Aalto University

Probabilistic machine learning | Intro (E)

Introduction to machine learning

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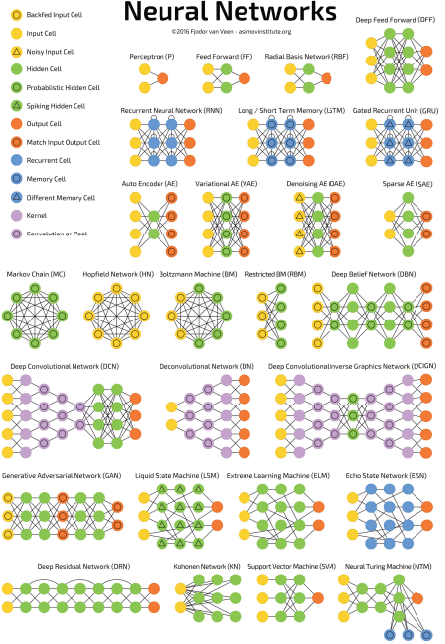


Intro

Many neural network models are made of neurons

⇝ A single lonely ☹ neuron can learn, too

It _must_ be interesting to understand it in detail

Formulation and training

The neuron

Formulation

The neuron

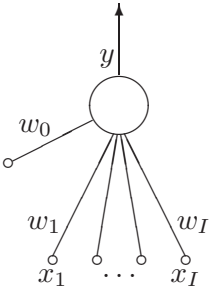
Formulation

Architecture

A neuron has a number I of inputs x_i and one output y

Associated with each input is a weight w_i $(i = 1, \ldots, I)$

- There may be an additional parameter w_0
- The bias, the weight for the input x_0
- Input x_0 is permanently set to 1



The neuron is a feedforward computational device

- Connections go from inputs to output

Formulation (cont.)

Activity

The activity of the neuron consists of two steps

1. In response to the presented input $\mathbf{x} = (x_1, \ldots, x_I)$, the **activation**

$$a = \sum_i w_i x_i$$

Sum is over $i = 0, \ldots, I$ if there is a bias
↝ $(i = 1, \ldots, I$ otherwise)

2. The output y, or **activity**, is set as a function $f(a)$ of the activation

$$y = f(a) = f(\sum_i w_i x_i)$$

There are several activation functions
↝ Deterministic and stochastic

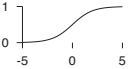
Formulation (cont.)

Popular activation functions (deterministic)

- Linear (identity)

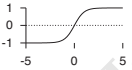
$$y(a) = a$$

- Sigmoid (logistic function)



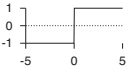
$$y(a) = \frac{1}{1 + e^{-a}}, \quad y \in (0, 1)$$

- Sigmoid (tanh)



$$y(a) = \tanh(a), \quad y \in (-1, +1)$$

- Threshold (sign)



$$y(a) = \text{sign}(a) = \begin{cases} +1, & a > 0 \\ -1, & a \leq 0 \end{cases}$$

Formulation (cont.)

Popular activation functions (stochastic)

Stochastic activation functions, y is randomly selected from $\{-1, +1\}$

- Heat bath

$$y(a) = \begin{cases} +1, & \text{with probability } \dfrac{1}{1+e^{-a}} \\ -1, & \text{with probability } 1 - \dfrac{1}{1+e^{-a}} \end{cases}$$

- ...

Formulation (cont.)

The neuron implements a function $y(\mathbf{x}|\mathbf{w}) = y[a(\mathbf{x}, \mathbf{w})]$, with $a = \sum_i w_i x_i$

The output y is often a nonlinear function of the inputs $\mathbf{x}$

- The function is parameterised by weights $\mathbf{w}$

The logistic sigmoid

We study a neuron which produces an output $y \in (0, 1)$, as function of $\mathbf{x}$

- We consider the logistic function (sigmoid)

$$y(\mathbf{x}|\mathbf{w}) = \frac{1}{1 + e^{-\mathbf{w}\cdot\mathbf{x}}}$$

Formulation (cont.)

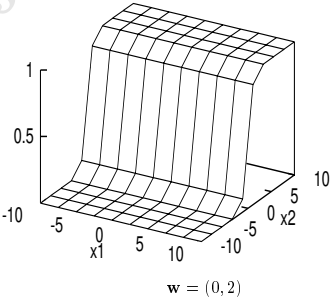
The case where input vector and parameter vector are two-dimensional

$$y(\mathbf{x}|\mathbf{w}) = \frac{1}{1 + e^{-\mathbf{w}\cdot\mathbf{x}}}$$

- $\mathbf{x} = (x_1, x_2)$ and $\mathbf{w} = (w_1, w_2)$
- The implemented function y

$$y(\mathbf{x}|\mathbf{w}) = \frac{1}{1 + e^{-(w_1 x_1 + w_2 x_2)}}$$

- (Temporarily, no bias)



Along a line perpendicular to the direction of $\mathbf{w}$, the output is constant

Along a line in the direction of $\mathbf{w}$, the output is a sigmoid function

Formulation (cont.)

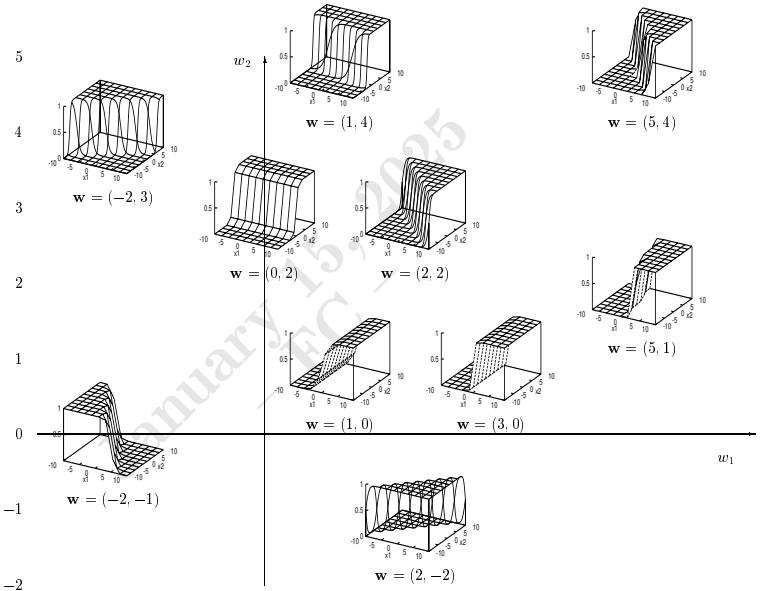
The weight space

The parameter/weight space of the neuron is a space whose dimensionality equals the number of weights and onto which weights can take on values

