Introduction

Numerical Methods for Deep Learning

Course Overview

- Module 1: Linear Models
  2. Linear Models and Least-Squares
  3. Iterative Methods for Least-Squares
  4. Linear Models for Classification
  5. Newton's Method for Classification
  6. Regularization for Image Classification

Course Overview

- Module 2: Neural Networks
    7. Introduction to Nonlinear Models
    8. Single Layer Neural Networks
    9. Training Algorithms for Single Layer Neural Networks
    10. Introduction to Deep Neural Networks
    11. Differentiating Deep Neural Networks
    12. Stochastic Gradient Descent and Variants
- Module 3: Parametric Models/Convolution Neural Networks
    13. Introduction to Parametric Models
    14. Application of CNN: Image Segmentation
    15. CNN and their relation to PDEs

Deep Neural Networks: History

- Neural Networks with a particular (deep) architecture
- Exist for a long time (70's and even earlier) [10, 11, 8]
- Recent revolution - computational power and lots of data [1, 9, 7]
- Can perform very well when trained with lots of data
- Applications
  - Image recognition [4, 6, 7], segmentation, natural language processing [2, 3, 5]

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- A few recent news articles:
  - Apple Is Bringing the AI Revolution to Your iPhone, WIRED 2016
  - Why Deep Learning Is Suddenly Changing Your Life, FORTUNE 2016
  - Data Scientist: Sexiest Job of the 21st Century, Harvard Business Rev '17

DNN - A Quick Overview - 1

Neural networks are data interpolator/classifier when the underlying model is unknown.

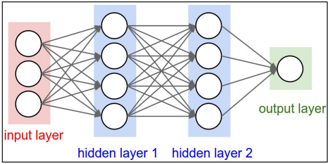
A generic way to write it is

$$\mathbf{c} = f(\mathbf{y}, \boldsymbol{\theta}).$$

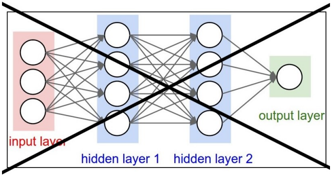
- the function f is the computational model
- $\mathbf{y} \in \mathbb{R}^{n_f}$ is the input data (e.g., an image)
- $\mathbf{c} \in \mathbb{R}^{n_c}$ is the output (e.g. class of the image)
- $\boldsymbol{\theta} \in \mathbb{R}^{n_p}$ are parameters of the model f

In supervised learning we have examples $\{(\mathbf{y}_j, \mathbf{c}_j) \; : \; j = 1, \ldots, n\}$ and the goal is to estimate or "learn" the parameters $\boldsymbol{\theta}$.

DNN - A Quick Overview - 2



DNN - A Quick Overview - 2



$$\begin{cases} \mathbf{y}_{l+1} & = & \sigma(\mathbf{K}_l \mathbf{y}_l + \mathbf{b}_l) \\ \mathbf{y}_{l+1} & = & \mathbf{y}_l + \sigma(\mathbf{K}_l \mathbf{y}_l + \mathbf{b}_l) \\ \mathbf{y}_{l+1} & = & \mathbf{y}_l + \sigma\left(\mathbf{L}_l \sigma(\mathbf{K}_l \mathbf{y}_l + \mathbf{b}_l)\right) \\ & \vdots & \end{cases}$$

Here:

- $l = 0, 1, 2, \ldots, N$ is the layer
- $\sigma : \mathbb{R} \to \mathbb{R}$ is the activation function
- $\mathbf{y}_0 = \mathbf{y} \in \mathbb{R}^{n_f}$ is the input data (e.g., an image)
- $\mathbf{c} \in \mathbb{R}^{n_c}$ is the output (e.g. class of the image)
- $\mathbf{L}_l, \mathbf{K}_l, \mathbf{b}_l$ are parameters of the model f

Learning From Data: The Core of Science - 1

Given inputs and outputs, how to choose f?

