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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 NGâĂŹs MOOC on Coursera will be in familiar territory)
-hyperparameters autotune with metaheuristic (PSO)
-experimental stuff and more to come (youâĂŹre welcome as coauthor!)

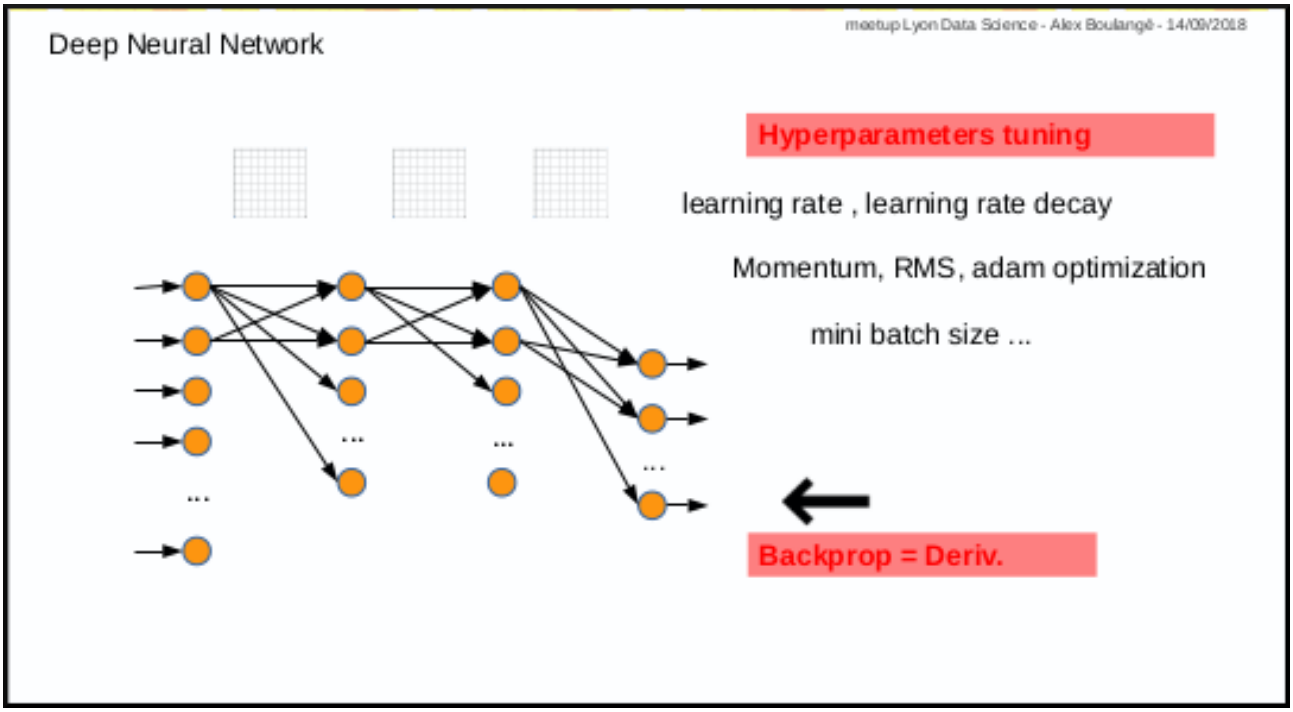
0.2 Why & how automl

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 !

