10-701: Introduction to Machine Learning

Lecture 18 – Pretraining, Fine-tuning & In-Context Learning

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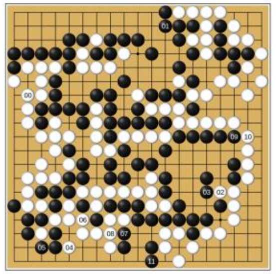
* Slides adopted from F24 offering of 10701 by Henry Chai.

Two big Q's

1. What can we do if the reward and/or transition functions/distributions are unknown?
    - Use online learning to gather data and learn $Q^*(s, a)$
2. How can we handle infinite (or just very large) state/action spaces?
    - Throw a neural network at it!



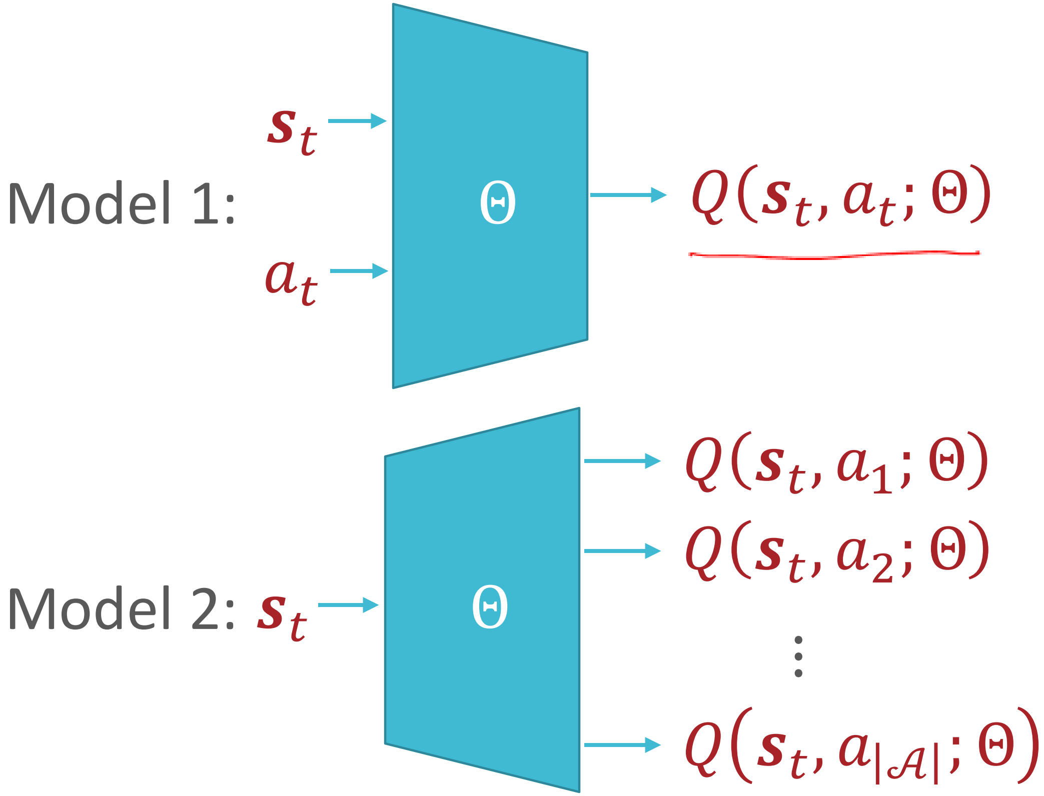
Deep Q-learning

Modeled by a DNN

- Use a parametric function, $Q(s, a; \Theta)$, to approximate $Q^*(s, a)$
  - Learn the parameters using *stochastic* gradient descent (SGD)
  - Training data $(\boldsymbol{s}_t, a_t, r_t, \boldsymbol{s}_{t+1})$ gathered online by the agent/learning algorithm

Deep Q-learning: Model

- 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



Deep Q-learning: Loss Function

- "True" loss

2. Don't know Q^*

$$\ell(\Theta) = \underbrace{\sum_{s \in \mathcal{S}}}_{} \sum_{a \in \mathcal{A}} \left(\overbrace{Q^*(s,a)}^{} - Q(s,a;\Theta)\right)^2$$

1. $\mathcal{S}$ too big to compute this sum

1. Use stochastic gradient descent: just consider one state-action pair in each iteration
2. Use temporal difference learning: (s_t, a_t, r_t, s_{t+1})
   - Given current parameters $\Theta^{(t)}$ the temporal difference target is

     current best guess of $Q^*(s_{t+1}, a')$

     $$Q^*(s_t, a_t) \approx \underbrace{r_t + \gamma \max_{a'} Q\left(s'_{t+1}, a'; \Theta^{(t)}\right)}_{} := y$$
   - Set the parameters in the next iteration $\Theta^{(t+1)}$ such that $Q\left(s, a; \Theta^{(t+1)}\right) \approx y$

     $$\ell\left(\Theta^{(t)}, \Theta^{(t+1)}\right) = \left(y - Q\left(s_t, a_t; \Theta^{(t+1)}\right)\right)^2$$

Deep Q-learning

Algorithm 4: Online learning (parametric form)

- Inputs: discount factor γ, an initial state s_0,

  learning rate α

- Initialize parameters $\Theta^{(0)}$

- For $t = 0, 1, 2, \ldots$
  - Gather training sample $\underline{(\boldsymbol{s}_t, \boldsymbol{a}_t, r_t, \boldsymbol{s}_{t+1})}$
  - Update $\underline{\Theta^{(t)}}$ by taking a step opposite the gradient

$$\Theta^{(t+1)} \leftarrow \Theta^{(t)} - \alpha \underline{\nabla_\Theta \ell(\Theta^{(t)}, \Theta)}$$

where

$$\nabla_\Theta \ell(\Theta^{(t)}, \Theta) = \underline{2(y - Q(s, a; \Theta)) \nabla_\Theta Q(s, a; \Theta)}$$

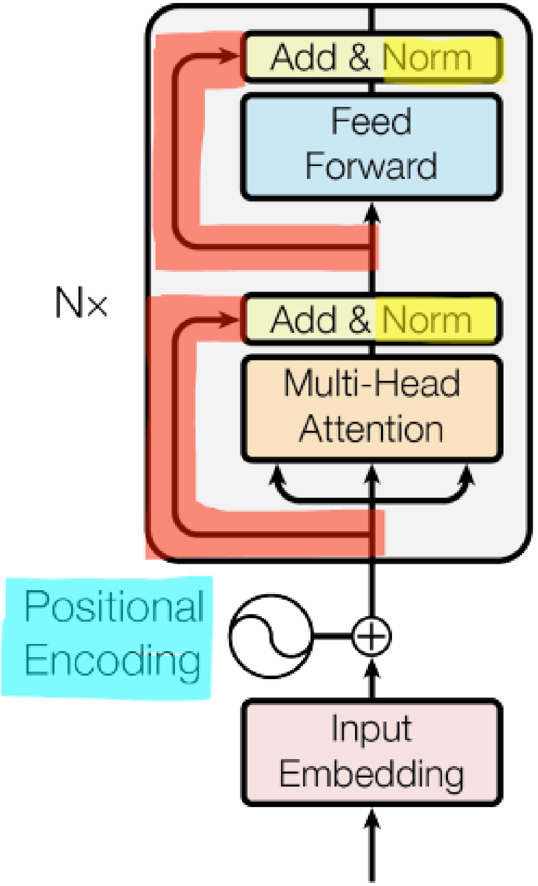
Deep Q-learning: Experience Replay

- SGD assumes i.i.d. training samples but in RL, samples are *highly* correlated
- Idea: keep a "replay memory" $\mathcal{D} = \{e_1, e_2, \dots, e_N\}$ of the N most recent experiences $e_t = (\boldsymbol{s}_t, \boldsymbol{a}_t, r_t, \boldsymbol{s}_{t+1})$ (Lin, 1992)
  - Also keeps the agent from "forgetting" about recent experiences
- Alternate between:
  1. Sampling some e_i uniformly at random from $\mathcal{D}$ and applying a Q-learning update (repeat T times)
  2. Adding a new experience to $\mathcal{D}$
- Can also sample experiences from $\mathcal{D}$ according to some distribution that prioritizes experiences with high error (Schaul et al., 2016)

Key Takeaways

- We can use (deep) Q-learning when the reward/transition functions are unknown and/or when the state/action spaces are too large to be modelled directly
  - Also guaranteed to converge under certain assumptions
  - Experience replay can help address non-i.i.d. samples

