Mathematics of Data: From Theory to Computation

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A lightning tour through the optimization of deep neural networks

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- This recitation

  1. Brief intro into tensors
  2. Backpropagation
  3. Automatic Differentiation & PyTorch
  4. Deep Learning Building Blocks

Outline

Recall: Definition and representation of deep neural networks

Training deep networks

Computational infrastructure

Deep Learning Toolkit

Tensors

- Tensors provide a natural and concise mathematical represention of **data** ($\mathbf{a}$) and **parameters** ($\mathbf{X}_l, \mu_l$ where l indicates the layers).
- Tensors are **multidimensional arrays** and are a generalization of:
  1. scalars - **tensors** with no *indices*; i.e., zeroth-rank tensor.
  2. vectors - **tensors** with exactly one *index*; i.e., first-rank tensor.
  3. matrices - **tensors** with exactly two *indices*; i.e., second-rank tensor.
  4. etc.

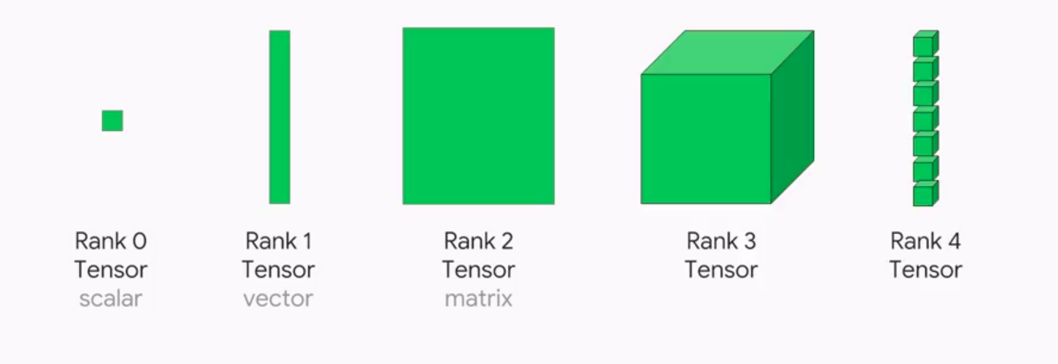

Figure: From [1]

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Recall: Basic Neural Network

1-hidden-layer neural network with m neurons (fully-connected architecture):

- Parameters: $\mathbf{X}_1 \in \mathbb{R}^{m \times d}$, $\mathbf{X}_2 \in \mathbb{R}^{c \times m}$ (weights), $\mu_1 \in \mathbb{R}^m, \mu_2 \in \mathbb{R}^c$ (biases)
- Activation function: $\sigma : \mathbb{R} \to \mathbb{R}$

$$h_{\mathbf{x}}(\mathbf{a}) := \begin{bmatrix} \ \mathbf{X}_2 \ \end{bmatrix} \underbrace{\overset{\text{activation}}{\overset{\downarrow}{\sigma}} \left(\overset{\text{weight}}{\overset{\downarrow}{\begin{bmatrix} \ \mathbf{X}_1 \ \end{bmatrix}}} \overset{\text{input}}{\overset{\downarrow}{\begin{bmatrix} \mathbf{a} \end{bmatrix}}} + \overset{\text{bias}}{\overset{\downarrow}{\begin{bmatrix} \mu_1 \end{bmatrix}}} \right)}_{\text{hidden layer = learned features}} + \overset{\text{bias}}{\overset{\downarrow}{\begin{bmatrix} \mu_2 \end{bmatrix}}}, \qquad \mathbf{x} := [\mathbf{X}_1, \mathbf{X}_2, \mu_1, \mu_2]$$

recursively repeat activation + affine transformation to obtain "deeper" networks.

Minimization of the loss function

In order to use first order methods, we need to derive the gradient

$$\nabla_{\boldsymbol{x}} R_n(\boldsymbol{x}) := \frac{1}{n}\sum_{i=1}^{n} \nabla_{\boldsymbol{x}} L(h(\boldsymbol{a}_i;\boldsymbol{x}), b_i) := \frac{1}{n}\sum_{i=1}^{n} \nabla_{\boldsymbol{x}} L_i(\boldsymbol{x}) \tag{1}$$

where $\boldsymbol{x} = [\mathbf{X}_1, \mu_1, \ldots, \mathbf{X}_k, \mu_k]$ are the weights and biases of the network. For convenience we sometimes also write $h_{\boldsymbol{x}}(\boldsymbol{a})$ instead of $h(\boldsymbol{a}; x)$.

