Analysing ensembles to improve forecast performance

```r
library(dplyr)
library(here)
library(stringr)
library(data.table)
library(scoringutils)
library(purrr)
library(tidyr)
library(ggplot2)
```

Model ensembles usually outperform individual models and forecasters in terms of predictive performance and therefore play an important role in any applied forecasting setting (e.g. epidemiology, finance, weather forecasting). Learned ensembles that adjust ensemble weights based on past performance hold great potential, but empirically it has proven surprisingly difficult to improve on simple mean or median ensembles. An important question therefore is what form of ensemble to choose.

Often, researchers have to decide on what kind of ensemble to use and can only know much later whether their choice was good. This research project aims to investigate model ensembles in an epidemiological setting and tries to establish heuristics for when to use which ensemble type.

(Possible) Objectives

- Analyse the performance of different ensemble techniques
- Specifically, analyse performance depending on different factors like
  - the number of available forecasting models
    - the degree of similarity between available forecasting models
    - the available training data
- Analyse how much do individual models contribute to an ensemble. Can a model be a valuable contribution to an ensemble, even though it is not a good forecasting model if looked at in isolation?
- Identify situations in which adding a model is beneficial or not
- Analyse how stable forecast performance of different ensemble types is

Data

All forecasts are made in a quantile-based format, meaning that forecasters provide a predictive distribution in the form of 23 quantiles (11 prediction intervals plus the median prediction), specifying how likely they think the true observed value will fall in a given range.

Human forecasts of COVID-19 made in the UK COVID-19 Forceasting Challenge

This data includes all forecasts as well as the true observations.

```r
uk_data <- fread("data/full-data-uk-challenge.csv")
```

The data has the following columns:

Column name	Column prediction
location_name	Name of the country
target_end_date	Date for which a forecast was made. This is always a Saturday

Column name	Column prediction
target_type	The target variable to be predicted, cases or deaths
true_value	The corresponding true observed value
population	population of the target country
forecast_date	Date on which a forecast was made. This is always a Monday
quantile	quantile-level of the predictive distribution
prediction	Predicted value corresponding to the quantile-level specified in ‘quantile’
model	Name of the forecaster
target	Summary of the prediction target variable (redundant information)
horizon	Forecast horizon
expert	Whether or not a forecaster self-identified as an expert

Potential difficulties are:

- there only is one location
- there are not a lot of observations
- many forecasters only submitted a few times and drop in and out

However, it is of particular interest to know

- how well different ensembles work in difficult settings where forecasters drop in and out
- whether aggregating human forecasts is different from aggregating model-based forecasts

Forecasts submitted to the European Forecast Hub

These forecasts were submitted to the European Forecast Hub by different research institutions. The file contains forecasts as well as true observations.

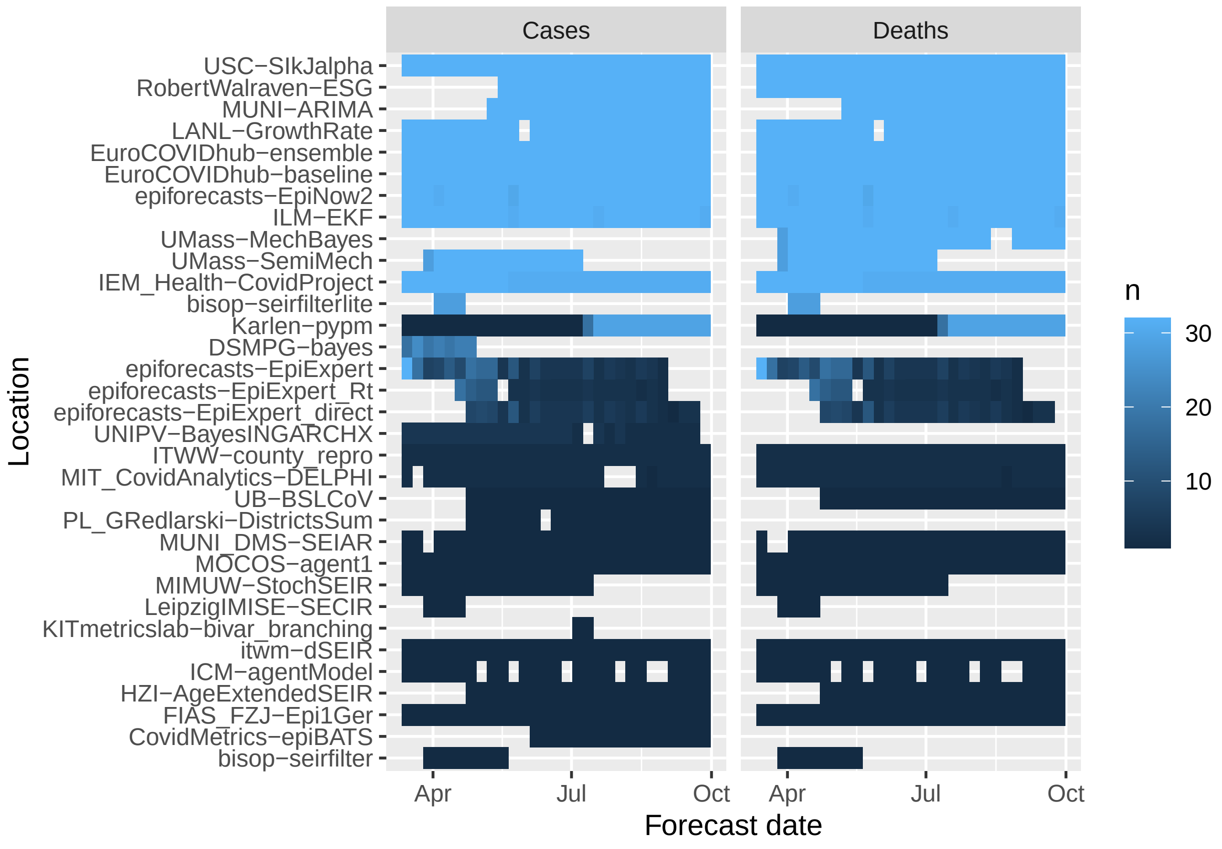
```
hub_data <- rbindlist(
  list(
    fread("data/full-data-european-forecast-hub-1.csv"),
    fread("data/full-data-european-forecast-hub-2.csv")
  )
)
```