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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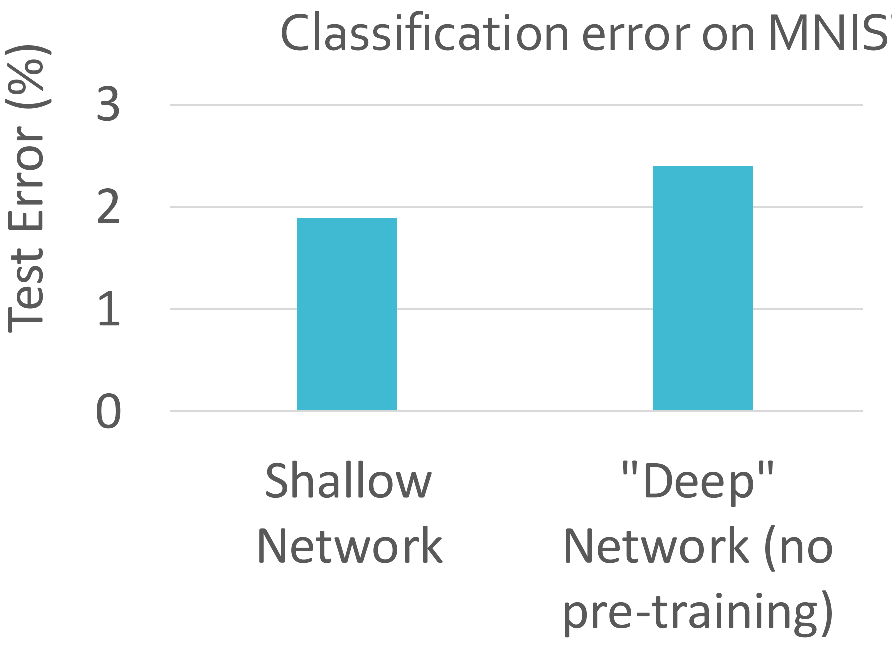
Traditional Supervised Learning

- 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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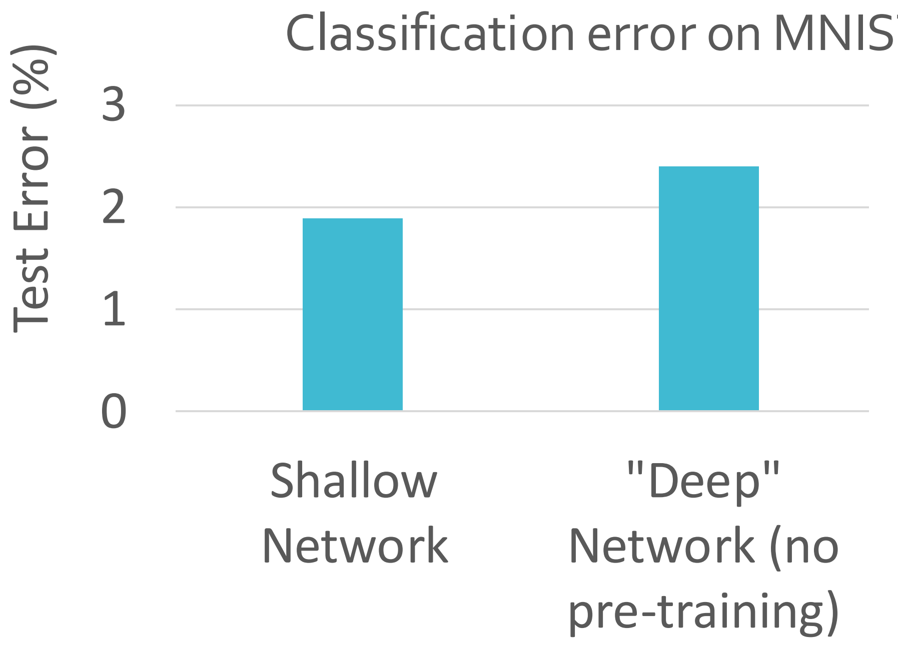
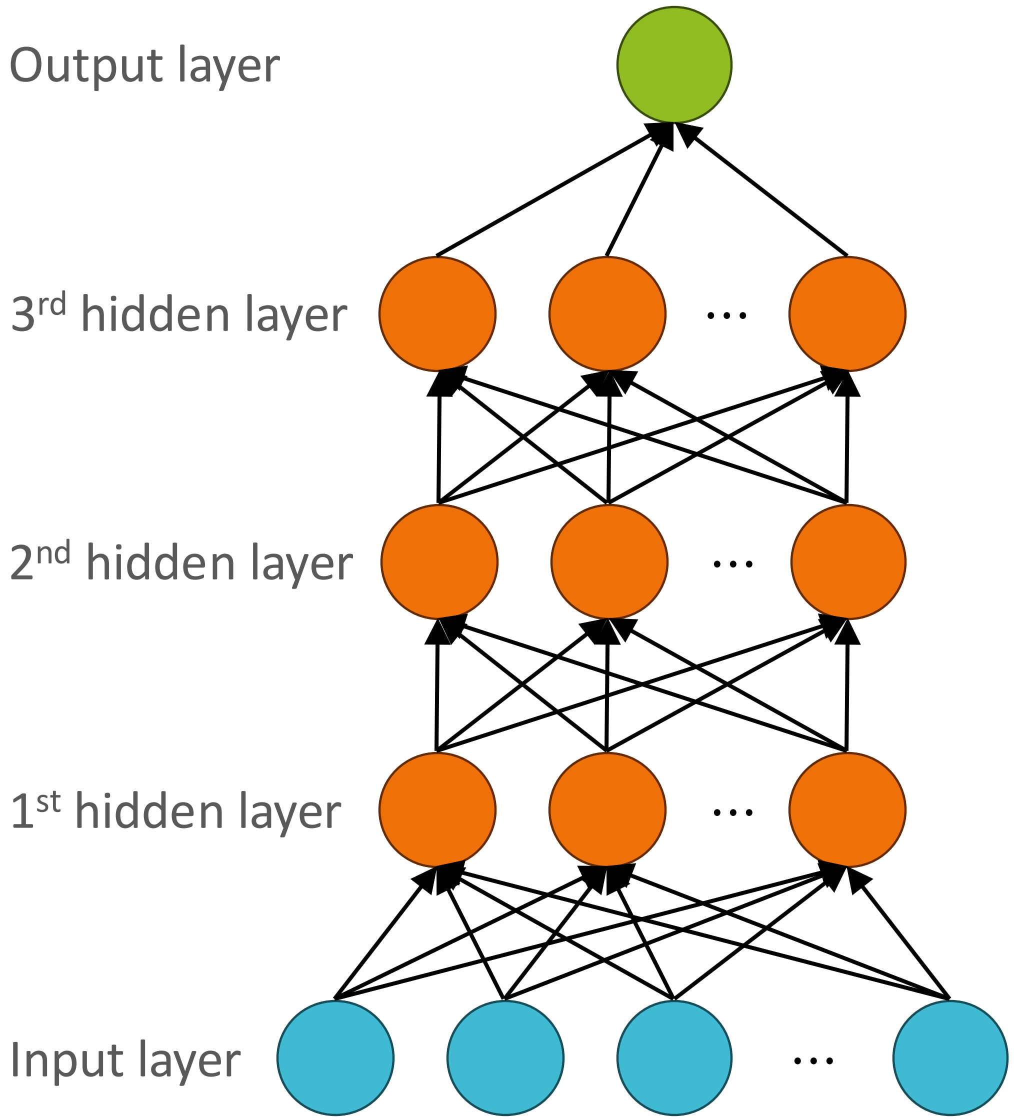


- Idea: if shallow networks are easier to train, let's just decompose our deep network into a series of shallow networks!

