EDAN96
Applied Machine Learning
Lecture 9: Training Techniques, Backward Propagation, and Automatic Differentiation

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Content

Overview and practice of some neural network architectures:

- Logistic loss
- The `Module` class
- Dense vectors
- A word on data loaders
- Backward propagation
- A word on automatic differentiation

Creating a Network with PyTorch

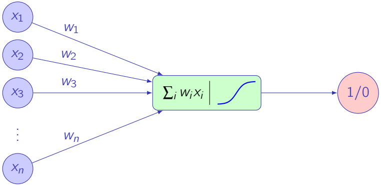
So far, we have used the `Sequential` class to create networks

For more complex architectures, we need to derive a class from `nn.Module`

This class must have the `__init__()` and `forward()` methods:

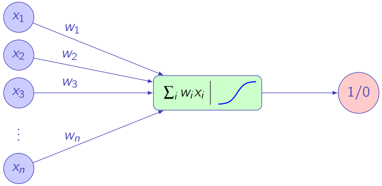
- In the `__init__()` constructor, you declare and create all the trainable parameters
- `forward()` implements the computation of the forward pass

Logistic Regression



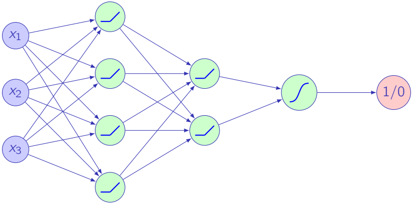

```
model = nn.Sequential(
    torch.nn.Linear(input_dim, 1),
    torch.nn.Sigmoid())
```

Logistic Regression



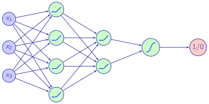

```
class Model(nn.Module):
    def __init__(self, input_dim):
        super().__init__()
        self.fc1 = nn.Linear(input_dim, 1)

    def forward(self, x):
        x = torch.sigmoid(self.fc1(x))
        return x
```

Neural Networks with Hidden Layers




```
model = nn.Sequential(
    nn.Linear(input_dim, 4),
    nn.ReLU(),
    nn.Linear(4, 2),
    nn.ReLU()
    nn.Linear(2, 1),
    torch.nn.Sigmoid()
    )
```

Neural Networks with Hidden Layers




```
class Model2(nn.Module):
    def __init__(self, input_dim):
        super().__init__()
        self.fc1 = nn.Linear(input_dim, 4)
        self.fc2 = nn.Linear(4, 2)
        self.fc3 = nn.Linear(2, 1)

    def forward(self, x):
        x = torch.relu(self.fc1(x))
        x = torch.relu(self.fc2(x))
        x = torch.sigmoid(self.fc3(x))
        return x
```

Code Example

Experiment: Deriving a class with a Jupyter Notebook:
https://github.com/pnugues/edan96/blob/main/programs/8-Salammbo_class_torch.ipynb

Problems with Softmax

The logistic and softmax functions are typical activations of the last layer
They are numerically unstable. Take for instance

$$softmax(1000.0, 1000.0, 1000.0) = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3}).$$

Now try to compute it from the formula:

$$softmax(x_i) = \frac{e^{x_i}}{\sum_j e^{x_j}}$$

Multiclass in PyTorch

To solve the numerical under or overflows, PyTorch integrates softmax in the cross entropy loss

It uses a specific function called LogSumExp . See
https://en.wikipedia.org/wiki/LogSumExp

See also:
https://gregorygundersen.com/blog/2020/02/09/log-sum-exp/

The last layer of a multiclass classification is typically a linear layer. For instance:

```
model = nn.Sequential(
    nn.Linear(input_dim, 5),
    nn.ReLU(),
    nn.Linear(5, 3)
    )
```

The layer outputs are called logits

The cross entropy loss uses a logit input in PyTorch: https://pytorch.org/docs/stable/generated/torch.nn.CrossEntropyLoss.html

Code Example

Experiment:
The code of a neural network with a sequential model is very close to that of logistic regression.
We just list the layers and activation functions
Jupyter Notebook: `https://github.com/pnugues/edan96/blob/main/programs/9-Salammbo_multi_torch.ipynb`