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Example (Naive computation of the gradient)

Let $h(\boldsymbol{a}; \boldsymbol{X}_1, \boldsymbol{X}_2) = \boldsymbol{X}_2^T \sigma(\boldsymbol{X}_1 \boldsymbol{a})$, and $L_i(\boldsymbol{X}_1, \boldsymbol{X}_2) = (b_i - \boldsymbol{X}_2^T \sigma(\boldsymbol{X}_1 \boldsymbol{a}_i))^2$ be the loss on a sample, then

$$\frac{\partial L_i}{\partial \boldsymbol{X}_2} = -2(b_i - \boldsymbol{X}_2^T \sigma(\boldsymbol{X}_1 \boldsymbol{a}_i))\sigma(\boldsymbol{X}_1 \boldsymbol{a}_i) \tag{2}$$

$$\frac{\partial L_i}{\partial \boldsymbol{X}_1} = -2(b_i - \boldsymbol{X}_2^T \sigma(\boldsymbol{X}_1 \boldsymbol{a}_i))\boldsymbol{X}_2 \odot \sigma'(\boldsymbol{X}_1 \boldsymbol{a}_i)\boldsymbol{a}_i^T \tag{3}$$

where $\odot$ denotes element-wise product of vectors.

Many similar terms in both derivatives $\Rightarrow$ Inefficient to compute them independently

Forward pass

Forward pass scheme
Input: $\boldsymbol{a}^{(\mathbf{0})} = \boldsymbol{a}$, $\mathbf{X}^{(l)}$ and $\mu^{(l)}$ for $l = 1, \ldots, k$.
1. **For** $l = 1, \ldots, k$ Compute $\boldsymbol{u}^{(l)} = \mathbf{X}^{(l)}\boldsymbol{a}^{(l-1)} + \mu^{(l)}$ Compute $\boldsymbol{a}^{(l)} = \sigma(\boldsymbol{u}^{(l)})$

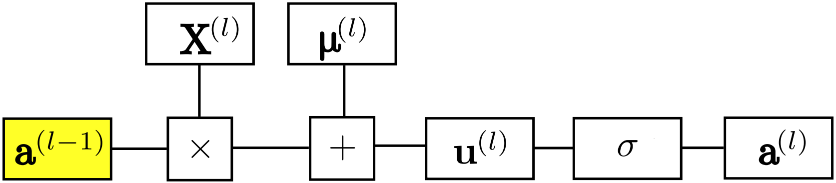

Figure: Computation of $\mathbf{u}^{(l)}$ and $\mathbf{a}^{(l)}$ starting from $\mathbf{a}^{(l-1)}$

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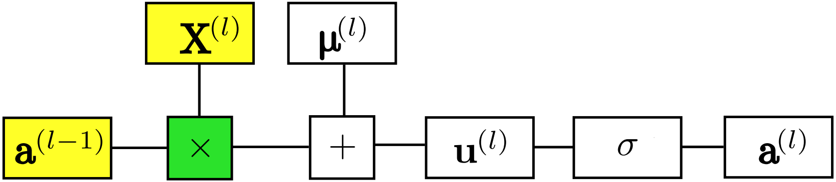

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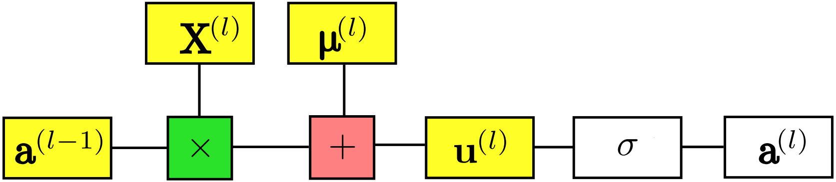

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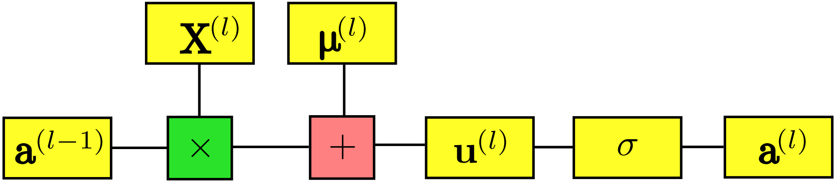

Figure: Computation of $\mathbf{u}^{(l)}$ and $\mathbf{a}^{(l)}$ starting from $\mathbf{a}^{(l-1)}$

Backward pass

Suppose $\frac{\partial L}{\partial \boldsymbol{a}^{(l)}}$ is given, as well as all pre-activation and hidden layer values.

