
In [ ]: #!pip install altair
```

```
In [2]: import h2o
        from h2o.estimators import (
            H2OGeneralizedLinearEstimator,
            H2ORandomForestEstimator,
            H2OGradientBoostingEstimator,
            H2ONaiveBayesEstimator,
            H2OStackedEnsembleEstimator,
            H2ODeepLearningEstimator
        )
        from h2o.frame import H2OFrame
        from sklearn.model_selection import train_test_split
        from sklearn.feature_extraction.text import TfidfVectorizer

        h2o.init()
```

Checking whether there is an H2O instance running at http://localhost:54321..... not found.

Attempting to start a local H2O server...

; OpenJDK 64-Bit Server VM JBR-11.0.13.7-1751.21-jcef (build 11.0.13+7-b1751.21, mixed mode)

Starting server from D:\Archivos de programa\Anaconda3\envs\Master_1\Lib\site-packages\h2o\backend\bin\h2o.jar

Ice root: C:\Users\david\AppData\Local\Temp\tmp73tmtmmz

JVM stdout: C:\Users\david\AppData\Local\Temp\tmp73tmtmmz\h2o_david_started_from_python.out

JVM stderr: C:\Users\david\AppData\Local\Temp\tmp73tmtmmz\h2o_david_started_from_python.err

Server is running at http://127.0.0.1:54321

Connecting to H2O server at http://127.0.0.1:54321 ... successful.

H2O_cluster_uptime:	04 secs
H2O_cluster_timezone:	Europe/Paris
H2O_data_parsing_timezone:	UTC
H2O_cluster_version:	3.46.0.6
H2O_cluster_version_age:	2 months and 4 days
H2O_cluster_name:	H2O_from_python_david_9k1xw8
H2O_cluster_total_nodes:	1
H2O_cluster_free_memory:	3.979 Gb
H2O_cluster_total_cores:	8
H2O_cluster_allowed_cores:	8
H2O_cluster_status:	locked, healthy
H2O_connection_url:	http://127.0.0.1:54321
H2O_connection_proxy:	{"http": null, "https": null}
H2O_internal_security:	False
Python_version:	3.10.13 final

GLOBAL PRESETS

```
In [696... import warnings
warnings.filterwarnings('ignore')

TEST_SIZE = 0.2
```

Throughout the project we reference many times the paper: **Practical considerations for specifying a super learner** <https://arxiv.org/pdf/2204.06139>

DATA LOADING AND PREPROCESSING

```
In [4]: from sklearn.datasets import fetch_openml
from sklearn.model_selection import train_test_split
import pandas as pd
```

```
In [865... spam_data = fetch_openml(data_id=44, as_frame=True)
spam_df = spam_data.frame

X = spam_df.iloc[:, :-1] # All columns except the last are features
y = spam_df.iloc[:, -1]  # The last column is the target (spam or not)
```

```
y = y.astype(int)

# Split the dataset into training (80%) and testing (20%)
X_temp, X_test, y_temp, y_test = train_test_split(X, y, test_size=0.2, random_state=42)

# We split the temporary dataset into training (80%) and validation (20% of temp, i.e. 16%)
X_train, X_val, y_train, y_val = train_test_split(X_temp, y_temp, test_size=0.2, random_state=42)

# Convert to H2O Frames
h2o_train = H2OFrame(pd.DataFrame(X_train).assign(label=y_train.values))
h2o_val = H2OFrame(pd.DataFrame(X_val).assign(label=y_val.values))
h2o_test = H2OFrame(pd.DataFrame(X_test).assign(label=y_test.values))

# Convert target columns to categorical
h2o_train['label'] = h2o_train['label'].asfactor()
h2o_val['label'] = h2o_val['label'].asfactor()
h2o_test['label'] = h2o_test['label'].asfactor()

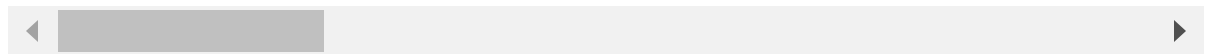
# Verify the splits
print("Training set size:", h2o_train.nrows)
print("Validation set size:", h2o_val.nrows)
print("Testing set size:", h2o_test.nrows)

# Example of dataset
X.head()
```

Out[388...

	word_freq_make	word_freq_address	word_freq_all	word_freq_3d	word_freq_our	w
count	4601.000000	4601.000000	4601.000000	4601.000000	4601.000000	
mean	0.104553	0.213015	0.280656	0.065425	0.312223	
std	0.305358	1.290575	0.504143	1.395151	0.672513	
min	0.000000	0.000000	0.000000	0.000000	0.000000	
25%	0.000000	0.000000	0.000000	0.000000	0.000000	
50%	0.000000	0.000000	0.000000	0.000000	0.000000	
75%	0.000000	0.000000	0.420000	0.000000	0.380000	
max	4.540000	14.280000	5.100000	42.810000	10.000000	

8 rows × 57 columns



Is SPAM class underrepresented?

In [649...

```
class_1 = len(spam_df[spam_df['class'] == '1'])
class_0 = len(spam_df[spam_df['class'] == '0'])
print(f"Records containing spam: {class_1}")
print(f"Records not containing spam: {class_0}")
```

Records containing spam: 1813

Records not containing spam: 2788

Computing the effective sample size n_{eff} (from paper)

We have binary data, the prevalence of Y is $p = \text{class_1} / \text{total_size}$, subsequently $n_{\text{rare}} = n * \min(p, 1-p)$, and finally $n_{\text{eff}} = \min(n, 5 * n_{\text{rare}})$

In [668...

```
n = len(spam_df)

p = class_1 / n
n_rare = n * min(p, 1-p)
n_eff = min(n, 5*n_rare)
n_eff
```

Out[668...

4601

Computing the V for V-fold cross-validation

Since $n_{\text{eff}} \geq 500$ but not ≥ 5000 we should select a value between 20 and 10. We take in account that n_{eff} is closer to 5000 and so we focus on V slightly higher than 10.

In [698...

```
N_FOLDS = 12
```

BASE LEARNERS - SPECIFICATION

When choosing the base learners for the first layer we have considered the properties of the dataset and the task in this case being binary classification. As the paper *Practical considerations for specifying a super learner* suggests "An ideal, rich library is diverse in its learning strategies, able to adapt to a range of underlying functional forms for the true prediction function, computationally feasible, and effective at handling high dimensional data. Diverse libraries include parametric learners, highly data-adaptive learners, multiple variants of the same learner with different tuning parameter specifications...". So the first layer should consist of diverse algorithms with different inductive biases to ensure a rich set of predictions for the metalearner".

We have selected:

Random Forest:

Because they are robust to overfitting on datasets with many features and they handle noisy or irrelevant features well, which is can be a thing in this case.

Generalized Linear Model - Logistic regression:

We chose to add it because it's a simple yet effective baseline model, especially logistic regression for binary classification. It should provide a low-variance learner to complement the other high-variance ones.

Deep Learning (H2O's MLP):

We add the neural networks, because of it's flexibility so it could capture non-linear relationships which should broaden the diversity of the stacks prediction.

Naive Bayes:

Why: Spam datasets often benefit from Naive Bayes since it assumes independence among features and thus might capture something more general than the other models.

Gradient Boosting Machines:

We choose them as another complement ensemble method that can capture rather complex relationship and so maybe overfit more to th data.

We assume the simpler models like naive bayes and logistic regression should bring in the stack a more general view without focusing too much on the quirks in the data and to balance it out we have selected a more accurate and flexible methods like MLP

Also we try various configurations of hyperparameters for each class of learners as the paper specifies: "*Since the true functional form is unknown, it is a good idea to consider a variety of base learners, and to construct multiple variations of the same base learner with different*

tuning specifications. There is no harm in including a learner that performs poorly in the library, as it will be given a weight of zero..." (or close to 0).

```
In [443... base_learners_simple01 = {
    "LogisticRegression": H2OGeneralizedLinearEstimator(family="binomial", nfolds=N
    "RandomForest": H2ORandomForestEstimator(ntrees=50, max_depth=10, nfolds=N_FOLD
    "GradientBoosting": H2OGradientBoostingEstimator(ntrees=50, max_depth=5, nfolds
    "NaiveBayes": H2ONaiveBayesEstimator(nfolds=N_FOLDS, seed=42, keep_cross_valida
}

# TODO consider balance_class=True

base_learners_mix_duplicates01 = {
    "LogisticRegression_binomial": H2OGeneralizedLinearEstimator(
        family="binomial", nfolds=N_FOLDS, seed=42, keep_cross_validation_predictio
    ),
    "RandomForest_50trees": H2ORandomForestEstimator(
        ntrees=50, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre
    ),
    "RandomForest_50trees_unbounded_D": H2ORandomForestEstimator(
        ntrees=50, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre
    ),
    "RandomForest_10trees": H2ORandomForestEstimator(
        ntrees=10, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre
    ),
    "RandomForest_10trees_unbounded_D": H2ORandomForestEstimator(
        ntrees=10, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre
    ),
    "GradientBoosting": H2OGradientBoostingEstimator(
        ntrees=50, max_depth=5, nfolds=N_FOLDS, seed=42, keep_cross_validation_pred
    ),
    "NaiveBayes": H2ONaiveBayesEstimator(
        nfolds=N_FOLDS, seed=42, keep_cross_validation_predictions=True
    ),
    "NeuralNetwork_32": H2ODeepLearningEstimator(
        hidden=[32], epochs=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pred
    ),
    "NeuralNetwork_32_16": H2ODeepLearningEstimator(
        hidden=[32, 16], epochs=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_
    )
}

base_learners_mix_rf_nns_01 = {
    "LogisticRegression_binomial": H2OGeneralizedLinearEstimator(
        family="binomial", nfolds=N_FOLDS, seed=42, keep_cross_validation_predictio
    ),
    "RandomForest_50trees": H2ORandomForestEstimator(
        ntrees=50, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre
    ),
    "RandomForest_50trees_unbounded_D": H2ORandomForestEstimator(
        ntrees=50, nfolds=N_FOLDS, seed=42, keep_cross_validation_predictions=True
    ),
    "RandomForest_10trees": H2ORandomForestEstimator(
        ntrees=10, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre
    ),
}
```

```

"RandomForest_10trees_unbounded_D": H2ORandomForestEstimator(
    ntrees=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_predictions=True
),
"GradientBoosting_10trees": H2OGradientBoostingEstimator(
    ntrees=10, max_depth=5, nfolds=N_FOLDS, seed=42, keep_cross_validation_pred
),
"GradientBoosting_50trees": H2OGradientBoostingEstimator(
    ntrees=50, max_depth=5, nfolds=N_FOLDS, seed=42, keep_cross_validation_pred
),
"NaiveBayes": H2ONaiveBayesEstimator(
    nfolds=N_FOLDS, seed=42, keep_cross_validation_predictions=True
),
"NeuralNetwork_32_16": H2ODeepLearningEstimator(
    hidden=[32, 16], epochs=300, nfolds=N_FOLDS, seed=42, keep_cross_validation
),
"NeuralNetwork_32_32": H2ODeepLearningEstimator(
    hidden=[32, 32], epochs=300, nfolds=N_FOLDS, seed=42, keep_cross_validation
),
"NeuralNetwork_32": H2ODeepLearningEstimator(
    hidden=[32], epochs=300, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre
)
}

```

BASE LEARNERS - TRAINING & EVALUATION

In [590...

