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About Index

The Annotated GPT-2

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- 1. Introduction
- 2. Prerequisites
- 3. Language Models are Unsupervised Multitask Learners
- 4. Abstract
- 5. Model Architecture (GPT-2)
- 6. Model Specifications (GPT)
- 7. Imports
- 8. Transformer Decoder inside GPT-2
 - i. CONV1D Layer Explained
 - ii. FEEDFORWARD Layer Explained
 - iii. ATTENTION Layer Explained
 - a. Scaled Dot-Product Attention
 - b. Multi-Head Attention
- 9. GPT-2 Model Architecture in Code
 - i. Transformer Decoder Block Explained
- 10. The GPT-2 Architecture Explained
 - i. Language Modeling or Classification
- 11. Sample text generation using Hugging Face Pretrained Weights
- 12. Extras
- 13. Credits
- 14 Feedback

Introduction

Welcome to "The Annotated GPT-2".

One of the most brilliant and well-explained articles I have ever read is The Annotated Transformer. It introduced **Attention** like no other post ever written. The simple idea was to present an "annotated" version of the paper Attention is all you need along with code.

Something I have come to realize with my little experience in Machine Learning, when you write things in code, the implementation and the secrets become clearer. It is not magic anymore.

There is nothing magic about magic. The magician merely understands something simple which doesn't appear to be simple or natural to the untrained audience. Once you learn how to hold a card while making your hand look empty, you only need practice before you, too, can "do magic."

- Jeffrey Friedl in the book Mastering Regular Expressions

The GPT-2 might seem like magic at first with all it's glitter and beauty too, but hopefully I would have uncovered that magic for you and revealed all the tricks by the time you finish reading this post. That is my goal. To make it as simple as possible for the keen to understand how the GPT-2 model works underneath.

Note: Pretty much the entirety of the code has been copied, inspired and referenced from Hugging Face's implementation of the GPT-2, keeping merely the essentials for simplicity. If you want to train the GPT-2 model on parallel GPUs, save checkpoints while fine-tuning, run inference tasks on multiple CPUs and much more, I would recommend using the Hugging Face API. A simple tutorial on how to do so was recently released by Hugging Face and can be found here.

In this post, I am not trying to reinvent the wheel, but merely bringing together a list of prexisting excellent resources to make it easier for the reader to grasp GPT-2. I leave it up to the reader to further build upon these foundations in any area they choose.

You can't build a great building on a weak foundation. You must have a solid foundation if you're going to have a strong superstructure.

- Gordon B. Hinckley

Prerequisites

This post assumes that the reader has a solid understanding of Attention and Transformers. The GPT-2 utilizes a 12-layer Decoder Only Transformer architecture. If you want a refresher or understand Attention and Transformers, here is an excellent list of resources to aid your understanding regarding:

- 1. The illustrated Transformer by Jay Alammar
- 2. The Annotated Transformer by Harvard NLP
- 3. Introduction to the Transformer by Rachel Thomas and Jeremy Howard

If you're just beginning your journey into NLP or you're an expert, I would definitely recommend the fast.ai NLP course taught by Rachel Thomas and Jeremy Howard. The course starts with the basics including Sentiment Classification using Naive Bayes and Logistic Regression, moves on to RNNs and also talks about Transfer Learning, ULMFiT, Seq2Seq translation and Transformers amongst other things. It is an excellent resource put together by the fast.ai team free of cost.

Another amazing resource on GPT-2 itself, is The Illustrated GPT-2 by Jay Alammar. This post starts with a basic introduction to Language Models and explains the GPT-2 model step-by-step in a very easy to understand manner. I would highly recommend the reader to give this post a read.

The Annotated Transformer by Harvard NLP implements the complete Transformer architecture using PyTorch and is great way to understand Attention in depth.

Let's then build upon these excellent existing resources and implement GPT-2 in code.

Language Models are Unsupervised Multitask Learners

Abstract

Natural language processing tasks, such as question answering, machine translation, reading comprehension, and summarization, are typically approached with supervised learning on taskspecific datasets. We demonstrate that language models begin to learn these tasks without any explicit supervision when trained on a new dataset of millions of webpages called WebText. Our largest model, GPT-2, is a 1.5B parameter Transformer that achieves state of the art results on 7 out of 8 tested language modeling datasets in a zero-shot setting but still underfits WebText. Samples from the model reflect these improvements and contain coherent paragraphs of text. These findings suggest a promising path towards building language processing systems which learn to perform tasks from their naturally occurring demonstrations.

A Zero-shot setting is one where you do not finetune the language model and directly run inference on the target dataset. For example, pretrain a LM on WebText and directly try and predict the next words of Amazon Movie reviews dataset.