Binary Classification from Logits

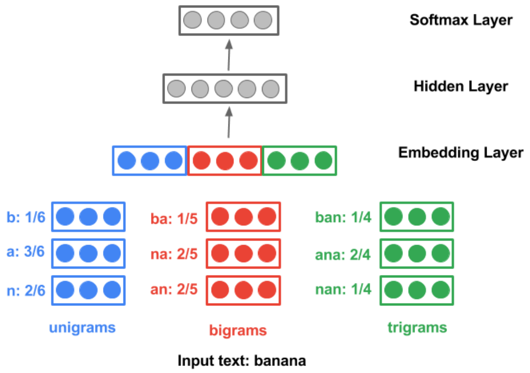
Binary and multiclass classifications have different architectures in PyTorch.
Maybe a bug in the API design?
We can use the `nn.BCEWithLogitsLoss()` to have a logit input:

```
model2 = nn.Sequential(
    nn.Linear(input_dim, 4),
    nn.ReLU(),
    nn.Linear(4, 2),
    nn.ReLU(),
    nn.Linear(2, 1)
)
```

Experiment: Deriving a class with a Jupyter Notebook:
https://github.com/pnugues/edan96/blob/main/programs/10-Salammbo_class_logits_torch.ipynb

Sum of Embeddings in CLD3

CLD3 computes the weighted sum of embeddings



Categorical Values: Multi-hot encoding

A collection of two documents D1 and D2:

D1: Chrysler plans new investments in Latin America.

D2: Chrysler plans major investments in Mexico.

Multi-hot encoding (also called a bag-of-words representation):

D.	america	chrysler	in	investments	latin	major	mexico	new	plans
1	1	1	1	1	1	0	0	1	1
2	0	1	1	1	0	1	1	0	1

This technique can create extremely large sparse vectors

Dense Vectors

We can replace one-hot vectors by dense ones using embeddings

A dense representation is a trainable vector of 10 to 300 dimensions.

The vector parameters are learned in the fitting procedure.

Dimensionality reduction inside a neural network or another procedure.

Example: GloVe file 100d.

Many techniques, often based on language modeling, here CBOW

Cloze Test

Guess a missing word given its context. Using the example:

Sing, O **goddess***, the anger of Achilles son of Peleus,*

Cloze test: A reader, given the incomplete phrase:

```
Sing, O ____, the anger of Achilles
```

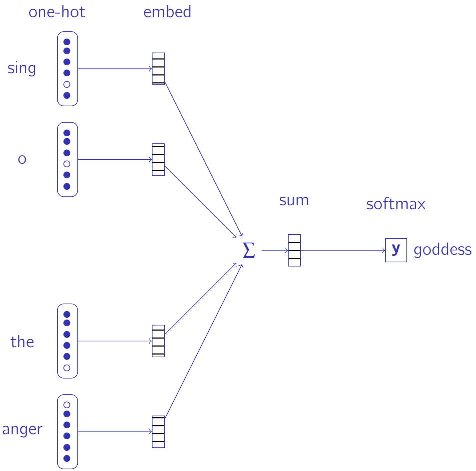
has to fill in the blank with the correct word, here **goddess**.

Easy to create a dataset for a Cloze test

$$X = \begin{bmatrix} \text{sing} & \text{o} & \text{the} & \text{anger} \\ \text{o} & \text{goddess} & \text{anger} & \text{of} \\ \text{goddess} & \text{the} & \text{of} & \text{achilles} \\ \text{the} & \text{anger} & \text{achilles} & \text{son} \\ \text{anger} & \text{of} & \text{son} & \text{of} \\ \text{of} & \text{achilles} & \text{of} & \text{peleus} \end{bmatrix}; \mathbf{y} = \begin{bmatrix} \text{goddess} \\ \text{the} \\ \text{anger} \\ \text{of} \\ \text{achilles} \\ \text{son} \end{bmatrix}$$

CBOW Architecture

Context words one-hot encoded, in practice just an index, followed by an **embedding layer.**



Embeddings in PyTorch

PyTorch has an `Embedding(num_embeddings, embedding_dim, ...)` class

An embedding object is a matrix from which we can extract embedding vectors using an index