```

def train_evaluate_stack(base_learners, metalearner, h2o_train, h2o_test, X_train):

    # TRAIN BASE LEARNERS
    print("\n>>> Training base learners:\n")
    for name, learner in base_learners.items():
        print(f"    Training {name} with {N_FOLDS}-fold cross-validation...")
        learner.train(x=list(range(X_train.shape[1])), y="label", training_frame=h2o_train)

    super_learner = H2OStackedEnsembleEstimator(
        base_models=list(base_learners.values()),
        metalearner_algorithm=metalearner
    )

    # TRAIN THE METALEARNER
    print("\n>>> Training super learner:\n")
    super_learner.train(x=list(range(X_train.shape[1])), y="label", training_frame=h2o_train)

    # EVAL BASE LEARNERS
    print("\n>>> Base learners' results:\n")
    results = {}
    for name, learner in base_learners.items():
        performance = learner.model_performance(test_data=h2o_test)
        f1_score = performance.F1()[0][1]
        auc_pr = performance.aucpr()
        accuracy = performance.accuracy()[0][1]
        results[name] = accuracy
        results[name] = {"F1-Score": f1_score, "AUC-PR": auc_pr, "Accuracy": accuracy}
        print(f"    {name} - F1-Score: {f1_score:.4f}, AUC-PR: {auc_pr:.4f}, Accuracy: {accuracy:.4f}")

    # EVAL THE METALEARNER
    print("\n>>> Metalearner's results:\n")

```

```

super_performance = super_learner.model_performance(test_data=h2o_test)
super_accuracy = super_performance.accuracy()[0][1]
super_f1 = super_performance.F1()[0][1]
super_auc_pr = super_performance.aucpr()
# print(f"\n    Super Learner - F1-Score: {super_f1:.4f}, AUC-PR: {super_auc_pr:.4f}")

# print("\nFinal Results Comparison:")
# for name, metrics in results.items():
#     print(f"{name} - F1-Score: {metrics['F1-Score']:.4f}, AUC-PR: {metrics['AUC-PR']:.4f}")

print(f"    Super Learner - F1-Score: {super_f1:.4f}, AUC-PR: {super_auc_pr:.4f}, Accuracy: {super_accuracy:.4f}")
return {"F1-Score": super_f1, "AUC-PR": super_auc_pr, "Accuracy": super_accuracy}

```

METALEARNER - TRAINING & EVALUATION

For the metalearner we principally selected two possible options for testing:

GLM:

We chose logistic regression because it is simple and interpretable and as a meta-learner we want it just combine the predictions of individual learners by weighting the them reducing the risk of overfitting when combining predictions. So in this case we are more focused on finding the best combination of predictions rather than adding more complexity.

Gradient Boosting Machine / MLP:

As an alternative second option we wanted something stronger, a bit of a bigger hammer sort to say, especially for our stacks which are more diverse in which case their predictions could be more complex, so they could capture non-linear relationships among them.

Evaluation metrics: In accordance with the paper where our task is binary classification of imbalanced classes we chose AUCPR as a primary evaluation metric. In addition as alternatives we provide F1 (once again due uneven class distribution) and finally accuracy as complement.

In [700... `train_evaluate_stack(base_learners_simple01, "glm", h2o_train, h2o_test, X_train)`


```
Training LogisticRegression_binomial with 5-fold cross-validation...  
glm Model Build progress: |██████████████████████████████████████████|  
(done) 100%  
  
    Training RandomForest_50trees with 5-fold cross-validation...  
drf Model Build progress: |██████████████████████████████████████████|  
(done) 100%  
  
        Training RandomForest_50trees_unbounded_D with 5-fold cross-validation...  
drf Model Build progress: |██████████████████████████████████████████|  
(done) 100%  
  
            Training RandomForest_10trees with 5-fold cross-validation...  
drf Model Build progress: |██████████████████████████████████████████|  
(done) 100%  
  
                Training RandomForest_10trees_unbounded_D with 5-fold cross-validation...  
drf Model Build progress: |██████████████████████████████████████████|  
(done) 100%  
  
                    Training NaiveBayes with 5-fold cross-validation...  
naivebayes Model Build progress: |██████████████████████████████████████████|  
(done) 100%  
  
                        Training NeuralNetwork with 5-fold cross-validation...  
deeplearning Model Build progress: |██████████████████████████████████████████|  
(done) 100%
```

```
stackensemble Model Build progress: |██████████|  
(done) 100%
```

```
LogisticRegression_binomial - F1-Score: 0.9125, AUC-PR: 0.9597, Accuracy (Test Set): 0.9251
RandomForest_50trees - F1-Score: 0.9375, AUC-PR: 0.9790, Accuracy (Test Set): 0.9479
RandomForest_50trees_unbounded_D - F1-Score: 0.9375, AUC-PR: 0.9790, Accuracy (Test Set): 0.9479
RandomForest_10trees - F1-Score: 0.9235, AUC-PR: 0.9688, Accuracy (Test Set): 0.9370
RandomForest_10trees_unbounded_D - F1-Score: 0.9235, AUC-PR: 0.9688, Accuracy (Test Set): 0.9370
NaiveBayes - F1-Score: 0.8303, AUC-PR: 0.8182, Accuracy (Test Set): 0.8588
NeuralNetwork - F1-Score: 0.9376, AUC-PR: 0.9743, Accuracy (Test Set): 0.9468
```

Super Learner - F1-Score: 0.9404, AUC-PR: 0.9818, Accuracy: 0.9490

```
train evaluate stack(base learners mix rf nns 01, "glm", h2o train, h2o test, X tra
```

```
>>> Training base learners:
```

```
Training LogisticRegression_binomial with 5-fold cross-validation...
```

[illegible]

Training RandomForest_50trees with 5-fold cross-validation...

[illegible]

Training RandomForest_50trees_unbounded_D with 5-fold cross-validation...

[illegible]

Training RandomForest_10trees with 5-fold cross-validation...

[illegible]

Training RandomForest_10trees_unbounded_D with 5-fold cross-validation...

```
drf Model Build progress: |██████████████████████████████████████|  
(done) 100%
```

```
Training GradientBoosting with 5-fold cross-validation...
```

[illegible]

```
Training NaiveBayes with 5-fold cross-validation...
```

```
naivebayes Model Build progress: ████████████████████████████████████  
(done) 100%
```

```
Training NeuralNetwork_32_16 with 5-fold cross-validation...
```

```
deeplearning Model Build progress: |██████████████████████████████████████|  
(done) 100%
```

```
Training NeuralNetwork 32 32 with 5-fold cross-validation...
```

```
deeplearning Model Build progress: |██████████████████████████████████████|  
(done) 100%
```

```
Training NeuralNetwork 32 with 5-fold cross-validation...
```

```
deeplearning Model Build progress: |████████████████████████████████████████|  
(done) 100%
```

```
>>> Training super learner:
```

```
stackensemble Model Build progress: |████████████████████████████████████████|  
(done) 100%
```

```
>>> Base learners' results:
```

LogisticRegression_binomial - F1-Score: 0.9125, AUC-PR: 0.9597, Accuracy (Test Set): 0.9251

RandomForest_50trees - F1-Score: 0.9375, AUC-PR: 0.9790, Accuracy (Test Set): 0.9479

RandomForest_50trees_unbounded_D - F1-Score: 0.9501, AUC-PR: 0.9839, Accuracy (Test Set): 0.9577

RandomForest_10trees - F1-Score: 0.9235, AUC-PR: 0.9688, Accuracy (Test Set): 0.9370

RandomForest_10trees_unbounded_D - F1-Score: 0.9300, AUC-PR: 0.9756, Accuracy (Test Set): 0.9425

GradientBoosting - F1-Score: 0.9452, AUC-PR: 0.9838, Accuracy (Test Set): 0.9533

NaiveBayes - F1-Score: 0.8303, AUC-PR: 0.8182, Accuracy (Test Set): 0.8588

NeuralNetwork_32_16 - F1-Score: 0.9274, AUC-PR: 0.9594, Accuracy (Test Set): 0.9

NeuralNetwork_32_32 - F1-Score: 0.9283, AUC-PR: 0.9676, Accuracy (Test Set): 0.9403

NeuralNetwork_32 - F1-Score: 0.9309, AUC-PR: 0.9660, Accuracy (Test Set): 0.9425

>>> Metalearner's results:

Super Learner - F1-Score: 0.9494, AUC-PR: 0.9875, Accuracy: 0.9577

In []:

In []:

Ablation studies

In the following we tried a more methodological way of building the stack. We tried two approaches and evaluated their effects on the final test metrics:

1) Building the stack from simpler models adding more complex ones:

In this method we start from a base consisting of simple models which we assume would capture the main / most general pattern in the data. Afterwards we gradually try adding more complex models to extend the stack capabilities to capture more finer intricacies and more complex (perhaps non-linear) relationships in the data and we observe the effect on the test metrics.

1) Building the stack from more complex models adding more general/simple ones: In

this method we start from a base consisting of more complex models which we assume would capture the complex relationships in data well and then we try to bring down the variance by adding simpler models that don't overfit to the data so much.