Model Architecture (GPT-2)

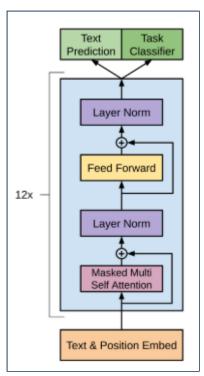
We use a Transformer (Vaswani et al., 2017) based architecture for our LMs. The model largely follows the details of the OpenAl GPT model (Radford et al., 2018) with a few modifications. Layer normalization (Ba et al., 2016) was moved to the input of each sub-block, similar to a preactivation residual network (He et al., 2016) and an additional layer normalization was added

after the final self-attention block. We scale the weights of residual layers at initialization by a factor of 1/VN where N is the number of residual layers. The vocabulary is expanded to 50,257 words. We also increase the context size from 512 to 1024 tokens and a larger batchsize of 512 is used.

This is the entirety of model explanation inside the GPT-2 research paper. This warrants a need for us to look at the architecture inside the GPT model.

Model Specifications (GPT)

Our model largely follows the original transformer work. We trained a 12-layer decoder-only transformer with masked self-attention heads (768 dimensional states and 12 attention heads). For the position-wise feed-forward networks, we used 3072 dimensional inner states. We used the Adam optimization scheme with a max learning rate of 2.5e-4. The learning rate was increased linearly from zero over the first 2000 updates and annealed to 0 using a cosine schedule. We train for 100 epochs on minibatches of 64 randomly sampled, contiguous sequences of 512 tokens. Since layernorm is used extensively throughout the model, a simple weight initialization of N(0, 0.02) was sufficient. We used a bytepair encoding (BPE) vocabulary with 40,000 merges and residual, embedding, and attention dropouts with a rate of 0.1 for regularization. We also employed a modified version of L2 regularization proposed in, with w = 0.01 on all non bias or gain weights. For the activation function, we used the Gaussian Error Linear Unit (GELU).



GPT Architecture

As can be seen from the GPT Architecture, to implement it, we will first need to implement Masked Self Attention and Feed Forward layer.

Imports

```
import torch
import copy
import torch.nn as nn
import torch.nn.functional as F
from torch.nn.modules import ModuleList
from torch.nn.modules.normalization import LayerNorm
import numpy as np
import os
from tqdm import tqdm_notebook, trange
import logging
logging.basicConfig(level = logging.INFO)
logger = logging.getLogger()
```

Transformer Decoder inside GPT-2

To re-use the terminology used to describe the Transformer, the attention is a function of a query (Q) and set of key (K) and value (V) pairs. To handle longer sequences, we modify the multi-head self-attention of the Transformer to reduce memory usage by limiting the dot products between Q and K in:

$$\operatorname{Attention}(Q,K,V) = \operatorname{softmax}(\frac{QK^T}{\sqrt{d_k}})V$$

Attention as a combination of query, key & value

```
class Conv1D(nn.Module):
    def __init__(self, nx, nf):
        super().__init__()
        self.nf = nf
        w = torch.empty(nx, nf)
        nn.init.normal_(w, std=0.02)
        self.weight = nn.Parameter(w)
        self.bias = nn.Parameter(torch.zeros(nf))

def forward(self, x):
```

```
size_out = x.size()[:-1] + (self.nf,)
x = torch.addmm(self.bias, x.view(-1, x.size(-1)), self.weight)
x = x.view(*size_out)
return x
```

CONV1D Layer Explained

The CONV1D layer can be thought of as a LINEAR layer itself. Essentially, it is casting an initial tensor x (having the final dimension of x.size(-1)) being passed to it to have a final dimension of size self.nf.

Here's an example output of the same:

As can be seen in the example above, the final dimension of tensor returned by CONV1D is 3 times the initial size. We do this to be able to cast the input to query, key and value matrices.

It is possible then to retrieve the query, key and value matrices like so:

```
query, key, value = x.split(d_model, dim=-1)
query.shape, key.shape, value.shape
>> (torch.Size([1, 4, 768]), torch.Size([1, 4, 768]), torch.Size([1, 4, 768]))
```

Another way to cast the input to Q, K and V matrices would have to been to have separate Wq, Wk and Wv matrices. I have explained this under the **EXTRA** section of this post at the bottom. I find this other approach more intuitive and relatable, but we use the CONVID layer in this post, because we reuse the CONVID pretrained weights from Hugging Face.

FEEDFORWARD Layer Explained

```
class FeedForward(nn.Module):
    def __init__(self, dropout, d_model=768, nx=768*4):
        super().__init__()
        self.c_fc = Conv1D(d_model, nx)
        self.c_proj = Conv1D(nx, d_model)
        self.act = F.gelu
        self.dropout = nn.Dropout(dropout)

def forward(self, x):
    return self.dropout(self.c_proj(self.act(self.c_fc(x))))
```

Something, that's just so well explained in Jay Alammar's post - also referenced above, is how the inputs are passed through ATTENTION layer first and then on to FEEDFORWARD layer. The Feedforward network, is a normal neural network that accepts the outputs from the ATTENTION layer (768), casts them to nx (768*4) dimension, adds an activation function self.act (GELU), casts them back to d_model (768) and adds dropout (0.1).

