International Master in Computer Vision

Fundamentals of machine

learning for computer vision

Eva Cernadas







Contents

- Machine learning theory (Dr. Jaime Cardoso)
- Linear regression and optimization (Dr. Jaime Cardoso)
- Clustering
- Model selection and evaluation
- Classical classification models
- Artificial neural networks
- Support vector machines (SVM)
- Ensembles: bagging, boosting and random forest

Artificial neural networks

• ANN: Artificial Neural Networks

- Neural network: combination of local processing units (**neurons**)
- Neuron: simple processing unit of various **inputs** and one **output**.
- Input connections with **weights** for each input.
- The output is determined by activation functions from the inputs and weights.
- The weights are **persistent**: they are the **memory** of the neural net.
- The weights are calculated to approximate *n*-dimensional functions.
- The neurons are grouped in **layers**: multi-layers networks: input, hidden (one or various) and output layers.

Neural network

- The term ANN are normally used to multi-layer perceptron (MLP).
- There are supervised and unsupervised neural networks.
- **Supervised** training: weights are calculated using training patterns and true outputs.
- Test pattern propagates through the net to calculate the output.
- The network **performance** is evaluated comparing true and predicted output using the previous measurements
- ANN may exhibit **overfitting**

Perceptron (I)

• One neuron with *n* inputs and one output, binary activation function (0,1), e.g. binary classification:

Step activation function

$$x_{i} \xrightarrow{W_{1}} \Sigma \xrightarrow{b} z z(x) = f\left(\sum_{i=1}^{n} w_{i}x_{i} - b\right) = f(w^{T}x - b) \quad f(t) = \begin{cases} 1 & t \ge 0 \\ -1 & t < 0 \end{cases}$$

- Need a threshold b (for example b=0.5) to calculate the output (-1 or 1). Varying b, a ROC curve is generated.
- Connection weights w₁...w_n: iteratively calculated
- A differential function *f*(*t*) may also be used

Perceptron (II)

• Gradient descent (training algorithm): searches to minimize the difference between the desired (y) and predicted (z) outputs, summed over the training set, μ is the learning speed = $\sum_{k=1}^{N} (y - z)^{2}$; $w(t + 1) = w(t) = u^{\partial J} = \partial J = \sum_{k=1}^{N} (y - z) f(z - z)$

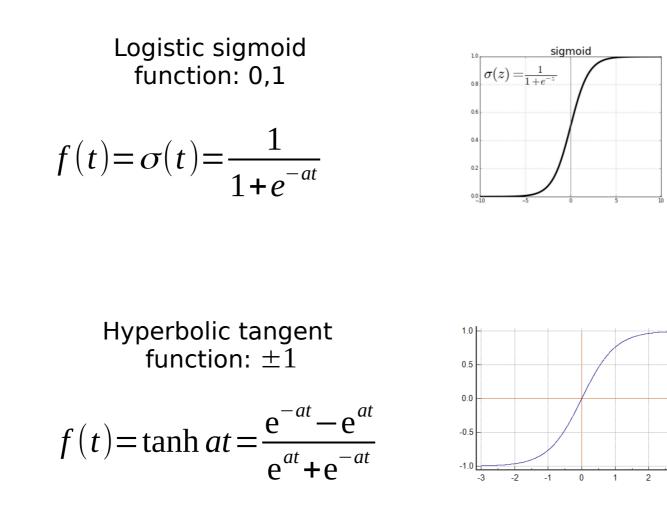
$$J = \sum_{i=1}^{N} (y_i - z_i)^2; \ \mathbf{w}(t+1) = \mathbf{w}(t) - \mu \frac{\partial J}{\partial \mathbf{w}}; \ \frac{\partial J}{\partial \mathbf{w}} = -\sum_{i=1}^{N} (y_i - z_i) f'(\mathbf{w}^T \mathbf{x}_i - b) \mathbf{x}_i$$
$$\mathbf{w}(t+1) = \mathbf{w}(t) + \mu \sum_{i=1}^{N} (y_i - z_i) f'(\mathbf{w}^T \mathbf{x}_i - b) \mathbf{x}_i$$

Note that $y_i - z_i \in \{0, \pm 1\}$

• If the data are linearly separable, this iterative training finds the separating hyperplane (**w**,b) for what $y_i z_i > 0$ for i=1..N.