```
In [766... simple_learners = [{
    "LogisticRegression_binomial": H2OGeneralizedLinearEstimator(
        family="binomial", nfolds=N_FOLDS, seed=42, keep_cross_vali
    )},
    {"NaiveBayes": H2ONaiveBayesEstimator(nfolds=N_FOLDS, seed=42, k

random_forests = {
    "RandomForest_10trees": H2ORandomForestEstimator(
        ntrees=10, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cros
    ),
    "RandomForest_20trees": H2ORandomForestEstimator(
        ntrees=20, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cros
    ),
    "RandomForest_50trees": H2ORandomForestEstimator(
        ntrees=50, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cros
    ),
    "RandomForest_10trees_unbounded_D": H2ORandomForestEstimator(
        ntrees=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_p
    ),
    "RandomForest_20trees_unbounded_D": H2ORandomForestEstimator(
        ntrees=20, nfolds=N_FOLDS, seed=42, keep_cross_validation_p
```

```

    ),
    "RandomForest_50trees_unbounded_D": H2ORandomForestEstimator(
        ntrees=50, nfolds=N_FOLDS, seed=42, keep_cross_validation_p
    )}

gradient_boostings = {

    "GradientBoosting_10trees": H2OGradientBoostingEstimator(
        ntrees=10, max_depth=5, nfolds=N_FOLDS, seed=42, keep_cross
    ),
    "GradientBoosting_20trees": H2OGradientBoostingEstimator(
        ntrees=20, max_depth=5, nfolds=N_FOLDS, seed=42, keep_cross
    ),
    "GradientBoosting_50trees": H2OGradientBoostingEstimator(
        ntrees=50, max_depth=5, nfolds=N_FOLDS, seed=42, keep_cross
    ),
    "GradientBoosting_10trees_unbounded_D": H2OGradientBoostingEsti
        ntrees=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_p
    ),
    "GradientBoosting_20trees_unbounded_D": H2OGradientBoostingEsti
        ntrees=20, nfolds=N_FOLDS, seed=42, keep_cross_validation_p
    ),
    "GradientBoosting_50trees_unbounded_D": H2OGradientBoostingEsti
        ntrees=50, nfolds=N_FOLDS, seed=42, keep_cross_validation_p
    )}

neural_networks = {
    "NeuralNetwork_6": H2ODeepLearningEstimator(
        hidden=[6], epochs=300, nfolds=N_FOLDS, seed=42, keep_cross
    ),
    "NeuralNetwork_16": H2ODeepLearningEstimator(
        hidden=[16], epochs=300, nfolds=N_FOLDS, seed=42, keep_cros
    ),
    "NeuralNetwork_32": H2ODeepLearningEstimator(
        hidden=[32], epochs=300, nfolds=N_FOLDS, seed=42, keep_cros
    ),
    "NeuralNetwork_32_16": H2ODeepLearningEstimator(
        hidden=[32, 16], epochs=300, nfolds=N_FOLDS, seed=42, keep_cros
    ),
    "NeuralNetwork_32_32": H2ODeepLearningEstimator(
        hidden=[32, 32], epochs=300, nfolds=N_FOLDS, seed=42, keep_
    ),
}

```

A more efficient variant would be training each model only once in case it is present in multiple combinations.

Due to the tradeoff between the scope of this project and time capabilities we perform only superficial overview. If the problem would be a topic of major research where the time needed to search the vast hypothesis space is available, we would suggest performing more extensive per-class tests with higher hyperparameter sampling granularity to better observe how they affect the models performance.

SIMPLE TO COMPLEX

To try all possible combinations would be computationally unfeasible. Therefore we chose a more naive tactic, where we examine the combination of a simple learner with the a few representative selections of a single class of complex learners and we choose the best performing options for combinations with others.

From the ablations we have selected the following configurations from each class:

RFs

```
In [797... random_forests = [{
    "RandomForest_10trees": H2ORandomForestEstimator(
        ntrees=10, max_depth=10, nfolds=N_FOLDS, seed=42, keep_
    ),
},
{
    "RandomForest_50trees": H2ORandomForestEstimator(
        ntrees=50, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre
    ),
},
{
    "RandomForest_10trees": H2ORandomForestEstimator(
        ntrees=10, max_depth=10, nfolds=N_FOLDS, seed=42, keep_
    ),
    "RandomForest_50trees": H2ORandomForestEstimator(
        ntrees=50, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre
    )
}]
```

GBM

```
In [800... gradient_boosting = [{
    "GradientBoosting_10trees": H2OGradientBoostingEstimator(
        ntrees=10, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre
    ),
    "GradientBoosting_50trees": H2OGradientBoostingEstimator(
        ntrees=50, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_predict
    ),
}, {
    "GradientBoosting_10trees": H2OGradientBoostingEstimator(
        ntrees=10, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre
    ),
    "GradientBoosting_20trees": H2OGradientBoostingEstimator(
        ntrees=20, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_predict
    ),
}]
```

MLP

```
In [803... mlp= [{
    "NeuralNetwork_10": H2ODeepLearningEstimator(
        hidden=[10], epochs=300, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre
    ),
}, {
    "NeuralNetwork_16": H2ODeepLearningEstimator(
        hidden=[16], epochs=300, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre
    ),
}]
```

```
In [858... from itertools import product

all_combinations = list(product(simple_learners, random_forests, gradient_boosting,
                                all_combinations

configurations = []
for combination in all_combinations:
    combined_config = {}
    for model_dict in combination:
        combined_config.update(model_dict) # Merge dictionaries
    configurations.append(combined_config)

print(f"Number of configurations: {len(configurations)}")
print("Sample configuration:", configurations[20])
```

Number of configurations: 24

Sample configuration: {'NaiveBayes': H2ONaiveBayesEstimator({'parms': {}}), 'RandomForest_10trees': H2ORandomForestEstimator({'parms': {}}), 'RandomForest_50trees': H2ORandomForestEstimator({'parms': {}}), 'GradientBoosting_10trees': H2OGradientBoostingEstimator({'parms': {}}), 'GradientBoosting_50trees': H2OGradientBoostingEstimator({'parms': {}}), 'NeuralNetwork_10': H2ODeepLearningEstimator({'parms': {}, 'supervised_learning': True})}

```
In [975... results = dict()

for i, stack in enumerate(configurations):
    results[i] = train_evaluate_stack(stack, "glm", h2o_train, h2o_val, X_train)
```



```
>>> Metalearner's results:
```

Super Learner - F1-Score: 0.9418, AUC-PR: 0.9813, Accuracy: 0.9538

```
>>> Training base learners:
```

Training LogisticRegression_binomial with 12-fold cross-validation...

[illegible]

Training RandomForest_10trees with 12-fold cross-validation...

[illegible]

Training GradientBoosting_10trees with 12-fold cross-validation...

[illegible]

Training GradientBoosting 20trees with 12-fold cross-validation...

[illegible]

Training NeuralNetwork 16 with 12-fold cross-validation...

```
deeplearning Model Build progress: |██████████████████████████████████████████|  
(done) 100%
```

```
>>> Training super learner:
```

```
stackensemble Model Build progress: |████████████████████████████████████████|  
(done) 100%
```

```
>>> Base learners' results:
```

LogisticRegression_binomial - F1-Score: 0.9160, AUC-PR: 0.9554, Accuracy (Test Set): 0.9334

RandomForest_10trees - F1-Score: 0.9310, AUC-PR: 0.9714, Accuracy (Test Set): 0.9457

```
GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Set): 0.9348
```

```
GradientBoosting_20trees - F1-Score: 0.9320, AUC-PR: 0.9788, Accuracy (Test Set): 0.9443
```

NeuralNetwork 16 - F1-Score: 0.9251, AUC-PR: 0.9590, Accuracy (Test Set): 0.9402

```
>>> Metalearner's results:
```

Super Learner - F1-Score: 0.9434, AUC-PR: 0.9825, Accuracy: 0.9552

```
>>> Training base learners:
```

Training LogisticRegression_binomial with 12-fold cross-validation...

[illegible]

```
Training RandomForest 50trees with 12-fold cross-validation...
```

```
drf Model Build progress: |██████████████████████████████████████|  
(done) 100%
```

Training GradientBoosting 10trees with 12-fold cross-validation...

[illegible]

Training GradientBoosting_50trees with 12-fold cross-validation...

```
gbm Model Build progress: |████████████████████████████████████████|
(done) 100%
    Training NeuralNetwork_10 with 12-fold cross-validation...
deeplearning Model Build progress: |██████████████████████████████████|
(done) 100%

>>> Training super learner:

stackedensemble Model Build progress: |██████████████████████████████████|
(done) 100%

>>> Base learners' results:

    LogisticRegression_binomial - F1-Score: 0.9160, AUC-PR: 0.9554, Accuracy (Test S
et): 0.9334
    RandomForest_50trees - F1-Score: 0.9298, AUC-PR: 0.9777, Accuracy (Test Set): 0.
9429
    GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Se
t): 0.9348
    GradientBoosting_50trees - F1-Score: 0.9472, AUC-PR: 0.9857, Accuracy (Test Se
t): 0.9579
    NeuralNetwork_10 - F1-Score: 0.9257, AUC-PR: 0.9665, Accuracy (Test Set): 0.9402

>>> Metalearner's results:

    Super Learner - F1-Score: 0.9477, AUC-PR: 0.9847, Accuracy: 0.9592

>>> Training base learners:

    Training LogisticRegression_binomial with 12-fold cross-validation...
glm Model Build progress: |████████████████████████████████████████|
(done) 100%
    Training RandomForest_50trees with 12-fold cross-validation...
drf Model Build progress: |████████████████████████████████████████|
(done) 100%
    Training GradientBoosting_10trees with 12-fold cross-validation...
gbm Model Build progress: |████████████████████████████████████████|
(done) 100%
    Training GradientBoosting_50trees with 12-fold cross-validation...
gbm Model Build progress: |████████████████████████████████████████|
(done) 100%
    Training NeuralNetwork_16 with 12-fold cross-validation...
deeplearning Model Build progress: |██████████████████████████████████|
(done) 100%

>>> Training super learner:

stackedensemble Model Build progress: |██████████████████████████████████|
(done) 100%

>>> Base learners' results:

    LogisticRegression_binomial - F1-Score: 0.9160, AUC-PR: 0.9554, Accuracy (Test S
et): 0.9334
    RandomForest_50trees - F1-Score: 0.9298, AUC-PR: 0.9777, Accuracy (Test Set): 0.
9429
```



