1]Alex BOULANGE - aboul@free.fr

automl R package vignette

[

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Contents

0.1 Introduction to automl package

This document is intended to answer the following questions; why & how automl and how to use it

automl package provides:
-Deep Learning last tricks (those who have taken Andrew NG's MOOC on Coursera will be in familiar territory)
-hyperparameters autotune with metaheuristic (PSO)
-experimental stuff and more to come (you're welcome as coauthor!)

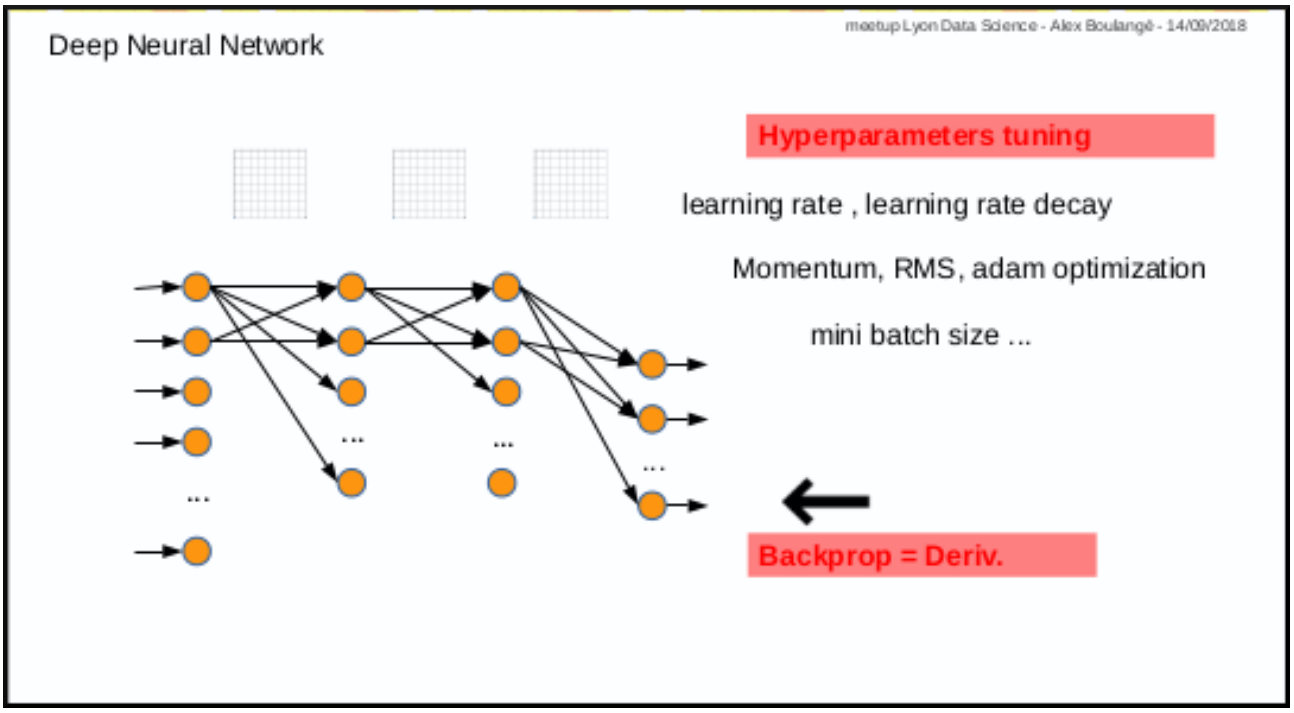
0.2 Why & how automl

0.2.1 Deep Learning existing frameworks, disadvantages

Deploying and maintaining most Deep Learning frameworks means: Python...
R language is so simple to install and maintain in production environments that it is obvious to use a pure R based package for deep learning !

