10-701: Introduction to Machine Learning Lecture 18 – Pretraining, Fine-tuning & In-Context Learning

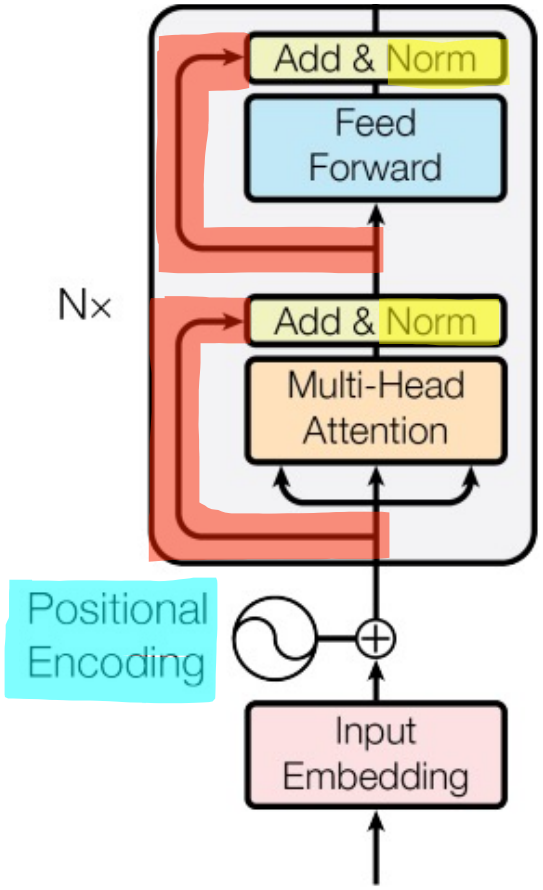
Henry Chai

3/25/24

Front Matter

- Announcements:
  - HW5 released 3/22, due 4/1 at 11:59 PM
  - Project mentors will be assigned later this week
    - Recitation on 3/29 is dedicated time to meet with your project mentors
    - **Your group must meet with your assigned project mentor and receive approval on your proposal to move forward to the next deliverable**
  - **Daniel is on leave and will be for an indeterminate amount of time, please direct all course requests/questions to Henry**

Okay, one massive detour later, how on earth do we go about training these things?



- 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: Mini-batch Stochastic Gradient Descent…

- Input: training dataset $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(i)}, y^{(i)}\right)\right\}_{i=1}^{N}$, step size γ, and batch size B

1. Randomly initialize the parameters $\boldsymbol{\theta}^{(0)}$ and set $t = 0$
2. While TERMINATION CRITERION is not satisfied
   a. Randomly sample B data points from $\mathcal{D}$, $\left\{\left(\boldsymbol{x}^{(b)}, y^{(b)}\right)\right\}_{b=1}^{B}$
   b. Compute the gradient of the loss w.r.t. the sampled *batch*, $\nabla J^{(B)}\left(\boldsymbol{\theta}^{(t)}\right)$
   c. Update $\boldsymbol{\theta}$: $\boldsymbol{\theta}^{(t+1)} \leftarrow \boldsymbol{\theta}^{(t)} - \gamma \nabla J^{(B)}\left(\boldsymbol{\theta}^{(t)}\right)$
   d. Increment t: $t \leftarrow t + 1$

- Output: $\boldsymbol{\theta}^{(t)}$

Mini-batch Stochastic Gradient Descent is a lie!

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Mini-batch Stochastic Gradient Descent is ~~a lie!~~ just the beginning!

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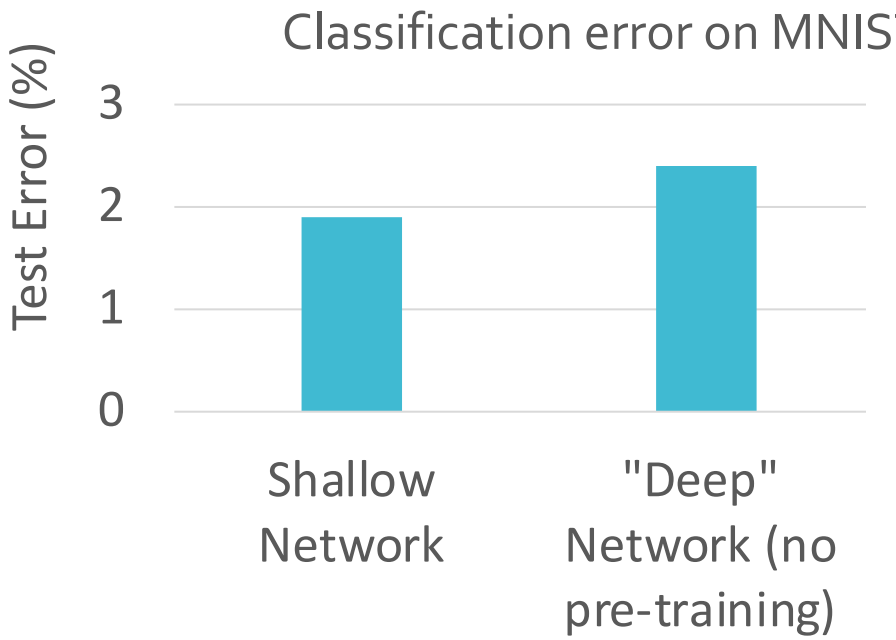
Traditional Supervised Learning

- 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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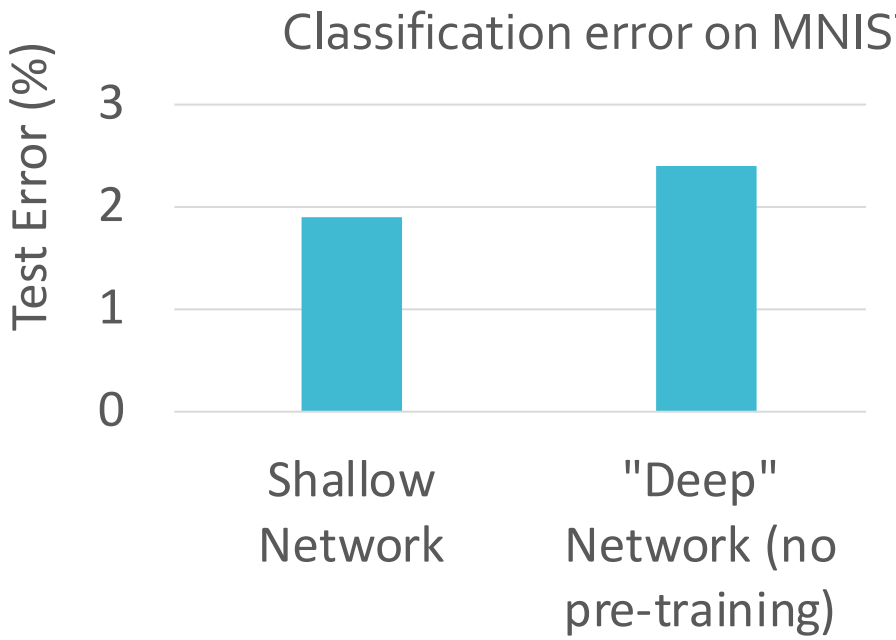
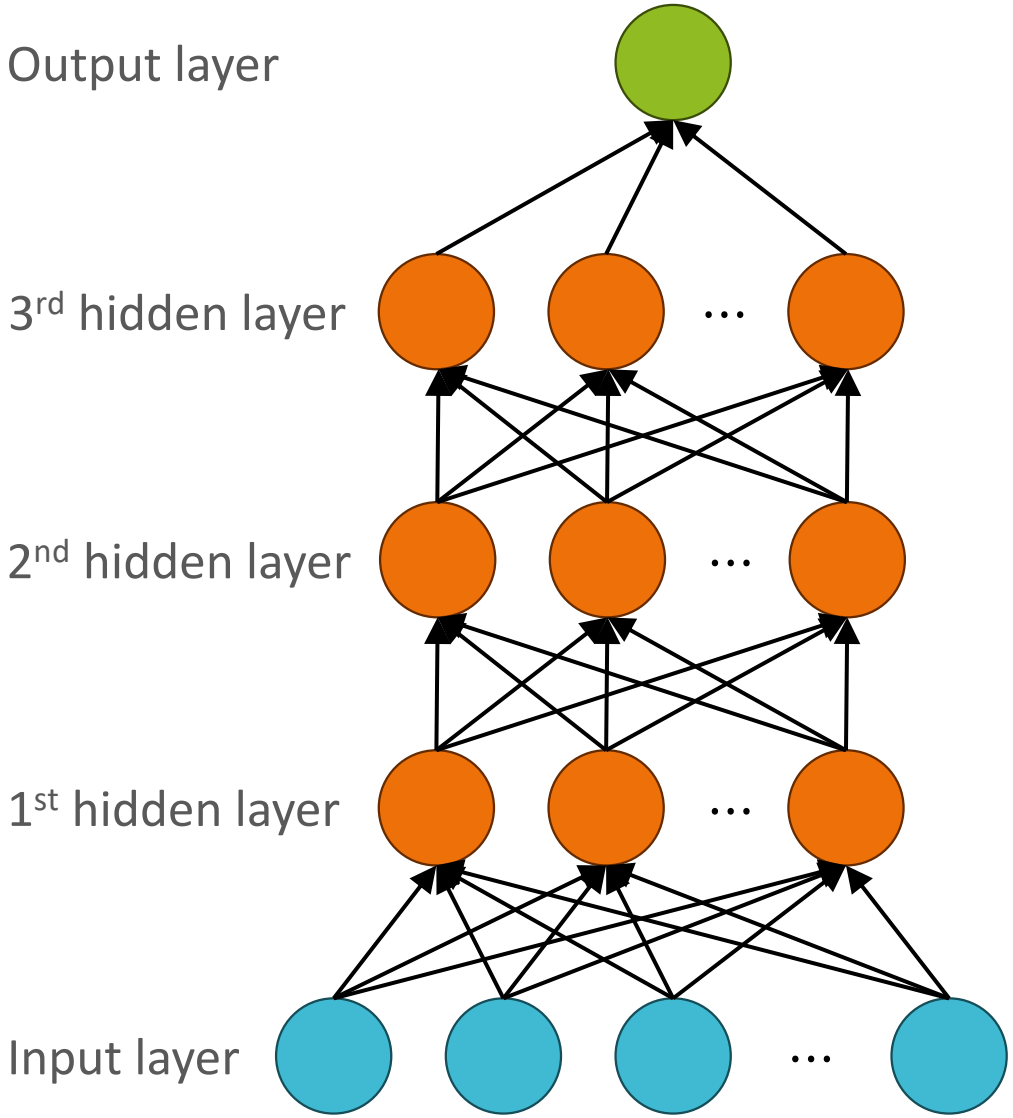


- Idea: if shallow networks are easier to train, let's just decompose our deep network into a series of shallow networks!