Optionally, the Hub data can be filtered to obtain a complete set of forecasts, as the current data set has missing forecasts:

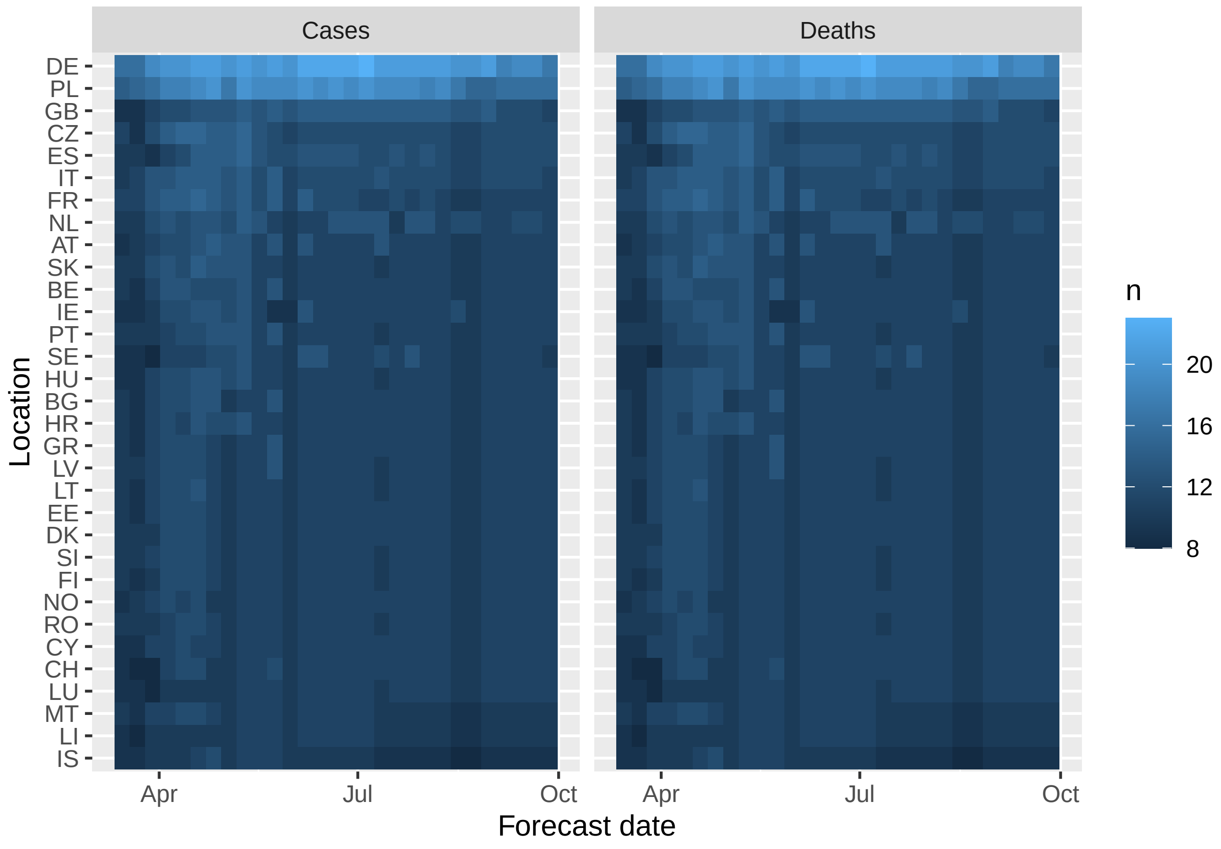
```
# helper functions for visualisation
plot_models_per_loc <- function(data) {
  data |>
    group_by(location, forecast_date) |>
    mutate(n = length(unique(model))) |>
    ggplot(aes(y = reorder(location, n), x = as.Date(forecast_date), fill = n)) +
    geom_tile() +
    facet_wrap(~ target_type) +
    labs(y = "Location", x = "Forecast date")
}

plot_locs_per_model <- function(data) {
  data |>
    group_by(model, forecast_date) |>
    mutate(n = length(unique(location))) |>
    ggplot(aes(y = reorder(model, n), x = as.Date(forecast_date), fill = n)) +
    geom_tile() +
    facet_wrap(~ target_type) +
```

```r
    labs(y = "Location", x = "Forecast date")
}
```