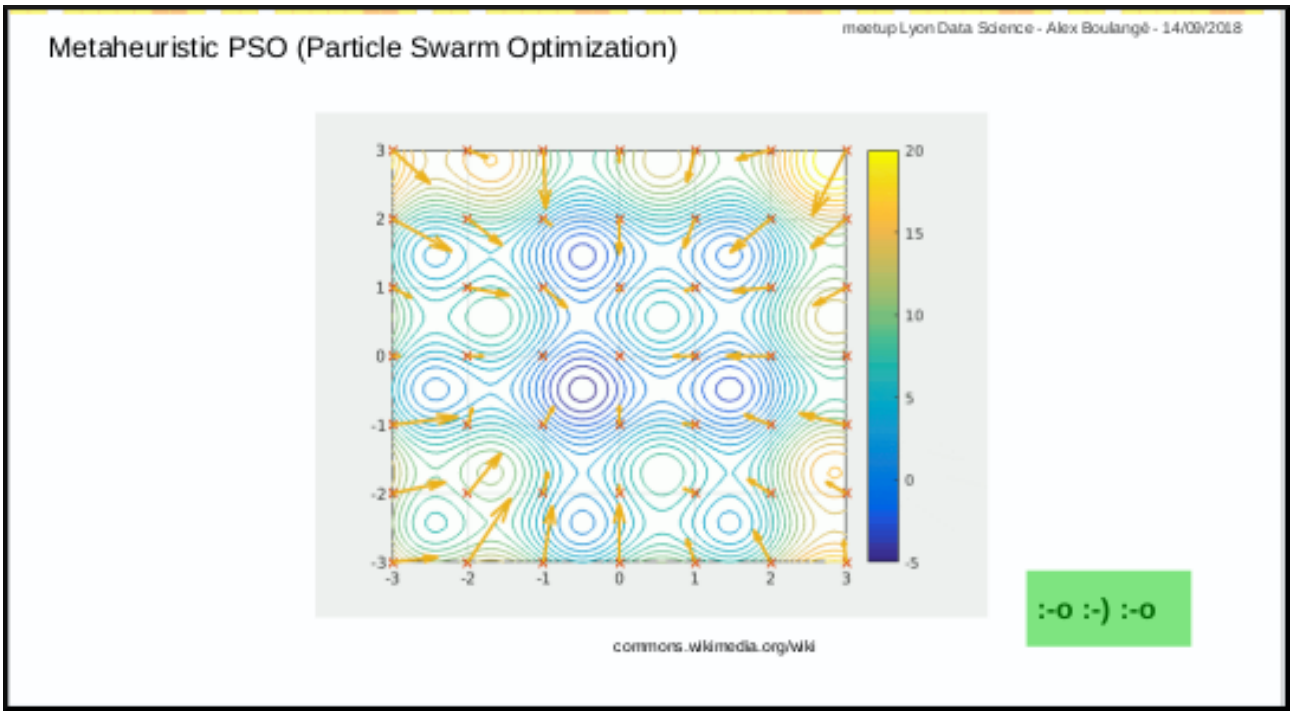
0.2.2 Neural Network - Deep Learning, disadvantages

Disadvantages :
1st disadvantage: you have to test manually different combinations of parameters (number of layers, nodes, activation function, etc ...) and then also tune manually hyper parameters for training (learning rate, momentum, mini batch size, etc ...)
2nd disadvantage: only for those who are not mathematicians, calculating derivative in case of new cost or activation function, may by an issue.



0.2.3 Metaheuristic - PSO, benefits

The Particle Swarm Optimization algorithm is a great and simple one.
In a few words, the first step consists in throwing randomly a set of particles in a space and the next steps consist in discovering the best solution while converging.