Option 1 (Fundamental(?) understanding): For example, Galileo's law of motion

$$x(t) = \frac{1}{2} g t^2,$$

with unknown parameter g.

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$$x(t) = \frac{1}{2} g t^2,$$

with unknown parameter g.
To estimate g observe falling object

t	x
0	0
1	4.9
2	20.1
3	44.1

Goal: Derive model from theory, calibrate it using data.

Learning From Data: The Core of Science - 2

Given inputs and outputs, how to choose f?

Option 2 (Phenomenological models): For example, Archie's law - what is the electrical resistivity of a rock and how it relates to its porosity, ϕ and saturation, S_w?

$$\rho(\phi, S_w) = a\phi^{n/2} S_w^p$$

a, n, p unknown parameters

Obtaining parameters from observed data and lab experiments on rocks.

Goal: Find model that consistent with fundamental theory, without directly deriving it from theory.

Phenomenological vs. Fundamental

Fundamental laws come from understanding(?) the underlying process. They are **assumed invariant** and can therefore be predictive(?).

Phenomenological models are data-driven. They “work” on some given data. Hard to know what their limitations are.

But ...

- models based on understanding can do poorly - weather, economics ...
- models based on data can sometimes do better
- how do we quantify understanding?

Generalization - 1

Suppose that we have examples $\{\mathbf{y}_j, \mathbf{c}_j\}, \quad j = 1, \ldots, n$, a model $f(\mathbf{y}, \boldsymbol{\theta})$ and some optimal parameter $\boldsymbol{\theta}^*$.
Let $\{(\mathbf{y}_j^t, \mathbf{c}_j^t) \ : \ j = 1, \ldots, s\}$ be some test set, that was not used to compute $\boldsymbol{\theta}^*$.

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For phenomenological models, there is no reason why the model should generalize, but in practice it often does.

Generalization - 2

Why would a model generalize poorly?

$$1 \ll \|f(\mathbf{y}_j^t, \boldsymbol{\theta}^*) - \mathbf{c}_j^t\|_p$$

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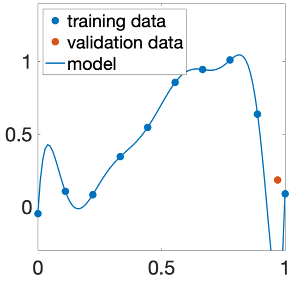

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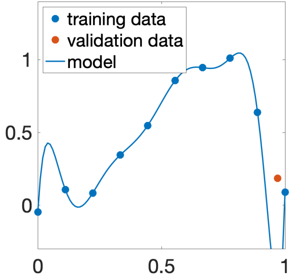

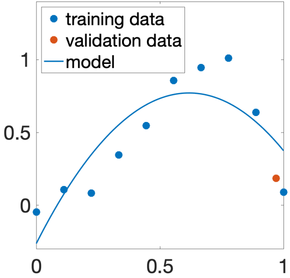

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Two common reasons:

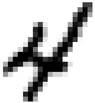
1. Our "optimal" $\boldsymbol{\theta}^*$ was optimal for the training but is less so for other data
2. The chosen computational model f is poor (e.g. quadratic model for a nonlinear function).

Example: Classification of Hand-written Digits

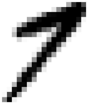
- Let $\mathbf{y}_j \in \mathbb{R}^{n_f}$ and let $\mathbf{c}_j \in \mathbb{R}^{n_c}$.
- The vector $\mathbf{c}$ is the probability of $\mathbf{y}$ belonging to a certain class. Clearly, $0 \leq \mathbf{c}_j \leq 1$ and $\sum_{j=1}^{n_c} \mathbf{c}_j = 1$.

