Deep Learning (BEV033DLE)
Lecture 2.

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- Neural networks are universal approximators
- Testing networks & loss functions
- Generalisation errors for neural classifiers & regressors

Neural networks as universal approximators

Neural networks are *universal approximators* if we do not restrict the network architecture

Boolean functions: Every boolean function $f\colon \{\pm 1\}^n \to \{\pm 1\}$ can be written in conjunctive normal form, i.e. as a conjunction over disjunctive clauses.

Theorem 1. *Every boolean function can be represented by a network with binary units and two layers.*

Remark 1. Notice, that the number of neurons in such a two layer network can grow exponentially with n. Implementing e.g. the parity function in DNF/CNF will require $\mathcal{O}(2^{n-1})$ neurons. It can be implemented much more efficiently by a deep network e.g. with $\mathcal{O}(n \log n)$ neurons if we do not restrict its depth.

Real valued functions: consider real valued functions $f\colon [0,1]^n \to \mathbb{R}$ that are Lipshitz continuous

$$|f(x) - f(x')| \leqslant \rho \|x - x'\| \quad \forall x, x' \in [0,1]^n.$$

To approximate such function by a network:

- Partition the domain : $[0,1]^n$ into sufficiently small boxes.
- Design a network that first decides which box the input vector belongs to and then predicts the average value of f at this box.

Neural networks as universal approximators

Theorem 2. *(Cybenko, 1989) Every smooth function on* $[0,1]^n$ *can be approximated arbitrarily well by a network with sigmoid units and two layers. In other words, given a smooth function* $f : [0,1]^n \to \mathbb{R}$ *and an* $\epsilon > 0$*, there is a sum*

$$G(x) = \sum_{j=1}^{N} \alpha_j \, \mathrm{S}(w_j^T x + b_j)$$

s.t. $|f(x) - G(x)| \leqslant \epsilon$ *for all* $x \in [0,1]^n$*.*

Remark 2.

- There are also "dual" universal approximation theorems that restrict the width of the network (i.e. number of units per layer) and allow arbitrary network depth.
- We limit the expressive power once we fix a network architecture.

Validating & testing neural networks

Given a network, we want to validate its performance on a test set. How *large* shall we choose this set & what *precisely* shall we measure?

- The relation between input features $x \in \mathcal{X}$ and hidden states $y \in \mathcal{Y}$ is given by a joint probability distribution $p(x, y)$, which is *unknown*.
- The network $h\colon \mathcal{X} \to \mathcal{Y}$ predicts hidden states y, given input features x.
- The loss $\ell(y, y')$ defines the cost incurred by a wrong prediction $y' = h(x)$, if the true hidden state was y. Examples:
  - classification, y is categorical: 0/1 loss $\ell(y, y') = [\![y \neq y']\!]$
  - classification, y is a sequence: Hamming distance $\ell(y, y') = \sum_i [\![y_i \neq y'_i]\!]$
  - regression, $y \in \mathbb{R}^n$: L1 norm $\ell(y, y') = \|y - y'\|_1$

We want to estimate the risk, i.e. the *expected loss*

$$R(h) = \sum_{x,y} p(x,y)\ell(y,h(x)) \approx \frac{1}{m} \sum_{(x,y)\in\mathcal{T}^m} \ell(y,h(x)) = R_{\mathcal{T}^m}(h)$$

where $\mathcal{T}^m = \{(x^j, y^j) \mid j = 1, \ldots, m\}$ is a test set of *i.i.d. examples* $x, y \sim p(x, y)$.

Validating & testing neural networks

How large shall we choose the size m of the test set $\mathcal{T}^m$?

Answer: Upper bound the deviation $|R_{\mathcal{T}^m}(h) - R(h)|$

$$\mathcal{T}^m \sim p(x,y) \;\; \Rightarrow \;\; \mathbb{P}\Big(|R(h) - R_{\mathcal{T}^m}(h)| > \varepsilon\Big) < ??$$

- Chebyshev inequality: $\mathbb{P}\Big(|R(h) - R_{\mathcal{T}^m}(h)| > \varepsilon\Big) < \frac{\mathbb{V}[\ell(y,h(x))]}{m\varepsilon^2}$, converges slowly for $m \to \infty$.
- Hoeffding inequality: $\mathbb{P}\Big(|R(h) - R_{\mathcal{T}^m}(h)| > \varepsilon\Big) < 2e^{-\frac{2m\varepsilon^2}{(\triangle\ell)^2}}$, where $\triangle\ell = \ell_{max} - \ell_{min}$.

