Lecture 18

Neural networks

Idea: make basis functions weight-dependent and fit those weights.

Previously, we considered

$$y(\vec{x}, \vec{w}) = f\left(\sum_{j=1}^{M} w_j \varphi_j(\vec{x})\right), \text{ where}$$

$f(\cdot)$ is identity for regression and non-linear activation f'n for classification.

Now, consider $(x_1, \ldots, x_D)$ ← input vector

$$a_j = \sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)} \qquad j = 1, \ldots, M$$

a_j: activation; $w_{ji}^{(1)}$: weights; $w_{j0}^{(1)}$: bias

Then, $z_j = h(a_j)$ ← non-linear activation f'n

$h(\cdot)$ can be $\sigma(\cdot)$ or $\tanh(\cdot)$

Next, $a_k = \sum_{j=1}^{M} w_{kj}^{(2)} z_j + w_{k0}^{(2)}$ $\qquad k = 1, \ldots, K$ ↗ total # outputs

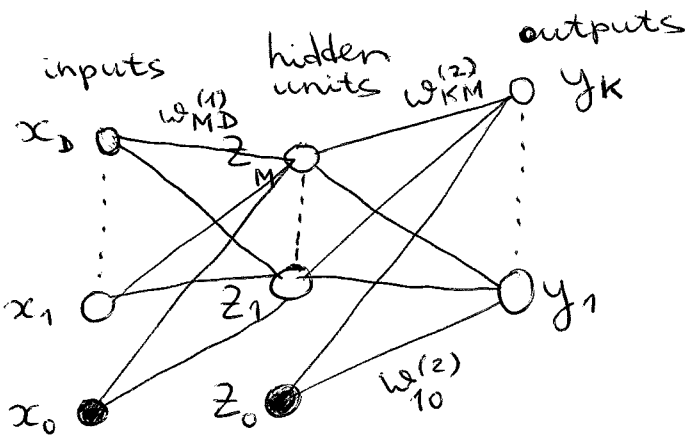
Finally, $y_k = \tilde{h}(a_k)$, where $\tilde{h}$ may be ($K=1$ or $K>1$) identity for regression, $\sigma(\cdot)$ for binary classification ($K=2$), etc.

y_k: output vector

We have:

$$y_k(\vec{x}, \vec{w}) = \sigma\left(\sum_{j=1}^{M} w_{kj}^{(2)} \underbrace{h\left(\sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)} \right)}_{z_j,\ j=1,\dots,M} + w_{k0}^{(2)} \right)$$

Note that it does not make sense to have $h(\cdot)$ as identity, since then the argument of the σ-function is just a linear model with various products of weights.



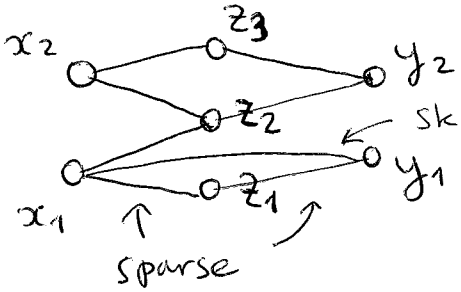
Define $x_0 = 1$ & $z_0 = 1$, then

$$y_k(\vec{x}, \vec{w}) = \sigma\left(\sum_{j=0}^{M} w_{kj}^{(2)} \underbrace{z_j}_{= \begin{cases} 1, & j=0 \\ h\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_i \right), & j=1,\dots,M \end{cases}} \right)$$

Generalizations: (1) multiple layers of hidden units

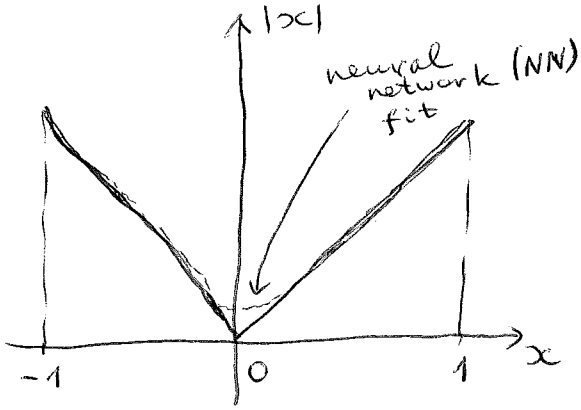
(2) sparse network architectures

(3) skip-layer connections:

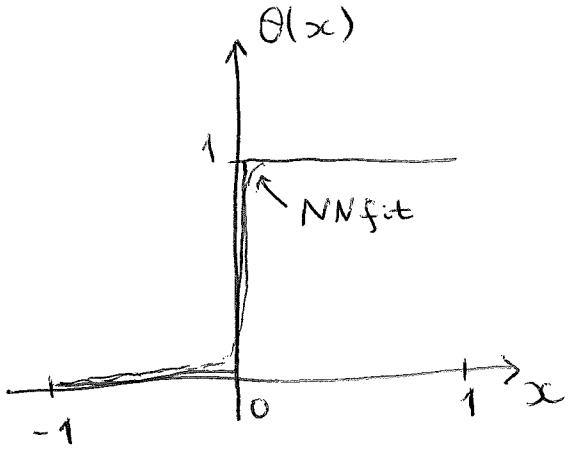


Note: feed-forward architectures only

Performance: can fit various functions fairly accurately



Sample $N = 50$ datapoints uniformly in $[-1, 1]$ interval, fit a two-layer network (input layer + hidden layer) discussed above:
3 hidden units,
tanh(·) activation f'n,
linear output units.



Weight-space symmetries:

with tanh(·) activation f's,

$$\tanh(-a) = -\tanh(a)$$, and

changing the sign of all weights (and the bias) leading into a unit can be compensated by the change in sign of all weights leading out of that unit.

M hidden units → 2^M equivalent weight vectors.

Similarly, can exchange weight values leading in and out of a hidden unit with another hidden unit ⇒ M! permutations

So we have $2^M M!$ symmetries for a two-layer network (can be easily generalized to other architectures and activation functions)

Network training

$n = 1, \ldots, N$: $\{\vec{x}_n\}$ $\{\vec{t}_n\}$

$\vec{x}_n$ ↑ inputs, $\vec{t}_n$ ↑ targets

Regression: (consider scalar targets $\{t_n\}$ for simplicity)

Assume $p(t|\vec{x}, \vec{w}, \beta) = \mathcal{N}(t|y(\vec{x}, \vec{w}), \beta^{-1})$

β = precision $\left(= \frac{1}{\sigma^2}\right)$

Output unit activation function = identity; single output unit.

As before,

$$\mathcal{J} = \prod_{n=1}^{N} p(t_n|\vec{x}_n, \vec{w}, \beta) \quad , \text{ or}$$

$$-\log \mathcal{J} = \frac{\beta}{2} \sum_{n=1}^{N} (y(\vec{x}_n, \vec{w}) - t_n)^2 + \frac{N}{2} \log(2\pi) - \frac{N}{2} \log \beta$$

$-\log \mathcal{J}$ = error f'n

Define $E(\vec{w}) = \frac{1}{2} \sum_n (y(\vec{x}_n, \vec{w}) - t_n)^2$,

then $\left.\frac{\partial E}{\partial \vec{w}}\right|_{\vec{w}_{ML}} = 0$ gives $\vec{w}_{ML}$.

ML approach → [or just minimizing $E(\vec{w})$] ↑ need numerical minimizer

given $\vec{w}_{ML}$, $\left.\frac{\partial E}{\partial \beta}\right|_{\beta_{ML}} = 0$ yields

$$\beta_{ML}^{-1} = \frac{1}{N} \sum_n (y(\vec{x}_n, \vec{w}_{ML}) - t_n)^2$$

$K=2$ classification:

$C_1: t=1 \qquad C_2: t=0$

as before, use $\sigma(\cdot)$ on the single output node, and define

$$\begin{cases} p(C_1|\vec{x}) = \underbrace{y(\vec{x}, \vec{w})}_{[0,1]} \\ p(C_2|\vec{x}) = 1 - p(C_1|\vec{x}) \end{cases}$$

Then $\mathcal{L} = \prod_n y_n^{t_n} (1-y_n)^{1-t_n}$, where

$$y_n = y(\vec{x}_n, \vec{w});$$

$$E(\vec{w}) = -\log \mathcal{L} = -\sum_n [t_n \log y_n + (1-t_n) \log(1-y_n)].$$

