

Task description

Given the present dataset on the behaviour and personal characteristics of the clients, build an ML model best suited to estimate future medical expenditures

Coming next:

Dataset inspection and preparation: >

Original dataset inspection

1338 observations of 8 variables

	Characteristics						
	Independent variables Dependent variable						
Name of the variable	age	sex	bmi	children	smoker	region	expenses
Values	Numeric	Male/female	Numeric	Numeric	Yes/No	Northeast/ northwest/ southeast/ southwest	Numeric

7IV's and 1 DV

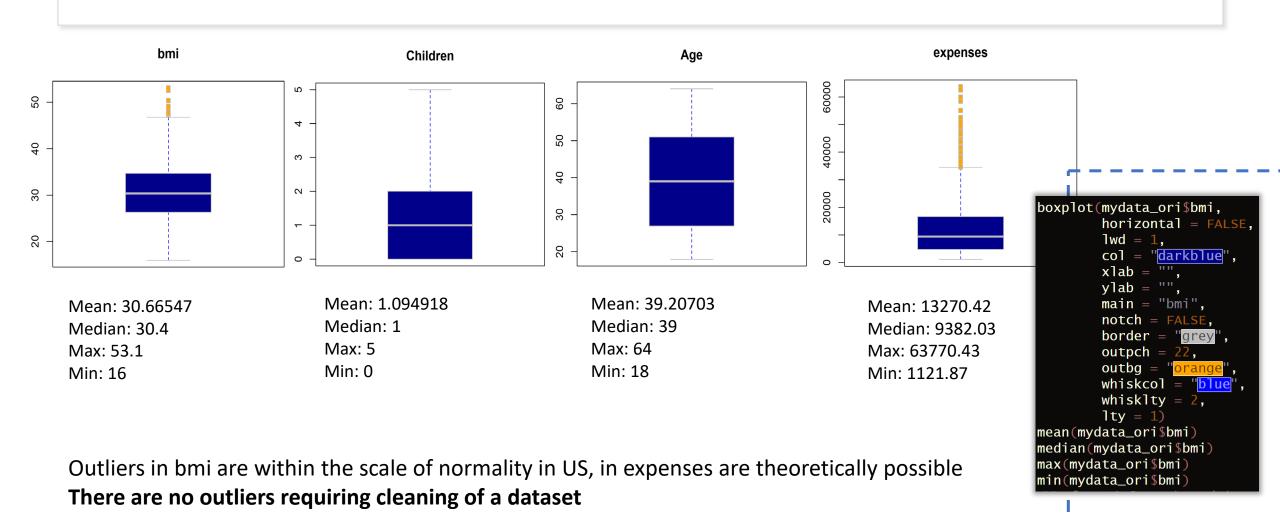
No N/A values

Factor variables: sex, smoker, region

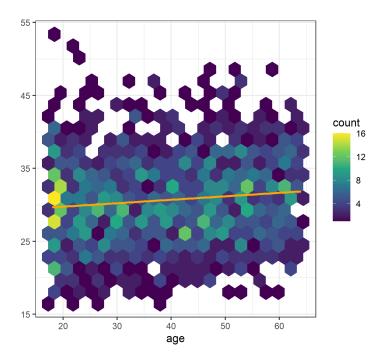
Creating dummy variables

age	sexmale	bmi	children	smokeryes	regionnorthwest	regionsoutheast	regionsouthwest	expenses
Numerio	If male = 1 If not =0	Numeric	Numeric	If smoker = 1 If not = 0	If northwest = 1 If not = 0	If southeast = 1 If not = 0	If southwest = 1 If not = 0	Numeric

Outliers research for nondummy variables



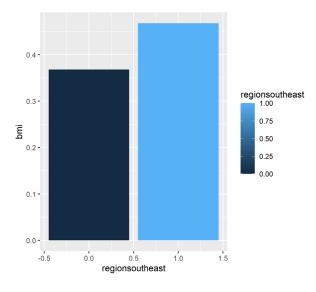
Biggest IV-correlations



Corr = 0.107457

Explainable by biological aspects

```
ggplot(mydata_v1, aes(x=age, y=bmi) )
+ geom_hex(bins = 20)
+ scale_fill_continuous(type = "viridis")
+ theme_bw()
+ geom_smooth(method = "lm", se = FALSE,col="orange")
```



Corr = 0.269927945

Explainable by regional cuisine: might be rational to retrieve more in-depth regional data

Or even conduct a field research!