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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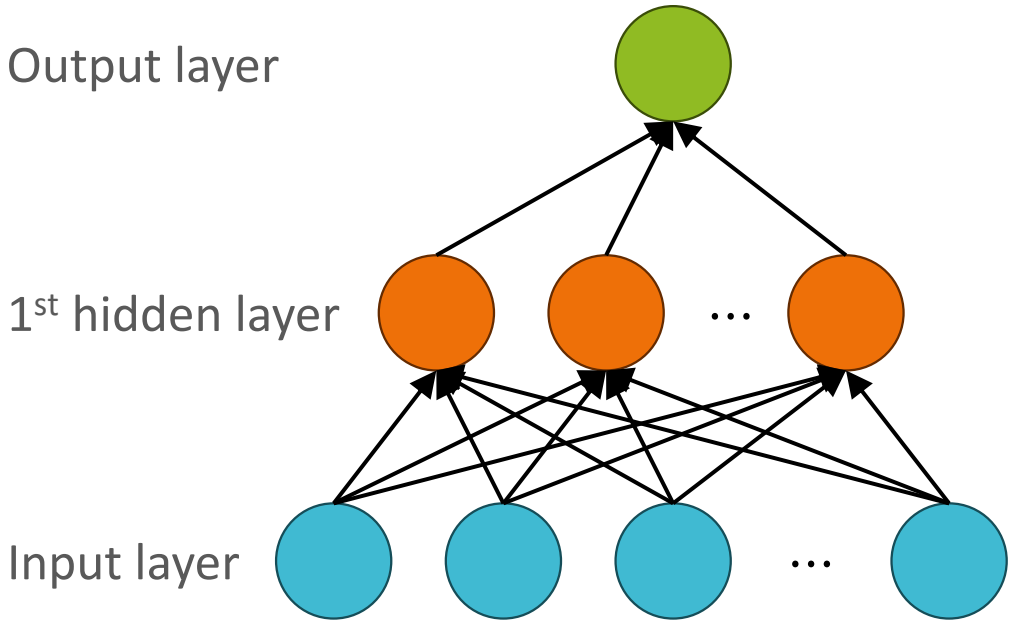

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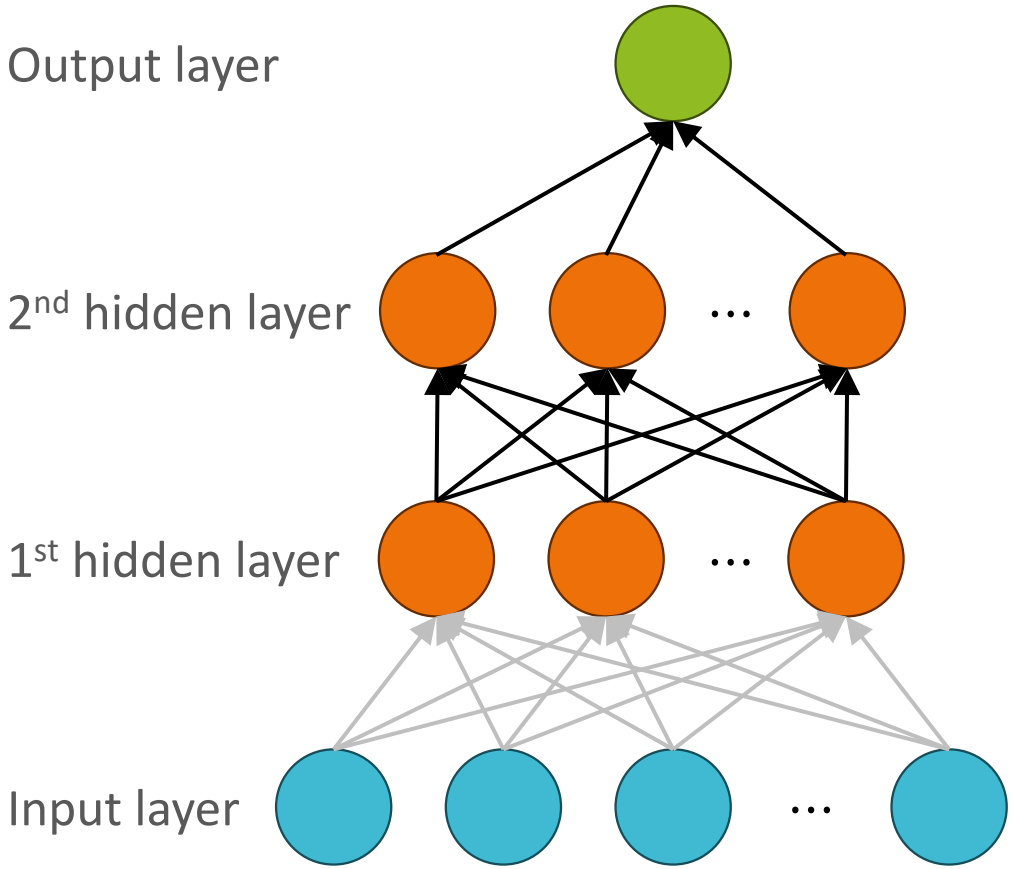

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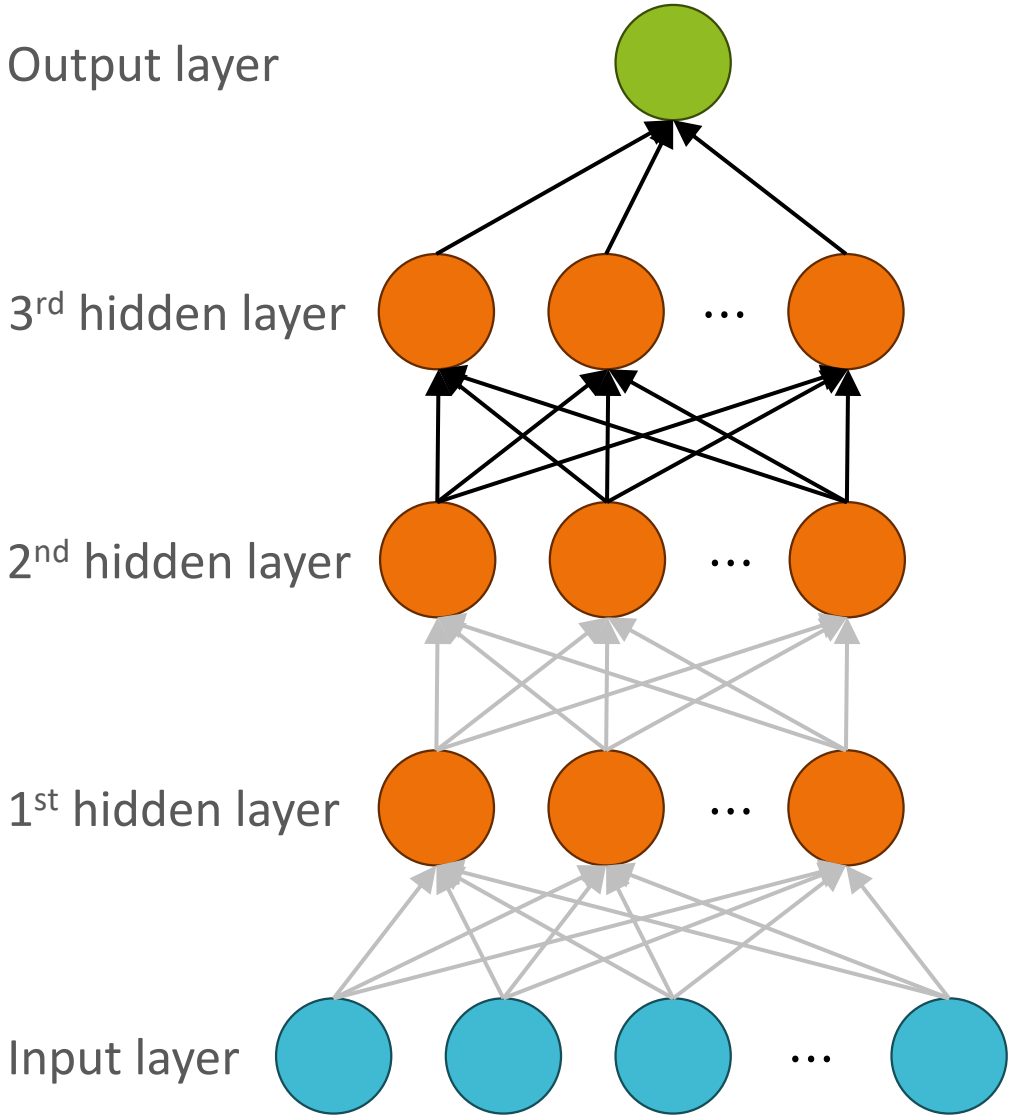

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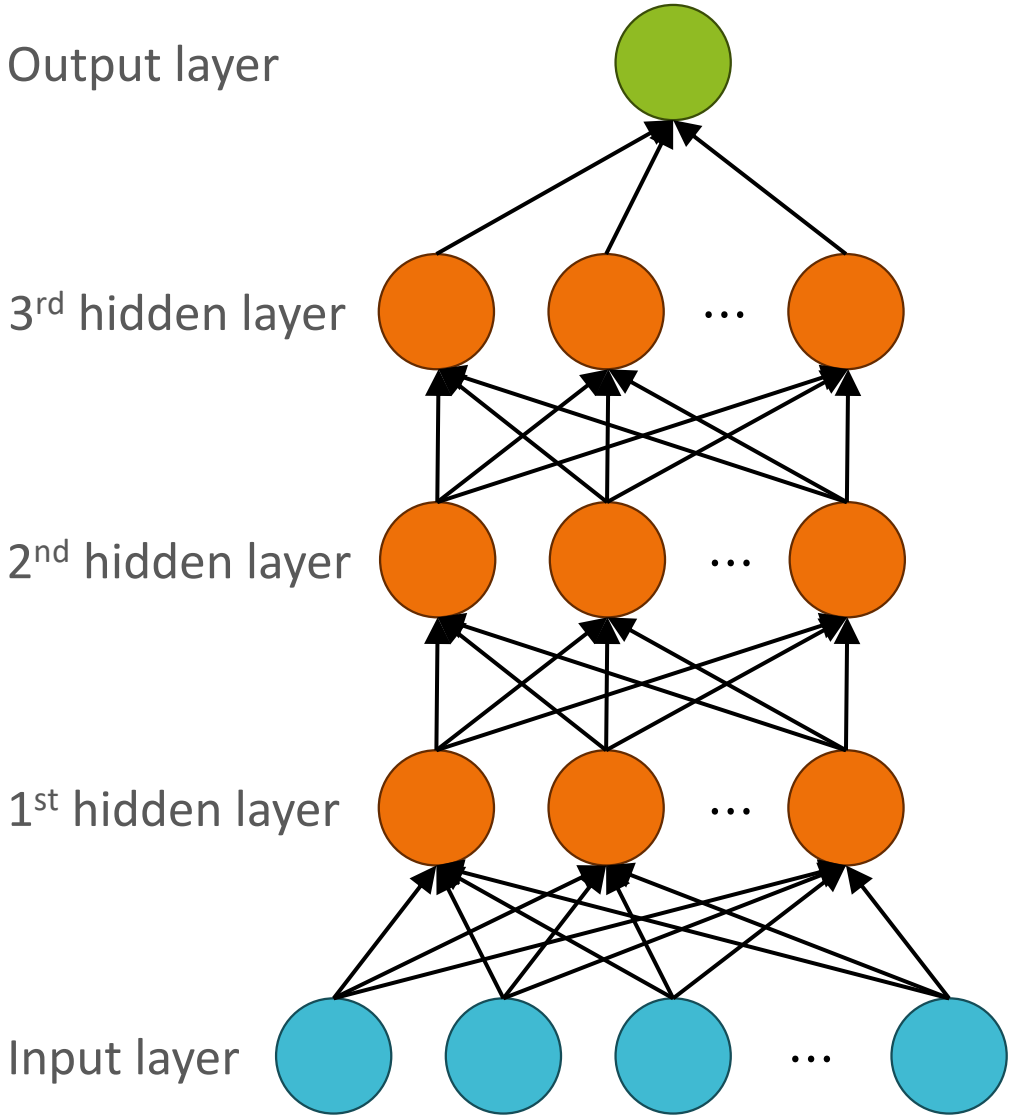
Fine-tuning (Bengio et al., 2006)

