MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC

COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

20 YEARS
1998-2018

Deep Learning: An Introduction for Applied Mathematicians

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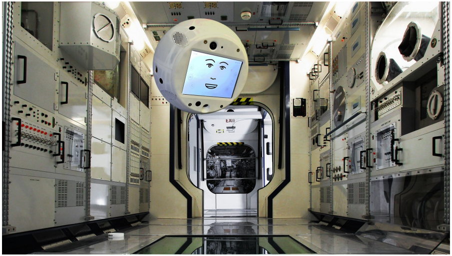
June 13, 2018

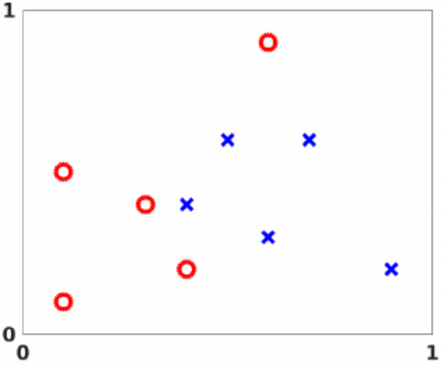
CSC Reading Group Seminar

Disclaimer



Claim: *I am not an expert in machine learning – But <u>we</u> are!*

Reference



C. F. Higham and D. J. Higham (2018). *Deep Learning: An Introduction for Applied Mathematicians.* arXiv:1801.05894v1.

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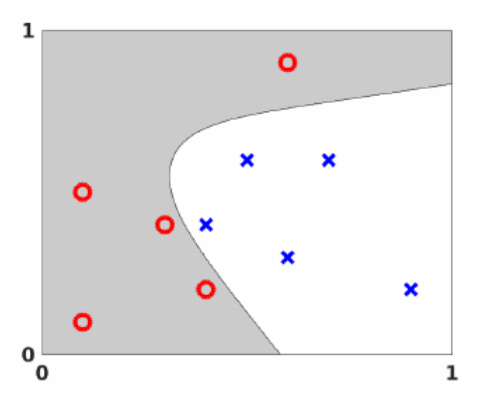

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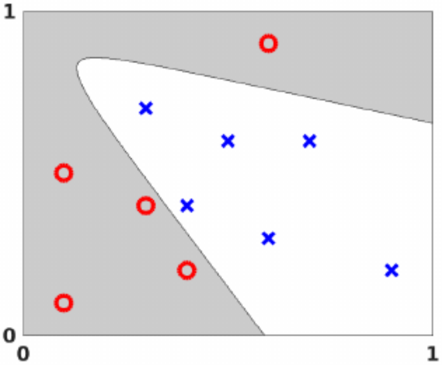

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Machine Learning	Numerical Analysis
neuron	smoothed step function

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???	model-order reduction

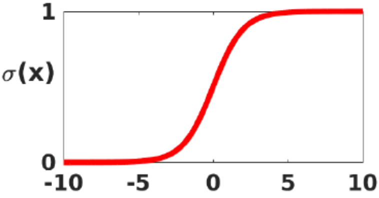
Overview

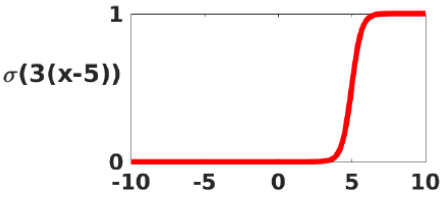
The General Set-up

The sigmoid function,

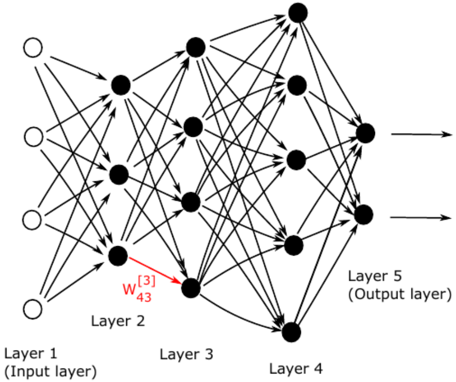
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

models the bahavior of a neuron in the brain.





