Neurons and neural networks I.
High-level vs. low level modeling

Previously in this course:

* Mechanistic description of neurons
* Descriptive models of neuronal operations

Goals of the next classes:

Are these models compatible with the neural architecture? How can neural computations interpreted in this framework?
Outline

- single neuron
- neural network
- supervised learning
- unsupervised learning
Neural networks, basic concepts

Goal of the neural network can be phrased:

- learning about its input
- forming memories

Address based memory

- not associative
- not fault tolerant
- not distributed

Biological memory

- associative
- error tolerant
  - cue error
  - hardware fault
- parallel and distributed
Terminology

Architecture: what variables are involved, how they interact (weights, activities)

Activity rule: short time-scale behavior
how activity of neurons depends on inputs

Learning rule: long time-scale behavior
how weights change as a function of activities of other neurons, time, or other factors
Terminology

**Supervised learning:** *labelled data* is provided, i.e. an input-output relationship is given; the ‘teacher’ tells whether the response of the neuron to a given input was correct.

**Unsupervised learning:** *unlabelled data* is available; learns the statistics of input: generating a table of occurrences; some more sophisticated *representation* is learned.
Single neuron as a classifier

**Definitions**

**Architecture:**  \( I \) inputs \( x_i \)
weights \( w_i \)

**Activity rule:**
1. activation is calculated
   \[
   a = \sum_{i} w_i x_i,
   \]
2. output is calculated
   - linear \( y(a) = a \).
   - logistic \( y(a) = \frac{1}{1 + e^{-a}} \).
   - tanh \( y(a) = \tanh(a) \).
   - threshold
      \[
      y(a) = \Theta(a) \equiv \begin{cases} 
      1 & a > 0 \\
-1 & a \leq 0
      \end{cases}
      \]
Single neuron as a classifier

Definitions

**Architecture:** $I$ inputs $x_i$
weights $w_i$

**Activity rule:**
1. activation is calculated
$$a = \sum_{i} w_i x_i,$$
2. output is calculated
   - linear
   - logistic
   - tanh
   - threshold

$$y(a) = a.$$ 

$$y(a) = \frac{1}{1 + e^{-a}}$$

$$y(a) = \tanh(a)$$

$$y(a) = \Theta(a) \equiv \begin{cases} 
1 & a > 0 \\
-1 & a \leq 0.
\end{cases}$$
Single neuron as a classifier
Concepts

Input space

\[ y(x; w) = \frac{1}{1 + e^{-(w_1 x_1 + w_2 x_2)}} \]
Single neuron as a classifier

Concepts

Input space

\[ y(x; w) = \frac{1}{1 + e^{-(w_1x_1 + w_2x_2)}} \]

\[ w = (0, 2) \]
Single neuron as a classifier

Concepts

Input space

\[ y(x; w) = \frac{1}{1 + e^{-(w_1x_1 + w_2x_2)}} \]

Weight space
Single neuron as a classifier

Concepts

The supervised learning paradigm:

given example inputs $x$ and target outputs $t$
learning the mapping between them

the trained network is supposed to give
‘correct response’ for any given input
stimulus

training is equivalent to learning the
appropriate weights

in order to achieve this, an objective
function (or error function) is defined,
which is minimized during training
Binary classification in a neuron

Error function:

$$G(w) = - \sum_n \left[ t^{(n)} \ln y(x^{(n)}; w) + (1 - t^{(n)}) \ln(1 - y(x^{(n)}; w)) \right]$$
Binary classification in a neuron

Error function:

\[ G(w) = - \sum_{n} \left[ t(n) \ln y(x(n); w) + (1 - t(n)) \ln (1 - y(x(n); w)) \right] \]

1. information content of outcomes
2. relative entropy of distributions \((t, 1-t)\) and \((y, 1-y)\)
Binary classification in a neuron

Error function:

\[ G(w) = - \sum_n \left[ t^{(n)} \ln y(x^{(n)}; w) + (1 - t^{(n)}) \ln (1 - y(x^{(n)}; w)) \right] \]

1. information content of outcomes
2. relative entropy of distributions \((t, 1-t)\) and \((y, 1-y)\)