Perceptron (III)

• Soft activation function *f*: sigmoid or hyperbolic tangent:



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Kernel perceptron

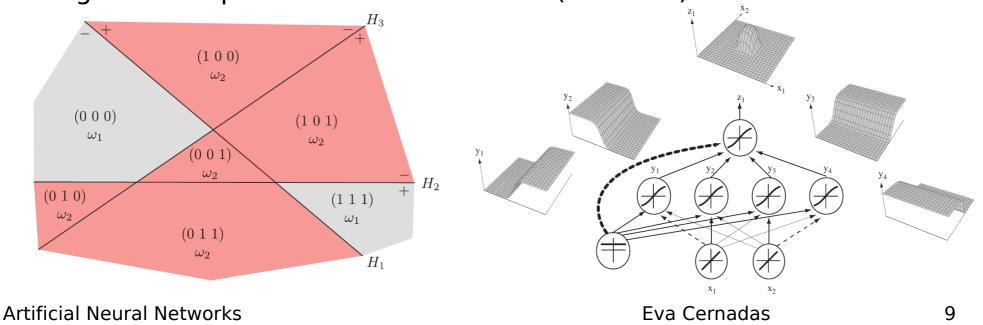
• Kernel perceptron: linear classification $z=f(w^T \vec{\Phi}(x)+b)$ in the multi-dimensional projected hidden space (f : step function) mapped by $\Phi(\mathbf{x})$:

$$\mathbf{w} = \sum_{i=1}^{N} a_i y_i \vec{\Phi}(\mathbf{x}_i) \qquad b = \sum_{i=1}^{N} a_i y_i$$

- Initially, $a_i=0$, i=1..N; $a_i=a_i+1$ if $y_i z_i<0$ (misclassified patted) until that $y_i z_i>0$ (pattern correctly classified) for i=1,...N
- For datasets that are not linearly separable. Artificial Neural Networks Eva Cernadas

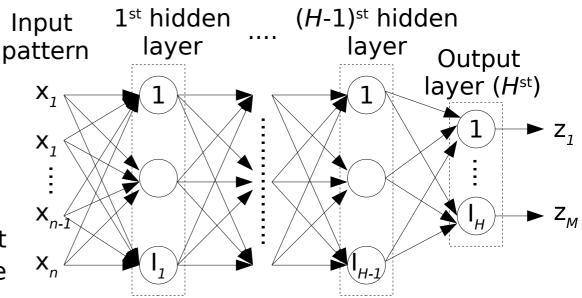
Multi-layer neural network (MLP)

- Each neuron is a linear classifier of the input space (hyperplane).
- Divides the space in two subspaces with outputs 0,1 (sigmoid function) or ± 1 (hiperbolic function).
- Joining various neurons into one layer, divides the space into regions with piecewise linear borders (surfaces).



Multi-layer Layer Perceptron

- Hidden layer: sigmoidal/tanh
 activation function
- Output layer: step activation for clasificación, linear for regression
- We need: training set, cost function, and derivable activation



- \mathbf{w}_{i}^{k} : weight vector of neuron $j=1..I_{k}$ in layer k=1..H
- $a_{ij}^{k} = (\mathbf{w}_{j}^{k})^{T} \mathbf{h}_{i}^{k-1} + b_{j}^{k}$, i = 1..N (pattern), k = 1..H (layer), $j = 1..I_{k}$ (neuron)
- \mathbf{h}_{i}^{k-1} : output of layer k-1 (\mathbf{I}_{k-1} values) for pattern \mathbf{x}_{i}
- \mathbf{h}_{i}^{k} : output of layer k for pattern \mathbf{x}_{i} : $\mathbf{h}_{ij}^{k} = f(\mathbf{a}_{ij}^{k})$ with $j = 1..I_{k}$
- y_{ij} = true output for *j*-th output neuron and training pattern \mathbf{x}_i

Backpropagation (I)

