Artificial intelligence in data science High level neural network implementations

Janos Török

Department of Theoretical Physics

October 6, 2022

Implementations

- ► SciKit-Learn
- ► Tensorflow
- ► Keras (Frontent for tensorflow and theano)
- pytorch

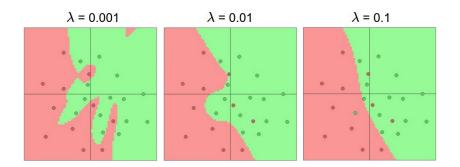
Differences

- SciKit-Learn
 - Easy use
 - ► Well integrated with other scientific methods
 - Limited capabilities
- Tensorflow
 - ► High performance
 - Deep flexibility
 - Can use multiple core and GPU
 - hard
 - very hard
- Keras (Frontent for tensorflow)
 - Easy
 - Supports tensorflow
 - Very flexible
- pytorch
 - ► Flexible
 - Supports GPU
 - complex



Overfitting

- ▶ Very often more parameters than data points
- ▶ Danger of overfitting (fits training perfectly but fails miserably on test)



Regularization

lackbox Do not allow weights to vary uncontrollably o add to the loss function the sum of the square of the norm of the weight matrix

$$J(W,b) = \frac{1}{m} \sum_{i=1}^{m} L(\hat{y}, y)$$

after regularization:

$$J(W,b) = \frac{1}{m} \sum_{i=1}^{m} L(\hat{y}, y) + \frac{\lambda}{2m} \sum_{l=1}^{L} ||w'||^{2}$$

$$\lambda = 0.001 \qquad \lambda = 0.01 \qquad \lambda = 0.1$$

Loss function

- SciKit-Learn:
 - Classification: Cross-Entropy

$$L(\hat{y}, y, W) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y}) + \alpha ||W||_2^2$$

► Regression: Square Error

$$L(\hat{y}, y, W) = \frac{1}{2}||\hat{y} - y||_2^2 + \alpha||W||_2^2$$

Keras:

Loss function

- SciKit-Learn:
 - Classification: Cross-Entropy
 - Regression: Square Error
- Keras:
 - mean square error
 - mean absolute error
 - hinge
 - Poisson
 - crossentropy
 - **.**...

Optimizer

- SciKit-Learn:
 - Ibfgs: is an optimizer in the family of quasi-Newton methods.
 - sgd: stochastic gradient descent
 - adam: stochastic gradient-based optimizer proposed by Kingma, Diederik, and Ba
- Keras:
 - sgd
 - adam
 - adagrad: adaptive gradient
 - rmsgrad: $E(g^2)$: moving average of squared gradients

$$E(g^{2})_{t} = \beta E(g^{2})_{t-1} + (1 - \beta) \left(\frac{\partial C}{\partial W}\right)^{2}$$

$$W_t = W_{t-1} - \frac{\eta}{\sqrt{E(g^2)}} \left(\frac{\partial C}{\partial W} \right)$$

. . .



Batch, epoch

- Batch: part of the training data used in an epoch
 - ► Gradient descent: batch = *N*
 - ► Stochastic gradient descent: batch = 1
 - ▶ Batch gradient descent: 0 <batch < N
- Epoch: one training session (one or more backpropagation)