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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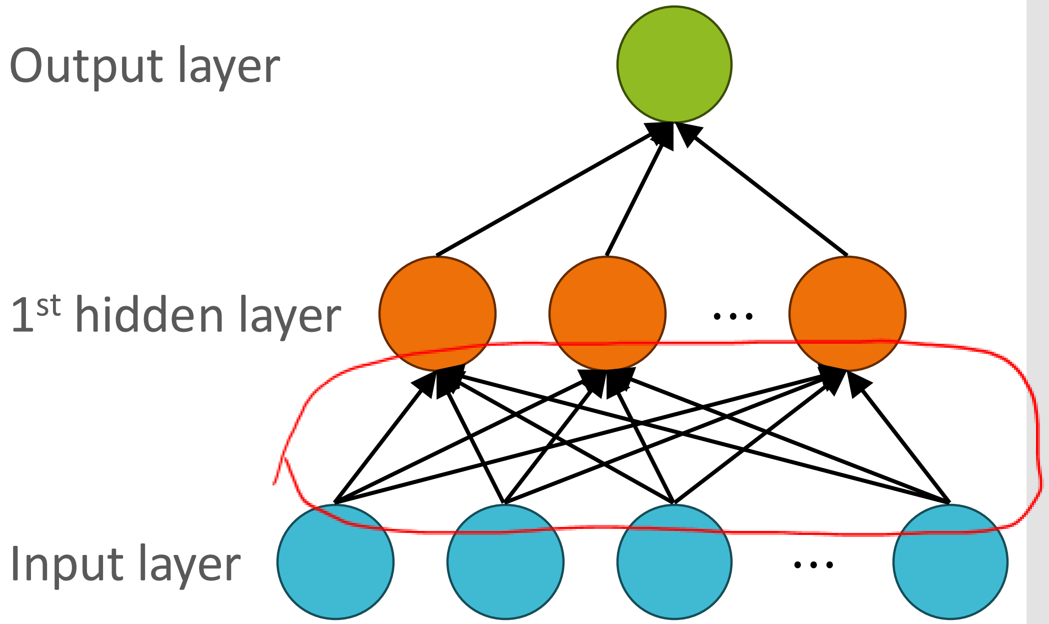

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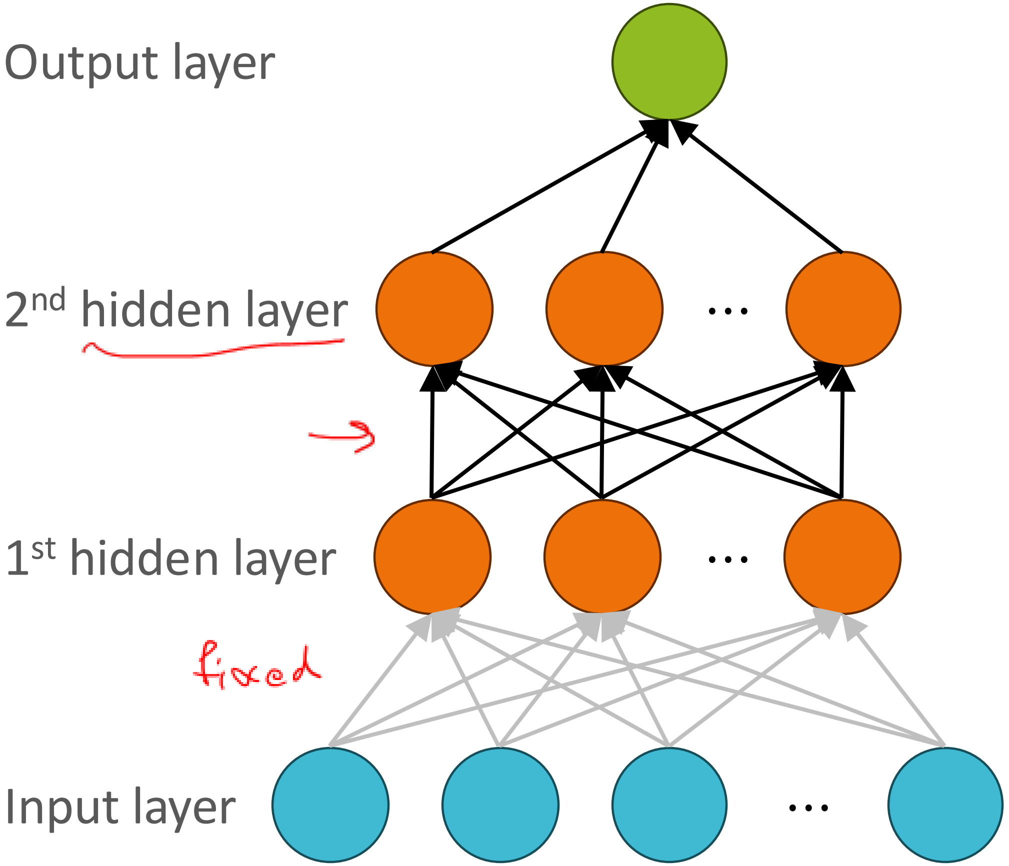

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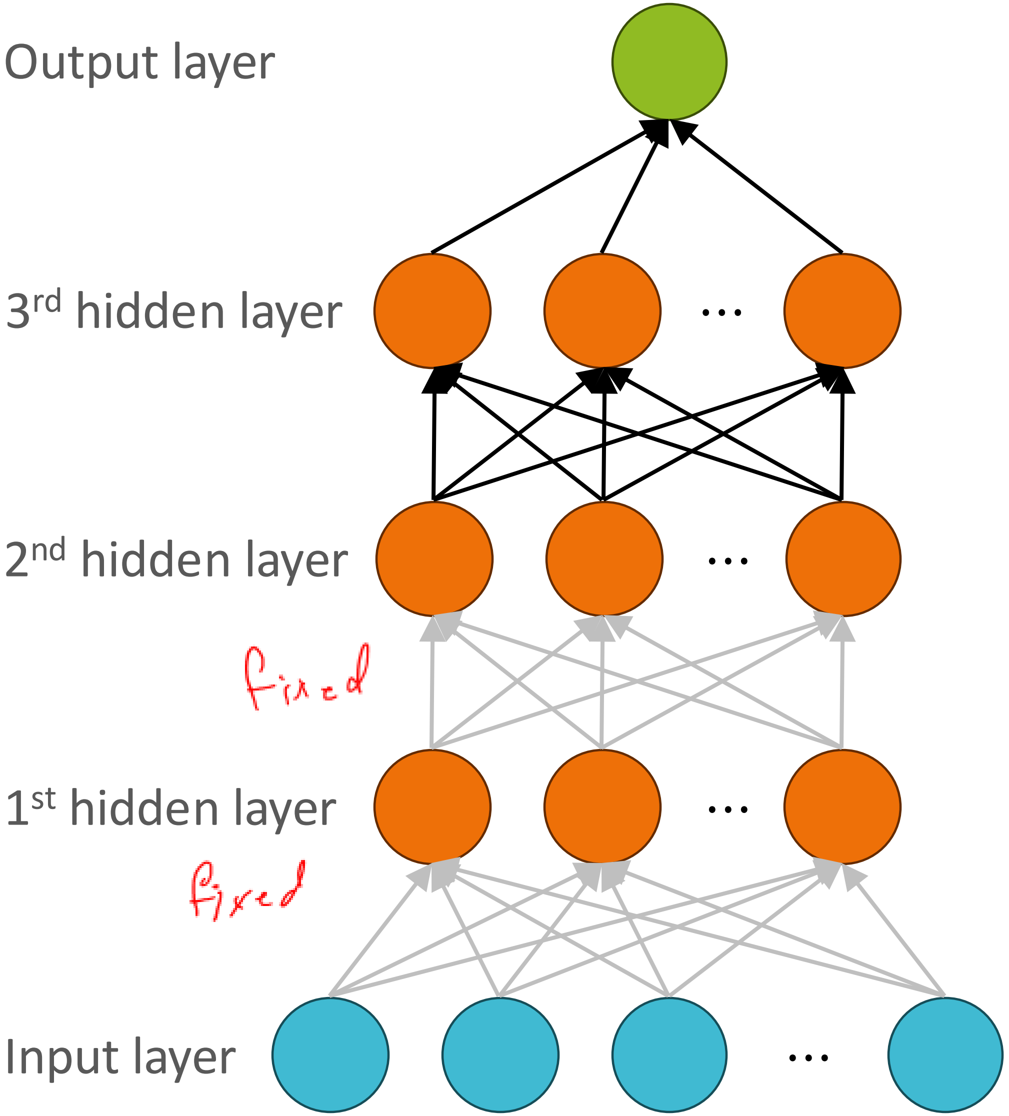