This is also mentioned in the **GPT** research paper referenced below.

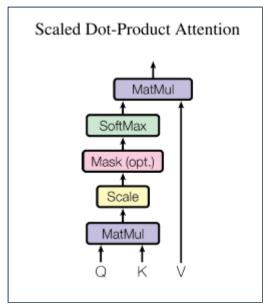
For the position-wise feed-forward networks, we used 3072 dimensional inner states

ATTENTION Layer Explained

The below extract is from the paper Attention is all you need.

Scaled Dot-Product Attention

We call our particular attention "Scaled Dot-Product Attention". The input consists of queries and keys of dimension dk, and values of dimension dv. We compute the dot products of the query with all keys, divide each by \sqrt{dk} , and apply a softmax function to obtain the weights on the values.



Attention Dot Product

In practice, we compute the attention function on a set of queries simultaneously, packed together into a matrix Q. The keys and values are also packed together into matrices K and V. We compute the matrix of outputs as:

$$\operatorname{Attention}(Q,K,V) = \operatorname{softmax}(\frac{QK^T}{\sqrt{d_k}})V$$

Output matrix as a combination of Q, K and V

The two most commonly used attention functions are additive attention, and dot-product (multiplicative) attention. Dot-product attention is identical to our algorithm, except for the scaling factor of 1/vdk. Additive attention computes the compatibility function using a feed-forward network with a single hidden layer. While the two are similar in theoretical complexity, dot-product attention is much faster and more space-efficient in practice, since it can be implemented using highly optimized matrix multiplication code. While for small values of dk the two mechanisms perform similarly, additive attention outperforms dot product attention without scaling for larger values of dk. We suspect that for large values of dk, the dot products grow large in magnitude, pushing the softmax function into regions where it has extremely small gradients. To counteract this effect, we scale the dot products by 1/vdk.

To implement the The Attention layer in code, we first utilize the $\boxed{\text{conv1D}}$ layer and $\boxed{\text{get the } q}$, $\boxed{\text{k}}$ and $\boxed{\text{v}}$ matrices as explained before.

Once we have the q, k and v matrices, we can perform attention using the function $_attn$. This function replicates the formula mentioned above inside $_attn$.

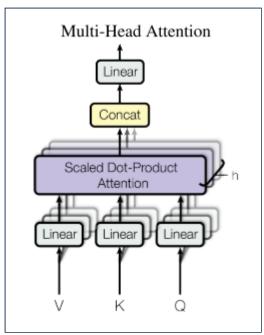
```
class Attention(nn.Module):
    def __init__(self, d_model=768, n_head=12, n_ctx=1024, d_head=64, bias=True,
        super(). init ()
        self.n head = n head
        self.d model = d model
        self.c attn = Conv1D(d model, d model*3)
        self.scale = scale
        self.softmax = nn.Softmax(dim=-1)
        self.register buffer("bias", torch.tril(torch.ones(n ctx, n ctx)).view(1,
        self.dropout = nn.Dropout(0.1)
        self.c proj = Conv1D(d model, d model)
    def split heads(self, x):
        "return shape [`batch`, `head`, `sequence`, `features`]"
        new_shape = x.size()[:-1] + (self.n_head, x.size(-1)//self.n_head)
        x = x.view(*new shape)
        return x.permute(0, 2, 1, 3)
    def attn(self, q, k, v, attn mask=None):
        scores = torch.matmul(q, k.transpose(-2, -1))
        if self.scale: scores = scores/math.sqrt(v.size(-1))
        nd, ns = scores.size(-2), scores.size(-1)
        if attn mask is not None: scores = scores + attn mask
        scores = self.softmax(scores)
        scores = self.dropout(scores)
        outputs = torch.matmul(scores, v)
        return outputs
    def merge heads(self, x):
                  = x.permute(0, 2, 1, 3).contiguous()
        new shape = x.size()[:-2] + (x.size(-2)*x.size(-1),)
        return x.view(*new shape)
    def forward(self, x):
                = self.c_attn(x) #new `x` shape - `[1,3,2304]`
        q, k, v = x.split(self.d model, dim=2)
        q, k, v = self.split heads(q), self.split heads(k), self.split heads(v)
                = self. attn(q, k, v)
        out
                = self.merge heads(out)
        out
                = self.c_proj(out)
        out
        return out
```

Another way to implement Attention is explained in the Extras section at the bottom of this blog. I find it to be more intuitive and easy to compare with the research paper. It utilizes Linear layers instead of CONVID to cast inputs to Q, K and V matrices. The reason why we haven't used it is because we use the pretrained weights for CONVID layer from Hugging Face.

