Neurons and neural networks II. Hopfield network
Perceptron recap

- key ingredient: adaptivity of the system
- unsupervised vs supervised learning
- architecture for discrimination: single neuron — perceptron
- error function & learning rule
- gradient descent learning & divergence
- regularisation
- learning as inference
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

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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

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in a compact form:

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

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

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Interpreting learning as inference

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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

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

the posterior distribution of $w$: $P(w | D, \alpha) = \frac{P(D | w) P(w | \alpha)}{P(D | \alpha)}$
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
Interpreting learning as inference

Demo

<table>
<thead>
<tr>
<th>Data set</th>
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<th>Probability of parameters</th>
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<tbody>
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<td>$N = 0$</td>
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![Graphs showing likelihood and probability of parameters]
Interpreting learning as inference

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$N = 2$

![Graphs and diagrams](image.png)
Interpreting learning as inference

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Interpreting learning as inference

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- $N = 2$

- $N = 4$

- $N = 6$
Interpreting learning as inference
Making predictions

Up to this point the goal was optimization: \[ M(w) = G(w) + \alpha E(w) \]
Interpreting learning as inference
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Are we equally confident in the two predictions?
Interpreting learning as inference
Making predictions

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Are we equally confident in the two predictions?

The Bayesian answer exploits the probabilistic interpretation:

\[
P(t^{(N+1)} | x^{(N+1)}, D, \alpha) = \int d^K w P(t^{(N+1)} | x^{(N+1)}, w, \alpha) P(w | D, \alpha)
\]
Interpreting learning as inference
Calculating Bayesian predictions

Predictive probability:

\[ P(t^{(N+1)} | x^{(N+1)}, D, \alpha) = \int d^K w \, P(t^{(N+1)} | x^{(N+1)}, w, \alpha) P(w | D, \alpha) \]
Interpreting learning as inference
Calculating Bayesian predictions

Predictive probability:

\[ P(t^{(N+1)} | x^{(N+1)}, D, \alpha) = \int d^K w \ P(t^{(N+1)} | x^{(N+1)}, w, \alpha) P(w | D, \alpha) \]

Likelihood:

\[ P(t^{(N+1)} = 1 | x^{(N+1)}, w, \alpha) = y(x^{(N+1)}; w) \]
\[ P(t^{(N+1)} = 0 | x^{(N+1)}, w, \alpha) = 1 - y(x^{(N+1)}; w) \]

Weight posterior

\[ P(w | D, \alpha) = \frac{1}{Z_M} \exp(-M(w)) \]

Partition function:

\[ Z_M = \int d^K w \exp(-M(w)) \]
Interpreting learning as inference
Calculating Bayesian predictions

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Weight posterior
\[ P(w | D, \alpha) = \frac{1}{Z_M} \exp(-M(w)) \]

Partition function:
\[ Z_M = \int d^K w \exp(-M(w)) \]

Finally:
\[ P(t^{(N+1)} = 1 | x^{(N+1)}, D, \alpha) = \int d^K w \ y(x^{(N+1)}; w) \frac{1}{Z_M} \exp(-M(w)) \]
Interpreting learning as inference
Calculating Bayesian predictions

\[ P(t^{(N+1)} = 1 \mid x^{(N+1)}, D, \alpha) = \int d^K w \ y(x^{(N+1)}; w) \frac{1}{Z_M} \exp(-M(w)) \]

How to solve the integral?
Interpreting learning as inference
Calculating Bayesian predictions

\[ P(t^{(N+1)} = 1 \mid x^{(N+1)}, D, \alpha) = \int d^K \mathbf{w} \ y(x^{(N+1)}; \mathbf{w}) \frac{1}{Z_M} \exp(-M(\mathbf{w})) \]

How to solve the integral?
Bad news: Monte Carlo integration is needed

\[ \langle f(\mathbf{w}) \rangle \simeq \frac{1}{R} \sum_r f(\mathbf{w}^{(r)}) \]
\begin{verbatim}
g = gradM(w);  # set gradient using initial w
M = findM(w);  # set objective function too

for l = 1:L  # loop L times
    p = randn(size(w));  # initial momentum is Normal(0,1)
    H = p' * p / 2 + M;  # evaluate H(w,p)

    * p = p - epsilon * g / 2;  # make half-step in p
    * wnew = w + epsilon * p;  # make step in w
    * gnew = gradM(wnew);  # find new gradient
    * p = p - epsilon * gnew / 2;  # make half-step in p