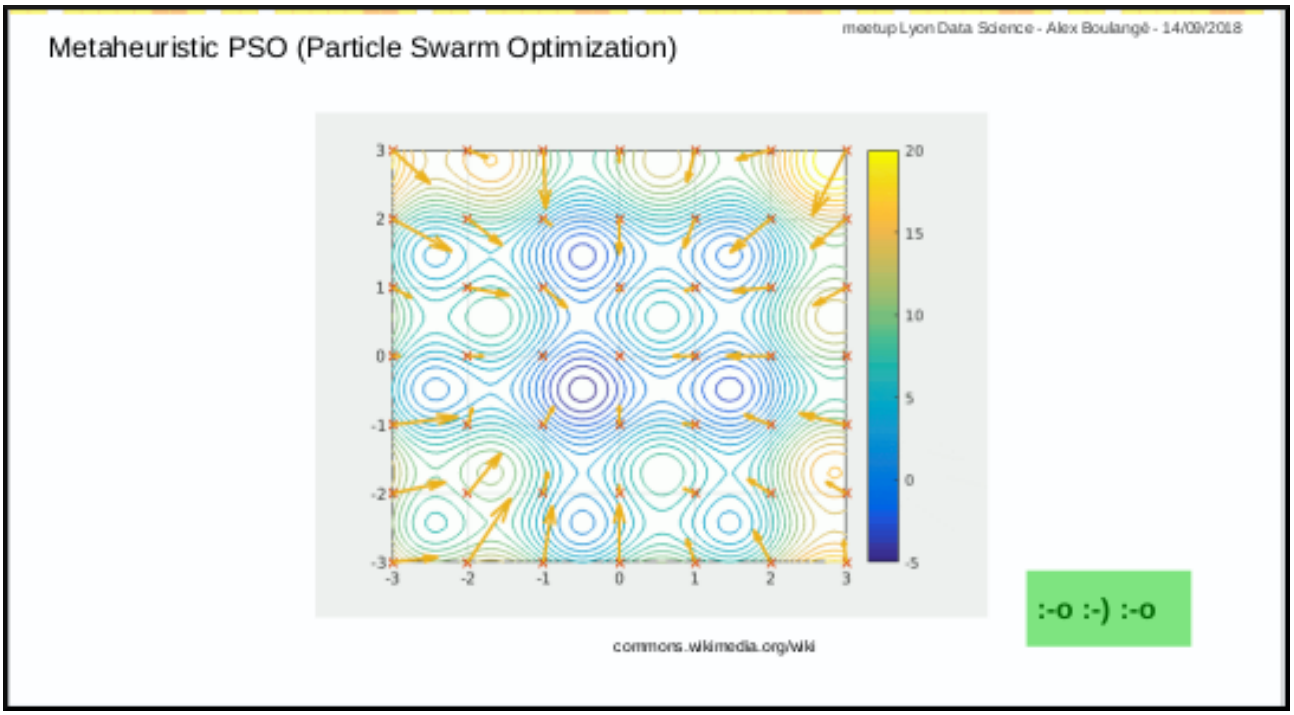
0.2.2 Neural Network - Deep Learning, disadvantages

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.



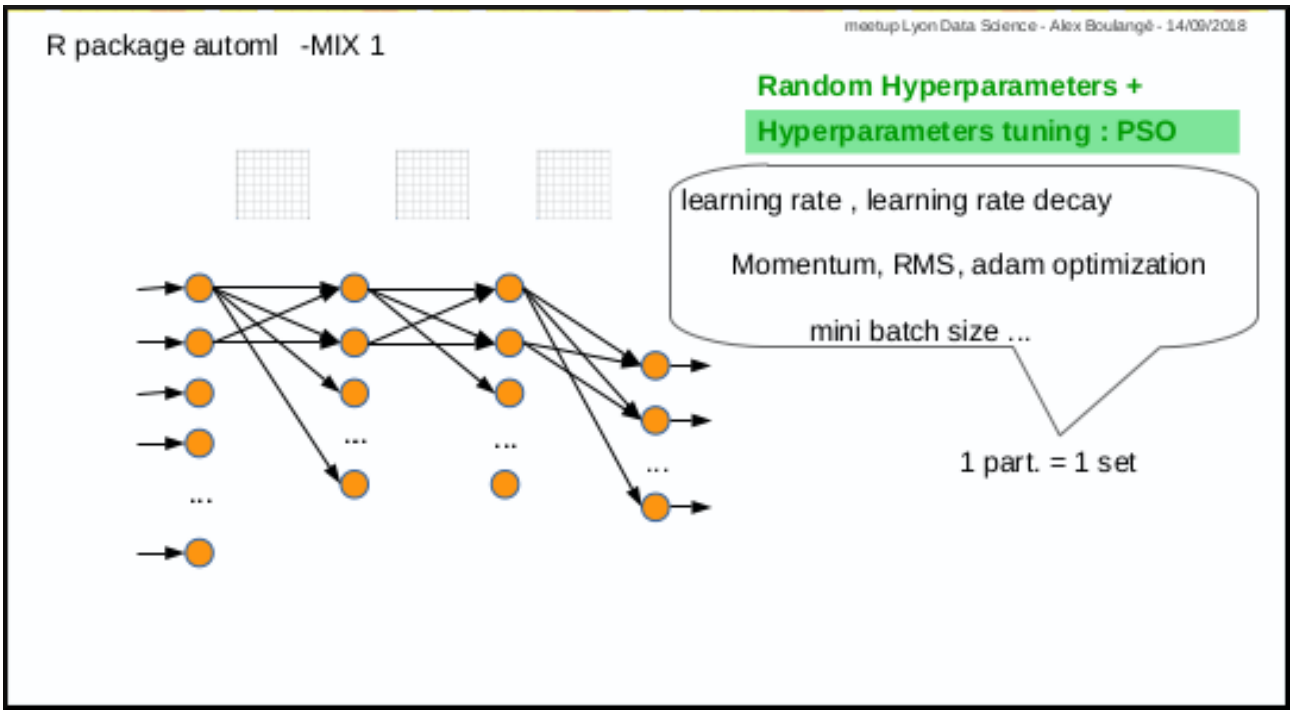
video tutorial from Yarpiz is a great ressource