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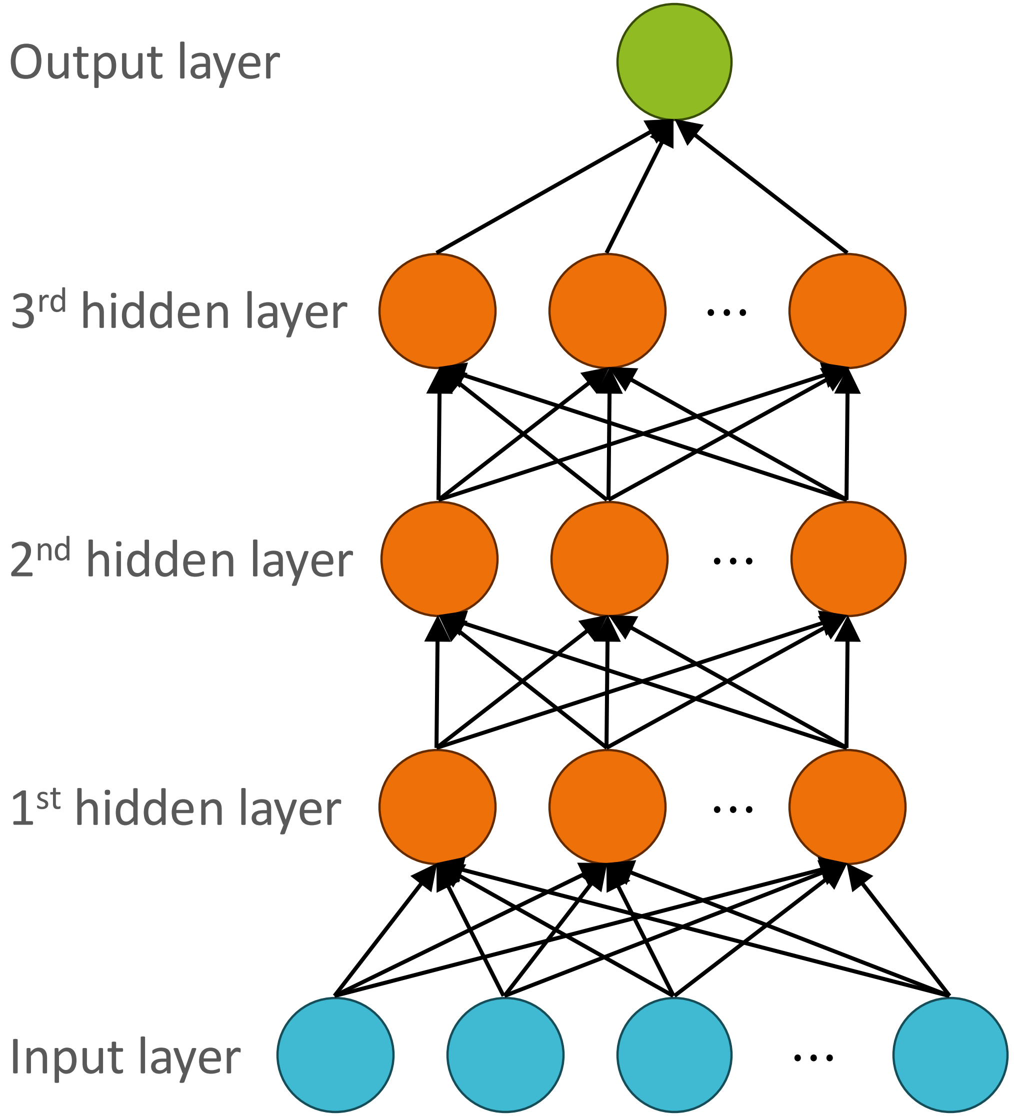
Fine-tuning (Bengio et al., 2006)

- 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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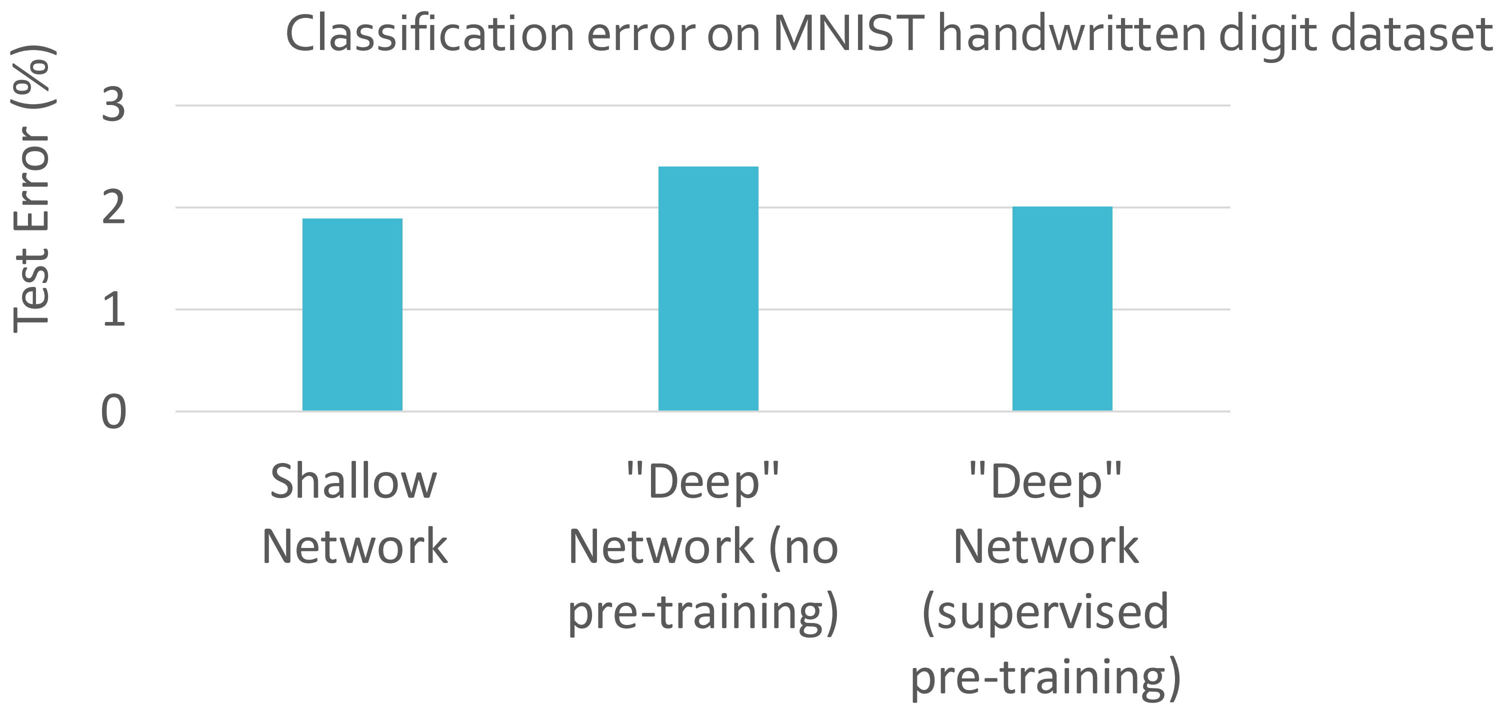

Supervised Pre-training (Bengio et al., 2006)

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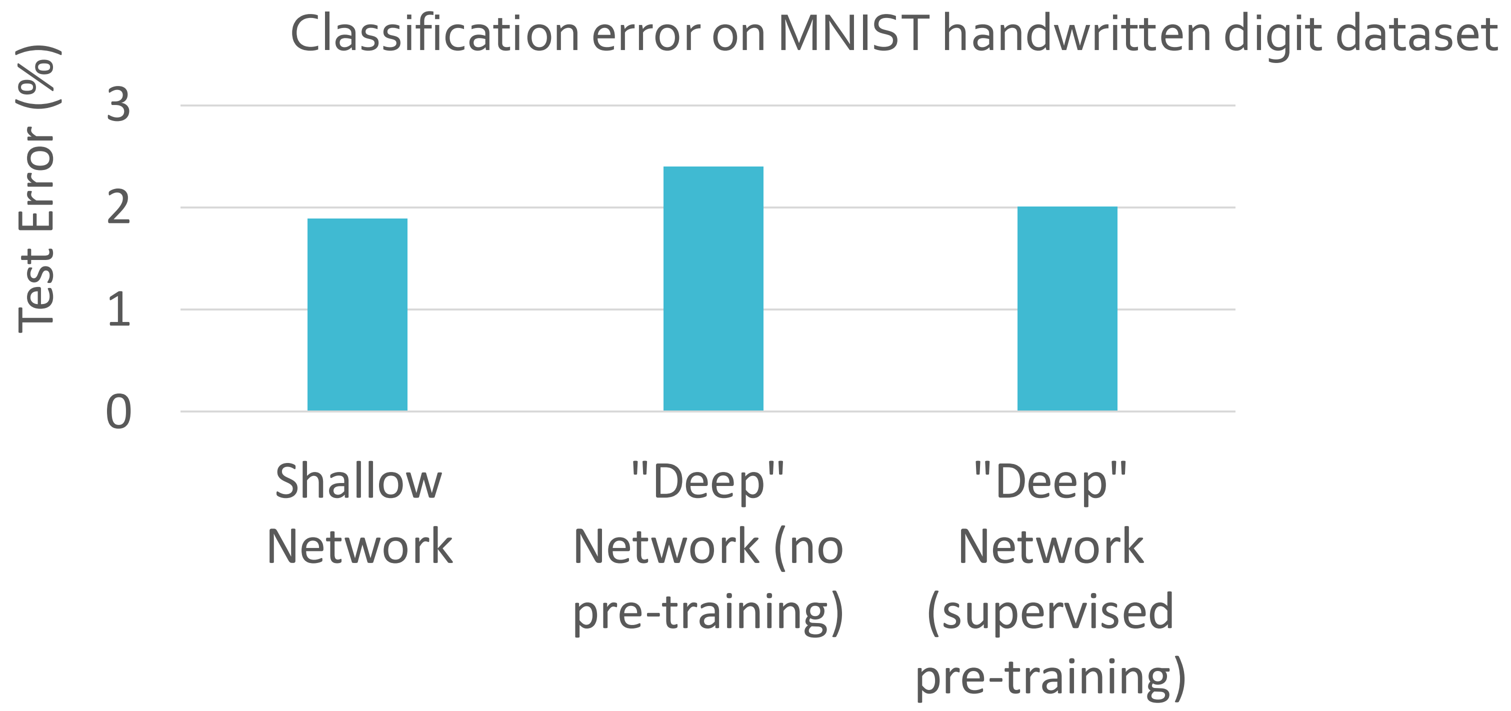

Is this the only thing we could do with the training data?

