Universality of Multi-Layer Perceptron

integral representaion and approximation bound

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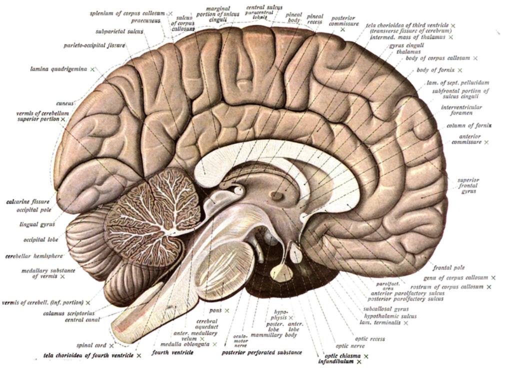
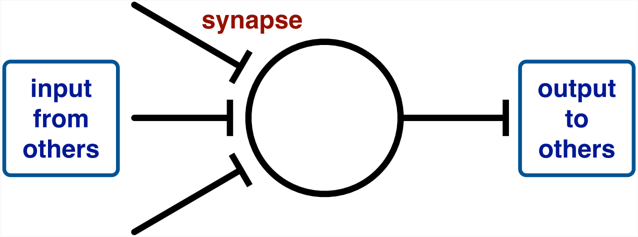
Introduction



An anatomical illustration from Sobotta's Human Anatomy 1908

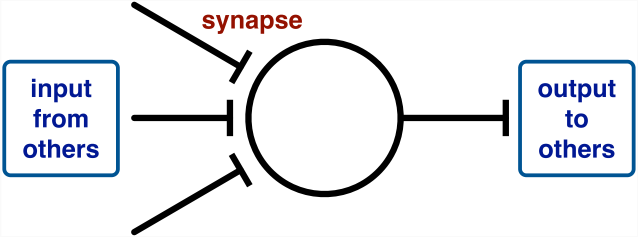
- weight: 1400g (2-3% of body)
- neurons:
  - cerebrum – 1.4×10^{10}
  - cerebellum – 1.0×10^{11}
- neuroglia:
  ten times of neurons
- synapses:
  10^3 – 10^5 per neuron
- energy consumption:
  - blood – 15%
  - oxygen – 20%
  - dextrose – 25%

output



- output: pulses from 0Hz to 500Hz
- normalize
  - max frequency: 500Hz $\mapsto 1$
  - min frequency: 0Hz $\mapsto 0$

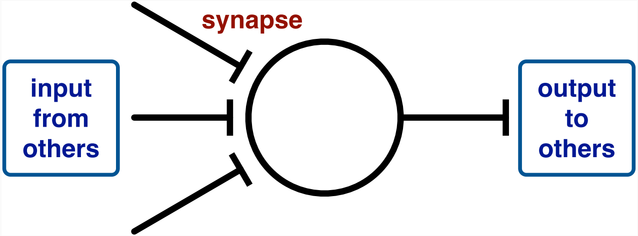
internal state



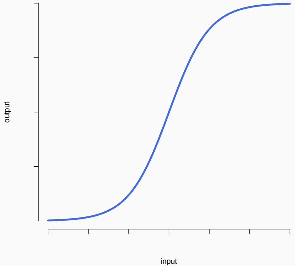
- input from other neuron: x_i
- strength of synapse: w_i
- internal state: weighted sum of inputs

$$u = \sum_i w_i x_i$$

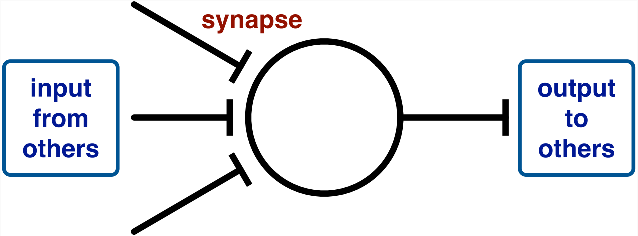
activation



- output a pulse when the internal state exceeds a certain constant: thresholding
- range from 0 to 1: non-linear transformation