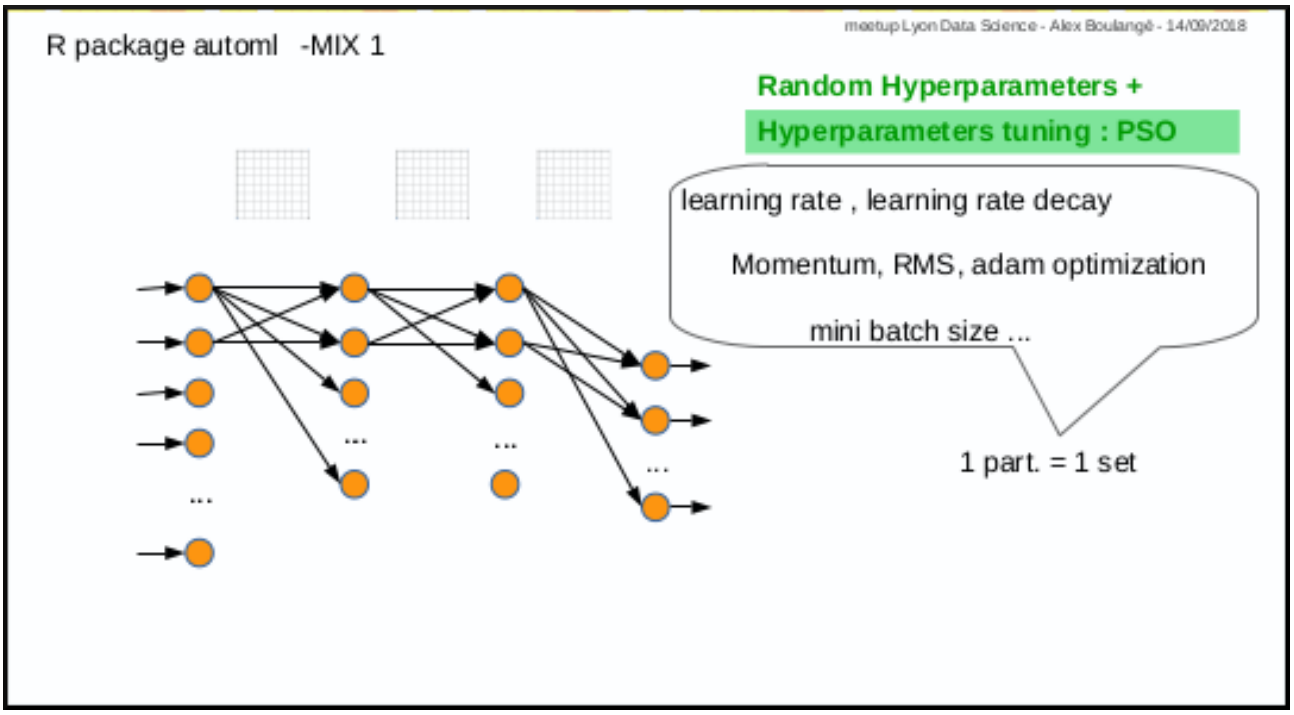
video tutorial from Yarpiz is a great ressource

0.2.4 Birth of automl package

automl package was born from the idea to use metaheuristic PSO to address the identified disadvantages above.
And last but not the least reason: use R and R only :-)
3 functions are available:
- automl_train_manual: the manual mode to train a model
- automl_train: the automatic mode to train model
- automl_predict: the prediction function to apply a trained model on datas