- Each point $\mathbf{w}$ in weight space corresponds to a function of $\mathbf{x}$

In our case study, there are two parameters (weights) w_1 and w_2

- The weight space is two-dimensional
- We see functions $y(\mathbf{x}|\mathbf{w})$ in place



Training

The E-uD-uE-uA-uF-AN(u)N

Training

The central idea of a supervised neuron (and also neural networks, I suppose)

⇝ Given examples of the relation between input vectors $\mathbf{x}$ and targets t

$$\{(\mathbf{x}^{(n)}, t^{(n)})\}_{n=1}^{N}$$

⇝ We wish to make the neuron $y(\mathbf{x}|\mathbf{w})$ learn the map from $\mathbf{x}$ to t

For any given $\mathbf{x}$, a successfully trained neuron will return some output y

- Output is expected to be close (in some sense) to target value t

---

Training the neuron means searching in weight space for some optimal $\hat{\mathbf{w}}$

- A value $\hat{\mathbf{w}}$ that produces a function $y(\mathbf{x}|\hat{\mathbf{w}})$ that fits the data well
- That is, output values y that are close to target values t

Training (cont.)

The error function

A function that measures how well a neuron with weights $\mathbf{w}$ solves the task

Often, the error function is a sum of terms, one for each input/target pair

- It measures how close output $y(\mathbf{x}|\mathbf{w})$ is to target t
- Each term is a function of $\mathbf{w}$, given the input $\mathbf{x}$

Training the neuron is an exercise in function minimisation (optimisation)

$\rightsquigarrow$ Find the $\mathbf{w}$ so that the error (objective) function is minimal

Training (cont.)

Binary classification

We have a lonely neuron whose output $y(\mathbf{x}, \mathbf{w})$ is bounded in $(0, 1)$

- The activation function is the logistic sigmoid

$$y(\mathbf{x}|\mathbf{w}) = \frac{1}{1 + e^{-\mathbf{w}\cdot\mathbf{x}}}$$

They gave us a set of input data with binary labels

$$\{(\mathbf{x}^{(n)}, t^{(n)})\}_{n=1}^{N}$$

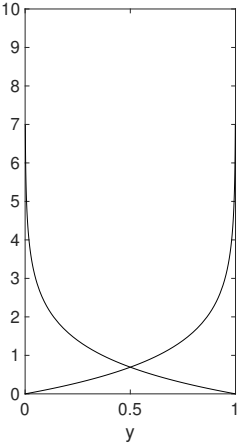
How do we train the neuron to binary classify the data?

- Firstly, we need to define some error function
- Then, we need to find a $\mathbf{w}$ that minimises it

Training (cont.)

We consider the following error function

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



The term in error function

- Bounded below, by zero
- When $y(\mathbf{x}^{(n)}|\mathbf{w}) = t^{(n)}$
- (for each n)

The neur(on)al model

$$y(\mathbf{x}|\mathbf{w}) = \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}}}$$

Training (cont.)

$$G(\mathbf{w}) = -\sum_n \left\{ t^{(n)} \ln \left[\underbrace{y(\mathbf{x}^{(n)}|\mathbf{w})}_{y^{(n)}} \right] + (1 - t^{(n)}) \ln \left[1 - \underbrace{y(\mathbf{x}^{(n)}|\mathbf{w})}_{y^{(n)}} \right] \right\}$$

The derivative $\mathbf{g} = (\cdots, g_j, \cdots)$ of $G(\mathbf{w})$ with respect to $\mathbf{w}$

$$\begin{aligned} g_j &= \frac{\partial G(\mathbf{w})}{\partial w_j} \\ &= \sum_{n=1}^{N} -\left[t^{(n)} - y^{(n)} \right] x_j^{(n)} \\ &= \sum_{n=1}^{N} -e^{(n)} x_j^{(n)} \end{aligned}$$

Quantity $e^{(n)} \equiv \left[t^{(n)} - y^{(n)} \right]$ is the mismatch on case n

The derivative $\dfrac{\partial G(\mathbf{w})}{\partial \mathbf{w}}$, the gradient $\nabla_{\mathbf{w}} G(\mathbf{w})$, is a sum of terms $\mathbf{g}^{(n)}$

$$g_j^{(n)} \equiv -\left[t^{(n)} - y^{(n)} \right] x_j^{(n)}, \text{ for } n = 1, \ldots, N$$

An online algorithm is designed by feeding each input to the neuron, one at a time, and then adjusting $\mathbf{w}$ a bit in the direction opposite to $\mathbf{g}^{(n)}$ (a stochastic gradient descent)

Training (cont.)

Sequential training

Architecture: A lonely ☹ neuron with I inputs x_i and one output y

- Associated with each input is a weight w_i $(i = 1, \ldots, I)$

Activity: In response to inputs $\mathbf{x}$, we compute the neuron activation

$$\begin{aligned} a &= \mathbf{w} \cdot \mathbf{x} \\ &= \sum_i w_i x_i \end{aligned}$$

The output y is set as a logistic sigmoid of the activation $a = \mathbf{w} \cdot \mathbf{x}$

$$y(\mathbf{x}, \mathbf{w}) = \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}}}$$

Training (cont.)