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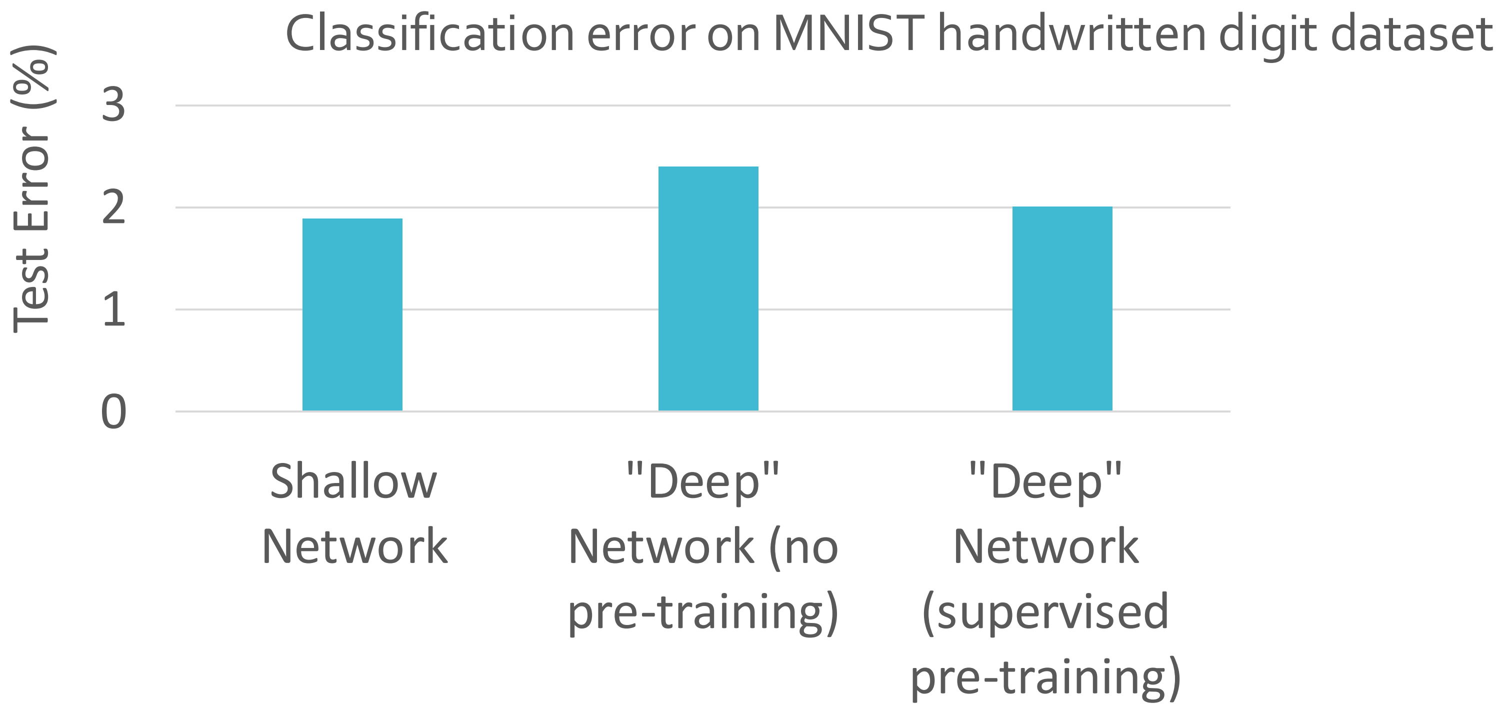
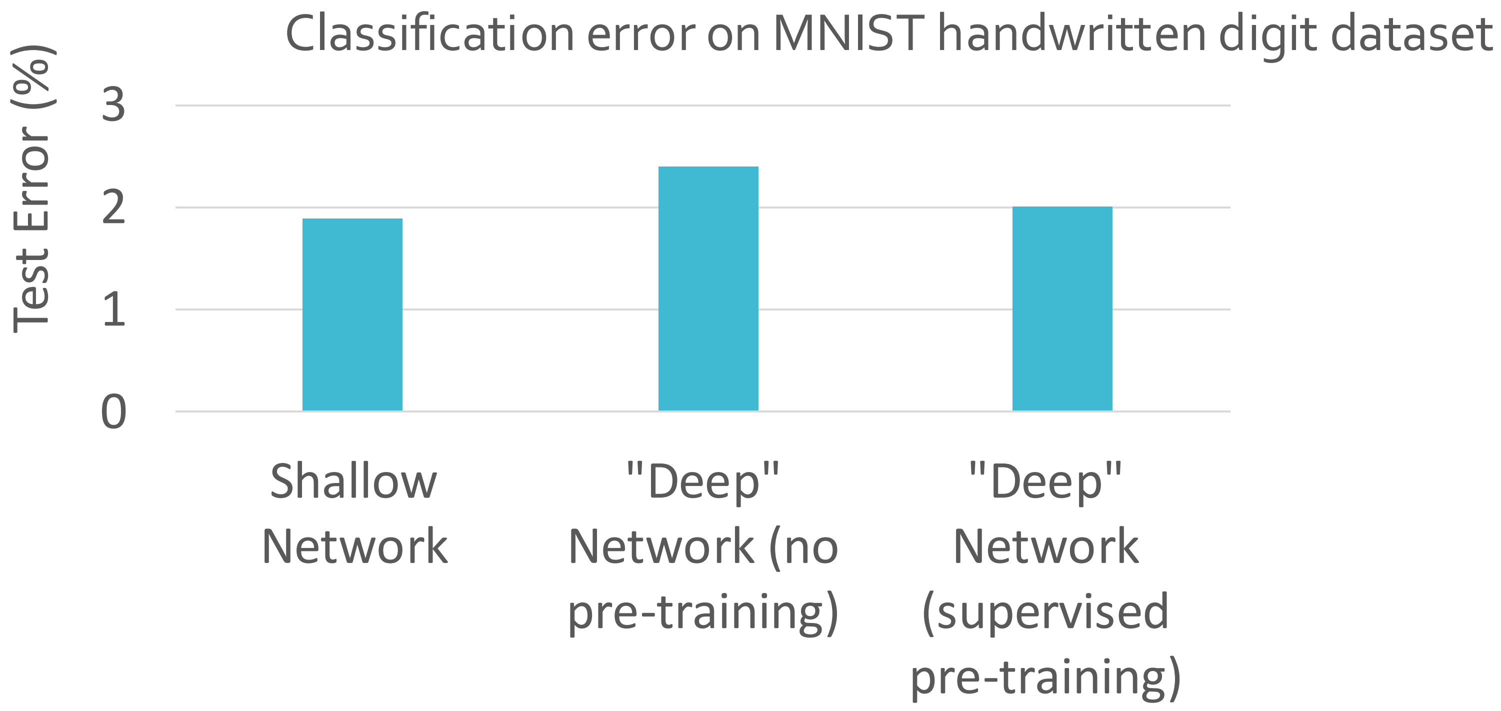
- Use the pre-trained weights as an initialization and *fine-tune* the entire network e.g., via SGD with the training dataset



