Machine Learning

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University of Illinois at Urbana-Champaign, 2018

L8: Deep Neural Networks.

Lecture outline.

- Review & motivation.
- Basic neural networks.
- Some modern usage.

Reading.

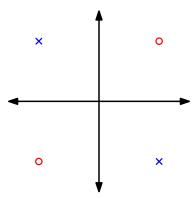
• I. Goodfellow et al.; Deep Learning; Chapters 6-9.

Review & Motivation.

Review.

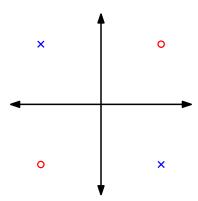
- Lecture 1. Basic ML; *k*-nn (*k* nearest neighbor).
- Lectures 2, 3, 6. Linear predictors (least squares, logistic regression, SVM).
- Lectures 4, 5. Convexity and optimization (e.g., *how we can learn* linear predictors).
 - Lecture 7. Multiclass and nonlinear (kernel) SVM.
 - Lecture 8. Deep neural networks.

Limitations of linear predictors?



No linear separator classifies perfectly!

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Magic fix:

$$\text{use features } \phi(\textbf{\textit{x}}) \coloneqq \textbf{\textit{x}}_1 \cdot \textbf{\textit{x}}_2, \\ \text{whereby } y = \text{sgn}\left(\textbf{\textit{w}}^\top \phi(\textbf{\textit{x}})\right) \text{ with } \textbf{\textit{w}} = [1] \in \mathbb{R}^1.$$

Kernel SVM can be trained in the dual kernels:

$$\begin{aligned} & \max_{\boldsymbol{\alpha} \in [0,C]^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \left\| \sum_{i=1}^n \alpha_i y^{(i)} \phi(\mathbf{x}^{(i)}) \right\|^2 \\ &= \max_{\boldsymbol{\alpha} \in [0,C]^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} (\phi(\mathbf{x}^{(i)}))^\top \phi(\mathbf{x}^{(j)}) \\ &= \max_{\boldsymbol{\alpha} \in [0,C]^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} \kappa(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}). \end{aligned}$$

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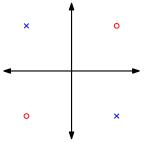
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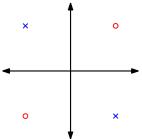
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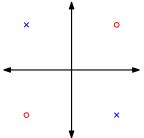
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• After lecture 4:



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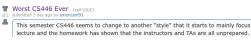
After lecture 6:



• After lecture 4:



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After lecture 8: ???

After lecture 4:



• After lecture 6:



After lecture 8: ???

Observations.

- Everything explicitly in threads.
- Implicit: communication insufficient (e.g., piazza).
- Implicit: homeworks not fun.
- What else?

Second aside: naming.

Artificial neural networks. (8 syllables.)

Neural networks. (4 syllables.)

Deep nets. (2 syllables.)

Basic neural networks.

Neural networks via features.

To make a linear predictor nonlinear, we rely upon feature mapping ϕ :

$$\mathbf{x} \mapsto \mathbf{w}^{\top} \mathbf{x}$$
 becomes $\mathbf{x} \mapsto \mathbf{w}^{\top} \phi(\mathbf{x})$.

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Why not *learn* ϕ ? e.g.,

$$\underset{\boldsymbol{w}}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \ell\left(y^{(i)} \boldsymbol{w}^{\top} \mathbf{x}^{(i)}\right) \quad \text{becomes} \quad \underset{\boldsymbol{w}, \phi \in \mathcal{F}}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \ell\left(y^{(i)} \boldsymbol{w}^{\top} \phi(\mathbf{x}^{(i)})\right)$$

where \mathcal{F} is some class of functions (why not every function?).

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with $\mathbf{w} \in \mathbb{R}^d$, $\mathbf{v} \in \mathbb{R}^m$, $\mathbf{A} \in \mathbb{R}^{m \times d}$, $\mathbf{b} \in \mathbb{R}^m$.