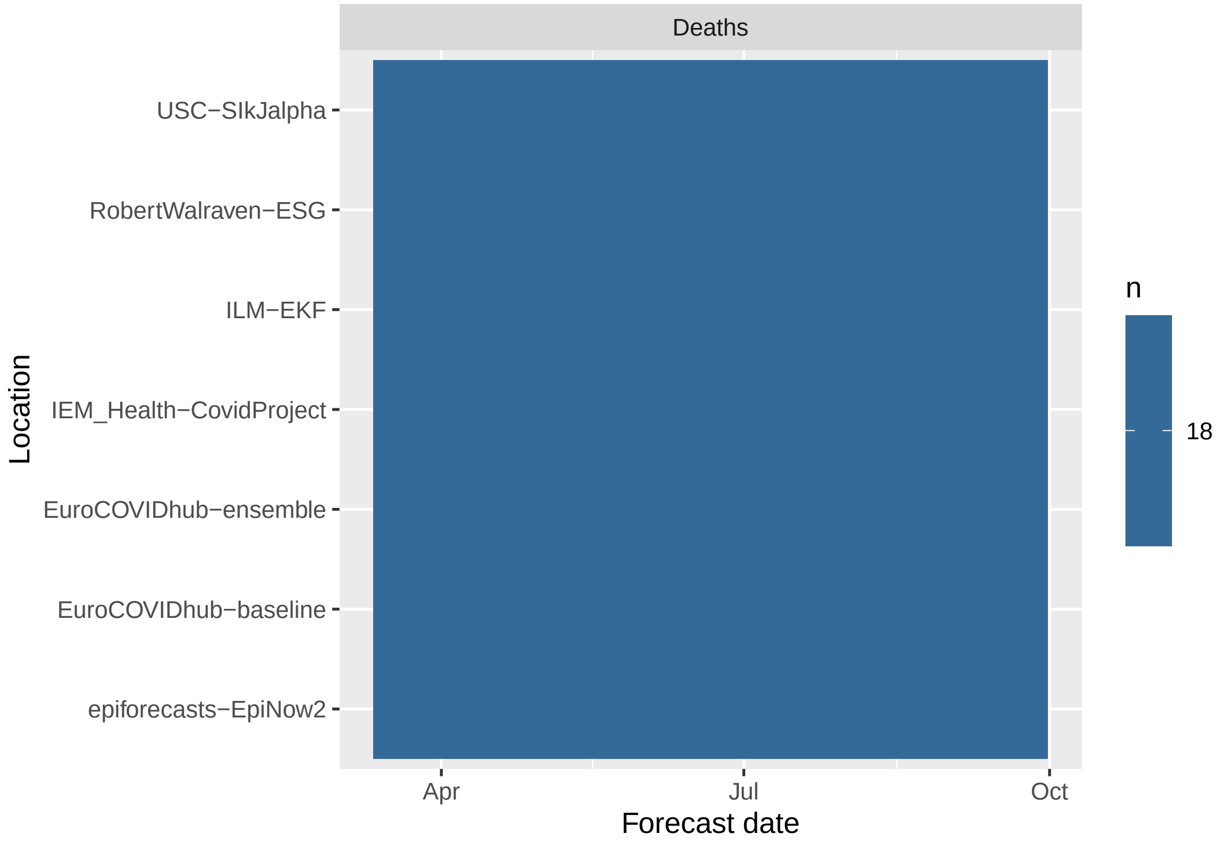
```r
plot_locs_per_model(hub_data)
```



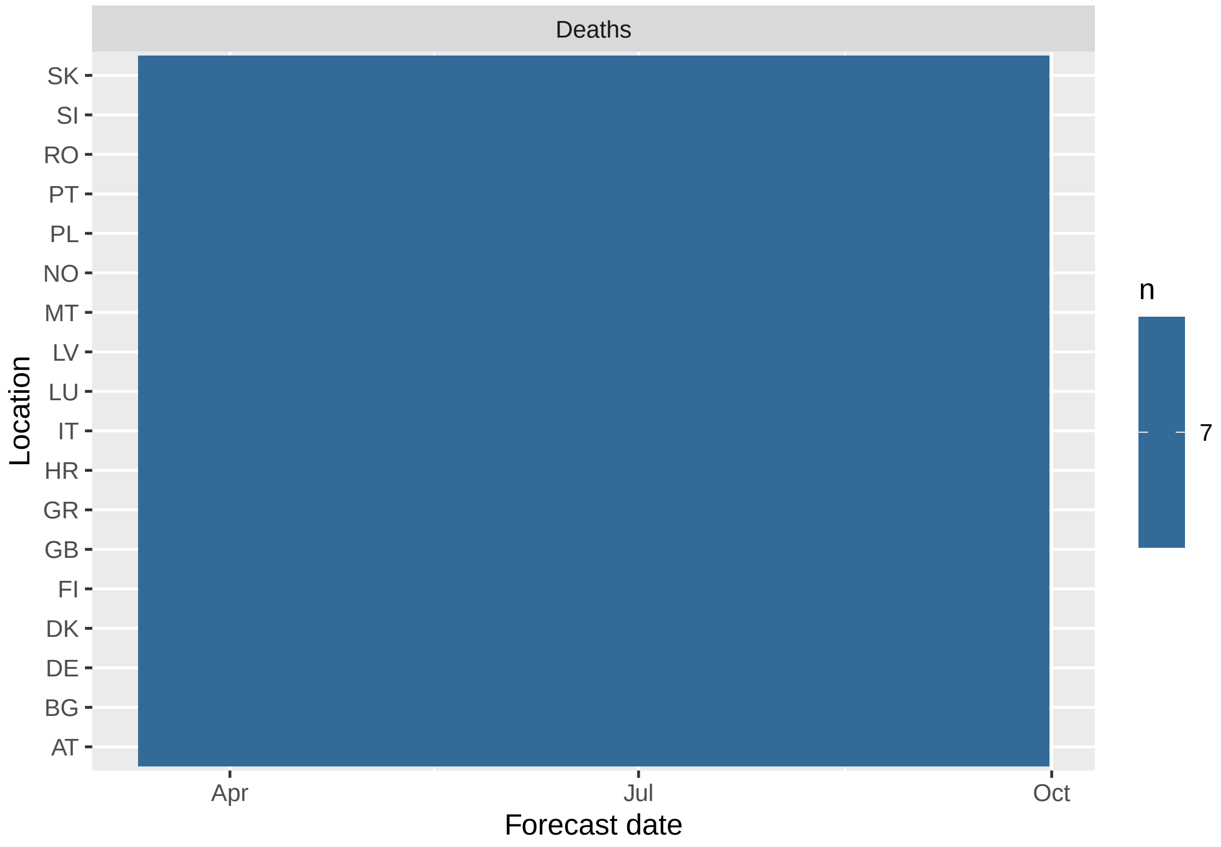
```r
plot_models_per_loc(hub_data)
```



```
# helper function to make a complete set. The data can be either complete
# per location (meaning that different locations will have different numbers of
# models) or it can be complete overall (removing models and locations)
make_complete_set <- function(hub_data,
                              forecast_dates = c("2021-03-15",
                                                 "2021-09-27"),
                              min_locations = 19,
                              per_location = FALSE) {

  # define the unit of a single forecast
  unit_observation <- c("location", "forecast_date", "horizon",
                        "model", "target_type")

  h <- hub_data |>
    # filter out models that don't have all forecast dates
    filter(forecast_date >= forecast_dates[1],
           forecast_date <= forecast_dates[2]) |>
    group_by_at(c(unit_observation)) |>
    ungroup(forecast_date) |>
    mutate(n = length(unique(forecast_date))) |>
    ungroup() |>
    filter(n == max(n))

  # per_location means a complete set per location, meaning that every location
  # has a complete set, but the numbers of models per location may be different
  # if this is not desired, we need to restrict the models and locations
  if (!per_location) {
    h <- h|>
      # filter out models that don't have at least min_locations
      group_by_at(unit_observation) |>
      ungroup(location) |>
      mutate(n = length(unique(location))) |>
      ungroup() |>
      filter(n >= min_locations) |>
      # filter out locations that don't have a full set of forecasts
      group_by(location, target_type) |>
      mutate(n = n()) |>
      ungroup() |>
      filter(n == max(n))
  }
  return(h)
}

hub_complete <- make_complete_set(hub_data)
print(plot_locs_per_model(hub_complete))
```

