10-301/601: Introduction to Machine Learning Lecture 19: Pretraining & Fine-tuning

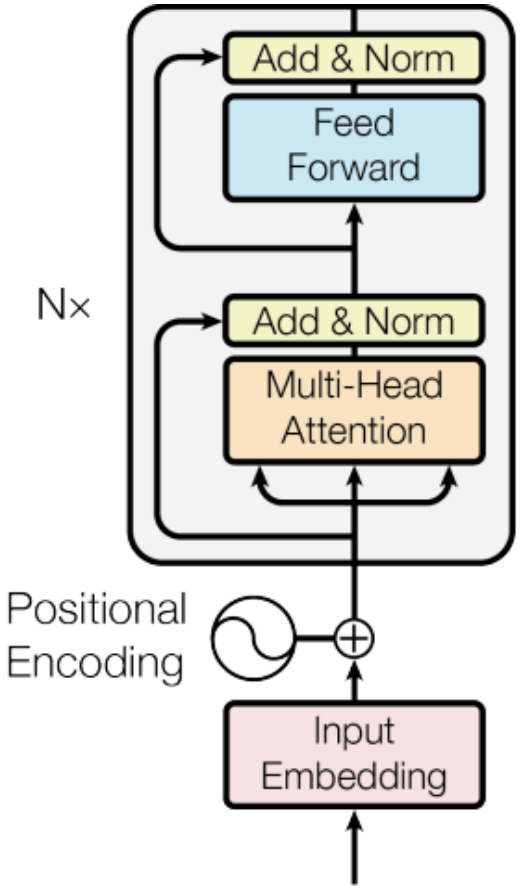
Matt Gormley & Henry Chai

3/24/25

Front Matter

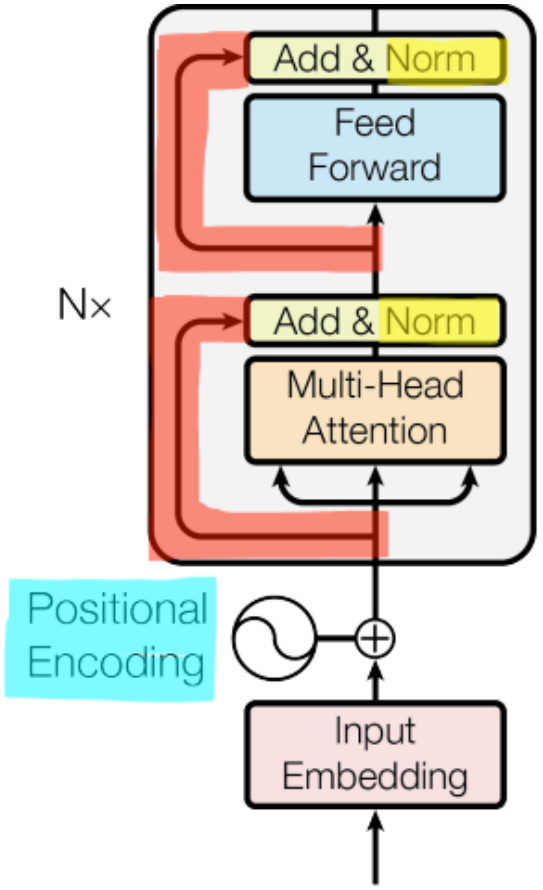
- Announcements
  - Exam 2 on 3/26 (Wednesday) from 7 – 9 PM
    - All topics from Lecture 8 to Lecture 16 (inclusive) **+ MLE/MAP portion of Lecture 17** are in-scope
    - Exam 1 content may be referenced but will not be the primary focus of any question
    - Please review the seating chart on Piazza and make sure you have a seat / know where you're going

Transformers



Source: https://arxiv.org/pdf/1706.03762.pdf

Transformers

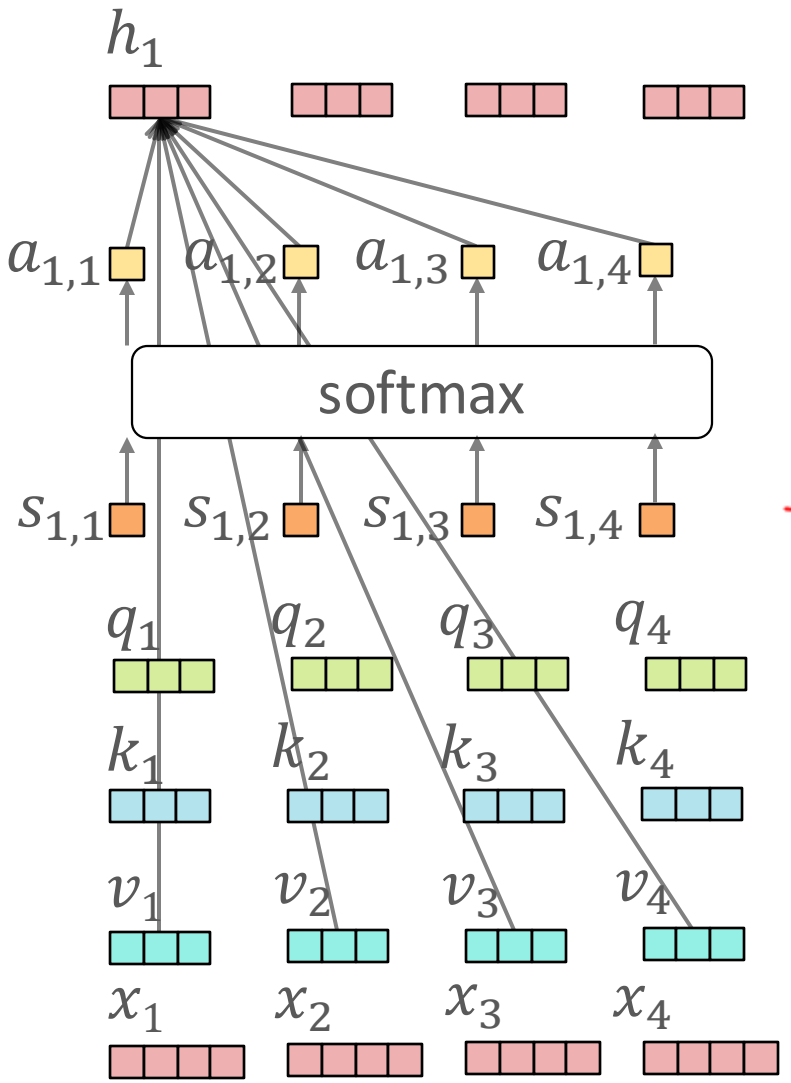


- In addition to multi-head attention, transformer architectures use
  1. Positional encodings
  2. Layer normalization
  3. Residual connections
  4. A fully-connected feed-forward network

Source: https://arxiv.org/pdf/1706.03762.pdf

Recall: Scaled Dot-product Attention

- Approach: compute a representation for each token in the *input sequence* by attending to all the input tokens



$$h_1 = \sum_{j=1}^{4} \text{softmax}(s_{1,j}) v_j$$

attention weights

scores: $s_{1,j} = \frac{k_j^T q_1}{\sqrt{d_k}}$

queries: $q_t = W_Q x_t$

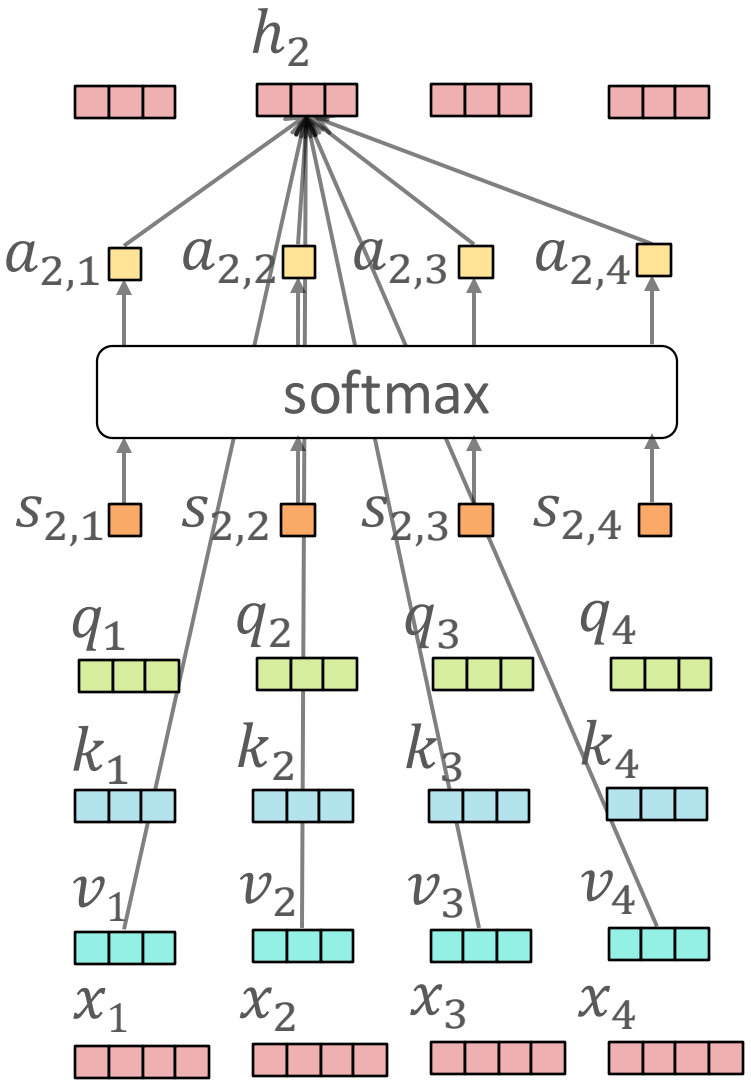
keys: $k_t = W_K x_t$

values: $v_t = W_V x_t$

input tokens

Recall: Scaled Dot-product Attention

- Approach: compute a representation for each token in the *input sequence* by attending to all the input tokens



$$h_2 = \sum_{j=1}^{4} \text{softmax}(s_{2,j}) v_j$$

attention weights

scores: $s_{2,j} = \frac{k_j^T q_2}{\sqrt{d_k}}$

queries: $q_t = W_Q x_t$

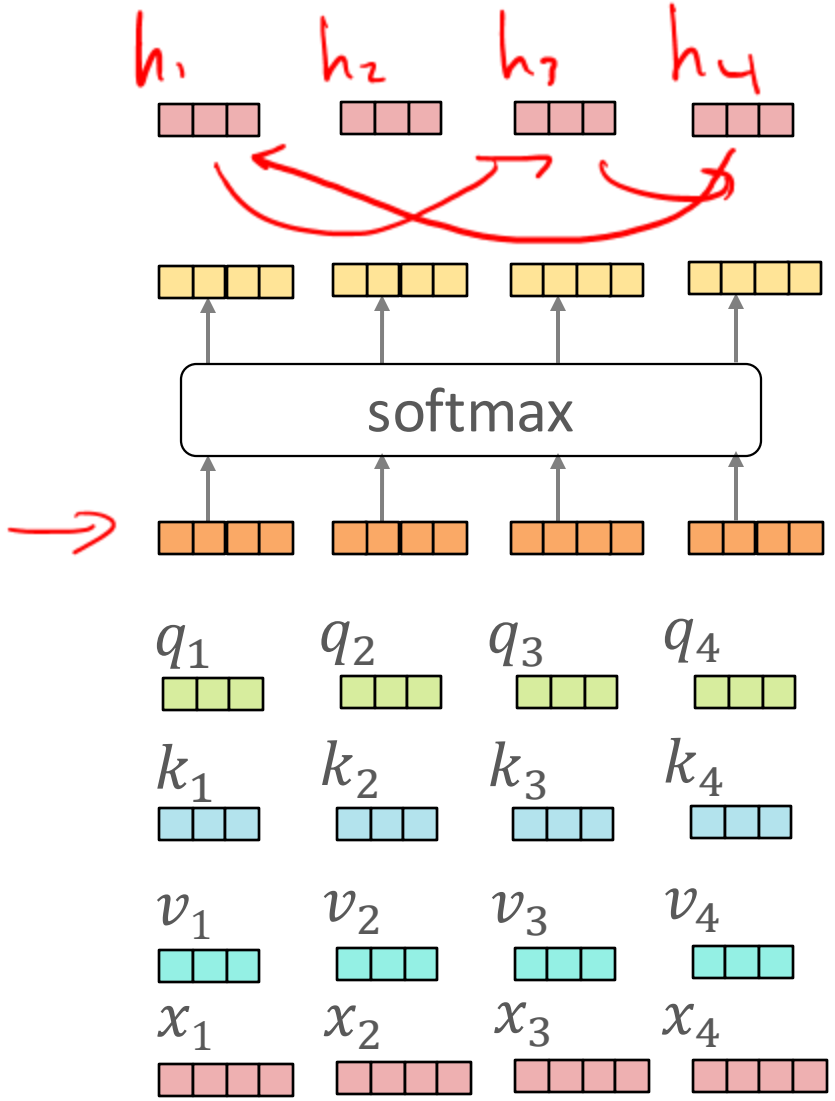
keys: $k_t = W_K x_t$

values: $v_t = W_V x_t$

input tokens

Scaled Dot-product Attention: Matrix Form

- Issue: if all tokens attend to every token in the sequence, then how does the model infer the order of tokens?



$$H = \text{softmax}(S)V \in \mathbb{R}^{N \times d_v}$$

attention weights

scores: $S = \frac{QK^T}{\sqrt{d_k}} \in \mathbb{R}^{N \times N}$

queries: $Q = XW_Q \in \mathbb{R}^{N \times d_k}$

keys: $K = XW_K \in \mathbb{R}^{N \times d_k}$

values: $V = XW_V \in \mathbb{R}^{N \times d_v}$

design matrix: $X \in \mathbb{R}^{N \times D}$

Positional Encodings

- Issue: if all tokens attend to every token in the sequence, then how does the model infer the order of tokens?
- Idea: add a position-specific embedding p_t to the token embedding x_t

$$\tilde{x}_t = x_t + p_t$$

- Positional encodings can be
  - *fixed* i.e., some predetermined function of t or *learned* alongside the token embeddings
  - *absolute* i.e., only dependent on the token's location in the sequence or *relative* to the query token's location

