Building GPT from scratch

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Credits to Andrej Kaparthy the GOAT for his amazing teaching!

Mini-shakespeare GPT

Hyperparameters

```
batch size = 32
block size
max iters
learning rate = 1e-3
n embd
n head = 2
```

Less good version

```
block_size = 8
max_iters = 5000
n_embd = 32

0.042369 M parameters
train loss 2.0616, val loss 2.1201
```

for arknois; of sund havinngbets.
I tontwers op-freatim inwat thee y matttheris's.

Rove have, take to word hof in me mea tir: Dull bethwit—the di!

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Thre Sink, heard so me'et tleit onotlous viers to, will doretese
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loughtry thee hive,
sweable
That hand nearth at in sild anved
I the comerce thess.
by will, pawt easisters, sake notos lake.

Better version

```
block_size = 16
max_iters = 13000
n_embd = 64

0.158913 M parameters
train loss 1.7365, val loss 1.8890
```

LAUNTIO:

This ghe altreaging donen fair lath, 'lls sore have and; Our know mine.

Firss? My have to lieves of this dO reath, for Counsameajing.

HESS ISABERBET:

my if were most my most of to sian,
The not all poble you with my cefor

The not all noble you, with my cefordoness, when fair, Leasiding, now, bey dentaae my than but my thou-bearn. DUCK:

No were sume me, you kners, 'lieved dear, ere of you day hearly mis $\mbox{On these my with told seerk.}$

Give is faireful didy foold belied; and You oher: reary ow any le

- Learnt shakespeare structure (NAME: speech)!
- ✓ More recognisable words!
- Starting new lines with capital letters!

Overview

Getting training data Slide 00 **Building attention head** Slide 00 **Building transformer block** Slide 00 Add section title Slide 00 Add section title Slide 00 Add section title Slide 00

Confidential Confi

1: Get training data

Raw data: We get 2 huge walls of encoded characters (integers), one set for training, one set for validation

```
# read and inspect
with open('input.txt', 'r', encoding='utf-8') as f:
   text = f.read()
# here are all the unique characters that occur in this text
chars = sorted(list(set(text)))
vocab_size = len(chars)
# create a mapping from characters to integers
stoi = { ch:i for i,ch in enumerate(chars) }
itos = { i:ch for i,ch in enumerate(chars) }
encode = lambda s: [stoi[c] for c in s] # encoder: take a string, output a list of integers
decode = lambda l: ''.join([itos[i] for i in l]) # decoder: take a list of integers, output a string
# encode data
data = torch.tensor(encode(text), dtype=torch.long)
                                                                  data.shape -> tensor([1115394])
# split data into train and validation
n = int(0.9 * len(data))
                                                                  encoded -> tensor([18, 47, 56, 57, 58,
train data = data[:n]
val_data = data[n:]
                                                                  14, 43, 44, 53, 56, 43)]
```

Confidential

Get training data

Training dataset: We get xb (inputs) and yb (targets). xb and yb each contain batches, each batch has block_size characters.

```
# data loading
def get_batch(split):
    # generate small batch of inputs x and targets y
    data = train_data if split == 'train' else val_data
    ix = torch.randint(len(data) - block_size, (batch_size,))
    x = torch.stack([data[i:i+block_size] for i in ix])
    y = torch.stack([data[i+1:i+1+block_size] for i in ix])
    x, y = x.to(device), y.to(device)
    return x, y
xb, yb = get_batch('train')
```

Each batch can make block_size examples. What we want to simulate through attention:

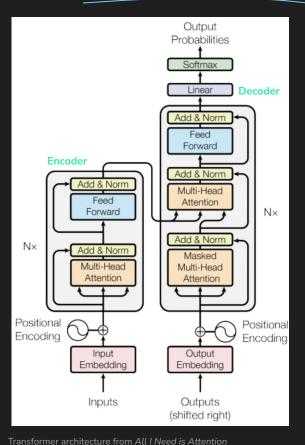
```
for b in range(batch_size): # batch dim
  for t in range(block_size): # time dim
    context = xb[b, :t+1]
    target = yb[b, t]
    print(f"when input is {context.tolist()}
    target: {target}")
```

What's happening?

