TabNet

TabNet was introduced in Arik and Pfister (2020). It is interesting for three reasons:

- It claims highly competitive performance on tabular data, an area where deep learning has not gained much of a reputation yet.
- TabNet includes interpretability[1] features by design.
- It is claimed to significantly profit from self-supervised pre-training, again in an area where this is anything but undeserving of mention.

In this post, we won't go into (3), but we do expand on (2), the ways TabNet allows access to its inner workings.

How do we use TabNet from R? The `torch` ecosystem includes a package – `tabnet` – that not only implements the model of the same name, but also allows you to make use of it as part of a `tidymodels` workflow.

tidymodels

To many R-using data scientists, the tidymodels framework will not be a stranger. `tidymodels` provides a high-level, unified approach to model training, hyperparameter optimization, and inference.

`tabnet` is the first (of many, we hope) `torch` models that let you use a `tidymodels` workflow all the way: from data pre-processing over hyperparameter tuning to performance evaluation and inference. While the first, as well as the last, may seem nice-to-have but not "mandatory", the tuning experience is likely to be something you'll won't want to do without!

Using tabnet with tidymodels

In this post, we first showcase a `tabnet`-using workflow in a nutshell, making use of hyperparameter settings reported in the paper.

Then, we initiate a `tidymodels`-powered hyperparameter search, focusing on the basics but also, encouraging you to dig deeper at your leisure.

Finally, we circle back to the promise of interpretability, demonstrating what is offered by `tabnet` and ending in a short discussion.

In the flow with TabNet

As usual, we start by loading all required libraries. We also set a random seed, on the R as well as the `torch` sides. When model interpretation is part of your task, you will want to investigate the role of random initialization.

```
library(torch)
library(tabnet)
library(tidyverse)
library(tidymodels)
library(finetune) # to use tuning functions from the new finetune
```

```
package
library(vip) # to plot feature importances

set.seed(777)
torch_manual_seed(777)
```

Next, we load the dataset.

```
# download from https://archive.ics.uci.edu/ml/datasets/HIGGS
higgs <- read_csv(
  "HIGGS.csv",
  col_names = c("class", "lepton_pT", "lepton_eta", "lepton_phi",
"missing_energy_magnitude",
                "missing_energy_phi", "jet_1_pt", "jet_1_eta",
"jet_1_phi", "jet_1_b_tag",
                "jet_2_pt", "jet_2_eta", "jet_2_phi", "jet_2_b_tag",
"jet_3_pt", "jet_3_eta",
                "jet_3_phi", "jet_3_b_tag", "jet_4_pt", "jet_4_eta",
"jet_4_phi", "jet_4_b_tag",
                "m_jj", "m_jjj", "m_lv", "m_jlv", "m_bb", "m_wbb",
"m_wwbb"),
  col_types = "fdddddddddddddddddddddddddddd"
  )
```

What's this about? In high-energy physics, the search for new particles takes place at powerful particle accelerators, such as (and most prominently) CERN's Large Hadron Collider. In addition to actual experiments, simulation plays an important role. In simulations, "measurement" data are generated according to different underlying hypotheses, resulting in distributions that can be compared with each other. Given the likelihood of the simulated data, the goal then is to make inferences about the hypotheses.

The above dataset (Baldi, Sadowski, and Whiteson (2014)) results from just such a simulation. It explores what features could be measured assuming two different processes. In the first process, two gluons collide, and a heavy Higgs boson is produced; this is the signal process, the one we're interested in. In the second, the collision of the gluons results in a pair of top quarks – this is the background process.

Through different intermediaries, both processes result in the same end products – so tracking these does not help. Instead, what the paper authors did was simulate kinematic features (momenta, specifically) of decay products, such as leptons (electrons and protons) and particle jets. In addition, they constructed a number of high-level features, features that presuppose domain knowledge. In their article, they showed that, in contrast to other machine learning methods, deep neural networks did nearly as well when presented with the low-level features (the momenta) only as with just the high-level features alone.

Certainly, it would be interesting to double-check these results on `tabnet`, and then, look at the respective feature importances. However, given the size of the dataset, non-negligible computing resources (and patience) will be required.