A neural network



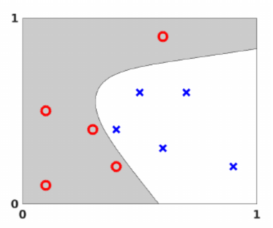
$$a^{[1]} = x \in \mathbb{R}^{n_1},$$

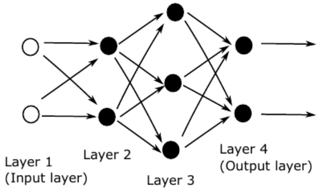
$$a^{[l]} = \sigma\left(W^{[l]} a^{[l-1]} + b^{[l]}\right) \in \mathbb{R}^{n_l}, \quad l = 2, 3, ..., L$$

The entering example

$$\min_{W^{[j]},b^{[j]}} \frac{1}{10}\sum_{i=1}^{10}\frac{1}{2}\|y(x^i)-F(x^i)\|_2^2, \quad j\in\{2,3,4\},$$

$$F(x)=\sigma\left(W^{[4]}\sigma\left(W^{[3]}\sigma\left(W^{[2]}x+b^{[2]}\right)+b^{[3]}\right)b^{[4]}\right)\in\mathbb{R}^2$$





The entering example

$$\min_{p\in\mathbb{R}^{23}} \frac{1}{10}\sum_{i=1}^{10}\frac{1}{2}\|y(x^i)-F(x^i)\|_2^2,$$

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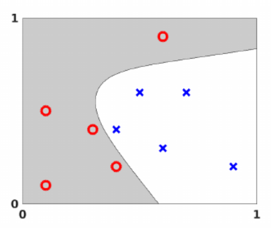

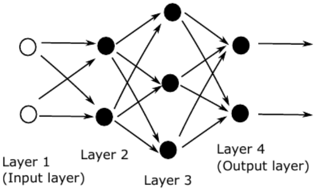

Stochastic Gradient

Objective function:

$$\mathcal{J}(p) = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2} \| y(x^i) - a^{[L]}(x^i, p) \|_2^2$$

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Steepest descent:

$$p \leftarrow p - \eta \nabla \mathcal{J}(p), \quad \eta \in \mathbb{R}_+ \text{ is called 'learning rate'.}$$

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Back Propagation (1/3)

Now, $p \sim \left\{ \left[W^{[l]}\right]_{j,k}, \left[b^{[l]}\right]_j \right\}$. Let $z^{[l]} := W^{[l]} a^{[l-1]} + b^{[l]}$ and $\delta_j^{[l]} := \frac{\partial C}{\partial z_j^{[l]}}$.

Lemma: Back Propagation

The partial derivatives are given by,

$$\delta^{[L]} = \sigma'(z^{[L]}) \cdot (a^{[L]} - y), \tag{1}$$

$$\delta^{[l]} = \sigma'(z^{[l]}) \cdot (W^{[l+1]})^T \delta^{[l+1]}, \quad 2 \leq l \leq L-1, \tag{2}$$

$$\frac{\partial C}{\partial b_j^{[l]}} = \delta_j^{[l]}, \quad 2 \leq l \leq L, \tag{3}$$

$$\frac{\partial C}{\partial w_{jk}^{[l]}} = \delta_j^{[l]} a_k^{[l-1]}, \quad 2 \leq l \leq L. \tag{4}$$

Back Propagation (2/3)

Proof.

We prove (1) component-wise:

$$\delta_j^{[L]} = \frac{\partial C}{\partial z_j^{[L]}} = \frac{\partial C}{\partial a_j^{[L]}} \frac{\partial a_j^{[L]}}{\partial z_j^{[L]}} = (a_j^{[L]} - y_j)\sigma'(z_j^{[L]}) = (a_j^{[L]} - y_j)(\sigma(z_j^{[L]}) - \sigma^2(z_j^{[L]}))$$

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Next, we prove (2) component-wise:

$$\delta_j^{[l]} = \frac{\partial C}{\partial z_j^{[l]}} = \sum_{k=1}^{n_{l+1}} \frac{\partial C}{\partial z_k^{[l+1]}} \frac{\partial z_k^{[l+1]}}{\partial z_j^{[l]}} = \sum_{k=1}^{n_{l+1}} \delta_k^{[l+1]} \frac{\partial z_k^{[l+1]}}{\partial z_j^{[l]}}$$
$$= \sum_{k=1}^{n_{l+1}} \delta_k^{[l+1]} w_{kj}^{[l+1]} \sigma'(z_j^{[l]}),$$

where $z_k^{[l+1]} = \sum_{s=1}^{n_l} w_{ks}^{[l+1]} \sigma(z_s^{[l]}) + b_k^{[l+1]}$.