Learning: back-propagation algorithm

\[ g_j = \frac{\partial G}{\partial w_j} = \sum_{n=1}^{N} -(t^{(n)} - y^{(n)}) x_j^{(n)} \]

Here \(e^{(n)} \equiv t^{(n)} - y^{(n)}\) is the error
Binary classification

The algorithm

1. Get the data
2. Calculate activations: $a = \sum_i w_i x_i$
3. Calculate the output of the neuron: $y(a) = \frac{1}{1 + e^{-a}}$
4. Calculate error: $e = t - y$
5. Update weight(s): $\Delta w_i = \eta e x_i$
Binary classification

The algorithm

1. Get the data
2. Calculate activations: \[ a = \sum_i w_i x_i, \]
3. Calculate the output of the neuron: \[ y(a) = \frac{1}{1 + e^{-a}} \]
4. Calculate error: \[ e = t - y \]
5. Update weight(s): \[ \Delta w_i = \eta e x_i \]

alternatively, batch learning can be done \[ g_i^{(n)} = -e^{(n)} x_i^{(n)}, \]
\[ \Delta w_i = -\eta \sum_n g_i^{(n)} \]
Binary classification

The algorithm

1. Get the data
2. Calculate activations: \( a = \sum_i w_i x_i \),
3. Calculate the output of the neuron: \( y(a) = \frac{1}{1 + e^{-a}} \)
4. Calculate error: \( e = t - y \)
5. Update weight(s): \( \Delta w_i = \eta ex_i \)

alternatively, batch learning can be done

\[
\begin{align*}
g_i^{(n)} &= -e^{(n)} x_i^{(n)}.
\end{align*}
\]

\[
\Delta w_i = -\eta \sum_n g_i^{(n)}
\]
Binary classification

The algorithm

1. Get the data
2. Calculate activations: \( a = \sum_i w_i x_i \)
3. Calculate the output of the neuron: \( y(a) = \frac{1}{1 + e^{-a}} \)
4. Calculate error: \( e = t - y \)
5. Update weight(s): \( \Delta w_i = \eta e x_i \)

alternatively, batch learning can be done

\[ g_i^{(n)} = -e^{(n)} x_i^{(n)} \]

\[ \Delta w_i = -\eta \sum_n g_i^{(n)} \]

gradient descent
Binary classification

The algorithm

1. Get the data
2. Calculate activations:  \[ a = \sum_i w_i x_i, \]
3. Calculate the output of the neuron:  \[ y(a) = \frac{1}{1 + e^{-a}} \]
4. Calculate error:  \[ e = t - y \]
5. Update weight(s):  \[ \Delta w_i = \eta e x_i \]

alternatively, batch learning can be done  \[ g_i^{(n)} = -e^{(n)} x_i^{(n)} \]

\[ \Delta w_i = -\eta \sum_n g_i^{(n)} \]

stochastic gradient descent

gradient descent
Binary classification
Demonstration
Binary classification Demonstration
Binary classification
Demonstration
Binary classification
Demonstration

Evolution of weights

(f) (g) (h) (i) (j) (k)
Binary classification Demonstration

Evolution of weights

Evolution of the error function

(f) (g) (c) (h) (i) (j) (k)
Binary classification
Are we happy?
Binary classification
Are we happy?

$w$’s seem to grow unbounded
Binary classification
Are we happy?

$w$’s seem to grow unbounded

Is this bad for us?
Binary classification
Are we happy?

$w$’s seem to grow unbounded

Is this bad for us?

Generic pain killer: *regularization*

$$M(w) = G(w) + \alpha E_W(w)$$

$$E_W(w) = \frac{1}{2} \sum_i w_i^2. \text{ (weight decay)}$$
Binary classification
Effect of regularization
Binary classification
Effect of regularization
Capacity of the neuron