• Gradient descent:

$$\Delta \mathbf{w}_{j}^{k} = -\mu \frac{\partial J}{\partial \mathbf{w}_{j}^{k}}, \Delta b_{j}^{k} = -\mu \frac{\partial J}{\partial b_{j}^{k}}, k = 1, \dots, H, j = 1, \dots, I_{k}$$

 Sum J of squared errors (SSE) J_i evaluated on output layer for the *i pattern*:

$$J = \sum_{i=1}^{N} J_{i} \qquad J_{i} = \frac{1}{2} \sum_{j=1}^{I_{H}} (y_{ij} - h_{ij}^{H})^{2} = \frac{|y_{i} - h_{i}^{H}|^{2}}{2}$$

• The derivative is:

$$\frac{\partial J_i}{\partial \boldsymbol{w}_j^k} = \frac{\partial J_i}{\partial a_{ij}^k} \frac{\partial a_{ij}^k}{\partial \boldsymbol{w}_j^k}, \frac{\partial J_i}{\partial b_j^k} = \frac{\partial J_i}{\partial a_{ij}^k} \frac{\partial a_{ij}^k}{\partial b_j^k}$$

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Backpropagation (II)

• Define:
$$\delta_{ij}^k \equiv \frac{\partial J_i}{\partial a_{ij}^k}$$

$$a_{ij}^{k} = (\mathbf{w}_{j}^{k})^{T} \mathbf{h}_{i}^{k-1} + \mathbf{b}_{j}^{k}$$

• Thus:
$$\frac{\partial a_{ij}^k}{\partial w_j^k} = h_i^{k-1}, \frac{\partial a_{ij}^k}{\partial b_j^k} = 1$$

• So:

$$\Delta \boldsymbol{w}_{j}^{k} = -\mu \sum_{i=1}^{N} \delta_{ij}^{k} \boldsymbol{h}_{i}^{k-1}; \Delta \boldsymbol{b}_{j}^{k} = -\mu \sum_{i=1}^{N} \delta_{ij}^{k}$$

Backpropagation (III)

• For the output layer (*k*=*H*):

$$\delta_{ij}^{k} \equiv \frac{\partial J_{i}}{\partial a_{ij}^{k}} \left[J_{i} = \frac{1}{2} \sum_{j=1}^{I_{H}} \left(y_{ij} - h_{ij}^{H} \right)^{2} \right]$$

 $\delta_{ij}^{H} = (y_{ij} - h_{ij}^{H})f'(a_{ij}^{H}) = \varepsilon_{ij}^{H}f'(a_{ij}^{H})$

$$h_{ij}^{k} = f(a_{ij}^{k})$$

$$\Delta \boldsymbol{w}_{j}^{k} = -\mu \sum_{i=1}^{N} \varepsilon_{ij}^{H} f'(\boldsymbol{a}_{ij}^{H}) \boldsymbol{h}_{ij}^{k-1}$$

$$\Delta b_j^k = -\mu \sum_{i=1}^N \varepsilon_{ij}^H f'(a_{ij}^H)$$

• For the layer *k*<*H*:

$$\delta_{ij}^{k} = \frac{\partial J_{i}}{\partial a_{ij}^{k}} = \sum_{l=1}^{I_{k+1}} \frac{\partial J_{i}}{\partial a_{il}^{k+1}} \frac{\partial a_{il}^{k+1}}{\partial a_{ij}^{k}} = \sum_{l=1}^{I_{k+1}} \delta_{il}^{k+1} \frac{\partial a_{il}^{k+1}}{\partial a_{ij}^{k}}$$

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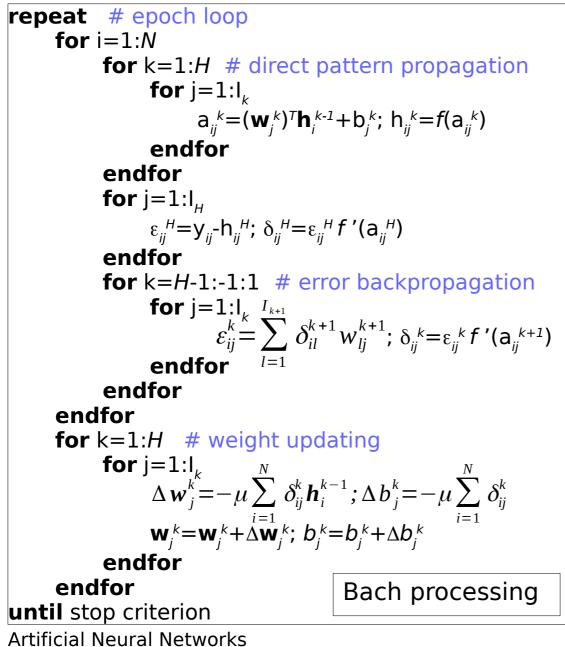
Backpropagation (IV)