- 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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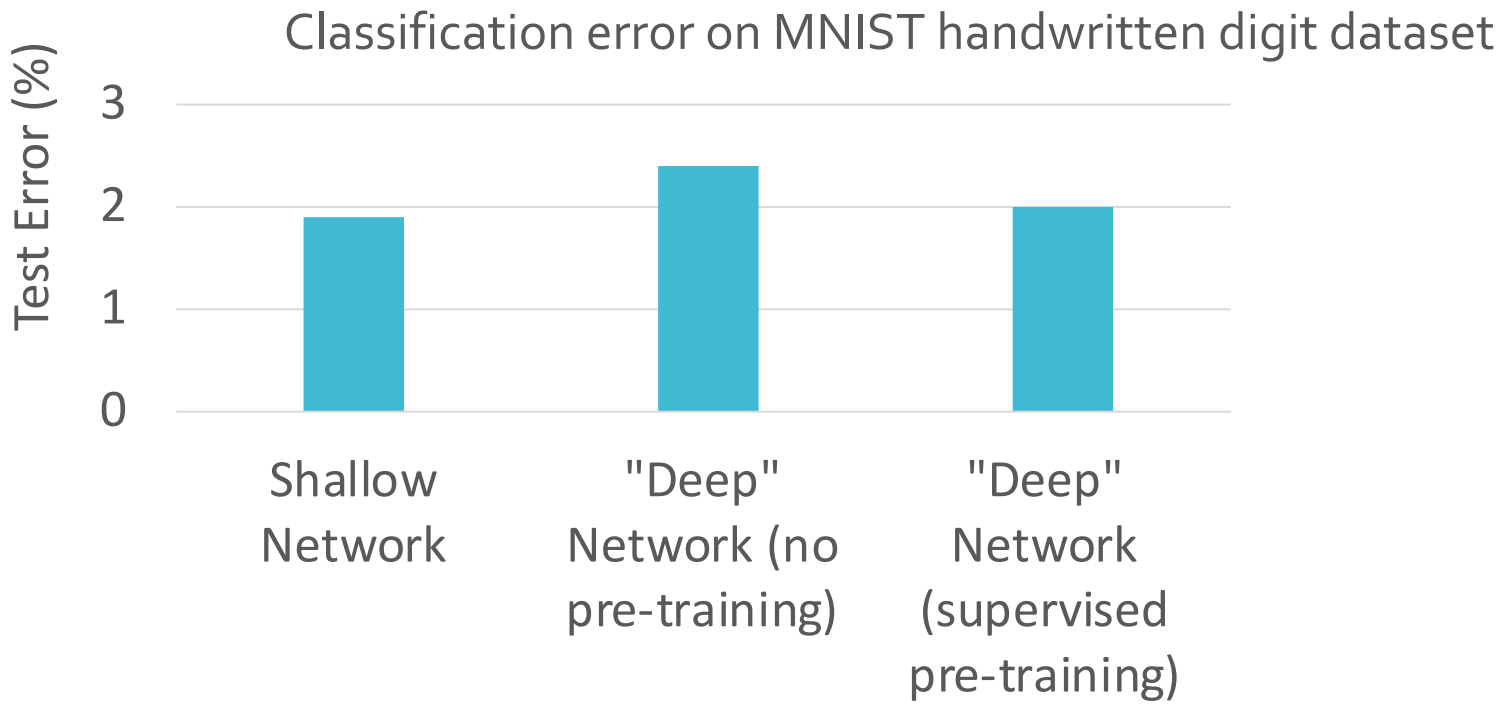

Supervised Pre-training (Bengio et al., 2006)

- Train each layer of the network iteratively using the training dataset *to predict the labels*
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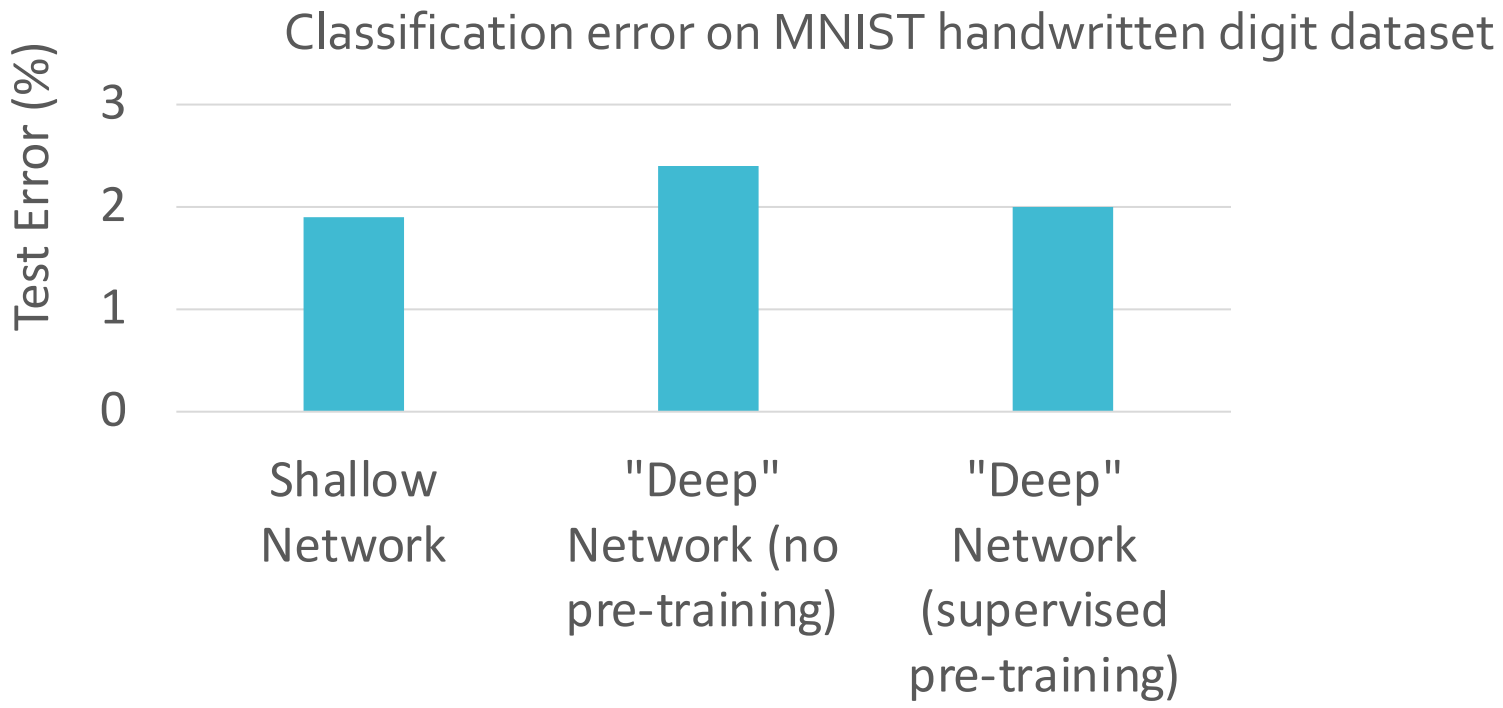
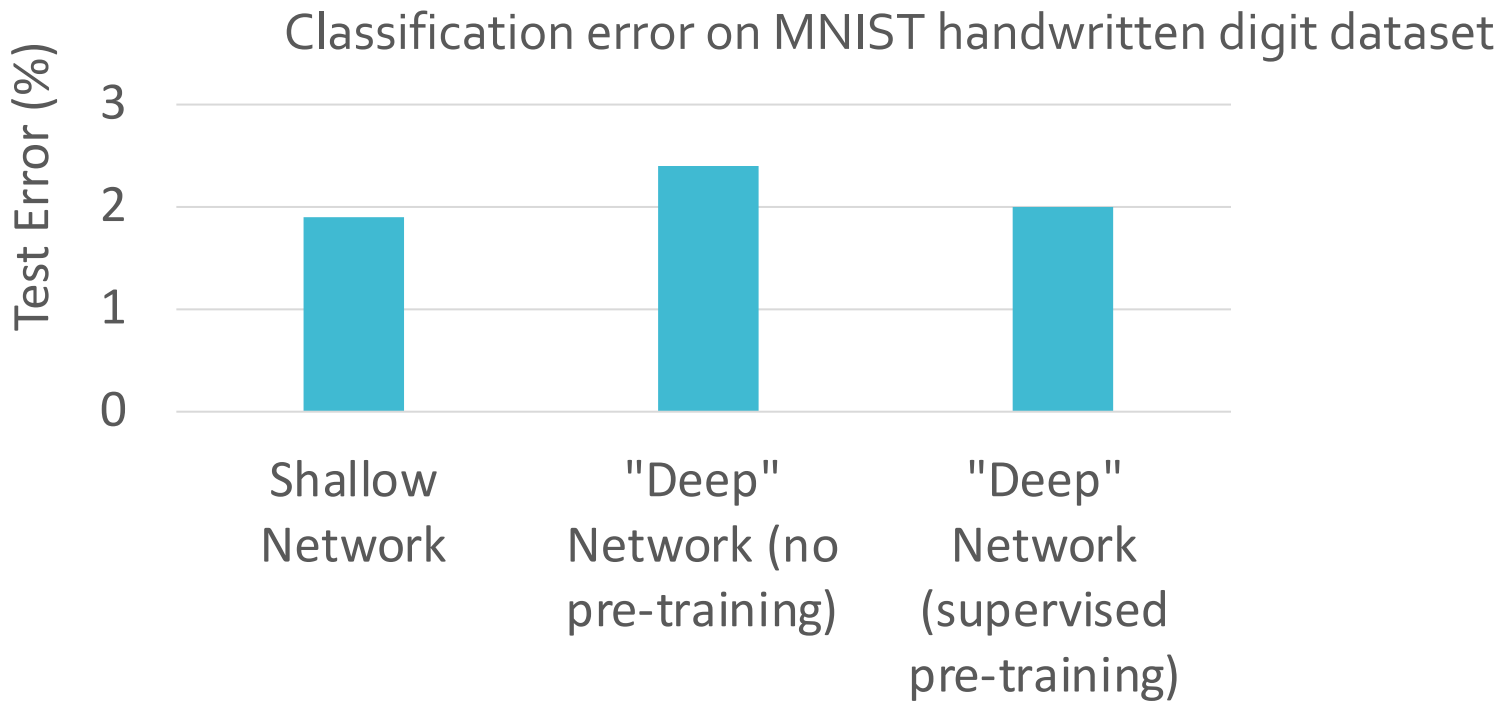


