Canadian climate: function-on-function regression

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The dataset was originally analyzed by Fuchs et al. (2015). The results of this vignette together with more explanations can be found in Brockhaus et al. (2015).

1 Load and plot data

Load FDboost package.
Load data and compute the first derivative.

```r
data(fuelSubset)
fuel <- fuelSubset
str(fuel)
```

List of 7

- `$heatan` : num [1:129] 26.8 27.5 23.8 18.2 17.5 ...
- `$h2o` : num [1:129] 2.3 3 2 1.85 2.39 ...
- `$nir.lambda` : num [1:231] 800 803 805 808 810 ...
- `$NIR` : num [1:129, 1:231] 0.2818 0.2916 -0.0042 -0.034 -0.1804 ...
- `$uvvis.lambda` : num [1:134] 250 256 261 267 273 ...
- `$UVVIS` : num [1:129, 1:134] 0.145 -1.584 -0.814 -1.311 -1.373 ...
- `$h2o.fit` : num [1:129] 2.58 3.43 1.83 2.03 3.07 ...

# normalize the wavelength to 0-1
# fuel$nir.lambda0 <- (fuel$nir.lambda - min(fuel$nir.lambda)) /
# (max(fuel$nir.lambda) - min(fuel$nir.lambda))
# fuel$uvvis.lambda0 <- (fuel$uvvis.lambda - min(fuel$uvvis.lambda)) /
# (max(fuel$uvvis.lambda) - min(fuel$uvvis.lambda))

# compute first derivatives as first order differences
fuel$dUVVIS <- t(apply(fuel$UVVIS, 1, diff))
fuel$dNIR <- t(apply(fuel$NIR, 1, diff))

# get the wavelength for the derivatives
fuel$duvvis.lambda <- fuel$uvvis.lambda[-1]
fuel$dnir.lambda <- fuel$nir.lambda[-1]

Compute the model to predict humidity. The predicted humidity is contained already in the dataset `fuel`.

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2 Model to predict humidity

We consider the following regression model to predict the humidity.

\[ E(Y_i) = \int \text{NIR}_i(s_1)\beta_1(s_1)ds_1 + \int \text{UVVIS}_i(s_2)\beta_2(s_2)ds_2 + \int d\text{NIR}_i(s_3)\beta_1(s_3)ds_3 + \int d\text{UVVIS}_i(s_4)\beta_2(s_4)ds_4, \]

with \( Y_i \) being the humidity and \( \text{NIR, UVVIS} \) are the spectra and \( d\text{NIR, dUVVIS} \) the respective derivatives, measured over \( s_1, \ldots, s_4 \) respectively. The optimal stopping iteration is determined by 10-fold bootstrap (better use multiple cores).

```r
modH2O <- FDboost(h2o ~ bsignal(UVVIS, uvvis.lambda, knots=40, df=4) + bsignal(NIR, nir.lambda, knots=40, df=4) + bsignal(dUVVIS, duvvis.lambda, knots=40, df=4) + bsignal(dNIR, dnir.lambda, knots=40, df=4), timeformula="bols(1), data=fuel")
```

```r
cvmH2O <- suppressWarnings(cvrisk(modH2O, grid=seq(100, 5000, by=100), folds=cv(model.weights(modH2O), type = "bootstrap", B = 10), mc.cores = 1))
```

```r
par(mfrow=c(1,2))
plot(cvmH2O)
modH2O[mstop(cvmH2O)]
#modH2O[2400]
```  

```r
### create new variable of predicted h2o
h2o.fit <- modH2O$fitted()
plot(fuel$h2o, h2o.fit)
aline(0,1)
```

3 Model to predict heat value

We consider the following regression model to predict the heat values.

\[ E(Y_i) = \int \text{NIR}_i(s_1)\beta_1(s_1)ds_1 + \int \text{UVVIS}_i(s_2)\beta_2(s_2)ds_2, \]

with \( Y_i \) being the heat value and \( \text{NIR and UVVIS} \) are the spectra, measured over \( s_1 \) and \( s_2 \) respectively.

```r
formula <- formula(heatan ~ bsignal(UVVIS, uvvis.lambda, knots=40, df=4.41) + bsignal(NIR, nir.lambda, knots=40, df=4.41))
## do a model fit:
mod <- FDboost(formula, timeformula="bols(1), data=fuel")
mod <- mod[198]
```

The optimal stopping iteration is determined by 50-fold bootstrap. We compute in each bootstrap-sample the coefficient functions to get an idea of the variability of the estimates (better use multiple cores).

```r
## get optimal mstop and do bootstrapping for coefficient estimates
set.seed(2703)
val <- validateFDboost(mod, folds=cv(model.weights(mod), type = "bootstrap", B = 50),
```

```r
```
Figure 1: Coefficient estimates for the effects of the two spectra.

Figure 2: Coefficient estimates for the effects of the two spectra.

```r
grid = 10:500, mc.cores = 1)

mopt <- val$grid[which.min(colMeans(val$oobrisk))]
print(mopt)
## use optimal mstop
mod <- mod[mopt] # 198

Plot the coefficient functions.

par(mfrow=c(1,2))
plot(mod, which=1, lwd=2, lty=5, rug=FALSE, ylab="", xlab="wavelength [nm]")

plot(mod, which=2, lwd=2, lty=5, rug=FALSE, ylab="", xlab="wavelength [nm]")
```
References
