10th Place Solution - ~350 oofs => 9 hillclimbing versions => Final Autogluon ensemble

Introduction

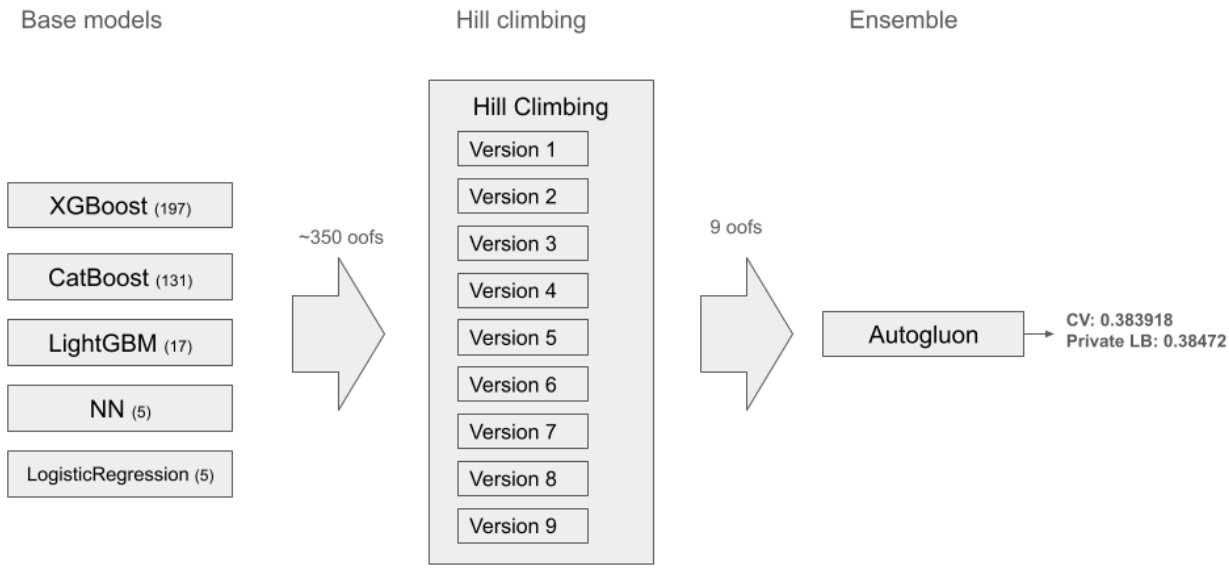
First and foremost, I want to extend a massive thank you to Kaggle for hosting the competition and to the community for sharing knowledge and creating interesting discussions. This was my first time working with the map@3 metric, and I found that ranking predictions give room for more creativity in the solutions.

Congratulations to the maestro himself @cdeotte for winning yet another playground competition and to @masayakawamata, @mahoganybuttstrings, @hahahaj and @optimistix for giving him a run for his money.

TL;DR

- Used standard models: XGBoost, CatBoost, LightGBM, NN, and Logistic Regression with minimal feature engineering.
- Generated ~350 Out-of-Fold (OOF) predictions. The best single model was an XGBoost with `CV=0.37799`, tuned with Optuna, using 6 fixed folds and sample weight bumping.
- Created 20 versions of hill climbing ensembles, with the best achieving a `CV=0.383830`.
- Used AutoGluon to ensemble the 9 best hill climbing results, reaching a final CV of `0.383918` and a Private LB score of `0.38472`.

Solution Overview



Each new version of hillclimbing had a larger set of oofs and the last one had ~350.

Base Models

XGBoost:

XGBoost performed the best, with the top single model achieving a `CV=0.37799`. Thanks to @ravi20076 for pointing out here in the early stage of the competition. The best parameters found were:

```
Params = {
'max_depth': 17,
'min_child_weight' : 4,
'subsample' : 0.8932774942420912,
'colsample_bytree' : 0.40035993059700825,
'gamma' : 0.44089845615519774,
'reg_alpha' : 3.0189326628791378,
'reg_lambda' : 1.0463133005441632,
'max_delta_step': 5}
```

This was achieved using sample weight bumping for 2nd, 3rd, and 4th places as described below. It is surprising that a depth of 17 was optimal, which I attribute to the synthetic nature of the data.

LightGBM/CatBoost:

Both were included for diversity, but they generally performed worse than XGBoost.

Neural Networks (NN):

I used a modified version of the excellent notebook by @paddykb: No Keras, No Loan. The best I could achieve was `CV=0.35097`.
I tried both cases using numeric features as numeric and categorical, and found the latter to perform best.