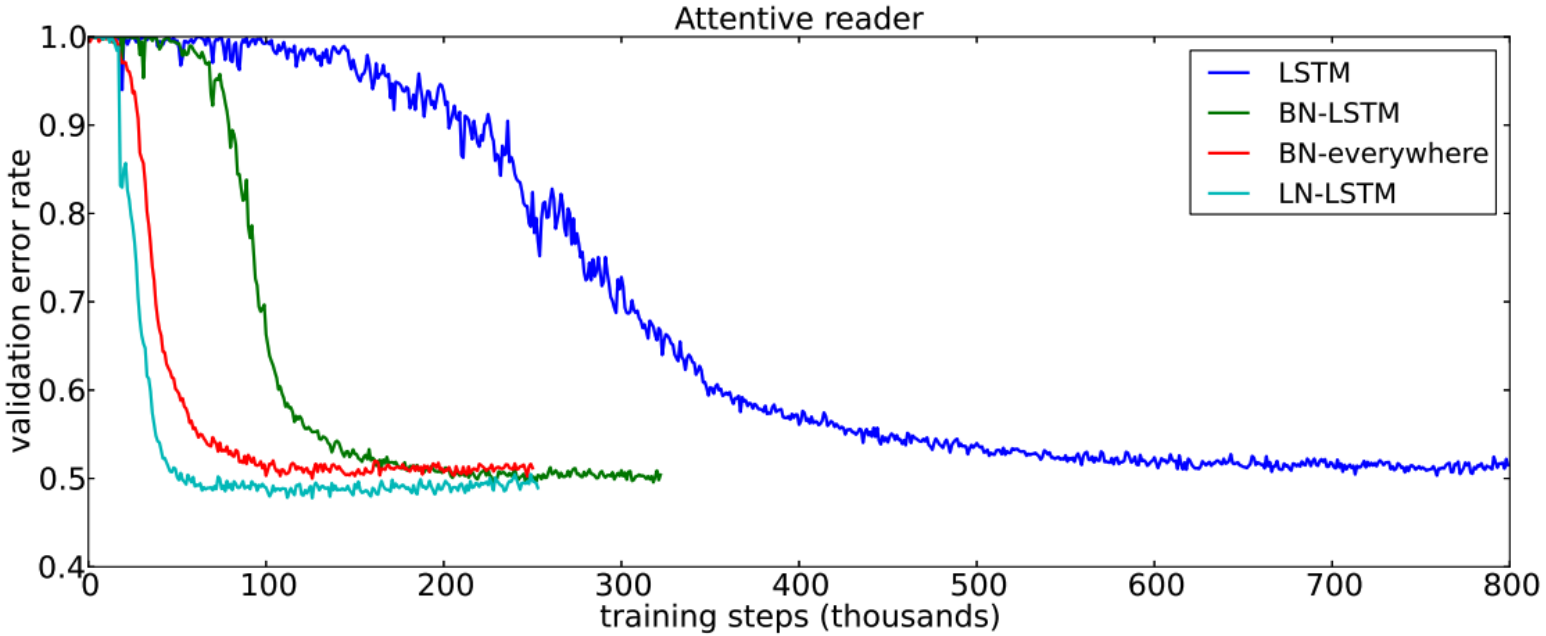
Layer Normalization

- Issue: for certain activation functions, the weights in later layers are **highly sensitive** to changes in the earlier layers
  - Small changes to weights in early layers are amplified so weights in deeper layers have to deal with massive dynamic ranges → slow optimization convergence
- Idea: normalize the output of a layer to always have the same (learnable) mean, β, and variance, γ^2

$$H' = \gamma\left(\frac{H - \mu}{\sigma}\right) + \beta$$

where μ is the mean and σ is the standard deviation of the values in the vector H

Layer Normalization



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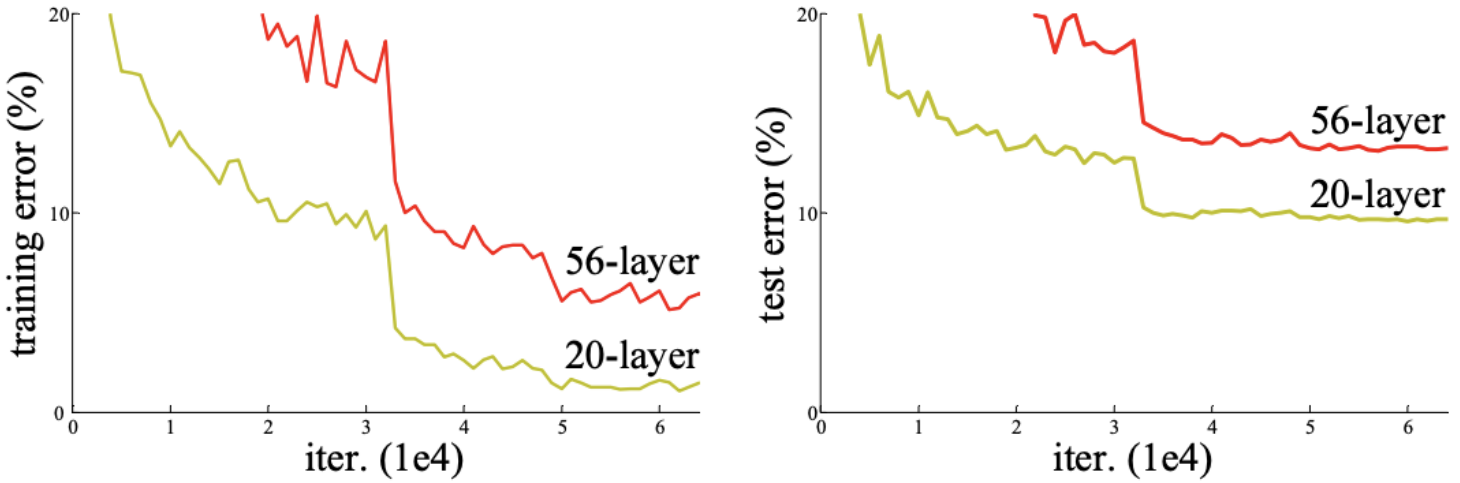
Source: https://arxiv.org/pdf/1607.06450.pdf

Residual Connections

- Observation: early deep neural networks suffered from the "degradation" problem where adding more layers actually made performance worse!



- Wait but this is ridiculous: if the later layers aren't helping, couldn't they just learn the identity transformation???
- Insight: neural network layers actually have a hard time learning the identity function

Source: https://arxiv.org/pdf/1512.03385.pdf

Residual Connections

- Observation: early deep neural networks suffered from the "degradation" problem where adding more layers actually made performance worse!
- Idea: add the input embedding back to the output of a layer

$$H' = H\left(x^{(i)}\right) + x^{(i)}$$

- Suppose the target function is f
  - Now instead of having to learn $f\left(x^{(i)}\right)$, the hidden layer just needs to learn the residual $r = f\left(x^{(i)}\right) - x^{(i)}$
  - If f is the identity function, then the hidden layer just needs to learn $r = 0$, which is easy for a neural network!

Residual Connections

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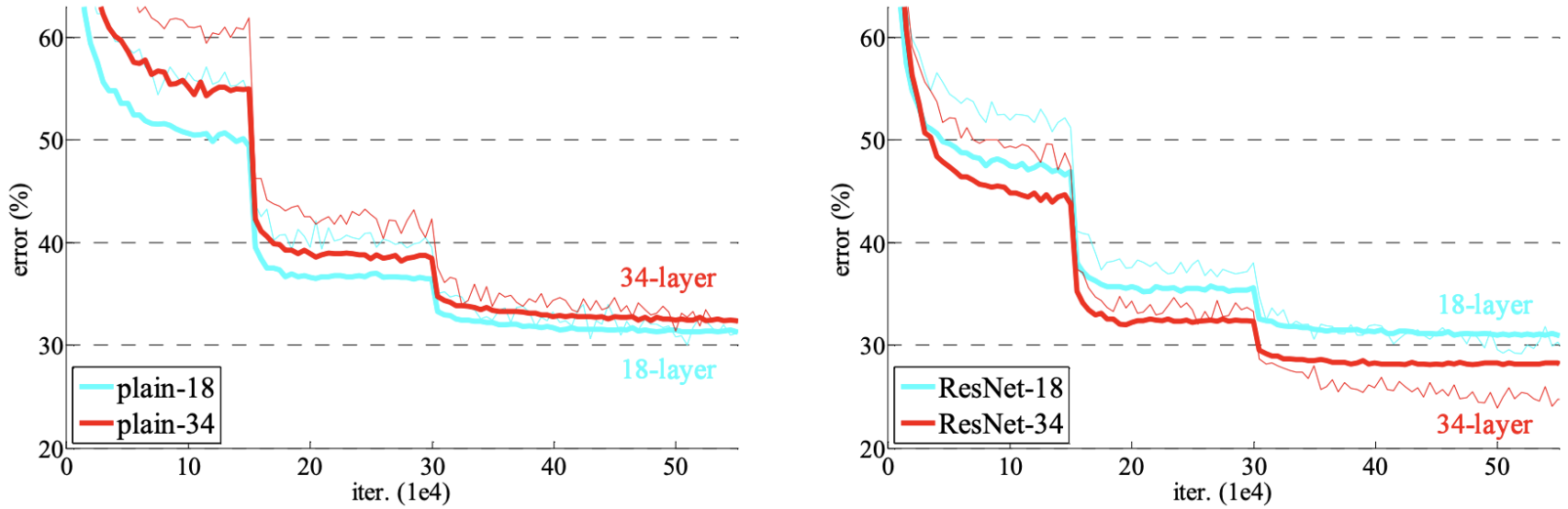

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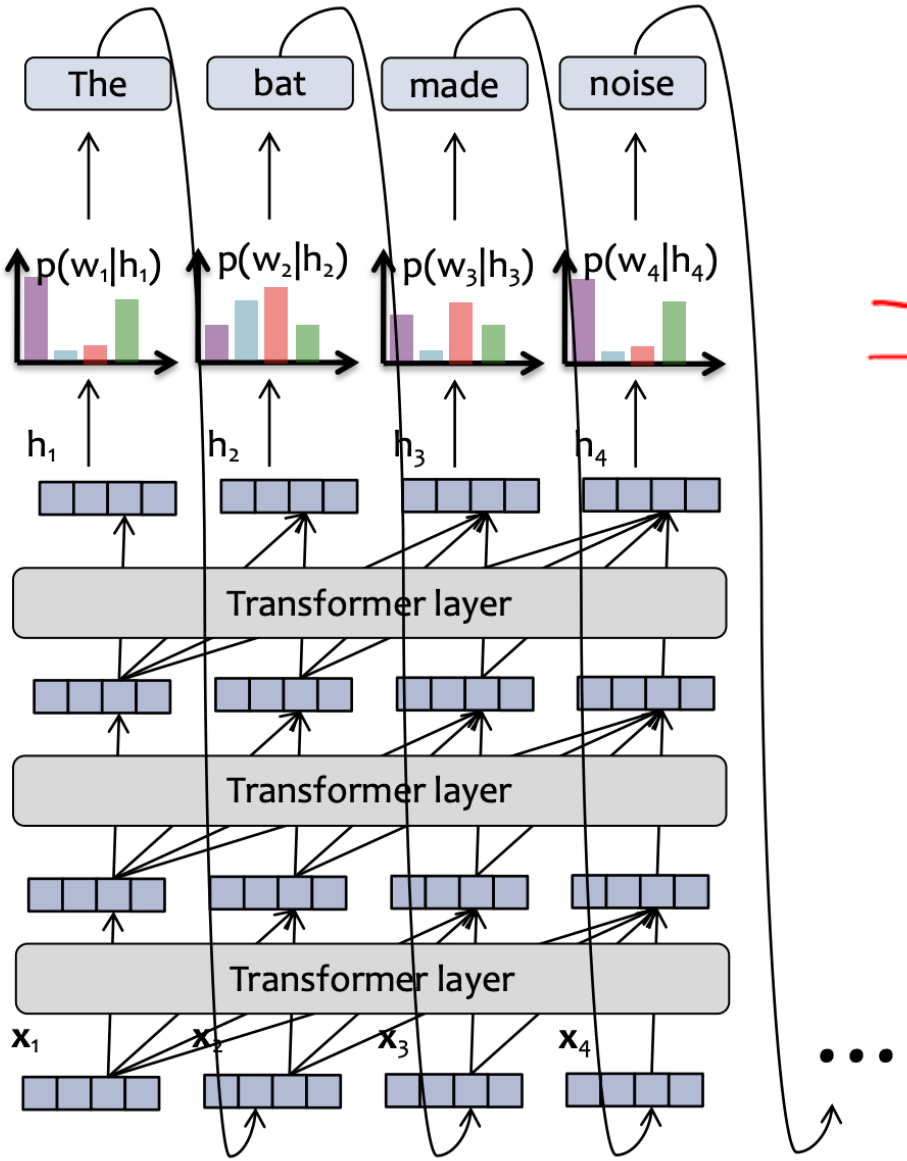


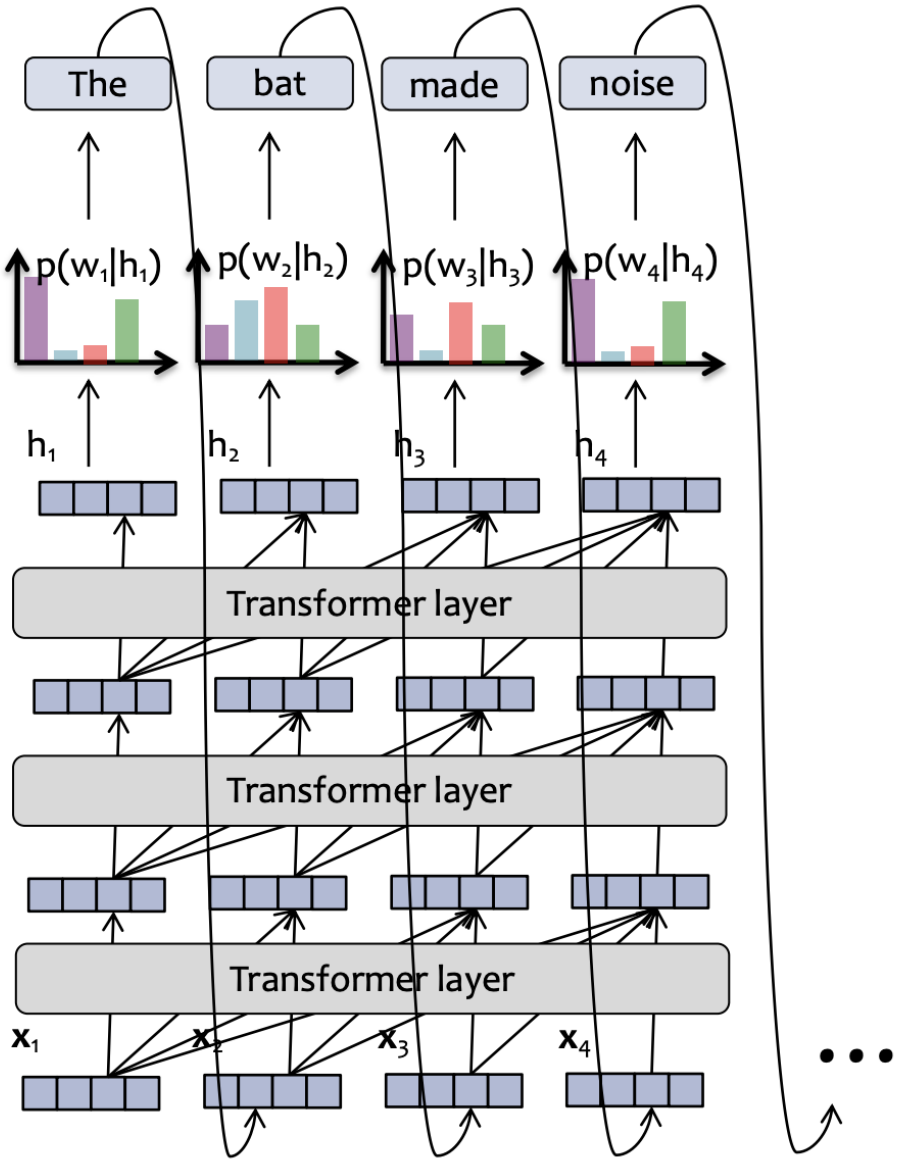
Each layer of a Transformer LM consists of several **sublayers:**

1. attention
2. feed-forward neural network
3. layer normalization
4. residual connections

Each hidden vector looks back at the hidden vectors of the **current and previous timesteps in the previous layer.**

The language model part is just like an RNN-LM.