```
(done) 100%
    Training GradientBoosting_10trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████|
(done) 100%
    Training GradientBoosting_20trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████|
(done) 100%
    Training NeuralNetwork_16 with 12-fold cross-validation...
deeplearning Model Build progress: |██████████████████████████████████████|
(done) 100%

>>> Training super learner:

stackedensemble Model Build progress: |██████████████████████████████████████|
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>>> Base learners' results:

    LogisticRegression_binomial - F1-Score: 0.9160, AUC-PR: 0.9554, Accuracy (Test Set): 0.9334
    RandomForest_50trees - F1-Score: 0.9298, AUC-PR: 0.9777, Accuracy (Test Set): 0.9429
    GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Set): 0.9348
    GradientBoosting_20trees - F1-Score: 0.9320, AUC-PR: 0.9788, Accuracy (Test Set): 0.9443
    NeuralNetwork_16 - F1-Score: 0.9368, AUC-PR: 0.9661, Accuracy (Test Set): 0.9497

>>> Metalearner's results:

    Super Learner - F1-Score: 0.9422, AUC-PR: 0.9828, Accuracy: 0.9538

>>> Training base learners:

    Training LogisticRegression_binomial with 12-fold cross-validation...
glm Model Build progress: |██████████████████████████████████████|
(done) 100%
    Training RandomForest_10trees with 12-fold cross-validation...
drf Model Build progress: |██████████████████████████████████████|
(done) 100%
    Training RandomForest_50trees with 12-fold cross-validation...
drf Model Build progress: |██████████████████████████████████████|
(done) 100%
    Training GradientBoosting_10trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████|
(done) 100%
    Training GradientBoosting_50trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████|
(done) 100%
    Training NeuralNetwork_10 with 12-fold cross-validation...
deeplearning Model Build progress: |██████████████████████████████████████|
(done) 100%

>>> Training super learner:

stackedensemble Model Build progress: |██████████████████████████████████████|
```


GradientBoosting_50trees - F1-Score: 0.9472, AUC-PR: 0.9857, Accuracy (Test Set): 0.9579

NeuralNetwork_16 - F1-Score: 0.9445, AUC-PR: 0.9751, Accuracy (Test Set): 0.9565

```
>>> Metalearner's results:
```

Super Learner - F1-Score: 0.9493, AUC-PR: 0.9854, Accuracy: 0.9592

```
>>> Training base learners:
```

```
Training LogisticRegression_binomial with 12-fold cross-validation...  
glm Model Build progress: |██████████████████████████████████████████|  
(done) 100%
```

```
Training RandomForest_10trees with 12-fold cross-validation...  
drf Model Build progress: |██████████████████████████████|  
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```

[illegible]

```
Training GradientBoosting_10trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████████|
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```

```
    Training GradientBoosting_20trees with 12-fold cross-validation...  
gbm Model Build progress: |██████████████████████████████████████|  
(done) 100%
```

```
Training NeuralNetwork_10 with 12-fold cross-validation...
deeplearning Model Build progress: |██████████████████████████████████████|
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```
>>> Training super learner:
```

```
stackensemble Model Build progress: ████████████████████████████████████████
(done) 100%
```

```
>>> Base learners' results:
```

LogisticRegression_binomial - F1-Score: 0.9160, AUC-PR: 0.9554, Accuracy (Test Set): 0.9334

RandomForest_10trees - F1-Score: 0.9310, AUC-PR: 0.9714, Accuracy (Test Set): 0.9457

RandomForest_50trees - F1-Score: 0.9298, AUC-PR: 0.9777, Accuracy (Test Set): 0.9429

GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Set): 0.9348

GradientBoosting_20trees - F1-Score: 0.9320, AUC-PR: 0.9788, Accuracy (Test Set): 0.9443

NeuralNetwork_10 - F1-Score: 0.9165, AUC-PR: 0.9590, Accuracy (Test Set): 0.9321

```
>>> Metalearner's results:
```

Super Learner - F1-Score: 0.9402, AUC-PR: 0.9825, Accuracy: 0.9524

```
>>> Training base learners:
```

```
Training LogisticRegression_binomial with 12-fold cross-validation...  
glm Model Build progress: |██████████|
```

```
(done) 100%  
Training RandomForest_10trees with 12-fold cross-validation...  
drf Model Build progress: |██████████████████████████████████████████|  
(done) 100%  
Training RandomForest_50trees with 12-fold cross-validation...  
drf Model Build progress: |██████████████████████████████████████████|  
(done) 100%  
Training GradientBoosting_10trees with 12-fold cross-validation...  
gbm Model Build progress: |██████████████████████████████████████████|  
(done) 100%  
Training GradientBoosting_20trees with 12-fold cross-validation...  
gbm Model Build progress: |██████████████████████████████████████████|  
(done) 100%  
Training NeuralNetwork_16 with 12-fold cross-validation...  
deeplearning Model Build progress: |██████████████████████████████████████|  
(done) 100%  
  
>>> Training super learner:  
  
stackedensemble Model Build progress: |██████████████████████████████████████|  
(done) 100%  
  
>>> Base learners' results:  
  
LogisticRegression_binomial - F1-Score: 0.9160, AUC-PR: 0.9554, Accuracy (Test Set): 0.9334  
RandomForest_10trees - F1-Score: 0.9310, AUC-PR: 0.9714, Accuracy (Test Set): 0.9457  
RandomForest_50trees - F1-Score: 0.9298, AUC-PR: 0.9777, Accuracy (Test Set): 0.9429  
GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Set): 0.9348  
GradientBoosting_20trees - F1-Score: 0.9320, AUC-PR: 0.9788, Accuracy (Test Set): 0.9443  
NeuralNetwork_16 - F1-Score: 0.9404, AUC-PR: 0.9692, Accuracy (Test Set): 0.9524  
  
>>> Metalearner's results:  
  
Super Learner - F1-Score: 0.9454, AUC-PR: 0.9842, Accuracy: 0.9565  
  
>>> Training base learners:  
  
Training NaiveBayes with 12-fold cross-validation...  
naivebayes Model Build progress: |██████████████████████████████████████|  
(done) 100%  
Training RandomForest_10trees with 12-fold cross-validation...  
drf Model Build progress: |██████████████████████████████████████████|  
(done) 100%  
Training GradientBoosting_10trees with 12-fold cross-validation...  
gbm Model Build progress: |██████████████████████████████████████████|  
(done) 100%  
Training GradientBoosting_50trees with 12-fold cross-validation...  
gbm Model Build progress: |██████████████████████████████████████████|  
(done) 100%  
Training NeuralNetwork_10 with 12-fold cross-validation...  
deeplearning Model Build progress: |██████████████████████████████████████|
```



```
Training NeuralNetwork_16 with 12-fold cross-validation...
deeplearning Model Build progress: |██████████████████████████████████████|
(done) 100%

>>> Training super learner:

stackedensemble Model Build progress: |██████████████████████████████████████|
(done) 100%

>>> Base learners' results:

NaiveBayes - F1-Score: 0.8303, AUC-PR: 0.7914, Accuracy (Test Set): 0.8628
RandomForest_10trees - F1-Score: 0.9310, AUC-PR: 0.9714, Accuracy (Test Set): 0.9457
GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Set): 0.9348
GradientBoosting_20trees - F1-Score: 0.9320, AUC-PR: 0.9788, Accuracy (Test Set): 0.9443
NeuralNetwork_16 - F1-Score: 0.9404, AUC-PR: 0.9726, Accuracy (Test Set): 0.9524

>>> Metalearner's results:

Super Learner - F1-Score: 0.9470, AUC-PR: 0.9827, Accuracy: 0.9579

>>> Training base learners:

Training NaiveBayes with 12-fold cross-validation...
naivebayes Model Build progress: |██████████████████████████████████████|
(done) 100%

Training RandomForest_50trees with 12-fold cross-validation...
drf Model Build progress: |██████████████████████████████████████|
(done) 100%

Training GradientBoosting_10trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████|
(done) 100%

Training GradientBoosting_50trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████|
(done) 100%

Training NeuralNetwork_10 with 12-fold cross-validation...
deeplearning Model Build progress: |██████████████████████████████████████|
(done) 100%

>>> Training super learner:

stackedensemble Model Build progress: |██████████████████████████████████████|
(done) 100%

>>> Base learners' results:

NaiveBayes - F1-Score: 0.8303, AUC-PR: 0.7914, Accuracy (Test Set): 0.8628
RandomForest_50trees - F1-Score: 0.9298, AUC-PR: 0.9777, Accuracy (Test Set): 0.9429
GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Set): 0.9348
GradientBoosting_50trees - F1-Score: 0.9472, AUC-PR: 0.9857, Accuracy (Test Set): 0.9579
```

NeuralNetwork_10 - F1-Score: 0.9210, AUC-PR: 0.9646, Accuracy (Test Set): 0.9375

```
>>> Metalearner's results:
```

Super Learner - F1-Score: 0.9509, AUC-PR: 0.9845, Accuracy: 0.9606

```
>>> Training base learners:
```

Training NaiveBayes with 12-fold cross-validation...

[illegible]

Training RandomForest_50trees with 12-fold cross-validation...

[illegible]

Training GradientBoosting_10trees with 12-fold cross-validation...

```
gbm Model Build progress: |██████████████████████████████████████████|  
(done) 100%
```

Training GradientBoosting_50trees with 12-fold cross-validation...

```
gbm Model Build progress: |██████████████████████████████████████|  
(done) 100%
```

Training NeuralNetwork_16 with 12-fold cross-validation...

```
deeplearning Model Build progress: |██████████████████████████████████████████|  
(done) 100%
```

```
>>> Training super learner:
```

```
stackensemble Model Build progress: |██████████|  
(done) 100%
```

```
>>> Base learners' results:
```

NaiveBayes - F1-Score: 0.8303, AUC-PR: 0.7914, Accuracy (Test Set): 0.8628

RandomForest_50trees - F1-Score: 0.9298, AUC-PR: 0.9777, Accuracy (Test Set): 0.9429

GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Set): 0.9348

GradientBoosting_50trees - F1-Score: 0.9472, AUC-PR: 0.9857, Accuracy (Test Set): 0.9579

NeuralNetwork_16 - F1-Score: 0.9347, AUC-PR: 0.9629, Accuracy (Test Set): 0.9484

```
>>> Metalearner's results:
```

Super Learner - F1-Score: 0.9542, AUC-PR: 0.9851, Accuracy: 0.9633

```
>>> Training base learners:
```

Training NaiveBayes with 12-fold cross-validation...