If we have K separate binary classifications to perform, K output nodes

$$t_k = \{0,1\}, \quad k = 1, \ldots, K$$

$$\mathcal{L} = \prod_{n=1}^{N} \prod_{k=1}^{K} y_{nk}^{t_{nk}} (1-y_{nk})^{1-t_{nk}}, \text{ where}$$

$$y_{nk} = y_k(\vec{x}_n, \vec{w})$$

$$E(\vec{w}) = -\log \mathcal{L} = -\sum_n \sum_k [t_{nk} \log y_{nk} + (1-t_{nk}) \log(1-y_{nk})]$$

$K > 2$ classification:

1-of-K coding scheme: $\underbrace{00\ldots1\ldots}_{K}$ ← class label

Then interpret $y_k(\vec{x}, \vec{w}) = p(t_k = 1 | \vec{x})$ ⇐ K output nodes

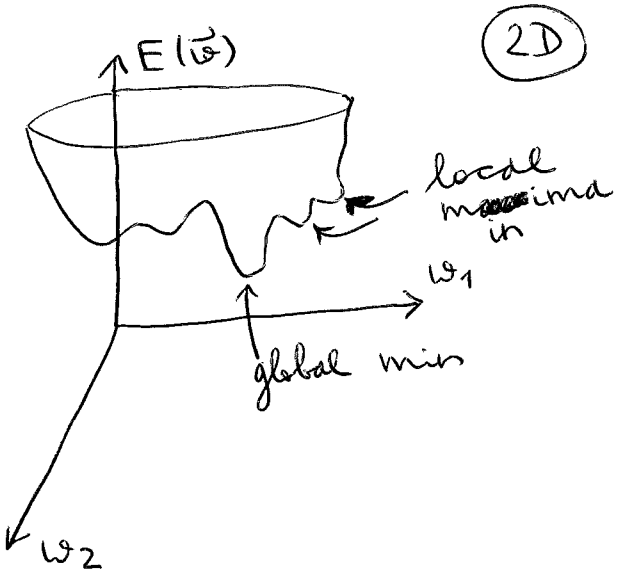
$$\mathcal{L} = \prod_{n=1}^{N} \prod_{k=1}^{K} y_{nk}^{t_{nk}}, \text{ or}$$

$$E(\vec{w}) = -\sum_n \sum_k t_{nk} \log y_{nk}$$

Output unit activation function = softmax:

$$y_k(\vec{x}, \vec{w}) = \frac{e^{a_k(\vec{x}, \vec{w})}}{\sum_{j=1}^{K} e^{a_j(\vec{x}, \vec{w})}}$$

Typically, $E(\vec{w})$ is non-trivial:



Prm optimization

If $\vec{\nabla} E(\vec{w})$ is available, could make small steps in the $-\vec{\nabla} E$ direction until $\vec{\nabla} E = 0 \Rightarrow$ steepest descent method.

This will only find a local min in general $\Rightarrow$ could run multiple times & compare the results (i.e., get the best one).

Besides, there're symmetries in weight space (e.g. $2^M M!$ equivalent minima in a 2-layer network with M hidden units).

Local quadratic approximation:

$$E(\vec{w}) \simeq E(\hat{\vec{w}}) + (\vec{w} - \hat{\vec{w}})^T \vec{b} + \frac{1}{2} (\vec{w} - \hat{\vec{w}})^T H (\vec{w} - \hat{\vec{w}})$$

↑ Taylor expansion around $\hat{\vec{w}}$

$$\vec{b} = \vec{\nabla} E \Big|_{\hat{\vec{w}}}, \quad H_{ij} = \frac{\partial^2 E}{\partial w_i \partial w_j} \Big|_{\hat{\vec{w}}} \qquad [H^T = H]$$

Then $\vec{\nabla} E_{(\vec{w})} \simeq \vec{b} + H(\vec{w} - \hat{\vec{w}})$

If $\hat{\vec{w}} = \vec{w}^*$ is a minimum, s.t. $\vec{b} = 0$, we get:

$$E(\vec{w}) \simeq E(\vec{w}^*) + \frac{1}{2} (\vec{w} - \vec{w}^*)^T H (\vec{w} - \vec{w}^*)$$

Consider $H\vec{u}_i = \lambda_i \vec{u}_i$ s.t. $\vec{u}_i^T \vec{u}_j = \delta_{ij}$

Now, expand $\vec{w} - \vec{w}^* = \sum_i \alpha_i \vec{u}_i$, s.t.