input-output

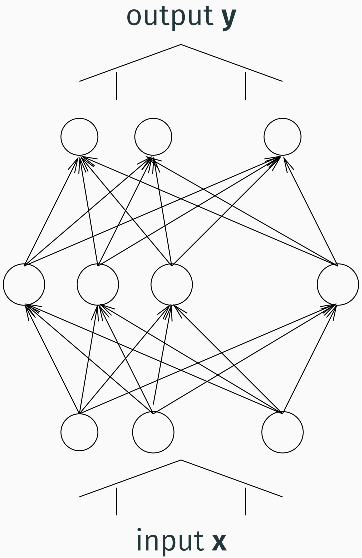


$$y = \psi\left(\sum_{i=1}^{m} w_i x_i - \theta\right) \qquad \text{(model of a neuron)}$$

y : output

θ : threshold

ψ : activation function



a simple calculation system consists of mathematical neurons

$$y_i = \sum_{j=1}^{h} c_{ij}\psi\left(\sum_{k=1}^{m} a_{jk}x_k - b_j\right), \quad (i = 1, \ldots, l)$$

(m-dim input, 1-dim output)

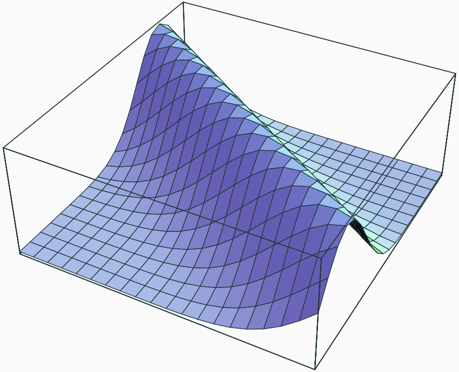
- easily implemented on computers because of homogeneously structured simple units
- simple and fast learning algorithms
  (error-backpropagation: gradient method calculated via chain rule)
- size of units and structure of network can be roughly designed without detailed prior knowledges
- learning from examples sometimes gives a unexpected result, which may include important information of data inside networks

Problem Formulation

Question

Find which class of functions can be well approximated by three layered perceptron with m-dim input and 1-dim output:

$$y = \sum_{j=1}^{h} c_j \psi \left(\sum_{k=1}^{m} a_{jk} x_k - b_j \right) .$$



ridge function on R^2

Definition

A function which is decribed with a vector $\mathbf{a} \in R^m$, a scalar $b \in R$ and a function $G : R \to R$ as

$$F(\mathbf{x}) = G(\mathbf{a} \cdot \mathbf{x} - b)$$

is called ridge function.

a

admissibility condition and transformation:

- suppose two functions $\phi_d, \phi_c \in L^1(R) \cap L^2(R)$ are bounded, and the following integral exists:

$$\int_{R^m} |\omega|^{-m} \hat{\phi}_d(\omega) \hat{\phi}_c(\omega) d\omega = 1$$

where $\hat{\cdot}$ denotes Fourier transform.

- define a transformation of f with ϕ_d by

$$T(\mathbf{a}, b) = \frac{1}{(2\pi)^m} \int_{R^m} \phi_d(\mathbf{a} \cdot \mathbf{x} - b) f(\mathbf{x}) d\mathbf{x}$$

kernel for composition

(combination of sigmoid functions)