Default prediction and default RSS and trControl

- default.pred (Mean of expenses): 0.1987984
- Default residual sum of squares (training): 41.37523
- Default residual sum of squares (test): 8.613895

trControl: repeated cross-validation: 10-fold, 2 repeats

We encountered instable results during grid selection for neural networks, so decided to improve stability with repeats

```
#Mean of the dependent variable:
default.pred <- mean(mydata_v3.train$expenses)
default.pred

#ESS for training and training set compared to default
default.train.rss <- sum((mydata_v3.train$expenses-default.pred)^2)
default.train.rss
default.test.rss <- sum((mydata_v3.test$expenses-default.pred)^2)
default.test.rss</pre>
```

Coming next:

Creating and adjusting models: >

OLS

Multiple R2:	
0.753285471	Values of coefficients
(Intercept)	-0.049353 (0.010757) ***
age	0.178726 (0.010023) ***
sexmale	-0.00346 (0.006042)
bmi	0.210286 (0.019317) ***
children	0.044712 (0.012472) ***
smokeryes	0.385820 (0.007342) ***
regionnorthwest	-0.00889 (0.008613)
regionsoutheast	-0.013671 (0.008647)
regionsouthwest	-0.015437 (0.008651)

R2 for training set: 0.7533

Pseudo R2 for test set: 0.7367

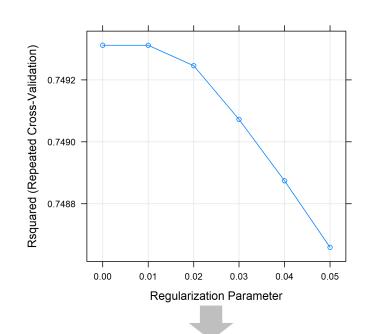
Not the best predictive quality: Highly likely that the relationship Is not linear.

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ''1

Ridge regression

Tuning grid (Alpha = 0)

Lambda	RMSE	Rsquared	MAE
0	0.09908424	0.749312	0.07016327
0.01	0.09908424	0.749312	0.07016327
0.02	0.09954816	0.7492457	0.07081842
0.03	0.10084844	0.7490722	0.07248005
0.04	0.10242469	0.7488739	0.07421301
0.05	0.10417994	0.7486586	0.07595175



Radical drop for Rsquared on training is observed after lambda>0.01

Best tune:

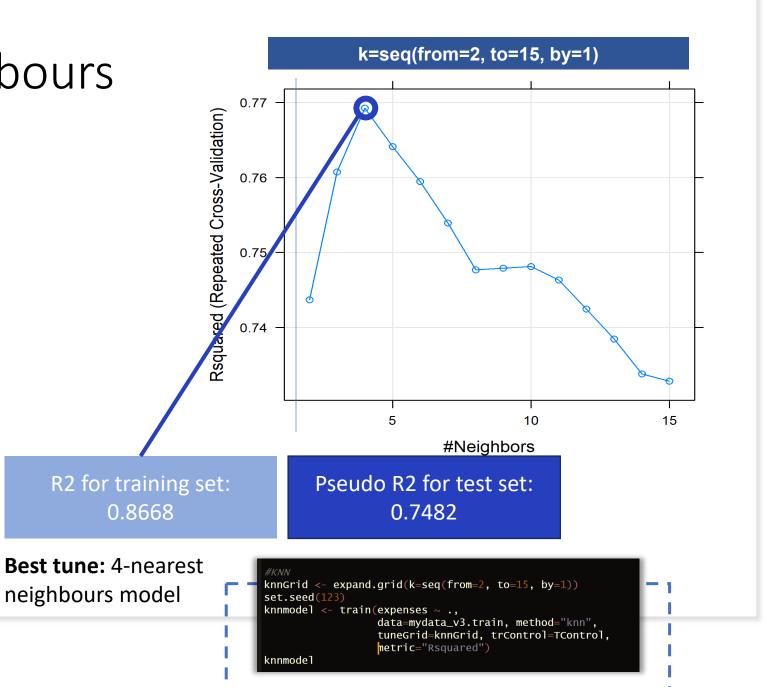
Alpha=0 Lambda = 0.01 R2 for training set: 0.7507

Pseudo R2 for test set: 0.7377

Did not improve the results radically, trying support vector regression.