Speaking of size, let's take a look:

```
higgs %>% glimpse()
Rows: 11,000,000
Columns: 29
```

```
$ class                     1.000000000000000000e+00, 1.000000…
$ lepton_pT                 0.8692932, 0.9075421, 0.7988347, 1…
$ lepton_eta                -0.6350818, 0.3291473, 1.4706388, …
$ lepton_phi                0.225690261, 0.359411865, -1.63597…
$ missing_energy_magnitude  0.3274701, 1.4979699, 0.4537732, 1…
$ missing_energy_phi        -0.68999320, -0.31300953, 0.425629…
$ jet_1_pt                  0.7542022, 1.0955306, 1.1048746, 1…
$ jet_1_eta                 -0.24857314, -0.55752492, 1.282322…
$ jet_1_phi                 -1.09206390, -1.58822978, 1.381664…
$ jet_1_b_tag               0.000000, 2.173076, 0.000000, 0.00…
$ jet_2_pt                  1.3749921, 0.8125812, 0.8517372, 2…
$ jet_2_eta                 -0.6536742, -0.2136419, 1.5406590,…
$ jet_2_phi                 0.9303491, 1.2710146, -0.8196895, …
$ jet_2_b_tag               1.107436, 2.214872, 2.214872, 2.21…
$ jet_3_pt                  1.1389043, 0.4999940, 0.9934899, 1…
$ jet_3_eta                 -1.578198314, -1.261431813, 0.3560…
$ jet_3_phi                 -1.04698539, 0.73215616, -0.208777…
$ jet_3_b_tag               0.000000, 0.000000, 2.548224, 0.00…
$ jet_4_pt                  0.6579295, 0.3987009, 1.2569546, 0…
$ jet_4_eta                 -0.01045457, -1.13893008, 1.128847…
$ jet_4_phi                 -0.0457671694, -0.0008191102, 0.90…
$ jet_4_btag                3.101961, 0.000000, 0.000000, 0.00…
$ m_jj                      1.3537600, 0.3022199, 0.9097533, 0…
$ m_jjj                     0.9795631, 0.8330482, 1.1083305, 1…
$ m_lv                      0.9780762, 0.9856997, 0.9856922, 0…
$ m_jlv                     0.9200048, 0.9780984, 0.9513313, 0…
$ m_bb                      0.7216575, 0.7797322, 0.8032515, 0…
$ m_wbb                     0.9887509, 0.9923558, 0.8659244, 1…
$ m_wwbb                    0.8766783, 0.7983426, 0.7801176, 0…
```

Eleven million "observations" (kind of) – that's a lot! Like the authors of the TabNet paper (Arik and Pfister (2020)), we'll use 500,000 of these for validation. (Unlike them, though, we won't be able to train for 870,000 iterations!)

The first variable, `class`, is either `1` or `0`, depending on whether a Higgs boson was present or not. While in experiments, only a tiny fraction of collisions produce one of those, both classes are about equally frequent in this dataset.

As for the predictors, the last seven are high-level (derived). All others are "measured".

Data loaded, we're ready to build a `tidymodels` *workflow*, resulting in a short sequence of concise steps.

First, split the data:

```
n <- 11000000
n_test <- 500000
test_frac <- n/n_all

split <- initial_time_split(higgs, prop = 1 - test_frac)
train <- training(split)
test  <- testing(split)
```

Second, create a `recipe`. We want to predict `class` from all other features present:

```
rec <- recipe(class ~ ., train)
```

Third, create a `parsnip` model specification of class `tabnet`. The parameters passed are those reported by the TabNet paper, for the S-sized model variant used on this dataset.[2]

```
# hyperparameter settings (apart from epochs) as per the TabNet paper
(TabNet-S)
mod <- tabnet(epochs = 3, batch_size = 16384, decision_width = 24,
attention_width = 26,
              num_steps = 5, penalty = 0.000001, virtual_batch_size =
512, momentum = 0.6,
              feature_reusage = 1.5, learn_rate = 0.02) %>%
  set_engine("torch", verbose = TRUE) %>%
  set_mode("classification")
```

Fourth, bundle recipe and model specifications in a workflow:

```
wf <- workflow() %>%
  add_model(mod) %>%
  add_recipe(rec)
```

Fifth, train the model. This will take some time. Training finished, we save the trained `parsnip` model, so we can reuse it at a later time.

```
fitted_model <- wf %>% fit(train)

# access the underlying parsnip model and save it to RDS format
# depending on when you read this, a nice wrapper may exist
# see https://github.com/mlverse/tabnet/issues/27
fitted_model$fit$fit$fit %>% saveRDS("saved_model.rds")
```

After three epochs, loss was at 0.609.

Sixth – and finally – we ask the model for test-set predictions and have accuracy computed.

```
preds <- test %>%
  bind_cols(predict(fitted_model, test))

yardstick::accuracy(preds, class, .pred_class)
# A tibble: 1 x 3
  .metric  .estimator .estimate

1 accuracy binary         0.672
```

We didn't quite arrive at the accuracy reported in the TabNet paper (0.783), but then, we only trained for a tiny fraction of the time.

In case you're thinking: *well, that was a nice and effortless way of training a neural network!* – just wait and see how easy hyperparameter tuning can get. In fact, no need to wait, we'll take a look right now.

TabNet tuning

For hyperparameter tuning, the `tidymodels` framework makes use of cross-validation. With a dataset of considerable size, some time and patience is needed; for the purpose of this post, I'll use 1/1,000 of observations.