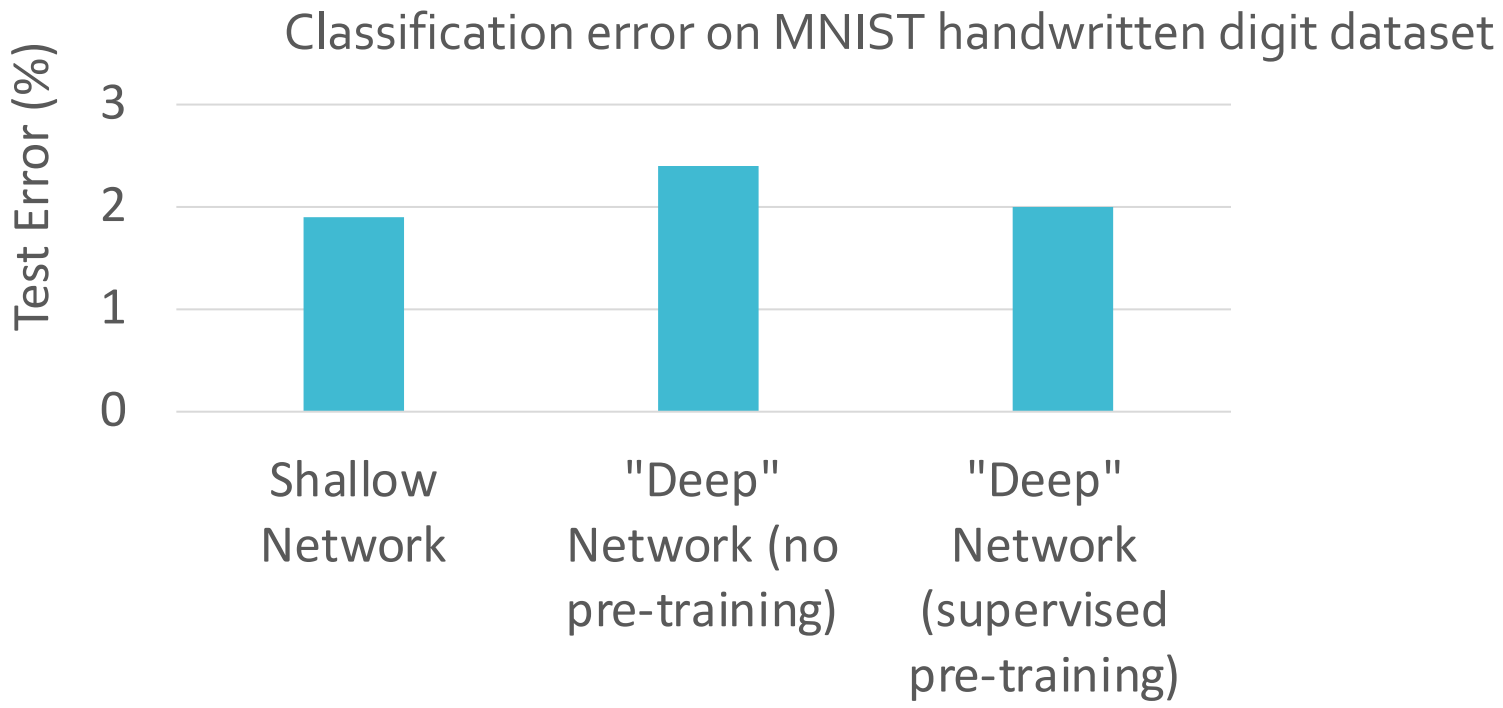
Is this the only thing we could do with the training data?

- 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



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

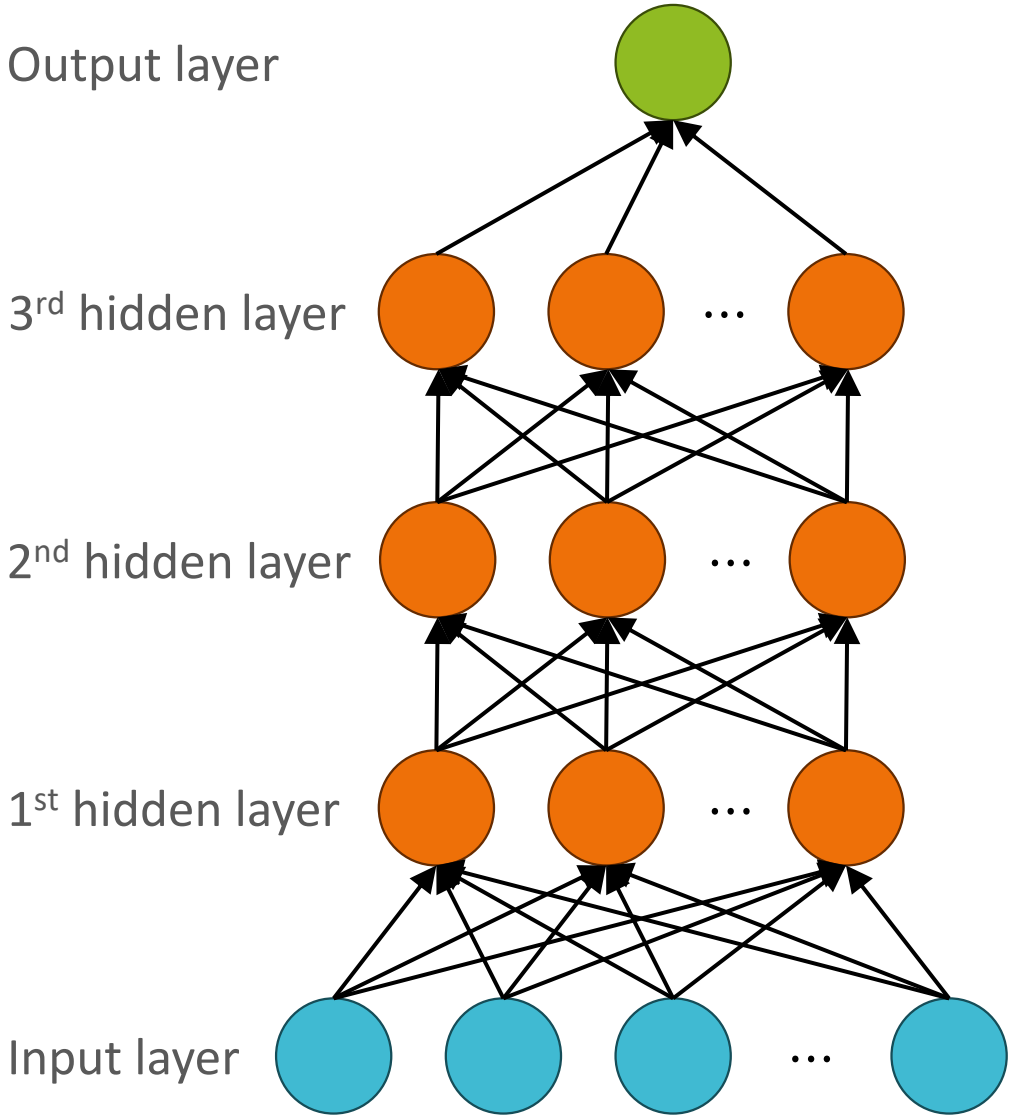
- Train each layer of the network iteratively using the training dataset *to learn useful representations*
- Idea: a good representation is one preserves a lot of information and could be used to recreate the inputs



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

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

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



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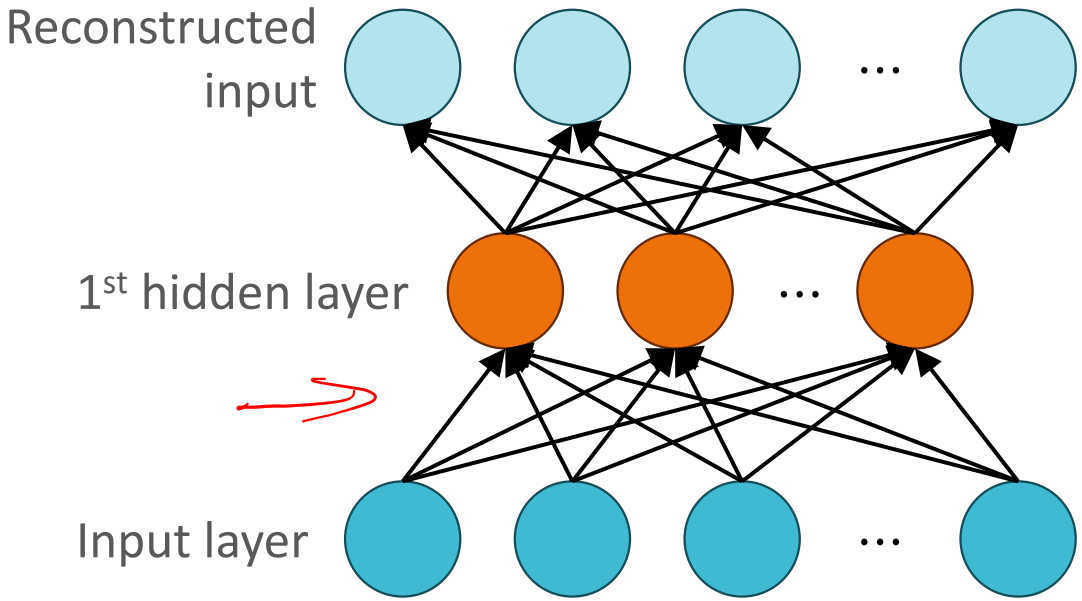
- This architecture/ objective defines an *autoencoder*



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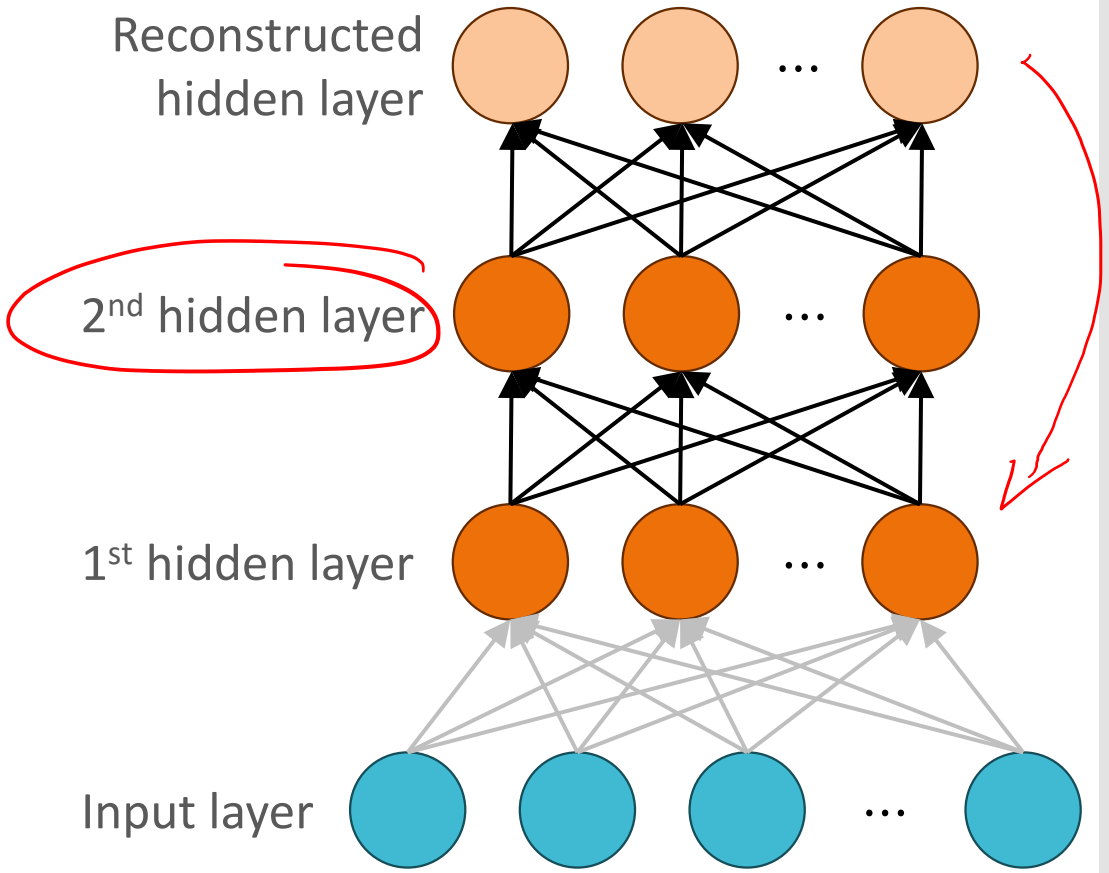