- **Goal**: obtain $\frac{\partial L}{\partial \mathbf{X}^{(l)}}$, $\frac{\partial L}{\partial \mu^{(l)}}$ and $\frac{\partial L}{\partial \boldsymbol{a}^{(l-1)}}$.

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$$\boldsymbol{u}^{(l)} = \mathbf{X}^{(l)} \boldsymbol{a}^{(l-1)} + \mu^{(l)} \Rightarrow \begin{cases} \frac{\partial L}{\partial \mathbf{X}^{(l)}} & = \frac{\partial L}{\partial \boldsymbol{u}^{(l)}} (\boldsymbol{a}^{(l-1)})^T \\ \frac{\partial L}{\partial \mu^{(l)}} & = \frac{\partial L}{\partial \boldsymbol{u}^{(l)}} \end{cases} \qquad \text{(chain rule)}$$

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$$\boldsymbol{a}^{(l)} = \sigma(\boldsymbol{u}^{(l)}) \Rightarrow \frac{\partial L}{\partial \boldsymbol{u}^{(l)}} = \frac{\partial L}{\partial \boldsymbol{a}^{(l)}} \odot \sigma'(\boldsymbol{u}^{(l)}) \qquad \text{(chain rule)}$$

Where $\odot$ is the Hadamard product (element-wise product).

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3. Finally we have
$$\boldsymbol{u}^{(l)} = \mathbf{X}^{(l)}\boldsymbol{a}^{(l-1)} + \mu^{(l)} \Rightarrow \frac{\partial L}{\partial \boldsymbol{a}^{(l-1)}} = (\mathbf{X}^{(l)})^T \frac{\partial L}{\partial \boldsymbol{u}^{(l)}} \qquad \text{(chain rule)}$$

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Backward pass scheme
Input: Gradient of the loss w.r.t. the last layer values $\partial L / \partial \boldsymbol{a}^{(k)}$
1. **For** $l = k, \ldots, 1$ Compute $\frac{\partial L}{\partial \boldsymbol{u}^{(l)}} = \frac{\partial L}{\partial \boldsymbol{a}^{(l)}} \odot \sigma'(\boldsymbol{u}^{(l)})$ Compute $\frac{\partial L}{\partial \mathbf{X}^{(l)}} = \frac{\partial L}{\partial \boldsymbol{u}^{(l)}} (\boldsymbol{a}^{(l-1)})^T, \frac{\partial L}{\partial \mu^{(l)}} = \frac{\partial L}{\partial \boldsymbol{u}^{(l)}}$ Compute $\frac{\partial L}{\partial \boldsymbol{a}^{(l-1)}} = (\mathbf{X}^{(l)})^T \frac{\partial L}{\partial \boldsymbol{u}^{(l)}}$

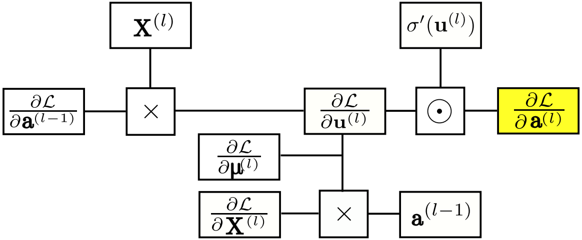

Figure: Computation of $\frac{\partial L}{\partial \mu^{(l)}}$, $\frac{\partial L}{\partial \mathbf{X}^{(l)}}$ and $\frac{\partial L}{\partial \boldsymbol{a}^{(l-1)}}$ starting from $\frac{\partial L}{\partial \boldsymbol{a}^{(l)}}$

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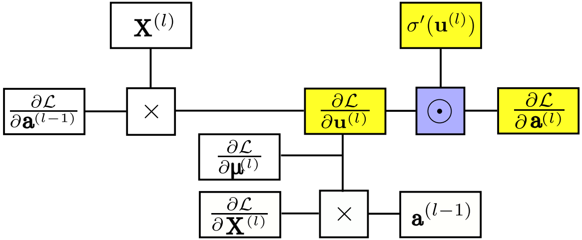

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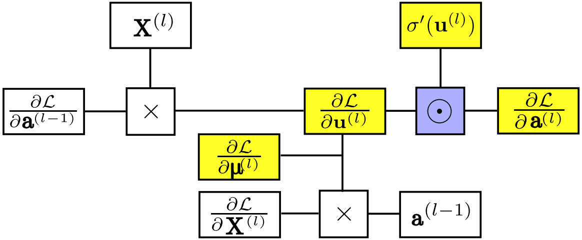

