

Readme for modeling 7Q10s using machine learning

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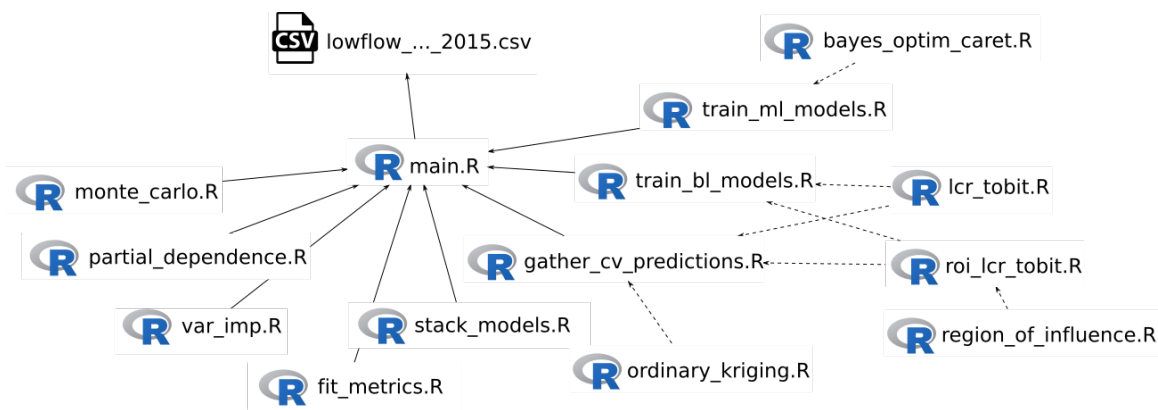
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Introduction

This readme file is intended to serve as a navigation guide for the model archive associated with the paper (citation information). The basic file contents and dependencies look like:



The arrows should be interpreted as “output dependency flow”. The steps should be run in roughly clockwise order. Each primary step can be run directly with “main.R” file via custom R functions that have the same name as the other R files in the figure above. Solid lines indicate primary functions that are sourced directly within “main.R” file, and the dashed lines indicate secondary functions that are sourced by the primary functions. For example, the “train_ml_models.R” file is sourced and run directly by “main.R”, but “train_ml_models.R” is dependent on “bayes_optim_caret.R”. The idea behind structuring the model archive in this way is that output dependencies can be traced directly back to the input data csv file titled “lowflow_sc_ga_al_gagesII_2015.csv”. The steps from the data file to the output should be completely reproducible¹ if functions are run in sequential order.

¹With the exception of possible stochastic differences in model training. This is discussed in more detail in lower sections

Quick start

Although all the scripts are included in the model archive, most of them need not be run to recreate a bulk of the important results. The quickest way to get started is by opening the “main.R” file and setting up the work environment. This includes installing packages and setting the working directory.

```
# Install all packages required for entire analysis. The libraries needed for
# each function are loaded in the function script.
install.packages(c("dplyr", "reshape2", "randomForest", "kknn", "caret",
                  "xgboost", "kernlab", "Cubist", "glmnet", "devtools", "AER",
                  "leaps", "doMC", "ICEbox", "geoR"))

# install PUBAD package off of github
devtools::install_github("wfarmer-usgs/PUBAD")

# load libraries needed for main.R script
library(dplyr); library(PUBAD)

# set working directory
setwd("~/set/working/directoy")
```

The next step is to load the csv file and prepare the data as input for the functions. The only packages that are required for this step are dplyr and PUBAD.

```
# Load csv file: note, data should be in a "data" folder in working directory
data_full <- read.csv("data/lowflow_sc_ga_al_gagesII_2015.csv",
                    header=T, na.strings = "-999") %>%
  setNames(tolower(names(.))) # make column names lower case

# Transform 7Q10 response variable
area <- data_full$drain_sqkm
ln7q10_da <- log((data_full$y7q10+0.001)/area)

# use functions from PUBAD to cull covariates
expVars <- data.frame(gages = data_full$staid) %>%
  getBasinChar()

# create model data using clean basin chars
model_data <- expVars$cleanBCs %>% # start with basin chars
  mutate(CLASS = as.integer(as.factor(CLASS))) %>% # change class to integer
  mutate_each(funs(as.numeric)) %>% # make everything numeric
  scale() %>% # convert to z-score: (x-mu)/sigma
  as.data.frame() %>% # make data frame
  setNames(tolower(names(.))) %>% # make sure colname are lower case
  mutate(y=ln7q10_da) %>% # add the transformed response variable from above
  select(y, class, lat_gage:aspect_eastness) # reorder column positions
```