Multi-Head Attention

The below extract is from the paper Attention is all you need.

Instead of performing a single attention function with dmodel-dimensional keys, values and queries, we found it beneficial to linearly project the queries, keys and values h times with different, learned linear projections to dk, dk and dv dimensions, respectively. On each of these projected versions of queries, keys and values we then perform the attention function in parallel, yielding dv-dimensional output values. These are **concatenated** and once again projected, resulting in the final values, as depicted in Figure below.



Multi Head Attention

Multi-head attention allows the model to jointly attend to information from different representation subspaces at different positions. With a single attention head, averaging inhibits this.

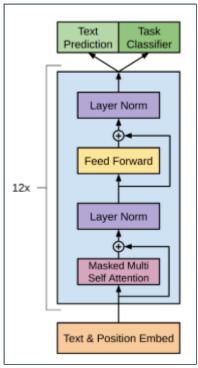
$$\begin{split} \text{MultiHead}(Q, K, V) &= \text{Concat}(\text{head}_1, ..., \text{head}_{\text{h}}) W^O \\ \text{where head}_{\text{i}} &= \text{Attention}(QW_i^Q, KW_i^K, VW_i^V) \end{split}$$

Multi Head Attention as an equation

In this work we employ h = 8 parallel attention layers, or heads. For each of these we use dk = dv = dmodel/h = 64. Due to the reduced dimension of each head, the total computational cost is similar to that of single-head attention with full dimensionality.

Not to be confused by this, in essence all that's being done is to add another dimension to the \mathbb{Q} , \mathbb{K} and \mathbb{V} matrices. That is, if the matrices were before of size [1, 4, 768] which represents $[bs, seq_len, d_model]$, these matrices are projected to dimension [1, 12, 4, 64] which represents $[bs, n_head, seq_len, d_model//n_head]$. GPT-2 utizes 12 parallel heads. We split the \mathbb{Q} , \mathbb{K} , \mathbb{V} matrices inside $[split_heads]$ function. Finally, once we get an output from applying parallel attentions we concatenate it inside $[bs, seq_len, d_model]$.

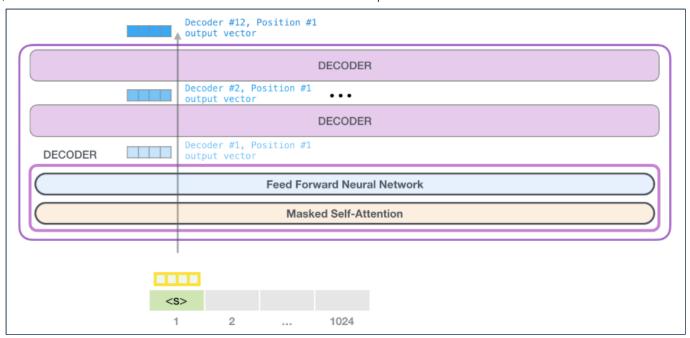
GPT-2 Model Architecture in Code



GPT Architecture

So far, we have implemented Multi Head Attention and FeedForward layers. The two layers form the building blocks of the Transformer Decoder block, shown in the picture above. The GPT-2 consists of 12 of these Transformer Blocks.

This has been shown in Jay Alammar's post like so:



GPT Architecture consisting of 12 Decoder Blocks

Transformer Decoder Block Explained

The Transformer Block consists of Attention and FeedForward Layers. As referenced from the GPT-2 Architecture Model Specification,

Layer normalization (Ba et al., 2016) was moved to the input of each sub-block Here are the sub-blocks are Attention and FeedForward.

Thus, inside a Transformer Decoder Block, essentially we first pass the inputs to a LayerNorm followed by the first sub-block Attention. Next, we pass the outputs of this sub-block to LayerNorm again and finally to FeedForward layer.

The GPT-2 Architecture Explained

As referenced from the GPT paper,

We trained a 12-layer decoder-only transformer with masked self-attention heads (768 dimensional states and 12 attention heads).

Thus, the complete GPT-2 architecture is the TransformerBlock copied over 12 times.