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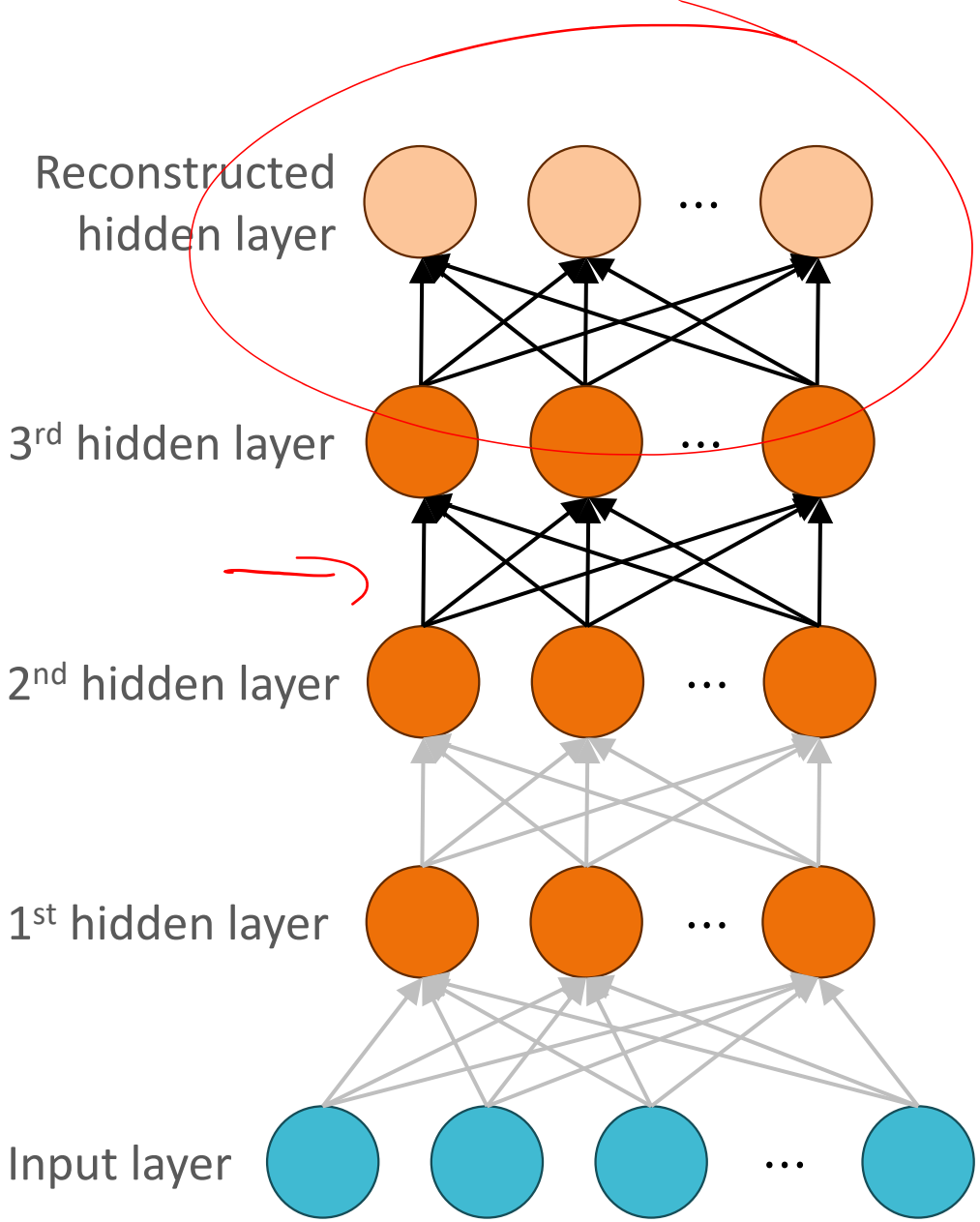

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Fine-tuning (Bengio et al., 2006)

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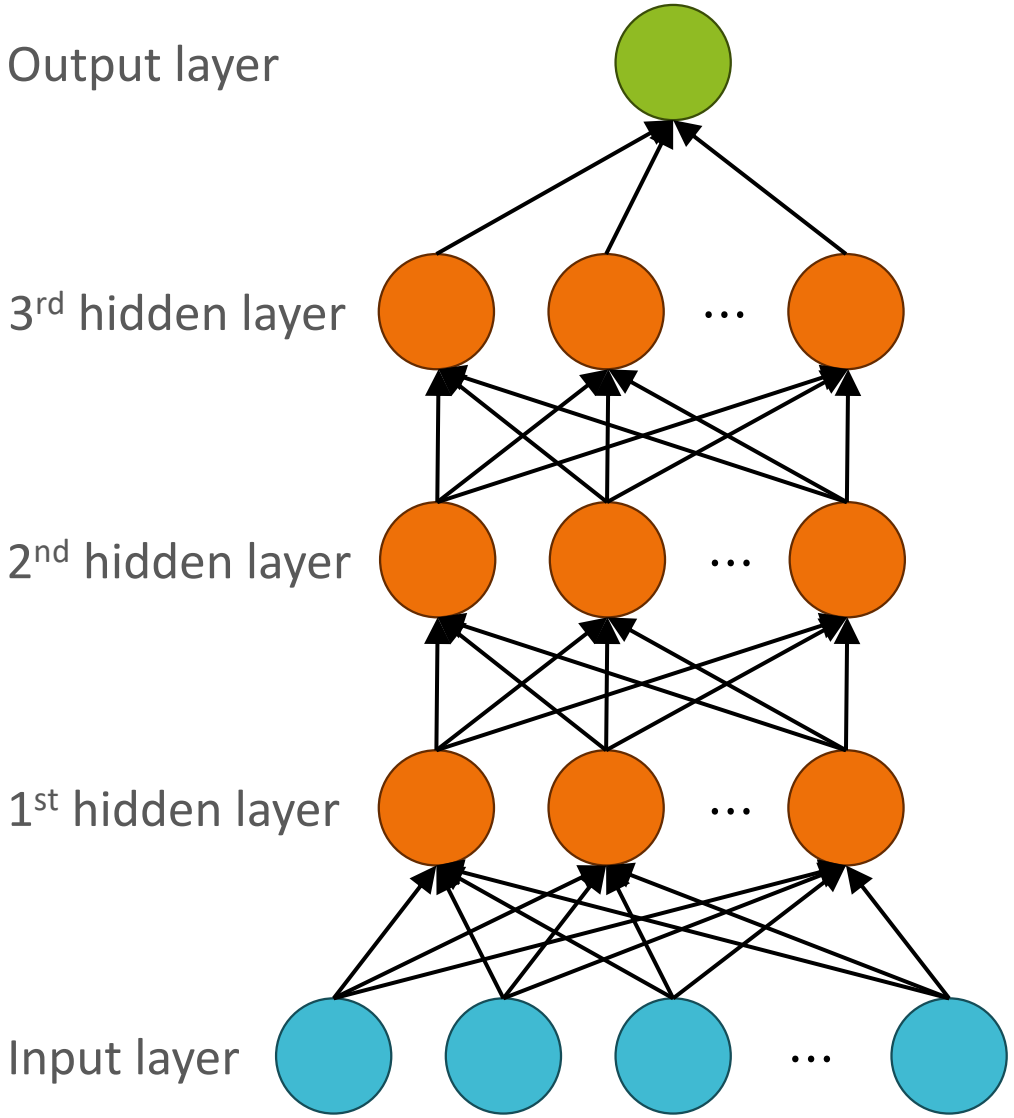
- When fine-tuning, we're effectively swapping out the last layer and fitting all the weights to the training dataset



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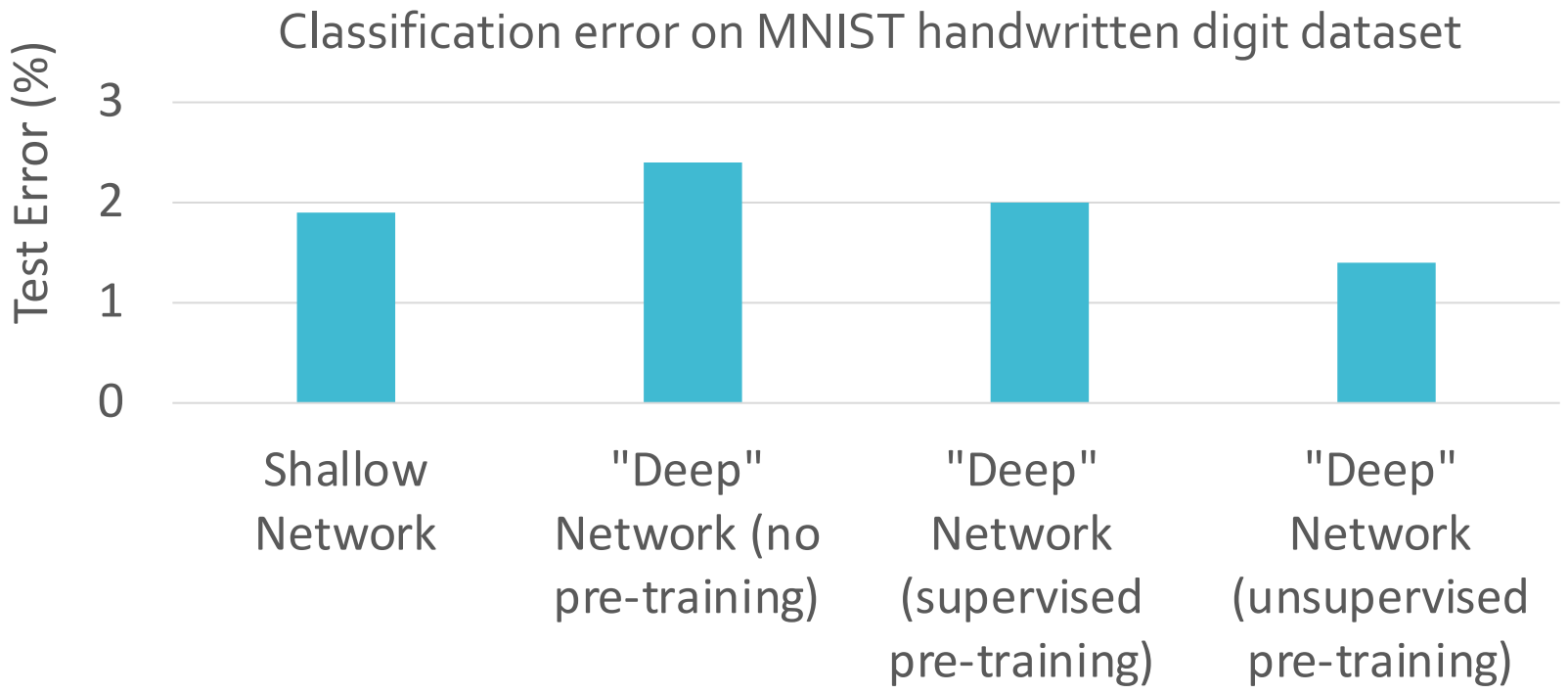

Another dose of Reality

- You have some niche task that you want to apply machine learning to e.g., predicting the author of children's books
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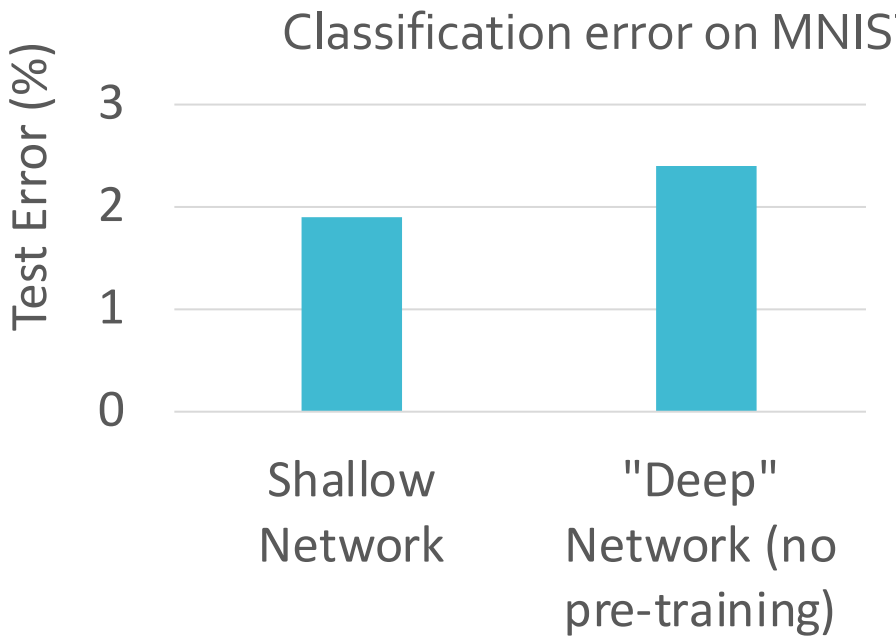

- Problem: what if you don't even have enough data to train a single layer/fine-tune the pre-trained network?