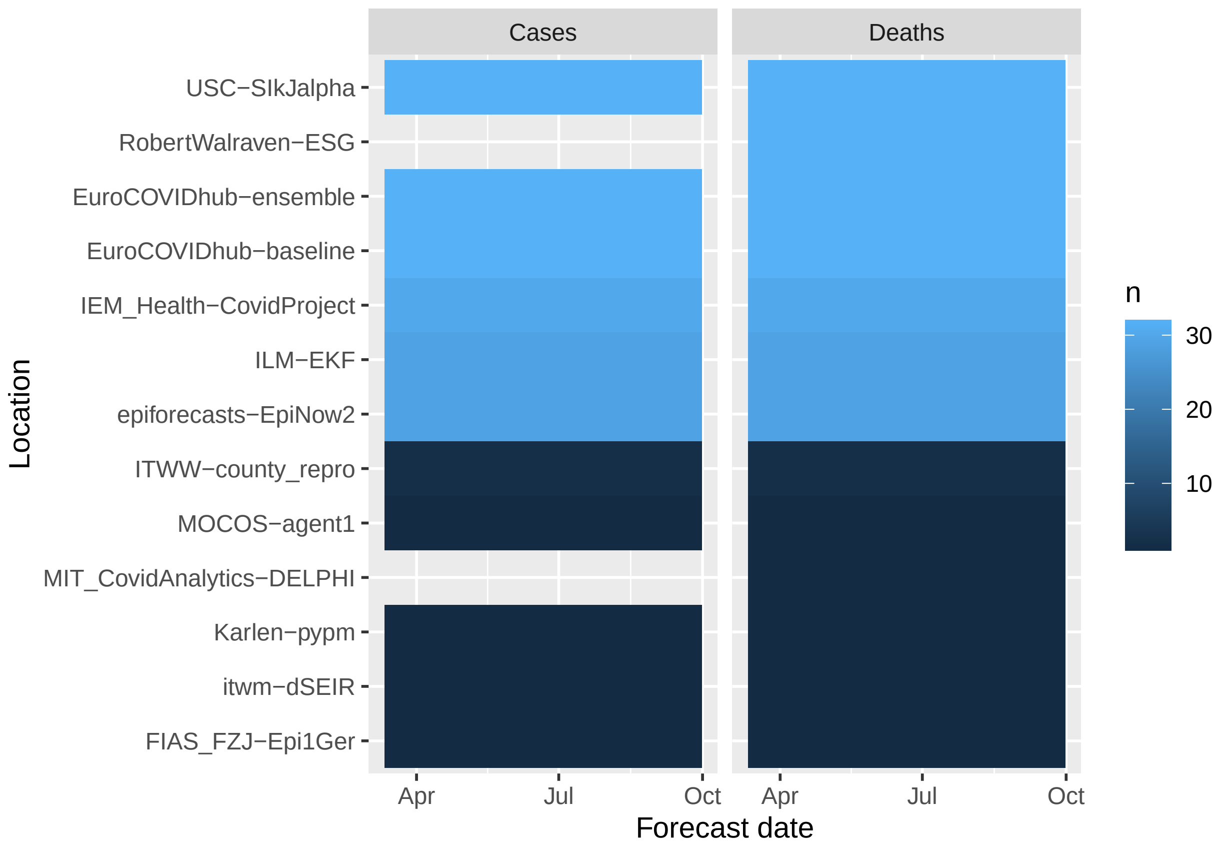


```
print(plot_models_per_loc(hub_complete))
```