$$\phi_c(z) = c\{\psi(z+h) - \psi(z-h)\}, \ (h > 0, c\text{: constant})$$

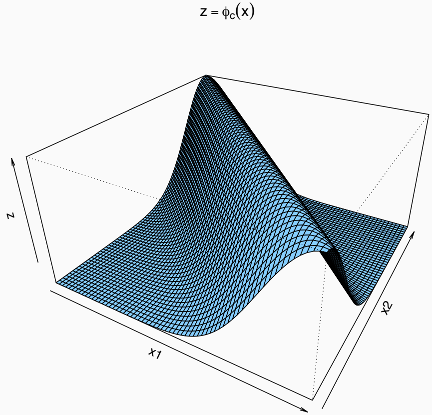
$$\psi(z) = \frac{1}{1+\exp(-z)}$$

kernel for decomposition

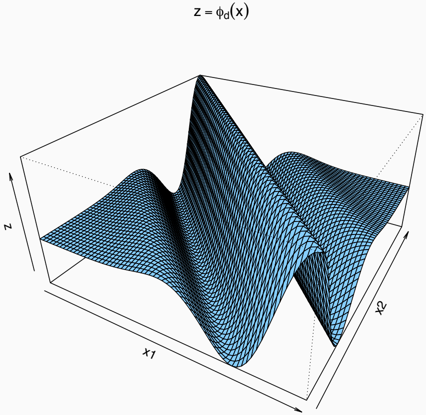
(generalized differential operator)

$$\phi_d(z) = \begin{cases} c\dfrac{d^m}{dz^m}\rho(z) & m\text{: even} \\ c\dfrac{d^{m+1}}{dz^{m+1}}\rho(z) & m\text{: odd} \end{cases}$$

$$\rho(z) = \begin{cases} e^{-1/(1-|z|^2)} & |z| < 1 \\ 0 & |z| \geq 1 \end{cases}$$



kernel for composition: ϕ_c



kernel for decomposition: ϕ_d
(differential operator)

Theorem (Murata 1996)

With transform T

$$\mathrm{T}(\mathbf{a}, b) = \frac{1}{(2\pi)^m} \int_{\mathbb{R}^m} \phi_d(\mathbf{a} \cdot \mathbf{x} - b) f(\mathbf{x}) d\mathbf{x},$$

function f is represented by

$$f(\mathbf{x}) = \lim_{\varepsilon \to 0} \int_{\mathbb{R}^{m+1}} \phi_c(\mathbf{a} \cdot \mathbf{x} - b) \mathrm{T}(\mathbf{a}, b) e^{-\varepsilon |\mathbf{a}|^2} d\mathbf{a} db.$$

If $f \in L^1(\mathbb{R}^m) \cap L^p(\mathbb{R}^m)$ $(1 \leq p < \infty)$, the above equation converges in terms of L^p-norm. If $f \in L^1(\mathbb{R}^m)$, bounded and uniformly continuous, the equation converges in terms of L^∞-norm.

- define:

$$f_\varepsilon(\mathbf{x}) = \int_{\mathbb{R}^m} \int_{\mathbb{R}} \int_{\mathbb{R}^m} f(\mathbf{y})\overline{\phi_d(\mathbf{a}\cdot\mathbf{y} - b)}\phi_c(\mathbf{a}\cdot\mathbf{x} - b)e^{-\varepsilon\|\mathbf{a}\|^2}d\mathbf{y}d\mathbf{a}db$$

- by Parseval's equality:

$$\int_{\mathbb{R}} \overline{\phi_d(\mathbf{a}\cdot\mathbf{y} - b)}\phi_c(\mathbf{a}\cdot\mathbf{x} - b)db = \int_{\mathbb{R}} \overline{\hat{\phi}_d(\omega)}\hat{\phi}_c(\omega)e^{i\omega\mathbf{a}\cdot(\mathbf{x}-\mathbf{y})}db$$

- thanks to the nature of Gaussian:

$$
\begin{aligned}
& f_\varepsilon(\mathbf{x}) \\
&= \int_{\mathbb{R}} \int_{\mathbb{R}^m} \int_{\mathbb{R}^m} \overline{\hat{\phi}_d(\omega)} \hat{\phi}_c(\omega) e^{i\omega \mathbf{a}\cdot(\mathbf{x}-\mathbf{y})} e^{-\varepsilon \|\mathbf{a}\|^2} f(\mathbf{y}) d\omega d\mathbf{y} d\mathbf{a} \\
&= (2\pi)^m \int_{\mathbb{R}^m} G_{1/2\varepsilon}\left(\mathbf{a} - i\omega(\mathbf{x}-\mathbf{y})/2\varepsilon\right) d\mathbf{a} \\
&\qquad \int_{\mathbb{R}} \int_{\mathbb{R}^m} |\omega|^{-m} \overline{\hat{\phi}_d(\omega)} \hat{\phi}_c(\omega) G_{2\varepsilon/\omega^2}\left(\mathbf{x}-\mathbf{y}\right) f(\mathbf{y}) d\omega d\mathbf{y} \\
&= (2\pi)^m \int_{\mathbb{R}} |\omega|^{-m} \overline{\hat{\phi}_d(\omega)} \hat{\phi}_c(\omega) G_{2\varepsilon/\omega^2} * f(\mathbf{x}) d\omega
\end{aligned}
$$