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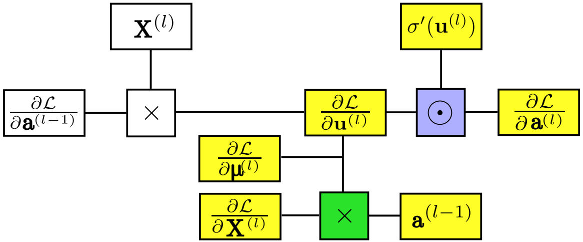

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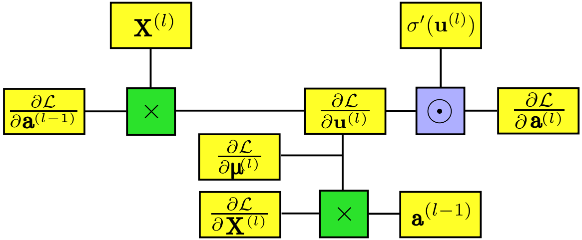

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Backpropagation

- Recursive computation of the derivative $\nabla_{\boldsymbol{x}} L_i(\boldsymbol{x})$

1. **Forward pass:** Compute all pre-activation and hidden layer values
2. **Backward pass:** Compute the derivative of L_i with respect to the weights and biases, from last to first layer.

Complexity of computing $\nabla_{\boldsymbol{x}} L_i(\boldsymbol{x})$

Method	Complexity
Naive derivative	$\mathcal{O}(k^2 m^2)$
Backpropagation	$\mathcal{O}(k m^2)$

Where m is number of neurons per layer and k is the number of layers.

Remarks:
- Complexity is reduced by reusing computations at each step (memoization).
- The backpropagation has the same complexity as the forward pass (but different constants).

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Automatic Differentiation

- *Automatic differentiation* is a computational technique to compute the *exact* gradient of a function by keeping track of its inputs and intermediate values

Automatic Differentiation

- *Automatic differentiation* is a computational technique to compute the *exact* gradient of a function by keeping track of its inputs and intermediate values
- This removes the tedious manual derivation of the gradient and if implemented in a certain way, also reduces the backward pass complexity from $\mathcal{O}(km^2)$ to $\mathcal{O}(km)$
- For a thorough survey and explanation, see [5]

Automatic Differentiation (AD)

Table: Reverse mode AD example, with $y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$ evaluated at $(x_1, x_2) = (2, 5)$. After the forward evaluation of the primals on the left, the adjoint operations on the right are evaluated in reverse. Note that both $\frac{\partial y}{\partial x_1}$ and $\frac{\partial y}{\partial x_2}$ are computed in the same reverse pass, starting from the adjoint $\bar{v}_5 = \bar{y} = \frac{\partial y}{\partial y} = 1$. From [5]

Forward Primal Trace

$$
\begin{array}{lll}
v_{-1} = x_1 & & = 2 \\
v_0 & = x_2 & = 5 \\
\hline
v_1 & = \ln v_{-1} & = \ln 2 \\
v_2 & = v_{-1} \times v_0 & = 2 \times 5 \\
v_3 & = \sin v_0 & = \sin 5 \\
v_4 & = v_1 + v_2 & = 0.693 + 10 \\
v_5 & = v_4 - v_3 & = 10.693 + 0.959 \\
\hline
y & = v_5 & = 11.652
\end{array}
$$

Reverse Adjoint (Derivative) Trace

$$
\begin{array}{llll}
\boldsymbol{\bar{x}_1} & \boldsymbol{= \bar{v}_{-1}} & & \boldsymbol{= 5.5} \\
\boldsymbol{\bar{x}_2} & \boldsymbol{= \bar{v}_0} & & \boldsymbol{= 1.716} \\
\hline
\bar{v}_{-1} & = \bar{v}_{-1} + \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}} & = \bar{v}_{-1} + \bar{v}_1 / v_{-1} & = 5.5 \\
\bar{v}_0 & = \bar{v}_0 + \bar{v}_2 \frac{\partial v_2}{\partial v_0} & = \bar{v}_0 + \bar{v}_2 \times v_{-1} & = 1.716 \\
\bar{v}_{-1} & = \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}} & = \bar{v}_2 \times v_0 & = 5 \\
\bar{v}_0 & = \bar{v}_3 \frac{\partial v_3}{\partial v_0} & = \bar{v}_3 \times \cos v_0 & = -0.284 \\
\bar{v}_2 & = \bar{v}_4 \frac{\partial v_4}{\partial v_2} & = \bar{v}_4 \times 1 & = 1 \\
\bar{v}_1 & = \bar{v}_4 \frac{\partial v_4}{\partial v_1} & = \bar{v}_4 \times 1 & = 1 \\
\bar{v}_3 & = \bar{v}_5 \frac{\partial v_5}{\partial v_3} & = \bar{v}_5 \times (-1) & = -1 \\
\bar{v}_4 & = \bar{v}_5 \frac{\partial v_5}{\partial v_4} & = \bar{v}_5 \times 1 & = 1 \\
\hline
\bar{v}_5 & = \bar{y} & = 1 &
\end{array}
$$