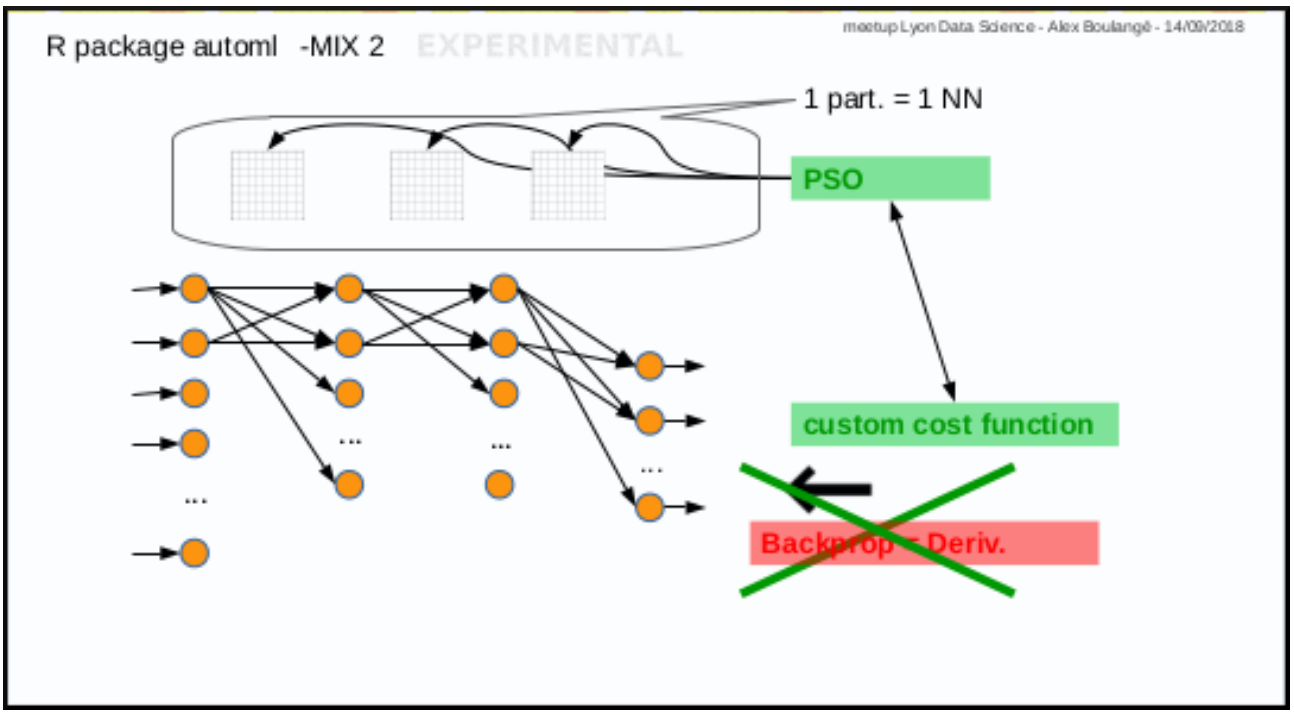
0.2.5 Mix 1: hyperparameters tuning with PSO

Mix 1 consists in using PSO algorithm to optimize the hyperparameters: each particle corresponds to a set of hyperparameters.
The automl_train function was made to do that.



0.2.6 Mix 2: PSO instead of gradient descent

Mix 2 is experimental, it consists in using PSO algorithm to optimize the weights of Neural Network in place of gradient descent: each particle corresponds to a set of neural network weights matrices.
The automl_train_manual function do that too.



0.3 First steps: How to

For those who will laugh at seeing deep learning with one hidden layer and the Iris data set of 150 records, I will say: you're perfectly right :-)
The goal at this stage is simply to take the first steps

0.3.1 fit a regression model manually (hard way)

Subject: predict Sepal.Length given other Iris parameters
1st with gradient descent and default hyperparameters value for learning rate (0.001) and mini batch size (32)

```
data(iris)
xmat <- cbind(iris[,2:4], as.numeric(iris$Species))
ymat <- iris[,1]
amlmodel <- automl_train_manual(Xref = xmat, Yref = ymat)
```

```
(cost: mse)
cost epoch10: 20.9340400047156 (cv cost: 25.205632342013) (LR:  0.001 )
cost epoch20: 20.6280923387762 (cv cost: 23.8214521197268) (LR:  0.001 )
cost epoch30: 20.3222407903838 (cv cost: 22.1899741289456) (LR:  0.001 )
cost epoch40: 20.0217966054298 (cv cost: 21.3908446693146) (LR:  0.001 )
cost epoch50: 19.7584058034009 (cv cost: 20.7170232035934) (LR:  0.001 )
   dim X: ...
```

```
res <- cbind(ymat, automl_predict(model = amlmodel, X = xmat))
colnames(res) <- c('actual', 'predict')
head(res)
```

```
     actual   predict
[1,]    5.1 -2.063614
[2,]    4.9 -2.487673
```

```
[3,]    4.7 -2.471912
[4,]    4.6 -2.281035
[5,]    5.0 -1.956937
[6,]    5.4 -1.729314
```

:-[] no pain, no gain ...