Logistic Regression:

This was adapted from @siukeitin's What if you can only use logistic regression…. With sample weight bumping, I achieved a `CV=0.37468`.

Ensembling Strategy

Hill Climbing:

I created 20 different versions using the GPU hill-climbing method by @cdeotte. My best hill climbing ensemble consisted of the following 14 OOF predictions:

```
- oof_model-1-15-w11-xgboost_trial_3_map3_0.37799.npy
- oof_model-13-3-w10-logisticregression_trial_0_map3_0.37530.npy
- oof_model-4-3-w10-NN_trial_0_map3_0.35016.npy
- oof_model-5-5-w10-catboost_trial_1_map3_0.34875.npy
- oof_model-12-1-w10-xgboost_index_0_map3_0.36555.npy
- oof_model-1-15-w11-xgboost_trial_0_map3_0.37737.npy
- oof_model-4-2-w10-NN_trial_3_map3_0.34908.npy
- oof_model-5-5-w10-catboost_trial_2_map3_0.35196.npy
- oof_model-12-1-w10-xgboost_index_67_map3_0.36579.npy
- oof_model-1-7-w10-xgboost_trial_0_map3_0.37640.npy
- oof_model-13-1-w10-logisticsregression_trial_0_map3_0.37411.npy
- oof_model-12-1-w10-xgboost_index_39_map3_0.36198.npy
- oof_model-3-2-w10-lightgbm_trial_2_map3_0.35041.npy
- oof_model-5-3-w10-catboost_trial_2_map3_0.34606.npy
```

This resulted in `CV=0.383830` and `Public LB=0.38268`. As @cdeotte has pointed out several times, the key is diversity in the models rather than high-performing single models.
On a side note, I think there is more to investigate with hill climbing (ideas, not used in this competition):

- Hill climb each fold separately, apply to the test set, and average the results.
- Experiment with starting the hill climb from different models, not just the best-performing one.

- Implement a tree-based search (e.g., using Alpha-beta pruning) to find an optimal set of models, rather than relying on a purely greedy approach.

During this competition, I noticed that sometimes adding a new OOF to the hill climb would significantly worsen the score, which makes me curious about potential improvements to the method.

Final Ensemble with AutoGluon:

The 9 best hill climbing ensembles were further ensembled using AutoGluon to produce the final submission with `CV=0.383918` and `Private LB=0.38472`.
Thanks to @ravaghi for pointing out how to use map@3 in AutoGluon here.

Other Techniques

1. Use Sample_Weight x4 for original data

Following a common technique from public notebooks, I set the `sample_weight` of the original data to 4x, which improved the score.

2. Use Sample_Weight to bump up 2nd, 3rd, and 4th placements

I analyzed OOF predictions to identify instances where the correct class was predicted as 2nd, 3rd, or 4th. I then retrained the models with increased `sample_weight` for these specific instances to encourage the model to rank them higher. The potential gain for moving up one place is:

- 2nd => 1st : 0.5 (from 0.5 to 1.0)
- 3rd => 2nd : 0.17 (from 0.33 to 0.5)
- 4th => 3rd : 0.33 (from 0.0 to 0.33)

I experimented with bumping the `sample_weight` for predictions where the probability difference between the two places where below a threshold (e.g., `0.02`). This technique yielded a `~0.001` CV improvement for many models. I tried bumping only the 2nd place predictions, as well as bumping all three ranks. I considered automating this with Optuna, but that will be a project for a future playground competition.

3. Using the same CV folds for everything

I used a fixed 6 Stratified-K-Fold strategy for all experiments. To ensure consistency and prevent data leakage between stages, I added a verification step to my scripts:

```
def verify_first_fold(val_idx):
    # Hardcoded first 10 indices of the first validation fold
```

```
    val_idx_expected = np.array([1, 2, 5, 8, 9, 14, 16, 23, 27, 30])
    if np.array_equal(val_idx[:10], val_idx_expected):
        return

    print("First fold validation indices do not match the expected values.")
    print("Expected:", val_idx_expected)
    print("Actual:", val_idx[:10])
    raise ValueError("Fold mismatch detected. Halting execution.")

# In the training loop
for fold, (train_idx, val_idx) in enumerate(kf.split(X=train_df, y=...)):
    if fold == 0:
        verify_first_fold(val_idx)
```

This is not a bulletproof method, but it saved me from polluting my OOFs on several occasions.