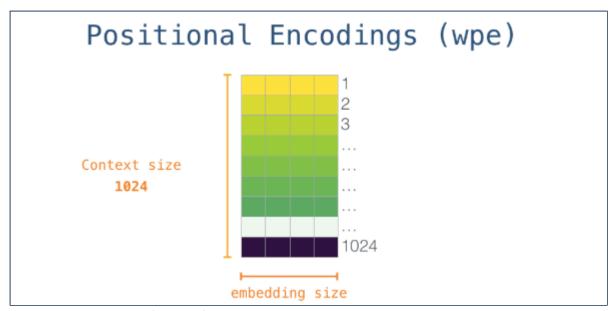
```
def _get_clones(module, n):
    return ModuleList([copy.deepcopy(module) for i in range(n)])
class GPT2(nn.Module):
    def init (self, nlayers=12, n ctx=1024, d model=768, vcb sz=50257):
        super(GPT2, self). init ()
        self.nlayers = nlayers
        block
                     = TransformerBlock(d model=768, n head=12, dropout=0.1)
        self.h
                     = get clones(block, 12)
        self.wte
                    = nn.Embedding(vcb_sz, d_model)
        self.wpe = nn.Embedding(n_ctx, d_model)
self.drop = nn.Dropout(0.1)
        self.ln f = LayerNorm(d model)
        self.out
                    = nn.Linear(d_model, vcb_sz, bias=False)
        self.loss fn = nn.CrossEntropyLoss()
        self.init_weights()
    def init_weights(self):
        self.out.weight = self.wte.weight
        self.apply(self._init_weights)
    def init weights(self, module):
        if isinstance(module, (nn.Linear, nn.Embedding, Conv1D)):
            module.weight.data.normal (mean=0.0, std=0.02)
            if isinstance(module, (nn.Linear, Conv1D)) and module.bias is not Nor
                module.bias.data.zero ()
        elif isinstance(module, nn.LayerNorm):
            module.bias.data.zero ()
            module.weight.data.fill_(1.0)
    def forward(self, src, labels=None, pos_ids=None):
        if pos_ids is None: pos_ids = torch.arange(0, src.size(-1)).unsqueeze(0)
        inp = self.drop((self.wte(src)+self.wpe(pos_ids)))
```

```
for i in range(self.nlayers): inp = self.h[i](inp)
inp = self.ln_f(inp)
logits = self.out(inp)
outputs = (logits,) + (inp,)

if labels is not None:
    shift_logits = logits[..., :-1, :].contiguous()
    shift_labels = labels[..., 1:].contiguous()
    loss = self.loss_fn(shift_logits.view(-1, shift_logits.size(-1)), shi
    outputs = (loss,) + outputs
    return outputs
return logits
```

Something I have not mentioned yet is Positional Encoding and Token Embeddings. Since, we cannot pass words such as "hey" or "hello" directly to the model, we first Tokenize our inputs. Next, we use Embeddings to represent the tokens as numbers. This post by Jay Alammar again explains Embeddings very well.

Also, since unlike the RNNs where the input words are passed sequentially, Transformers take input matrices in parallel thus losing the sense of position for the words being input. To make up for the loss, before handling the Token Embeddings to the model, we add Positional Encoding - a signal that indicates the order of the words in the sequence. Since, as mentioned before, the context size of GPT-2 is 1024, the positional encodings are of dimensions [1024, 768].



Positional Encodings referenced from [The Illustrated GPT-2](http://jalammar.github.io/illustrated-gpt2/)

Thus, the inputs to the GPT-2 architecture is the sum of Token Embeddings and Positional Encodings passed through a Dropout, to add regularization. Once, we have the input matrix,

we pass this through each of the 12 Layers of the GPT-2 architecure, where each layer is a Transformer Decoder Block that consists of two sublayers - Attention and FeedForward Network.

Language Modeling or Classification

When using GPT-2 as a language model, we pass the inputs to a final LayerNorm and through a Linear layer with a final dimension of size [768, vocab_sz] (50257) and get an output of size [1, 4, 50257]. This output represents the next word logits and we can very easily now pass this through a Softmax layer and take argmax to get the positional of the word inside the vocabulary with the highest probability.

For classification task, we can pass the outputs received from the GPT-2 architecture through a Linear layer with a dimension of size [768, n] to get probabilities for each category (where n represents number of categories), pass it through a softmax, get the highest predicted category and use CrossEntropyLoss to train the architecture to do classification.

And that's really all the magic behind GPT-2. It's a Decoder only Transformer Based architecture that takes inputs parallely with Positional Encodings unlike RNNs, passes them through each of it's 12 Transformer Decoder layers (which consist of Multi head Attention and FeedForward Network) to return the final output.

Let's see this model in action in a language model task.