where

$$
G_{\sigma^2(\mathbf{x})} = \frac{1}{\sqrt{2\pi\sigma^2}^m} \exp\left(-\frac{\|\mathbf{x}\|^2}{2\sigma^2}\right)
$$

- by Hölder's inequality:

$$
\begin{aligned}
&\left\|f_\varepsilon - f\right\| \\
&= \left\|(2\pi)^m \int_{\mathbb{R}} |\omega|^{-m} \overline{\hat{\phi}_d(\omega)} \hat{\phi}_c(\omega) \left(G_{2\varepsilon/\omega^2} * f - f\right) d\omega\right\| \\
&\leq (2\pi)^m \int_{\mathbb{R}} \left|\omega^{-m} \overline{\hat{\phi}_d(\omega)} \hat{\phi}_c(\omega)\right| \left\|G_{2\varepsilon/\omega^2} * f - f\right\| d\omega \\
&= (2\pi)^m \left[\int_{|\omega| \geq \gamma} + \int_{|\omega| < \gamma}\right] \\
&\qquad \left|\omega^{-m} \overline{\hat{\phi}_d(\omega)} \hat{\phi}_c(\omega)\right| \left\|G_{2\varepsilon/\omega^2} * f - f\right\| d\omega
\end{aligned}
$$

Question

Suppose a function f is represented by a transform T as

$$f(x) = \int T(\mathbf{a}, b)\phi_c(\mathbf{x}; \mathbf{a}, b) d\mathbf{a} db.$$

Evaluate the accuracy of a finte sum of ϕ_c

$$f_n(\mathbf{x}) = \sum_i^n c_i \phi_c(\mathbf{x}; \mathbf{a}_i, b_i).$$

- a function f is represented by a transform T as

$$f(x) = \int T(\mathbf{a}, b)\phi_c(\mathbf{x}; \mathbf{a}, b) d\mathbf{a} db.$$

- consider a finite sum of ϕ_c:

$$f_n(\mathbf{x}) = \sum_i^n c_i \phi_c(\mathbf{x}; \mathbf{a}_i, b_i).$$

- suppose inputs $\mathbf{x} \in R^m$ are generated subject to a probability density $\mu(\mathbf{x})$, evaluate the approximation by n units with the following norm:

$$\|f_n(\mathbf{x}) - f(\mathbf{x})\|^2_{L^2(R^m, \mu)} = \int_{R^m} (f_n(\mathbf{x}) - f(\mathbf{x}))^2 \mu(\mathbf{x}) d\mathbf{x}$$

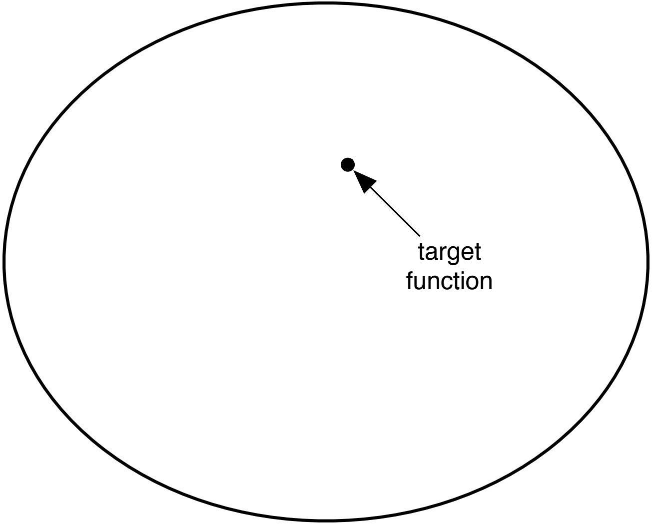
Theorem (Murata 1996)