Changes to the above workflow start at model specification. Let's say we'll leave most settings fixed, but vary the TabNet-specific hyperparameters `decision_width`, `attention_width`, and `num_steps`, as well as the learning rate:[3]

```
mod <- tabnet(epochs = 1, batch_size = 16384, decision_width = tune(),
attention_width = tune(),
              num_steps = tune(), penalty = 0.000001,
virtual_batch_size = 512, momentum = 0.6,
              feature_reusage = 1.5, learn_rate = tune()) %>%
  set_engine("torch", verbose = TRUE) %>%
  set_mode("classification")
```

Workflow creation looks the same as before:

```
wf <- workflow() %>%
  add_model(mod) %>%
  add_recipe(rec)
```

Next, we specify the hyperparameter ranges we're interested in, and call one of the grid construction functions from the `dials` package to build one for us. If it wasn't for demonstration purposes, we'd probably want to have more than eight alternatives though, and pass a higher `size` to `grid_max_entropy()` .

```
grid <-
  wf %>%
  parameters() %>%
  update(
    decision_width = decision_width(range = c(20, 40)),
    attention_width = attention_width(range = c(20, 40)),
    num_steps = num_steps(range = c(4, 6)),
    learn_rate = learn_rate(range = c(-2.5, -1))
  ) %>%
  grid_max_entropy(size = 8)

grid
# A tibble: 8 x 4
  learn_rate decision_width attention_width num_steps

1    0.00529             28              25         5
2    0.0858              24              34         5
3    0.0230              38              36         4
4    0.0968              27              23         6
5    0.0825              26              30         4
6    0.0286              36              25         5
7    0.0230              31              37         5
8    0.00341             39              23         5
```

To search the space, we use `tune_race_anova()` from the new finetune package, making use of five-fold cross-validation:

```
ctrl <- control_race(verbose_elim = TRUE)
folds <- vfold_cv(train, v = 5)
set.seed(777)

res <- wf %>%
    tune_race_anova(
    resamples = folds,
    grid = grid,
    control = ctrl
  )
```

We can now extract the best hyperparameter combinations:

```
res %>% show_best("accuracy") %>% select(- c(.estimator, .config))
# A tibble: 5 x 8
  learn_rate decision_width attention_width num_steps .metric   mean
n std_err

1     0.0858             24              34         5 accuracy 0.516
5 0.00370
2     0.0230             38              36         4 accuracy 0.510
5 0.00786
3     0.0230             31              37         5 accuracy 0.510
5 0.00601
4     0.0286             36              25         5 accuracy 0.510
5 0.0136
5     0.0968             27              23         6 accuracy 0.498
5 0.00835
```

It’s hard to imagine how tuning could be more convenient!

Now, we circle back to the original training workflow, and inspect TabNet’s interpretability features.

TabNet interpretability features

TabNet’s most prominent characteristic is the way – inspired by decision trees – it executes in distinct steps. At each step, it again looks at the original input features, and decides which of those to consider based on lessons learned in prior steps. Concretely, it uses an attention mechanism to learn sparse *masks* which are then applied to the features.

Now, these masks being “just” model weights means we can extract them and draw conclusions about feature importance. Depending on how we proceed, we can either

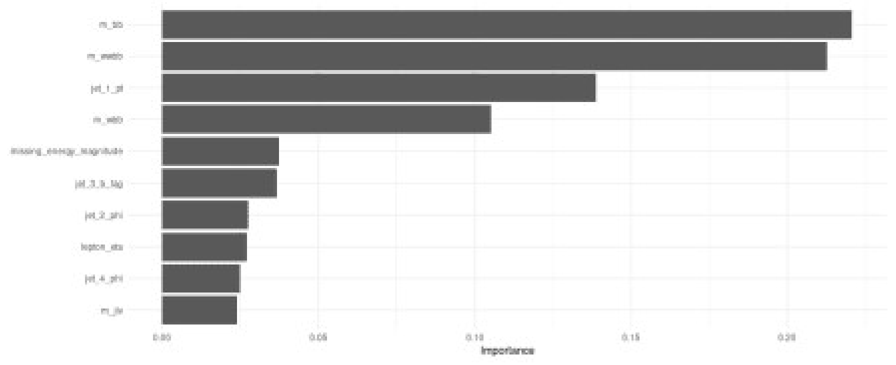
- aggregate mask weights over steps, resulting in global per-feature importances;
- run the model on a few test samples and aggregate over steps, resulting in observation-wise feature importances; or
- run the model on a few test samples and extract individual weights observation- as well as step-wise.

This is how to accomplish the above with `tabnet`.

Per-feature importances

We continue with the `fitted_model` workflow object we ended up with at the end of part 1. `vip::vip` is able to display feature importances directly from the `parsnip` model:

```
fit <- pull_workflow_fit(fitted_model)
vip(fit) + theme_minimal()
```



(#fig:unnamed-chunk-16)Global feature importances.