Okay, but how on earth do we go about training these things?



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Backpropagation: Procedural Method

Algorithm 1 Forward Computation

procedure NNFORWARD(Training example $(\mathbf{x}, \mathbf{y})$, Params $\boldsymbol{\alpha}, \boldsymbol{\beta}$)
  $\mathbf{a} = \boldsymbol{\alpha}\mathbf{x}$
  $\mathbf{z} = \sigma(\mathbf{a})$
  $\mathbf{b} = \boldsymbol{\beta}\mathbf{z}$
  $\hat{\mathbf{y}} = \text{softmax}(\mathbf{b})$
  $J = -\mathbf{y}^T \log \hat{\mathbf{y}}$
  $\mathbf{o} = \texttt{object}(\mathbf{x}, \mathbf{a}, \mathbf{z}, \mathbf{b}, \hat{\mathbf{y}}, J)$
  return intermediate quantities $\mathbf{o}$

Algorithm 2 Backpropagation

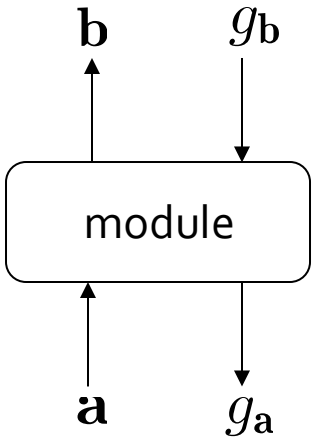
procedure NNBACKWARD(Training example $(\mathbf{x}, \mathbf{y})$, Params $\boldsymbol{\alpha}, \boldsymbol{\beta}$, Intermediates $\mathbf{o}$)
  Place intermediate quantities $\mathbf{x}, \mathbf{a}, \mathbf{z}, \mathbf{b}, \hat{\mathbf{y}}, J$ in $\mathbf{o}$ in scope
  $\mathbf{g}_{\hat{\mathbf{y}}} = -\mathbf{y} \div \hat{\mathbf{y}}$
  $\mathbf{g}_{\mathbf{b}} = \mathbf{g}_{\hat{\mathbf{y}}}^T \left(\text{diag}(\hat{\mathbf{y}}) - \hat{\mathbf{y}}\hat{\mathbf{y}}^T\right)$
  $\mathbf{g}_{\boldsymbol{\beta}} = \mathbf{g}_{\mathbf{b}}^T \mathbf{z}^T$
  $\mathbf{g}_{\mathbf{z}} = \boldsymbol{\beta}^T \mathbf{g}_{\mathbf{b}}^T$
  $\mathbf{g}_{\mathbf{a}} = \mathbf{g}_{\mathbf{z}} \odot \mathbf{z} \odot (1 - \mathbf{z})$
  $\mathbf{g}_{\boldsymbol{\alpha}} = \mathbf{g}_{\mathbf{a}} \mathbf{x}^T$
  return parameter gradients $\mathbf{g}_{\boldsymbol{\alpha}}, \mathbf{g}_{\boldsymbol{\beta}}$

Issues:

1. Hard to reuse / adapt for other models
2. Hard to optimize individual steps
3. Hard to debug using the finite-difference check

Module-based AutoDiff

- Key Idea:
  - componentize the computation of the neural-network into layers
  - each layer consolidates multiple **real-valued nodes** in the computation graph (a subset of them) into one **vector-valued node** (aka. a **module**)
- Each **module** is capable of two actions:
  - **Forward computation of the output given some input**
  - **Backward computation of the gradient with respect to the input given the gradient with respect to the output**



Module-based AutoDiff

Linear Module The linear layer has two inputs: a vector $\mathbf{a}$ and parameters $\omega \in \mathbb{R}^{B \times A}$. The output $\mathbf{b}$ is not used by LINEARBACKWARD, but we pass it in for consistency of form.

procedure LINEARFORWARD($\mathbf{a}$, ω)
  $\mathbf{b} = \omega\mathbf{a}$
  return $\mathbf{b}$
procedure LINEARBACKWARD($\mathbf{a}$, ω, $\mathbf{b}$, $\mathbf{g_b}$)
  $\mathbf{g}_\omega = \mathbf{g_b}\mathbf{a}^T$
  $\mathbf{g_a} = \omega^T\mathbf{g_b}$
  return $\mathbf{g}_\omega, \mathbf{g_a}$

Softmax Module The softmax layer has only one input vector $\mathbf{a}$. For any vector $\mathbf{v} \in \mathbb{R}^D$, we have that $\text{diag}(\mathbf{v})$ returns a $D \times D$ diagonal matrix whose diagonal entries are $v_1, v_2, \ldots, v_D$ and whose non-diagonal entries are zero.

procedure SOFTMAXFORWARD($\mathbf{a}$)
  $\mathbf{b} = \text{softmax}(\mathbf{a})$
  return $\mathbf{b}$
procedure SOFTMAXBACKWARD($\mathbf{a}$, $\mathbf{b}$, $\mathbf{g_b}$)
  $\mathbf{g_a} = \mathbf{g_b}^T\left(\text{diag}(\mathbf{b}) - \mathbf{b}\mathbf{b}^T\right)$
  return $\mathbf{g_a}$

Sigmoid Module The sigmoid layer has only one input vector $\mathbf{a}$. Below σ is the sigmoid applied element-wise, and $\odot$ is element-wise multiplication s.t. $\mathbf{u} \odot \mathbf{v} = [u_1 v_1, \ldots, u_M v_M]$.

procedure SIGMOIDFORWARD($\mathbf{a}$)
  $\mathbf{b} = \sigma(\mathbf{a})$
  return $\mathbf{b}$
procedure SIGMOIDBACKWARD($\mathbf{a}$, $\mathbf{b}$, $\mathbf{g_b}$)
  $\mathbf{g_a} = \mathbf{g_b} \odot \mathbf{b} \odot (1 - \mathbf{b})$
  return $\mathbf{g_a}$

Cross-Entropy Module The cross-entropy layer has two inputs: a gold one-hot vector $\mathbf{a}$ and a predicted probability distribution $\hat{\mathbf{a}}$. It's output $b \in \mathbb{R}$ is a scalar. Below $\div$ is element-wise division. The output b is not used by CROSSENTROPYBACKWARD, but we pass it in for consistency of form.

procedure CROSSENTROPYFORWARD($\mathbf{a}$, $\hat{\mathbf{a}}$)
  $b = -\mathbf{a}^T \log \hat{\mathbf{a}}$
  return $\mathbf{b}$
procedure CROSSENTROPYBACKWARD($\mathbf{a}$, $\hat{\mathbf{a}}$, b, g_b)
  $\mathbf{g}_{\hat{\mathbf{a}}} = -g_b(\mathbf{a} \div \hat{\mathbf{a}})$
  return $\mathbf{g_a}$

Module-based AutoDiff

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procedure NNFORWARD(Training example $(\mathbf{x}, \mathbf{y})$, Parameters $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$)
  $\mathbf{a} = \text{LINEARFORWARD}(\mathbf{x}, \boldsymbol{\alpha})$
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  $\mathbf{b} = \text{LINEARFORWARD}(\mathbf{z}, \boldsymbol{\beta})$
  $\hat{\mathbf{y}} = \text{SOFTMAXFORWARD}(\mathbf{b})$
  $J = \text{CROSSENTROPYFORWARD}(\mathbf{y}, \hat{\mathbf{y}})$
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  Place intermediate quantities $\mathbf{x}, \mathbf{a}, \mathbf{z}, \mathbf{b}, \hat{\mathbf{y}}, J$ in $\mathbf{o}$ in scope
  $g_J = \frac{dJ}{dJ} = 1$ ▷ Base case
  $\mathbf{g}_{\hat{\mathbf{y}}} = \text{CROSSENTROPYBACKWARD}(\mathbf{y}, \hat{\mathbf{y}}, J, g_J)$
  $\mathbf{g}_{\mathbf{b}} = \text{SOFTMAXBACKWARD}(\mathbf{b}, \hat{\mathbf{y}}, \mathbf{g}_{\hat{\mathbf{y}}})$
  $\mathbf{g}_{\boldsymbol{\beta}}, \mathbf{g}_{\mathbf{z}} = \text{LINEARBACKWARD}(\mathbf{z}, \mathbf{b}, \mathbf{g}_{\mathbf{b}})$
  $\mathbf{g}_{\mathbf{a}} = \text{SIGMOIDBACKWARD}(\mathbf{a}, \mathbf{z}, \mathbf{g}_{\mathbf{z}})$
  $\mathbf{g}_{\boldsymbol{\alpha}}, \mathbf{g}_{\mathbf{x}} = \text{LINEARBACKWARD}(\mathbf{x}, \mathbf{a}, \mathbf{g}_{\mathbf{a}})$ ▷ We discard $\mathbf{g}_{\mathbf{x}}$
  return parameter gradients $\mathbf{g}_{\boldsymbol{\alpha}}, \mathbf{g}_{\boldsymbol{\beta}}$

1. Easy to reuse / adapt for other models
2. Individual layers are easier to optimize
3. Simple to debug: just run a finite-difference check on each layer separately

Module-based AutoDiff (OOP Version)

Object-Oriented Implementation:

- Let each module be an object and allow the **control flow** of the program to define the computation graph
- **No longer need to implement NNBackward(·)**, just follow the computation graph in reverse topological order

```
class Sigmoid(Module)
    method forward(a)
        b = σ(a)
        return b
    method backward(a, b, g_b)
        g_a = g_b ⊙ b ⊙ (1 − b)
        return g_a
```

```
class Softmax(Module)
    method forward(a)
        b = softmax(a)
        return b
    method backward(a, b, g_b)
        g_a = g_b^T (diag(b) − bb^T)
        return g_a
```

```
class Linear(Module)
    method forward(a, ω)
        b = ωa
        return b
    method backward(a, ω, b, g_b)
        g_ω = g_b a^T
        g_a = ω^T g_b
        return g_ω, g_a
```

```
class CrossEntropy(Module)
    method forward(a, â)
        b = −a^T log â
        return b
    method backward(a, â, b, g_b)
        g_â = −g_b(a ÷ â)
        return g_a
```

Module-based AutoDiff (OOP Version)

```
1  class NeuralNetwork(Module):
2
3      method init()
4          lin1_layer = Linear()
5          sig_layer = Sigmoid()
6          lin2_layer = Linear()
7          soft_layer = Softmax()
8          ce_layer = CrossEntropy()
9
10     method forward(Tensor x, Tensor y, Tensor α, Tensor β)
11         a =lin1_layer.apply_fwd(x, α)
12         z =sig_layer.apply_fwd(a)
13         b =lin2_layer.apply_fwd(z, β)
14         ŷ =soft_layer.apply_fwd(b)
15         J =ce_layer.apply_fwd(y, ŷ)
16         return J.out_tensor
17
18     method backward(Tensor x, Tensor y, Tensor α, Tensor β)
19         tape_bwd()
20         return lin1_layer.in_gradients[1], lin2_layer.in_gradients[1]
```

Module-based AutoDiff (OOP Version)

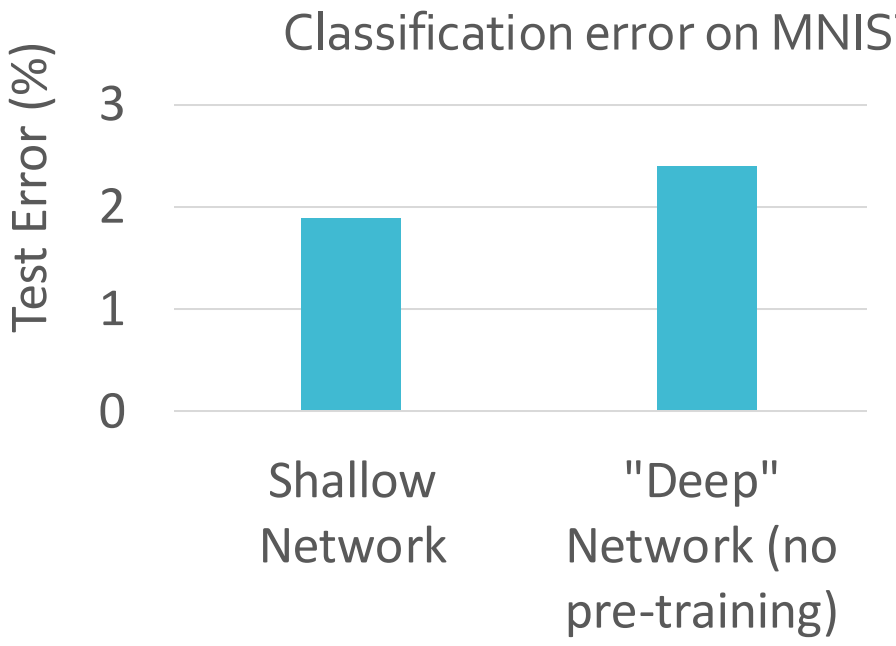
```
1  global tape = stack()
2
3  class Module:
4
5      method init()
6          out_tensor = null
7          out_gradient = 1
8
9      method apply_fwd(List in_modules)
10         in_tensors = [x.out_tensor for x in in_modules]
11         out_tensor = forward(in_tensors)
12         tape.push(self)
13         return self
14
15     method apply_bwd():
16         in_gradients = backward(in_tensors, out_tensor, out_gradient)
17         for i in 1,..., len(in_modules):
18             in_modules[i].out_gradient += in_gradients[i]
19         return self
20
21 function tape_bwd():
22     while len(tape) > 0
23         m = tape.pop()
24         m.apply_bwd()
```

Traditional Supervised Learning

- You have some task that you want to apply machine learning to
- You have a labelled dataset to train with
- You fit a deep learning model to the dataset

Reality

- You have some niche task that you want to apply machine learning to e.g., predicting the author of children's books
- You have a tiny labelled dataset to train with
- You fit a massive deep learning model to the dataset
- Surprise, surprise: it overfits and your test error is super high



- "gradient-based optimization starting from random initialization appears to often get stuck in poor solutions for such deep networks."