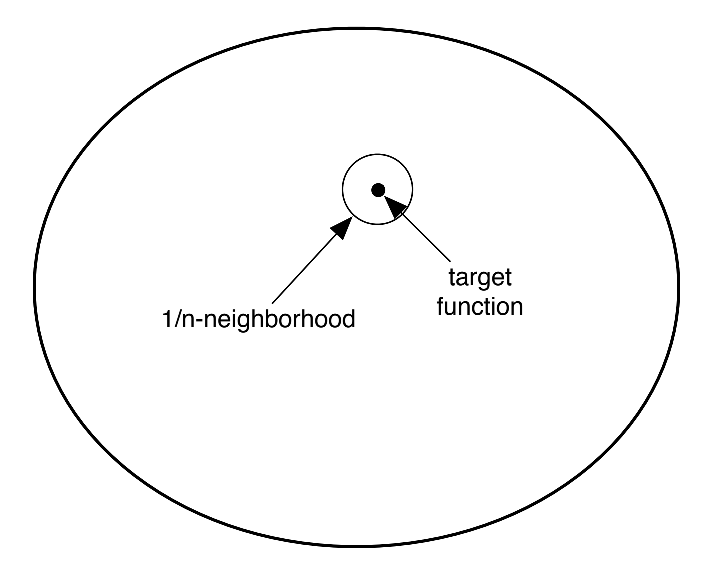
Suppose a function f is represented by a transform T as

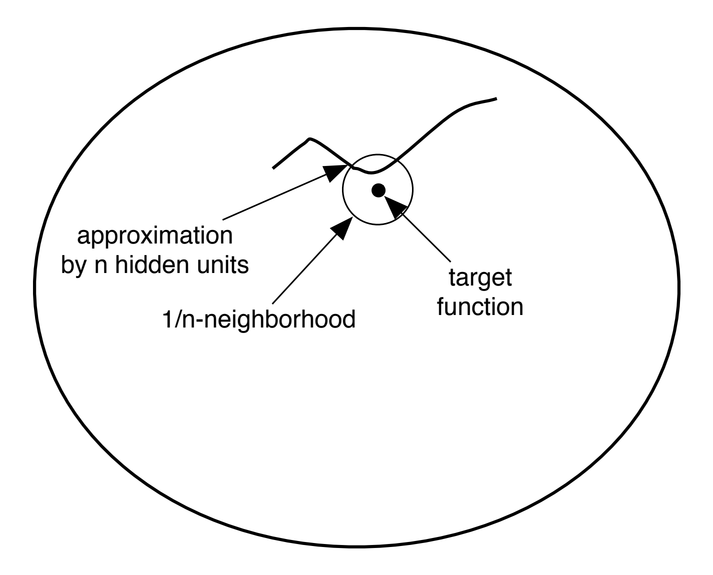
$$f(x) = \int T(\mathbf{a}, b)\phi_c(\mathbf{x}; \mathbf{a}, b) d\mathbf{a} db.$$