Example 1. Consider a classifier with 0/1 loss. What test set size m ensures that $R_{\mathcal{T}^m}(h) - 0.01 < R(h) < R_{\mathcal{T}^m}(h) + 0.01$ with probability 95%?
Answer: By using Hoeffding inequality, we get $m \approx 2 \cdot 10^4$.

Learning neural networks: generalisation & overfitting

Given an i.i.d. training set $\mathcal{T}^m = \{(x^j, y^j) \mid j = 1, \ldots, m\}$, we want to train a network $y = h(x, w)$ by minimising its *empirical risk*, i.e. expected loss on the training set

$$\frac{1}{m} \sum_{(x,y) \in \mathcal{T}^m} \ell\big(y, h(x, w)\big) \to \min_w$$

Often we can not minimise this objective by gradient descent: e.g. classification with 0/1 loss. Let us make a virtue of necessity and consider another *learning criterion*: the negative log-likelihood.

- last layer of the network: class scores + softmax, its outputs $h_k(x, w)$ are interpreted as *conditional class probabilities* $h_k(x, w) = p_w(y = k \,|\, x)$
- the learning criterion (NLL) reads

$$-\frac{1}{m} \sum_{(x,y) \in \mathcal{T}^m} \log p_w(y \,|\, x) = -\frac{1}{m} \sum_{(x,y) \in \mathcal{T}^m} \log h_y(x, w) \to \min_w$$

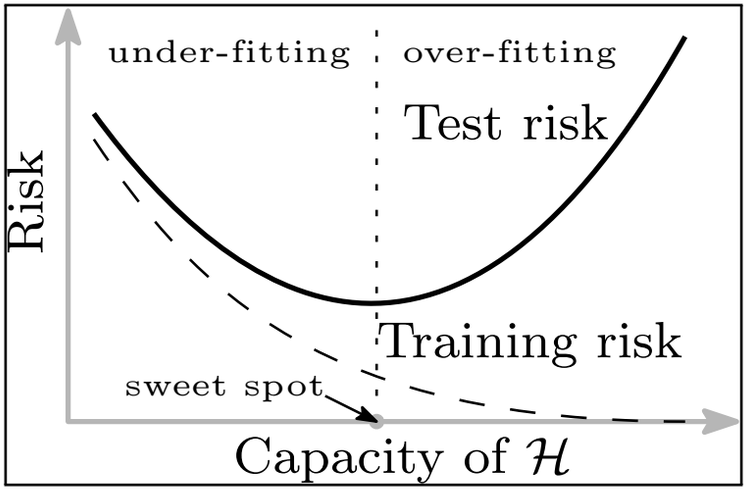
  and is differentiable in w.

Advantage: we can estimate the prediction uncertainty.

Learning neural networks: generalisation & overfitting

Generalisation error (bounds) We fix a network architecture. This defines an infinite network class $\mathcal{H}$. We choose the network $h_m \in \mathcal{H}$ with the best performance on a training set $\mathcal{T}^m$. For this we minimise the learning criterion by *stochastic gradient descent* (SGD).

We would expect the following behaviour for training sets $\mathcal{T}^m$ with fixed size m.



Can we bound the generalisation error of the network $h_m = \arg\min_{h \in \mathcal{H}} R_{\mathcal{T}^m}(h)$?

$$\mathcal{T}^m \sim p(x,y) \;\Rightarrow\; \mathbb{P}\Big(|R(h_m) - R_{\mathcal{T}^m}(h_m)| > \varepsilon\Big) < ??$$

- We can not apply the Hoeffding inequality here (why?)

Learning neural networks: generalisation & overfitting

ML theory provides generalisation bounds assuming that we can *uniformly* bound the deviation between risk and empirical risk, i.e. $\sup_{h\in\mathcal{H}}|R(h) - R_{\mathcal{T}^m}(h)|$

Finite $\mathcal{H}$: We train a network and keep several checkpoints with best training accuracy. Then we want to choose the best network from this set $\mathcal{H}$ by comparing their performance on some validation set $\mathcal{T}^m$. How large shall we choose m?
Answer: use the generalised Hoeffding inequality for a finite set of predictors

