12DL:: Notation

Note: The lecture uses many examples from maths, statistics and machine learning. Therefore notation may overlap, but the context should make clear how to uncerstand the notation. If notation is unclear nevertheless, please contact the instructors.

Data

 $\mathcal{X} \subseteq \mathbb{R}^p$: p-dimensional **feature space** / input space Usually we assume categorical features to be numerically encoded.

\mathcal{Y} : target space

e.g.: $\mathcal{Y}=\mathbb{R}$ for regression, $\mathcal{Y}=\{0,1\}$ or $\mathcal{Y}=\{-1,+1\}$ for binary classification, $\mathcal{Y} = \{1, \dots, g\}$ for multi-class classification with g classes

 $\mathbf{x} = (x_1, \dots, x_p)^{\top} \in \mathcal{X}$: feature vector / covariate vector

 $y \in \mathcal{Y}$: target variable / output variable Concrete samples are called labels

 $(\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{X} \times \mathcal{Y} : i$ -th **observation** / sample / instance / example

 $\mathcal{D}=\left(\left(\mathbf{x}^{(1)},y^{(1)}\right),\ldots,\left(\mathbf{x}^{(n)},y^{(n)}\right)
ight)\in\mathbb{D}_n:$ data set of size n. An n-tuple, a family indexed by $\{1,\ldots,n\}$. We use \mathcal{D}_n to emphasize its size.

 $\mathcal{D}_{\mathsf{train}}, \ \mathcal{D}_{\mathsf{test}} \subseteq \mathcal{D}$: data sets for training and testing Often: $\mathcal{D} = \mathcal{D}_{\mathsf{train}} \ \dot{\cup} \ \mathcal{D}_{\mathsf{test}}$

 $\mathcal{D}_{subtrain}$, $\mathcal{D}_{val} \subseteq \mathcal{D}_{train}$: data sets in the context of early stopping Note: Sophisticated forms also apply cross-validation

Loss, Risk and ERM

 $L: \mathcal{Y} \times \mathbb{R}^g \to \mathbb{R}_0^+:$ loss function: Quantifies "quality" $L(y, f(\mathbf{x}))$ of prediction $f(\mathbf{x})$.

(Theoretical) risk: $\mathcal{R}:\mathcal{H}\to\mathbb{R}$, $\mathcal{R}(f)=\mathbb{E}_{((\mathbf{x},y)\sim\mathbb{P}_{xy})}[L\left(y,f(\mathbf{x})\right)]$

Empirical risk: $\mathcal{R}_{\mathsf{emp}}$: \mathcal{H} \to \mathbb{R} , $\mathcal{R}_{\mathsf{emp}}$: Θ \to \mathbb{R} ; $\mathcal{R}_{\mathsf{emp}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right)$

Empirical risk minimization (ERM): $\hat{\theta} \in \arg\min_{\theta \in \Theta} \mathcal{R}_{emp}(\theta)$

Regularized risk: $\mathcal{R}_{\text{reg}}: \mathcal{H} \to \mathbb{R}, \mathcal{R}_{\text{reg}}(f) = \mathcal{R}_{\text{emp}}(f) + \lambda \cdot J(f)$ with regularizer J(f), complexity control parameter $\lambda > 0$ (analogous for θ).

Gradient based Optimization

 $\hat{\theta}^{[t]}$: t-th step of an optimizer $\alpha \in \mathbb{R}_+$: step-size / learning rate $\mathbf{d} \in \mathbb{R}^d$: descent direction in $\hat{oldsymbol{ heta}}$ $J_1, ..., J_K$: mini-batches of fixed size m with $k \in \{1, ..., K\}$

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(Feedforward) Neural Network
(F)NN: f(\mathbf{x}) = \tau \circ \phi \circ \sigma^{(\prime)} \circ \phi^{(\prime)} \circ \sigma^{(\prime-1)} \circ \phi^{(\prime-1)} \circ \dots \circ \sigma^{(1)} \circ \phi^{(1)}, with
    \phi^{(i)}: affine transformation in hidden layer i
    \sigma^{(i)}: activation function in hidden layer i
    \phi: affine function in output layer
     \tau: activation function in output layer
Hidden layer i, i \in \{1...l\} with m^{(i)} = \text{nmb.} of neurons in i
    \mathbf{W}^{(i)}: weight matrix (m^{(i-1)} \times m^{(i)})
     If \mathbf{x}^{(p\times 1)}:
       \mathbf{b}^{(i)}: bias
       \mathbf{z}^{(i)} = \mathbf{z}_{out}^{(i)} = \sigma^{(i)}(\phi^{(i)}) = \sigma^{(i)}(\mathbf{z}_{in}^{(i)}) = \sigma^{(i)}(\mathbf{W}^{(i)})^{T} \mathbf{z}^{(i-1)} + \mathbf{b}^{(i)}:
        activation
   If \mathbf{X}^{(n\times p)}.
       \mathbf{B}^{(i)}: bias (n \times m)
       \mathbf{Z}^{(i)} = \mathbf{Z}_{out}^{(i)} = \sigma^{(i)}(\phi^{(i)}) = \sigma^{(i)}(\mathbf{Z}_{in}^{(i)}) = \sigma^{(i)}(\mathbf{Z}^{(i-1)}\mathbf{W}^{(i)} + \mathbf{B}^{(i)}):
        activation
Neuron j, j \in \{1 ... m^{(i)}\}:
   \mathbf{W}_{i}^{(i)}: column j (m^{(i-1)} \times 1) of weight matrix
     If \mathbf{x}^{(p\times 1)}:
       \mathbf{z}_{i}^{(i)} = \mathbf{z}_{i,out}^{(i)} = \sigma^{(i)}(\phi_{i}^{(i)}) = \sigma^{(i)}(\mathbf{z}_{i,in}^{(i)}) = \sigma^{(i)}(\mathbf{W}_{i}^{(i)T}\mathbf{z}^{(i-1)} + b_{i}^{(i)}):
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Convolutional Neural Networks

Recurrent Neural Networks