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

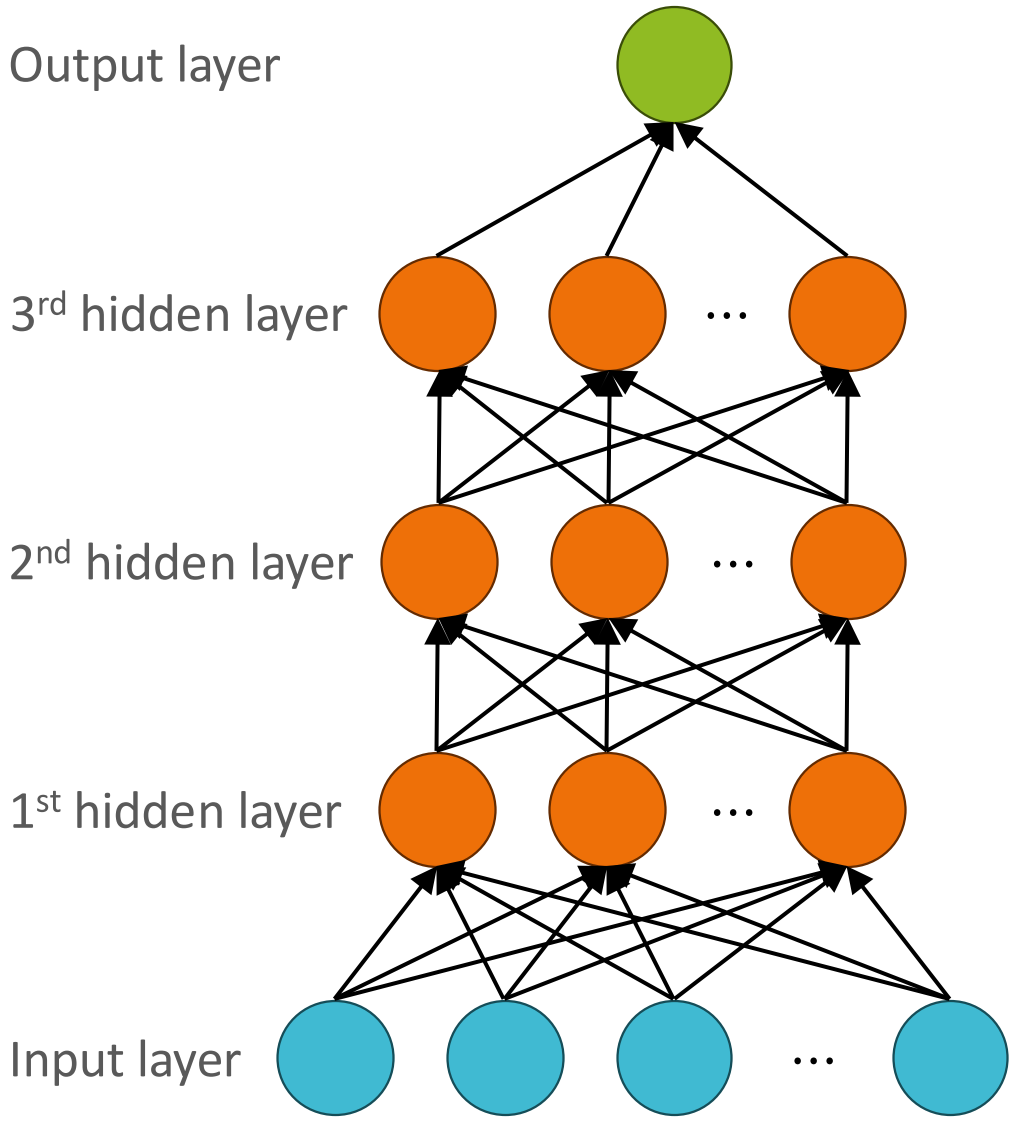
- Train each layer of the network iteratively using the training dataset *to learn useful representations*
- Idea: a good representation is one preserves a lot of information and could be used to recreate the inputs



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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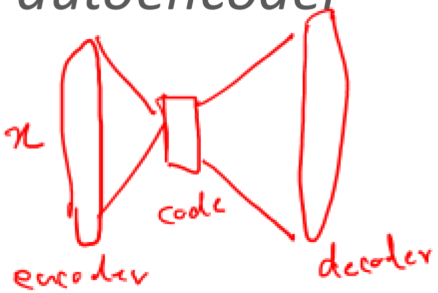
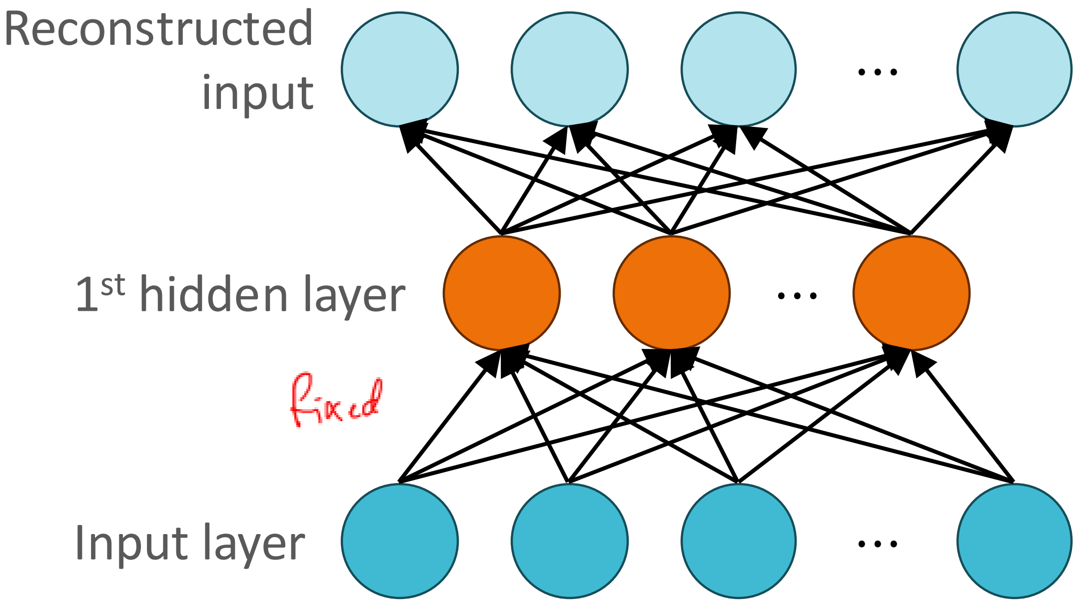
- This architecture/ objective defines an *autoencoder*





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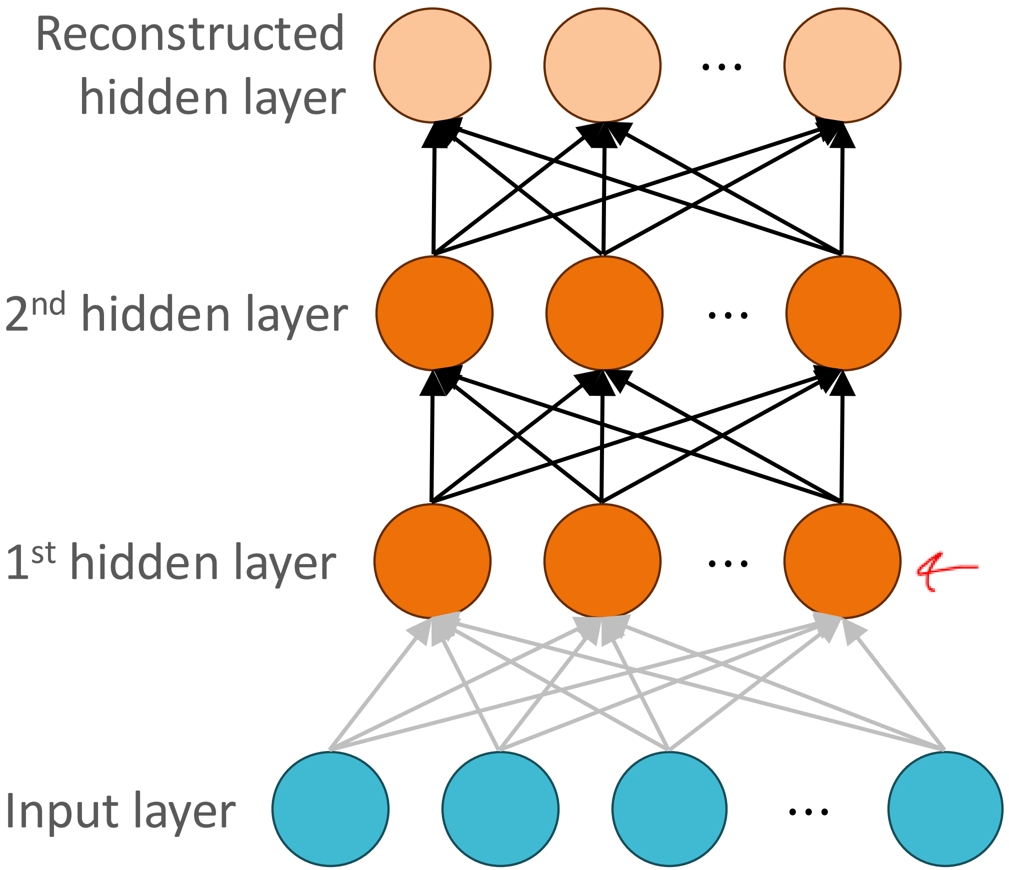