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

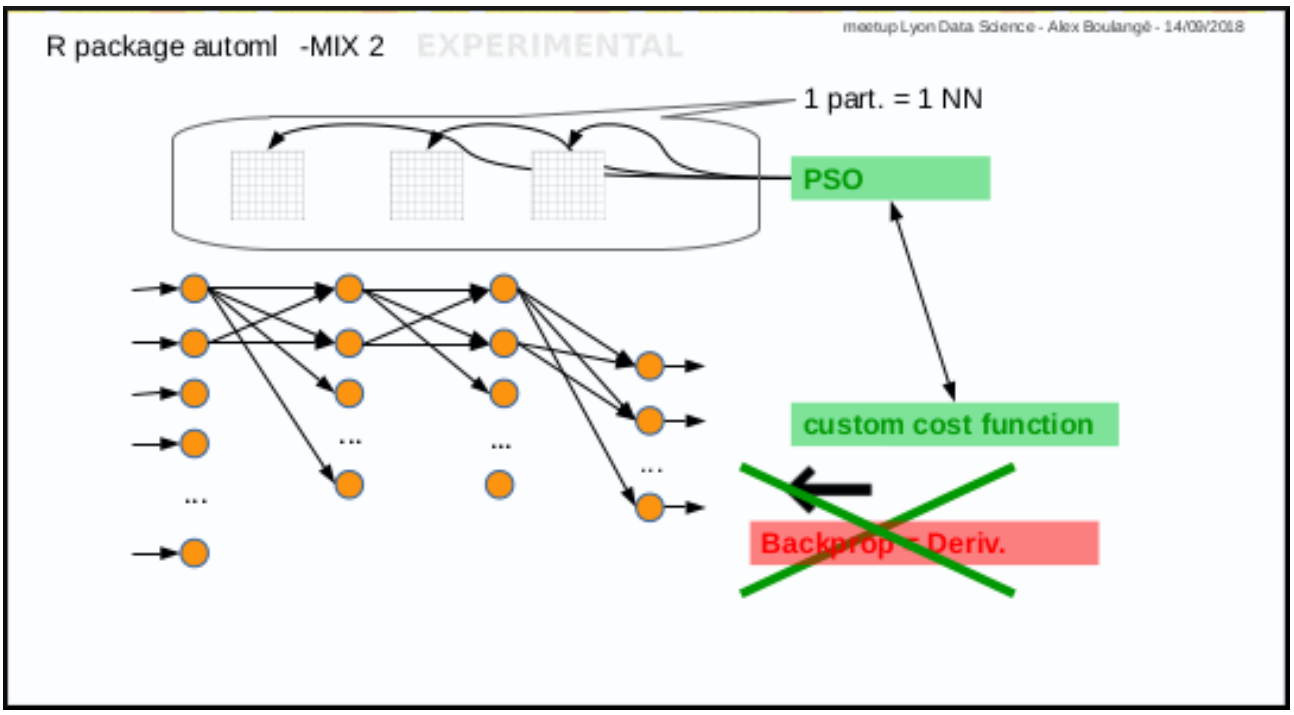
0.2.5 Mix 1: hyperparameters tuning with PSO

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,
                                        auto_layers_max = 1,
                                        nbcores = 4))
end.time <- Sys.time()
cat(paste('time ellapsed:', end.time - start.time, '\n'))
```