- Since $a_{il}^{k+1} = (\mathbf{w}_{l}^{k+1})^{T} \mathbf{h}_{i}^{k} + \mathbf{b}_{l}^{k+1}$ and $\mathbf{h}_{ij}^{k} = f(a_{ij}^{k})$, then: $a_{il}^{k+1} = \sum_{m=1}^{I_{k}} w_{lm}^{k+1} f(a_{im}^{k}) + b_{l}^{k+1}$ $\frac{\partial a_{il}^{k+1}}{\partial a_{ij}^{k}} = w_{lj}^{k+1} f'(a_{ij}^{k})$
- So $\delta_{ij}^{\ k}$ is a recursive function depending on $\delta_{ij}^{\ k+1}$ and $\mathbf{w}_{i}^{\ k+1}$:

$$\delta_{ij}^{k} = \sum_{l=1}^{I_{k+1}} \delta_{il}^{k+1} w_{lj}^{k+1} f'(a_{ij}^{k}) = f'(a_{ij}^{k}) \sum_{l=1}^{I_{k+1}} \delta_{il}^{k+1} w_{lj}^{k+1}, k = K-1, \dots, 1$$

- Denoting $\varepsilon_{ij}^k = \sum_{l=1}^{I_{k+1}} \delta_{il}^{k+1} w_{lj}^{k+1}$, we obtain: $\delta_{ij}^k = \varepsilon_{ij}^k f'(a_{ij}^k)$
- The derivatives are, respectively, f'(t)=af(t)[1-f(t)] and $f'(t)=a[1-f^2(t)]$ for sigmoid and tanh activation functions.

Backpropagation (V)



- Initial random low weights w^k_j and biases b^k_j
- Epoch: processing of the whole training set
- Stop criterion: 1) J or gradient of J below a threshold; 2) maximum of epochs
- Speed μ with intermediate values: avoid slowness and oscilations
- Select the best among different initializations in order to avoid falls into local minima with high J
- Weight updating pattern by pattern (online): it can avoid local minimums and converges faster

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Enhancements over backpropagation (I)

- **Preprocessing**: inputs using 0 mean and the same variance as the activation range *f*(*t*).
- **Symmetrical activation** (tanh) instead of the sigmoid function.
- **Moment** (α): inertia in the learning:

$$\Delta \boldsymbol{w}_{j}^{k}(t+1) = \alpha \Delta \boldsymbol{w}_{j}^{k}(t) - \mu \sum_{i=1}^{N} \delta_{ij}^{k} \boldsymbol{h}_{i}^{k-1}$$

t=iteration; $\alpha \in [0.7-0.95]$; $\Delta \mathbf{w}_i^k$ reduce approx. in 1- α

Enhancements over backpropagation (II)

 RMSProp (root mean square propagation): use a second order moment instead of first order moment; η,β: hyperparameters
 epoch=presentation of training set

 $S_{w} = 0; S_{b} = 0$

for epoch=1:nepoch

calculate $\Delta \boldsymbol{w}$ and $\Delta \boldsymbol{b}$

Use the squared gradient to scale the learning speed.

$$S_{w} = \beta S_{w} + (1-\beta) |\Delta w|^{2}; S_{b} = \beta S_{b} + (1-\beta) \Delta b^{2}$$

$$w(t+1) = w(t) - \frac{\eta \Delta w}{\varepsilon + \sqrt{S_w}}; b(t+1) = b(t) - \frac{\eta \Delta b}{\varepsilon + \sqrt{S_b}}$$

endfor

Enhancements over backpropagation (III)