Training

The teacher supplies a target value $t \in \{0, 1\}$

- The correct label t of input $\mathbf{x}$

We compute the neuron error with weights $\mathbf{w}$

$$e = t - y$$

We adjust all the weights to reduce the error

$$\Delta w_i = \eta \underbrace{(t - y) x_i}_{-g_i^{(\cdot)}}$$

- They call η the 'step-size'

Activity and training are repeated for each supplied pair $(\mathbf{x}, t)$

- A change in weight is made after every pair is presented

With fixed-size sets of data, we can cycle thru multiple times

Training (cont.)

An alternative training paradigm is to go through a batch of examples

- Compute all the outputs $y^{(n)}$ and errors $e^{(n)}$
- Accumulate all the changes, $\Delta w_i = \eta e x_i$
- Apply cumulative change at the end

Batch training

For each input-output pair $\{\mathbf{x}^{(n)}, t^{(n)}\}$, we compute $y^{(n)} = y(\mathbf{x}^{(n)}|\mathbf{w})$

$$y(\mathbf{x}|\mathbf{w}) = \frac{1}{1 + \exp\left(-\sum_i w_i x_i\right)}$$

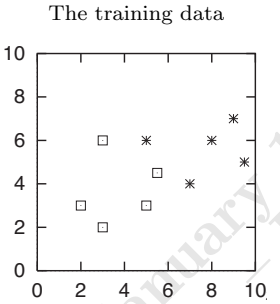
Define the term $e^{(n)} = \left[t^{(n)} - y^{(n)}\right]$ and compute for each weight w_i

$$g_i^{(n)} = -e^{(n)} x_i^{(n)}$$

Then, let

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

Training (cont.)



Batch-mode (gradient descent)

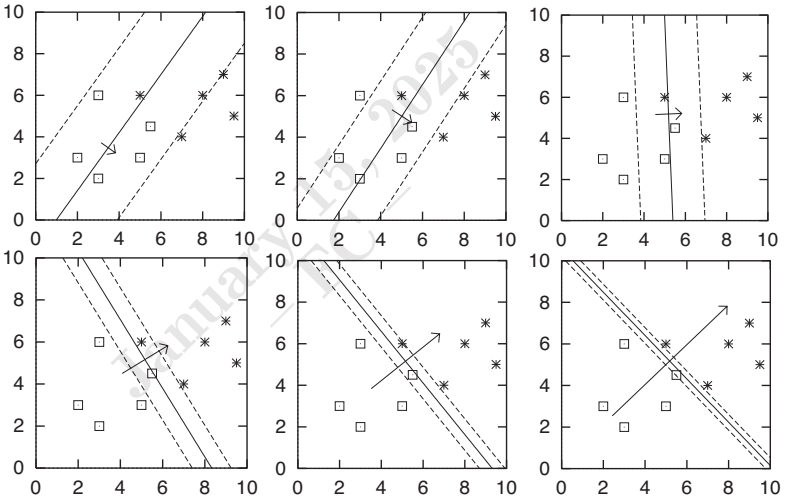
- Step-size $\eta = 0.01$

Each data point consists of a two-dimensional input vector $\mathbf{x}$ and a t value

- $\times$ for $t = 1$
- $\square$ for $t = 0$

Training (cont.)

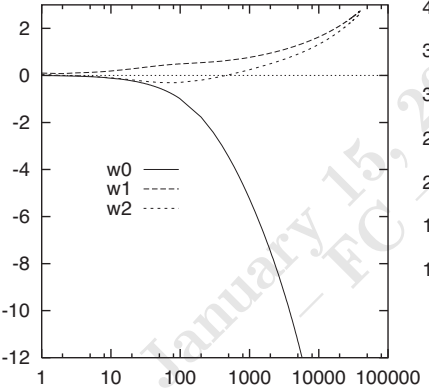
The performed function after 30, 80, 500, 3K, 10K and 40K iterations

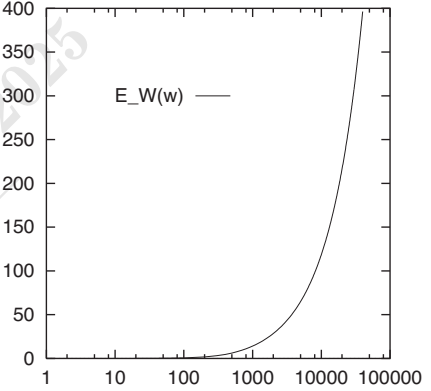


Contours correspond to $a \in \{-1, 0, +1\}$, namely at $y \in \{0.27, 0.50, 0.73\}$

Training (cont.)

(a) Evolution of the weights as a function of the (log) number of iterations





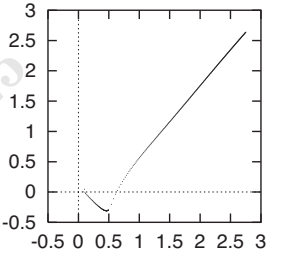
(b) Magnitude of the weights as a function of the (log) number of iterations

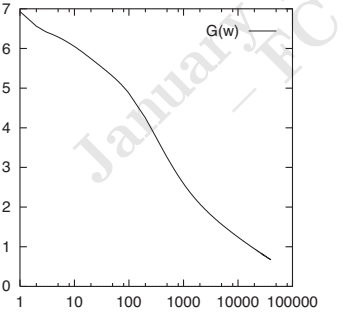
$$E_W(\mathbf{w}) = 1/2 \sum_i {w_i}^2$$

Training (cont.)

Evolution of the weights

- In weight-space





The error function as a function of number of iterations (on log scale)

Training (cont.)

This training algorithm works, if η is set to an appropriate value

- It finds a $\mathbf{w}$ that correctly classifies examples

For linearly separable examples, the neuron finds the separation

- With time, weights diverge to ever-larger values
- It is a manifestation of overfitting (undesirable)

Note to self: It's dumb to early-stop an algorithm meant to do minimisation

- It is more principled to use regularisation

Training (cont.)