```
(cost: mse)
iteration 1 particle 1 weighted err: 22.20611 (train: 20.93004 cvalid: 17.73985 ) BEST MODEL KEPT
iteration 1 particle 2 weighted err: 21.48398 (train: 20.87709 cvalid: 19.35987 ) BEST MODEL KEPT
iteration 1 particle 3 weighted err: 22.98075 (train: 20.96822 cvalid: 15.9369 )
iteration 1 particle 4 weighted err: 22.64428 (train: 21.44958 cvalid: 22.19627 )
iteration 1 particle 5 weighted err: 22.03677 (train: 20.83123 cvalid: 17.81739 )
iteration 1 particle 6 weighted err: 22.30679 (train: 21.02051 cvalid: 17.80482 )
iteration 1 particle 7 weighted err: 22.15835 (train: 20.67513 cvalid: 16.96709 )
iteration 1 particle 8 weighted err: 21.04265 (train: 20.1281 cvalid: 17.84174 ) BEST MODEL KEPT
```

```
iteration 1 particle 9 weighted err: 21.0425 (train: 20.72162 cvalid: 19.91941 ) BEST MODEL KEPT
iteration 1 particle 10 weighted err: 13.78127 (train: 13.54355 cvalid: 12.94923 ) BEST MODEL KEPT
iteration 1 particle 11 weighted err: 20.34595 (train: 19.54807 cvalid: 17.55337 )
iteration 1 particle 12 weighted err: 21.86865 (train: 20.99222 cvalid: 18.80114 )
iteration 1 particle 13 weighted err: 14.11782 (train: 13.54468 cvalid: 12.11184 )
iteration 1 particle 14 weighted err: 23.71203 (train: 20.88439 cvalid: 13.81528 )
iteration 1 particle 15 weighted err: 22.20701 (train: 20.90727 cvalid: 17.65792 )
...
iteration 4 particle 1 weighted err: 12.94662 (train: 4.40029 cvalid: 9.74174 )
iteration 4 particle 2 weighted err: 18.67702 (train: 17.28413 cvalid: 18.15469 )
iteration 4 particle 3 weighted err: 0.76426 (train: 0.01617 cvalid: 0.48373 )
iteration 4 particle 4 weighted err: 11.2243 (train: 11.00578 cvalid: 10.45947 )
iteration 4 particle 5 weighted err: 1.93528 (train: 0.00141 cvalid: 1.21008 )
iteration 4 particle 6 weighted err: 17.89662 (train: 17.65917 cvalid: 17.06555 )
iteration 4 particle 7 weighted err: 0.49851 (train: 0.42819 cvalid: 0.47214 ) BEST MODEL KEPT
...
time ellapsed: 1.84548579454422
```

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

```
     actual  predict
[1,]    5.1 4.975551
[2,]    4.9 4.667541
[3,]    4.7 4.735524
[4,]    4.6 4.784364
[5,]    5.0 5.037152
[6,]    5.4 5.325999
```

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)))
```

```
(cost: crossentropy)
cost epoch10: 2.41256625698174 (cv cost: 1.52787772773656) (LR:  0.001 )
cost epoch20: 2.39487960709668 (cv cost: 1.30539484912328) (LR:  0.001 )
```

```
cost epoch30: 2.37790838174604 (cv cost: 0.914874371089546) (LR:  0.001 )
cost epoch40: 2.36237291354489 (cv cost: 1.23368286521283) (LR:  0.001 )
cost epoch50: 2.34978864866666 (cv cost: 1.26105975399258) (LR:  0.001 )
   dim X: ...
```

```
amlmodelsaved <- amlmodel
```

We saved the model to continue training later (see below in next section)

0.3.7 continue training on saved model (fine tuning ...)