Examples (MNIST):

$\mathbf{y}_1$



$\mathbf{y}_2$



$\mathbf{c}_1 = [0, 0, 0, 0, 1, 0, 0, 0, 0, 0]^\top \quad \mathbf{c}_2 = [0, 0.3, 0, 0, 0, 0, 0, 0.7, 0, 0]^\top$

Example: Classification of Natural Images

Image classification of natural images

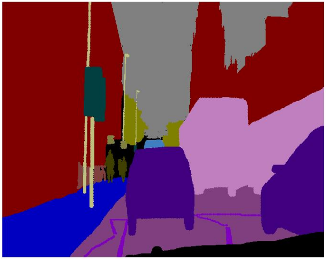
Examples (CIFAR-10):

Example: Semantic Segmentation - 1

- let $\mathbf{y}_j \in \mathbb{R}^n$ be an RGB or grey valued image.
- let the pixels in $\mathbf{c}_j \in \{1, 2, 3, \ldots\}^k$ denote the labels.

$\mathbf{y}$, input image

$\mathbf{c}$, segmentation (labeled image)



Goal: Find map $\mathbf{c} = f(\mathbf{y}, \boldsymbol{\theta})$

Example: Semantic Segmentation - 2

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- extract features from the image
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Reduce the problem of learning from the image to feature detection and classification

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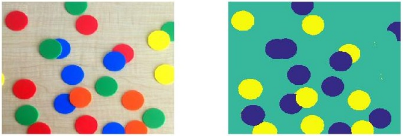
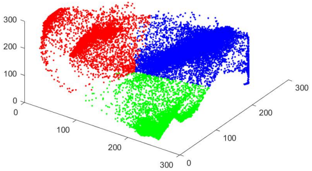
Example: Semantic Segmentation - 3

Simpler setup

- data, **y** is the RGB value of the pixel (and its neighbors?)
- **c** is a labeled pixel
- The map $\mathbf{c} = f(\mathbf{y}, \boldsymbol{\theta})$



input image and segmentation



3D representation of RGB values

References

[1] Y. Bengio et al. Learning deep architectures for AI. *Foundations and trends® in Machine Learning*, 2(1):1–127, 2009.

[2] A. Bordes, S. Chopra, and J. Weston. Question Answering with Subgraph Embeddings. *arXiv preprint arXiv:1406.3676*, 2014.

[3] R. Collobert, J. Weston, L. Bottou, M. Karlen, K. Kavukcuoglu, and P. Kuksa. Natural Language Processing (Almost) from Scratch. *Journal of Machine Learning Research*, 12:2493–2537, 2011.

[4] G. Hinton, L. Deng, D. Yu, G. E. Dahl, A.-r. Mohamed, N. Jaitly, A. Senior, V. Vanhoucke, P. Nguyen, T. N. Sainath, et al. Deep neural networks for acoustic modeling in speech recognition: The shared views of four research groups. *IEEE Signal Processing Magazine*, 29(6):82–97, 2012.

[5] S. Jean, K. Cho, R. Memisevic, and Y. Bengio. On Using Very Large Target Vocabulary for Neural Machine Translation. *arXiv preprint arXiv:1412.2007*, 2014.

[6] A. Krizhevsky, I. Sutskever, and G. Hinton. Imagenet classification with deep convolutional neural networks. *Advances in neural information processing systems*, 61:1097–1105, 2012.

[7] Y. LeCun, Y. Bengio, and G. Hinton. Deep learning. *Nature*, 521(7553):436–444, 2015.

[8] Y. LeCun, B. E. Boser, and J. S. Denker. Handwritten digit recognition with a back-propagation network. In *Advances in neural information processing systems*, pages 396–404, 1990.

References (cont.)

[9] R. Raina, A. Madhavan, and A. Y. Ng. Large-scale deep unsupervised learning using graphics processors. In *the 26th Annual International Conference*, pages 873–880. ACM, June 2009.

[10] F. Rosenblatt. The perceptron: A probabilistic model for information storage and organization in the brain. *Psychological review*, 65(6):386–408, 1958.

[11] D. Rumelhart, G. Hinton, and J. Williams, R. Learning representations by back-propagating errors. *Nature*, 323(6088):533–538, 1986.