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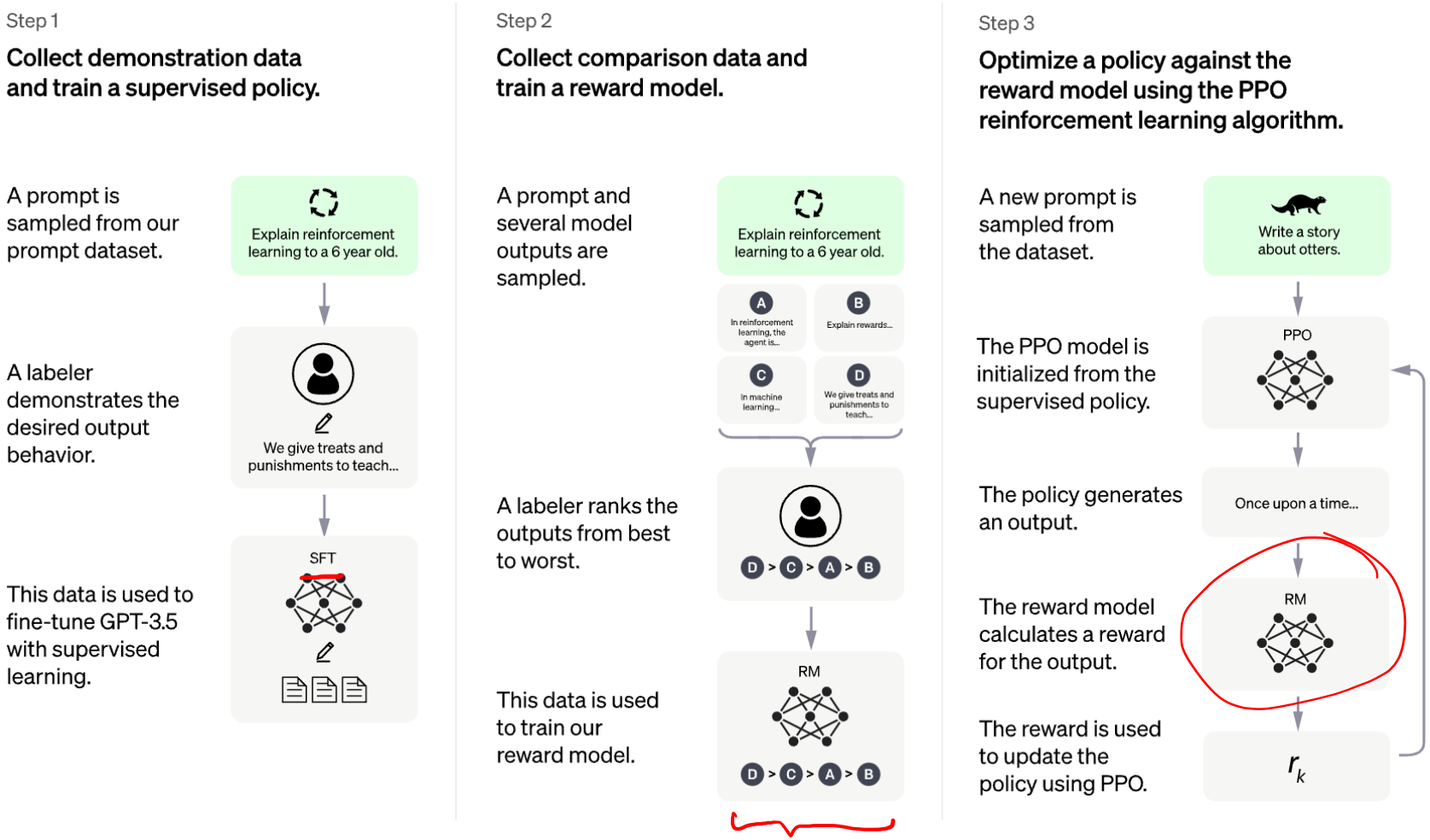
- You fit a massive deep learning model to the dataset
- Surprise, surprise: it overfits and your test error is super high
- Key observation: you can pre-train on basically any labelled or unlabelled dataset!
- Okay that's great for pre-training and all, but what if
  A. the concept of labelled data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

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)

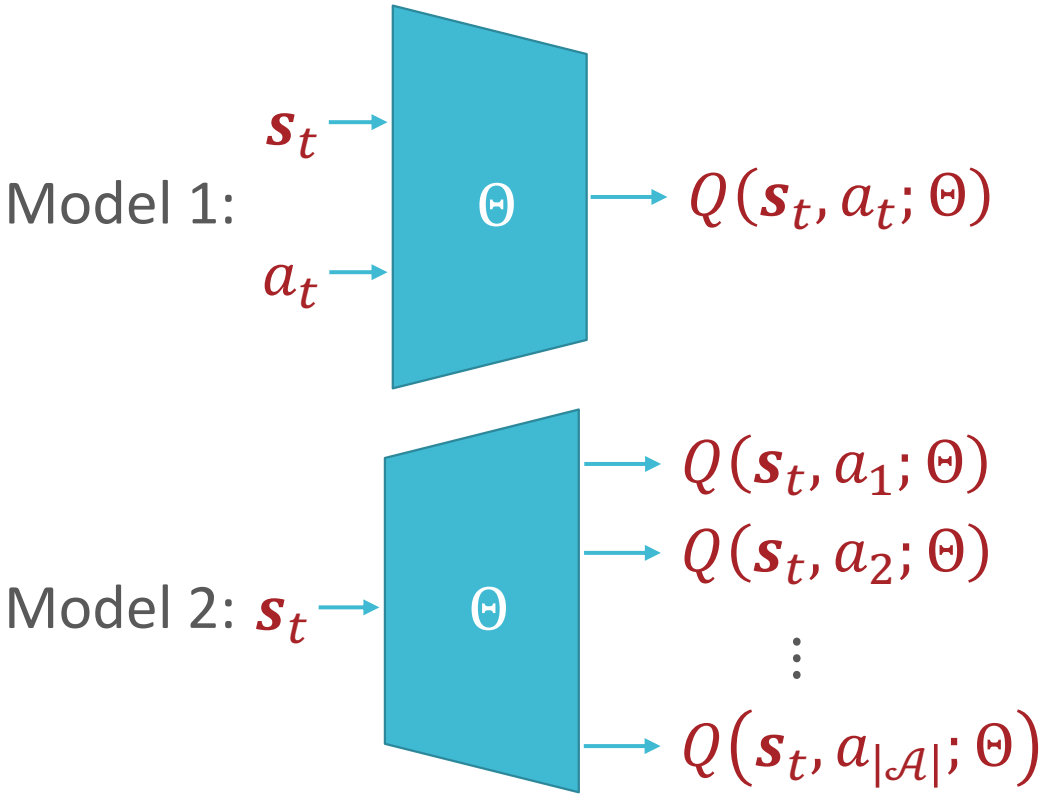


- RLHF is a special form of fine-tuning that uses *proximal policy optimization* (PPO)

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

Recall: Deep Q-learning

- Represent states using some feature vector $\boldsymbol{s}_t \in \mathbb{R}^M$
  e.g. for Go, $\boldsymbol{s}_t = [1, 0, -1, \dots, 1]^T$
- Define a *differentiable* function that approximates Q



What if instead of optimizing the Q-function, we could optimize the policy directly?

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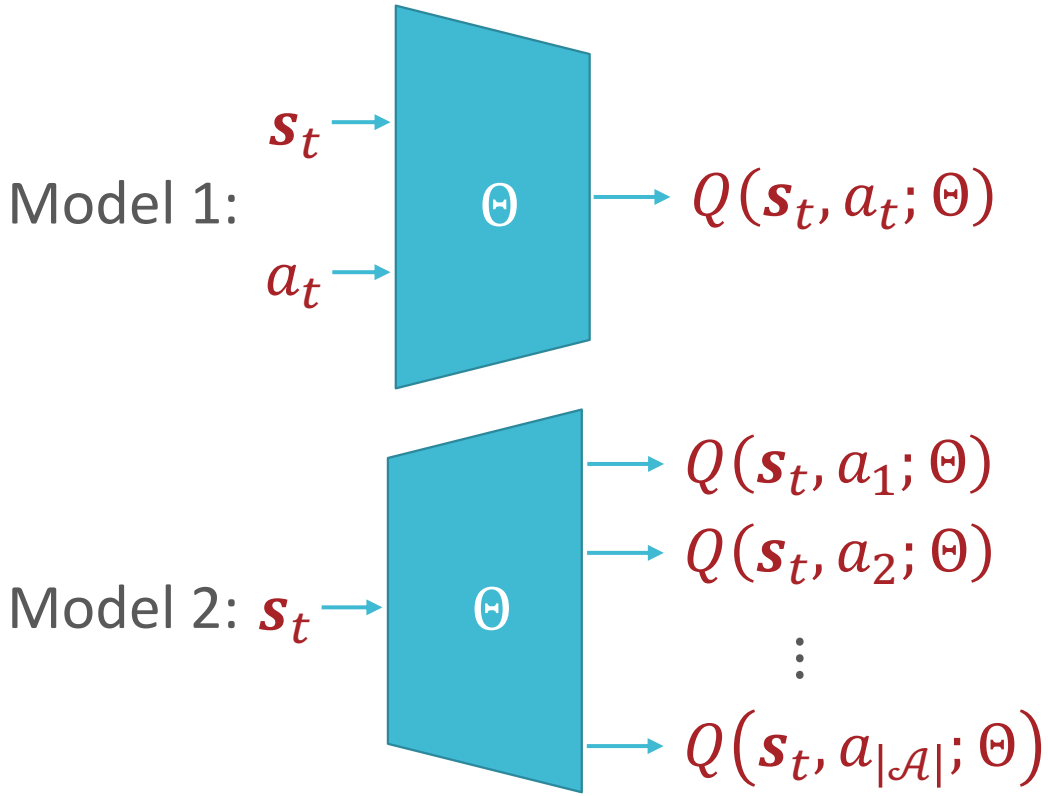
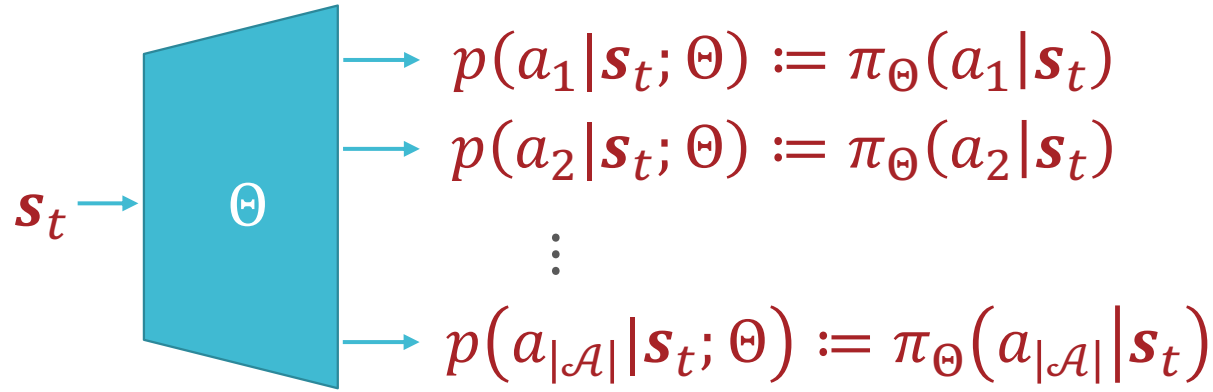