- ix: randomly index into our wall of encoded characters to form random batches with *block_size* characters
- With a batch of X numbers, we can form X training examples

```
xb[:4, :] inputs:
           torch.Size([32, 16])
           tensor([[21, 27, 24, 13, 26, 33, 31, 10, 0, 32, 59, 57, 46, 6, 1, 58],
                   [53, 59, 57, 1, 51, 43, 52, 0, 13, 56, 43, 1, 39, 58, 1, 58],
                   [50, 6, 1, 57, 47, 56, 8, 1, 18, 39, 56, 43, 1, 63, 53, 59].
                   [58, 46, 1, 57, 53, 6, 1, 46, 53, 50, 63, 1, 57, 47, 56, 11]])
yb[:4, :] targets
           torch.Size([32, 16])
           tensor([[27, 24, 13, 26, 33, 31, 10, 0, 32, 59, 57, 46, 6, 1, 58, 59],
                   [59, 57, 1, 51, 43, 52, 0, 13, 56, 43, 1, 39, 58, 1, 58, 46],
                   [6, 1, 57, 47, 56, 8, 1, 18, 39, 56, 43, 1, 63, 53, 59, 1],
                   [46, 1, 57, 53, 6, 1, 46, 53, 50, 63, 1, 57, 47, 56, 11, 1]])
           when input is [21] target: 27
           when input is [21, 27] target: 24
           when input is [21, 27, 24] target: 13
            when input is [21, 27, 24, 13] target: 26
           when input is [21, 27, 24, 13, 26] target: 33
           when input is [21, 27, 24, 13, 26, 33] target: 31
            when input is [21, 27, 24, 13, 26, 33, 31] target: 10
            when input is [21, 27, 24, 13, 26, 33, 31, 10] target: 0
            when input is [21, 27, 24, 13, 26, 33, 31, 10, 0] target: 32
            when input is [21, 27, 24, 13, 26, 33, 31, 10, 0, 32] target: 59
           when input is [21, 27, 24, 13, 26, 33, 31, 10, 0, 32, 59] target: 57
           when input is [21, 27, 24, 13, 26, 33, 31, 10, 0, 32, 59, 57] target: 46
           when input is [21, 27, 24, 13, 26, 33, 31, 10, 0, 32, 59, 57, 46] target: 6
```

Our Autoregressive Model



What are autoregressive models?

- Autoregressive models like GPT are designed to generate output one token at a time, using only past context
- It uses only a decoder, which is causal (masked self-attention so tokens can only see past tokens)

Encoder	Looks at the full input sequence (bidirectional - use case: sentiment analysis)
Decoder	Looks only at past tokens (causal, autoregressive: use case: language modelling)

What is in a decoder?

- Many blocks which consist of:
- 1) Attention layer:
 - Allows tokens to 'look' at one another and gain information from context
 - Linear combination of input vectors (focus on rships btw tokens)
- 2) Feedforward:
 - Processes each token independently
 - Non-linear transformations to individual token

transformer architecture from Att i Need is Attention

Building an attention head

Simplified version: Within 1 example, we want each token to **get information from the previous tokens** to make a prediction on the next one. One simple way is to multiply with the **average of past tokens**.

Code

```
B,T,C = 4,8,2 # batch, time, channels
x = torch.randn(B,T,C)

# v1: using matrix multiply for a weighted aggregation
wei = torch.tril(torch.ones(T, T))
wei = wei / wei.sum(1, keepdim=True)
xbow1 = wei @ x # (B, T, T) @ (B, T, C) ----> (B, T, C)

# v2: use Softmax
tril = torch.tril(torch.ones(T, T))
wei2 = torch.zeros((T,T))
wei2 = wei2.masked_fill(tril == 0, float('-inf'))
wei2 = F.softmax(wei2, dim=-1)
xbow2 = wei2 @ x

wei, wei2
```

What's happening

wei = affinities, tell us how much each token from the past contributes to our average