4. Optuna - Tricks

- I consolidated all hyperparameter tuning runs in the Optuna Dashboard for better tracking. All the results are stored in local sqlite3 databases for each notebook and I use a separate consolidation script to merge into a single db:

```
def merge_optuna_studies(
  source_storages: List[str],
  output_storage: str,
  min_trials: int = 10,
  name_prefix: str = ""
) -> int:
    """Merge studies from multiple Optuna storages into one."""
    copied_studies = 0

    for source_storage in source_storages:
        try:
            # Get all study summaries from the source storage
            study_summaries =
optuna.study.get_all_study_summaries(storage=source_storage)

            if len(study_summaries) == 0:
                print(f"No studies found in {source_storage}. Skipping.")
                continue
```

```
            print(f"Found {len(study_summaries)} studies in {source_storage}")

            # Process each study
            for summary in study_summaries:
                study_name = summary.study_name
                n_trials = summary.n_trials

                if n_trials < min_trials:
                    print(f"Skipping study '{study_name}' with only {n_trials} trials (minimum
required: {min_trials})")
                    continue

                print(f"Copying study '{study_name}' with {n_trials} trials")

                optuna.study.copy_study(from_study_name=study_name,
                                        from_storage=source_storage,
                                        to_storage=output_storage,
                                        to_study_name=study_name)

                copied_studies += 1

        except Exception as e:
            print(f"Error processing {source_storage}: {str(e)}")

    return copied_studies
```

- I used `WilcoxonPruner` to reduce computational effort, though this resulted in fewer OOFs being generated. Here is the setup:

```
# Pruner setup
p_threshold = 0.08  # p-value threshold for pruning
n_startup_steps = 2  # Number of trials to complete before pruning begins
pruner = optuna.pruners.WilcoxonPruner(
    p_threshold=p_threshold,
    n_startup_steps=n_startup_steps
)

# Create the Optuna study
study = optuna.create_study(
```

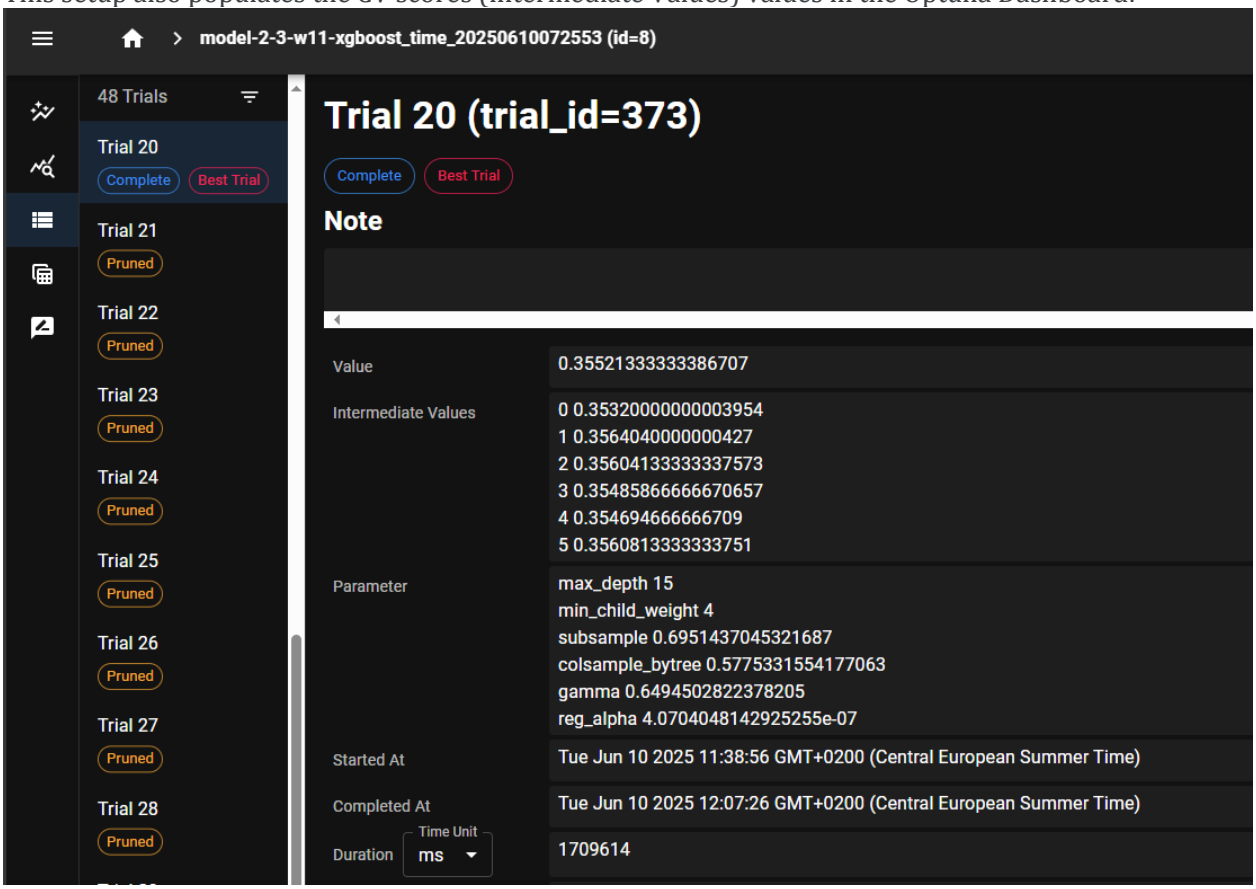
```
    direction="maximize",
    pruner=pruner
)

def objective(trial):
    # ...
    # Within the CV loop, report the intermediate score to Optuna
        # ... train and evaluate on fold ...
        trial.report(map3_score, step=fold)

        # Prune the trial if it is unpromising unless on the last fold.
        if trial.should_prune() and fold < total_folds - 1:
            raise optuna.TrialPruned()

    return final_cv_score
```