Source: https://www.cs.toronto.edu/~larocheh/publications/dbn_supervised_tr1282.pdf

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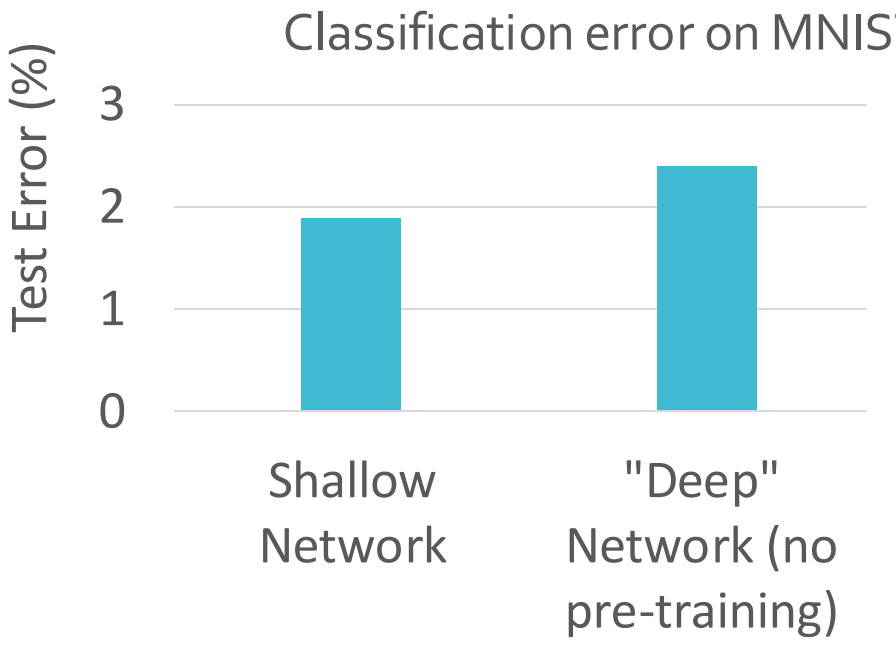
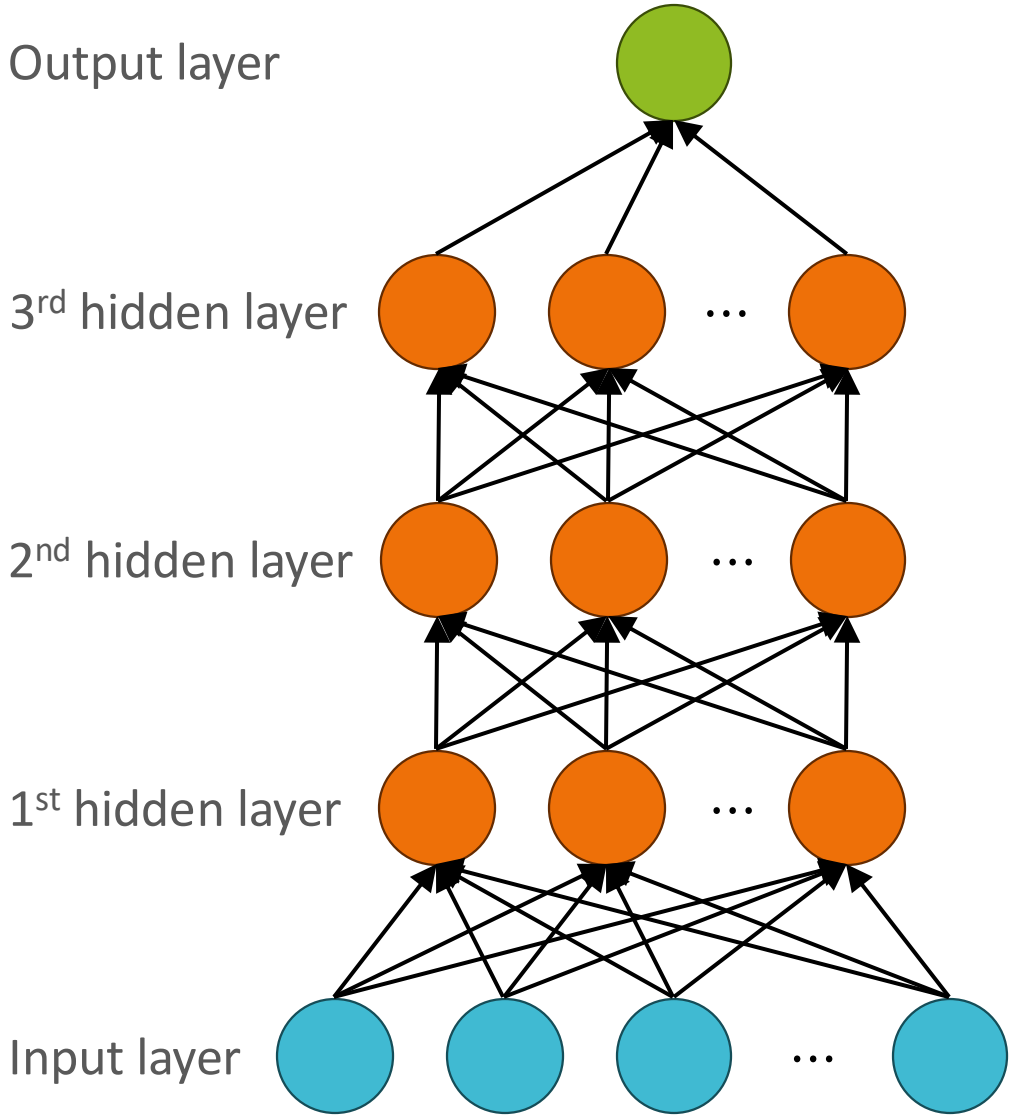


- Idea: if shallow networks are easier to train, let's just decompose our deep network into a series of shallow networks!

Source: https://www.cs.toronto.edu/~larocheh/publications/dbn_supervised_tr1282.pdf

Pre-training (Bengio et al., 2006)

- Train each layer of the network iteratively using the training dataset
- Start at the input layer and move towards the output layer
- Once a layer has been trained, fix its weights and use those to train subsequent layers



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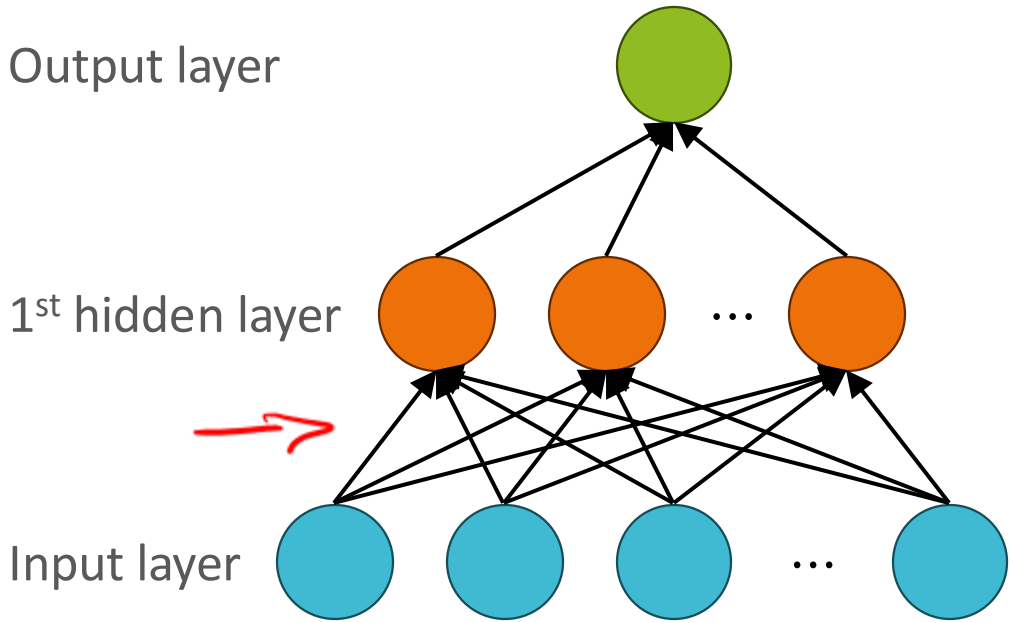

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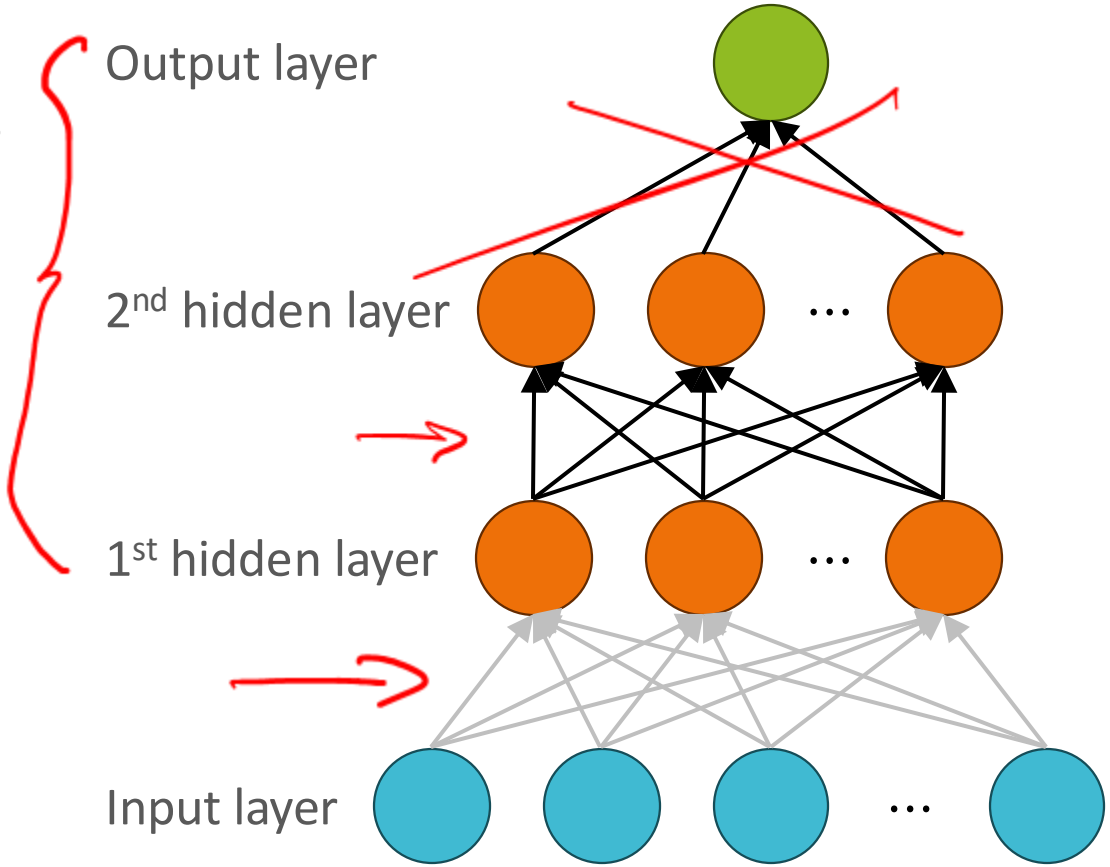

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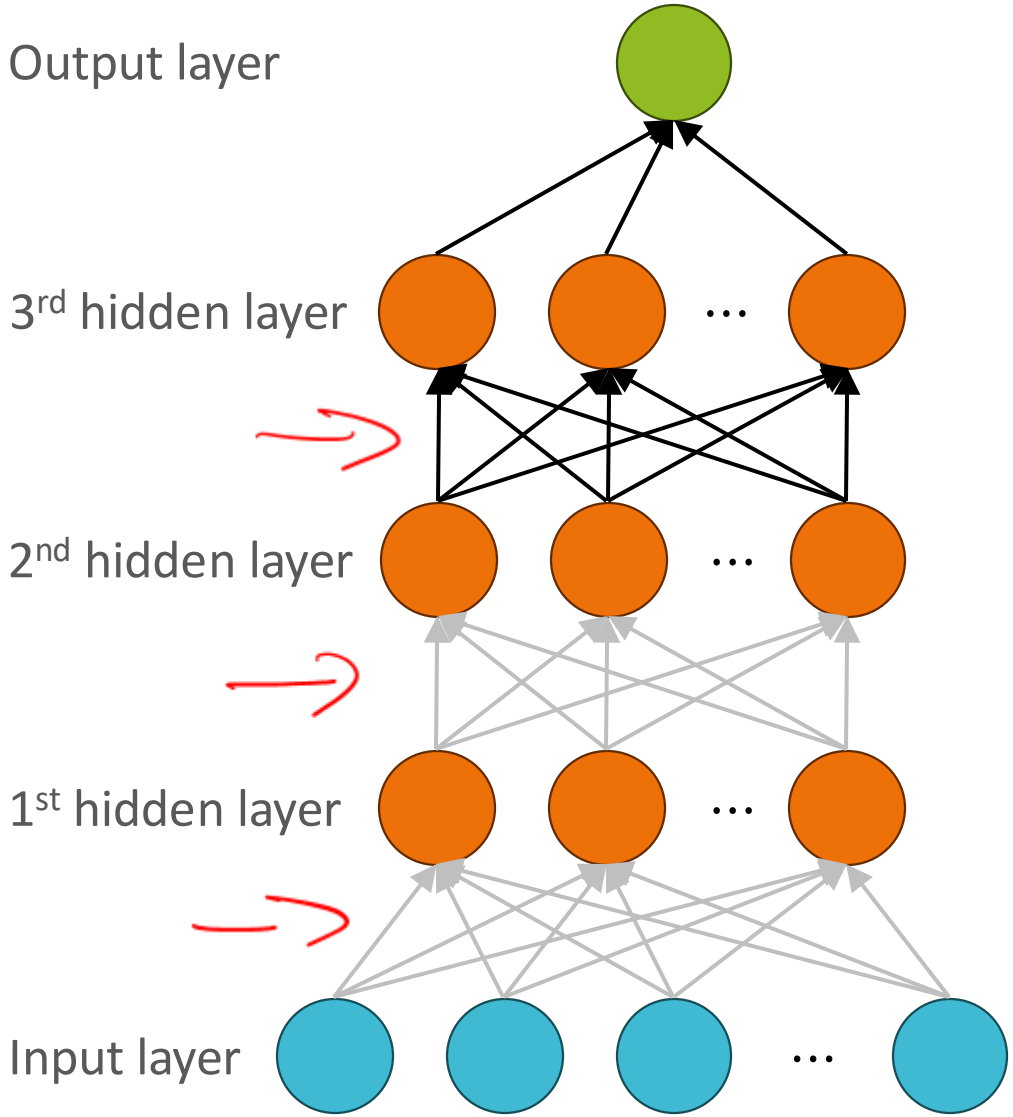