How much information can the neuron transmit?
Interpreting learning as inference

So far: optimization wrt. an objective function

\[ M(w) = G(w) + \alpha E_W(w) \]

where

\[ G(w) = - \sum_n \left[ t^{(n)} \ln y(x^{(n)}; w) + (1 - t^{(n)}) \ln(1 - y(x^{(n)}; w)) \right] \]

\[ E_W(w) = \frac{1}{2} \sum_i w_i^2. \]
Interpreting learning as inference

So far: optimization wrt. an objective function

\[ M(w) = G(w) + \alpha E_W(w) \]

where

\[ G(w) = -\sum_n \left[ t^{(n)} \ln y(x^{(n)}; w) + (1 - t^{(n)}) \ln (1 - y(x^{(n)}; w)) \right] \]

\[ E_W(w) = \frac{1}{2} \sum_i w_i^2. \]

What’s this quirky regularizer, anyway?
Interpreting learning as inference

Let’s interpret $y(x,w)$ as a probability:

$$P(t = 1 \mid w, x) = y$$
$$P(t = 0 \mid w, x) = 1 - y$$
Interpreting learning as inference

Let’s interpret $y(x, w)$ as a probability:

$$P(t = 1 \mid w, x) = y$$
$$P(t = 0 \mid w, x) = 1 - y$$

in a compact form:

$$P(t \mid w, x) = y^t (1 - y)^{1-t} = \exp[t \ln y + (1 - t) \ln(1 - y)]$$
Interpreting learning as inference

Let’s interpret $y(x, w)$ as a probability:

\[
P(t = 1 \mid w, x) = y \\
P(t = 0 \mid w, x) = 1 - y
\]

in a compact form:

\[
P(t \mid w, x) = y^t (1 - y)^{1-t} = \exp[t \ln y + (1 - t) \ln(1 - y)]
\]

the **likelihood** of the input data can be expressed with the original error function function

\[
P(D \mid w) = \exp[-G(w)]
\]
Interpreting learning as inference

Let’s interpret $y(x,w)$ as a probability:

\[
P(t = 1 \mid w, x) = y \\
P(t = 0 \mid w, x) = 1 - y
\]

in a compact form:

\[
P(t \mid w, x) = y^t (1 - y)^{1-t} = \exp[t \ln y + (1 - t) \ln(1 - y)]
\]

the **likelihood** of the input data can be expressed with the original error function function

\[
P(D \mid w) = \exp[-G(w)]
\]

the regularizer has the form of a prior!

\[
P(w \mid \alpha) = \frac{1}{Z_W(\alpha)} \exp(-\alpha E_W).
\]
Interpreting learning as inference

Let’s interpret \( y(x,w) \) as a probability:

\[
P(t = 1 \mid w, x) = y \\
P(t = 0 \mid w, x) = 1 - y
\]

in a compact form:

\[
P(t \mid w, x) = y^t (1 - y)^{1-t} = \exp[t \ln y + (1 - t) \ln(1 - y)]
\]

the **likelihood** of the input data can be expressed with the original error function function

\[
P(D \mid w) = \exp[-G(w)]
\]

the regularizer has the form of a prior!

\[
P(w \mid \alpha) = \frac{1}{Z_W(\alpha)} \exp(-\alpha E_W).
\]

what we get in the objective function \( M(w) \):

the posterior distribution of \( w \):

\[
P(w \mid D, \alpha) = \frac{P(D \mid w)P(w \mid \alpha)}{P(D \mid \alpha)}
\]
Interpreting learning as inference

Relationship between $M(w)$ and the posterior

$$P(w \mid D, \alpha) = \frac{P(D \mid w)P(w \mid \alpha)}{P(D \mid \alpha)}$$

$$= \frac{e^{-G(w)} e^{-\alpha E_w(w)}/Z_W(\alpha)}{P(D \mid \alpha)}$$

$$= \frac{1}{Z_M} \exp(-M(w)).$$

**Interpretation:** minimizing $M(w)$ leads to finding the maximum a posteriori estimate $w_{MP}$

The log probability interpretation of the objective function retains:
- additivity of errors, while
- keeping the multiplicativity of probabilities
Interpreting learning as inference
Properties of the Bayesian estimate
Interpreting learning as inference

Properties of the Bayesian estimate

• The probabilistic interpretation makes our assumptions explicit: by the regularizer we imposed a soft constraint on the learned parameters, which expresses our prior expectations.

• An additional plus:

   beyond getting $w_{MP}$ we get a measure for learned parameter uncertainty