Mnew = findM(wnew);  # find new objective function
Hnew = p' * p / 2 + Mnew;  # evaluate new value of H
dH = Hnew - H;  # decide whether to accept
if (dH < 0) accept = 1;
elseif (rand() < exp(-dH)) accept = 1;  # compare with a uniform
else accept = 0;  # variate
endif
if (accept) g = gnew;  w = wnew;  M = Mnew;  endif
endfor

function gM = gradM(w)  # gradient of objective function
    a = x * w;  # compute activations
    y = sigmoid(a);  # compute outputs
    e = t - y;  # compute errors
    g = -x' * e;  # compute the gradient of G(w)
gM = alpha * w + g;
endfunction

function M = findM(w)  # objective function
    G = -(t' * log(y) + (1-t') * log(1-y));
    EW = w' * w / 2;
    M = G + alpha * EW;
endfunction
\end{verbatim}
Interpreting learning as inference
Calculating Bayesian predictions
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Original estimate
Interpreting learning as inference
Calculating Bayesian predictions

Original estimate

Bayesian estimate
Interpreting learning as inference

Gaussian approximation

\[ P(t^{(N+1)} = 1 \mid x^{(N+1)}, D, \alpha) = \int d^K w \ y(x^{(N+1)}; w) \frac{1}{Z_M} \exp(-M(w)) , \]

Taylor expansion around the MAP estimate

\[ M(w) \simeq M(w_{\text{MP}}) + \frac{1}{2} (w - w_{\text{MP}})^T A (w - w_{\text{MP}}) + \cdots , \]

\[ A_{ij} \equiv \left. \frac{\partial^2}{\partial w_i \partial w_j} M(w) \right|_{w=w_{\text{MP}}} \]
Interpreting learning as inference

Gaussian approximation

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Taylor expansion around the MAP estimate

\[ M(w) \approx M(w_{MP}) + \frac{1}{2}(w - w_{MP})^\top A(w - w_{MP}) + \cdots, \]

\[ A_{ij} \equiv \frac{\partial^2}{\partial w_i \partial w_j} M(w) \bigg|_{w=w_{MP}} \]

The Gaussian approximation:

\[ Q(w; w_{MP}, A) = [\det(A/2\pi)]^{1/2} \exp \left[ -\frac{1}{2}(w - w_{MP})^\top A(w - w_{MP}) \right] \]
Interpreting learning as inference

**Gaussian approximation**

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Neural networks

Unsupervised learning

Capacity of a single neuron is limited: certain data can only be learned. So far, we used a supervised learning paradigm: a teacher was necessary to teach an input-output relation.

*Hopfield networks* try to cure both.

**Unsupervised learning:** what is it about?

Hebb rule: an enlightening example

assuming 2 neurons and a weight modification process:

\[
\frac{dw_{ij}}{dt} \sim \text{Correlation}(x_i, x_j)
\]

This simple rule realizes an associative memory!
Neural networks
The Hopfield network

Architecture: a set of $I$ neurons
connected by symmetric synapses of weight $w_{ij}$
no self connections: $w_{ii} = 0$
output of neuron $i$: $x_i$

Activity rule:
$$x(a) = \Theta(a) \equiv \begin{cases} 
1 & a \geq 0 \\
-1 & a < 0.
\end{cases}$$

Synchronous/ asynchronous update

Learning rule:
$$w_{ij} = \eta \sum_n x_i^{(n)} x_j^{(n)} ,$$
Neural networks
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Synchronous/ asynchronous update

Learning rule:
$$w_{ij} = \eta \sum_n x_i^{(n)} x_j^{(n)},$$

alternatively, a continuous network can be defined as:
$$a_i = \sum_j w_{ij} x_j; \quad x_i = \tanh(a_i).$$
Neural networks
Stability of Hopfield network

Are the memories stable?

\[ E(x, w) = -\frac{1}{2} \sum_{m,n} w_{mn} x_m x_n - \sum_n w_{0n} x_n \]

Necessary conditions: symmetric weights; asynchronous update
Neural networks
Stability of Hopfield network

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Necessary conditions: symmetric weights; asynchronous update

Robust against perturbation of a subset of weights
Neural networks

Capacity of Hopfield network

How many traces can be memorized by a network of \( I \) neurons?

Desired memories: D J C M S
Neural networks
Capacity of Hopfield network

\[ a_i = \sum_j w_{ij} x_j^{(n)}, \]

\[ w_{ij} = x_i^{(n)} x_j^{(n)} + \sum_{m \neq n} x_i^{(m)} x_j^{(m)}. \]

\[
a_i = \sum_{j \neq i} x_i^{(n)} x_j^{(n)} x_j^{(n)} + \sum_{j \neq i} \sum_{m \neq n} x_i^{(m)} x_j^{(m)} x_j^{(n)} = (I - 1)x_i^{(n)} + \sum_{j \neq i} \sum_{m \neq n} x_i^{(m)} x_j^{(m)} x_j^{(n)}. \]

\[ P(i \text{ unstable}) = \Phi \left( -\frac{I}{\sqrt{IN}} \right) = \Phi \left( -\frac{1}{\sqrt{N/I}} \right), \]