This is just a lookup table

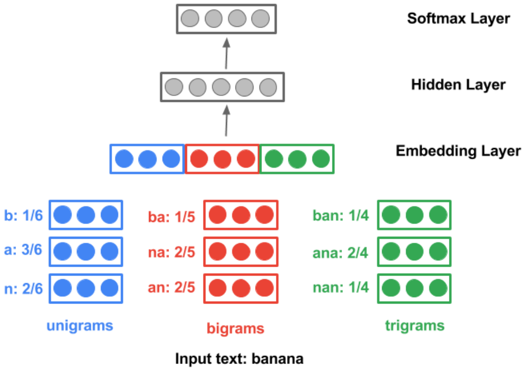
```
# Creates trainable vectors of size 64
embedding_chars = nn.Embedding(MAX_CHARS, 64)

# Extracts embeddings in rows 3 and 2,
# corresponding to two characters
embedding_chars(torch.LongTensor([3, 2]))
```

Code Example

Experiment: Embeddings with a Jupyter Notebook:
`https://github.com/pnugues/edan96/blob/main/programs/11-pytorch_embeddings.ipynb`
To create a batch, we would need to pad the character, bigram, and trigram hash codes.

Sum of Embeddings in CLD3

CLD3 computes the weighted sum (mean) of the embeddings



Embedding Bags in PyTorch

`EmbeddingBags` class creates embedding objects.

```
embedding_bag = nn.EmbeddingBag(MAX_CHARS, 64) # default mean
embedding_bag = nn.EmbeddingBag(MAX_CHARS, 64, mode='sum')
```

Given a list of embeddings (a list of rows) as input, an embedding bag returns:

1. The mean,
2. The sum, or
3. The weighted sum of the embeddings.

We specify the weights with a `per_sample_weights` parameter.
`https://pytorch.org/docs/stable/generated/torch.nn.EmbeddingBag.html`

Programming Embedding Bags in PyTorch (I)

```
embedding_bag = nn.EmbeddingBag(MAX_CHARS, 64, mode='sum')

# Computes the sum of rows 1 and 2 and rows 3 and 4
# The result is a matrix of two rows
embedding_bag(torch.tensor([[1, 2], [3, 4]]))

embedding_bag(torch.tensor([[1, 2], [3, 4]]),
           per_sample_weights=torch.tensor([[0.5, 0.5],
           [0.2, 0.8]]))
```

Programming Embedding Bags in PyTorch (II)

With bags of unequal sizes, we have to use a list of offsets

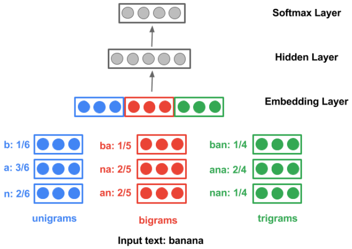
```
embedding_bag(torch.tensor([1, 2, 3, 4]),
       offsets=torch.tensor([0, 2]),
       per_sample_weights=torch.tensor([0.5, 0.5, 0.2, 0.8]))
```

Adding the embeddings

Describe a language detector: Given a string predict the language:

- *Bonjour* –> French
- Guten Tag –> German

Follow the complete compact language detector (CLD3)
`https://github.com/google/cld3`



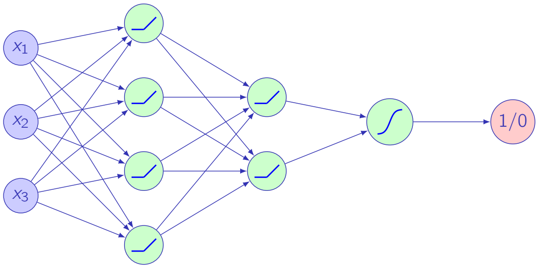
Code Example

Experiment: Classification with embedding bags Jupyter Notebook:
`https://github.com/pnugues/pnlp/blob/main/notebooks/11_07_language_detector.ipynb`

Data Loaders

- Current datasets have now terabytes of data
- Impossible to fit into memory (even Tatoeba)
- For real world applications, you will have to use or write a data loader that can create smaller, processable batches from your storage
- This involves the `Dataset` and `DataLoader` classes
- Beyond the scope of this lecture
- Read on this here: `https://pytorch.org/blog/efficient-pytorch-io-library-for-large-datasets-many-file`