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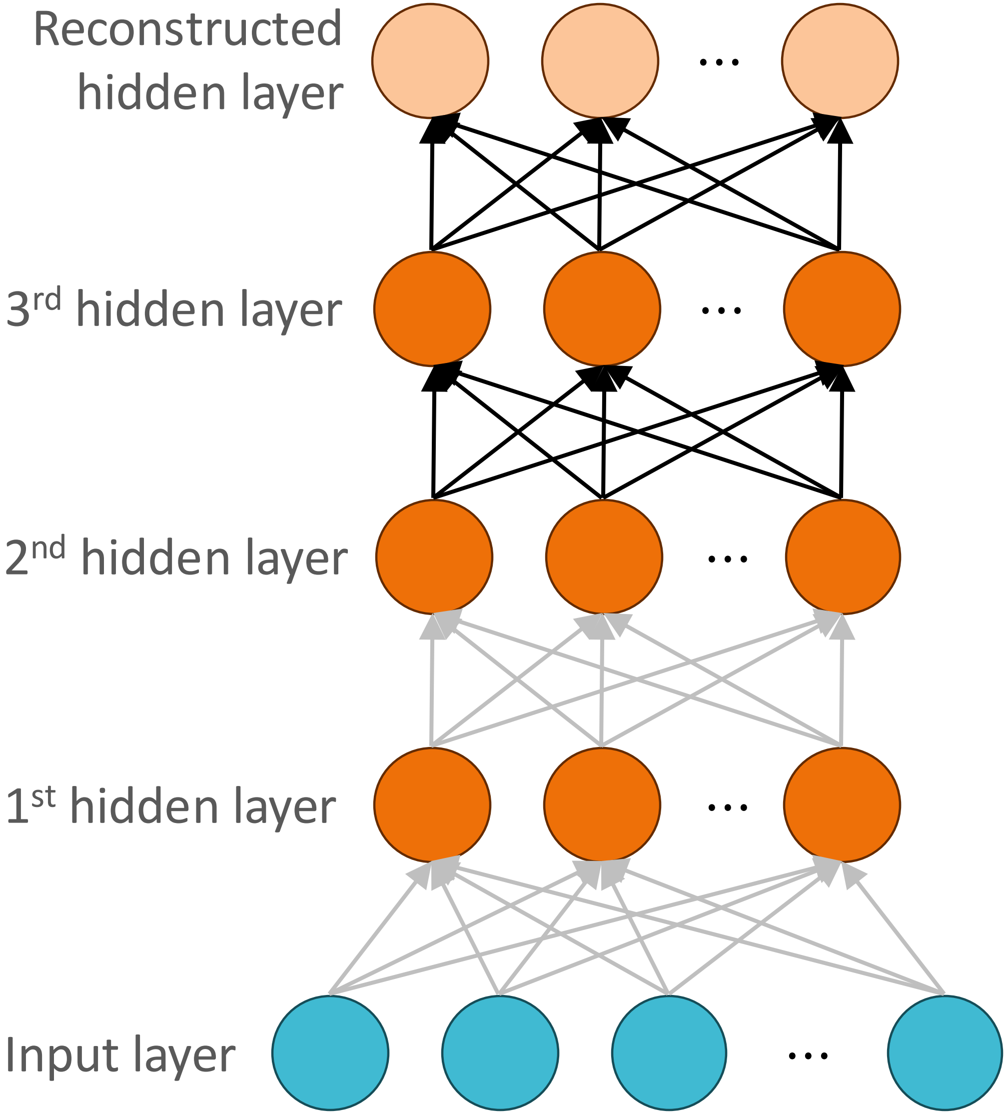

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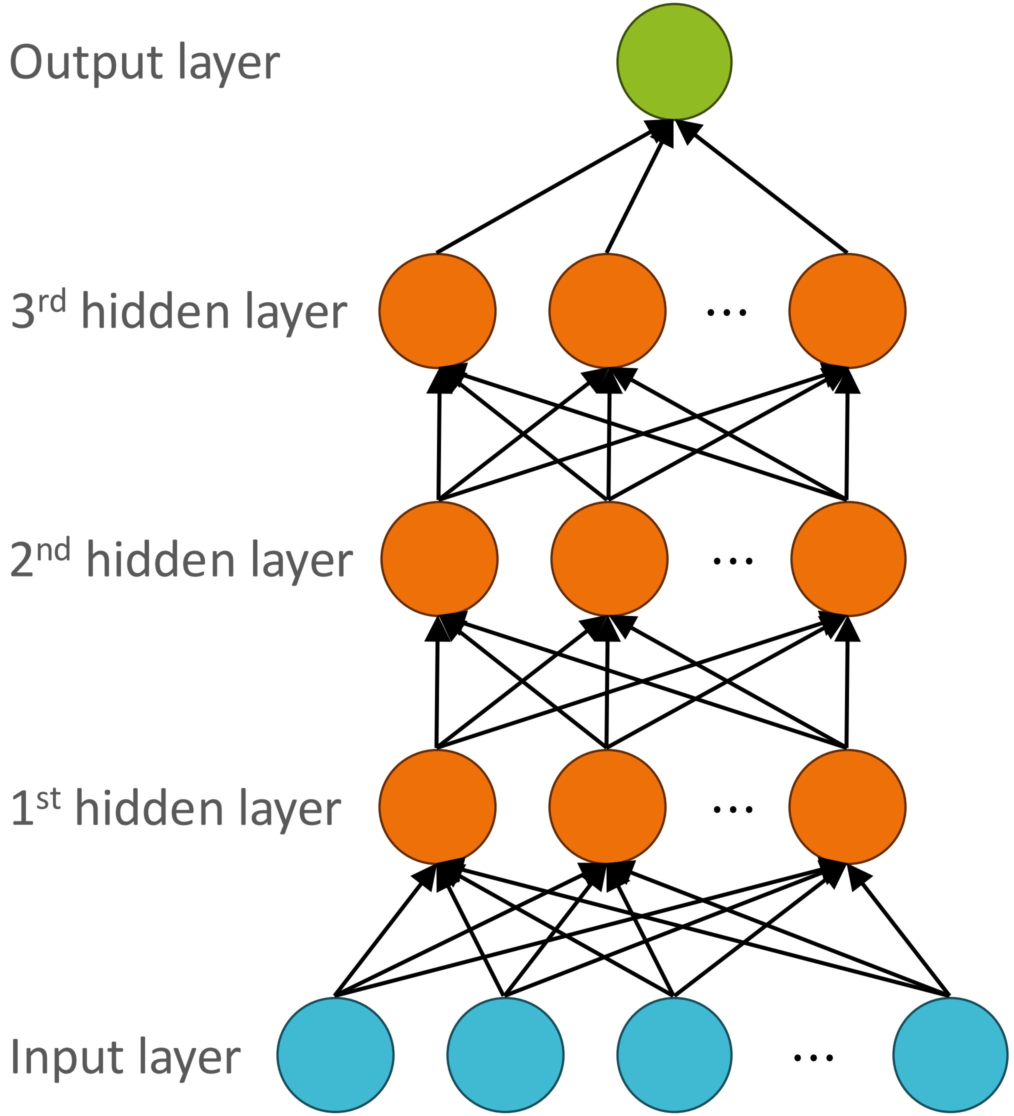
Fine-tuning (Bengio et al., 2006)