```
naivebayes Model Build progress: ██████████  
(done) 100%
```

Training RandomForest 50trees with 12-fold cross-validation...

```
drf Model Build progress: |██████████|  
(done) 100%
```

Training GradientBoosting 10trees with 12-fold cross-validation...

[illegible]

Training GradientBoosting 20trees with 12-fold cross-validation...

```
gbm Model Build progress: |████████████████████████████████████████|  
(done) 100%  
    Training NeuralNetwork_10 with 12-fold cross-validation...  
deeplearning Model Build progress: |████████████████████████████████████████|  
(done) 100%  
  
>>> Training super learner:  
  
stackedensemble Model Build progress: |████████████████████████████████████████|  
(done) 100%  
  
>>> Base learners' results:  
  
NaiveBayes - F1-Score: 0.8303, AUC-PR: 0.7914, Accuracy (Test Set): 0.8628  
RandomForest_50trees - F1-Score: 0.9298, AUC-PR: 0.9777, Accuracy (Test Set): 0.  
9429  
GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Se  
t): 0.9348  
GradientBoosting_20trees - F1-Score: 0.9320, AUC-PR: 0.9788, Accuracy (Test Se  
t): 0.9443  
NeuralNetwork_10 - F1-Score: 0.9160, AUC-PR: 0.9633, Accuracy (Test Set): 0.9334  
  
>>> Metalearner's results:  
  
Super Learner - F1-Score: 0.9452, AUC-PR: 0.9822, Accuracy: 0.9565  
  
>>> Training base learners:  
  
    Training NaiveBayes with 12-fold cross-validation...  
naivebayes Model Build progress: |████████████████████████████████████████|  
(done) 100%  
        Training RandomForest_50trees with 12-fold cross-validation...  
drf Model Build progress: |████████████████████████████████████████|  
(done) 100%  
            Training GradientBoosting_10trees with 12-fold cross-validation...  
gbm Model Build progress: |████████████████████████████████████████|  
(done) 100%  
                Training GradientBoosting_20trees with 12-fold cross-validation...  
gbm Model Build progress: |████████████████████████████████████████|  
(done) 100%  
                    Training NeuralNetwork_16 with 12-fold cross-validation...  
deeplearning Model Build progress: |████████████████████████████████████████|  
(done) 100%  
  
>>> Training super learner:  
  
stackedensemble Model Build progress: |████████████████████████████████████████|  
(done) 100%  
  
>>> Base learners' results:  
  
NaiveBayes - F1-Score: 0.8303, AUC-PR: 0.7914, Accuracy (Test Set): 0.8628  
RandomForest_50trees - F1-Score: 0.9298, AUC-PR: 0.9777, Accuracy (Test Set): 0.  
9429  
GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Se  
t): 0.9348
```

```
GradientBoosting_20trees - F1-Score: 0.9320, AUC-PR: 0.9788, Accuracy (Test Set): 0.9443
NeuralNetwork_16 - F1-Score: 0.9329, AUC-PR: 0.9641, Accuracy (Test Set): 0.9470

>>> Metalearner's results:

Super Learner - F1-Score: 0.9470, AUC-PR: 0.9833, Accuracy: 0.9579

>>> Training base learners:

Training NaiveBayes with 12-fold cross-validation...
naivebayes Model Build progress: |██████████████████████████████████████|
(done) 100%
Training RandomForest_10trees with 12-fold cross-validation...
drf Model Build progress: |███████████████████████████████████████████|
(done) 100%
Training RandomForest_50trees with 12-fold cross-validation...
drf Model Build progress: |███████████████████████████████████████████|
(done) 100%
Training GradientBoosting_10trees with 12-fold cross-validation...
gbm Model Build progress: |███████████████████████████████████████████|
(done) 100%
Training GradientBoosting_50trees with 12-fold cross-validation...
gbm Model Build progress: |███████████████████████████████████████████|
(done) 100%
Training NeuralNetwork_10 with 12-fold cross-validation...
deeplearning Model Build progress: |██████████████████████████████████████|
(done) 100%

>>> Training super learner:

stackedensemble Model Build progress: |██████████████████████████████████████|
(done) 100%

>>> Base learners' results:

NaiveBayes - F1-Score: 0.8303, AUC-PR: 0.7914, Accuracy (Test Set): 0.8628
RandomForest_10trees - F1-Score: 0.9310, AUC-PR: 0.9714, Accuracy (Test Set): 0.9457
RandomForest_50trees - F1-Score: 0.9298, AUC-PR: 0.9777, Accuracy (Test Set): 0.9429
GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Set): 0.9348
GradientBoosting_50trees - F1-Score: 0.9472, AUC-PR: 0.9857, Accuracy (Test Set): 0.9579
NeuralNetwork_10 - F1-Score: 0.9207, AUC-PR: 0.9644, Accuracy (Test Set): 0.9375

>>> Metalearner's results:

Super Learner - F1-Score: 0.9513, AUC-PR: 0.9840, Accuracy: 0.9606

>>> Training base learners:

Training NaiveBayes with 12-fold cross-validation...
naivebayes Model Build progress: |██████████████████████████████████████|
(done) 100%
```

```
Training RandomForest_10trees with 12-fold cross-validation...
drf Model Build progress: |██████████████████████████████████████████████████████████████████████████████|
(done) 100%
    Training RandomForest_50trees with 12-fold cross-validation...
drf Model Build progress: |██████████████████████████████████████████████████████████████████████████████|
(done) 100%
    Training GradientBoosting_10trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████████████████████████████████████████████|
(done) 100%
    Training GradientBoosting_50trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████████████████████████████████████████████|
(done) 100%
    Training NeuralNetwork_16 with 12-fold cross-validation...
deeplearning Model Build progress: |██████████████████████████████████████████████████████████████████████████████|
(done) 100%

>>> Training super learner:

stackedensemble Model Build progress: |██████████████████████████████████████████████████████████████████████████████|
(done) 100%

>>> Base learners' results:

NaiveBayes - F1-Score: 0.8303, AUC-PR: 0.7914, Accuracy (Test Set): 0.8628
RandomForest_10trees - F1-Score: 0.9310, AUC-PR: 0.9714, Accuracy (Test Set): 0.9457
RandomForest_50trees - F1-Score: 0.9298, AUC-PR: 0.9777, Accuracy (Test Set): 0.9429
GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Set): 0.9348
GradientBoosting_50trees - F1-Score: 0.9472, AUC-PR: 0.9857, Accuracy (Test Set): 0.9579
NeuralNetwork_16 - F1-Score: 0.9275, AUC-PR: 0.9690, Accuracy (Test Set): 0.9416

>>> Metalearner's results:

Super Learner - F1-Score: 0.9527, AUC-PR: 0.9849, Accuracy: 0.9620

>>> Training base learners:

    Training NaiveBayes with 12-fold cross-validation...
naivebayes Model Build progress: |██████████████████████████████████████████████████████████████████████████████|
(done) 100%
    Training RandomForest_10trees with 12-fold cross-validation...
drf Model Build progress: |██████████████████████████████████████████████████████████████████████████████|
(done) 100%
    Training RandomForest_50trees with 12-fold cross-validation...
drf Model Build progress: |██████████████████████████████████████████████████████████████████████████████|
(done) 100%
    Training GradientBoosting_10trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████████████████████████████████████████████|
(done) 100%
    Training GradientBoosting_20trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████████████████████████████████████████████|
(done) 100%
    Training NeuralNetwork_10 with 12-fold cross-validation...
```



```

RandomForest_50trees - F1-Score: 0.9298, AUC-PR: 0.9777, Accuracy (Test Set): 0.9429
GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Set): 0.9348
GradientBoosting_20trees - F1-Score: 0.9320, AUC-PR: 0.9788, Accuracy (Test Set): 0.9443
NeuralNetwork_16 - F1-Score: 0.9226, AUC-PR: 0.9693, Accuracy (Test Set): 0.9375

```

>>> Metalearner's results:

```
Super Learner - F1-Score: 0.9424, AUC-PR: 0.9836, Accuracy: 0.9538
```

Results achieved from combinations built on single primitive model

In [988...

```

import altair as alt

labels = []
for conf in configurations:
    label = "_".join(conf.keys())
    label = label.replace("LogisticRegression_binomial", "LR")
    label = label.replace("RandomForest", "RF")
    label = label.replace("GradientBoosting", "GB")
    label = label.replace("NeuralNetwork", "MLP")
    label = label.replace("trees", "")
    label = label.replace("NaiveBayes", "NB")
    labels.append(label)