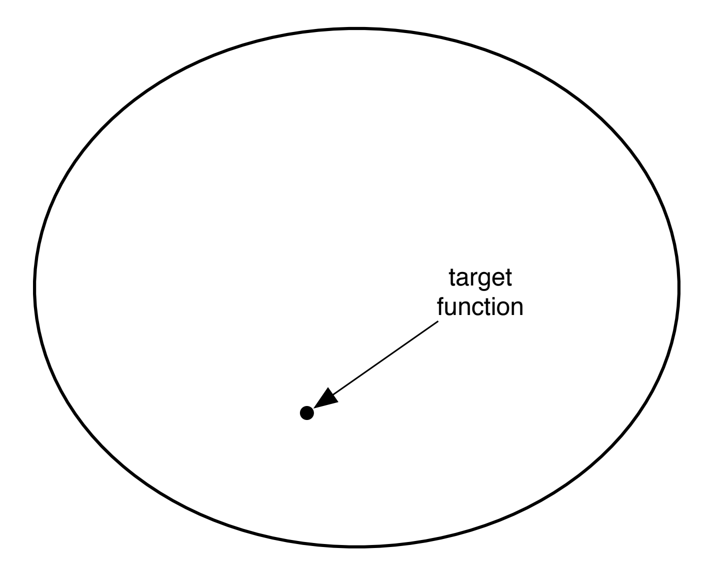
If the L_1-norm (absolute integral) of T, $\|T\|_{L^1}$, is bounded, there exists an approximation f_n with a sum of n ϕ_c's which satisfies

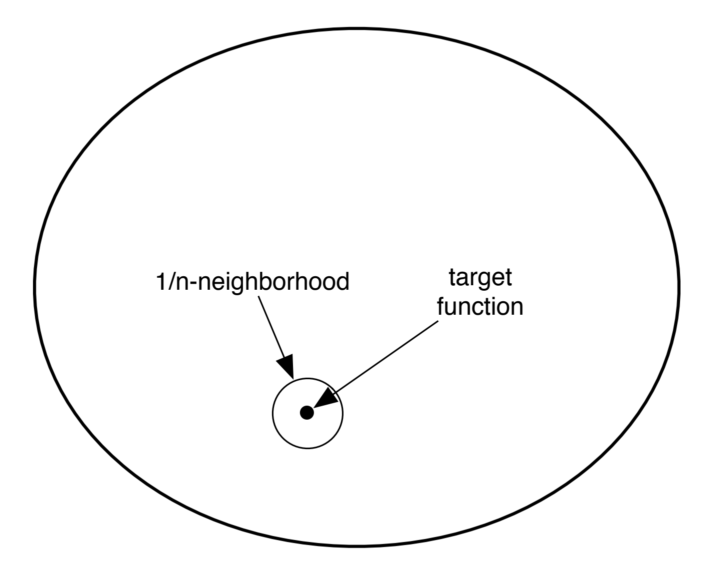
$$\|f_n(\mathbf{x}) - f(\mathbf{x})\|^2_{L^2(R^m,\mu)} \leq \frac{1}{n}\|T\|^2_{L^1}.$$

