Chapter 7. Neural Networks

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Chapter 11. only focus on Feedforward NNs.
Related to projection pursuit regression:
\[ f(x) = \sum_{m=1}^{M} g_m(w'_m x), \]
where each \( w_m \) is a vector of weights and \( g_m \) is a smooth nonparametric function; to be estimated.

Two high waves in 1960s and late 1980s-90s.

A biological neuron vs an artificial neuron (perceptron). Google: images biological neural network tutorial
Minsky & Papert’s (1969) XOR problem:
\[ XOR(X_1, X_2) = 1 \text{ if } X_1 \neq X_2; = 0 \text{ o/w. } X_1, X_2 \in \{0, 1\}. \]
Perceptron: \[ f = I(\alpha_0 + \alpha'X > 0). \]
McCulloch & Pitts model (1943):
\[ n_j(t) = I(\sum_{i \rightarrow j} w_{ij}n_i(t - 1) > \theta_j). \]
\( w_{ij} \) can be > 0 (excitatory) or < 0 (inhibitory).

Feldman’s (1985) “one hundred step program”: at most 100 steps within a human reaction time.
because a human can recognize another person in 100 ms, while the processing time of a neuron is 1ms. \( \implies \) human brain works in a massively parallel and distributed way.

Cognitive science: human vision is performed in a series of layers in the brain.

Human can learn.

Hebb (1949) model:
\[ w_{ij} \leftarrow w_{ij} + \eta y_i y_j, \]
reinforcing learning by simultaneous activations.
Feed-forward NNs

- **Fig 11.2**

- **Input**: $X$

- A hidden layer (or layers): for $m = 1, \ldots, M$, 
  
  $Z_m = \sigma(\alpha_0 + \alpha'_m X), \ Z = (Z_1, \ldots, Z_M)'$.
  
  e.g. $\sigma(v) = 1/(1 + \exp(-v))$, sigmoid (or logit$^{-1}$) function.

- **Output**: $f_1(X), \ldots, f_K(X)$.

  $T_k = \beta_{0k} + \beta'_k Z, \ T = (T_1, \ldots, T_K)'$

  $f_k(X) = g_k(T)$.

  e.g. regression: $g_k(T) = T_k$;

  classification: $g_k(T) = \exp(T_k) / \sum_{j=1}^K \exp(T_j)$; softmax or multi-logit$^{-1}$ function.
FIGURE 11.2. Schematic of a single hidden layer, feed-forward neural network.
FIGURE 11.3.  Plot of the sigmoid function $\sigma(v) = 1/(1 + \exp(-v))$ (red curve), commonly used in the hidden layer of a neural network. Included are $\sigma(sv)$ for $s = 1/2$ (blue curve) and $s = 10$ (purple curve). The scale parameter $s$ controls the activation rate, and we can see that large $s$ amounts to a hard activation at $v = 0$. Note that $\sigma(s(v - v_0))$ shifts the activation threshold from 0 to $v_0$. 
How to fit the model?

Given training data: \((Y_i, X_i), \ i = 1, \ldots, n\).

For regression, minimize
\[
R(\theta) = \sum_{k=1}^{K} \sum_{i=1}^{n} (Y_{ik} - f_k(X_i))^2.
\]

For classification, minimize
\[
R(\theta) = -\sum_{k=1}^{K} \sum_{i=1}^{n} Y_{ik} \log f_k(X_i).
\]
And \(G(x) = \arg \max f_k(x)\).

Can use other loss functions.

How to minimize \(R(\theta)\)?
Gradient descent, called back-propagation.
§11.4
Very popular and appealing! recall Hebb model

Other algorithms: Newton’s, conjugate-gradient, ...
Back-propagation algorithm

- Given: training data \((Y_i, X_i), i = 1, ..., n\).
- Goal: estimate \(\alpha\)'s and \(\beta\)'s.
  
  Consider \(R(\theta) = \sum_i \sum_k (Y_{ik} - f_k(X_i))^2 := \sum_i R_i\).

- Denote \(Z_{mi} = \sigma(\alpha_0m + \alpha_m'X_i), Z_i = (Z_{1i}, ..., Z_{Mi})',\)

\[
\frac{\partial R_i}{\partial \beta_{km}} = -2(Y_{ik} - f_k(X_i))g'_k(\beta'_kZ_i)Z_{mi} := \delta_{ki}Z_{mi},
\]

\[
\frac{\partial R_i}{\partial \alpha_{ml}} = -\sum_k 2(Y_{ik} - f_k(X_i))g'_k(\beta'_kZ_i)\beta_{km}\sigma'(\alpha_m'X_i)X_{il} := s_{mi}X_{il}.
\]

where \(\delta_{ki}, s_{mi}\) are “errors” from the current model.