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Gained nothing! $\mathbf{v}^{\top}(\mathbf{A}\mathbf{x} + \mathbf{b}) = (\mathbf{A}^{\top}\mathbf{v})^{\top}\mathbf{x} + \mathbf{v}^{\top}\mathbf{b}$.

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Fix: introduce **nonlinearity/transfer/activation** $\sigma : \mathbb{R}^m \to \mathbb{R}^m$:

$$\phi(\mathbf{x}) := \sigma(\mathbf{A}\mathbf{x} + \mathbf{b}).$$

We will predict with

$$\mathbf{x} \mapsto \mathbf{w}^{\top} \phi(\mathbf{x})$$
 where $\phi(\mathbf{x}) = \sigma(\mathbf{A}\mathbf{x} + \mathbf{b})$.

We will train with

$$\underset{\boldsymbol{w} \in \mathbb{R}^{m}, \boldsymbol{A} \in \mathbb{R}^{m \times d}, \boldsymbol{b} \in \mathbb{R}^{m}}{\arg \min} \frac{1}{n} \sum_{i=1}^{n} \ell \left(y^{(i)} \boldsymbol{w}^{\top} \sigma \left(\boldsymbol{A} \boldsymbol{x}^{(i)} + \boldsymbol{b} \right) \right).$$

(Question: which training procedure? Why does it work?)

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Why stop there? We can also do

$$\mathbf{x} \mapsto \mathbf{w}^{\top} \sigma_1 \left(\mathbf{A}_1 \phi(\mathbf{x}) + \mathbf{b}_1 \right)$$
 where $\phi(\mathbf{x}) = \sigma_2 \left(\mathbf{A}_2 \mathbf{x} + \mathbf{b}_2 \right)$,

and iterate further.

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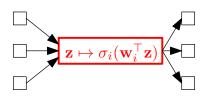
and iterate further. This is a neural network.

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Node *j* in this graph:

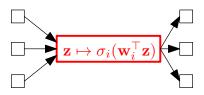
- Collects a vector z from its in-edges;
- Computes $\mathbf{z} \mapsto \sigma_j(\mathbf{w}_i^{\top} \mathbf{z} + b_j)$;
- Propagates this value along its out-edges.



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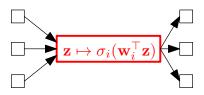


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Tensorflow computation graphs: everything needed to train is in the graph; e.g., parameters get nodes.

Neural networks as functions.

A linear predictor (one layer network) has the form

$$\mathbf{x} \mapsto \mathbf{w}^{\top} \mathbf{x}$$
.

A two layer network has the form

$$\mathbf{x} \mapsto \mathbf{w}^{\top} \sigma_1 \left(\mathbf{A}_1 \mathbf{x} + \mathbf{b}_1 \right).$$

Iterating, a multi-layer network has the form

$$\mathbf{x} \mapsto \mathbf{w}^{\top} \sigma_1 \left(\mathbf{A}_1 \sigma_2 \left(\cdots \mathbf{A}_{L-2} \sigma_{L-1} \left(\mathbf{A}_{L-1} \mathbf{x} + \mathbf{b}_{L-1} \right) + \mathbf{b}_{L-2} \cdots \right) + \mathbf{b}_1 \right).$$

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ERM now takes the form

$$\underset{\boldsymbol{w},\boldsymbol{A}_{1},\ldots,\boldsymbol{A}_{L-1},\boldsymbol{b}_{1},\ldots,\boldsymbol{b}_{L-1}}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \ell\left(y^{(i)} \boldsymbol{w}^{\top} \sigma_{1} \left(\cdots \sigma_{L-1} (\boldsymbol{A}_{L-1} \boldsymbol{x}^{(i)} + \boldsymbol{b}_{L-1})\cdots\right)\right).$$

Neural network (univariate) activations.

We mentioned that **nodes** compute

$$\mathbf{z} \mapsto \sigma \left(\mathbf{v}^{\top} \mathbf{z} \right),$$

where activation/transfer/nonlinearity $\sigma: \mathbb{R} \to \mathbb{R}$ is:

- ReLU (Rectified Linear Unit) $z \mapsto \max\{0, z\}$;
- Sigmoid $z \mapsto \frac{1}{1 + \exp(-z)}$;
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By
$$\mathbf{z}\mapsto\sigma(\mathbf{A}\mathbf{z}+\mathbf{b}),$$

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Soon we will see multivariate nonlinearities, sometimes with output dimension \neq input dimension!