Autograd and Differentiable Programming

- Automatic differentiation + automatic construction of a computational graph from code
- Pedagogic version of autograd (with very readable code) available on github
- Industrial strength implementations used by Facebook and Google also available
- For cool applications on the extreme end see differentiable graphic rendering and differentiable convex optimization solvers.

Outline

Pytorch

- Popular machine learning framework developed by Facebook
- Key innovations: APIs (module structure, dataset) and dynamic graphs (helps debugging, later adopted by tensorflow as well)
- Other frameworks worth mentioning: tensorflow (Google), mxnet (Microsoft) and Flux.jl (for julia)
- *very good* manual and tutorial at https://pytorch.org/docs/stable/index.html
- Two introductory notebooks are provided in this supplementary

Deep Learning Building Blocks: Linear Layers

- $f_l : \mathbb{R}^n \to \mathbb{R}^m$
- $f_l(\mathbf{a}) = \mathbf{X}_l \mathbf{a} + \mu_l$
- Question: How shall we modify the previous 'Bias' class to implement a linear layer?

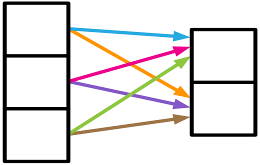


Figure: Linear Layer, from [4]

Deep Learning Building Blocks: Linear Layers

- $f_l : \mathbb{R}^n \to \mathbb{R}^m$
- $f_l(\mathbf{a}) = \mathbf{X}_l\mathbf{a} + \mu_l$
- pytorch implementation: `torch.nn.Linear`
- Multi-layer perceptron (MLP): Stack several (≥ 2) llinear layers, interleaved with activation functions.

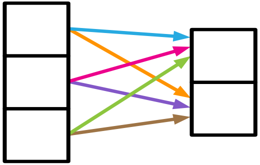
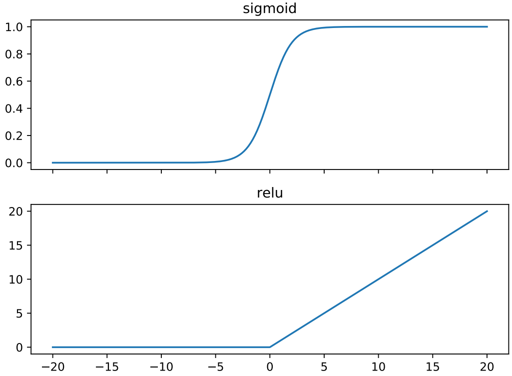


Figure: Linear Layer, from [4]

Deep Learning Building Blocks: Activation functions

- Non-linear functions that are applied element-wise and give the neural network its expressivity
- MLP without nonlinearity is just a factored linear layer
  $f_{\text{total}}(\boldsymbol{a}) = \mathbf{X}_{\text{total}}\boldsymbol{a} + \mu_{\text{total}} = \mathbf{X}_2\mathbf{X}_1\boldsymbol{a} + \mathbf{X}_2\mu_1 + \mu_2$
- Historically sigmoid $\sigma(x) = \frac{1}{1+e^{-x}}$ was common,but due to optimization issues, nowadays the **re**ctified **l**inear **u**nit (RELU) $\sigma(x) = \mathrm{relu}(x) = \max(x, 0)$ is the most common
- $f_{\text{total}}(\boldsymbol{a}) = \mathbf{X}_2\sigma(\mathbf{X}_1\boldsymbol{a} + \mu_1) + \mu_2$ is the minimal "deep" neural network, the "deep" refers to the nonlinearity "hiding" the inner projection
- `torch.nn.ReLu` and `torch.nn.Sigmoid` respectively
- Question: How can we implement an MLP class?