• Masked with lower triangle bc future tokens don't contribute

Now we see that wei is all uniform, but we don't actually want it to be uniform because some tokens will find others more interesting, and we want it to be data dependent. Eg. vowel interested in consonants in the past.

```
wei, wei2
[1.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000], the store
[0.5000, 0.5000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000], the store
[0.3333, 0.3333, 0.3333, 0.0000, 0.0000, 0.0000, 0.0000], 0.0000, 0.2500, 0.2500, 0.2500, 0.0000, 0.0000, 0.0000, 0.0000], 1 the store
[0.2500, 0.2500, 0.2500, 0.2500, 0.0000, 0.0000, 0.0000], 0.0000, 0.0000], 1 the store
[0.1667, 0.1667, 0.1667, 0.1667, 0.1667, 0.0000, 0.0000], 1 the store
[0.1429, 0.1429, 0.1429, 0.1429, 0.1429, 0.0000], 1 the store
[0.1250, 0.1250, 0.1250, 0.1250, 0.1250, 0.1250, 0.1250]] fruit fresh fresh fresh fruit
```

Building an attention head

Proper version: Within 1 example, we want each token to **get information from the previous tokens** to make a prediction on the next one. Use **keys, queries** and **values**

Code

```
B,T,n \text{ embd} = 4,8,32
x = torch.randn(B,T,n\_embd) # x (B, T, n\_embd)
# v3: self-attention (s)
head size = 16
key = nn.Linear(n embd, head size, bias=False)
query = nn.Linear(n_embd, head_size, bias=False)
value = nn.Linear(n embd, head size, bias=False)
# linear proj of n embd → head size (B,T,n embd) @ (n embd, hs)->(B,T,hs)
k = key(x) # k (B, T, hs)
q = query(x) # q (B, T, hs)
v = value(x) # v (B, T, hs)
# compute affinities
wei = q @ k.transpose(-2, -1) * k.shape[-1]**0.5 # (B,T,hs) @ (B,hs,T) \rightarrow (B,T,T)
# for each token in the sequence, get dot pdts btw its guery and each key
# wei[b, i, j] = how much token i should pay attention to token j in that batch
# Scaled attention divides wei by 1/sqrt(head_size), wei is unit variance
# apply causual mask + softmax
tril = torch.tril(torch.ones(T, T))
wei = wei.masked fill(tril == 0, float('-inf'))
wei = F.softmax(wei, dim=-1)
out = wei @ v # (B,T,T)@(B,T,hs) \rightarrow (B,T,hs)
out.shape
```

What's happening

wei = affinities, tell us how much each token from the past contributes to our average → make this non-uniform (data dependent)

Self attention does it by having every node emit 3 vectors:

- * query what am i looking for
- * key what do i contain (acts like a label)
- * wei dot product of each token's query and all tokens' key to give a relevance score how much does this key match what i'm looking for? Mask to only include past tokens
- * value the actual info retrieved once a you decide which tokens are relevant
- * **out** dot product of each token's wei with query and all tokens' key to give a relevance score

head_size - dimensionality of attention mechanism (q,k,v vectors)- how much detail or nuance each attention head can capture in its comparisons

Building an attention head

Layer - Head

```
class Head(nn.Module):
   def __init (self, head size):
       super(). init ()
       self.key = nn.Linear(n_embd, head_size, bias=False) # weight matrix (n_embd, hs)
       self.query = nn.Linear(n embd, head size, bias=False)
       self.value = nn.Linear(n_embd, head_size, bias=False)
       self.register_buffer('tril', torch.tril(torch.ones(block_size, block_size)))
       self.dropout = nn.Dropout(dropout)
   def forward(self,x):
       B, T, C = x.shape \# \times (B, T, n \text{ embd})
       k = self.kev(x)
                           # k (B, T, hs)
       q = self.query(x) # q (B, T, hs)
       v = self.value(x) # v (B, T, hs)
       # linear proj n_embd → head_size (B,T,n_embd)@(n_embd, hs)->(B,T,hs)
       # compute affinities
       wei = q @ k.transpose(-2, -1) * k.shape[-1]**0.5 # (B,T,hs) @ (B,hs,T) \rightarrow (B,T,T)
       # for each token in the sequence, get dot pdts btw its query and each key
       # wei[b, i, j] = how much token i should pay attention to token j in that batch
       # Scaled attention divides wei by 1/sqrt(head_size), wei is unit variance
       # apply causual mask + softmax
       wei = wei.masked fill(self.tril[:T, :T] ==0, float('-inf'))
       wei = F.softmax(wei. dim=-1)
       wei = self.dropout(wei)
       out = wei @ v
                            # (B, T, T) @ (B, T, hs) -> (B, T, hs)
       # each token's output is a weighted average of value vectors
       return out
```