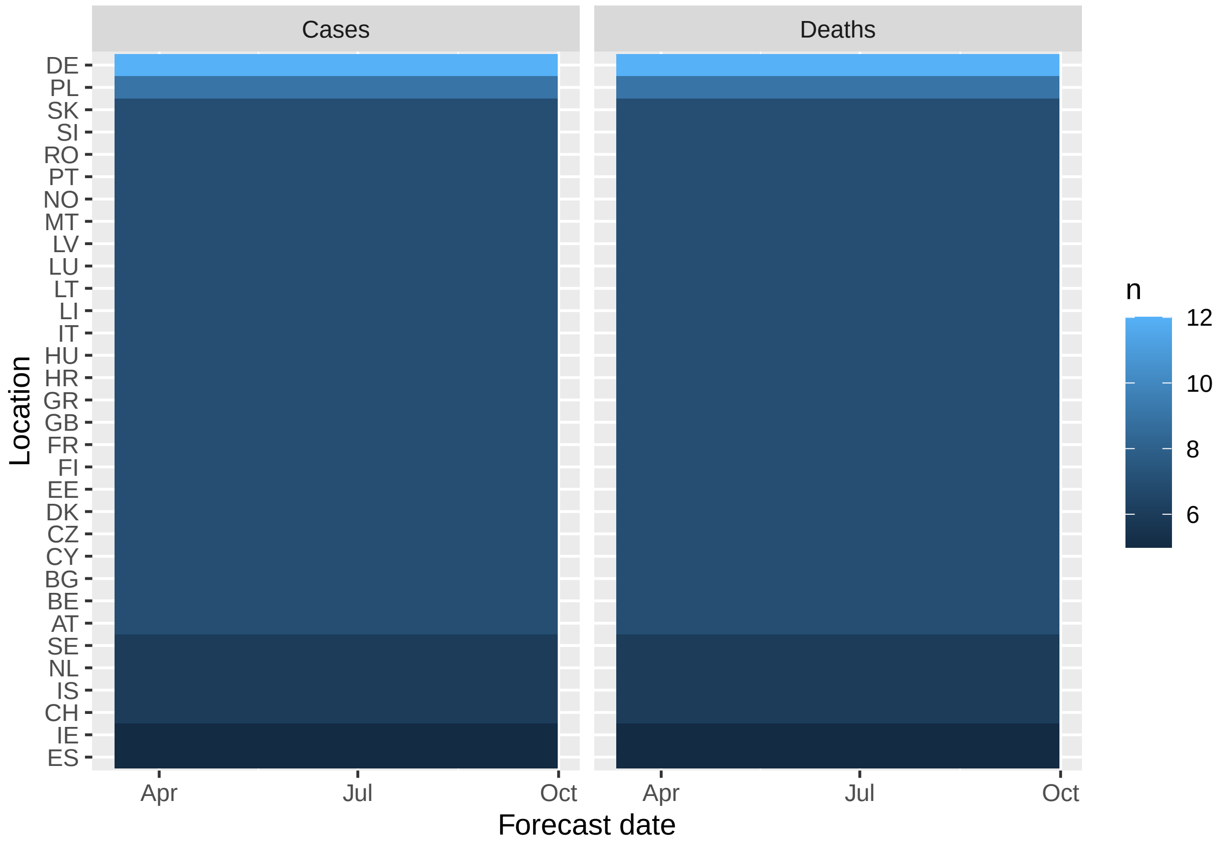


Or allowing different numbers of models per location:

```
hub_complete_loc <- make_complete_set(hub_data, per_location = TRUE)
print(plot_locs_per_model(hub_complete_loc))
```



```
plot_models_per_loc(hub_complete_loc)
```



Updating the European Forecast Hub data (probably not necessary) To update the data, clone the whole repository or use subversion (svn) to only download the relevant folder. Run

```
git clone https://github.com/epiforecasts/covid19-forecast-hub-europe/
```

or

```
svn checkout https://github.com/epiforecasts/covid19-forecast-hub-europe/trunk/data-processed
```