The raw 7Q10s are divided by the drainage area of the basin and log transformed prior to modelling. Because some of the 7Q10's are zero, a small, arbitrary constant of 0.001 was added to each 7Q10 value prior to taking the log transform. This data transformation for the baseline models is slightly different, and is explained in the “Description of train_bl_models” section below. After the data is loaded, the first steps is to find the optimal hyperparameters of for all of the models using random search and bayesian optimization. This process will take over 24 hours for all of the models, and we already provide the optimal values in the “gather_cv_predictions.R” file. You can go ahead and jump straight to this step. The gather_cv_predictions() function calculates

prediction for each basin and model in a leave-one-out cross validation framework. With that being said, this function will still take ~45 minutes to run.

```
# gather cross validation predictions
source("scripts/gather_cv_predictions.R")
cv_preds <- gather_cv_predictions(model_data,data_full)
```

The next step is to build the ensemble-stacked model using the cross validated predictions calculated in the step above. The output, `all_preds`, is a matrix of the cross validation predictions for all the models and the actual observations. This is the result that is used for the bulk of the analysis.

```
# stacked regression
source("scripts/stack_models.R")
all_preds <- stack_models(cv_preds)
```

Calculate fit metrics using the the cross validation predictions,

```
# calculate fit metrics
source("scripts/fit_metrics.R")
model_error <- fit_metrics(all_preds,data_full)
```

The final steps for this truncated version of the analysis is to calculate variable importance, partial dependence, and make some plots. The paper includes a monte carlo analysis. I do not suggest you try to run the full monte carlo², but the script is included for inspection.

```
# calculate variable importance
source("scripts/var_imp.R")
var_imp_overall <- var_imp(model_data)

# calculate partial dependence
source("scripts/partial_dependence.R")
pdp_data <- partial_dependence(model_data,var_imp_overall)
```

Note that the variable importance and partial dependence don't actually require direct inputs from the other functions above. However, the model selections for the variable importance are based off pieces of the earlier analysis. The very last step is to create plots from the paper:

```
# generate list of plots
source("scripts/make_plots.R")
plots <- make_plots(all_preds,model_error,var_imp_overall,pdp_data)

# display the plots
plots$rmse_vs_unitrmse
plots$pred_vs_obs
plots$error_decomp
plots$var_imp
plots$partial_dep
```

²The monte carlo analysis requires 800 models for all 6 model types using loo-cv cross validation = over 100,000 models

Extended analysis

This section includes more information about determining the hyperparameters of the models and the monte carlo analysis.

Description of train_bl_models

We classified multivariate regression and geostatistical models as “baseline” methods. This classification scheme is used as a way to compare groups of models and does not reflect the complexity, accuracy, or robustness of the method. The models include two versions of censored regression, ordinary kriging, and a unit-area discharge null model. The first thing to note is that the response variable is slightly different for the censored regression models.

```
model_data <- expVars$cleanBCs %>% # start with basin chars
  setNames(tolower(names(.))) %>% # make sure colname are lower case
  mutate(class = as.integer(as.factor(class))) %>% # change class to integer
  mutate(drain_sqkm = log(drain_sqkm)) %>%
  mutate_each(funs(as.numeric)) %>% # make everything numeric
  scale() %>% # convert to z-score: (x-mu)/sigma
  as.data.frame() %>% # make data frame
  mutate(y=data_full$y7q10+0.001) %>%
  mutate(y=log(y)) %>%
  select(y, class:aspect_eastness)
```

If you compare this setup to the `model_data` setup above, you will notice that the response variable is slightly different. This is because the the censored regression functions require a unique censoring value. In raw 7Q10 space, this is normally just zero. If we add a small constant to the 7Q10's and normalize them by their drainage basins, then there is no longer a unique censoring value (because the drainage basin areas are different). Therefore, we just take the natural log of the $7Q10 + 0.001$ and censor as $\ln(0.001)$.