Deep Learning Building Blocks: Loss functions

- Express the task that your model is intended to perform on the data
- For regression, a sensible default is the mean square error $MSE(a,b) = \frac{1}{N}\sum_{i=1}^{N}(a_i - b_i)^2$
- For classification, a sensible default is cross-entropy $H(a,b) = -\sum_{i=1}^{N} a_i \log b_i$ with $a, b \in [0,1]$
- `torch.nn.MSELoss` and `torch.nn.CrossEntropyLoss` respectively

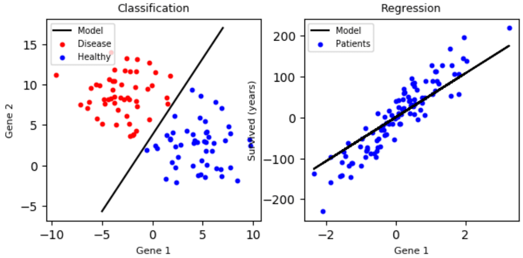


Figure: From [7]

Deep Learning Building Blocks: Convolutional Layers

- apply an MLP across spatial locations of an image to learn a filter
- $f_l : \mathbb{R}^{n \times H \times W} \to \mathbb{R}^{m \times H-k+1 \times W-k+1}$
- $f_l(\mathbf{a}) = \begin{bmatrix} \sum_{i=1}^{n} X_{l,1,i} \star a_i + \mu_1 \\ \vdots \\ \sum_{i=1}^{n} X_{l,o,i} \star a_i + \mu_o \end{bmatrix}$
- $x \star a$ denotes the cross correlation operator, i.e. a sliding window inner product: $(x \star a)_i = \sum_{j=1}^{k} x_{i+j-1} a_j$. The window size k is also called kernel size
- *reduces* spatial dimensions, effectively *subsampling* the input, other parameters include stride and dilation (can find explanations online)
- PyTorch implementation: `torch.nn.ConvNd` for $N \in \{1, 2, 3\}$ dimensional convolution

Convolution layer

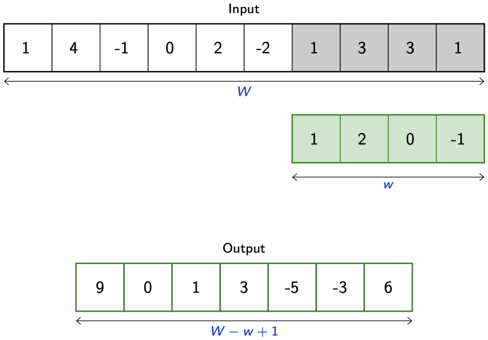


Figure: Convolution operation, from [6]

Deep Learning Building Blocks: Attention Layers

- $f_l : \mathbb{R}^{T,n} \to \mathbb{R}^{T,m}$,explicitly maps between sets
- $f_l(\mathbf{a}) = \mathrm{Attention}(\mathbf{a})X_v\mathbf{a}$
- where the $\mathrm{Attention}(mba)$ is a weight matrix defined rowise as $\mathrm{Attention}(\mathbf{a})_r = \mathrm{softmax}\left(\left(X_q\mathbf{a}\mathbf{a}^T X_k^T\right)_r\right)$
- originally conceived to help RNNs with long range dependencies, requires explicit order encoding
- currently *dominates* both RNNs and CNNs for sequence and vision tasks
- computationally and memory heavy in the original form$\mathcal{O}(T^2)$ but recent work improved this to $\approx \mathcal{O}(T)$.

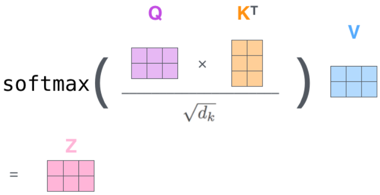


Figure: Attention Layer, from [3]

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Automatic differentiation in machine learning: a survey, 2018.
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[7] petercour.
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Advanced material

Optional reading material for additional building blocks and the complexity of backpropagation.

Deep Learning Building Blocks: Recurrent Layers

- introduces hidden state $h_t \in R^H$ into the training process, generally trained through unrolling the computation graph across time steps T
- $f_l : \mathbb{R}^n \times \mathbb{R}^H \to \mathbb{R}^m \times \mathbb{R}^H$, but when training implicitly $\mathbb{R}^{T,n} \to \mathbb{R}^{T,m} \times \mathbb{R}^{T,H}$ since we unroll through time
- $f_l(\mathbf{a}_t), h_t = g(\mathbf{a}_{t-1}, h_{t-1})$
- h_0 is some initial value,often the zero vector
- $g(\dot{)}$ is usually the GRU or LSTM unit which uses an MLP to predict updates to the hidden state as well as the output