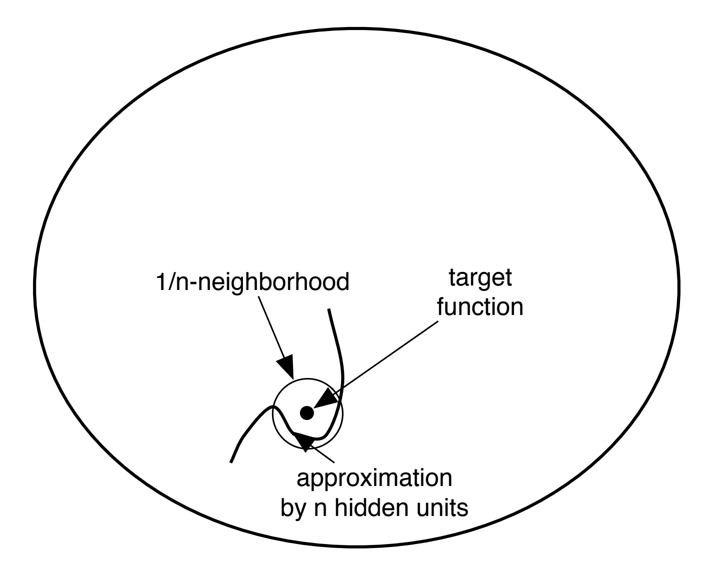

target
function

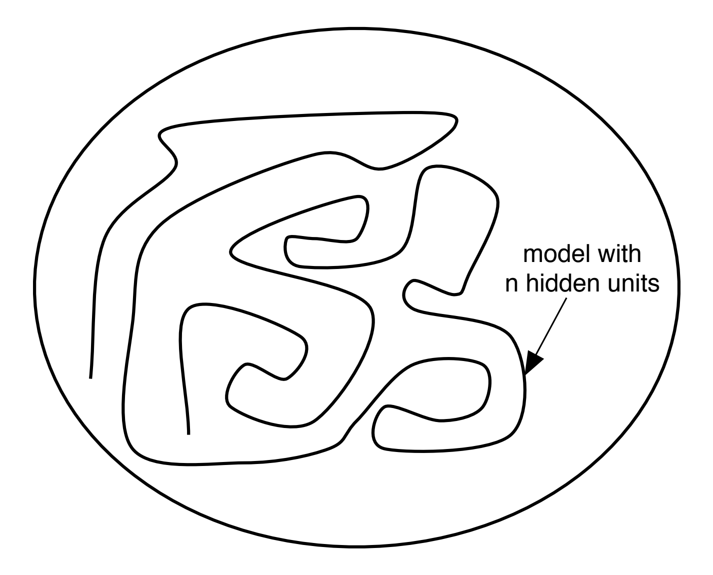

1/n-neighborhood
target
function


approximation
by n hidden units
1/n-neighborhood
target
function


target
function

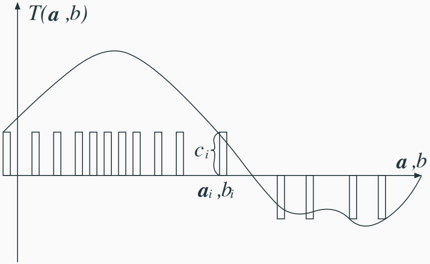

1/n-neighborhood
target
function


1/n-neighborhood
target
function
approximation
by n hidden units


model with
n hidden units

- since f and ϕ_c are real-valued functions, T is real.
- normalize T and construct a probability distribution on $(\mathbf{a}, b)$.

$$p(\mathbf{a}, b) = \frac{|T(\mathbf{a}, b)|}{\|T\|_{L^1}},$$



random coding

- select n pairs of $(\mathbf{a}, b)$ independently subject to $p(\mathbf{a}, b)$, and construct

$$f_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n} c_i \phi_c(\mathbf{a}_i \cdot \mathbf{x} - b_i),$$

where $c_i = \operatorname{sign}(T(\mathbf{a}_i, b_i)) \cdot \|T\|_{L^1}$.

- for fixed x, consider a random variable

$$X_i = c_i \phi_c(\mathbf{a}_i \cdot \mathbf{x} - b_i),$$

then

$$EX_i = f(x), \; V(X_i) \le \|T\|_{L^1}^2 \cdot \left(\max_z \phi_c(z)\right)^2.$$

in the following discussion, assume $|\phi_c| < 1$.

- mean squared error of function f_n is evaluated as

$$E \int (f_n(\mathbf{x}) - f(\mathbf{x}))^2 \mu(\mathbf{x}) d\mathbf{x} = \int V(f_n(\mathbf{x})) \mu(\mathbf{x}) d\mathbf{x}$$
$$= \int V\left(\frac{1}{n}(X_1 + X_2 + \cdots + X_n)\right) \mu(\mathbf{x}) d\mathbf{x} \le \frac{1}{n} \|T\|_{L^1}^2.$$

example of function spaces with $O(1/n)$-rate convergence

function space	approximation	
$\int \lvert\hat{f}(\omega)\rvert d\omega < \infty$	$\sum_{i=1}^{n} c_i \sin(\mathbf{a}_i \cdot \mathbf{x} - b_i)$	(Jones 1992)
$\int \lvert\omega\rvert\lvert\hat{f}(\omega)\rvert d\omega < \infty$	$\sum_{i=1}^{n} c_i \sigma(\mathbf{a}_i \cdot \mathbf{x} - b_i)$	(Barron 1993)
m-th Hölder continuous	$\sum_{i=1}^{n} c_i \sigma(\mathbf{a}_i \cdot \mathbf{x} - b_i)$	(Murata 1996)
$H^{2p,1}(R^m),\ 2p > m$	$\sum_{i=1}^{n} c_i e^{-\lvert\mathbf{x}-\mathbf{a}_i\rvert^2/b_i^2}$	(Girosi 1993)

where σ is the sigmoid function, $H^{2p,1}(R^m)$ is the Sobolev space of $2p$-th order differentiable.