Backpropagation: The Forward Pass



The forward pass:

1. Layer 1 $f^{(1)}(W^{(1)}\mathbf{x})$, where $f^{(1)}$ is the activation function.
2. For the second layer, $f^{(2)}(W^{(2)}f^{(1)}(W^{(1)}x))$,
3. Last layer (L) and output the prediction:

$$\hat{y} = f^{(L)}(W^{(L)}...f^{(2)}(W^{(2)}f^{(1)}(W^{(1)}\mathbf{x}))...).$$

4. For the figure $\hat{y} = f^{(3)}(W^{(3)}W^{(2)}W^{(1)}\mathbf{x})$, where $f^{(3)}(x)$ is the logistic function.

Naive Gradient Descent

Try to minimize the difference between the predicted and observed annotations: $Loss(y, \hat{y})$.

$$\mathbf{w}_{(k+1)} = \mathbf{w}_{(k)} - \alpha_{(k)} \nabla Loss(\mathbf{w}_{(k)}).$$

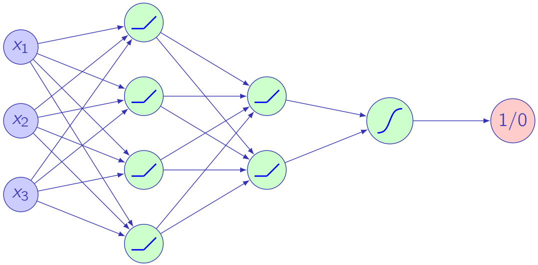
We compute the gradient:

$$\begin{aligned}
\frac{\partial Loss(\mathbf{w})}{\partial w_{ij}^{(l)}} &= \frac{\partial(-y \ln \hat{y} - (1-y)\ln(1-\hat{y}))}{\partial w_{ij}^{(l)}} \\
&= \frac{\partial(-y \ln f^{(3)}(W^{(3)}W^{(2)}W^{(1)}\mathbf{x}) - (1-y)\ln(1-f^{(3)}(W^{(3)}W^{(2)}W^{(1)}\mathbf{x})))}{\partial w_{ij}^{(l)}},
\end{aligned}$$

for all the weights $w_{ij}^{(l)}$.
Method impractical in real cases (billions of weights)

Breaking Down the Computation

We first compute the gradient with respect to the inputs.



$$
\begin{aligned}
\hat{y} &= \mathbf{a}^{(L)}, \\
&= f^{(L)}(\mathbf{z}^{(L)}), \\
&= f^{(L)}(W^{(L)}\mathbf{a}^{(L-1)})
\end{aligned}
$$

Gradient with Respect to the Input

For a given layer, we have:

$$\begin{aligned}\mathbf{z}^{(l)} &= W^{(l)}\mathbf{a}^{(l)}, \\ &= W^{(l)}f(\mathbf{z}^{(l-1)})\end{aligned}$$

We compute:

$$\frac{\partial \mathbf{z}^{(l)}}{\partial \mathbf{z}^{(l-1)}}$$

and we can show that this relation applies for any pair of adjacent layers l and $l-1$ in the network:

$$\nabla_{\mathbf{z}^{(l-1)}}\mathbf{z}^{(l)} = f^{(l-1)\prime}(\mathbf{z}^{(l-1)})^{\intercal} \odot W^{(l)}.$$

Recurrence Relation

Using the chain rule:

$$
\begin{aligned}
\nabla_{\mathbf{x}} Loss(\hat{y}, y) &= \nabla_{\mathbf{x}} Loss(f^{(L)}(W^{(L)} \ldots f^{(2)}(W^{(2)} f^{(1)}(W^{(1)}\mathbf{x}))\ldots), y),\\
&= \frac{\partial Loss(\hat{y}, y)}{\partial \mathbf{z}^{(L)}} \frac{\partial \mathbf{z}^{(L)}}{\partial \mathbf{z}^{(L-1)}} \frac{\partial \mathbf{z}^{(L-1)}}{\partial \mathbf{z}^{(L-2)}} \cdots \frac{\partial \mathbf{z}^{(2)}}{\partial \mathbf{z}^{(1)}} \frac{\partial \mathbf{z}^{(1)}}{\partial \mathbf{x}},
\end{aligned}
$$