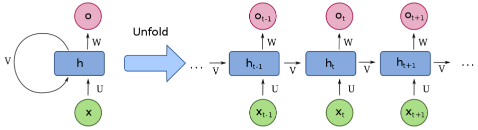

Figure: Recurrent Layer, from [2]

Deep Learning Building Blocks: Transposed-Convolutional Layers

- apply an MLP across spatial locations of an image to learn a filter
- $f_l : \mathbb{R}^{n \times H \times W} \to \mathbb{R}^{m \times H+k-1 \times W+k-1}$
- $f_l(\mathbf{a}) = \begin{bmatrix} \sum_{i=1}^{n} X_{l,1,i} \star a_i + \mu_1 \\ \vdots \\ \sum_{i=1}^{n} X_{l,o,i} \star a_i + \mu_o \end{bmatrix}$
- $x \star a$ denotes the transposed cross correlation operator: $(x \star a)_i = \sum_{j=1}^{k} x_j a_{i+j-1}$.
- *increases* spatial dimensions, effectively *oversampling* the input, other parameters include stride and dilation (can find explanations online)
- PyTorch implementation: `torch.nn.ConvTransposeNd` for $N \in \{1, 2, 3\}$ dimensional transposed convolution

Transposed convolution layer

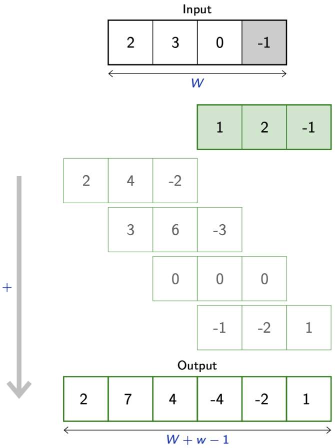

Figure: Transposed convolution operation, from [6]

Deep Learning Building Blocks: Graphical Layers

- generalizes attention to sparse,non-euclidean geometry and variable cardinality sets of inputs
- $f_l : E_{l-1}, V_{-1}, u_{-1} \to E_l, V_l, u^l$ where the E_i, V_i are the sets of edge and node attribute tensors respectively and u is a graph level attribute tensor (from [4])
- updates to e, v, u tensors follow the template $x = \mathrm{Agg}(\mathrm{Proj}(\mathrm{Neigh}(x)))$ i.e. we **agg**regate the **proj**ected elements of the **neigh**ourhood set of an element x.
- Examples for Agg are `sum`,`mean`,`max`, Proj is usually a neural network and the Neigh set are the nodes connected by an edge, to a node by various edges or all elements in the graph respectively for e, v, u.

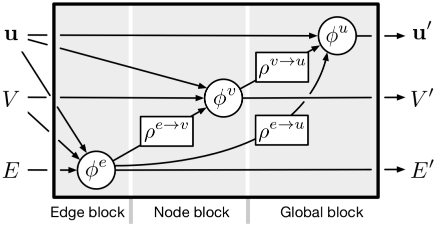

Figure: Graphical Layer, from [4]

Using networks for multi-class classification

Definition (Score-based classifier)

For a network $h : \mathbb{R}^d \to \mathbb{R}^c$ define the score-based classifier $i_h : \mathbb{R}^d \to \{1, \ldots, c\}$ as

$$i_h(\mathbf{a}) = \arg\max_{i \in \{1,\ldots,c\}} [h(\mathbf{a})]_i$$

One output per class, choose the class corresponding to the maximum output. Example:

$$f(\mathbf{x}_0) = \begin{bmatrix} 0.1 \\ -0.8 \\ \mathbf{1.4} \\ 1.1 \end{bmatrix} \qquad \Longrightarrow i_f(\mathbf{a}) = 3$$

Definition (Cross-entropy loss)

Let $\mathbf{a} \in \mathbb{R}^d$ be a sample with label $b \in \{1, \ldots, c\}$

$$L(h(\mathbf{a}), b) = -\log\left(\frac{\exp(h(\mathbf{a})_b)}{\sum_{j=1}^{c} \exp(h(\mathbf{a})_j)}\right)$$

$\mathbf{e}_i \in \mathbb{R}^c$ denotes the i-th canonical vector.

Most common loss for classification via ERM with neural networks. Example:

$$h(\mathbf{a}) = \begin{bmatrix} 0.1 \\ \mathbf{-0.8} \\ \mathbf{1.4} \\ 1.1 \end{bmatrix} \quad \begin{array}{l} L(f(\mathbf{a}), 2) = 2.95 \\ \\ L(f(\mathbf{a}), 3) = 0.75 \end{array}$$

Complexity of Backpropagation

The size of each layer (including input) is $\mathcal{O}(m)$, and the number of layers is $\mathcal{O}(k)$.