The only two models that require tuning are the two versions of the censored regression models. For example, the full censored regression model requires selecting a subset of predictors using best subset selection. It is impossible to know which predictors or the best selection algorithm to select apriori, so this is tunes using cross validation. The first step is to create a grid of possible values:

```
# tune parameter grid for lcr_tobit
lcr_grid <- expand.grid(subset_method=c("forward", "backward"),
  subset_number=c(2,4,8,10,12))

print(lcr_grid)
```

##	subset_method	subset_number
## 1	forward	2
## 2	backward	2
## 3	forward	4
## 4	backward	4
## 5	forward	8
## 6	backward	8
## 7	forward	10
## 8	backward	10
## 9	forward	12
## 10	backward	12

and in this case, 10 different models are built inside a loo-cv framework and the RMSE is recorded for each

model. The model with the lowest RMSE is selected as the final model. This process is referred to a “grid search”.

```
lcr_tune_error <- numeric()
for (i in 1:nrow(lcr_grid)){

  # fit model with values from grid
  fit <- lcr.tobit(model_data,
                  subset_method=as.character(lcr_grid[i,1]),
                  subset_number=lcr_grid[i,2],
                  thold=log(0.001))

  # record rmse for ith model
  lcr_tune_error[i] <- sqrt(mean((fit$obs-fit$pred)^2,na.rm=T))
}
```

A similar process is done for the region of influenced censored regression model, but with an additional “neighbors” hyperparameters.

```
# tune parameter grid for ROI lcr_tobit
roi_grid <- expand.grid(neighbors=seq(25,200,25),
                      subset_method=c("forward","backward"),
                      subset_number=c(2,4,8,10,12))

roi_tune_error <- numeric()
for (i in 1:nrow(roi_grid)){

  # fit model with values from grid
  fit <- roi.lcr.tobit(model_data,
                     neighbors=roi_grid[i,1],
                     subset_method=as.character(roi_grid[i,2]),
                     subset_number=roi_grid[i,3],
                     thold=log(0.001))

  # record rmse for ith model
  roi_tune_error[i] <- sqrt(mean((fit$obs-fit$pred)^2,na.rm=T))
}
```

Description of train_ml_models

The process for the machine learning models is conceptually similar to the baseline models, but is much more computationally expensive. This basic pipeline involves (1) generating a bunch of points in hyperparameters and RMSE space to be used as substrate for a gaussian process model, and (2) use bayesian optimization to estimate the functional relationship between the hyperparameters and the RMSE. The gaussian process model attempts to discover a function that relates values of the hyperparameters to an output, in this case, the RMSE. Then an optimization function is used to seek for the combination of parameters where the function is maximized. Theoretically this should result in a set of optimal hyperparameters for a given model. Below is an example using a cubist model. There are only two hyperparameters for a cubist model, the number of *neighbors* and the number of *committees*. The number of nodes used in the smoothed-prediction process is referred to as *neighbors*. The predictions from single-tree cubist model can be improved using a boosting-like ensemble method where subsequent trees are built using the residuals from the single tree. The number of trees used in the ensemble is referred to as *committees*. We don't know what values to select apriori, so we use the steps above. I have automated this process using a custom function that is a wrapper

around both the `train` function from the `caret` package and the `BayesianOptimization` function from the `rBayesianOptimization` package.

```
library(caret)
source('scripts/bayes_optim_caret.R')

# list of parameter boundaries
cubist_bounds <- list(committees = c(1L,100L),
                      neighbors = seq(0L,9L))

# pass to custom function
cubist_params <- bayes_optim_caret(model_data, 'cubist', cubist_bounds, iter=30)
```