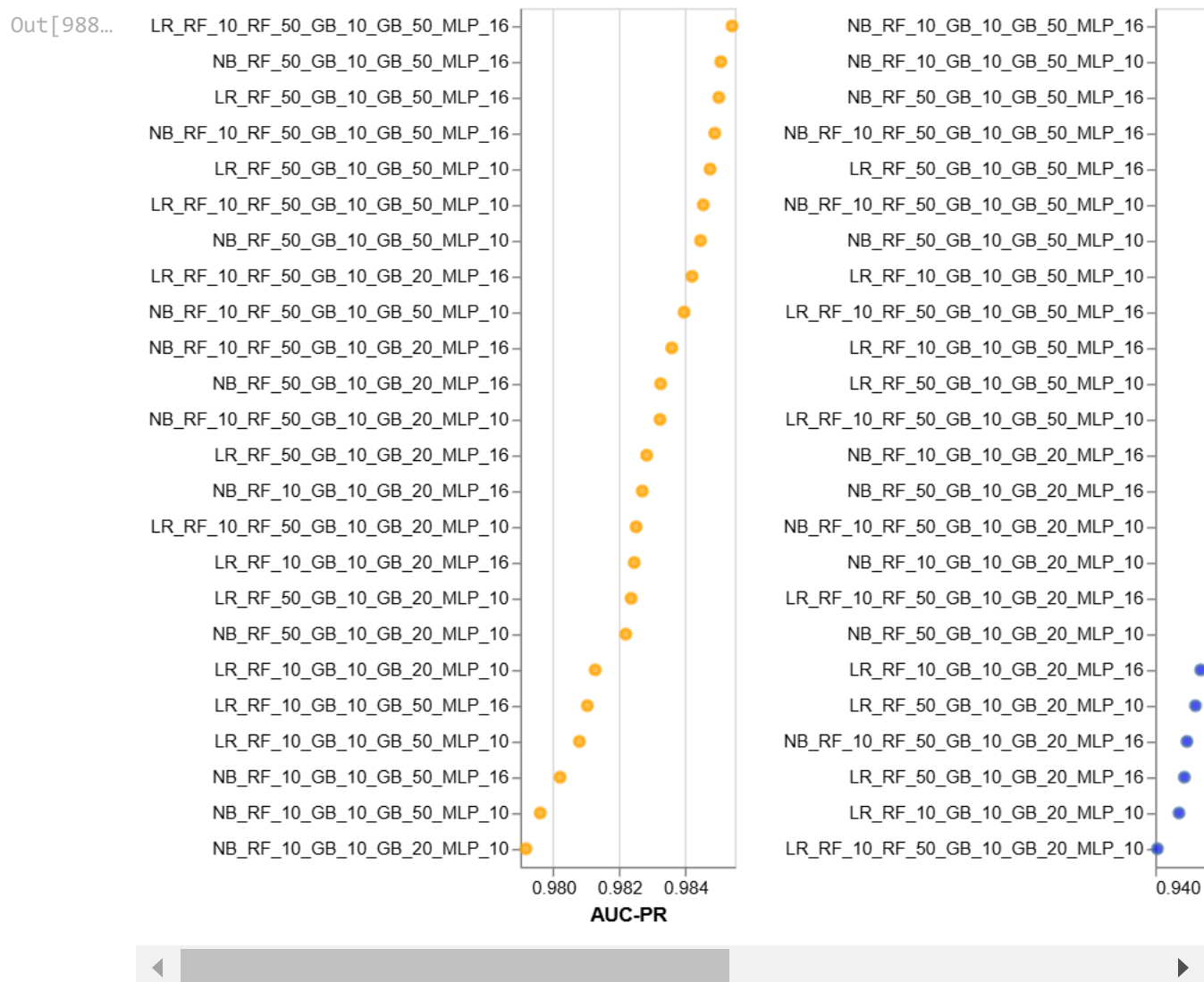
data_single = []
for label, record in zip(labels, results.values()):
    record["Configuration"] = label
    data_single.append(record)
data
df = pd.DataFrame(data_single)

f1_chart = alt.Chart(df).mark_point(fill="blue").encode(
    y=alt.Y('Configuration', sort="-x", axis=alt.Axis(title=None)),
    x=alt.X('F1-Score').scale(zero=False)
).properties(width=120)

aucpr_chart = alt.Chart(df).mark_point(fill="orange", stroke="orange").encode(
    y=alt.Y('Configuration', sort="-x", axis=alt.Axis(title=None)),
    x=alt.X('AUC-PR').scale(zero=False)
).properties(width=120)

accuracy_chart = alt.Chart(df).mark_point(fill="purple", stroke="purple").encode(
    y=alt.Y('Configuration', sort="-x", axis=alt.Axis(title=None)),
    x=alt.X('Accuracy').scale(zero=False)
).properties(width=120)
(aucpr_chart | f1_chart | accuracy_chart).configure_axis(labelLimit=1000)

```



Now we also add combinations using both LR and NB

```
In [945... simple_learners_combined = [{
    "LogisticRegression_binomial": H2OGeneralizedLinearEstimator(
        family="binomial", nfolds=N_FOLDS, seed=42, keep_cross_vali
    ),
    "NaiveBayes": H2ONaiveBayesEstimator(nfolds=N_FOLDS, seed=42, ke

all_combinations_combined = list(product(simple_learners_combined, random_forests,

configurations_combined = []
for combination in all_combinations_combined:
    combined_config = {}
    for model_dict in combination:
        combined_config.update(model_dict) # Merge dictionaries
    configurations_combined.append(combined_config)
```

```
print(f"Number of configurations: {len(configurations_combined)}")  
# print("Sample configuration:", configurations_combined[2])
```

Number of configurations: 12

In [941...

```
results_combined = dict()  
  
for i, stack in enumerate(configurations_combined):  
    results_combined[i] = train_evaluate_stack(stack, "glm", h2o_train, h2o_val, X_
```



```
(done) 100%
    Training GradientBoosting_50trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████████|
(done) 100%
    Training NeuralNetwork_16 with 12-fold cross-validation...
deeplearning Model Build progress: |██████████████████████████████████████|
(done) 100%

>>> Training super learner:

stackedensemble Model Build progress: |██████████████████████████████████████|
(done) 100%

>>> Base learners' results:

    LogisticRegression_binomial - F1-Score: 0.9160, AUC-PR: 0.9554, Accuracy (Test S
et): 0.9334
    NaiveBayes - F1-Score: 0.8303, AUC-PR: 0.7914, Accuracy (Test Set): 0.8628
    RandomForest_10trees - F1-Score: 0.9310, AUC-PR: 0.9714, Accuracy (Test Set): 0.
9457
    GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Se
t): 0.9348
    GradientBoosting_50trees - F1-Score: 0.9472, AUC-PR: 0.9857, Accuracy (Test Se
t): 0.9579
    NeuralNetwork_16 - F1-Score: 0.9390, AUC-PR: 0.9707, Accuracy (Test Set): 0.9511

>>> Metalearner's results:

    Super Learner - F1-Score: 0.9488, AUC-PR: 0.9812, Accuracy: 0.9592

>>> Training base learners:

    Training LogisticRegression_binomial with 12-fold cross-validation...
glm Model Build progress: |██████████████████████████████████████████|
(done) 100%
    Training NaiveBayes with 12-fold cross-validation...
naivebayes Model Build progress: |██████████████████████████████████████|
(done) 100%
    Training RandomForest_10trees with 12-fold cross-validation...
drf Model Build progress: |██████████████████████████████████████████|
(done) 100%
    Training GradientBoosting_10trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████████|
(done) 100%
    Training GradientBoosting_20trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████████|
(done) 100%
    Training NeuralNetwork_10 with 12-fold cross-validation...
deeplearning Model Build progress: |██████████████████████████████████████|
(done) 100%

>>> Training super learner:

stackedensemble Model Build progress: |██████████████████████████████████████|
(done) 100%
```



```
GradientBoosting_20trees - F1-Score: 0.9320, AUC-PR: 0.9788, Accuracy (Test Set): 0.9443
NeuralNetwork_16 - F1-Score: 0.9356, AUC-PR: 0.9689, Accuracy (Test Set): 0.9484

>>> Metalearner's results:

Super Learner - F1-Score: 0.9440, AUC-PR: 0.9829, Accuracy: 0.9552

>>> Training base learners:

Training LogisticRegression_binomial with 12-fold cross-validation...
glm Model Build progress: |██████████████████████████████████████|
(done) 100%
Training NaiveBayes with 12-fold cross-validation...
naivebayes Model Build progress: |██████████████████████████████████████|
(done) 100%
Training RandomForest_10trees with 12-fold cross-validation...
drf Model Build progress: |██████████████████████████████████████|
(done) 100%
Training RandomForest_50trees with 12-fold cross-validation...
drf Model Build progress: |██████████████████████████████████████|
(done) 100%
Training GradientBoosting_10trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████|
(done) 100%
Training GradientBoosting_50trees with 12-fold cross-validation...
gbm Model Build progress: |██████████████████████████████████████|
(done) 100%
Training NeuralNetwork_10 with 12-fold cross-validation...
deeplearning Model Build progress: |██████████████████████████████████████|
(done) 100%

>>> Training super learner:

stackedensemble Model Build progress: |██████████████████████████████████████|
(done) 100%

>>> Base learners' results:

LogisticRegression_binomial - F1-Score: 0.9160, AUC-PR: 0.9554, Accuracy (Test Set): 0.9334
NaiveBayes - F1-Score: 0.8303, AUC-PR: 0.7914, Accuracy (Test Set): 0.8628
RandomForest_10trees - F1-Score: 0.9310, AUC-PR: 0.9714, Accuracy (Test Set): 0.9457
RandomForest_50trees - F1-Score: 0.9298, AUC-PR: 0.9777, Accuracy (Test Set): 0.9429
GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Set): 0.9348
GradientBoosting_50trees - F1-Score: 0.9472, AUC-PR: 0.9857, Accuracy (Test Set): 0.9579
NeuralNetwork_10 - F1-Score: 0.9291, AUC-PR: 0.9676, Accuracy (Test Set): 0.9429

>>> Metalearner's results:

Super Learner - F1-Score: 0.9492, AUC-PR: 0.9851, Accuracy: 0.9592
```



```
Training RandomForest_10trees with 12-fold cross-validation...
drf Model Build progress: |████████████████████████████████████████|
(done) 100%
    Training RandomForest_50trees with 12-fold cross-validation...
drf Model Build progress: |████████████████████████████████████████|
(done) 100%
    Training GradientBoosting_10trees with 12-fold cross-validation...
gbm Model Build progress: |████████████████████████████████████████|
(done) 100%
    Training GradientBoosting_20trees with 12-fold cross-validation...
gbm Model Build progress: |████████████████████████████████████████|
(done) 100%
    Training NeuralNetwork_10 with 12-fold cross-validation...
deeplearning Model Build progress: |██████████████████████████████████|
(done) 100%

>>> Training super learner:

stackedensemble Model Build progress: |██████████████████████████████|
(done) 100%

>>> Base learners' results:

LogisticRegression_binomial - F1-Score: 0.9160, AUC-PR: 0.9554, Accuracy (Test S
et): 0.9334
NaiveBayes - F1-Score: 0.8303, AUC-PR: 0.7914, Accuracy (Test Set): 0.8628
RandomForest_10trees - F1-Score: 0.9310, AUC-PR: 0.9714, Accuracy (Test Set): 0.
9457
RandomForest_50trees - F1-Score: 0.9298, AUC-PR: 0.9777, Accuracy (Test Set): 0.
9429
GradientBoosting_10trees - F1-Score: 0.9186, AUC-PR: 0.9722, Accuracy (Test Se
t): 0.9348
GradientBoosting_20trees - F1-Score: 0.9320, AUC-PR: 0.9788, Accuracy (Test Se
t): 0.9443
NeuralNetwork_10 - F1-Score: 0.9193, AUC-PR: 0.9737, Accuracy (Test Set): 0.9375