For our network:

$$
\begin{aligned}
\nabla_{\mathbf{x}} Loss(y, \hat{y}) &= -\frac{\partial(y \ln \hat{y} + (1-y)\ln(1-\hat{y}))}{\partial \mathbf{x}},\\
&= -\frac{y-\hat{y}}{\hat{y}(1-\hat{y})}\hat{y}(1-\hat{y}) W^{(3)} W^{(2)} W^{(1)},\\
&= (\hat{y}-y) W^{(3)} W^{(2)} W^{(1)},\\
&= (f^{(3)}(W^{(3)} W^{(2)} W^{(1)}\mathbf{x}) - y) W^{(3)} W^{(2)} W^{(1)}.
\end{aligned}
$$

Gradient with Respect to the Weights

We now compute the gradient with respect to $W^{(l)}$, l being the index of any layer. From the chain rule, for the last layer, L, we have:

$$\nabla_{W^{(L)}} Loss(y, \hat{y}) = \frac{\partial Loss(y, \hat{y})}{\partial \mathbf{z}^{(L)}} \frac{\partial \mathbf{z}^{(L)}}{\partial W^{(L)}}$$

and

$$\begin{aligned} \mathbf{z}^{(L)} &= W^{(L)} f^{(L-1)}(\mathbf{z}^{(L-1)}), \\ &= W^{(L)} \mathbf{a}^{(L-1)}. \end{aligned}$$

The partial derivatives of $\mathbf{z}^{(L)}$ with respect to $W^{(L)}$ simply consist of the transpose of $\mathbf{a}^{(L-1)}$. Then, we have:

$$\frac{\partial \mathbf{z}^{(L)}}{\partial W^{(L)}} = \mathbf{a}^{(L-1)\intercal}.$$

We can show:

$$\nabla_{W^{(l)}} Loss(y, \hat{y}) = \nabla_{\mathbf{z}^{(l)}} Loss(y, \hat{y}) \mathbf{a}^{(l-1)\intercal}.$$

Code Example

Experiment: Checking the gradient with PyTorch Jupyter Notebook:
https://github.com/pnugues/edan96/blob/main/programs/backprop_mse_test.ipynb

Backward Differentiation

A generalization of backpropagation

PyTorch records all the operations in the forward pass

It then computes the graph of derivatives using the chain rule proceeding backwards

1. https://pytorch.org/blog/overview-of-pytorch-autograd-engine/
2. https://docs.pytorch.org/docs/stable/notes/autograd.html
3. https://github.com/pytorch/pytorch/blob/master/tools/autograd/derivatives.yaml

Using PyTorch's example:

$$f(x, y) = \log xy$$

We have:

$$g(x, y) = xy$$

$$\begin{aligned}
\frac{\partial f}{\partial x} &= \frac{\partial f}{\partial g}\frac{\partial g}{\partial x} = \frac{1}{xy}y = \frac{1}{x} \\
\frac{\partial f}{\partial y} &= \frac{\partial f}{\partial g}\frac{\partial g}{\partial y} = \frac{1}{xy}x = \frac{1}{y}
\end{aligned}$$

Code Example

Experiment: Checking the gradient with PyTorch Jupyter Notebook:
`https://github.com/pnugues/edan96/blob/main/programs/14-autodiff.ipynb`

Further Reading

1. For a video overview: https://www.youtube.com/playlist?list=PLZHQObOWTQDNU6R1_67000Dx_ZCJB-3pi, especially the two last lectures;
2. PyTorch https://pytorch.org/tutorials/beginner/blitz/autograd_tutorial.html
3. Functions: https://github.com/pytorch/pytorch/blob/master/tools/autograd/derivatives.yaml
4. For a description of it in Tensorflow, see https://www.tensorflow.org/guide/autodiff
5. For a description of the `tf.gradients` class: https://www.tensorflow.org/api_docs/python/tf/gradients
6. For a more elaborate description: http://www.cs.toronto.edu/~rgrosse/courses/csc421_2019/slides/lec06.pdf