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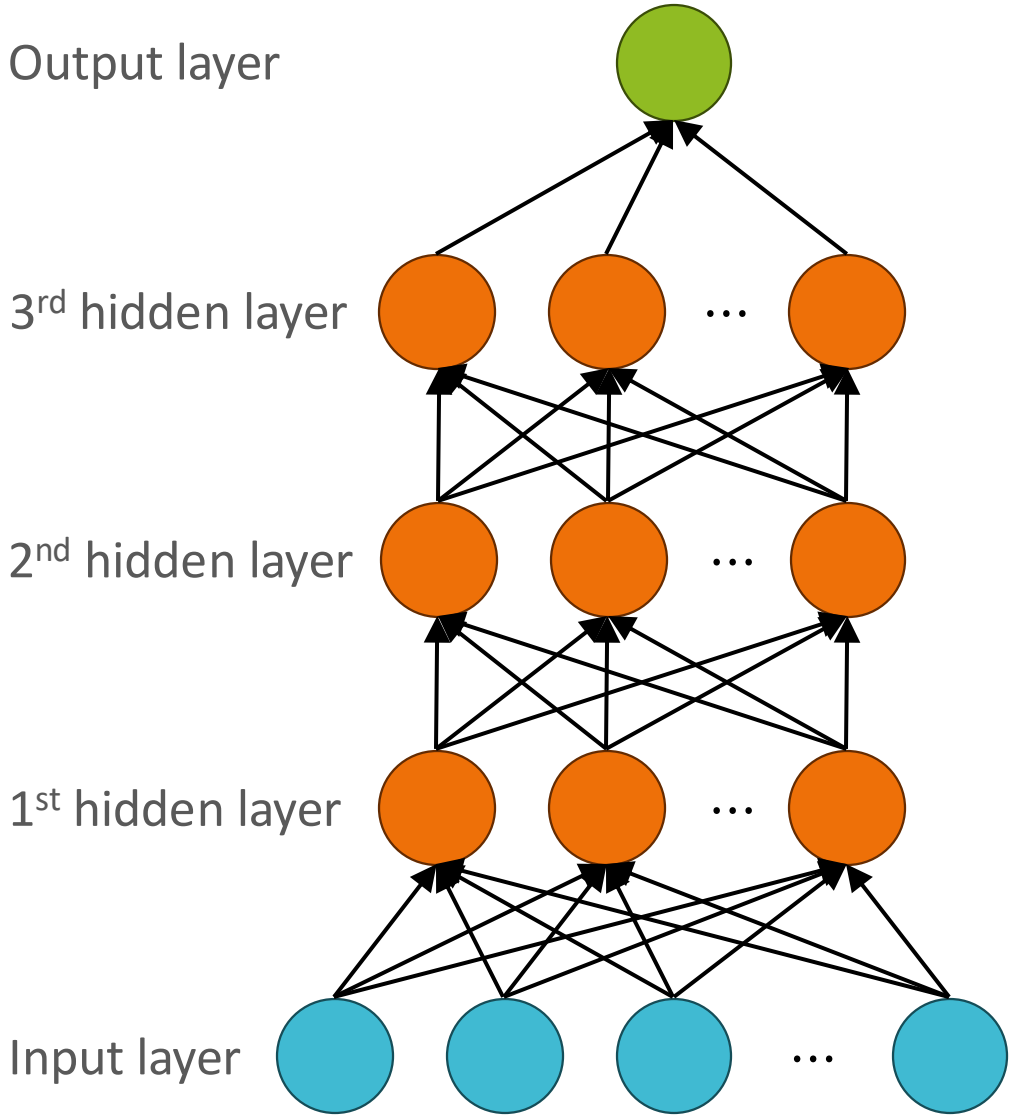
Fine-tuning (Bengio et al., 2006)

- Train each layer of the network iteratively using the training dataset
- Use the pre-trained weights as an initialization and *fine-tune* the entire network e.g., via SGD with the training dataset



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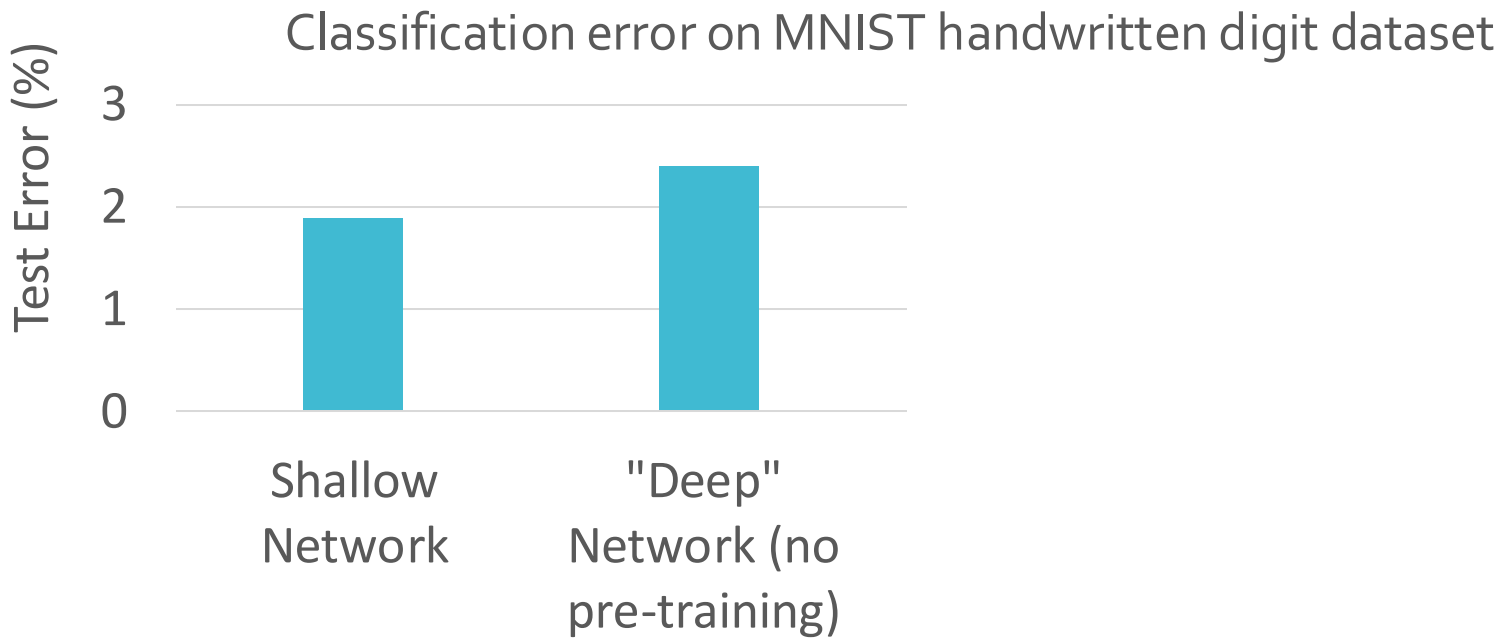
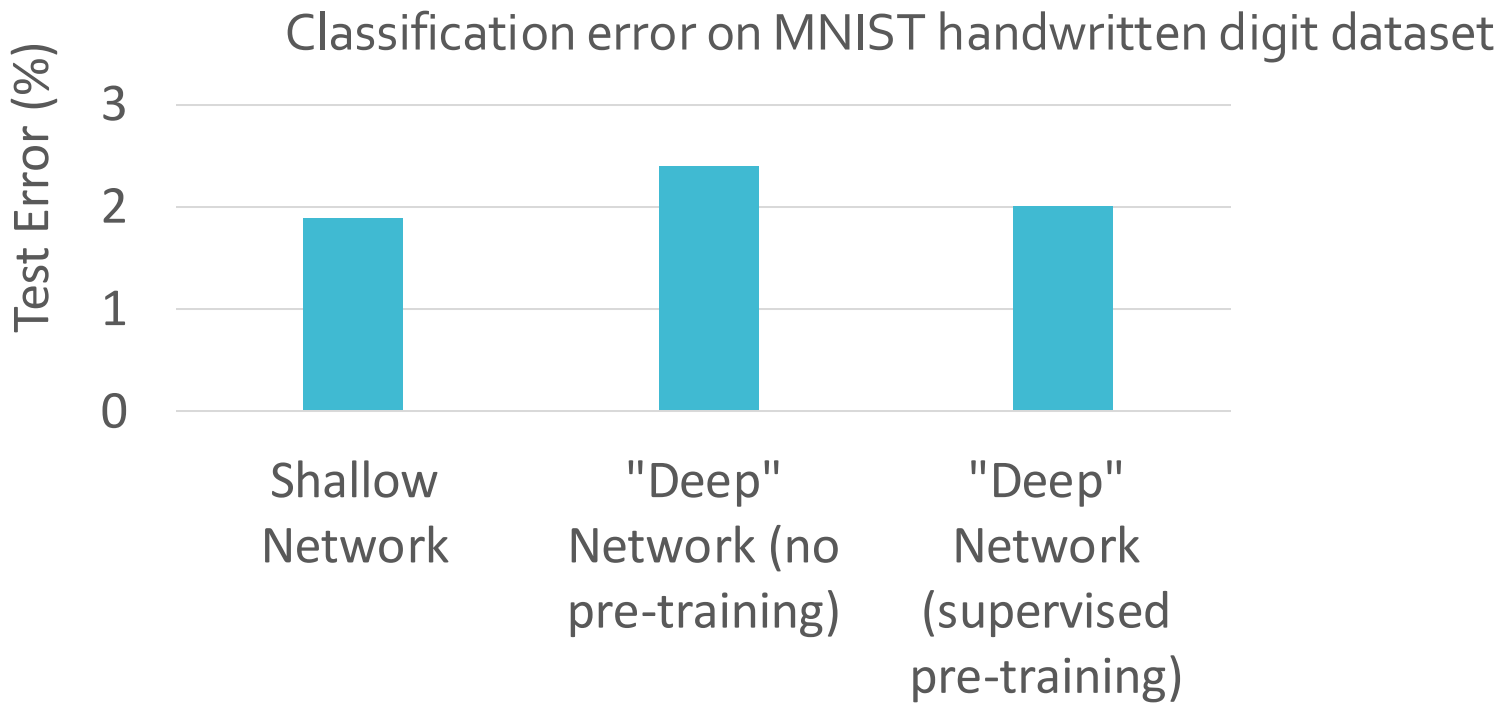


Supervised Pre-training (Bengio et al., 2006)

- Train each layer of the network iteratively using the training dataset *to predict the labels*
- Use the pre-trained weights as an initialization and *fine-tune* the entire network e.g., via SGD with the training dataset



Is this the only thing we could do with the training data?

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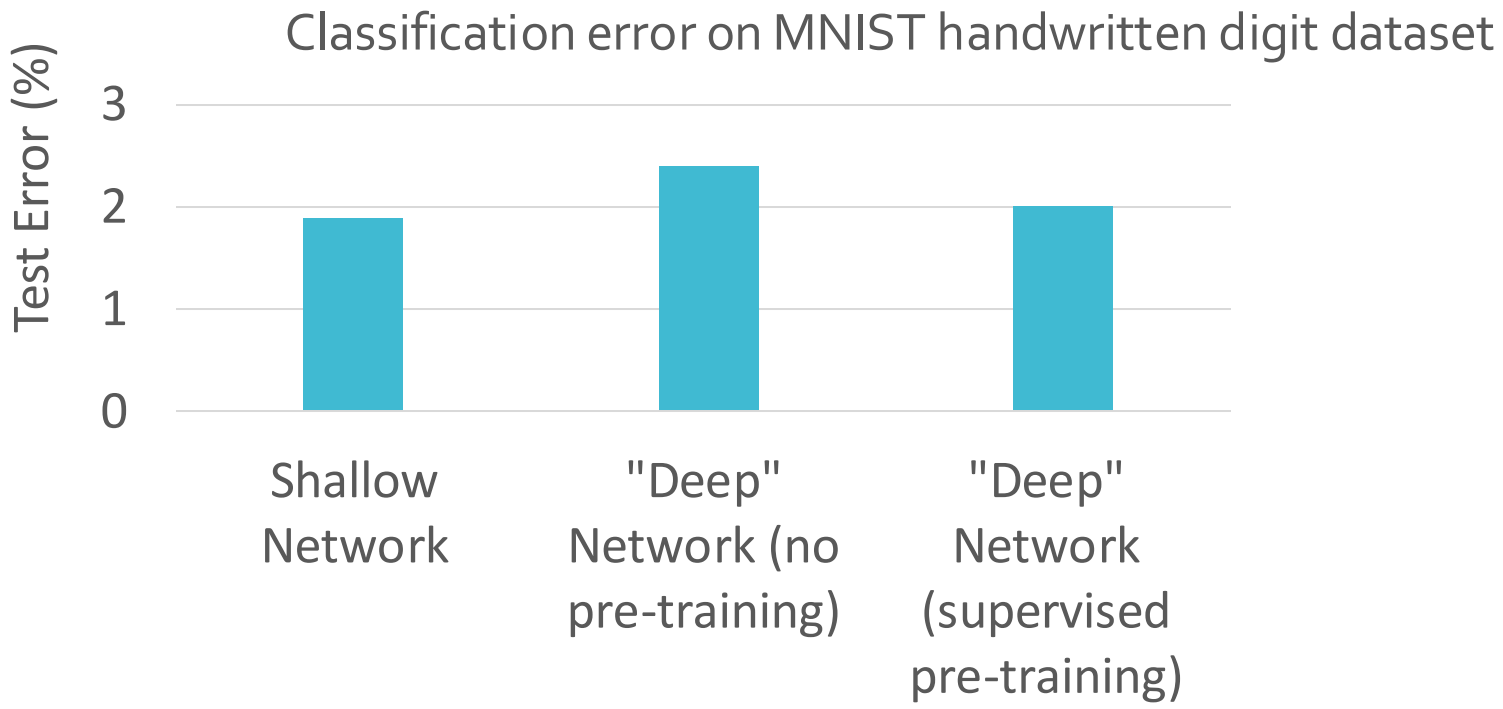
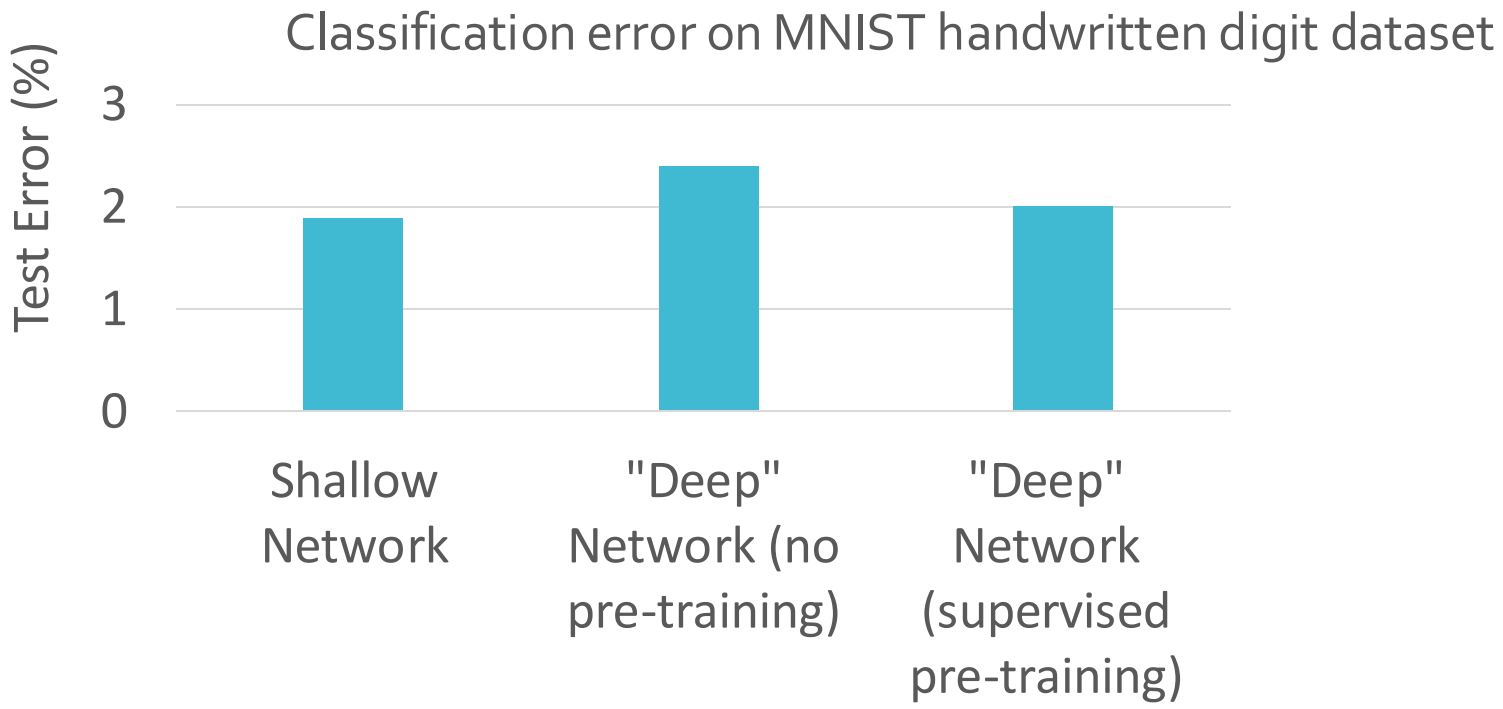