Parametrized Stochastic Policies

- Represent states using some feature vector $\boldsymbol{s}_t \in \mathbb{R}^M$
  e.g. for Go, $\boldsymbol{s}_t = [1, 0, -1, \ldots, 1]^T$
- Define a *differentiable* function that specifies a *stochastic* policy π_Θ
- Minimize the negative expected total reward w.r.t. Θ

$$\ell(\Theta) = -\mathbb{E}_{\pi_\Theta}\left[\sum_{t=0}^{\infty} \gamma^t r_t\right]$$

Model:



Okay… but how on earth do we compute the gradient of this thing?

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  e.g. for Go, $\boldsymbol{s}_t = [1, 0, -1, \dots, 1]^T$
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$$\ell(\Theta) = -\mathbb{E}_{\pi_\Theta}\left[\mathbb{E}_{p(s'|s,a)}\left[\sum_{t=0}^{\infty}\gamma^t r_t\right]\right]$$

reward

model trained on human feedback

Model: $\boldsymbol{s}_t \rightarrow \Theta$

$$p(a_1|\boldsymbol{s}_t;\Theta) \coloneqq \pi_\Theta(a_1|\boldsymbol{s}_t)$$
$$p(a_2|\boldsymbol{s}_t;\Theta) \coloneqq \pi_\Theta(a_2|\boldsymbol{s}_t)$$
$$\vdots$$
$$p(a_{|\mathcal{A}|}|\boldsymbol{s}_t;\Theta) \coloneqq \pi_\Theta(a_{|\mathcal{A}|}|\boldsymbol{s}_t)$$

Trajectories

- A *trajectory* $\mathrm{T} = \{\boldsymbol{s}_0, a_0, \boldsymbol{s}_1, a_1, \ldots, \boldsymbol{s}_T\}$ is one run of an agent through an MDP ending in a terminal state, $\boldsymbol{s}_T$
- Our stochastic policy and the transition distribution induce a distribution over trajectories

$$p_\Theta(\mathrm{T}) = p(\{s_0, a_0, s_1, a_1, \ldots, s_T\})$$
$$= p(s_0) \prod_{t=0}^{T-1} \pi_\Theta(a_t|s_t)\, p(s_{t+1}|s_t, a_t)$$

- If all runs end at a terminal state, then we can rewrite the negative expected total reward as

$$\ell(\Theta) = -\mathbb{E}_{p_\Theta(\mathrm{T}=\{\boldsymbol{s}_0, a_0, \ldots, \boldsymbol{s}_T\})}\left[\sum_{t=0}^{T-1} \gamma^t R(\boldsymbol{s}_t, a_t)\right] := -\mathbb{E}_{p_\Theta(\mathrm{T})}[R(\mathrm{T})]$$

Likelihood Ratio Method a.k.a. REINFORCE (Williams, 1992)

$$\nabla_\Theta \ell(\Theta) = \nabla_\Theta\left(-\mathbb{E}_{p_\Theta(\mathrm{T})}[R(\mathrm{T})]\right) = \nabla_\Theta\left(-\int R(\mathrm{T}) p_\Theta(\mathrm{T})\, d\mathrm{T}\right)$$

$$= -\int R(\mathrm{T}) \nabla_\Theta p_\Theta(\mathrm{T})\, d\mathrm{T}$$

$$= -\int R(\mathrm{T}) \nabla_\Theta \left(p(\boldsymbol{s}_0) \prod_{t=0}^{T-1} p(s_{t+1}|s_t, a_t)\, \pi_\Theta(a_t|\boldsymbol{s}_t) \right) d\mathrm{T}$$

- Issues:
  - The transition probabilities $p(s_{t+1}|s_t, a_t)$ are unknown a priori
  - Computing $\nabla_\Theta p_\Theta(\mathrm{T})$ involves taking the gradient of a product

Source: https://citeseerx.ist.psu.edu/doc/10.1.1.129.8871

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- Insight:

$$\nabla_\Theta P_\Theta(\tau) = \frac{P_\Theta(\tau)}{P_\Theta(\tau)} \nabla_\Theta P_\Theta(\tau) = P_\Theta(\tau) \nabla_\Theta \log P_\Theta(\tau)$$

$$\log P_\Theta(\tau) = \log p(s_0) + \sum_{t=0}^{T-1} \log p(s_{t+1}|s_t, a_t) + \sum_{t=0}^{T-1} \log \pi_\Theta(a_t|s_t)$$

$$\nabla_\Theta \log P_\Theta(\tau) = \sum_{t=0}^{T-1} \nabla_\Theta \log \pi_\Theta(a_t|s_t)$$

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$$\nabla_\Theta \ell(\Theta) = \nabla_\Theta\left(-\mathbb{E}_{p_\Theta(\mathrm{T})}[R(\mathrm{T})]\right) = \nabla_\Theta\left(-\int R(\mathrm{T}) p_\Theta(\mathrm{T})\, d\mathrm{T}\right)$$

$$= -\int R(\mathrm{T}) \nabla_\Theta p_\Theta(\mathrm{T})\, d\mathrm{T} = -\int R(\mathrm{T}) \nabla_\Theta (\log p_\Theta(\mathrm{T})) p_\Theta(\mathrm{T}) d\mathrm{T}$$

$$= -\mathbb{E}_{p_\Theta(\mathrm{T})}[R(\mathrm{T}) \nabla_\Theta (\log p_\Theta(\mathrm{T}))]$$

$$\approx -\frac{1}{N} \sum_{n=1}^{N} R\left(\mathrm{T}^{(n)}\right) \nabla_\Theta \left(\log p_\Theta\left(\mathrm{T}^{(n)}\right)\right)$$

(where $\mathrm{T}^{(n)} = \left\{\boldsymbol{s}_0^{(n)}, a_0^{(n)}, \boldsymbol{s}_1^{(n)}, a_1^{(n)}, \ldots, \boldsymbol{s}_{T^{(n)}}^{(n)}\right\}$ is a sampled trajectory)

$$= -\frac{1}{N} \sum_{n=1}^{N} \left(\sum_{t=0}^{T^{(n)}-1} \gamma^t R\left(\boldsymbol{s}_t^{(n)}, a_t^{(n)}\right) \right) \left(\sum_{t=0}^{T^{(n)}-1} \nabla_\Theta \log \pi_\Theta \left(a_t^{(n)} \middle| \boldsymbol{s}_t^{(n)} \right) \right)$$

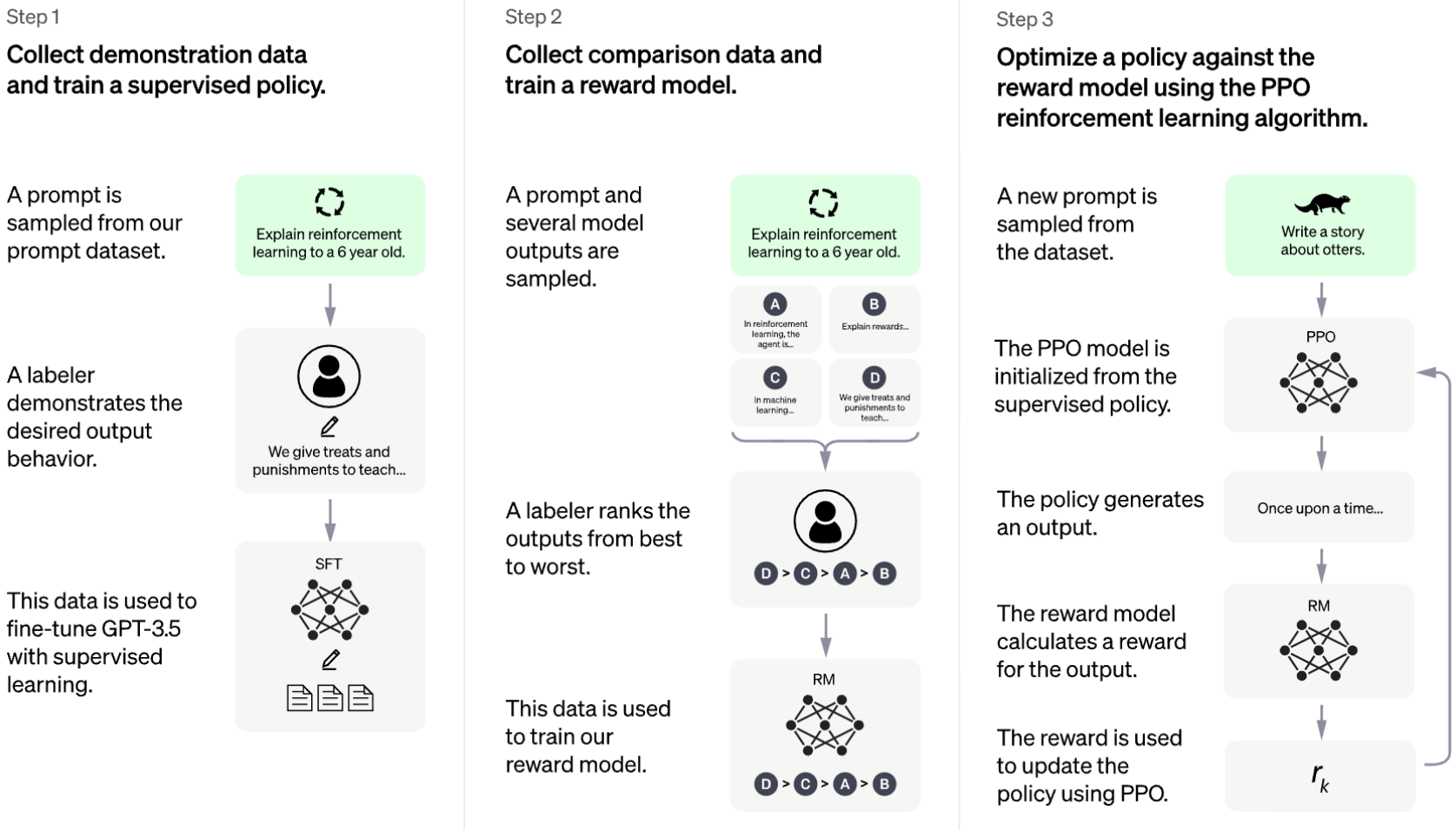
Policy Gradient Methods

- Practical considerations:
  - Not compatible with deterministic policies (would require knowledge of the transition probabilities)
  - Sampled trajectories/rewards can be highly variable, which leads to unstable estimates of the expectation
    - Can compare sampled rewards against a constant *baseline* to get an *advantage function* (Peters and Schaal, 2008): $A(\mathrm{T}) = R(\mathrm{T}) - B$

Policy Gradient Methods

- Practical considerations:
  - Policy gradient methods are *on-policy*: they require using the current (potentially bad) policy to sample (a lot of) trajectories…
    - *Trust region methods* (Schulman et al., 2015) impose a constraint on how far the policy distribution can shift from one iteration to the next (in terms of a KL divergence)
    - *Proximal policy optimization* (Schulman et al., 2017) limits how much the magnitude of the objective function can change from one iteration to the next via clipping

Okay, so this is great if our problem is subjective, but again, what can we do for objective tasks where training data is scarce?