>>> Metalearner's results:

Super Learner - F1-Score: 0.9485, AUC-PR: 0.9820, Accuracy: 0.9592

>>> Training base learners:

    Training LogisticRegression_binomial with 12-fold cross-validation...
glm Model Build progress: |████████████████████████████████████████|
(done) 100%
    Training NaiveBayes with 12-fold cross-validation...
naivebayes Model Build progress: |████████████████████████████████████|
(done) 100%
    Training RandomForest_10trees with 12-fold cross-validation...
drf Model Build progress: |████████████████████████████████████████|
(done) 100%
    Training RandomForest_50trees with 12-fold cross-validation...
drf Model Build progress: |████████████████████████████████████████|
(done) 100%
    Training GradientBoosting_10trees with 12-fold cross-validation...
gbm Model Build progress: |████████████████████████████████████████|
```

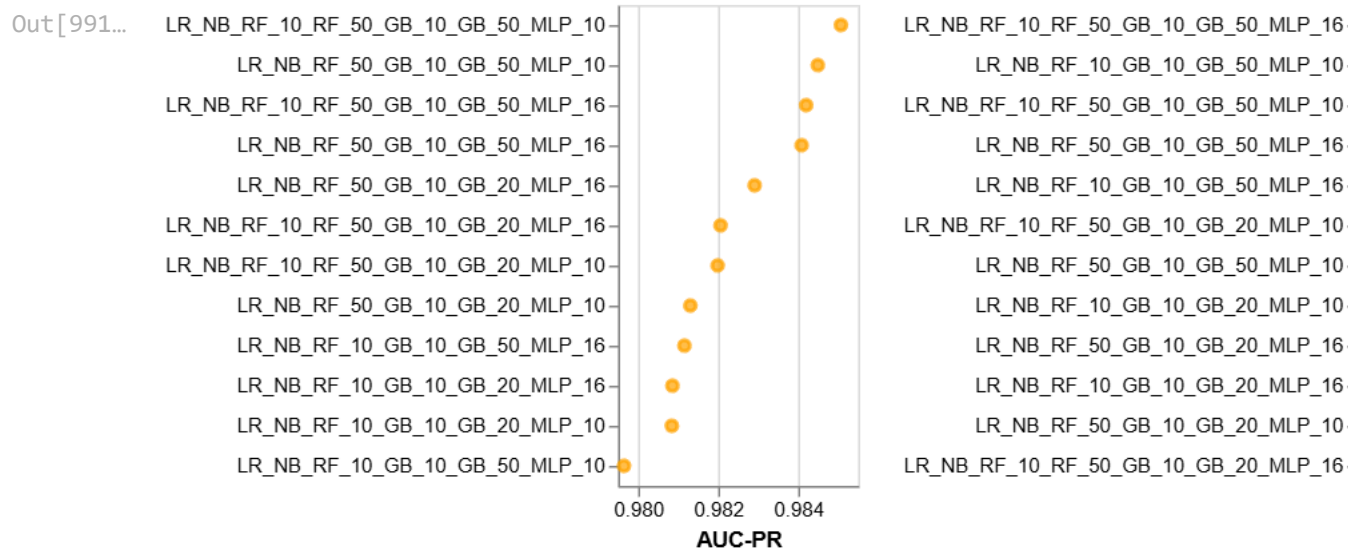


```

y=alt.Y('Configuration', sort="-x", axis=alt.Axis(title=None)),
x=alt.X('AUC-PR').scale(zero=False)
).properties(width=120)

accuracy_chart = alt.Chart(df).mark_point(fill="purple", stroke="purple").encode(
    y=alt.Y('Configuration', sort="-x", axis=alt.Axis(title=None)),
    x=alt.X('Accuracy').scale(zero=False)
).properties(width=120)
(aucpr_chart | f1_chart | accuracy_chart).configure_axis(labelLimit=1000)

```



Putting the results together

```

In [997... data = data_single + data_combined

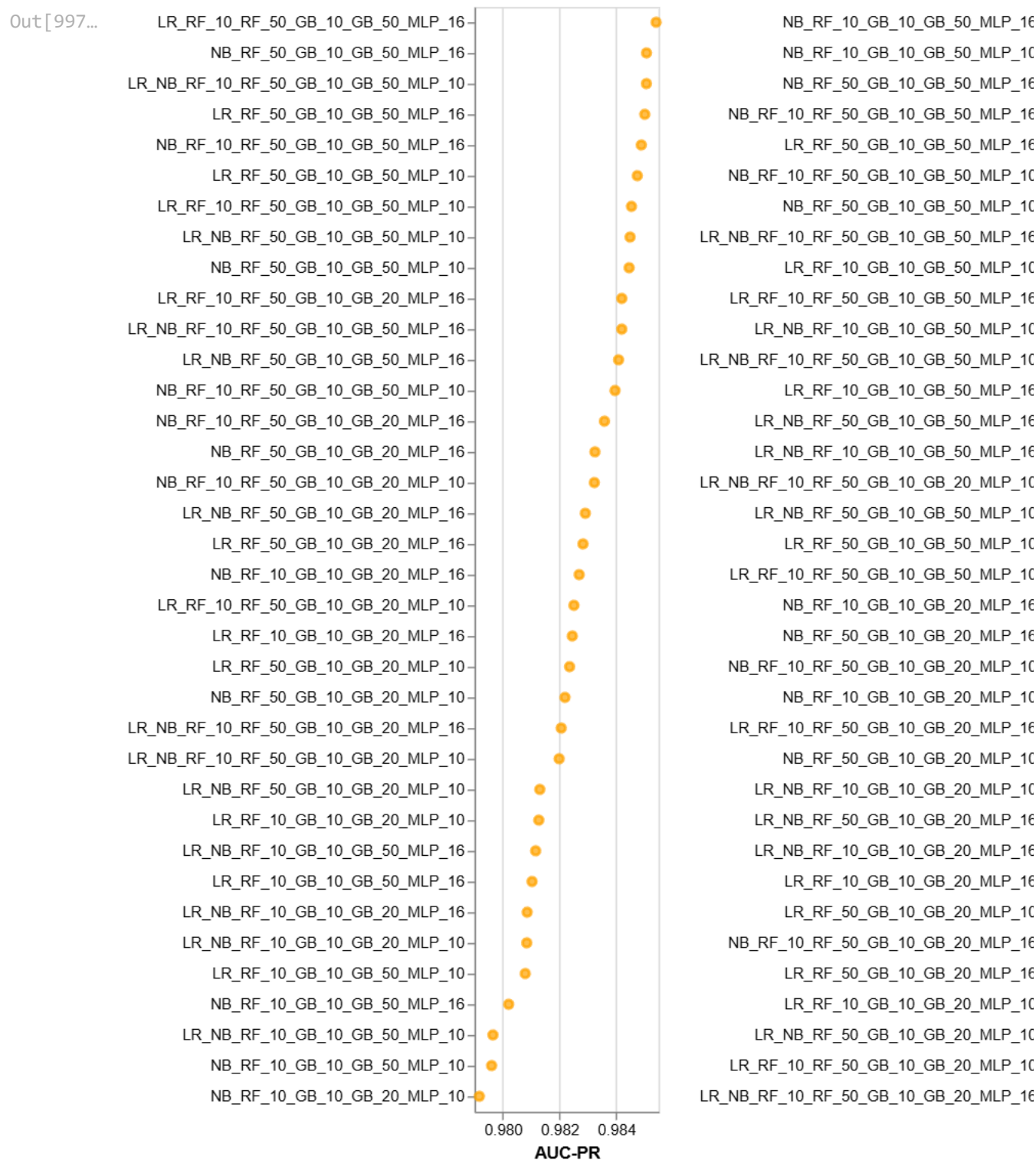
df = pd.DataFrame(data)

f1_chart = alt.Chart(df).mark_point(fill="blue").encode(
    y=alt.Y('Configuration', sort="-x", axis=alt.Axis(title=None)),
    x=alt.X('F1-Score').scale(zero=False)
).properties(width=120)

aucpr_chart = alt.Chart(df).mark_point(fill="orange", stroke="orange").encode(
    y=alt.Y('Configuration', sort="-x", axis=alt.Axis(title=None)),
    x=alt.X('AUC-PR').scale(zero=False)
).properties(width=120)

accuracy_chart = alt.Chart(df).mark_point(fill="purple", stroke="purple").encode(
    y=alt.Y('Configuration', sort="-x", axis=alt.Axis(title=None)),
    x=alt.X('Accuracy').scale(zero=False)
).properties(width=120)
(aucpr_chart | f1_chart | accuracy_chart).configure_axis(labelLimit=1000)

```



We must note that all of the models perform comparably with the differences being minuscule. Even still we selected a subset of representative examples. From the following results we select:

Naive Bayes + Random Forest 50 trees + Gradient Boosting 10 trees + Gradient Boosting 50 trees + MLP with 16 neurons in 1 hidden layer as second best performing (yet not the most complex) model according to the AUC-PR metric.

Naive Bayes + Random Forest 10 trees + Gradient Boosting 10 trees + Gradient Boosting 50 trees + MLP with 16 neurons in 1 hidden layer as the best performing according to the F1 and Accuracy scores.

Logistic Regression + Random Forest 10 trees + Gradient Boosting 10 trees + Gradient Boosting 50 trees + MLP with 16 neurons in 1 hidden layer as the model well balancing all the metrics.

Additionally we add a **simple stack** without tuned hyperparameters consisting of one version of each learner without MLP.