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$$= \sum_{k=1}^{n_{l+1}} \delta_k^{[l+1]} w_{kj}^{[l+1]} \sigma'(z_j^{[l]}),$$

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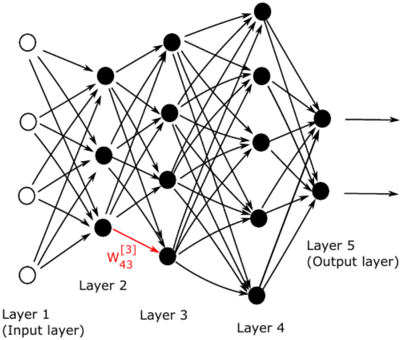
(3) and (4) similar. □

Back Propagation (3/3)

Interpretation:

- Evaluation of $a^{[L]}$ requires a so-called forward pass: $a^{[1]}, z^{[2]} \to a^{[2]}, z^{[3]} \to ... \to a^{[L]}$
- Compute: $\sigma^{[L]}$ via (1)
- Compute: backward pass (2) $\sigma^{[L]} \to \sigma^{[L-1]} \to ... \to \sigma^{[2]}$
- Gradients via (3)-(4)



MATLAB Example

Acknowledgements

We are grateful to the MatConvNet team for making their package available under a permissive BSD license. The MATLAB code in Listings 6.1 and 6.2 can be found at

`http://personal.strath.ac.uk/d.j.higham/algfiles.html`

as well as an exteneded version that produces Figures 7 and 8, and a MATLAB code that uses `lsqnonlin` to produce Figure 4.

personal.strath.ac.uk/d.j.higham/algfiles.html

See the book Matlab Guide for more info about MATLAB.

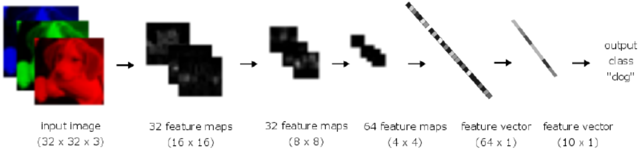
MATLAB files from **Deep Learning: An Introduction for Applied Mathematicians,** by C. F. Higham and D. J. Higham, manuscript, 2018.

- netbp.m from Listing 6.1
- netbpfull.m extended version of netbp.m that produces the figure
- activate.m from Listing 6.2
- nlsrun.m code from section 2 that uses MATLAB's lsqnonlin optimizer

Some more details

Convolutional Neural Network:

- Presented approach unfeasible for large data ($W^{[l]}$ is dense).
- Layers can be pre- and post-precessing steps used in image analysis; *filtering*, *max pooling*, *average pooling*, ...



Avoiding Overfitting:

- Trained network works well on given data, but *not* on new data.
- Splitting: *training* – *validation* data
- Dropout: independently remove neurons

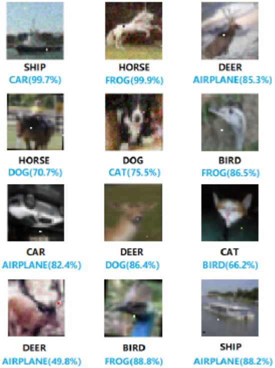
Current Research Directions

Research directions:

- proofs – e.g. when data is assumed to be i.i.d.
- in practice: design of *layers*
- perturbation theory: update trained network
- autoencoders: $\|x - G(F(x))\|_2^2 \to \min$

Two software examples:

- `http://www.vlfeat.org/matconvnet/`
- `http://scikit-learn.org/`



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artificial intelligence	$f_p(x)$
PCA	POD

Further readings

- Andrew Ng. *Coursera Machine Learning* (online courses)
- M. Nielsen, *Neural Networks and Deep Learning*, Determination Press, 2015.
- I. Goodfellow, Y. Bengio, and A. Courville, *Deep Learning*, MIT Press, Boston, 2016.
- Y. LeCun, Y. Bengio, and G. Hinton, *Deep learning*, Nature, 521 (2015), pp. 436444.
- S. Mallat, *Understanding deep convolutional networks*, Philosophical Transactions of the Royal Society of London A, 374 (2016).