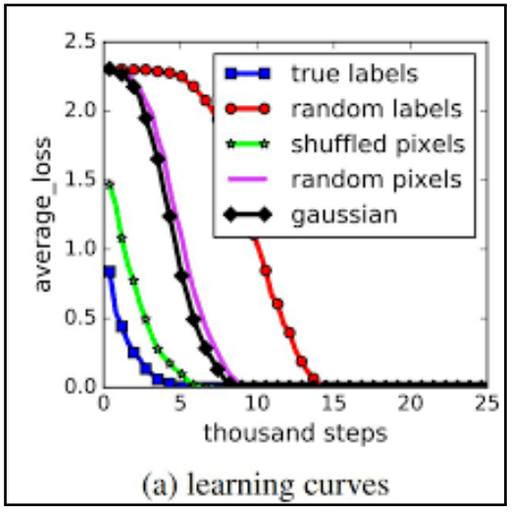
$$\mathbb{P}\Big(\max_{h\in\mathcal{H}}|R(h) - R_{\mathcal{T}^m}(h)| > \varepsilon\Big) < 2|\mathcal{H}|e^{-\frac{2m\varepsilon^2}{(\triangle\ell)^2}}$$

Infinite $\mathcal{H}$: Vapnik-Cervonenkis theory provides such a uniform bound in terms of VC-dimension, i.e. the size of the largest set of data points x that can be classified by predictors from $\mathcal{H}$ in any possible way (the set is *shattered* by $\mathcal{H}$)

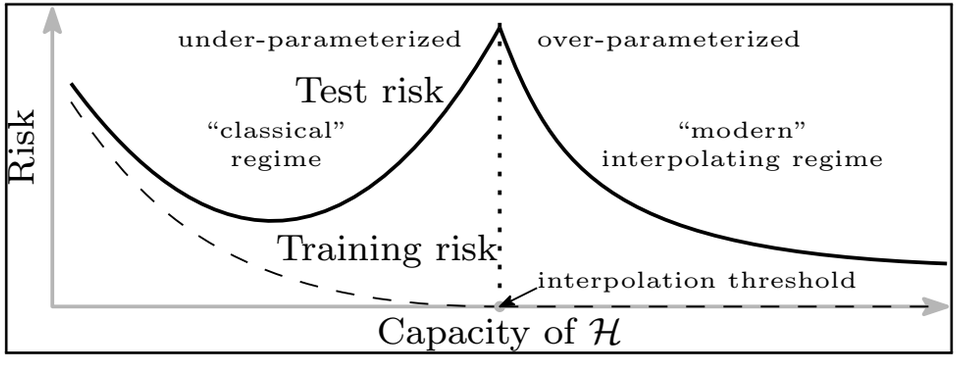
These bounds are however not tight enough for deep networks. Large networks with $> 10^6$ parameters would require billions of training examples. Neural networks in typical applications are in an *over-parametrised* regime outside of the plot in the previous slide.

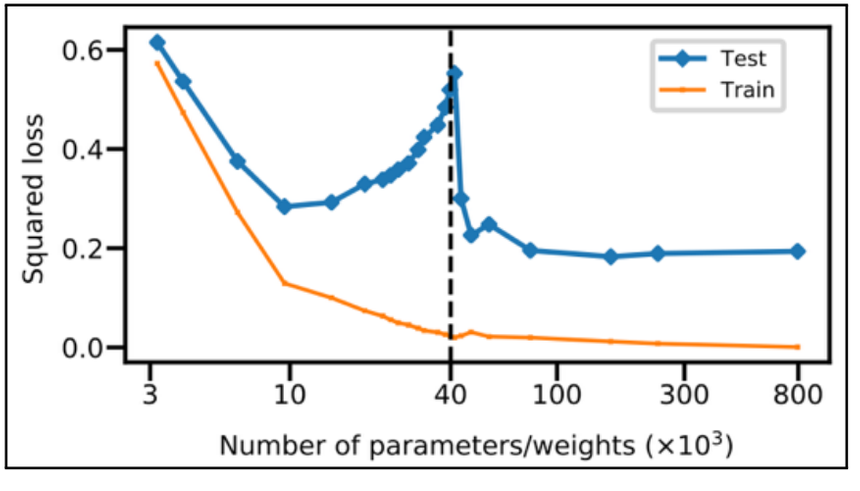
Learning neural networks: generalisation & overfitting

Example 2 (Zhang et al., ICLR, 2018)**.** Image classification on CIFAR (10 classes, $\sim 5 \cdot 10^4$ training examples, tackled by networks with $\sim 10^5$ parameters. The networks learned by SGD and additional regularisers (e.g. data augmentation, dropout, etc.) Achieved accuracy $> 95\%$, generalisation error $< 5\%$. *Such networks can learn data with random labels!* I.e. the training set is shattered by $\mathcal{H}$.



Double descent phenomenon: Current ongoing research seems to indicate that SGD, when used for training over-parametrised networks, is choosing smooth predictors with small norm. This leads to the following unexpected behaviour:





Belkin et al., PNAS, 2019: network with a single hidden layer learned on MNIST