Regularisation

We augment the error function so that we penalise solutions we dislike (large weights)

- Them sharp boundaries arising from large weight values
- We penalise large (half-)norms of the parameter vector

$$E_W(\mathbf{w}) = \frac{1}{2}\sum_i {w_i}^2$$

$$= \frac{1}{2}||\mathbf{w}||_2^2$$

We augment the error function $G(\mathbf{w})$ with a weight-decay regulariser $E_W(\mathbf{w})$

$$M(\mathbf{w}) = G(\mathbf{w}) + \alpha E_W(\mathbf{w})$$

- α is a regularisation constant (it is a hyper-parameter)

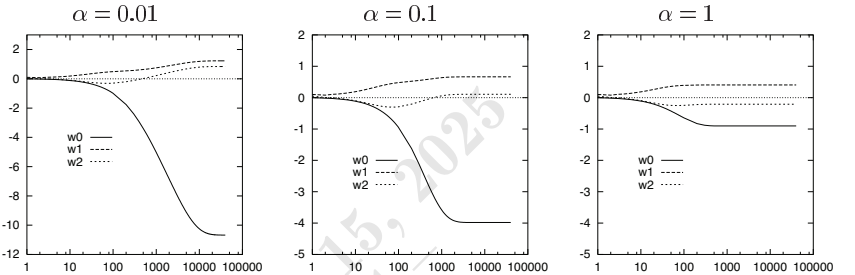
Training (cont.)

$$M(\mathbf{w}) = \underbrace{-\sum_n \left\{ t^{(n)} \ln \left[y(\mathbf{x}^{(n)}|\mathbf{w}) \right] + (1 - t^{(n)}) \ln \left[1 - y(\mathbf{x}^{(n)}|\mathbf{w}) \right] \right\}}_{\text{Error function: } G(\mathbf{w})} + \alpha \underbrace{\frac{1}{2} \sum_i {w_i}^2}_{\text{Regularizer: } E_W(\mathbf{w})}$$

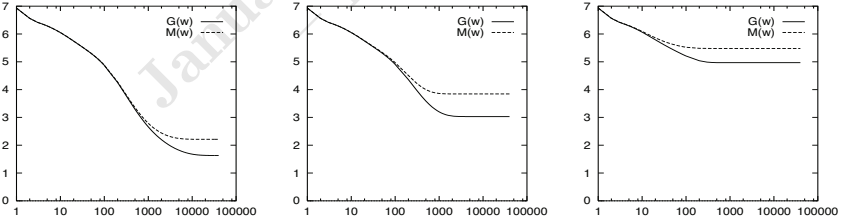
Influence of weight decay on the neuron batch training, gradient descent

- $\alpha \in \{0.01, 0.1, 1\}$

Training (cont.)



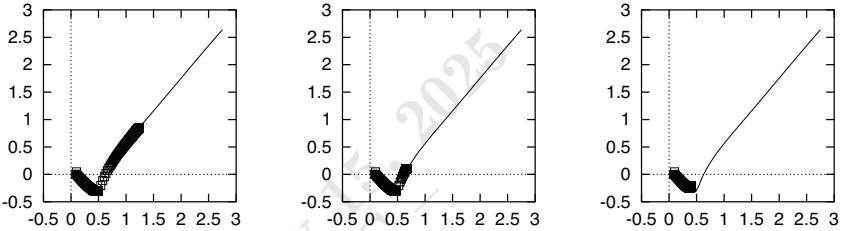
(a) Evolution of weights w_0, w_1 and w_2, as a function of number of iterations



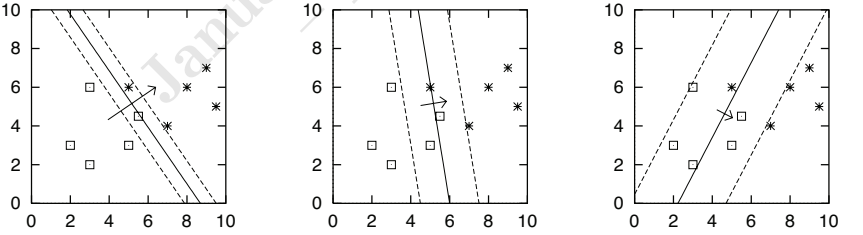
(c) Objective $M(\mathbf{w})$ and error function $G(\mathbf{w})$, against number of iterations

Training (cont.)

(b) In weight space, with trajectory in the case of zero weight-decay



(d) The function performed by the neuron, after 40 000 iterations



Learning and predictions

The neuron

Learning

The neuron

Learning

We trained the neuron to behave as a linear classifier

- Minimisation of an objective function

$$M(\mathbf{w}) = \underbrace{-\sum_n \left\{ t^{(n)} \ln \left[y(\mathbf{x}^{(n)}|\mathbf{w}) \right] + (1 - t^{(n)}) \ln \left[1 - y(\mathbf{x}^{(n)}|\mathbf{w}) \right] \right\}}_{\text{Error function: } G(\mathbf{w})} + \alpha \underbrace{\frac{1}{2} \sum_i {w_i}^2}_{\text{Regularizer: } E_W(\mathbf{w})}$$

The neuron's output $y(\mathbf{x}, \mathbf{w})$ defines the probability that an input $\mathbf{x}$ belongs to class $t = 1$, rather than to the alternative $t = 0$, when the parameter values $\mathbf{w}$ are all given

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Values of $\mathbf{w}$ define the different hypothesis about the probability of class 1

- Relative to class 0, as function of input $\mathbf{x}$

Learning (cont.)

Assume the inputs $\{\mathbf{x}_n\}_{n=1}^N$ to be given (sure variables, not to be modelled)

Let D be the observed target data $D = \{t_n\}_{n=1}^N$

To infer parameters $\mathbf{w}$ given data D, we require a likelihood function

- The joint probability of all of the data, given parameters

Plus some prior probability over $\mathbf{w}$

Learning (cont.)

