Topics:

- Our prediction schema
- K-fold cross-validation
- Forward and Backward phase
- Chain Rule (on board)
- Derivation how compute partial derivatives for quadratic Loss
- Source code with which you figure out "What it do?"

Our Prediction Schema

$$\widehat{F}(x; \mathbf{a}, \mathbf{b}) = \sum_{m=0}^{M} b_m \cdot S_m(\sum_{j=0}^{n} a_{jm} x_j)$$

1.
$$S_0(z) = 1$$
 always.
And $=> S'_0 = 0 = S_0(1 - S_0)$
1. $S(z)' = S(z)(1 - S(z))$

K fold cross-validation

- One way to mitigate problems with simple cross-validation is use K-fold cross-validation.
- This technic allow to have a data manipulating schema when number of observation is not very big or even limited and we can not make train set and test set as big as we want.

Algorithm:

1. Split available data into K disjoint folds(or groups, or subsets): $D_1, D_2, ..., D_k$ which are in the union gives original available data. For example typical case K = 10

2. For $= \overline{1,K}$:

Train each Predictor (or Model) on Train $(\bigcup_i D_i)/D_i$ and evaluate empirical loss on Test D_i .

3. For each predictor average empirical loss on all test set D_j . It is an estimation of generalization error.

Here cross-validation estimate the performance of the actual predicting.

4. Select a model with lowest generalization error. One possible way of doing things if there are several models with small generalization error - select "simplest" one

What is forward propagation?

- Take out model and substitute x and evaluate $\widehat{F}(x; a, b)$
- If need store some intermediate results then do it

Motivation video with "Do it"

Loss function for regression for NN

- $L = \frac{1}{N} \sum_{i=1}^{N} \left(y_i \widehat{F}(x_i) \right)^2$ and even more $\frac{1}{N}$ multiplier can be omitted.
- And also people who create neural networks approximations consider

$$L = \frac{1}{2} \sum_{i=1}^{N} \left(y_i - \widehat{F}(x_i) \right)^2.$$

 For differentiable function negative gradient show a direction to fastest local descend of function value if choose direction from unit norm sphere where norm is Euclidian norm.

Chain Rule

- In board discuss Chain Rule
- Gradients
- Linearity of apply derivative
- Difference between Gradient and Jacobian

Derivative to compute partial derivatives

For single layer network and for single observation we have

$$r_{i} = y_{i} - \widehat{F}(x_{i})$$

$$L = \frac{1}{2} \left(y_{i} - \widehat{F}(x_{i}) \right)^{2} = \frac{1}{2} r^{2}$$

$$\frac{dL}{dx} = \frac{2}{3} r = r = (y_{i} - \widehat{F}(x_{i}))$$

$$\widehat{F}(x; \boldsymbol{a}, \boldsymbol{b}) = \sum_{m=0}^{M} b_m \cdot S_m(\sum_{j=0}^{n} a_{jm} x_j)$$

$$\frac{\partial L}{\partial b_m} = \frac{dL}{dr} \cdot \frac{\partial r}{\partial b_m} = \left(y_i - \widehat{F}(x_i) \right) \cdot \frac{d\left(-\widehat{F}(x_i) \right)}{db_m} = \left(\widehat{F}(x_i) - y_i \right) \cdot S_m \left(\sum_{j=0}^n a_{jm} x_j \right)$$

 $\frac{\partial L}{\partial b_m}$ = "error" · "output of the m'th internal node"

Derivative to compute partial derivatives

For single layer network and for single observation we have

 $\mathbf{r}_i = \mathbf{y}_i - \widehat{F}(\mathbf{x}_i)$

$$L = \frac{1}{2} \left(y_i - \widehat{F}(x_i) \right)^2 = \frac{1}{2} r^2$$

$$\frac{dL}{dr} = \frac{2}{2} r = r = (y_i - \widehat{F}(x_i))$$

$$\widehat{F}(x; \mathbf{a}, \mathbf{b}) = \sum_{m=0}^{M} b_m \cdot S_m \left(\sum_{j'=0}^{n} a_{j'm} x_{j'} \right)$$

$$\frac{\partial L}{\partial a_{jm}} = \frac{dL}{dr} \frac{\partial r}{\partial a_{jm}} = (y_i - \widehat{F}(x_i)) \frac{\partial (y_i - \widehat{F}(x_i))}{\partial a_{jm}} = \left(\widehat{F}(x_i) - y_i \right) b_m \cdot \frac{\partial \left(S_m \left(\sum_{j'=0}^{n} a_{j'm} x_{j'} \right) \right)}{\partial a_{jm}}$$

$$\frac{\partial L}{\partial a_{im}} = (\widehat{F}(x_i) - y_i) b_m \cdot S \left(\sum_{j'=0}^{n} a_{j'm} x_{j'} \right) \left(1 - S \left(\sum_{j'=0}^{n} a_{j'm} x_{j'} \right) \right) \cdot x_j$$

Practice

- L4_single_nn_compute_gradient_of_loss.py
- Read it and fill comments (In Russian on English)