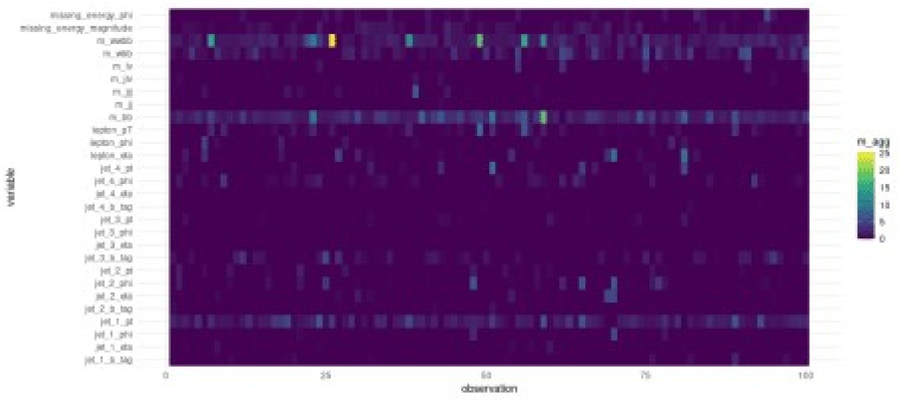
Together, two high-level features dominate, accounting for nearly 50% of overall attention. Along with a third high-level feature, ranked in place four, they occupy about 60% of “importance space”.

Observation-level feature importances

We choose the first hundred observations in the test set to extract feature importances. Due to how TabNet enforces sparsity, we see that many features have not been made use of:

```
ex_fit <- tabnet_explain(fit$fit, test[1:100, ])

ex_fit$M_explain %>%
  mutate(observation = row_number()) %>%
  pivot_longer(-observation, names_to = "variable", values_to = 
"m_agg") %>%
  ggplot(aes(x = observation, y = variable, fill = m_agg)) +
  geom_tile() +
  theme_minimal() +
  scale_fill_viridis_c()
```

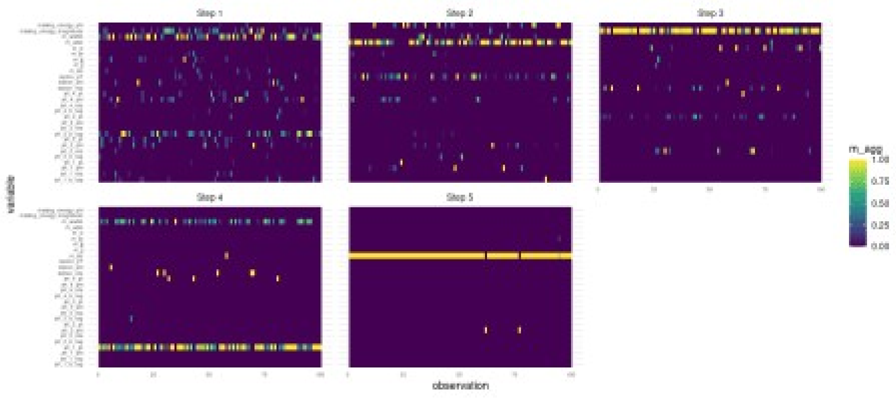


(#fig:unnamed-chunk-18)Per-observation feature importances.

Per-step, observation-level feature importances

Finally and on the same selection of observations, we again inspect the masks, but this time, per decision step:

```
ex_fit$masks %>%
  imap_dfr(~mutate(
    .x,
    step = sprintf("Step %d", .y),
    observation = row_number()
  )) %>%
  pivot_longer(-c(observation, step), names_to = "variable", values_to
= "m_agg") %>%
  ggplot(aes(x = observation, y = variable, fill = m_agg)) +
  geom_tile() +
  theme_minimal() +
  theme(axis.text = element_text(size = 5)) +
  scale_fill_viridis_c() +
  facet_wrap(~step)
```



(#fig:unnamed-chunk-20)Per-observation, per-step feature importances.

This is nice: We clearly see how TabNet makes use of different features at different times.

So what do we make of this? It depends. Given the enormous societal importance of this topic – call it interpretability, explainability, or whatever – let's finish this post with a short discussion.

Interpretable, explainable, …? Beyond the arbitrariness of definitions

An internet search for "interpretable vs. explainable ML" immediately turns up a number of sites confidently stating "interpretable ML is …" and "explainable ML is …", as though there were no arbitrariness in common-speech definitions. Going deeper, you find articles such as Cynthia Rudin's "Stop Explaining Black Box Machine Learning Models for High Stakes Decisions and Use Interpretable Models Instead" (Rudin (2018)) that present you with a clear-cut, deliberate, instrumentalizable distinction that can actually be used in real-world scenarios.