Sample text generation using Hugging Face Pretrained Weights

First, let's initialize the model with the Pretrained Weights already provided by Hugging Face.

```
model = GPT2()
# load pretrained_weights from hugging face
# download file https://s3.amazonaws.com/models.huggingface.co/bert/gpt2-pytorch_
model_dict = model.state_dict() #currently with random initialization
state_dict = torch.load("./gpt2-pytorch_model.bin") #pretrained weights

old_keys = []
new_keys = []
for key in state_dict.keys():
    if "mlp" in key: #The hugging face state dict references the feedforward netw
    new_key = key.replace("mlp", "feedforward")
```

```
new_keys.append(new_key)
    old_keys.append(key)

for old_key, new_key in zip(old_keys, new_keys):
    state_dict[new_key]=state_dict.pop(old_key)

pretrained_dict = {k: v for k, v in state_dict.items() if k in model_dict}

model_dict.update(pretrained_dict)
model.load_state_dict(model_dict)
model.eval() #model in inference mode as it's now initialized with pretrained wei
```

Let's now generate text. We will utilize Hugging Face's pretrained Tokenizer to convert words to input embeddings.

```
from transformers import GPT2Tokenizer
tokenizer = GPT2Tokenizer.from pretrained("gpt2")
context
          = torch.tensor([tokenizer.encode("The planet earth")])
def generate(context, ntok=20):
    for _ in range(ntok):
        out = model(context)
        logits = out[:, -1, :]
        indices_to_remove = logits < torch.topk(logits, 10)[0][..., -1, None]</pre>
        logits[indices_to_remove] = np.NINF
        next tok = torch.multinomial(F.softmax(logits, dim=-1), num samples=1).sd
        context = torch.cat([context, next_tok.unsqueeze(-1)], dim=-1)
    return context
out = generate(context, ntok=20)
tokenizer.decode(out[0])
>> 'The planet earth is the source of all of all the light," says the study that
```

Extras

Another way to implement Attention as shown in the NLP Course by fast.ai referenced from here, that I find to be more intuitive is as below:

```
class Attention FASTAI(nn.Module):
    def __init__(self, d_model=768, n_head=12, d_head=64, n_ctx=1024, bias=True,
        super(). init ()
        self.n head = n head
        self.d head
                     = d head
        self.softmax = nn.Softmax(dim=-1)
        self.scale
                     = scale
        self.atn drop = nn.Dropout(0.1)
        self.wq, self.wk, self.wv = [nn.Linear(d model, n head*d head,
                                               bias=bias) for o in range(3)]
    def split_heads(self, x, layer, bs):
        x = layer(x)
        return x.view(bs, x.size(1), self.n_head, self.d_head).permute(0,2,1,3)
    def attn(self, q, k, v, attn mask=None):
        scores = torch.matmul(q, k.transpose(-2, -1))
        if self.scale: scores = scores/math.sqrt(v.size(-1))
        if attn mask is not None:
            scores = scores.float().masked fill(attn mask, -float('inf')).type as
        attn prob = self.atn drop(self.softmax(scores))
        attn vec = attn prob @ v
        return attn vec
    def merge_heads(self, x, bs, seq_len):
                  = x.permute(0, 2, 1, 3).contiguous()
        return x.view(bs, seq_len, -1)
    def forward(self, q, k, v, mask=None):
        bs, seq len = q.size(0), q.size(1)
        wq, wk, wv = map(lambda o:self.split heads(*o, bs),
                        zip((q,k,v), (self.wq, self.wk, self.wv)))
                   = self. attn(wq, wk, wv)
        attn vec
                    = self.merge heads(attn vec, bs, seq len)
        attn vec
        return attn vec
```

The key difference between the implementation above and the one we have used is that this implementation does not use CONV1D. Instead, we first pass the input x to self.wq, self.wk and self.wv Linear Layers to get wq, wk and wv matrices and then perform attention as before.

Credits

I just want to take the time to thank Rachel Thomas and Jeremy Howard for a great NLP course and the fast.ai course in general, which has helped me bolster my understanding of RNNs, GRUs, AWD-LSTM and Transformers. Also, a special thanks to Hugging Face for creating an open source NLP library and providing a number of Pretrained Models to use. As mentioned the code in this blog post comes directly from the Hugging Face library. And, Jay Alammar for the excellent work that he has been doing to Visualise machine learning concepts. The Illustrated GPT-2 is one of the most comprehensive blog posts on GPT-2. Finally, to Harvard NLP, for The Annotated Transformer, a beautiful and easy to follow implementation of Transformers in PyTorch.