Forward pass scheme
1. For $l = 1, \ldots, k$ ▶ $\boldsymbol{u}^{(l)} = X^{(l)}\boldsymbol{a}^{(l-1)} + \mu^{(l)}$ ▶ $\boldsymbol{a}^{(l)} = \sigma(\boldsymbol{u}^{(l)})$

Backward pass scheme
1. For $l = k, \ldots, 1$ ▶ $\frac{\partial L}{\partial \boldsymbol{u}^{(l)}} = \frac{\partial L}{\partial \boldsymbol{a}^{(l)}} \odot \sigma'(\boldsymbol{u}^{(l)})$ ▶ $\frac{\partial L}{\partial X^{(l)}} = \frac{\partial L}{\partial \boldsymbol{u}^{(l)}}(\boldsymbol{a}^{(l-1)})^T$ ▶ $\frac{\partial L}{\partial \mu^{(l)}} = \frac{\partial L}{\partial \boldsymbol{u}^{(l)}}$ ▶ $\frac{\partial L}{\partial \boldsymbol{a}^{(l-1)}} = (X^{(l)})^T \frac{\partial L}{\partial \boldsymbol{u}^{(l)}}$

Complexity of Backpropagation

The size of each layer (including input) is $\mathcal{O}(m)$, and the number of layers is $\mathcal{O}(k)$.

Forward pass scheme
1. For $l = 1, \ldots, k$ ▶ $\boldsymbol{u}^{(l)} = X^{(l)}\boldsymbol{a}^{(l-1)} + \mu^{(l)} \Rightarrow \mathcal{O}(m^2)$ ▶ $\boldsymbol{a}^{(l)} = \sigma(\boldsymbol{u}^{(l)}) \Rightarrow \mathcal{O}(m)$

Forward pass is $\mathcal{O}(km^2)$

Backward pass scheme
1. For $l = k, \ldots, 1$ ▶ $\frac{\partial L}{\partial \boldsymbol{u}^{(l)}} = \frac{\partial L}{\partial \boldsymbol{a}^{(l)}} \odot \sigma'(\boldsymbol{u}^{(l)})$ ▶ $\frac{\partial L}{\partial X^{(l)}} = \frac{\partial L}{\partial \boldsymbol{u}^{(l)}} (\boldsymbol{a}^{(l-1)})^T$ ▶ $\frac{\partial L}{\partial \mu^{(l)}} = \frac{\partial L}{\partial \boldsymbol{u}^{(l)}}$ ▶ $\frac{\partial L}{\partial \boldsymbol{a}^{(l-1)}} = (X^{(l)})^T \frac{\partial L}{\partial \boldsymbol{u}^{(l)}}$

Complexity of Backpropagation

The size of each layer (including input) is $\mathcal{O}(m)$, and the number of layers is $\mathcal{O}(k)$.

Forward pass scheme

1. **For** $l = 1, \ldots, k$
   - $\boldsymbol{u}^{(l)} = X^{(l)}\boldsymbol{a}^{(l-1)} + \mu^{(l)} \Rightarrow \mathcal{O}(m^2)$
   - $\boldsymbol{a}^{(l)} = \sigma(\boldsymbol{u}^{(l)}) \Rightarrow \mathcal{O}(m)$

Forward pass is $\mathcal{O}(km^2)$

Backward pass scheme

1. **For** $l = k, \ldots, 1$
   - $\frac{\partial L}{\partial \boldsymbol{u}^{(l)}} = \frac{\partial L}{\partial \boldsymbol{a}^{(l)}} \odot \sigma'(\boldsymbol{u}^{(l)}) \Rightarrow \mathcal{O}(m)$
   - $\frac{\partial L}{\partial X^{(l)}} = \frac{\partial L}{\partial \boldsymbol{u}^{(l)}} (\boldsymbol{a}^{(l-1)})^T \Rightarrow \mathcal{O}(m^2)$
   - $\frac{\partial L}{\partial \mu^{(l)}} = \frac{\partial L}{\partial \boldsymbol{u}^{(l)}} \Rightarrow \mathcal{O}(1)$
   - $\frac{\partial L}{\partial \boldsymbol{a}^{(l-1)}} = (X^{(l)})^T \frac{\partial L}{\partial \boldsymbol{u}^{(l)}} \Rightarrow \mathcal{O}(m^2)$

Backward pass is $\mathcal{O}(km^2)$