After some manual fine tuning on learning rate, mini batch size and iterations number (epochs):

```
data(iris)
xmat <- cbind(iris[,2:4], as.numeric(iris$Species))
ymat <- iris[,1]
amlmodel <- automl_train_manual(Xref = xmat, Yref = ymat,
                                hpar = list(learningrate = 0.01,
                                            minibatchsize = 2^2,
                                            numiterations = 30))
```

```
(cost: mse)
cost epoch10: 5.55679482839698 (cv cost: 4.87492997304325) (LR:  0.01 )
cost epoch20: 1.64996951479802 (cv cost: 1.50339773126712) (LR:  0.01 )
cost epoch30: 0.647727077375946 (cv cost: 0.60142564484723) (LR:  0.01 )
   dim X: ...
```

```
res <- cbind(ymat, automl_predict(model = amlmodel, X = xmat))
colnames(res) <- c('actual', 'predict')
head(res)
```

```
     actual  predict
[1,]    5.1 4.478478
[2,]    4.9 4.215683
[3,]    4.7 4.275902
[4,]    4.6 4.313141
[5,]    5.0 4.531038
[6,]    5.4 4.742847
```

Better result, but with human efforts!

0.3.2 fit a regression model automatically (easy way, Mix 1)

Same subject: predict Sepal.Length given other Iris parameters

```
data(iris)
xmat <- as.matrix(cbind(iris[,2:4], as.numeric(iris$Species)))
ymat <- iris[,1]
start.time <- Sys.time()
amlmodel <- automl_train(Xref = xmat, Yref = ymat,
                         autopar = list(psopartpopsize = 15,
                                        numiterations = 5,
                                        nbcores = 4))
end.time <- Sys.time()
cat(paste('time ellapsed:', end.time - start.time, '\n'))
```

```
(cost: mse)
iteration 1 particle 1 weighted err: 23.08807 (train: 20.43233 cvalid: 13.79297 ) BEST MODEL KEPT
iteration 1 particle 2 weighted err: 23.29786 (train: 20.80544 cvalid: 14.57438 )
iteration 1 particle 3 weighted err: 21.37242 (train: 20.49244 cvalid: 18.29247 ) BEST MODEL KEPT
iteration 1 particle 4 weighted err: 22.44818 (train: 21.07049 cvalid: 17.62624 )
iteration 1 particle 5 weighted err: 25.90267 (train: 20.79786 cvalid: 23.98837 )
iteration 1 particle 6 weighted err: 23.10971 (train: 21.0241 cvalid: 22.3276 )
iteration 1 particle 7 weighted err: 20.63938 (train: 20.56765 cvalid: 20.38834 ) BEST MODEL KEPT
iteration 1 particle 8 weighted err: 25.00172 (train: 20.13291 cvalid: 23.17591 )
iteration 1 particle 9 weighted err: 22.1777 (train: 20.7751 cvalid: 17.26859 )
```

```
iteration 1 particle 10 weighted err: 15.92525 (train: 13.59336 cvalid: 15.05079 ) BEST MODEL KEPT
iteration 1 particle 11 weighted err: 19.86139 (train: 19.28898 cvalid: 17.85796 )
iteration 1 particle 12 weighted err: 21.90814 (train: 21.05856 cvalid: 18.93462 )
iteration 1 particle 13 weighted err: 13.64409 (train: 12.87311 cvalid: 10.94568 ) BEST MODEL KEPT
iteration 1 particle 14 weighted err: 23.06805 (train: 20.8384 cvalid: 15.26429 )
iteration 1 particle 15 weighted err: 22.33673 (train: 20.87946 cvalid: 17.23627 )
...
iteration 3 particle 1 weighted err: 4.51508 (train: 0.12889 cvalid: 2.87026 )
iteration 3 particle 2 weighted err: 1.0349 (train: 0.81318 cvalid: 0.25888 ) BEST MODEL KEPT
iteration 3 particle 3 weighted err: 0.16113 (train: 0.15751 cvalid: 0.14845 ) BEST MODEL KEPT
iteration 3 particle 4 weighted err: 17.98279 (train: 16.49247 cvalid: 12.76667 )
iteration 3 particle 5 weighted err: 7.11793 (train: 0.12653 cvalid: 4.49615 )
iteration 3 particle 6 weighted err: 22.29957 (train: 20.53873 cvalid: 21.63925 )
iteration 3 particle 7 weighted err: 1.11164 (train: 0.99896 cvalid: 1.06938 )
iteration 3 particle 8 weighted err: 11.17099 (train: 10.35378 cvalid: 8.31077 )
iteration 3 particle 9 weighted err: 0.11955 (train: 0.11199 cvalid: 0.09308 ) BEST MODEL KEPT
...
time ellapsed: 2.54119062026342
```

```
res <- cbind(ymat, automl_predict(model = amlmodel, X = xmat))
colnames(res) <- c('actual', 'predict')
head(res)
```

```
     actual  predict
[1,]    5.1 4.906462
[2,]    4.9 4.891540
[3,]    4.7 4.877194
[4,]    4.6 4.897768
[5,]    5.0 4.921673
[6,]    5.4 5.053157
```