The likelihood measures how well various parameters $\mathbf{w}$ predict the observed data

- It is the probability assigned by the model to the observed data t

$$p(t=1|\mathbf{w},\mathbf{x}) = y(\mathbf{w},\mathbf{x})$$
$$p(t=0|\mathbf{w},\mathbf{x}) = 1 - y(\mathbf{w},\mathbf{x})$$

Each observed datum is assumed to be Bernoulli with parameter y

$$\begin{aligned} p(t|\mathbf{w},\mathbf{x}) &= y^t(1-y)^{1-t} \\ &= \exp\left[t\ln(y) + (1-t)\ln(1-y)\right] \end{aligned}$$

For independent and identically distributed data, the probability of the data

$$\begin{aligned} p(\{t\}|\mathbf{w},\{\mathbf{x}\}) &= \prod_n \left\{ y(\mathbf{w},\mathbf{x}_n)^{t_n} \left[1 - y(\mathbf{w},\mathbf{x}_n)\right]^{t_n} \right\} \\ &= \prod_n e^{\left\{ t_n \ln\left[y(\mathbf{w},\mathbf{x}_n)\right] + (1-t_n)\ln\left[1-y(\mathbf{w},\mathbf{x}_n)\right] \right\}} \\ &\rightsquigarrow \exp\Bigg(\underbrace{\sum_n \left\{ t_n \ln\left[y(\mathbf{w},\mathbf{x}_n)\right] + (1-t_n)\ln\left[1-y(\mathbf{w},\mathbf{x}_n)\right] \right\}}_{-G(\mathbf{w})} \Bigg) \end{aligned}$$

Learning (cont.)

$$p(\{t\}|\mathbf{w}, \{\mathbf{x}\}) = \exp\Big(\underbrace{\sum_n \{t_n \ln[y(\mathbf{w}, \mathbf{x}_n)] + (1 - t_n) \ln[1 - y(\mathbf{w}, \mathbf{x}_n)]\}}_{-G(\mathbf{w})}\Big)$$

This is the probabilistic interpretation of the cross-entropy objective

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The error function $G(\mathbf{w})$ can be interpreted as negative log likelihood

$$p(\{t\}|\mathbf{w}) = \exp\big[-G(\mathbf{w})\big]$$

Learning (cont.)

The regulariser is interpreted as log prior probability over the parameters $\mathbf{w}$

$$P(\mathbf{w}|\alpha) = \frac{1}{Z_W(\alpha)} \exp\Big[-\alpha E_W\Big]$$

If E_W is quadratic, then the corresponding prior distribution is Gaussian

$$\begin{aligned} P(\mathbf{w}|\alpha) &= \frac{1}{Z_W(\alpha)} \exp\Big[-\alpha E_W\Big] \\ &= \frac{1}{Z_W(\alpha)} \exp\Big[-\frac{\alpha}{2}\sum_i {w_i}^2\Big] \end{aligned}$$

- I is the number of parameters in $\mathbf{w}$
- $Z_W^{-1}(\alpha)$ is equal to $(\alpha/2\pi)^{I/2}$
- The variance $\sigma_W^2 = 1/\alpha$
- The mean $\boldsymbol{\mu} = \mathbf{0}$

Learning (cont.)

Why is it natural to interpret the error functions as log probabilities?

- Probabilities are multiplicative, for independent events
- Error functions are often additive, over multiple data
- The log fixes the correspondence

Generalised Gaussian priors

$$E_W(\mathbf{w}) = \frac{1}{2}\sum_i |w_i|^q$$

If E_W is a q-norm, the prior distribution is a generalised Gaussian

$$p(\mathbf{w}|\alpha) = \Big[\frac{q}{2}\Big(\frac{\alpha}{2}\Big)^{1/q}\frac{1}{\Gamma(1/q)}\Big]^I \exp\Big[-\frac{\alpha}{2}\sum_i |w_i|^q\Big]$$

Learning (cont.)

The objective function $M(\mathbf{w})$ is inference of parameters $\mathbf{w}$, given data D

$$\begin{aligned} P(\mathbf{w}|D,\alpha) &= \frac{P(D|\mathbf{w})P(\mathbf{w}|\alpha)}{P(D|\alpha)} \\ &= \frac{1}{P(D|\alpha)} e^{-G(\mathbf{w})} \frac{1}{Z_W(\alpha)} e^{-\alpha E_W(\mathbf{w})} \\ &= \frac{1}{Z_M(\alpha)} \exp\big[-M(\mathbf{w})\big] \end{aligned}$$

The $\mathbf{w}$ by minimising $M(\mathbf{w})$ is interpreted as the most probable vector $\hat{\mathbf{w}}$

The partition function (normalisation constant)

$$Z_M(\alpha) = \int \mathrm{d}\mathbf{w} \exp\big[-M(\mathbf{w})\big]$$

Learning (cont.)

Estimator $\hat{\mathbf{w}}$, the product of traditional learning is a point in the weight-space

- $\hat{\mathbf{w}}$ maximises the posterior probability density

In a sensible sense, the product of learning is an ensemble of plausible values

- We do not choose one particular hypothesis $\mathbf{w}$
- We rather evaluate the posterior probabilities

The posterior distribution, the likelihood times a prior distribution over $\mathbf{w}$

Learning (cont.)

For a neuron with two inputs and no bias

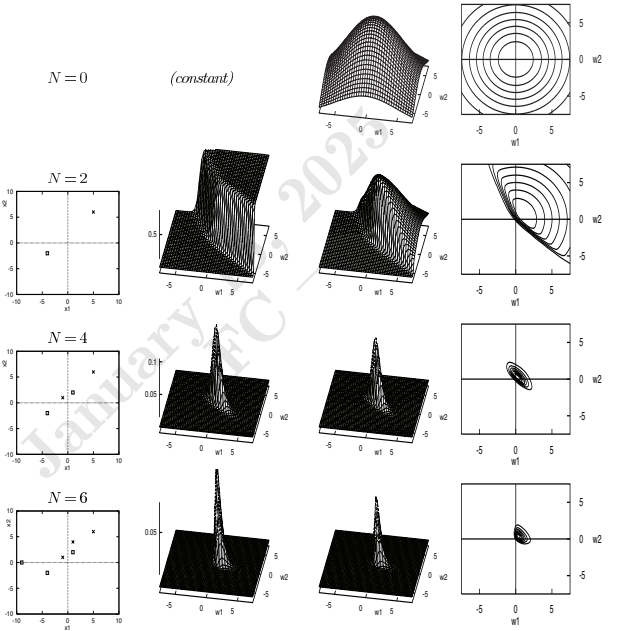
$$y(\mathbf{x}|\mathbf{w}) = \frac{1}{1 + e^{-(w_1 x_1 + w_2 x_2)}}$$