This setup also populates the CV scores (intermediate Values) values in the Optuna Dashboard:



- I always enqueued default parameters or other strong baseline configurations as the first trial.

5. Feature Engineering Search

Mid-competition, I fixed my best XGBoost parameters and systematically tested ~200 engineered features, calculating the map@3 for each. Some examples:


```
{
   "tested_features":  {
      "Potassium_binned":  0.36687777777820074,
      "Humidity_x_Moisture_x_Potassium":  0.36101355555603537,
      "Humidity_x_Potassium":  0.36245444444491326,
      "Humidity_x_Moisture":  0.36123777777825505,
      "log_Temparature":  0.3660744444448719,
      "Temparature_x_Nitrogen_div_Humidity":  0.36036377777826734,
      "sqrt_Phosphorous":  0.36733622222264173,
      "Temparature_x_Humidity_div_Nitrogen":  0.3603313333338274,
```


Not a single feature improved the result over the baseline without feature engineering. This is consistent with other competitors' findings. However, some of these OOFs were still selected by the hill climbing algorithm due to the diversity they added. I am aware of @cdeotte's advice to add all features and then remove them one by one, but I lacked the computational resources for that approach. I had to remove some of the oofs due to memory limitation of the number of oofs possible to hillclimb on my pc.

What Did Not Work / Future Improvements

TabTransformer:

I spent some time trying to get a network based on the TabTransformer library to work, but could only achieve a `CV=0.31`. I later discovered the excellent notebook
by @omidbaghchehsaraei TabTransformer but did not have time to incorporate his work.

Identify DAP/Urea in a separate model:

Analyzing the per-class map@3 score from several of my OOFs, I found that DAP and Urea had poor results compared to other classes:

CLASS-WISE MAP@3 CONTRIBUTION: (final oof)
`Class 14-25-14: MAP@3=0.432626`, Contribution=0.066011 (114,436 samples)
`Class 10-26-26: MAP@3=0.408642`, Contribution=0.062052 (113,887 samples)
`Class 17-17-17: MAP@3=0.426334`, Contribution=0.063923 (112,453 samples)
`Class 28-28: MAP@3=0.372506`, Contribution=0.055209 (111,158 samples)
`Class 20-20: MAP@3=0.369162`, Contribution=0.054581 (110,889 samples)

`Class DAP: MAP@3=0.341869`, Contribution=0.043240 (94,860 samples)
`Class Urea: MAP@3=0.315330`, Contribution=0.038814 (92,317 samples)
I tried to train a separate binary classification model to identify DAP/Urea and use its predictions as a feature for the main models, but this did not improve my score. I also tried using `sample_weight` to specifically bump up DAP/Urea, but that only resulted in a much worse CV.

Lessons Learned

- Trust your local CV.
- Prioritize model diversity for ensembling.
- Learn from discussion and other notebooks
- I used the same seed for all models. However, as @cdeotte mentioned in his 1st place solution, map@3 can be sensitive to randomness in training, so perhaps there was an element of luck involved. :)

This was my first attempt at a write-up. Thank you to the Kaggle Community for all the lessons learned, and I'm looking forward to the next playground competition. Happy Kaggling!