It's even better, with no human efforts but machine time
Windows users won't benefit from parallelization, the function uses parallel package included with R base...

0.3.3 fit a regression model experimentally (experimental way, Mix 2)

Same subject: predict Sepal.Length given other Iris parameters

```
data(iris)
xmat <- as.matrix(cbind(iris[,2:4], as.numeric(iris$Species)))
ymat <- iris[,1]
amlmodel <- automl_train_manual(Xref = xmat, Yref = ymat,
                                hpar = list(modexec = 'trainwpso',
                                            numiterations = 30,
                                            psopartpopsize = 50))
```

```
(cost: mse)
cost epoch10: 0.113576786377019 (cv cost: 0.0967069106128153) (LR:  0 )
cost epoch20: 0.0595472259640828 (cv cost: 0.0831404427407914) (LR:  0 )
cost epoch30: 0.0494578776185938 (cv cost: 0.0538888075333611) (LR:  0 )
   dim X: ...
```

```
res <- cbind(ymat, automl_predict(model = amlmodel, X = xmat))
colnames(res) <- c('actual', 'predict')
head(res)
```

```
     actual  predict
[1,]    5.1 5.028114
[2,]    4.9 4.673366
[3,]    4.7 4.738188
[4,]    4.6 4.821392
[5,]    5.0 5.099064
[6,]    5.4 5.277315
```

Pretty good too, even better!

0.3.4 fit a regression model with custom cost (experimental way, Mix 2)

Same subject: predict Sepal.Length given other Iris parameters
Let's try with Mean Absolute Percentage Error instead of Mean Square Error

```
data(iris)
xmat <- as.matrix(cbind(iris[,2:4], as.numeric(iris$Species)))
ymat <- iris[,1]
f <- 'J=abs((y-yhat)/y)'
f <- c(f, 'J=sum(J[!is.infinite(J)],na.rm=TRUE)')
f <- c(f, 'J=(J/length(y))')
f <- paste(f, collapse = ';')
amlmodel <- automl_train_manual(Xref = xmat, Yref = ymat,
                                hpar = list(modexec = 'trainwpso',
                                            numiterations = 30,
                                            psopartpopsize = 50,
                                            costcustformul = f))
```

```
(cost: custom)
cost epoch10: 0.901580275333795 (cv cost: 1.15936129555304) (LR:  0 )
cost epoch20: 0.890142834441629 (cv cost: 1.24167078564786) (LR:  0 )
cost epoch30: 0.886088388448652 (cv cost: 1.22756121243449) (LR:  0 )
   dim X: ...
```

```
res <- cbind(ymat, automl_predict(model = amlmodel, X = xmat))
colnames(res) <- c('actual', 'predict')
head(res)
```

```
     actual  predict
[1,]    5.1 4.693915
[2,]    4.9 4.470968
[3,]    4.7 4.482036
[4,]    4.6 4.593667
[5,]    5.0 4.738504
[6,]    5.4 4.914144
```

0.3.5 fit a classification model with softmax (Mix 2)