We can plot the posterior probability of $\mathbf{w}$

$$p(\mathbf{w}|D, \alpha) \propto \exp\big[- M(\mathbf{w})\big]$$

Each data point consists of a two-dimensional input vector $\mathbf{x}$ and a t value

- $\times$ for $t = 1$
- $\square$ for $t = 0$



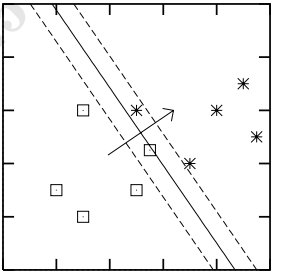
Prediction

The neuron

Prediction

The task is making predictions using the neuron we trained as classifier

$$y(\mathbf{x}, \mathbf{w}) = \frac{1}{1 + e^{-(w_1 x_1 + w_2 x_2)}}$$

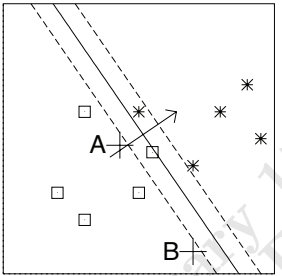


Training by minimising $M(\mathbf{w}) = G(\mathbf{w}) + \alpha E(\mathbf{w})$, optimized for $\alpha = 0.01$

We consider the task of predicting class $\mathbf{t}^{(N+1)}$ for a new input $\mathbf{x}^{(N+1)}$

- We could just use the neuron, weights set to $\hat{\mathbf{w}}$

Prediction (cont.)



Consider two new data points

- A and B

Both are assigned to class 1

- With probability 0.2
- $\hat{\mathbf{w}}\mathbf{x}^{(\mathsf{A})} = \hat{\mathbf{w}}\mathbf{x}^{(\mathsf{B})}$

These predictions would be correct, if we really really knew $\mathbf{w}$ was $\hat{\mathbf{w}}$

- But we do not, parameters are uncertain
- We placed a prior over them
- We even got its posterior

Prediction (cont.)

Prediction of a new datum $\mathbf{t}^{(n)}$ involves marginalising over the parameters

- Well, over anything else that is endowed with uncertainty
- We assume that we only have the weight $\mathbf{w}$ uncertain
- Weight-decay α and model $\mathcal{H}$ are assumed to be sure

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

Predictions are weighted by weighting the predictions, for all possible $\mathbf{w}$

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

The weights are given by the posterior probabilities of $\mathbf{w}$

- $P(\mathbf{w}|D, \alpha) = 1/Z_M \exp[-M(\mathbf{w})]$
- $Z_M = \int d^K \mathbf{w} \exp[-M(\mathbf{w})]$

Prediction (cont.)

We get predictions if we find a way of computing the integral

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

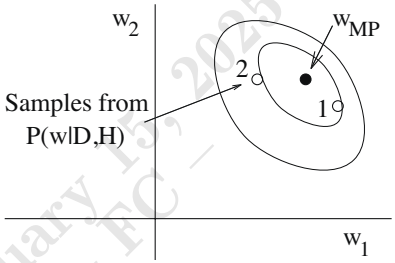
Expectation of function y under the posterior distribution

$$\langle y(\mathbf{w}) \rangle \simeq \frac{1}{R} \sum_r y(\mathbf{w}_r)$$

Average the output at $\mathbf{x}^{(N+1)}$, under the posterior of $\mathbf{w}$

$$\{\mathbf{w}_r\}_{r=1}^R, \quad \text{simulated}$$

Prediction (cont.)



We average together predictions made by each possible value of weights **w**

- Each value receives a(nother) weight proportional to its probability
- The probability is under the posterior ensemble

Simulation

The neuron

Simulation

Simulation

Need to simulate a density $P(\mathbf{x})$, known to within a multiplicative constant

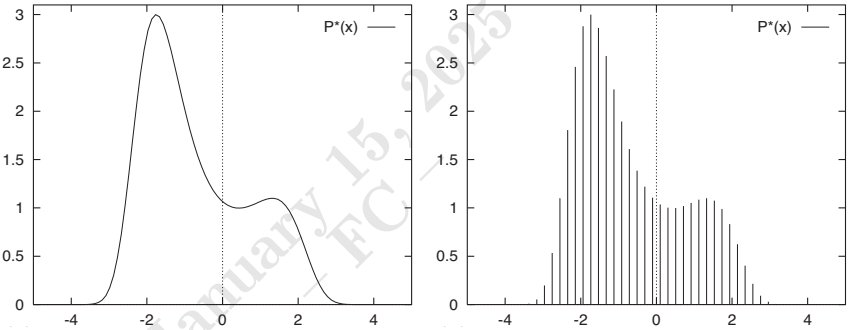
- We can evaluate a function $P^*(\mathbf{x})$ such that $P(\mathbf{x}) = P^*(\mathbf{x})/Z$

$Z = \int d^N\mathbf{x} P^*(\mathbf{x})$ is unknown, and even if we knew it we would not know how to simulate P w/o listing ALL states (may take a few universe ages)

- Best evaluations come from places where P is big

Simulation (cont.)

We wish to draw samples from some $P(x) = P^*(x)/Z$, we can plot $P^*(x)$



Potentially, we could discretise the support of variable x, and ask for samples from the discrete probability distribution over the finite set of uniformly spaced points $\{x_i\}$, no?