• Adaptive learning speed: $\mu(t=0) \in [0.03 - 0.1]$

-
$$\mu(t+1) = (1+\epsilon_i)\mu(t)$$
 if $J(t+1) < J(t)$

-
$$\mu(t+1) = (1-\epsilon_d)\mu(t)$$
 and $a=0$ if $J(t+1) > (1+\epsilon_c)J(t)$, with
 $\epsilon_i = 0.05$, $\epsilon_d = 0.3$ e $\epsilon_c = 0.04$

• **Speed reduction**: *t*=epoch; μ₀,β,*k*: hyper-parameters

$$\mu(t) = \frac{\mu_0}{1 + t \beta} \qquad \mu(t) = 0.95^t \mu_0 \qquad \mu(t) = \frac{k \mu_0}{\sqrt{t}}$$

Enhancements over backpropagation (IV)

- Different speed for each weight: increase μ when the gradient of that weight has the same sign in two iteractions.
- Desired outputs y_{ij} corresponding with activation function (sigmoid or hyperbolic).
- If $y_{ij} \in [0,1]$, they can be seen as probabilities and **cross entropy** can be used as cost function instead of SSE:

$$J = -\sum_{i=1}^{N} \sum_{j=1}^{I_{H}} \left[y_{ij} \ln h_{ij}^{H} + (1 - y_{ij}) \ln (1 - h_{ij}^{H}) \right]$$

Enhancements over backpropagation (V)

• Karhunen-Loewe divergence or relative entropy, using softmax activation function for the output, can also be used as a cost function: a^{μ}

$$J = -\sum_{i=1}^{N} \sum_{j=1}^{I_{H}} y_{ij} \ln \frac{h_{ij}^{H}}{y_{ij}} \qquad h_{ij}^{H} = \frac{e^{a_{ij}}}{\sum_{l=1}^{I_{H}} e^{a_{il}^{H}}}$$

- The number H of layers and neurons I_k in each layer k=1..H must be decided: tunable hyper-parameter
- With many neurons (and weights \mathbf{w}_{j}^{k} , that are trainable parameters), produces overfitting.

Enhancements over backpropagation (VI)

- In practice, it was demostrated that backpropagation did not provide good solutions using various hidden layers.
- It was demostrated Mathematically that ANN with only one hidden layer is a universal approximator of any function.
- But this affects the training error, not test error: overfitting
- Number of neurons by layer: start with many neurons and use regularization to remove the less informative weights (pruning).

Enhancements over backpropagation (VII)

- Weight reduction: use J'(W)=J(W)+λ|W|² regularizated by the squared norm of the weight matrix W={w_j^k}, k=1..H,
 j=1..l_ν
- Alternative to |**W**|²:

$$\sum_{l=1}^{N_w} \frac{\theta_l^2}{\theta_h^2 + \theta_l^2}$$

being θ_l the *l*th weight (*l*=1..N_w) and θ_h the threshold: removes the weights $\theta_l < \theta_h$

Enhancements over backpropagation (VIII)

- Sensitivity analysis: the weights θ_{I} with low saliency $s_{I} = h_{II} \theta_{I}^{2}/2$ are periodically removed. h_{II} measures the effect over J of removing θ_{I}): $h_{II} = \frac{\partial^{2} J}{\partial \theta_{I}^{2}}$
- **Early stopping**: each epoch, the network is tested over a separated validation set
- Training is stopped when the validation error starts to increase (overfitting).

Enhancements over backpropagation (IX)

- Shared weights: some conections are enforced to share weight values to guarantee certain in-variances (ex: translation, rotation and scale in images).
- Alternative: to use input features which are invariants to these transformations.

Limitations of MLP (I)

- Slow training, stucking in non-optimal local minima, most frequently with several hidden layers
- Many tunable hyper-parameters: number of hidden layers
 (*H*), number of neurons in each layer (I₁..I_H), learning speed
 (μ), momentum (α), etc.
- For some time, the multilayer networks (H>2) were discarded instead of one hidden layer (H=2) networks, that are universal approximators.