Unsupervised Pre-training (Bengio et al., 2006)

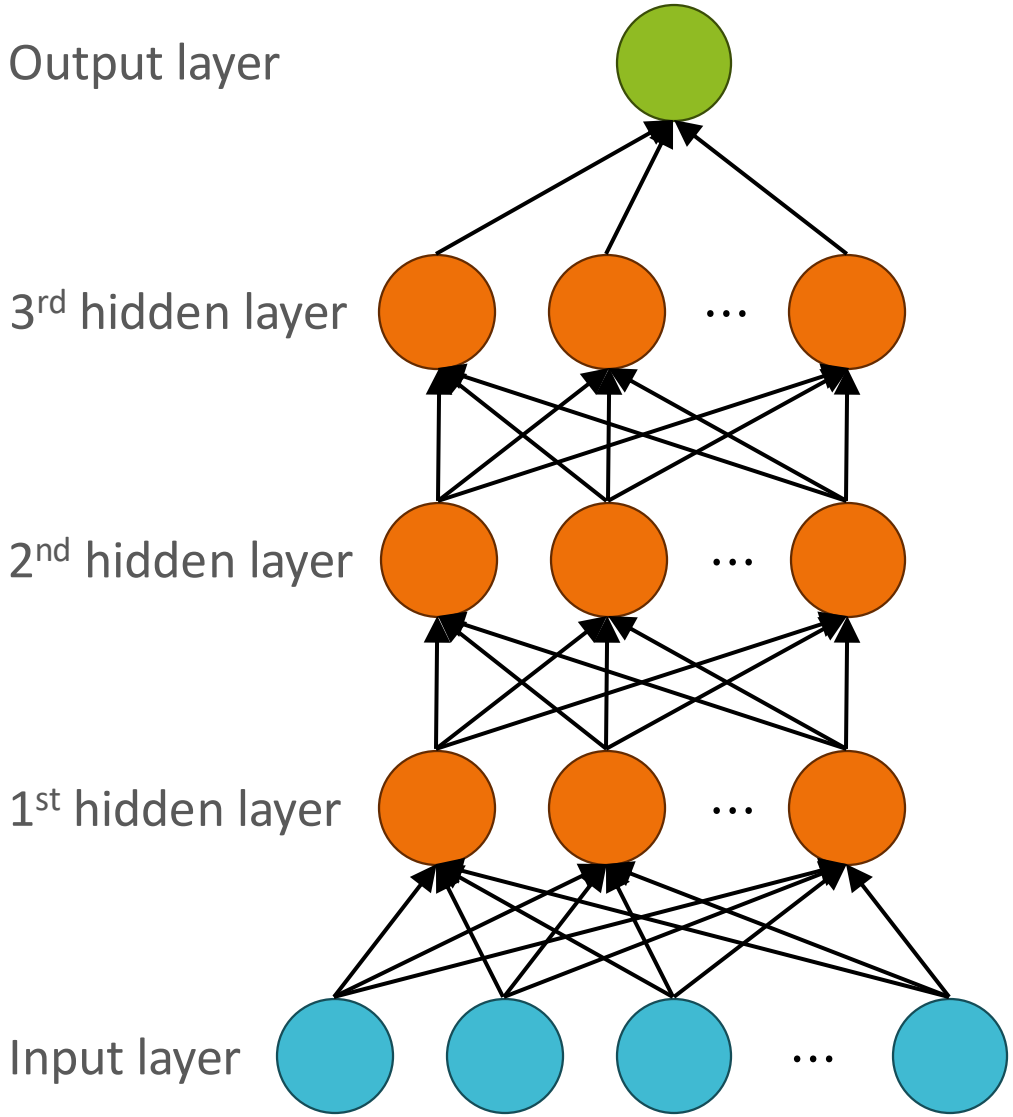
- Train each layer of the network iteratively using the training dataset *to learn useful representations*
- Idea: a good representation is one preserves a lot of information and could be used to recreate the inputs



Unsupervised Pre-training (Bengio et al., 2006)

- Train each layer of the network iteratively using the training dataset by minimizing the *reconstruction error*

$$\|\boldsymbol{x} - h(\boldsymbol{x})\|_2$$



Source: https://www.cs.toronto.edu/~larocheh/publications/dbn_supervised_tr1282.pdf

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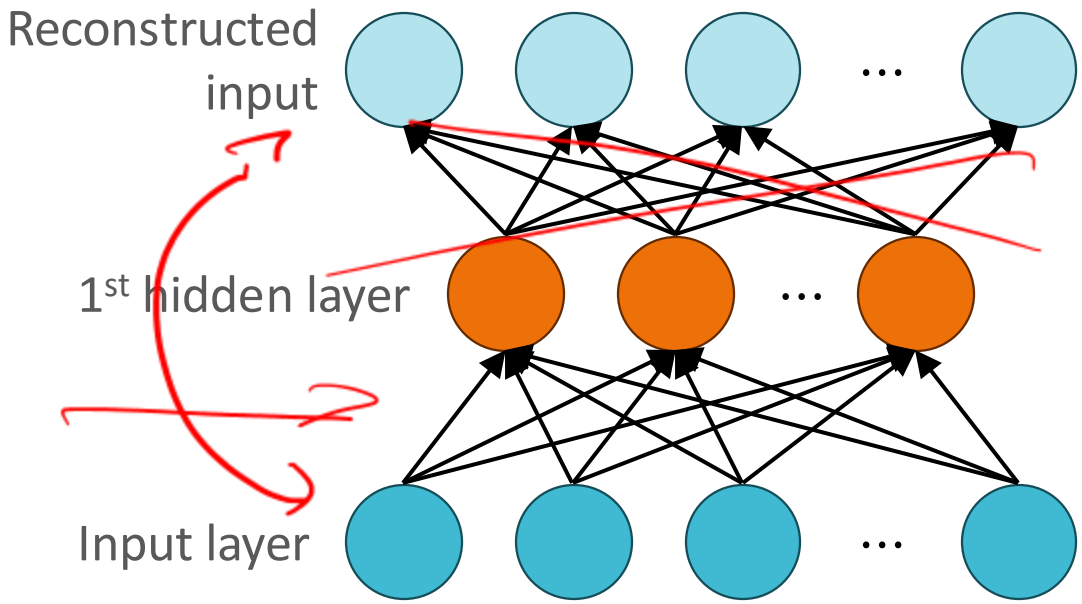
- This architecture/ objective defines an *autoencoder*



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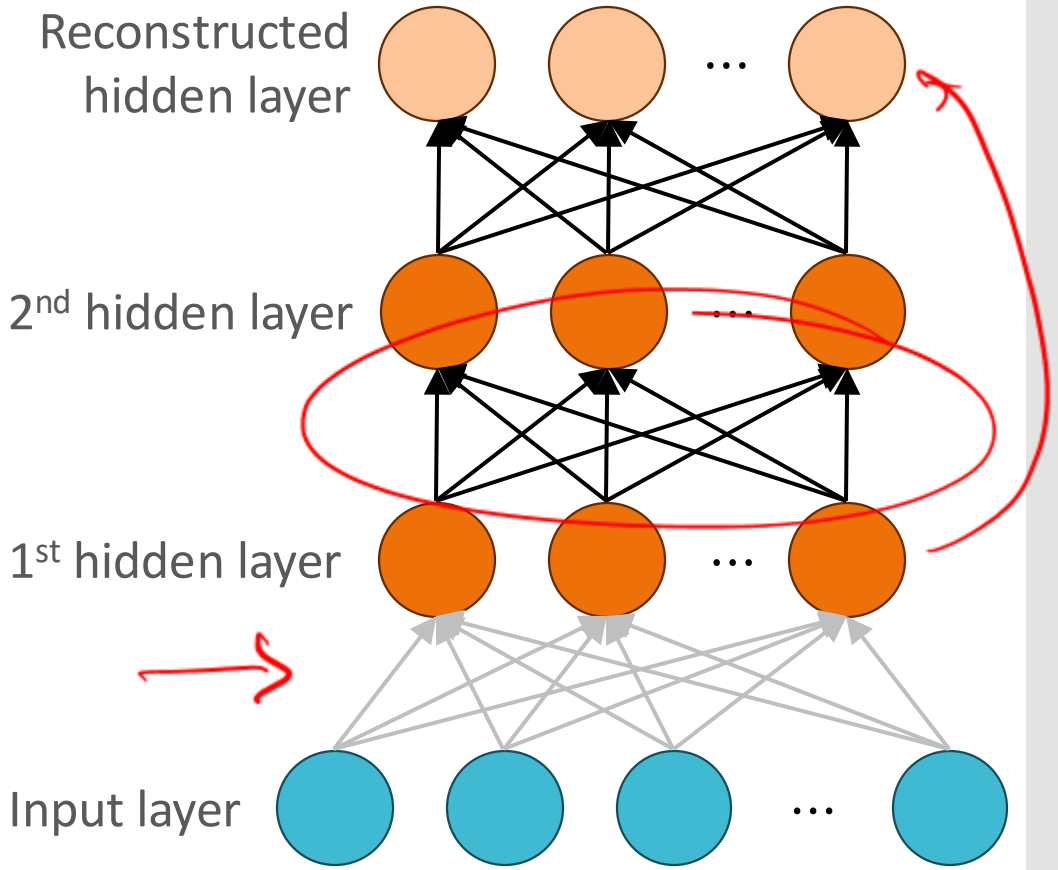

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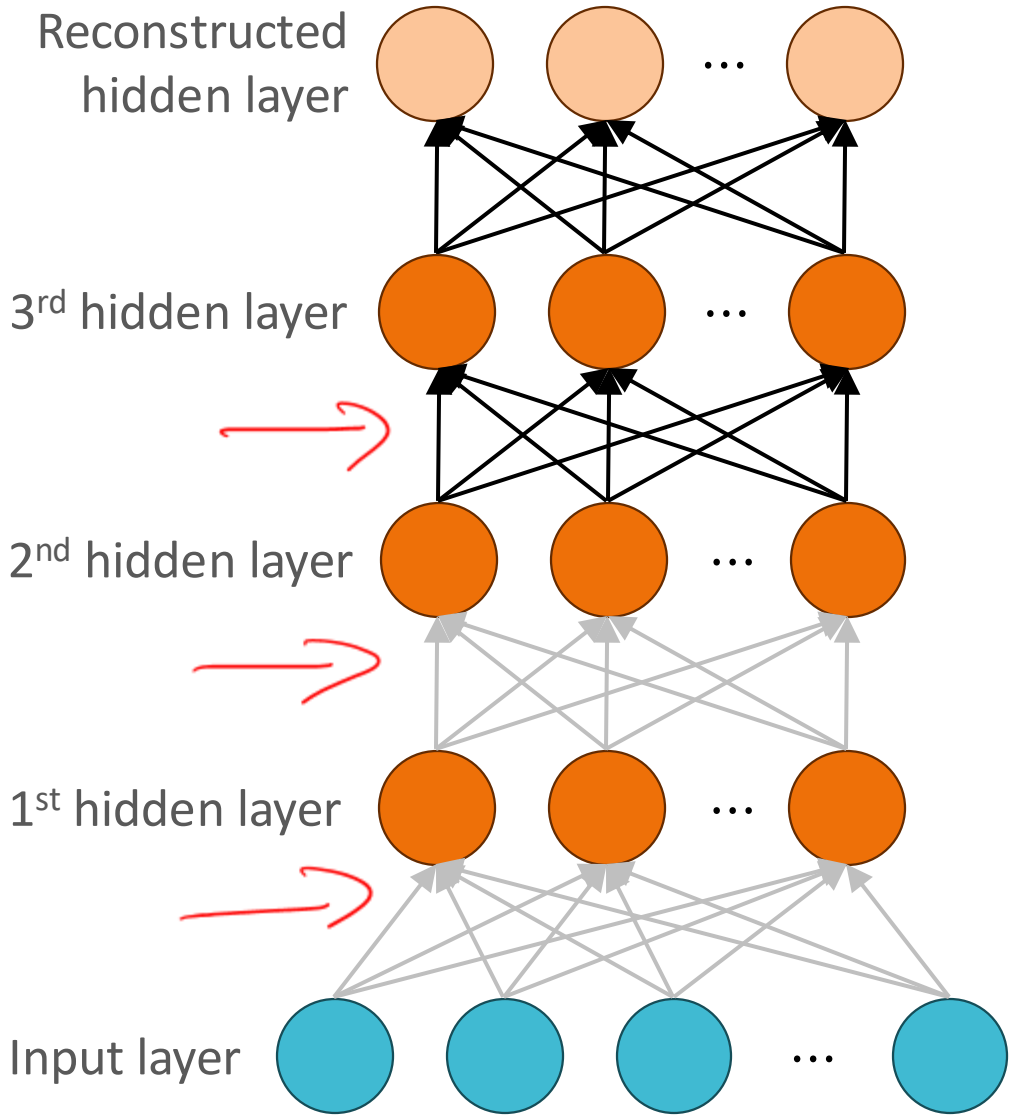

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Fine-tuning (Bengio et al., 2006)