- $p_i^* = P^*(x_i) \quad \longrightarrow Z \simeq \sum_i p_i^* \quad \longrightarrow p_i = p_i^*/Z$

$\rightsquigarrow$ Samples from the empirical distribution $\{p_i\}$

Simulation (cont.)

What's the cost of evaluating (just) Z?

- We have to visit every site x_i?
- Yes! Well, 50 P^* evaluations

- In 1000 dimensions, 50^{1000}
- We do not need a 50-grid!
- A 2-grid is good enough
- 2^{1000}, a lot better
- Not really!

1. **Energy-based simulations**
2. **Shape-based simulations**

Energy-based simulation

The neuron

Energy-based simulations

We do not simulate $P(\mathbf{w}|D,\alpha)$, but another (simpler) density $Q(\mathbf{w}|\Theta)$

- $Q(\mathbf{w}|\Theta)$ must be easy to simulate and similar to $P(\mathbf{w}|D,\alpha)$
- We pick a new $Q(\mathbf{w}|\Theta)$ at each simulated state $\mathbf{w}_r$

The $Q(\mathbf{w}|\Theta,\mathbf{w}_r)$ depends on the system's energy

$$H(\mathbf{w},\mathbf{p}) = \underbrace{E(\mathbf{w})}_{\mathbf{w}^T\mathbf{x}} + \underbrace{K(\mathbf{p})}_{\mathbf{p}^T\mathbf{p}/2}$$

$\mathbf{p}$ are momentum variables

Energy-based simulations

Langevin thermostats

We create, asymptotically, samples from the joint distribution

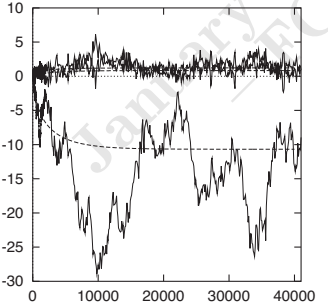
$$P_H(\mathbf{w},\mathbf{p}) = \frac{1}{Z_H}\exp\left[-H(\mathbf{w},\mathbf{p})\right]$$
$$= \underbrace{\frac{1}{Z_H}\exp\left[-E(\mathbf{w})\right]}_{\text{desired density}}\exp\left[-K(\mathbf{p})\right]$$

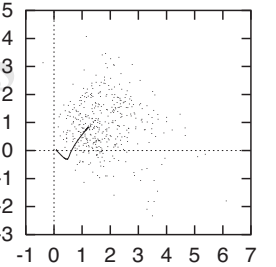
1. Draw $\mathbf{p} \sim \mathcal{N}(\mathbf{p}|\boldsymbol{\mu}, \mathbf{I})$
2. Calculate gradient $\mathbf{g} = \partial E(\mathbf{w})/\partial \mathbf{w}$
3. Make a step in $\mathbf{w}$-space $\Delta\mathbf{w} = -\gamma^2\mathbf{w} + 2\gamma\mathbf{p}$
4. Accept/reject proposal $\mathbf{w}$ based on changes in $M(\mathbf{w})$ and $\mathbf{g}$

Energy-based simulations (cont.)

Weights' 'evolution'

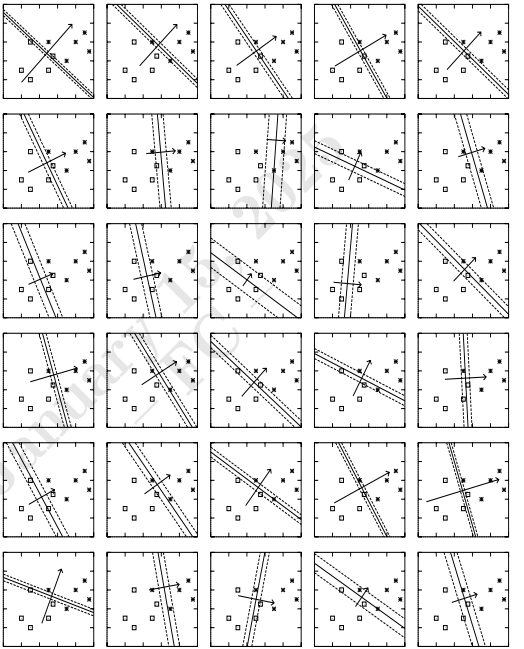
- In weight-space





Energy-based samples

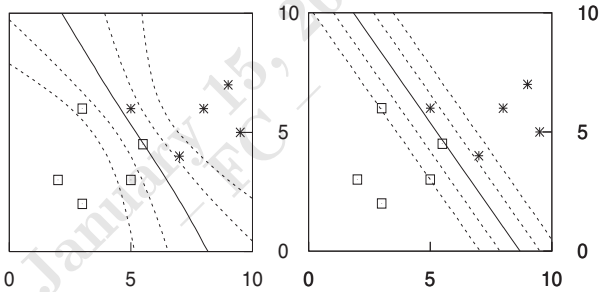
- Convergence in 10 K
- Acceptance rate 93%



Energy-based simulation (cont.)

Samples from iteration 10 000 to 40 000, every 1000 iterations

(a) The predictive function by averaging predictions from 30 samples



- Contours at $a = \{0, \pm 1, \pm 2\}$, $y = \{0.5, 0.27, 0.73, 0.12, 0.88\}$

(b) Predictions by the 'most probable' setting of neuron parameters

Energy-based simulation (cont.)

The behaviour of functions $G(\mathbf{w})$ and $M(\mathbf{w})$ during sampling

- Compared with values of G and M at $\hat{\mathbf{w}}$

Function $G(\mathbf{w})$ fluctuates around $G(\hat{\mathbf{w}})$, unsymmetrically

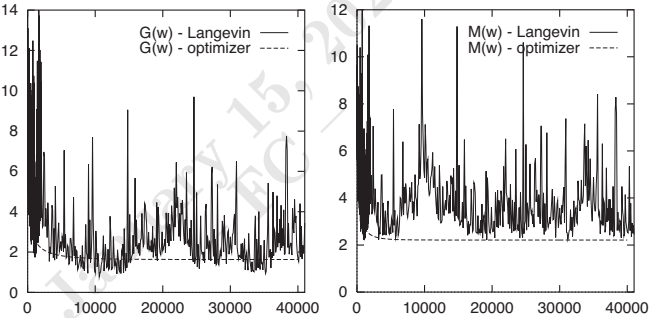
Function $M(\mathbf{w})$ also fluctuates, but not around $M(\hat{\mathbf{w}})$

- It cannot go lower than the optimum
- Actually, it rarely even gets closer

Energy-based simulations (cont.)