Some modern usage.

Multiclass output.

Modern networks often end with **softmax** nonlinearity:

$$\mathbf{z} \mapsto \sum_{i=1}^k \frac{\exp(\mathbf{z}_i)\mathbf{e}_i}{\sum_{j=1}^k \exp(\mathbf{z}_j)}$$

(where \mathbf{e}_i is i^{th} standard basis vector.) Output is now a probability vector!

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Alternate notation: output vector $\mathbf{v}_i \propto \exp(\mathbf{z}_i)$.

Cross-entropy loss.

Given one hot $\mathbf{y} \in \{\mathbf{e}_1, \dots, \mathbf{e}_k\}$ and probability vector $\hat{\mathbf{y}} \in \mathbb{R}^k$,

$$\ell(y,\hat{y}) = -\sum_{i=1}^k \mathbf{y}_i \ln(\hat{\mathbf{y}}).$$

Combined with softmax $\hat{\boldsymbol{y}} \propto \exp(\boldsymbol{z})$:

$$-\sum_{i=1}^k \boldsymbol{y}_i \ln \left(\frac{\exp(\boldsymbol{z}_i)}{\sum_j \exp(\boldsymbol{z}_j)} \right) = -\sum_{i=1}^k \boldsymbol{y}_i \boldsymbol{z}_i + \ln \left(\sum_{i=1}^k \exp(\boldsymbol{z}_i) \right).$$

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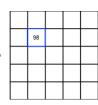
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Question: since last expression is convex in *z*, is the corresponding ERM problem convex?

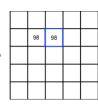
120	190	140	150	200
17	21	30	8	27
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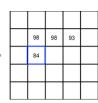
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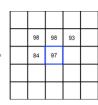
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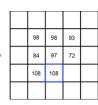
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	108			

,
3
3
7





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Written as matrix-vector product **Ax**:

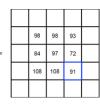
$$\begin{bmatrix} \text{offset 0} \\ \text{offset 1} \\ \text{offset 2} \\ \text{offset 3} \end{bmatrix} \begin{bmatrix} \uparrow \\ \mathbf{x} \\ \downarrow \end{bmatrix}.$$



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Why? Major space savings (#params = filter size). Magical effectiveness on real-world data.

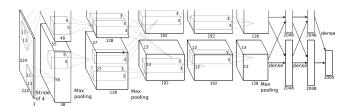
Pooling.

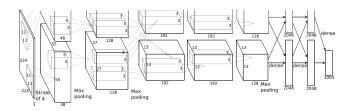
Again slide a window over the input; now take average or maximum.

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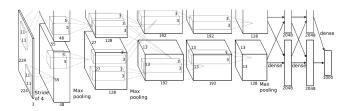
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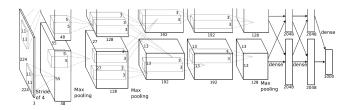




... What? Modern version:



... What? Modern version: 2dconv, relu, 2dmaxpool; 2dconv, relu, 2dmaxpool; dense, relu; dense, relu; dense, softmax.



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2dconv, relu, 2dmaxpool;

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dense, relu;

dense, relu;

dense, softmax.

Differences with original: no "two "tubes" (there for GPUs), no normalization, filter size and stride tweaks...

Regularization.

- "Weight decay": $+\frac{\lambda}{2} ||\mathbf{v}||^2$ in objective (\mathbf{v} = all params).
- Dropout: randomly nullify node outputs in training.
- Batch normalization: "standardize" node output distribution.
- Use SGD! (Implicit regularization.)

Advanced topics.

- Recurrent links; loops.
- Conditional execution.
- "Differentiable" programming.

Summary.

Deep networks

as learning features; iterated linear predictors; graphs.

Cross-entropy loss, convolution layers, max-pooling.