Feedback

Comments or feedback? Please tweet me at @amaarora

Jeremy Howard



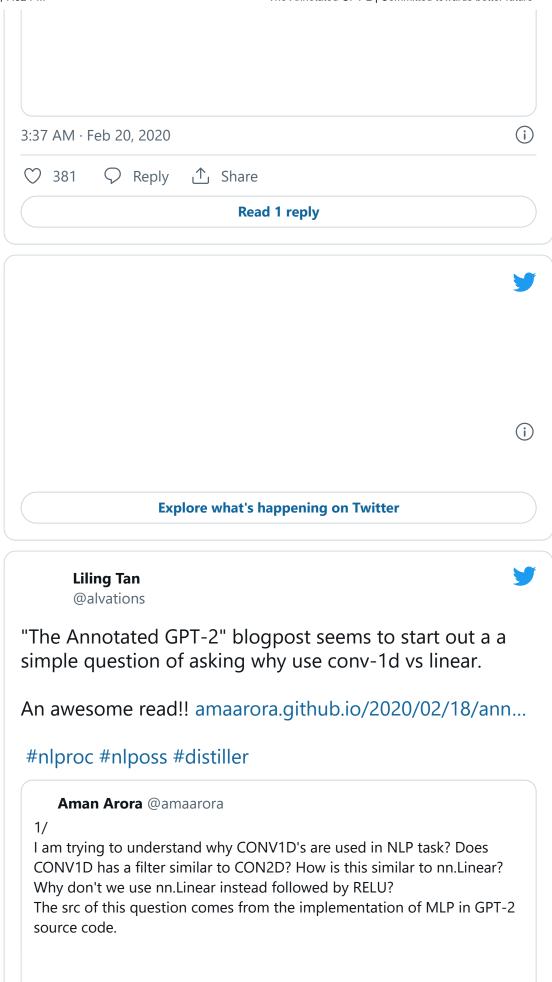
This is a really wonderful resource, and draws together many very nice pieces of work.

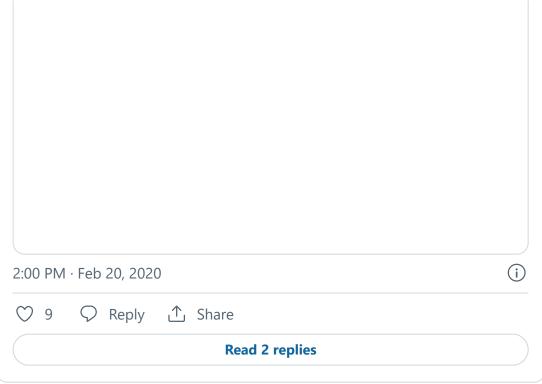
Aman Arora @amaarora

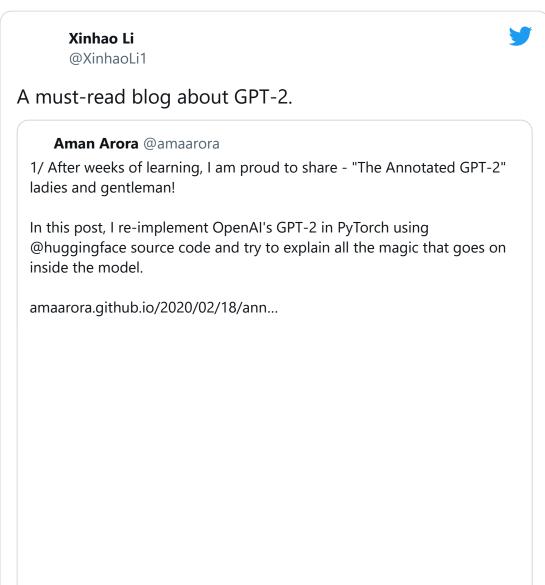
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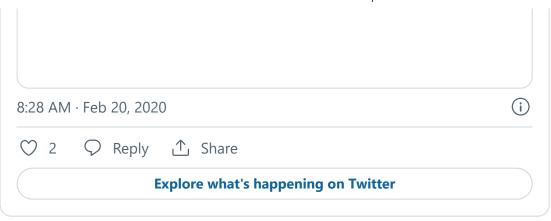
In this post, I re-implement OpenAI's GPT-2 in PyTorch using @huggingface source code and try to explain all the magic that goes on inside the model.

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Sanyam Bhutani



@bhutanisanyam1

One of the best NLP Blogposts I've read: A definitive and complete writeup.

This is a blog, I wish I had when I was tinkering with the GPT-2.

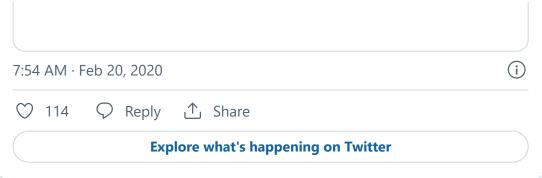
Must read for everyone:

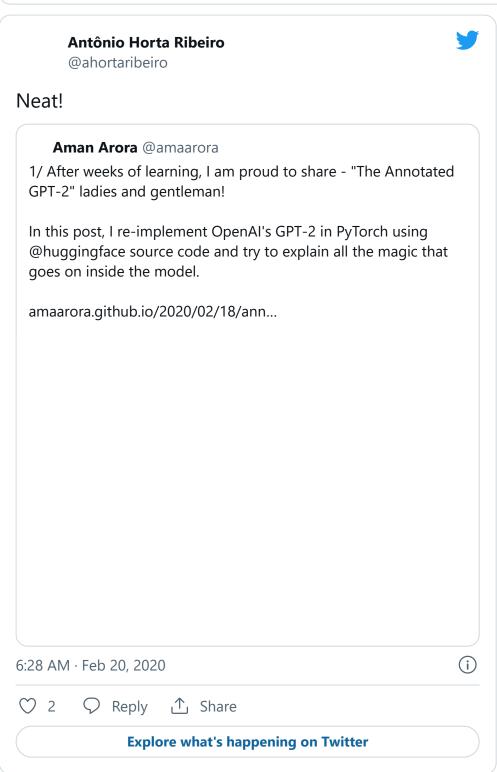
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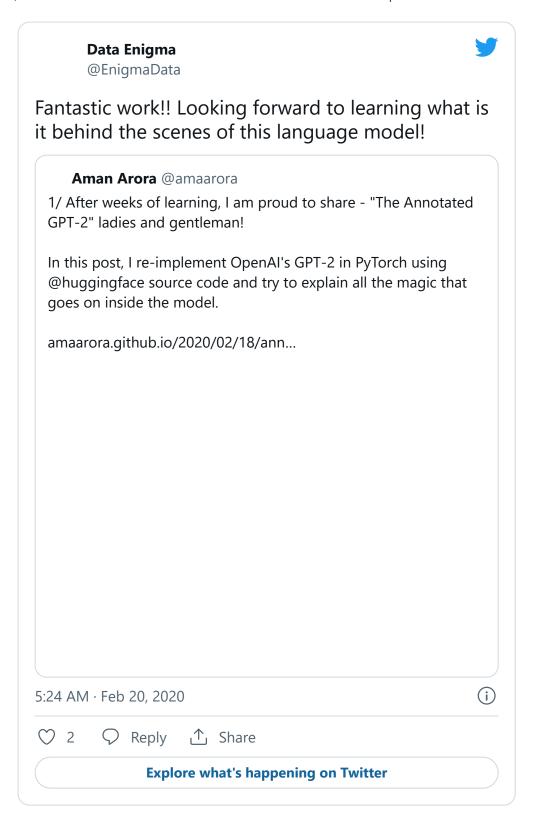
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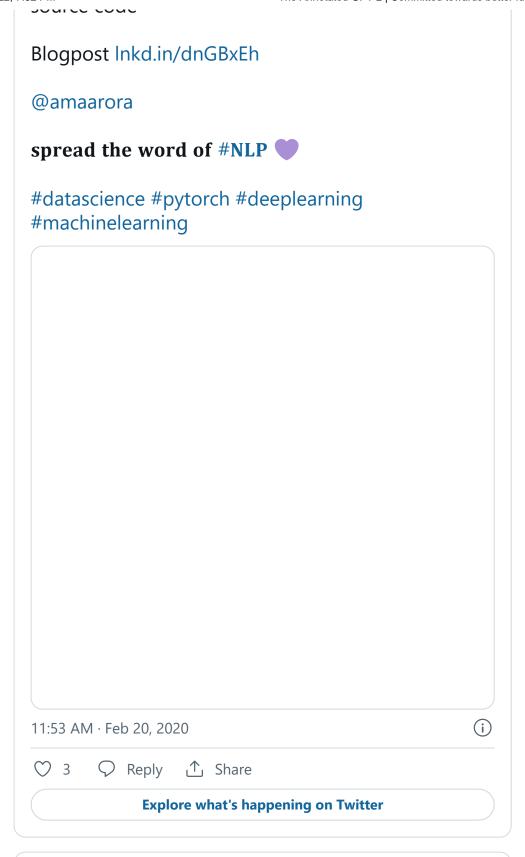








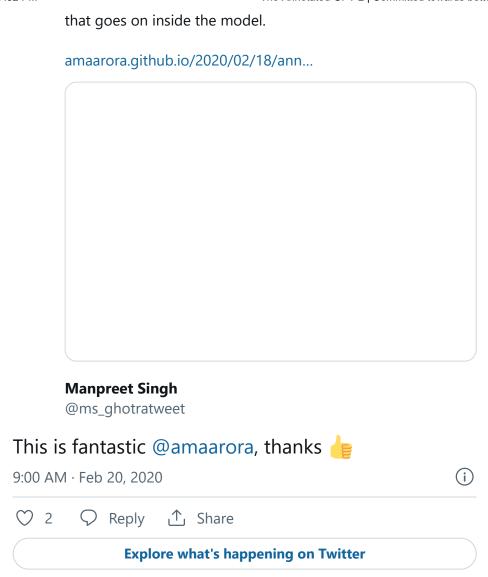
The Annotated GPT-2 - Understand how the GPT-2 model works underneath with explanations and source code



Aman Arora @amaarora · Feb 20, 2020

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This is a place where I write freely and try to uncomplicate the complicated for myself and everyone else through Python code.