(a) The error function as a function of the (log) number of iterations

- The error function during optimisation



(b) The objective function as a function of the (log) number of iterations

- The objective function during optimisation

Shape-based simulation

The neuron

Near-Gaussian simulations

An old trick with nonlinearities is to take them and locally linearise them

An old trick with distributions is to approximate them with Gaussians

- Such approximations may be a good alternative to evaluate

$$p(\mathbf{t}^{(N+1)}|\mathbf{x}^{(N+1)}, D, \alpha) = \int \mathrm{d}^K \mathbf{w}\, y(\mathbf{x}^{(N+1)}|\mathbf{w}) \frac{1}{Z_M} \exp\left[-M(\mathbf{x})\right]$$

⇝ The actual name of the method is saddle-point approximation
⇝ The actual name of the method is Laplace's approximation
⇝ The actual name of the method is Gaussian approximation

Near-Gaussian simulations

Interest in an unnormalised probability density $P^*(x)$, peak at some x_0

- $Z_P \equiv \int P^*(x)\mathrm{d}x$ is the normalising constant

We Taylor-expand the logarithm of $P^*(x)$ around its peak

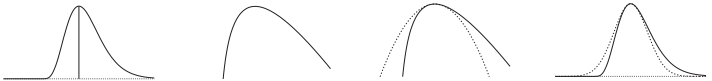
$$\ln\left[P^*(x)\right] \simeq \ln\left[P^*(x_0)\right] - \frac{1}{2}\Big\{\underbrace{-\frac{\partial^2}{\partial x^2}\ln[P^*(x)]\Big|_{x_0}}_{c}\Big\}(x-x_0)^2 + \cdots$$

$$\simeq \ln\left[P^*(x_0)\right] - \frac{c}{2}(x-x_0)^2 + \cdots$$

We approximate $P^*(x)$ by an unnormalised Gaussian

$$Q^*(x) \equiv P^*(x_0)\exp\Big[-\frac{c}{2}(x-x_0)^2\Big]$$

Z_P is approximated by its normalising constant $\quad Z_Q \equiv P^*(x_0)\sqrt{\dfrac{2\pi}{c}}$



Shape-based simulations (cont.)

We start by making a Gaussian approximation to the posterior probability

- We go to the bottom of $M(\mathbf{w})$ and there we Taylor-expand it

$$M(\mathbf{w}) \simeq M(\hat{\mathbf{w}}) + \frac{1}{2}(\mathbf{w}-\hat{\mathbf{w}})^{\mathsf{T}}\mathbf{A}(\mathbf{w}-\hat{\mathbf{w}}) + \text{ h.o.t.}$$

  $\mathbf{A}$ is the matrix of second derivatives (the Hessian) of $M(\mathbf{w})$

$$A_{ij} = \frac{\partial^2}{\partial w_i \partial w_j} M(\mathbf{w})\Big|_{\hat{\mathbf{w}}}$$

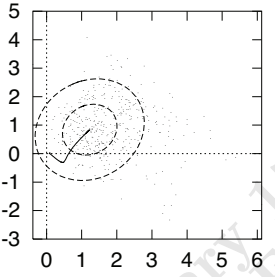
- Then, we define the Gaussian approximation

$$Q(\mathbf{w}|\hat{\mathbf{w}}, \mathbf{A}) = \Big[\det\Big(\frac{\mathbf{A}}{2\pi}\Big)\Big]^{1/2} \exp\Big[-\frac{1}{2}(\mathbf{w}-\hat{\mathbf{w}})^{\mathsf{T}}\mathbf{A}(\mathbf{w}-\hat{\mathbf{w}})\Big]$$

  Q is a normal with covariance matrix $\mathbf{A}^{-1}$

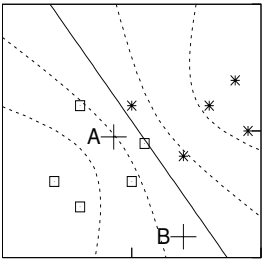
Shape-based simulations (cont.)

(a) A projection of the Gaussian approximation onto the (w_1, w_2)-plane



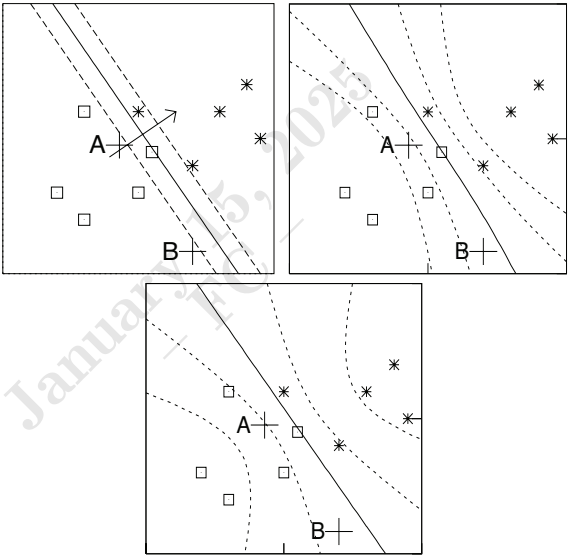
- One and two standard deviation contours
- The trajectory of the optimizer
- Near-normal samples

$p(\mathbf{t}^{(N+1)}|\mathbf{x}^{(N+1)}, D, \alpha)$



(b) The predictive function obtained from the Gaussian approximation

Wrap-up



Outro

The neuron