Limitations of MLP (II)

- However, the neurons required with one layer is higher than with various layers
- Backpropagation is based on f'(a_{ij}^{k+1}), where f is sigmoid or tanh and exhibits null derivative in most its domain
- This leads to null gradients stopping training and generating many problems.

MLP in Python

Class **MLPClassifier** implements a multi-layer perceptron (MLP) algorithm that trains using Backpropagation.

MLP trains on two arrays: array X of size (n_samples, n_features), which holds the training samples represented as floating point feature vectors; and array y of size (n_samples,), which holds the target values (class labels) for the training samples:

```
>>> from sklearn.neural_network import MLPClassifier
>>> X = [[0., 0.], [1., 1.]]
>>> y = [0, 1]
>>> clf = MLPClassifier(solver='lbfgs', alpha=1e-5,
... hidden_layer_sizes=(5, 2), random_state=1
...
>>> clf.fit(X, y)
MLPClassifier(alpha=1e-05, hidden_layer_sizes=(5, 2), random_stat
solver='lbfgs')
```

After fitting (training), the model can predict labels for new samples:

```
>>> clf.predict([[2., 2.], [-1., -2.]])
array([1, 0])
```

MLP in octave

- Package **nnet** in octave: https://octave.sourceforge.io/nnet/
 - prestd(): preprocesses the data so that the mean is 0 and the standard deviation is 1.
 - trastd(): preprocess additional data for neural network simulation (for example the test set).
 - newff(): create a feed-forward backpropagation network.
 - **train()**: a neural feed-forward network will be trained.
 - sim(): is usuable to simulate a before defined and trained neural network.
- Similar functions in the Matlab Neural Network Toolbox

MLP in R

Package nnet in R: https://cran.r-project.org/web/packages/nnet/index.html

nnet	Fit Neural Networks

Description

Fit single-hidden-layer neural network, possibly with skip-layer connections.

Usage

```
nnet(x, ...)
## S3 method for class 'formula'
nnet(formula, data, weights, ...,
    subset, na.action, contrasts = NULL)
## Default S3 method:
nnet(x, y, weights, size, Wts, mask,
    linout = FALSE, entropy = FALSE, softmax = FALSE,
    censored = FALSE, skip = FALSE, rang = 0.7, decay = 0,
    maxit = 100, Hess = FALSE, trace = TRUE, MaxNWts = 1000,
    abstol = 1.0e-4, reltol = 1.0e-8, ...)
```

Extreme Learning Machine (ELM)

- Network with H=2 layers: only one hidden layer, direct propagation
- Input weights W¹={w_{jk}¹} and biases {b_j}, with j=1..l₁ and k=1..n, initialized with random values.
- Output weights $\mathbf{W}^2 = \{\mathbf{w}_{jk}^2\}$ and biases $\{\mathbf{b}_j\}$, with $j=1..l_2$ ($l_2=C$, no. classes, for classification) and $k=1..l_1$
- W² calculated using the pseudo inverse of activity matrix H and the desired outputs Y as W²=Y H⁺: direct and efficient for small datasets and networks

•
$$\mathbf{W}^2 = (\mathbf{I}_2 \times \mathbf{I}_1), \mathbf{Y} = (\mathbf{I}_2 \times N), \mathbf{H} = (\mathbf{I}_1 \times N), \mathbf{H}^{\dagger} = (N \times \mathbf{I}_1)$$

Extreme Learning Machine (II)

- It was proved that training error converges to zero when $I_1 \rightarrow N$
- The activation function for the output layer is linear (for regression) or sigmoid+softmax (for classification):

Linear
activation:
$$z_{ij} = w_{jl}^2 f\left(\sum_{m=1}^n w_{lm}^1 x_{im} + b_j^1\right)$$
 $i=1, \dots, N; j=1...I_2$
Sigmoid+
softmax $h_{ij}^2 = f\left[w_{jl}^2 f\left(\sum_{m=1}^n w_{lm}^1 x_{im} + b_l^1\right) + b_j^2\right]$ $z_{ij} = \frac{e^{h_{ij}^2}}{\sum_{k=1}^{I_2} e^{h_{kj}^2}}$

The number I_1 of hidden neurons is a tunable hyper-• parameter, with best values lower than the number N of training patterns Artificial Neural Networks