More on Attention

Input: x (B, T, n_embd); Output per head: out (B, T, hs) n_embd = hs * num_heads

<u>Attention</u> is a communication mechanism. Each token's output is a weighted average of all past token's value vectors (weighted by how much attention it pays to each token)

• There is no notion of space, hence need to positional encoding later

<u>Self attention</u> means <u>keys</u> and <u>values</u> are produced from the same source as <u>queries</u>. In <u>Cross-attention</u>, queries are from x, but the keys and values come from some other, external source (e.g. encoder module)

<u>Decoders</u> have triangular masking that causes tokens to only be able to see past tokens; used in autoregressive settings like language modelling.

<u>Encoders</u> exclude this, allowing all tokens to communicate; used in sentiment analysis all tokens can talk to predict the overall sentiment.

<u>Scaled attention</u> additionally divides wei by 1/sqrt(head_size), which makes wei unit variance, so softmax does not saturate too much.

- Without scaled attention: k.var() = 1, $q.var() = 1 \rightarrow wei.var() = hs$
- After scaling: wei.var() = 1

<u>Dropout</u> is a regularisation technique that randomly zeros some wei in each forward pass, prevents overfitting and forces the model to not rely too heavily on any single neuron.

 Eg. `dropout = nn.Dropout(p=0.1)` - each wei has a probability p of being zeroed out. Remaining elements scale up by 1/(1-p).

Building a transformer block

Layers - MultiHead Attention & Feedforward

```
class MultiHeadAttention(nn.Module):
    "multiple heads of self-attention in parallel"

def __init__(self, num_heads, head_size):
    super().__init__()
    self.heads = nn.ModuleList([Head(head_size) for _ in range(num_heads)])
    self.proj = nn.Linear(head_size * num_heads, n_embd)
    # concatenate attn outputs across multi heads &
    # & project back to n_embd to enable subsequent layers to consume result
    self.dropout = nn.Dropout(dropout)

def forward(self, x):
    out = torch.cat([h(x) for h in self.heads], dim=-1) # (B, T, hs * num_heads)
    out = self.dropout(self.proj(out)) # (B, T, n_embd)
    return out
```


What's happening

Blocks consist of:

1) Multi head Attention layer:

- Allows tokens to 'look' at one another and gain information from context
- Linear combination of input vectors (focus on rships btw tokens)

How it happens:

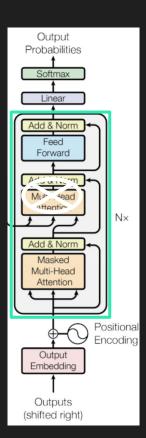
- Inputs into each Head(x) (B, T, n_embd)
- Outputs (B, T, hs) from each head are concatenated (B, T, hs * num_heads), then passed through a linear layer to project back to original shape (B, T, n_embd)

2) Feedforward

• Processes each token independently via non-linear transformations

How

- Project the embedding into a higher-dimensional space, apply a non-linearity, and then project it back. This allows the model to learn more expressive transformations.
- The intermediate dimension (4 * n_embd) gives the model room to mix and recombine features.



Building a transformer block

Layers - Block (MultiHead Attention + Feedforward)

```
class Block(nn.Module):
    "Block: communication followed by computation"

def __init__(self, n_embd, n_head):
    super().__init__()
    head_size = n_embd // n_head
    self.sa = MultiHeadAttention(n_head, head_size)
    self.ffwd = FeedForward(n_embd)
    self.ln1 = nn.LayerNorm(n_embd)
    self.ln2 = nn.LayerNorm(n_embd)

def forward(self, x):
    x = x + self.sa(self.ln1(x))
    x = x + self.ffwd(self.ln2(x))
    return x
```

What's happening

Block consist of:

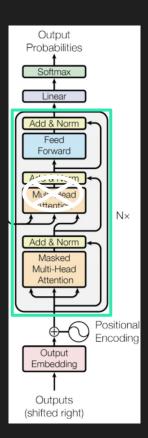
x -> LayerNorm -> Multi head Attention layer -> Residual connection -> LayerNorm -> Feedforward layer -> Residual connection

LayerNorm: Transformers use LayerNorm instead of BatchNorm

- For input x: (B, T, n_embd)
- LN works across n_embd per-token normalization across features
- BN works across B –, per-batch normalisation. Doesn't work as transformers have variable batch sizes and even batch size = 1. BN needs multiple samples to compute statistics

Residual connection: When applying a transformation F(x) to input x, instead of `out = F(x)`, do `out = x + F(x)`. Helps with:

- Gradient flow: In deep networks, gradients can vanish. Skip connection allows gradient of x to flow directly to out, stabilising training
- Let model learn an adjustment instead of full transformation:
 Eq. if model must learn out = x
 - o Without residuals, model must learn $F(x) \approx x$. learn the full identity map F(x) to rebuild x from scratch
 - o With residuals, out = $x + F(x) \rightarrow$ model must learn $F(x) \approx 0$. If the best thing the layer can do is "do nothing," it only needs to output zeros, or it can learn small tweaks. This is way easier than learning to rebuild x



Putting it all into GPT model

GPTModel definition

```
class GPTLanguageModel(nn.Module):
    def __init__(self):
        super(). init ()
        self.token_embedding_table = nn.Embedding(vocab_size, n_embd)
        self.position embedding table = nn.Embedding(block size. n embd)
       self.blocks = nn.Sequential(*[Block(n_embd, n_head = n_head) for _ in range(n_layer)])
       self.ln f = nn.LayerNorm(n embd)
       self.lm_head = nn.Linear(n_embd, vocab_size)
       # initialise weights & biases in layers
       self.apply(self._init_weights)
   # initialise linear & embedding layer: weights to small normal distrib; bias to 0
    def _init_weights(self, module):
       if isinstance(module, nn.Linear):
            torch.nn.init.normal (module.weight, mean=0.0, std=0.02)
            if module.bias is not None:
                torch.nn.init.zeros (module.bias)
        elif isinstance(module, nn.Embedding):
            torch.nn.init.normal_(module.weight, mean=0.0, std=0.02)
```

GPTModel definition

```
def forward(self, idx, targets = None):
    B, T = idx.shape # idx (B, T): current context
    tok emb = self.token embedding table(idx) # (B, T, n embd)
    pos_emb = self.position_embedding_table(torch.arange(T, device=device)) # (T, n_embd)
    x = tok emb + pos emb
                                                                   Probabilities
    x = self.blocks(x) # transformer block (B, T, n_embd)
    x = self.ln_f(x) # layernorm (B, T, n_embd)
                                                                     Softmax
    logits = self.lm_head(x) # lm_head (B, T, vocab_size)
                                                                     Linear
    # get loss
    if targets is None:
                                                                   Add & Norm
        loss = None
                                                                      Feed
    else:
                                                                     Forward
        B, T, C = logits.shape
        logits = logits.view(B*T, C)
                                                                   Add & Norm
        targets = targets.view(B*T)
                                                                    Multi-Head
                                                                     Attention
        loss = F.cross_entropy(logits, targets)
                                                                                   N×
    return logits, loss
                                                                   Add & Norm
                                                                    Multi-Head
                                                                     Attention
                                                                               Positional
                                                                               Encodina
                                                                     Output
                                                                    Embeddina
                                                                    Outputs
```

Putting it all into GPT model

Code

```
model = GPTLanguageModel()
m = model.to(device)
# print number of params
print(sum(p.numel() for p in m.parameters())/1e6, 'M parameters')
# optimise
optimiser = torch.optim.AdamW(model.parameters(), lr=learning rate)
for iter in range(max iters):
    # every once in a while evaluate loss on train and val sets
    if iter % eval interval == 0 or iter == max iters-1:
        losses = estimate loss()
        print(f"step {iter}: train loss {losses['train']:.4f}, val loss {losses['val']:.4f}")
    # sample a batch of data
    xb, yb = get batch('train')
    # evaluate loss
    logits, loss = model(xb, yb)
    optimiser.zero_grad(set_to_none= True)
    loss.backward()
    optimiser.step()
```

