Chapter 7. Neural Networks

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Introduction

- 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:
  $XOR(X_1, X_2) = 1$ if $X_1 \neq X_2$; $= 0$ o/w. $X_1, X_2 \in \{0, 1\}$.
  Percepton: $f = I(\alpha_0 + \alpha' X > 0)$.

- McCulloch & Pitts model (1943):
  $n_j(t) = I(\sum_{i \to j} w_{ij} n_i(t-1) > \theta_j)$.
  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. $\Longrightarrow$ 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 $m = 1, ..., M$,
  $Z_m = \sigma(\alpha_{0m} + \alpha_m' X)$, $Z = (Z_1, ..., Z_M)'$.
  e.g. $\sigma(v) = 1/(1 + \exp(-v))$, sigmoid (or logit^{-1}) function.
- Output: $f_1(X), ..., f_K(X)$.
  $T_k = \beta_{0k} + \beta_k' Z$, $T = (T_1, ..., T_K)'$,
  $f_k(X) = g_k(T)$.
  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-$\text{logit}^{-1}$ function.

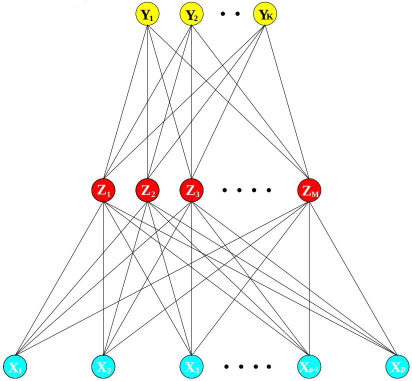


FIGURE 11.2. *Schematic of a single hidden layer, feed-forward neural network.*

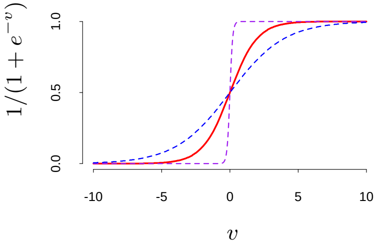


FIGURE 11.3. *Plot of the sigmoid function* $\sigma(v) = 1/(1+\exp(-v))$ *(red curve), commonly used in the hidden layer of a neural network. Included are* $\sigma(sv)$ *for* $s = \frac{1}{2}$ *(blue curve) and* $s = 10$ *(purple curve). The scale parameter* s *controls the activation rate, and we can 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), $i = 1, ..., n$.
- 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 α's and β's.
  Consider $R(\theta) = \sum_i \sum_k (Y_{ik} - f_k(X_i))^2 := \sum_i R_i$.
- Denote $Z_{mi} = \sigma(\alpha_{0m} + \alpha_m' X_i)$, $Z_i = (Z_{1i}, ..., Z_{Mi})'$,

$$\frac{\partial R_i}{\partial \beta_{km}} = -2(Y_{ik} - f_k(X_i)) g_k'(\beta_k' Z_i) Z_{mi} := \delta_{ki} Z_{mi},$$

$$\frac{\partial R_i}{\partial \alpha_{ml}} = -\sum_k 2(Y_{ik} - f_k(X_i)) g_k'(\beta_k' Z_i) \beta_{km} \sigma'(\alpha_m' X_i) X_{il} := s_{mi} X_{il}.$$

  where δ_{ki}, s_{mi} are "errors" from the current model.
- Update at step $r + 1$:

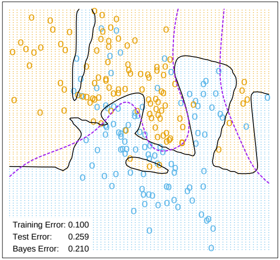
$$\beta_{km}^{(r+1)} = \beta_{km}^{(r)} - \gamma_r \sum_i \left. \frac{\partial R_i}{\partial \beta_{km}} \right|_{\beta^{(r)}, \alpha^{(r)}}, \quad \alpha_{ml}^{(r+1)} = \alpha_{ml}^{(r)} - \gamma_r \sum_i \left. \frac{\partial R_i}{\partial \alpha_{ml}} \right|_{\beta^{(r)}, \alpha^{(r)}}.$$

  γ_r: learning rate; can be fixed or selected by a line search.
- training epoch: a cycle of updating
- $+$: simple and intuitive; -: slow

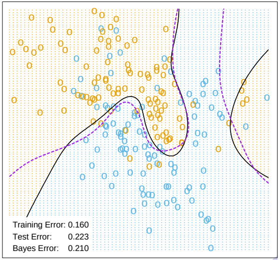
Some issues

- 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
  $R(\theta) + \lambda J(\theta)$ 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



Neural Network - 10 Units, Weight Decay=0.02



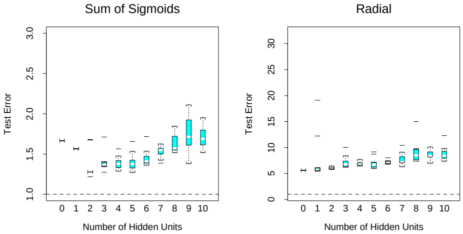


FIGURE 11.6. *Boxplots of test error, for simulated data example, relative to the Bayes error (broken horizontal line). True function is a sum of two sigmoids on the left, and a radial function is on the right. The test error is displayed for* 10 *different starting weights, for a single hidden layer neural network with the number of units as indicated.*

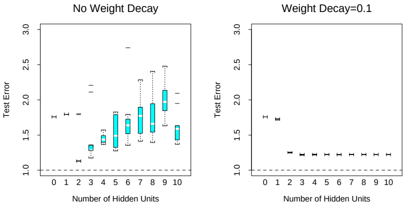


FIGURE 11.7. *Boxplots of test error, for simulated data example, relative to the Bayes error. True function is a sum of two sigmoids. The test error is displayed for ten different starting weights, for a single hidden layer neural network with the number units as indicated. The two panels represent no weight decay (left) and strong weight decay* $\lambda = 0.1$ *(right).*

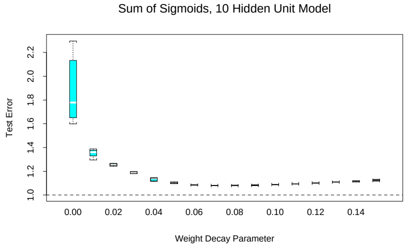


FIGURE 11.8. *Boxplots of test error, for simulated data example. True function is a sum of two sigmoids. The test error is displayed for ten different starting weights, for a single hidden layer neural network with ten hidden units and weight decay parameter value as indicated.*

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 witha 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

- LeCun et al (1998, *Proc of the IEEE*);
- 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,

$$\mathrm{ReLU}(x) = \max(0, x).$$

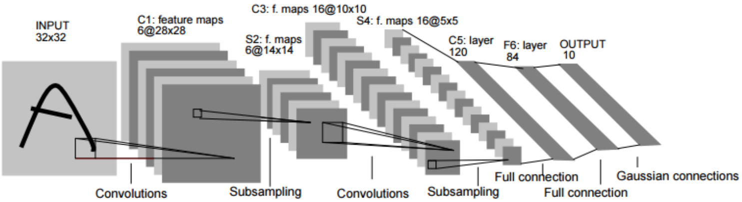


Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.