K-Nearest neighbours

k	RMSE	Rsquared
2	0.100108	0.743676
3	0.096258	0.760743
4	0.094312	0.769267
5	0.095359	0.764131
6	0.096407	0.759458
7	0.097445	0.753921
8	0.098635	0.747705
9	0.098612	0.747886
10	0.098622	0.748135
11	0.099009	0.746331
12	0.099753	0.742467
13	0.100556	0.738475
14	0.101373	0.733812
15	0.101613	0.732828



Kernel regressions

Linear

Tuning grid (eps <- 0.1)

J
0.01
0.11
0.21
0.31
0.41
0.51
0.61
0.71

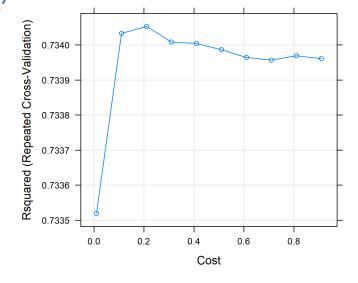
0.81

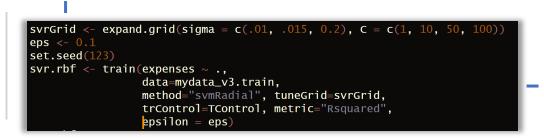
0.91

Best tune: c = 0.21

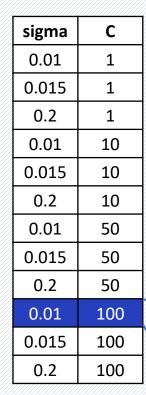
R2 for training set: 0.6999

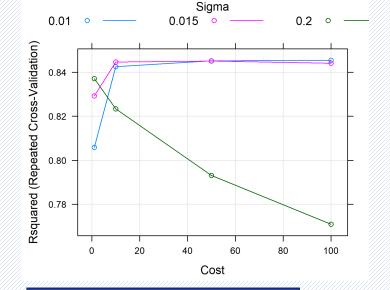
Pseudo R2 for test set: 0.6685





Radial





Pseudo R2 for test set: 0.8307

R2 for training set: 0.8523

Best tune:

sigma = 0.01C = 100

Conclusions so far

Radial Kernel regression gives the best results: it means that the relationship is not linear. Using neural network-based regressions might be useful

For this the authors use not only Caret package, but also "NeuralNetTools", for the intermediary visualization of the trees

Coming next:

Neural network-based regressions: >

Neural network – 1 hidden layer

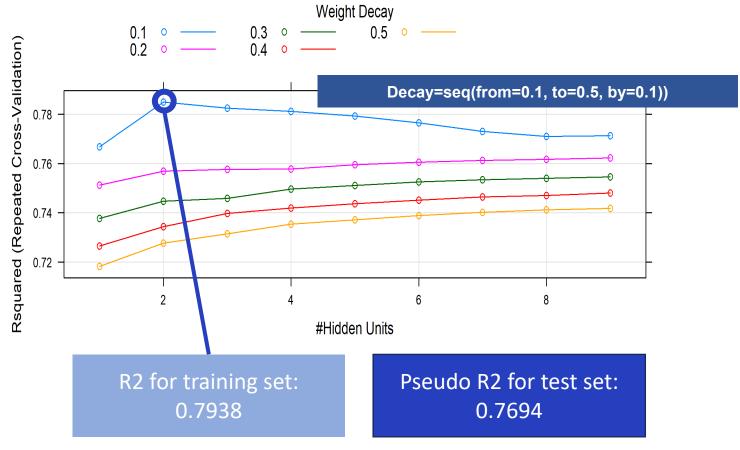
Tuning grid:

Hidden layer size: from 1 to 8

Decay: 0.1,0.2,0.3,0.5

Proposal for adjustment:

To provide more detailed research on decay hyperparameter



Best tune: (8)-2-(1) Neural network with decay = 0.1

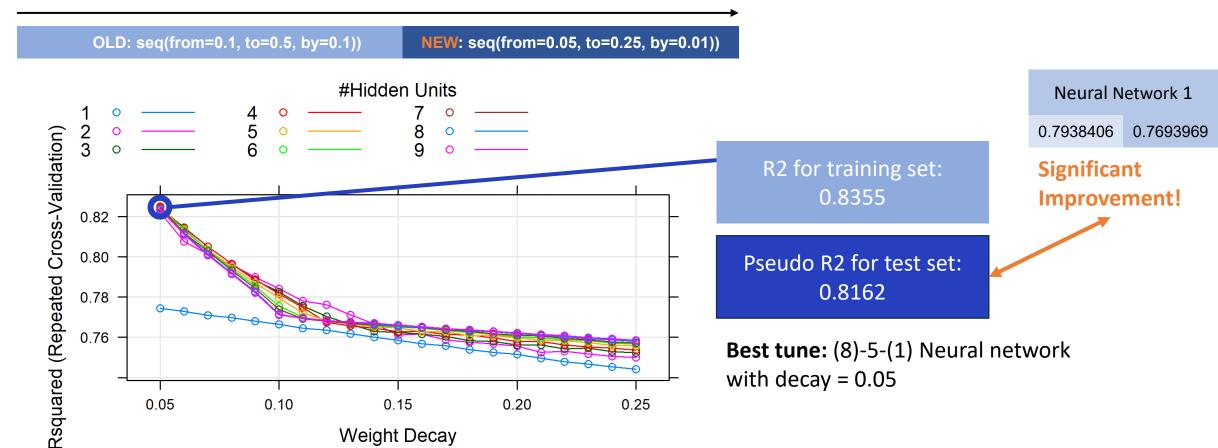
Neural network – 1 hidden layer + decay

adjusted

nnGrid_1 <- expand.grid(size=1:8,</pre> decay = seq(from = 0.05, to = 0.25, by = 0.01))



Weight Decay



Neural network – multiple layers

Tuning grid:

Layer 1: from 0 to 8 layers

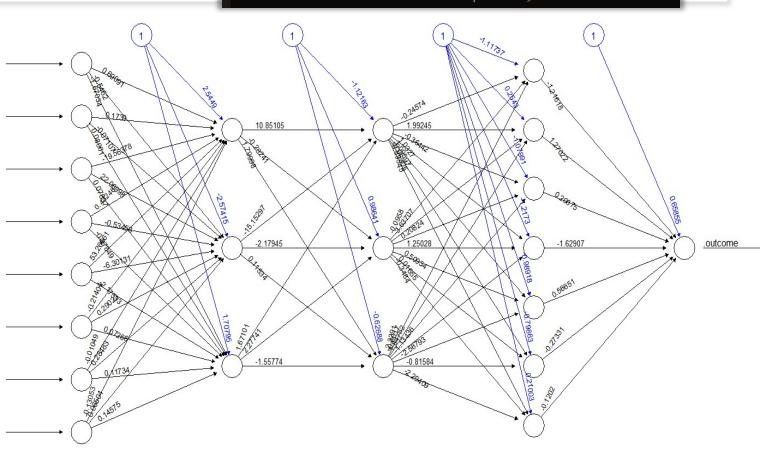
Layer 2: from 1 to 8 layers

Layer 3: from 1 to 8 layers

R2 for training set: 0.8673

Pseudo R2 for test set: 0.8531

Best tune: (8)-3-3-8-(1) Neural network



Random forest — without optimization

Tuning grid: Standard: mtry = 2,5,8

mtry	RMSE	Rsquared	MAE
2	0.084449	0.842333	0.057702
5	0.074729	0.852679	0.041999
8	0.076909	0.844876	0.043334

Best tune: mtry = 5

Model is overfit.

Is there an opportunity to optimize the result?

R2 for training set: 0.9573

Pseudo R2 for test set: 0.8481

Coming next:

Deep-Dark forest: →

Deep-Dark Forest: logic of optimization

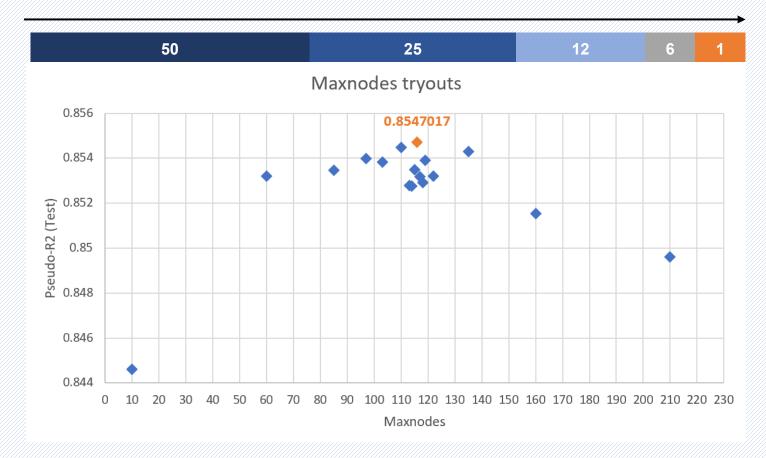
Usually to optimize Random Forest, the cycle is used to find optimal "maxnodes" hyperparameter.