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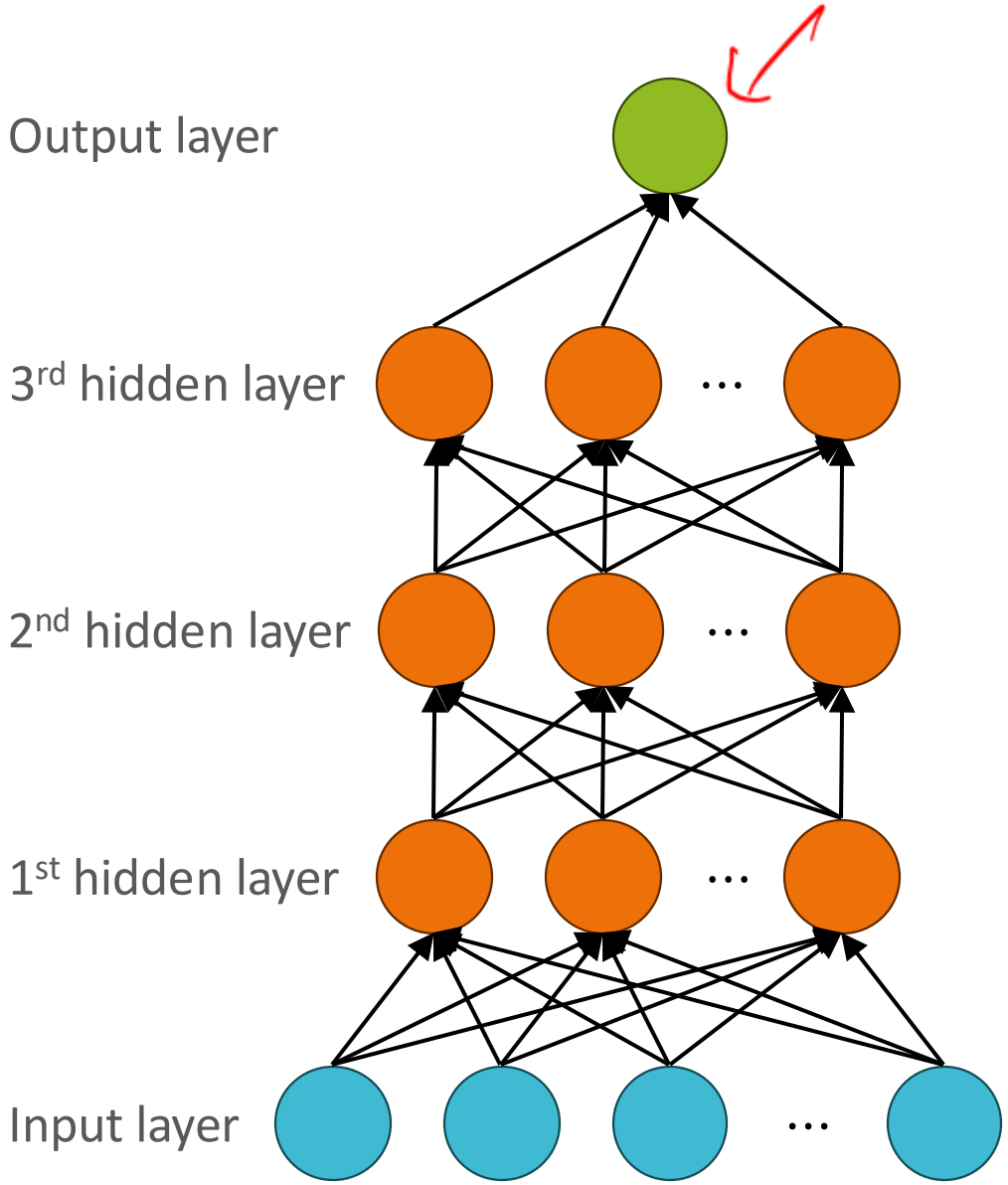
- When fine-tuning, we're effectively swapping out the last layer and fitting all the weights to the training dataset



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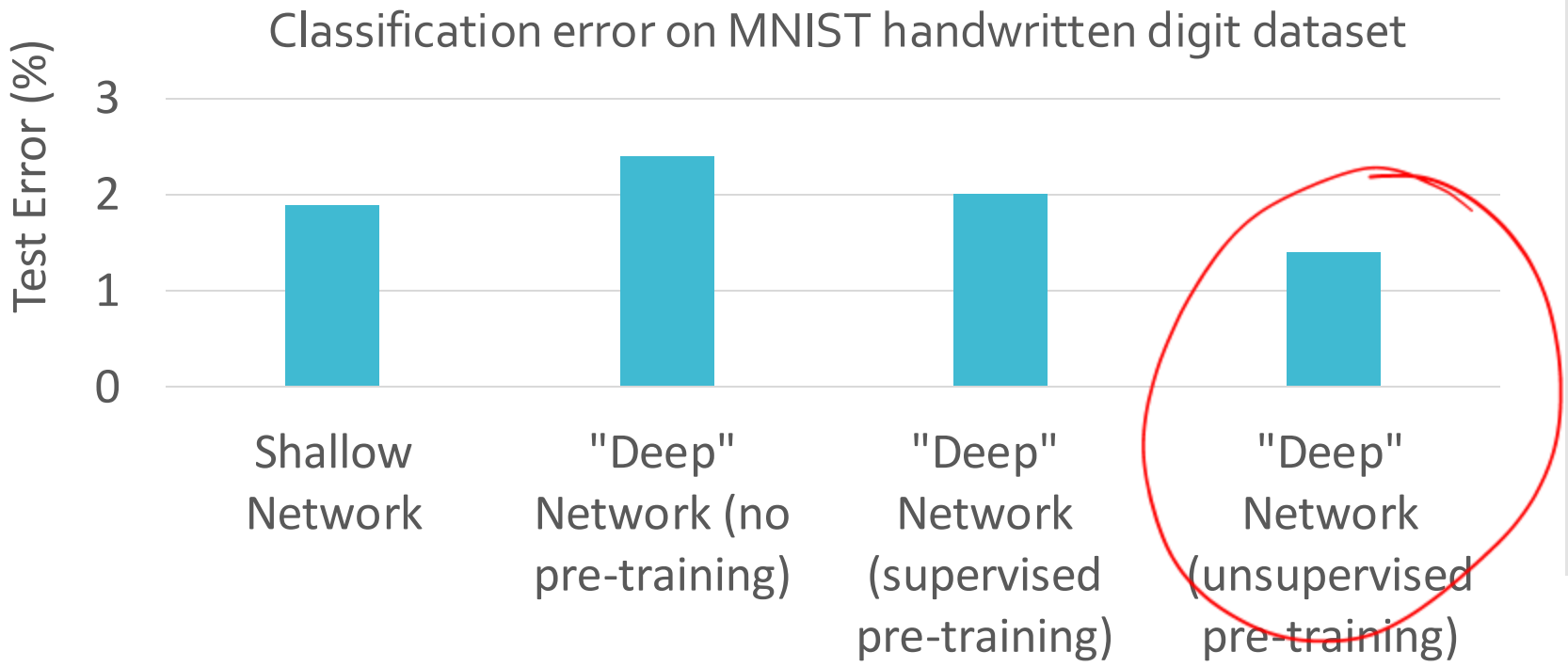
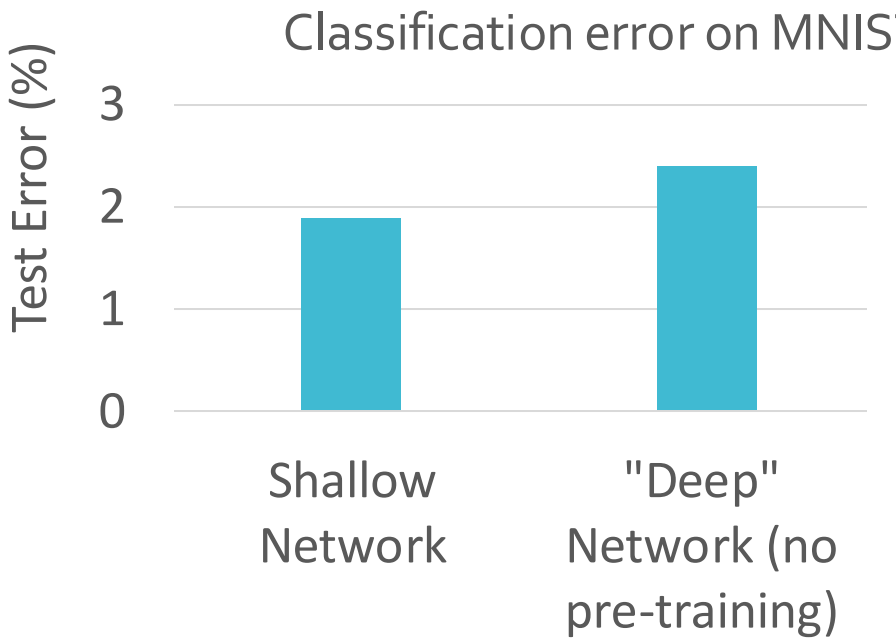


Another dose of Reality

- You have some niche task that you want to apply machine learning to e.g., predicting the author of children's books
- You have a tiny labelled dataset to train with
- You fit a massive deep learning model to the dataset
- Surprise, surprise: it overfits and your test error is super high



- Problem: what if you don't even have enough data to train a single layer/fine-tune the pre-trained network?

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- Key observation: you can pre-train on basically any labelled or unlabelled dataset!
  - Ideally, you want to use a *large* dataset *related* to your goal task

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  - GPT-3 pre-training data:

Dataset	Quantity (tokens)	Weight in training mix
Common Crawl (filtered)	410 billion	60%
WebText2	19 billion	22%
Books1	12 billion	8%
Books2	55 billion	8%
Wikipedia	3 billion	3%

Source: https://arxiv.org/pdf/2005.14165.pdf

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- Surprise, surprise: it overfits and your test error is super high
- Key observation: you can pre-train on basically any labelled or unlabelled dataset!
- Okay that's great for pre-training and all, but what if
  A. you don't have enough data to fine-tune your model?
  B. the concept of labelled data doesn't apply to your task i.e., not every input has a "correct" label e.g., chatbots?

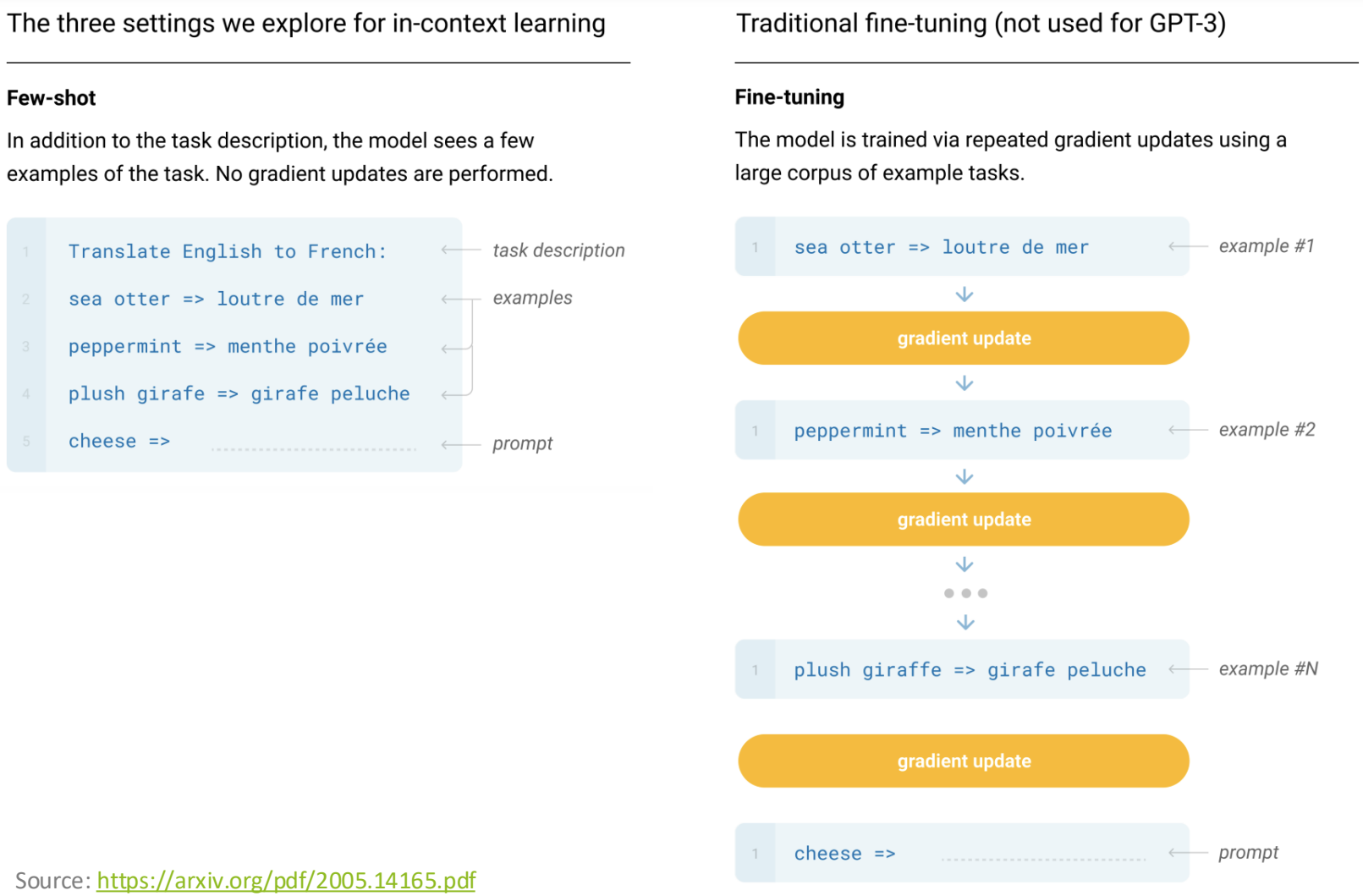
In-context Learning

- Problem: given their size, effectively fine-tuning LLMs can require lots of labelled data points.
- Idea: leverage the LLM's context window by passing a few examples to the model as input, *without performing any updates to the parameters*
- Intuition: during training, the LLM is exposed to a *massive* number of examples/tasks and the input conditions the model to "locate" the relevant concepts

Source: https://arxiv.org/pdf/2111.02080.pdf

Few-shot, One-shot & Zero-shot (in-context) Learning

- Idea: leverage the LLM's context window by passing a few examples to the model as input, *without performing any updates to the parameters*



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Few-shot, One-shot & Zero-shot (in-context) Learning

- Idea: leverage the LLM's context window by passing ~~a~~ ~~few~~ one examples~~s~~ to the model as input, *without performing any updates to the parameters*

The three settings we explore for in-context learning

One-shot

In addition to the task description, the model sees a single example of the task. No gradient updates are performed.

```
1  Translate English to French:        ← task description
2  sea otter => loutre de mer          ← example
3  cheese =>                           ← prompt
```