Subject: continue training on saved model (model saved above in last section)

```
amlmodel <- automl_train_manual(Xref = xmat, Yref = ymat,
                                hpar = list(numiterations = 100,
                                            psopartpopsize = 50),
                                mdlref = amlmodelsaved)
```

```
(cost: crossentropy)
cost epoch10: 2.33948479711291 (cv cost: 1.3572198299724) (LR:  0.001 )
cost epoch20: 2.32669285753264 (cv cost: 1.30152708067868) (LR:  0.001 )
cost epoch30: 2.31504805288479 (cv cost: 1.29552449383989) (LR:  0.001 )
cost epoch40: 2.30430035748777 (cv cost: 1.29397405747142) (LR:  0.001 )
cost epoch50: 2.29430374216071 (cv cost: 1.29240693651625) (LR:  0.001 )
cost epoch60: 2.28495815493859 (cv cost: 1.29246202979512) (LR:  0.001 )
cost epoch70: 2.27608005019126 (cv cost: 1.29620090185108) (LR:  0.001 )
cost epoch80: 2.26753980962059 (cv cost: 1.3019296243155) (LR:  0.001 )
cost epoch90: 2.25934270485252 (cv cost: 1.30591289162664) (LR:  0.001 )
cost epoch100: 2.25229290115905 (cv cost: 1.30730635529277) (LR:  0.001 )
   dim X: ...
```

We can see the error continuing to decrease from last training
The training continued with the same parameters, but notice that we were able to change the number of iterations

0.3.8 use the 2 steps automatic approach

Same subject: predict Species given other Iris parameters
Let's try the automatic approach in 2 steps with the same Logistic Regression architecture;
1st step goal is performance, overfitting
2nd step is robustness, regularization

```
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(Xref = xmat, Yref = ymat,
                                hpar = list(layersshape = c(0),
                                            layersacttype = c('sigmoid'),
                                            layersdropoprob = c(0)),
                                autopar = list(auto_runtype = '2steps'))
```

```
STEP: 1 (overfitting)
(cost: crossentropy)
iteration 1 particle 1 weighted err: 2.42056 BEST MODEL KEPT
iteration 1 particle 2 weighted err: 2.40494 BEST MODEL KEPT
iteration 1 particle 3 weighted err: 2.41726
iteration 1 particle 4 weighted err: 2.42334
iteration 1 particle 5 weighted err: 2.4091
iteration 1 particle 6 weighted err: 2.41962
```

```
iteration 1 particle 7 weighted err: 2.40137 BEST MODEL KEPT
iteration 1 particle 8 weighted err: 2.34594 BEST MODEL KEPT
...
iteration 3 particle 1 weighted err: 2.39013
iteration 3 particle 2 weighted err: 2.36849
iteration 3 particle 3 weighted err: 2.23385 BEST MODEL KEPT
iteration 3 particle 4 weighted err: 2.40762
iteration 3 particle 5 weighted err: 2.33986
iteration 3 particle 6 weighted err: 2.39917
iteration 3 particle 7 weighted err: 2.38197
iteration 3 particle 8 weighted err: 2.34594
STEP: 2 (regularization)
(cost: crossentropy)
iteration 1 particle 1 weighted err: 2.70508 (train: 2.24474 cvalid: 1.09389 ) BEST MODEL KEPT
iteration 1 particle 2 weighted err: 2.71015 (train: 2.2452 cvalid: 1.08283 )
iteration 1 particle 3 weighted err: 2.2944 (train: 2.23677 cvalid: 2.0927 ) BEST MODEL KEPT
iteration 1 particle 4 weighted err: 2.6911 (train: 2.23902 cvalid: 1.1088 )
iteration 1 particle 5 weighted err: 2.69633 (train: 2.24061 cvalid: 1.10131 )
iteration 1 particle 6 weighted err: 2.68252 (train: 2.24303 cvalid: 1.14432 )
iteration 1 particle 7 weighted err: 2.75194 (train: 2.24576 cvalid: 0.98029 )
iteration 1 particle 8 weighted err: 4.64173 (train: 2.23456 cvalid: 3.73904 )
...
iteration 2 particle 1 weighted err: 2.70508 (train: 2.24474 cvalid: 1.09389 )
iteration 2 particle 2 weighted err: 2.71015 (train: 2.2452 cvalid: 1.08283 )
iteration 2 particle 3 weighted err: 2.24647 (train: 2.23637 cvalid: 2.21111 ) BEST MODEL KEPT
...
```

Compared to the last runs (in previous sections above), difference between train and cross validation errors is much more tenuous
Automatically :-)

0.4 ToDo List idea

- review the code to object oriented
- manage transfert learning from existing frameworks
- implement CNN
- implement RNN
- ...

-> I won't do it alone, let's create a team !
https://aboulaboul.github.io/automl
https://github.com/aboulaboul/automl