$$E(\vec{w}) \simeq E(\vec{w}^*) + \frac{1}{2} \sum_{kl} (w_k - w_k^*) H_{kl} (w_l - w_l^*) =$$

$$= E(\vec{w}^*) + \frac{1}{2} \sum_{kl} \sum_{ij} \alpha_i \alpha_j u_{i,k} \underbrace{\sum_l H_{kl} u_{j,l}}_{\lambda_j u_{j,k}} =$$

$$= E(\vec{w}^*) + \frac{1}{2} \sum_{ij} \alpha_i \alpha_j \lambda_j \underbrace{\sum_k u_{i,k} u_{j,k}}_{\delta_{ij}} =$$

$$= E(\vec{w}^*) + \frac{1}{2} \sum_i \alpha_i^2 \lambda_i$$

H is pos.-definite iff $\vec{v}^T H \vec{v} > 0$, $\forall \vec{v}$.

Using $\vec{v} = \sum_i c_i \vec{u}_i$, we obtain:

$$\vec{v}^T H \vec{v} = \sum_{ij} v_i H_{ij} v_j = \sum_{ij} \left(\sum_k c_k u_{k,i} \right) \times$$

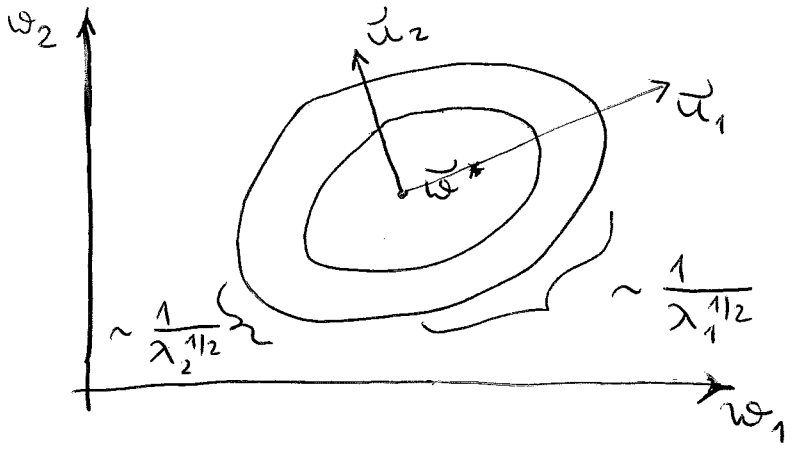
$$\times H_{ij} \left(\sum_l c_l u_{l,j} \right) =$$

$$= \sum_{kl} c_k c_l \lambda_l \underbrace{\left(\sum_i u_{k,i} u_{l,i} \right)}_{\delta_{kl}} = \sum_l c_l^2 \lambda_l .$$

↑ $\sum_j H_{ij} u_{l,j} = \lambda_l u_{l,i}$

Thus H is pos-def iff $\lambda_i > 0$, $\forall i$.
This is a requirement for $\vec{w}^*$ to be a minimum, rather than a max or a saddle point.

Contours of $E(\vec{w})$:



Suppose $E(\vec{w}) - E(\vec{w}^*) = \Delta$, then

$$E(\vec{w}) - E(\vec{w}^*) = \frac{1}{2}\sum_i \lambda_i \alpha_i^2 = \Delta.$$

If $\vec{w} = \vec{w}^* + \underbrace{\alpha_i \vec{u}_i}_{\text{along } \vec{u}_i} \Rightarrow 2\Delta = \lambda_i \alpha_i^2$, or $\alpha_i \sim \frac{1}{\lambda_i^{1/2}}$.

Steepest descent:

$$\vec{w}^{(\tau+1)} = \vec{w}^{(\tau)} - \eta \vec{\nabla} E(\vec{w}^{(\tau)})$$

(τ: step #; η: learning rate)

Note that $E(\vec{w}) = \sum_{n=1}^{N} E_n(\vec{w})$, so that, alternatively, we can do

$$\vec{w}^{(\tau+1)} = \vec{w}^{(\tau)} - \eta \vec{\nabla} E_n(\vec{w}^{(\tau)})$$

↑ sequential gradient descent [cycle through datapoints]

This is a diff. algorithm b/c a local min for the whole dataset ≠ local min for each individual datapoint.