- aim: minimize approximation errors of a contaminated function $y = f(\mathbf{x}) + \xi$
  - $f_{n,opt}$ – not obtainable

$$\text{minimize } \|y - f_n\|^2 = E_{\mathbf{x},y}(y - f_n(\mathbf{x}))^2$$

  - $f_{n,t}$ – obtainable

$$\text{minimize } \frac{1}{t}\sum_{j=1}^{t}(y_j - f_n(\mathbf{x}_j))^2$$

- error decomposition:

$$\|y - f_{n,t}\|^2 \Rightarrow \underbrace{\|y - f_{n,opt}\|^2}_{\text{structural error}} + \underbrace{\|f_{n,opt} - f_{n,t}\|^2}_{\text{learning error}}$$

- errors caused by model structure:

$$\begin{aligned}\|y - f_{n,opt}\|^2 &= E_{\mathbf{x},y}(y - f_{n,opt}(\mathbf{x}))^2 \\ &= E_{\mathbf{x},\xi}(f(\mathbf{x}) + \xi - f_{n,opt}(\mathbf{x}))^2 \\ &= E_{\xi}(\xi^2) + E_{\mathbf{x}}(f(\mathbf{x}) - f_{n,opt}(\mathbf{x}))^2 \\ &= V(\xi) + \|f_{n,opt} - f\|^2_{L^2(R^m,\mu)} \\ &\leq \sigma^2 + \frac{2\|T\|^2_{L^1}}{n},\end{aligned}$$

where σ^2 is the variance of an additive noise ξ.

- errors caused by training from examples:

$$E\left[\|y-f_{n,t}\|^2\right] = \|y-f_{n,opt}\|^2 + \frac{1}{2t}\mathrm{tr}GH^{-1} + o\left(\frac{1}{t}\right)$$
$$V\left[\|y-f_{n,t}\|^2\right] = \frac{1}{2t^2}\mathrm{tr}GH^{-1}GH^{-1} + o\left(\frac{1}{t^2}\right),$$

where ij-elemensts of G and H are given by using the partial derivative with respect to the i-th element, ∂_i, as

$$G_{ij} = E_{\mathbf{x},y}(\partial_i(y-f_n(\mathbf{x}))^2\partial_j(y-f_n(\mathbf{x}))^2)$$
$$H_{ij} = E_{\mathbf{x},y}(\partial_i\partial_i(y-f_n(\mathbf{x}))^2).$$

Theorem

The squared error of three-layered perceptron is asymptotically bound by

$$\begin{aligned}\|y - f_{n,t}\|^2 \leq \sigma^2 + \frac{2\|T\|_{L^1}^2}{n} \\ + \frac{1}{t}\left(\frac{\mathrm{tr} GH^{-1}}{2} + \sqrt{\frac{\mathrm{tr} GH^{-1}GH^{-1}}{2\delta}}\right) \\ + o\left(\frac{1}{n}\right) + o\left(\frac{1}{t}\right)\end{aligned}$$

with probability $1 - \delta$.

Concluding Remarks

we have investigated:

- integral representation of three-layered perceptron
- approximation bounds of some function spaces

further works are done on:

- specifying classes of activation functions
- investigating reproducing kernel Hilbert spaces

References

Murata, Noboru (Aug. 1996). "An Integral Representation of Functions Using Three-layered Networks and Their Approximation Bounds." In: Neural Networks 9 (6), pp. 947–956. DOI: 10.1016/0893-6080(96)00000-7.