- RLHF is a special form of fine-tuning, used to fine-tune GPT-3.5 into ChatGPT

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

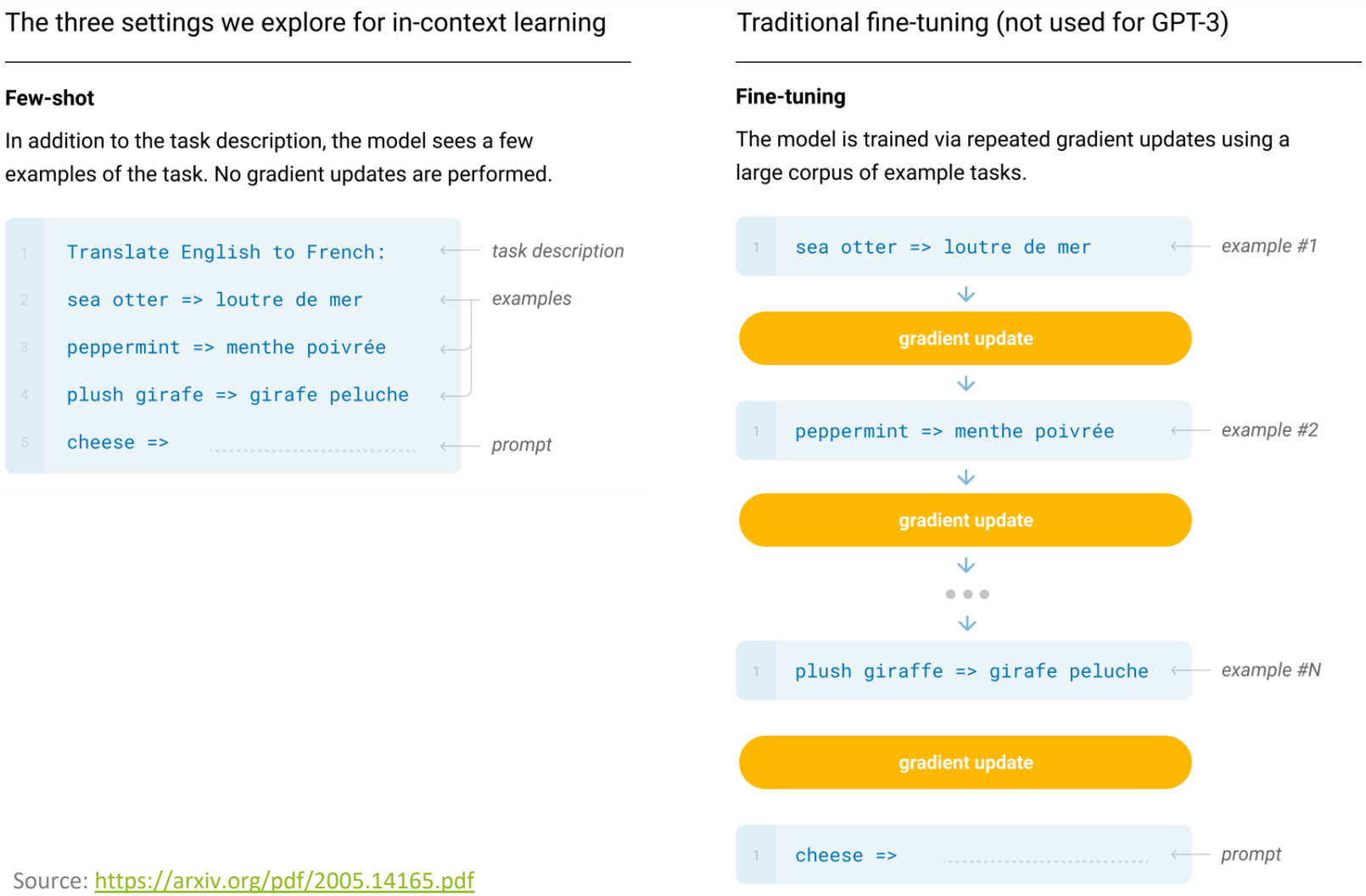
In-context Learning

- 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*



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

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
```

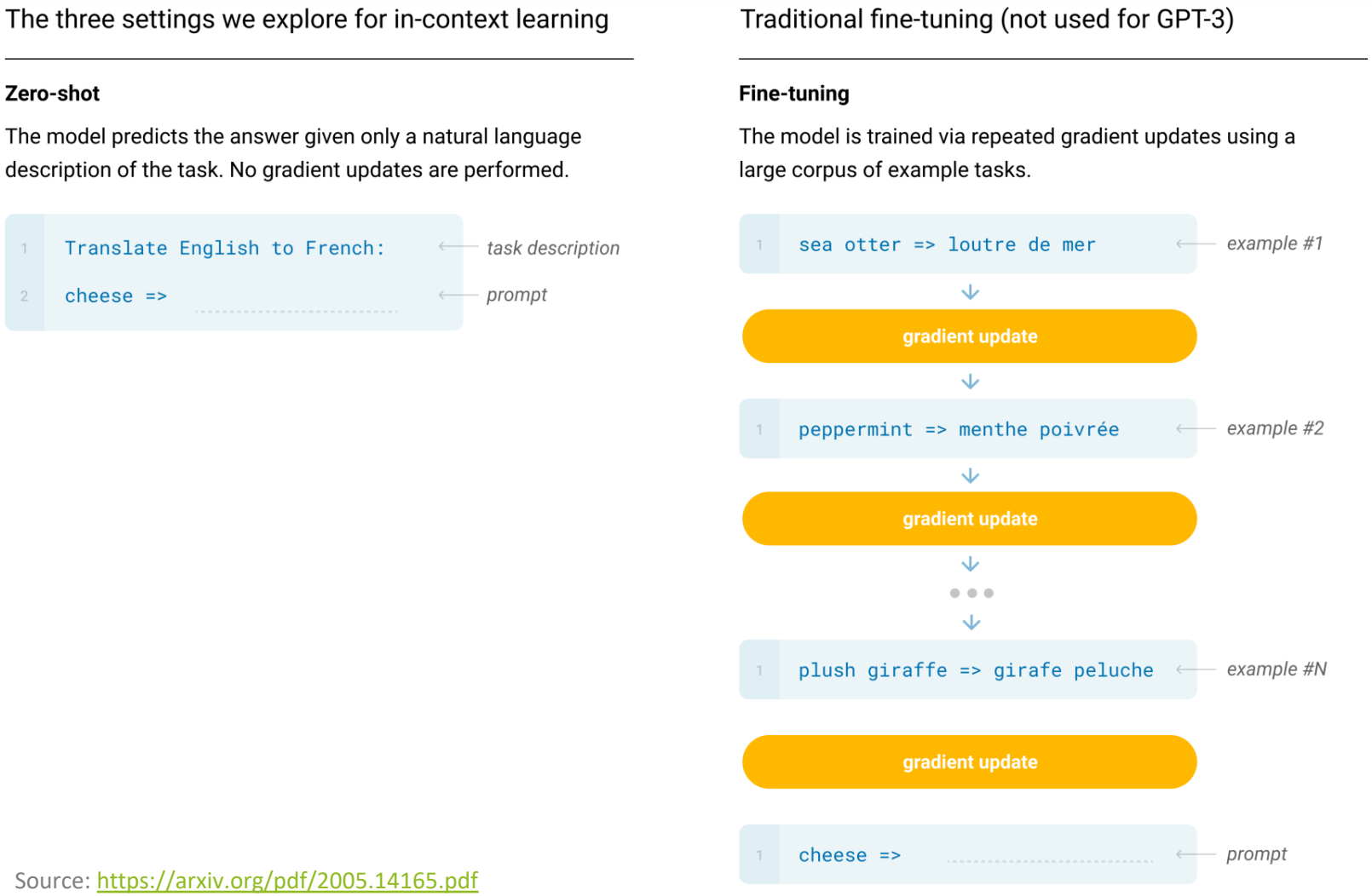
gradient update

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

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

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

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



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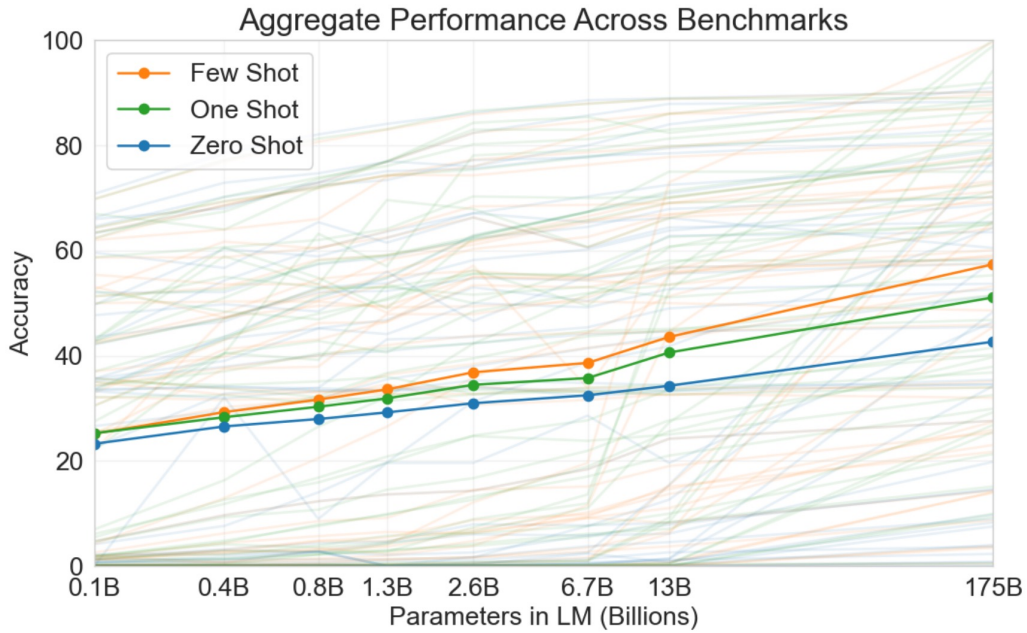

- Key Takeaway: LLMs can perform well on novel tasks without having to fine-tune the model, sometimes even with just one or zero labelled training data points!

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

Key Takeaways

- Instead of random initializations, modern deep learning typically initializes weights via pretraining, then fine-tunes them to the specific task
  - Supervised vs. unsupervised fine-tuning
  - Pretraining need not occur on the task of interest
- For tasks with subjective outputs, models can be fine-tuned using reinforcement learning with human feedback
  - Uses (proximal) policy optimization to optimize a parametrized policy directly
- Some tasks can be performed by a pretrained LLM without any fine-tuning via in-context learning