What's happening

Training:

- 1. Set an AdamW optimiser that knows which parameters to update and at what learning rate.
- 2. Get a batch of data xb and yb (B, T) each
- 3. Evaluate loss
- 4. Using optimiser:
 - a. Set all gradients of params to zero
 - b. Use loss.backwards() to calculate gradients
 - c. Use .step() to update params with gradients
- For every eval_intervaliterations, print average loss of training and validation sets across eval iters

```
def estimate_loss():
    # average the loss for both train and val over a few iter
    out = {}
    model.eval()
                                                0.158913 M parameters
    for split in ['train', 'val']:
        losses = torch.zeros(eval iters)
                                                 step 500: train loss 2.2663, val loss 2.2690
        for k in range(eval iters):
            X, Y = get_batch (split)
                                                 step 2000: train loss 2.0090, val loss 2.0685
            logits, loss = model(X, Y)
                                                 step 2500: train loss 1.9944, val loss 2.0705
            losses[k] = loss.item()
                                                 step 3000: train loss 1.9626, val loss 2.0436
        out[split] = losses.mean()
                                                 step 3500: train loss 1.9322, val loss 2.0284
    model.train()
    return out
```

Building GPT model!

GPTLanguageModel definition

```
class GPTLanguageModel(nn.Module):
  def generate(self, idx, max new tokens):
       # idx is (B, T) array of indices in current context
       for __in range(max new tokens):
           # crop idx to last block size tokens (pos emb only has up to block size embeddings)
           idx cond = idx[:, -block size:]
           # get predictions for each time step in input
           logits, loss = self(idx_cond)
           # logits[:, 0, :] - prediction for what comes aft token 1
           # logits[:, 1, :] - prediction for what comes aft token 1, 2
           # logits[:, 2, :] - prediction for what comes aft token 1, 2, 3
           # get predictions for next token after all tokens in input
           logits = logits[:, -1, :] # (B,C)
           # apply softmax to get probabilities
           probs = F.softmax(logits, dim=-1)
           # sample from distribution
           idx_next = torch.multinomial(probs, num_samples=1) # (B, 1)
           # append sampled index to the running sequence
           idx = torch.cat((idx, idx_next), dim=1) # (B, T+1)
       return idx
```

Code

```
# generate from the model
context = torch.zeros((1, 1), dtype = torch.long, device = device)
print(decode(m.generate(context, max new tokens=500)[0].tolist()))
```

context = torch.zeros((1, 1), dtype=torch.long, device=device)

- Creates a starting input tensor for the model.
- Shape $(1, 1) \rightarrow$ batch size of 1, sequence length of 1.
- The value is 0, which corresponds to the first token in your vocabulary.
- •

m.generate(context, max_new_tokens=500)

- Calls the model's generate method to predict the next token 500 times
- It maintains the last block_size tokens as context (due to the positional embedding limits)

[0].tolist()

- The output of generate is a tensor of shape (1, 501) (original + 500 new tokens).
- [0] extracts the first (and only) sequence from the batch.
- .tolist() converts the tensor to a Python list of integers to then be decoded

Mini-shakespeare GPT

Hyperparameters

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block size
max iters
learning rate = 1e-3
n embd
n head = 2
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Less good version

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Thre Sink, heard so me'et tleit onotlous viers to, will doretese
Ay: marter? foullove
loughtry thee hive,
sweable
That hand nearth at in sild anved
I the comerce thess.
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Better version

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block_size = 16
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```

LAUNTIO:

This ghe altreaging donen fair lath, 'lls sore have and; Our know mine.

Firss? My have to lieves of this dO reath, for Counsameajing.

HESS ISABERBET:

my if were most my most of to sian,

The not all noble you, with my cefordoness, when fair, Leasiding, now, bey dentaae my than but my thou-bearn.

No were sume me, you kners, 'lieved dear, ere of you day hearly mis On these my with told seerk.

Give is faireful didy foold belied; and You oher: reary ow any le

- Learnt shakespeare structure (NAME: speech)!
- ✓ More recognisable words!
- ✓ Starting new lines with capital letters!