To load the forecasts and truth data and to update the csv files, run

```
# load truth data using the covidHubutils package ------------------------------
devtools::install_github("reichlab/covidHubUtils")
library(covidHubUtils)

truth <- covidHubUtils::load_truth(hub = "ECDC") |>
  filter(target_variable %in% c("inc case", "inc death")) |>
  mutate(target_variable = ifelse(target_variable == "inc case",
                                  "Cases", "Deaths")) |>
  rename(target_type = target_variable,
         true_value = value) |>
  select(-model)

fwrite(truth, "data/weekly-truth-Europe.csv")

# get the correct file paths to all forecasts ----------------------------------
folders <- here("data-processed", list.files("data-processed"))
folders <- folders[
```

```r
  !(grepl("\\.R", folders) | grepl(".sh", folders) | grepl(".csv", folders))
]

file_paths <- purrr::map(folders,
                         .f = function(folder) {
                           files <- list.files(folder)
                           out <- here::here(folder, files)
                           return(out)}) %>%
  unlist()
file_paths <- file_paths[grepl(".csv", file_paths)]

# load all past forecasts ------------------------------------------------------
# ceate a helper function to get model name from a file path
get_model_name <- function(file_path) {
  split <- str_split(file_path, pattern = "/")[[1]]
  model <- split[length(split) - 1]
  return(model)
}

# load forecasts
prediction_data <- map_dfr(file_paths,
                           .f = function(file_path) {
                             data <- fread(file_path)
                             data[, `:=`(
                               target_end_date = as.Date(target_end_date),
                               quantile = as.numeric(quantile),
                               forecast_date = as.Date(forecast_date),
                               model = get_model_name(file_path)
                             )]
                             return(data)
                           }) %>%
  filter(grepl("case", target) | grepl("death", target)) %>%
  mutate(target_type = ifelse(grepl("death", target),
                              "Deaths", "Cases"),
         horizon = as.numeric(substr(target, 1, 1))) %>%
  rename(prediction = value) %>%
  filter(type == "quantile",
         grepl("inc", target)) %>%
  select(location, forecast_date, quantile, prediction,
         model, target_end_date, target, target_type, horizon)

# merge forecast data and truth data and save
hub_data <- merge_pred_and_obs(prediction_data, truth,
                               by = c("location", "target_end_date",
                                      "target_type")) |>
  filter(target_end_date >= "2021-01-01") |>
  select(-location_name, -population, -target)

# split forecast data into two to reduce file size
split <- floor(nrow(hub_data) / 2)

# harmonise forecast dates to be the date a submission was made
hub_data <- mutate(hub_data,
                   forecast_date = calc_submission_due_date(forecast_date))

# function that performs some basic filtering to clean the data
filter_hub_data <- function(hub_data) {

  # define the unit of a single forecast
  unit_observation <- c("location", "forecast_date", "horizon", "model", "target_type")

  h <- hub_data |>
    # filter out unnecessary horizons and dates
    filter(horizon <= 4,
           forecast_date > "2021-03-08") |>
    # filter out all models that don't have all quantiles
    group_by_at(unit_observation) |>
    mutate(n = n()) |>
    ungroup() |>
    filter(n == max(n)) |>
    # filter out models that don't have all horizons
    group_by_at(unit_observation) |>
    ungroup(horizon) |>
    mutate(n = length(unique(horizon))) |>
    ungroup() |>
    filter(n == max(n))

  return(h)
}

hub_data <- filter_hub_data(hub_data)

fwrite(hub_data[1:split, ],
       file = "data/full-data-european-forecast-hub-1.csv")
fwrite(hub_data[(split + 1):nrow(hub_data), ],
       file = "data/full-data-european-forecast-hub-2.csv")
```

Data from the US Forecast Hub

Let me know if you're interested in that as well. The US data set is larger (more models and more locations) and has more models that submitted forecasts for all 50 states.

(Possible) Methods

Potential ensemble types to consider

Mean ensemble (untrained) Quantiles of the predictive distribution are computed as an unweighted mean of the corresponding quantiles of all member models. E.g. the 80%-quantile of the ensemble is the mean of all 80% quantiles of all preditive distributions.

Simple example for a mean ensemble:

```
mean_ensemble <- hub_data %>%
  group_by(location, target_type, target_end_date, true_value, horizon, quantile) %>%
  summarise(prediction = mean(prediction)) %>%
  mutate(model = "mean-ensemble")

scores_mean <- mean_ensemble %>%
```

```r
  eval_forecasts(summarise_by = c("target_type", "model"))
```

Median ensemble (untrained) Quantiles of the predictive distribution are computed as the mean of the corresponding quantiles of all member models.

Simple example for a median ensemble:

```r
median_ensemble <- hub_data %>%
  group_by(location, target_type, target_end_date, horizon, true_value, quantile) %>%
  summarise(prediction = median(prediction)) %>%
  mutate(model = "median-ensemble")

scores_median <- median_ensemble %>%
  eval_forecasts(summarise_by = c("target_type", "model"))
```

Hayman-type ensembles (untrained or potentially trained) In the easy version, essentially quantiles of the predictive distribution are generated by throwing all quantiles from all member forecasts together, sorting them, and taking the desired quantiles of that forecast distribution. This is completely valid approach (with a small caveat in that it assumes equally spaced quantiles).

I need to do some more reading on the more sophisticated versions and can provide some more information.

Mean or median ensembles based on the top X past forecasters (semi-trained) The idea is that you select the best forecasters over a certain training window and then obtain the ensemble as an unweighted mean or median of all forecasts.

Inverse score ensembles For every forecaster, past forecasts are evaluated using the weighted interval score (see below). Forecasters then receive a weight that is equal to the inverse of their weighted interval score over the training period.

Quantile regression averaging (trained) Quantiles of the predictive distribution are computed as a linear combination of the quantiles of all member models. LInear combinations are optimised to minimise the weighted interval score (see below).

In R, this can be done using the `quantgen` package.

Weighted mean ensemble as used by the US Forecast Hub (trained) Need to look up the details and obtain their code.

Weighted median ensemble as used by the US Forecast Hub (trained) Need to look up the details and obtain their code.