Quick ELM (I)

- Problems of ELM with large datasets:
 - The activity **H** matrix is of order $I_1 \times N$. With large datasets, it does not fit in memory
 - If **H** fits in memory, calculation of \mathbf{H}^{\dagger} is not possible
 - Tuning of hidden layer size I_1 requires to repeat training many times, that is not possible
- Solution: Quick ELM
 - Quick extreme learning machine for large-scale classification. Audi Albtoush, Manuel Fernández-Delgado, Eva Cernadas and Senén Barro. Neural Computing and Applications, Vol. 34, pp. 5923–5938 (2022). DOI: 10.1007/s00521-021-06727-8

Quick ELM (II)

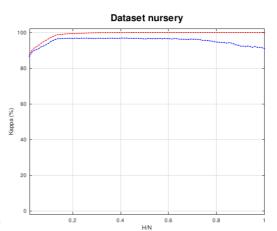
- Quick ELM: efficient approach for classification
- 1) Avoids tuning of I_1 by estimating it from N
- 2) Bounds the size of matrix **H** for large datasets
- 3) Replaces patterns by prototypes to calculate ${\ensuremath{\textbf{H}}}$
- Works on datasets with 31 million patterns, 30,000 inputs and 130 classes
- Estimation of *I*₁:

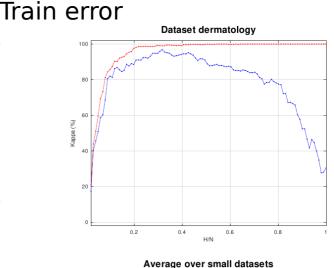
```
I_1 = [\eta \min(N, N_0)], \eta = 0.15, N_0 = 15000
```

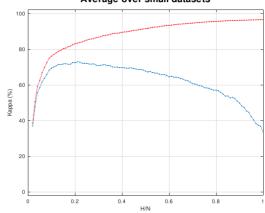
Quick ELM (III)

- Based on behavior of performance vs I₁ / N
- The optimal I₁ is increasing with N
- Performance reduces when $I_1 \rightarrow N$
- Overtraining
- Empirically, we observed that I₁ about 0.15N is a good choice
- Upper bounded by N_o









Quick ELM (IV)

- Replaces \mathbf{x}_n by \mathbf{p}_{cl} (prototype) for $H_{kn} = g(\mathbf{w}_k^{\ 1} \mathbf{x}_n + b_k)$ in matrix **H**
- Limited collection of prototypes $\{\mathbf{p}_{cl}\}\$ with $c=1..C, l=1..L_{c}$
- The maximum number L_c of prototypes per class depends on the class population N_c , with $L_c < 100$
- The total number of prototypes is bounded to allow H fits in memory and be pseudo-inverted
- Each prototype **p**_{cl} is iteratively updated with its nearest training patterns of its class c:

$$\boldsymbol{p}_{cl}(t+1) = \left[1 - \frac{1}{N_{cl}(t)}\right] \boldsymbol{p}_{cl}(t) + \frac{\boldsymbol{x}_n}{N_{cl}(t)} \qquad c = y_n \qquad N_{cl}(t+1) = N_{cl}(t) + 1$$
$$l = \underset{j=1..L_c}{argmin} \left\{|\boldsymbol{p}_{cj} - \boldsymbol{x}_n|\right\}$$

 $N_{cl}(t)$: no. training patterns nearest to *l*-th prototype of class *c* Artificial Neural Networks Eva Cernadas

Other neural networks

- Radial Basis Function (RBF) neural network
- Recursive networks: with feedback from outputs to inputs
- Self-Organized Map (SOM): non-supervised learning
- Learning vector quantization (LVQ): SOM with supervised learning
- Boltzmann machine

Deep Learning

- Networks with many hidden layers:
 - Deep neural network (DNN)
 - Deep belief network (DBN)
 - Convolutional neural network (CNN)
 - Deep autoencoder network (DAN)
- Non-supervised pre-training for each layer separately: restricted Boltzman machine (RBM). Unsupervised. Locates the starting weights in areas of the weight space with good solutions
- **Supervised training** of the output weights
- Fine training of intermediate and output weights using back-propagation