Traditional fine-tuning (not used for GPT-3)

Fine-tuning

The model is trained via repeated gradient updates using a large corpus of example tasks.

```
1  sea otter => loutre de mer          ← example #1
```

gradient update

```
1  peppermint => menthe poivrée        ← example #2
```

gradient update

...

```
1  plush giraffe => girafe peluche     ← example #N
```

gradient update

```
1  cheese =>                           ← prompt
```

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Few-shot, One-shot & Zero-shot (in-context) Learning

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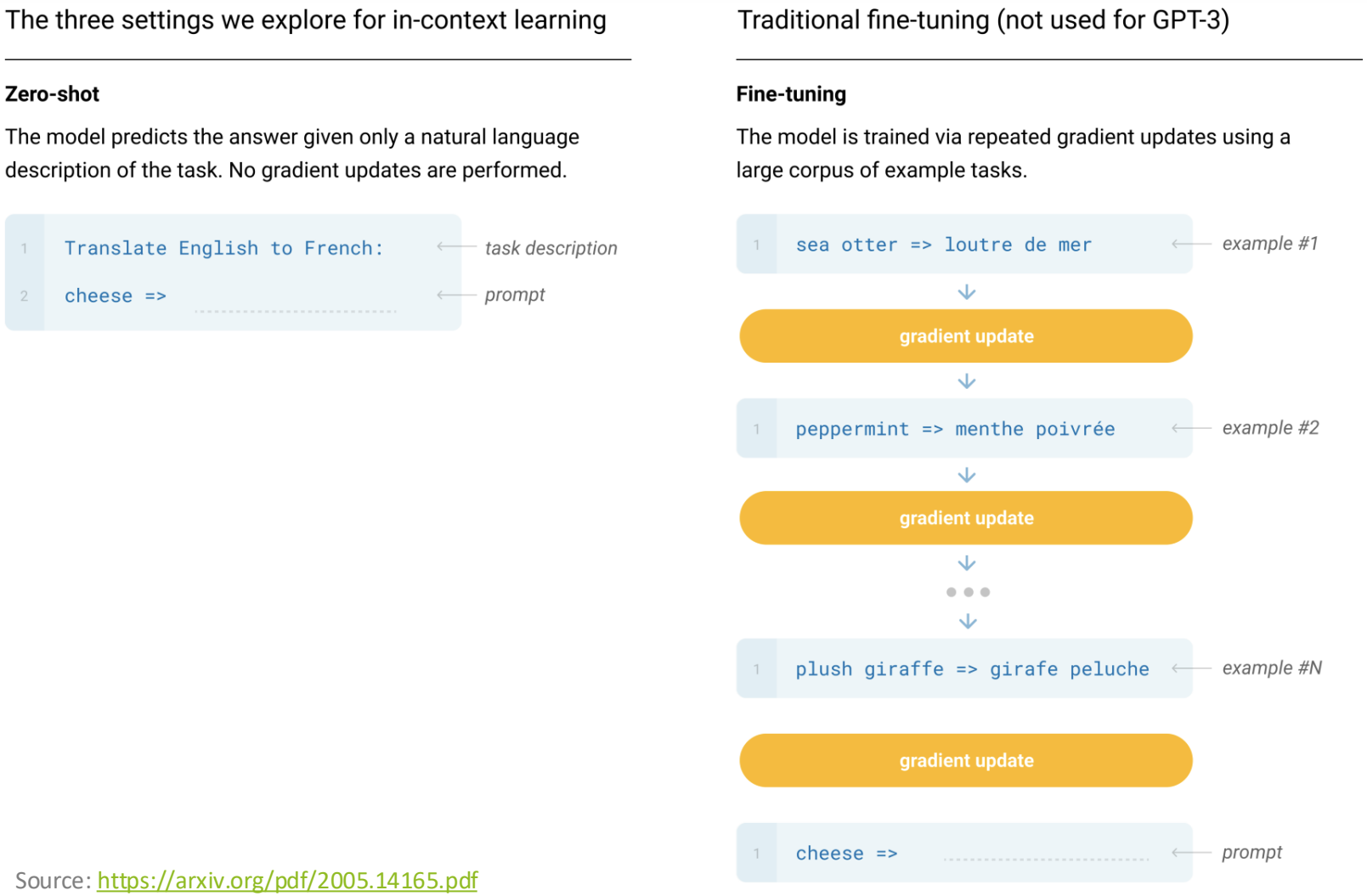

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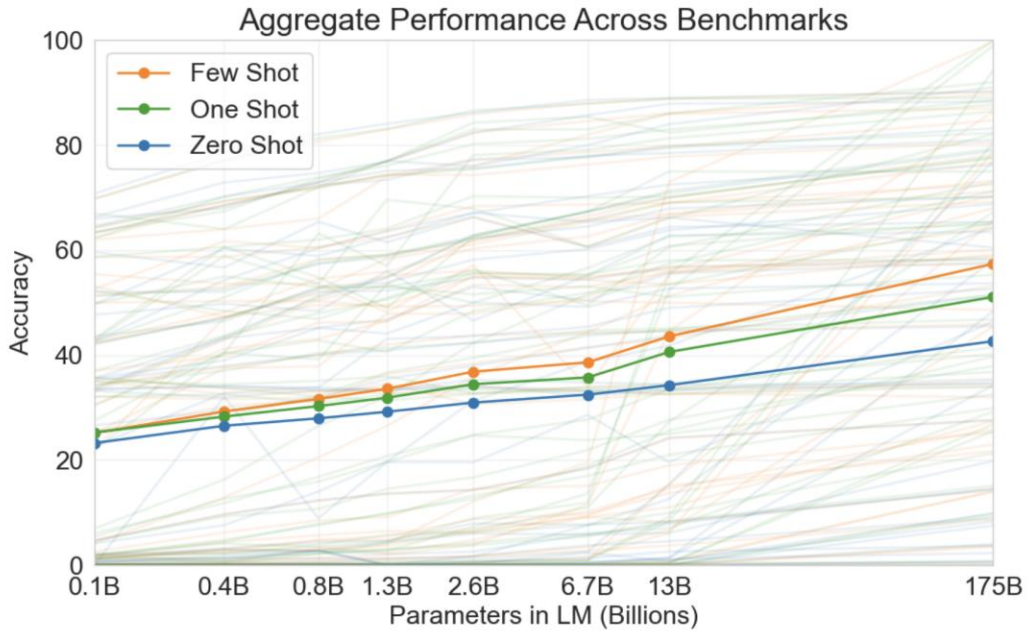


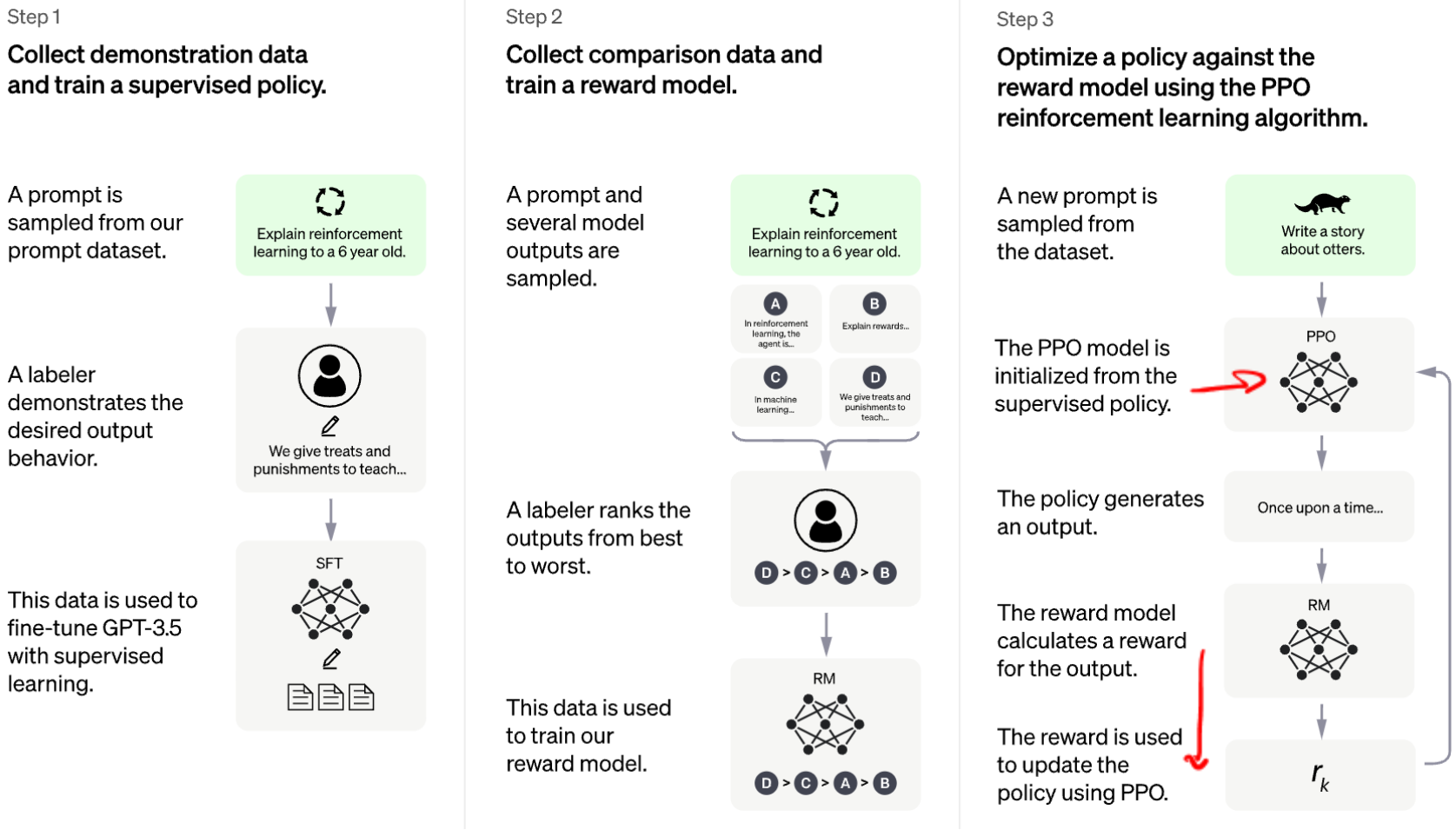
- Key Takeaway: LLMs can perform well on novel tasks without having to fine-tune the model, sometimes even with just one or zero labelled training data points!

Source: https://arxiv.org/pdf/2005.14165.pdf

Reinforcement Learning from Human Feedback (RLHF)

- Insight: for many machine learning tasks, there is no universal ground truth, e.g., there are lots of possible ways to respond to a question or prompt.
- Idea: use human feedback to determine how good or bad some prediction/response is!
- Issue: if the input space is huge (e.g., all possible chat prompts), to train a good model, we might need tons and tons of (potentially expensive) human annotation…
- Idea: use a small number of annotations to learn a "reward" function!

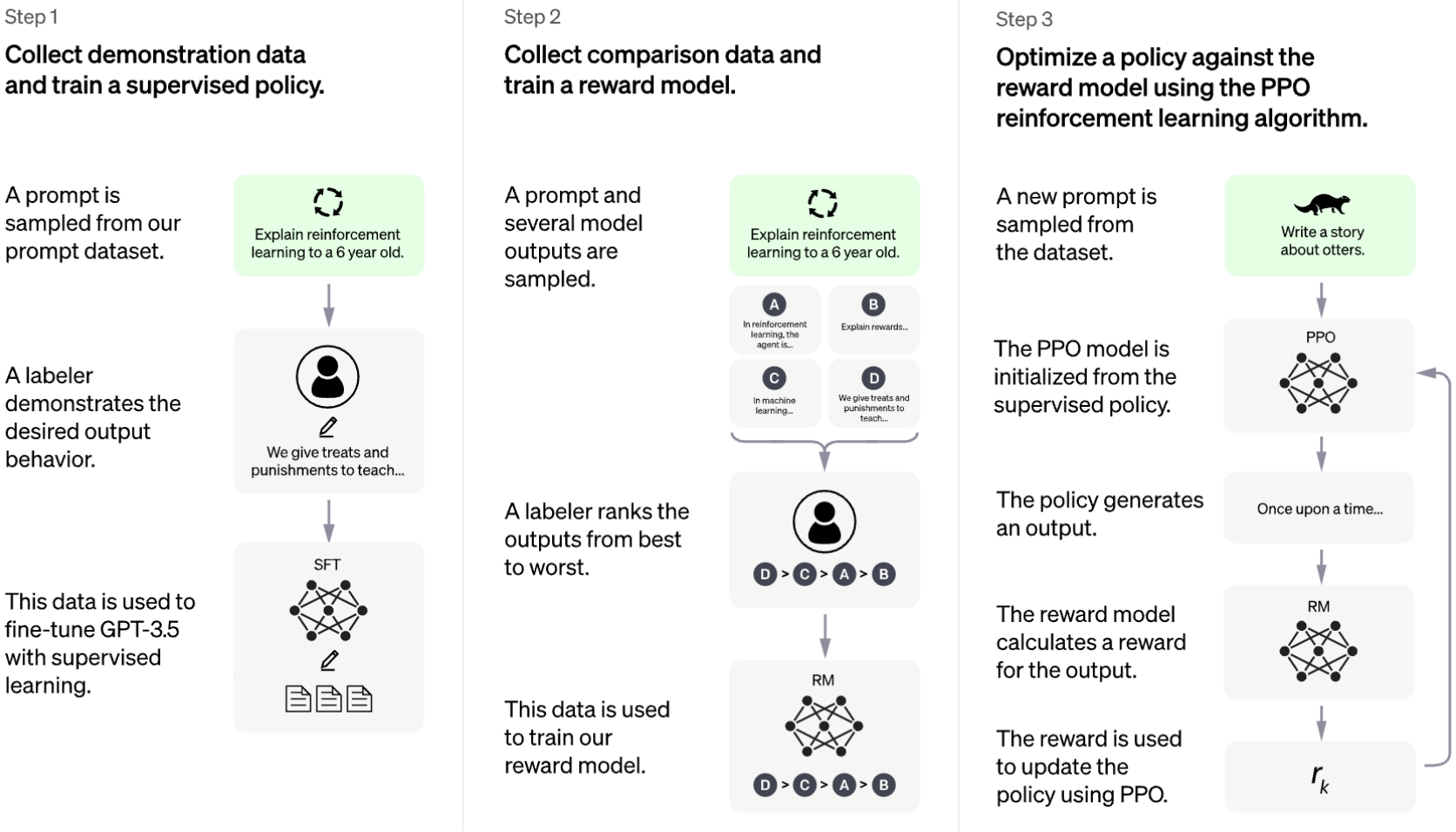
Reinforcement Learning from Human Feedback (RLHF)



- RLHF is a form of fine-tuning that uses reinforcement learning where the reward function is learned from human preferences

Source: https://openai.com/blog/chatgpt

What the heck is "Reinforcement Learning"?



- RLHF is a form of fine-tuning that uses *reinforcement learning* where the reward function is learned from human preferences

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