Potential analyses

The first step is presumably to set up a framework for generating ensembles (ideally in a way that you could just add / replace different ensembling techniques) and scoring performance.

Evaluating performance depending on the number of member models To that end, one could iteratively sample n models, create an ensemble using those n models and evaluate this ensembles. Then, scores obtained by all possible combinations of those n models get averaged and we can compare average performance for different n.

How does performance of the ensemble variants change if we include or exclude models? Does that differ for different ensemble types?

```
# helper function
create_mean_ensemble <- function(data, members) {
  data %>%
  filter(model %in% members) %>%
  group_by(location, target_end_date, horizon, true_value, target_type, quantile) %>%
  summarise(prediction = mean(prediction)) %>%
  mutate(model = "mean-ensemble")
}

score_forecasts <- function(data) {
  score <- data %>%
    eval_forecasts(summarise_by = c("target_type", "model"))
  return(score$interval_score)
}


models_germany <- hub_data %>%
  filter(location == "DE",
         model != "") %>%
  pull(model) %>%
  unique()

n <- 5

models <- list()
models[[1]] <- sample(models_germany, size = 5)
models[[2]] <- sample(models_germany, size = 5)
#...
# get all posisble combinations

scores <- list()

data_germany <- hub_data %>%
  filter(location == "DE")

for (i in 1:length(models)) {
  ensemble <- create_mean_ensemble(data_germany, members = models[[i]])
  scores[[i]] <- score_forecasts(ensemble)
}

scores
```

Evaluating performance depending on the training period for trained ensembles Shorter training period means an ensemble can adapt more quickly to changing conditions. A longer training period makes sure it doesn't over-correct to past errors and is able to pick up consistently good performance.

Analyse performance of an ensemble depending on the similarity of its member models For every ensemble, a similarity score could be computed by calculating the pairwise Cramér-distance (need to look for available code) between any two member models and taking the average distance across all positive pairs.

Do ensembles which have a higher average distance perform better?

Analyse the impact of adding a model to an ensemble By creating leave-one-out ensembles (the same ensemble with a given model included or excluded) one could analyse the impact that model has on an ensemble. How that impact differ for different ensemble types? Can we identify situations in which a model is beneficial or not? Can a model be beneficial even if it is not a good model?

One potential aspect to look at could again be similarity between models. Does a model contribute more to an ensemble if it is very different from existing models? Does that differ for different ensemble types?

Analyse how stable different ensemble types are Are some ensemble types more or less prone to bad outlier or does performance fluctuate more in general?

Forecast evaluation

Proper scoring rules Forecasts in a quantile-based forecast can be evaluated using the weighted interval score (WIS, lower values are better), a proper scoring rule. Proper scoring rules incentivise the forecaster to state their true best belief and cannot be 'cheated'.

The WIS can be decomposed into three components: a penalty for dispersion (i.e. large forecast uncertainty) as well as penalties for over- and underprediction.

WIS = Dispersion + Over-prediction + Under-prediction

For a single prediction interval, the interval score is computed as

$$IS_\alpha(F, y) = (u - l) + \frac{2}{\alpha} \cdot (l - y) \cdot 1(y \leq l) + \frac{2}{\alpha} \cdot (y - u) \cdot 1(y \geq u),$$

where $1()$ is the indicator function, y is the true value, and l and u are the $\frac{\alpha}{2}$ and $1 - \frac{\alpha}{2}$ quantiles of the predictive distribution F, i.e. the lower and upper bound of a single prediction interval. For a set of K prediction intervals and the median m, the WIS is computed as a weighted sum,

$$WIS = \frac{1}{K + 0.5} \cdot \left(w_0 \cdot |y - m| + \sum_{k=1}^{K} w_k \cdot IS_\alpha(F, y)\right),$$

where w_k is a weight for every interval. Usually, $w_k = \frac{\alpha_k}{2}$ and $w_0 = 0.5$

The WIS is closely related to the absolute error. Over- and under-prediction should therefore also be understood as a form of absolute forecasting error.

Forecast calibration **Coverage** In addition to the WIS it makes sense to look at forecast calibration in terms of interval coverage. On average, all 50% or 90% prediction intervals should ideally cover 50% or 90% of the true observations. By comparing nominal and empirical coverage we can quickly determine whether a model is over- or underconfident.

Bias The over- and under-prediction penalties of the WIS capture absolute forecasting errors. In addition we can examine whether a forecast has relative tendency to over- or under-predict. This is less susceptible to large outlier predictions

PIT histograms

Probability integral transform (PIT) histograms are another way of examining forecast calibration

Evaluating forecasts in R Forecasts can be evaluated in R using the `scoringutils` package.

```r
scores <- eval_forecasts(uk_data,
                         summarise_by = c("model", "target_type"))

scores
```