Subject: predict Species given other Iris parameters
Softmax is available with PSO, no derivative needed ;-)

```
data(iris)
xmat = iris[,1:4]
lab2pred <- levels(iris$Species)
lghlab <- length(lab2pred)
iris$Species <- as.numeric(iris$Species)
ymat <- matrix(seq(from = 1, to = lghlab, by = 1), nrow(xmat), lghlab, byrow = TRUE)
ymat <- (ymat == as.numeric(iris$Species)) + 0
amlmodel <- automl_train_manual(Xref = xmat, Yref = ymat,
                                hpar = list(modexec = 'trainwpso',
                                            layersshape = c(10, 0),
                                            layersacttype = c('relu', 'softmax'),
                                            layersdropoprob = c(0, 0),
                                            numiterations = 50,
                                            psopartpopsize = 50))
```

```
(cost: crossentropy)
cost epoch10: 0.373706545886467 (cv cost: 0.36117608867856) (LR:  0 )
cost epoch20: 0.267034060152876 (cv cost: 0.163635821437066) (LR:  0 )
cost epoch30: 0.212054571476337 (cv cost: 0.112664100290429) (LR:  0 )
cost epoch40: 0.154158717402463 (cv cost: 0.102895917099299) (LR:  0 )
cost epoch50: 0.141037927317585 (cv cost: 0.0864623836595045) (LR:  0 )
   dim X: ...
```

```
res <- cbind(ymat, automl_predict(model = amlmodel, X = xmat))
colnames(res) <- c(paste('act',lab2pred, sep = '_'),
 paste('pred',lab2pred, sep = '_'))
head(res)
tail(res)
```

```
  act_setosa act_versicolor act_virginica pred_setosa pred_versicolor pred_virginica
1          1              0             0   0.9863481     0.003268881    0.010383018
2          1              0             0   0.9897295     0.003387193    0.006883349
3          1              0             0   0.9856347     0.002025946    0.012339349
4          1              0             0   0.9819881     0.004638452    0.013373451
5          1              0             0   0.9827623     0.003115452    0.014122277
6          1              0             0   0.9329747     0.031624836    0.035400439

    act_setosa act_versicolor act_virginica pred_setosa pred_versicolor pred_virginica
145          0              0             1  0.02549091    2.877957e-05      0.9744803
146          0              0             1  0.08146753    2.005664e-03      0.9165268
147          0              0             1  0.05465750    1.979652e-02      0.9255460
148          0              0             1  0.06040415    1.974869e-02      0.9198472
149          0              0             1  0.02318048    4.133826e-04      0.9764061
150          0              0             1  0.03696852    5.230936e-02      0.9107221
```

0.3.6 change the model parameters (shape ...)

Same subject: predict Species given other Iris parameters
1st example: with gradient descent and 2 hidden layers containing 10 nodes, with various activation functions for hidden layers

```
data(iris)
xmat = iris[,1:4]
lab2pred <- levels(iris$Species)
lghlab <- length(lab2pred)
iris$Species <- as.numeric(iris$Species)
ymat <- matrix(seq(from = 1, to = lghlab, by = 1), nrow(xmat), lghlab, byrow = TRUE)
ymat <- (ymat == as.numeric(iris$Species)) + 0
amlmodel <- automl_train_manual(
                Xref = xmat, Yref = ymat,
                hpar = list(
                    layersshape = c(10, 10, 0),
                    layersacttype = c('tanh', 'relu', ''),
                    layersdropoprob = c(0, 0, 0)
                    )
                )
```

nb: last activation type may be left to blank (it will be set automatically)

2nd example: with gradient descent and no hidden layer (logistic regression)

```
data(iris)
xmat = iris[,1:4]
lab2pred <- levels(iris$Species)
lghlab <- length(lab2pred)
iris$Species <- as.numeric(iris$Species)
ymat <- matrix(seq(from = 1, to = lghlab, by = 1), nrow(xmat), lghlab, byrow = TRUE)
ymat <- (ymat == as.numeric(iris$Species)) + 0
amlmodel <- automl_train_manual(Xref = xmat, Yref = ymat,
                                hpar = list(layersshape = c(0),
                                            layersacttype = c('sigmoid'),
                                            layersdropoprob = c(0)))
```

0.4 ToDo List

- transfert learning from existing frameworks
- CNN
- RNN

-> join the team !
https://github.com/aboulaboul/automl