However, usually steps which are used are large.

By using repeatedcy, we allowed ourselves **the stability** to make the cycle step smaller. But not **the time**.

So we thought of a logic of recursively decreasing steps to "scope in" to the optimal result of maxnodes. (see on the right)

Navigating by decreasing steps to find the optimized number of max nodes



Deep-Dark Forest: logic of optimization

```
for (maxnodes in c(10,60,110,160,210)) { set.seed(123) rfmodel <- train(expenses \sim ., data=myda for (maxnodes in c(60,85,110,135,160)) { set.seed(123) rfmodel <- train(expenses \sim ., data=myda
```

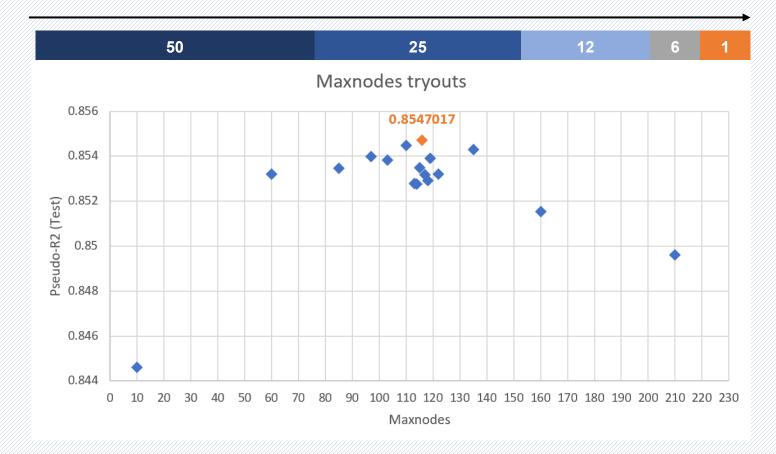
As a result, optimal number of maxnodes was found at maxnodes=116, which allowed to receive the following results:

R2 for training set: 0.9274

Pseudo R2 for test set: 0.8547

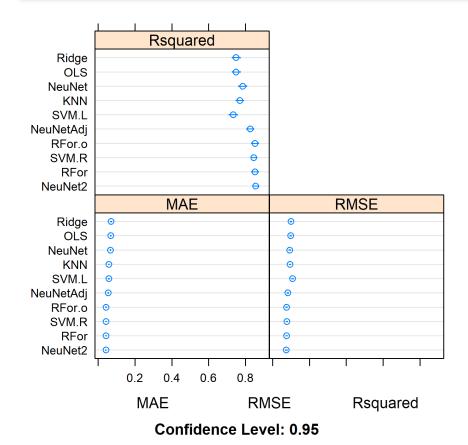
Best tune: maxnodes = 116

This result can be perceived as overfit, however the method used might be relevant for future optimization problems Navigating by decreasing steps to find the optimized number of max nodes



Final results

- Optimized Random Forest seems overfit, however still performs on test set
- The optimal algorithm is thus multi-layered Neural network (neuralnet method) with (8)-3-3-8-(1) configuration



Model	R2.Train	R2.Test	Hyperparameters
Random Forest optimized	0.927427	0.854702	maxnodes = 116
Neural Network Multi- Layer	0.867340	0.853113	(8)-3-3-8-(1) Neuralnet
Random Forest	0.957386	0.848082	mtry=5
Radial SVR	0.852334	0.830719	sigma = 0.01, Cost = 100
Neural Network Single-	0.835498	0.816199	(8)-5-(1) Nnet
Layer Adjusted Decay			decay = 0.05
Neural Network Single-	0.793841	0.769397	(8)-2-(1) Nnet
Layer			decay = 0.1
k-NN	0.866813	0.748233	k=4
Linear Regression	0.753285	0.736734	ı
Ridge Regression	0.750788	0.736660	Alpha=0, Lambda = 0.01
Linear SVR	0.699909	0.668502	c = 0.21

Thank you for the attention!

We are open for questions!