- Update at step \(r + 1:\)

\[
\beta_{km}^{(r+1)} = \beta_{km}^{(r)} - \gamma_r \sum_i \frac{\partial R_i}{\partial \beta_{km}}\bigg|_{\beta^{(r)}, \alpha^{(r)}}, \quad \alpha_{ml}^{(r+1)} = \alpha_{ml}^{(r)} - \gamma_r \sum_i \frac{\partial R_i}{\partial \alpha_{ml}}\bigg|_{\beta^{(r)}, \alpha^{(r)}}.
\]

\(\gamma_r\): learning rate; can be fixed or selected by a line search.

- training epoch: a cycle of updating
- +: simple and intuitive; -: slow
Some issues

- Starting values:
  Existence of many local solutions.
  Multiple tries; model averaging, ...

- Over-fitting?
  Old days: adding more and more units and hidden layers ...
  Early stopping!
  Regularization: add a penalty term, e.g. Ridge; use
  \[ R(\theta) + \lambda J(\theta) \text{ with } J(\theta) = \sum_{km} \beta_{km}^2 + \sum_{ml} \alpha_{ml}^2; \]
  called weight decay; Fig 11.4.

- Performance: Fig 11.6-8

- Example code: ex7.1.r
Neural Network - 10 Units, No Weight Decay

Training Error: 0.100
Test Error: 0.259
Bayes Error: 0.210

Neural Network - 10 Units, Weight Decay=0.02

Training Error: 0.160
Test Error: 0.223
Bayes Error: 0.210
**FIGURE 11.6.** Boxplots of test error, for simulated data example, relative to the Bayes error (broken horizontal line). True function is a sum of two sigmoids on the left, and a radial function is on the right. The test error is displayed for 10 different starting weights, for a single hidden layer neural network with the number of units as indicated.
FIGURE 11.7. Boxplots of test error, for simulated data example, relative to the Bayes error. True function is a sum of two sigmoids. The test error is displayed for ten different starting weights, for a single hidden layer neural network with the number units as indicated. The two panels represent no weight decay (left) and strong weight decay $\lambda = 0.1$ (right).
FIGURE 11.8. Boxplots of test error, for simulated data example. True function is a sum of two sigmoids. The test error is displayed for ten different starting weights, for a single hidden layer neural network with ten hidden units and weight decay parameter value as indicated.
Current and future ...

- Deep learning: deep NNs (Wikipedia; google)
  Facebook hired Yann LeCun;
  Google hired Geoffrey Hinton;
  Baidu hired Andrew Ng; ...

- Impressive applications: imaging recognition (Krizhevsky et al); playing the game of Go (Silver et al 2016, *Nature*); ...

- Keys: Krizhevsky et al,
  “60 million parameters ... of five convolutional layers ... three fully-connected layers with a final 1000-way softmax.”
  “there are roughly 1.2 million training images, 50,000 validation images, and 150,000 testing images.”
  Needs **regularization** too!

- Qs: another wave? over-stated?
Convolutional NNs

- Keys: “to ensure some degree of shift, scale, and distortion invariance: *local receptive fields, shared weights ... and spatial or temporal sub-sampling.*”
- “Local correlations are the reasons for the well-known advantages of extracting and combining *local* features ...”
- Hubel and Wiesel (1962): locally-sensitive, orientation-selective neurons in the cat’s visual system.
- New: a convolution layer uses rectified linear function,

\[
\text{ReLU}(x) = \max(0, x).
\]
Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.

Figure: LeCun et al 1998, *Proc of the IEEE.*
Figure: Angermueller et al 2016, Mol Sys Biol.
Resources

- Python library:
  1. Theano: on top, Keras;
  2. Caffe: by Berkeley Vision and Learning Center (BVLC);
     Google’s DeepDream is based on it.
     http://caffe.berkeleyvision.org/
- Matlab: ConvNet, DeepLearnToolBox, MatConvNet, ...
- Java: Deeplearning4j, ...
- Others: Torch, ...
- R packages: deepnet, darch, mxnet, h2o; really?
- Reusing trained networks: why?
  DeCAF:
Revolution of Depth

152 layers

ILSVRC'15 ResNet ILSVRC'14 GoogleNet ILSVRC'14 VGG ILSVRC'13 ILSVRC'12 AlexNet ILSVRC'11 ILSVRC'10

ImageNet Classification top-5 error (%)

3.57 6.7 7.3 11.7 16.4 25.8 28.2 shallow

(slide from Kaiming He’s recent presentation)