```
In [103... learner01 = {"NaiveBayes": H2ONaiveBayesEstimator(nfolds=N_FOLDS, seed=42, keep_cross_validation_pre=0),
              "RandomForest_50trees": H2ORandomForestEstimator(ntrees=50, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre=0),
              "GradientBoosting_10trees": H2OGradientBoostingEstimator(ntrees=10, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre=0),
              "GradientBoosting_50trees": H2OGradientBoostingEstimator(ntrees=50, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre=0),
              "NeuralNetwork_16": H2ODeepLearningEstimator(hidden=[16], epochs=300, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre=0),
            }
learner02 = {"NaiveBayes": H2ONaiveBayesEstimator(nfolds=N_FOLDS, seed=42, keep_cross_validation_pre=0),
              "RandomForest_10trees": H2ORandomForestEstimator(ntrees=10, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre=0),
              "GradientBoosting_10trees": H2OGradientBoostingEstimator(ntrees=10, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre=0),
              "GradientBoosting_50trees": H2OGradientBoostingEstimator(ntrees=50, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre=0),
              "NeuralNetwork_16": H2ODeepLearningEstimator(hidden=[16], epochs=300, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre=0),
            }
learner03 = {"LogisticRegression_binomial": H2OGeneralizedLinearEstimator(family="binomial", nfolds=N_FOLDS, seed=42, keep_cross_validation_pre=0),
              "RandomForest_50trees": H2ORandomForestEstimator(ntrees=50, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre=0),
              "GradientBoosting_10trees": H2OGradientBoostingEstimator(ntrees=10, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre=0),
              "GradientBoosting_50trees": H2OGradientBoostingEstimator(ntrees=50, max_depth=10, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre=0),
              "NeuralNetwork_16": H2ODeepLearningEstimator(hidden=[16], epochs=300, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre=0),
            }
```



```

        hidden=[16], epochs=300, nfolds=N_FOLDS, seed=42, keep_cross_validation_pre
    ),
}

learner04 = {
    "LogisticRegression": H2OGeneralizedLinearEstimator(family="binomial", nfolds=N
    "RandomForest": H2ORandomForestEstimator(ntrees=50, max_depth=10, nfolds=N_FOLD
    "GradientBoosting": H2OGradientBoostingEstimator(ntrees=50, max_depth=5, nfolds
    "NaiveBayes": H2ONaiveBayesEstimator(nfolds=N_FOLDS, seed=42, keep_cross_valida
}

learners = [learner01, learner02, learner03, learner04]

```

First we compare the results without any changes

In [100...

```

results_final4 = dict()

for i, stack in enumerate(learners):
    results_final4[i] = train_evaluate_stack(stack, "glm", h2o_train, h2o_val, X_tr

```



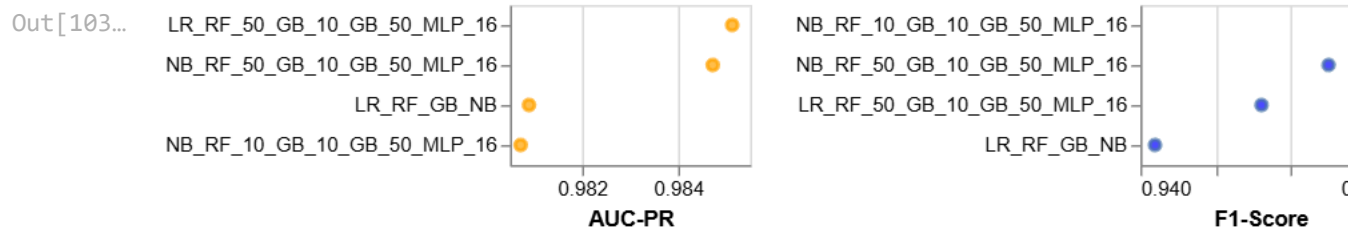
```

x=alt.X('F1-Score').scale(zero=False)
).properties(width=120)

aucpr_chart = alt.Chart(df).mark_point(fill="orange", stroke="orange").encode(
    y=alt.Y('Configuration', sort="-x", axis=alt.Axis(title=None)),
    x=alt.X('AUC-PR').scale(zero=False)
).properties(width=120)

accuracy_chart = alt.Chart(df).mark_point(fill="purple", stroke="purple").encode(
    y=alt.Y('Configuration', sort="-x", axis=alt.Axis(title=None)),
    x=alt.X('Accuracy').scale(zero=False)
).properties(width=120)
(aucpr_chart | f1_chart | accuracy_chart).configure_axis(labelLimit=1000)

```



Second we try deeplearning as a choice of classifier

```

In [101... results_final4_dl = dict()

for i, stack in enumerate(learners):
    results_final4_dl[i] = train_evaluate_stack(stack, "deeplearning", h2o_train, h

```



```

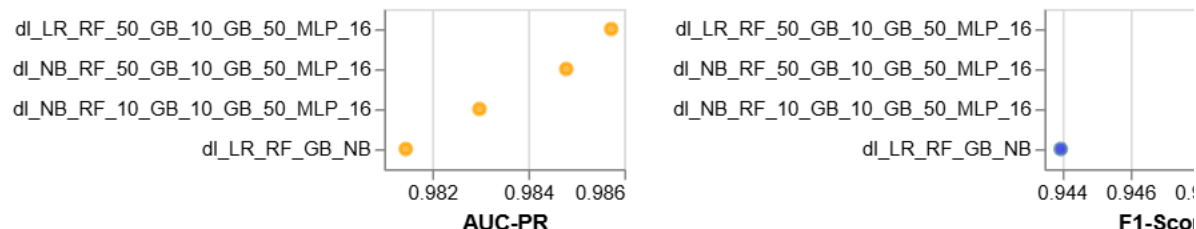
x=alt.X('F1-Score').scale(zero=False)
).properties(width=120)

aucpr_chart = alt.Chart(df).mark_point(fill="orange", stroke="orange").encode(
    y=alt.Y('Configuration', sort="-x", axis=alt.Axis(title=None)),
    x=alt.X('AUC-PR').scale(zero=False)
).properties(width=120)

accuracy_chart = alt.Chart(df).mark_point(fill="purple", stroke="purple").encode(
    y=alt.Y('Configuration', sort="-x", axis=alt.Axis(title=None)),
    x=alt.X('Accuracy').scale(zero=False)
).properties(width=120)
(aucpr_chart | f1_chart | accuracy_chart).configure_axis(labelLimit=1000)

```

Out[104...



Additionally we could try applying option of balancing classes and stratified fold assignment since we have inbalanced dataset

However due to the results we have already obtained we don't apply those.

Final results comparison

```
In [105... data = data_final4 + data_final4_d1
```

```

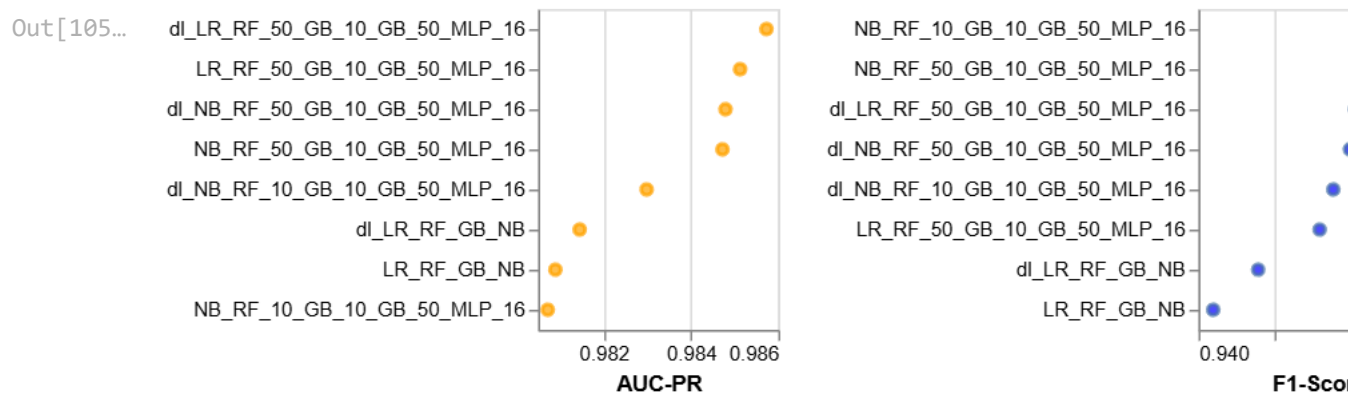
In [105... df = pd.DataFrame(data)

f1_chart = alt.Chart(df).mark_point(fill="blue").encode(
    y=alt.Y('Configuration', sort="-x", axis=alt.Axis(title=None)),
    x=alt.X('F1-Score').scale(zero=False)
).properties(width=120)

aucpr_chart = alt.Chart(df).mark_point(fill="orange", stroke="orange").encode(
    y=alt.Y('Configuration', sort="-x", axis=alt.Axis(title=None)),
    x=alt.X('AUC-PR').scale(zero=False)
).properties(width=120)

accuracy_chart = alt.Chart(df).mark_point(fill="purple", stroke="purple").encode(
    y=alt.Y('Configuration', sort="-x", axis=alt.Axis(title=None)),
    x=alt.X('Accuracy').scale(zero=False)
).properties(width=120)
(aucpr_chart | f1_chart | accuracy_chart).configure_axis(labelLimit=1000)

```



Even though deeplearning metalearner performs the best on AUC-PR we choose the model **Naive Bayes + Random Forest 50 trees + Gradient Boosting 10 trees + Gradient Boosting 50 trees + MLP with 1 hidden layer with 16 neurons** as the model which best balances all metrics but primarily performs among the best on AUC-PR and F1-Score.

```
In [106... best_model = train_evaluate_stack(learner01, "glm", h2o_train, h2o_test, X_train)
```


- We note that as expected choice of a single simple model LR or NB performed significantly worse compared to any other stack.
- Stacks in general surpassed the results of the individual methods although the change was not too big so the original base learners probably manage to

capture the relationships in the data well enough.

- In the AUC-PR and F1-Score matrix which we have selected to account for imbalanced classes, most of the stacks perform very pretty similarly on AUC-PR with highest differences present in F1-Score results. In terms of accuracy they also varied minimally.
- Even though we have imbalanced dataset accuracy is not significantly worse than the other metrics that take in account the imbalance.
- High AUC-PR should signify that method manages very well the classification of the minority class - in this case spam.
- High F1 also means it balanced pretty well precision and recall although in real life false positives and false negatives might not have similar consequences and we might focus more on rather not detecting good email as spam.
- Surprisingly the inclusion of both simple methods (NB and LR) didn't significantly improve the results or perform in general better than the single simple method combinations.
- The best stack combines Random Forest and Gradient Boosting, both with 50 trees which are both the default configurations that we would select if using these methods in separate.
- Depth unbounded tree based ensembles performed worse in general compared to the ones bounded with max tree depth 10.