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

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

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



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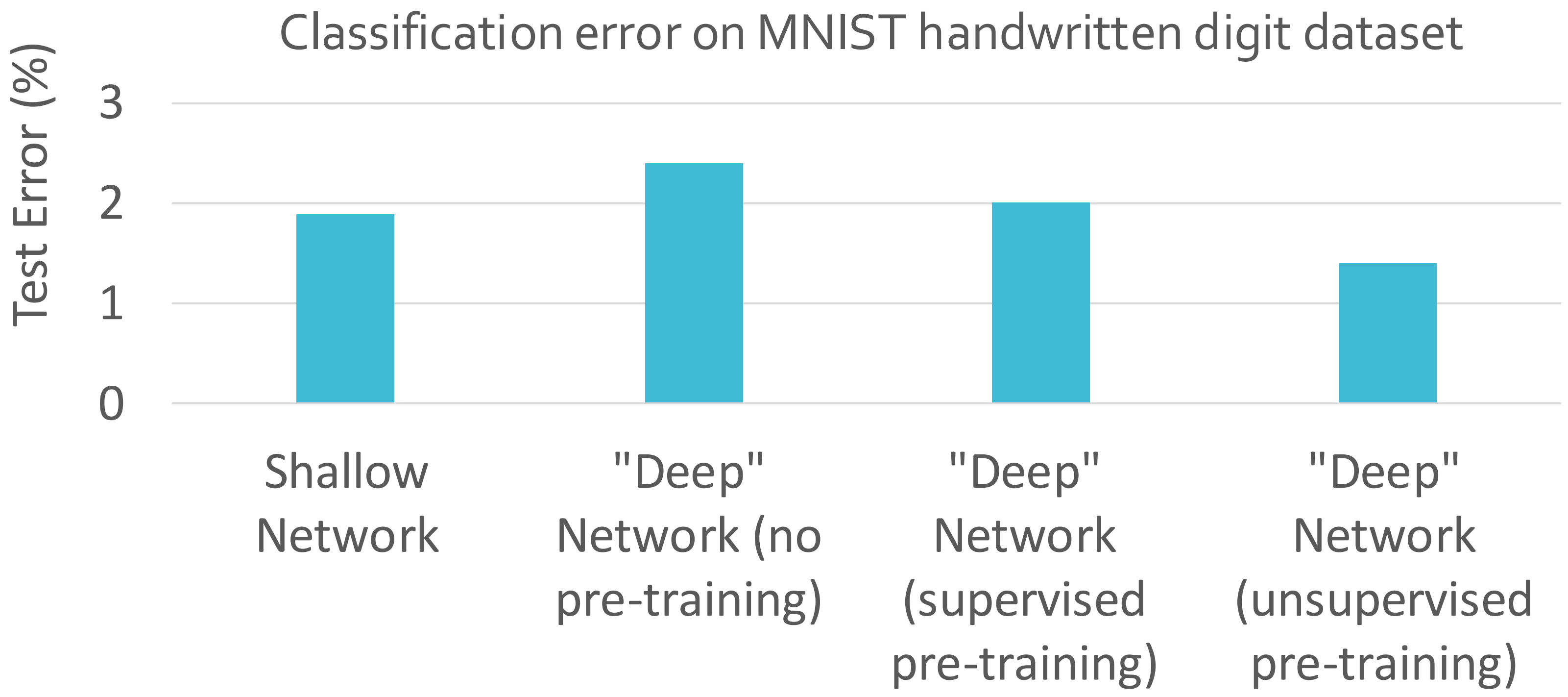
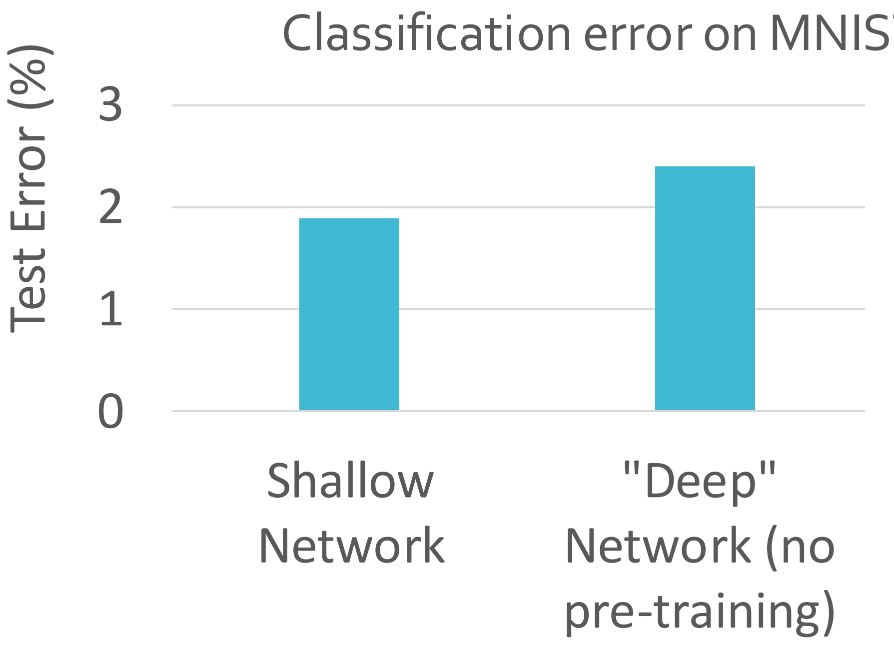


Another dose of Reality

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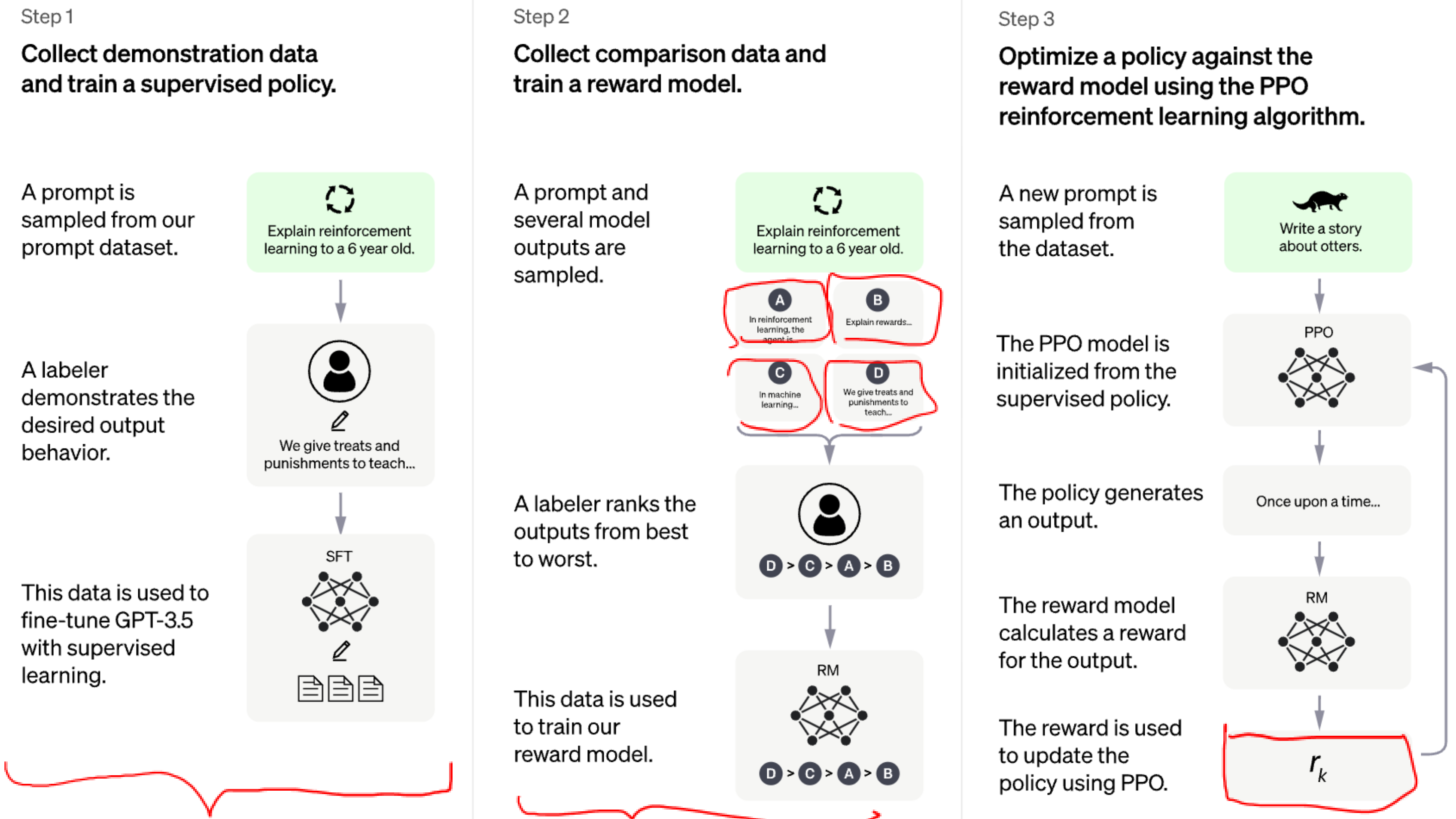
- Surprise, surprise: it overfits and your test error is super high
- Key observation: you can pre-train on basically any labelled or unlabelled dataset!
- Okay that's great for pre-training and all, but what if
  A. the concept of labelled data doesn't apply to your task i.e., not every input has a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



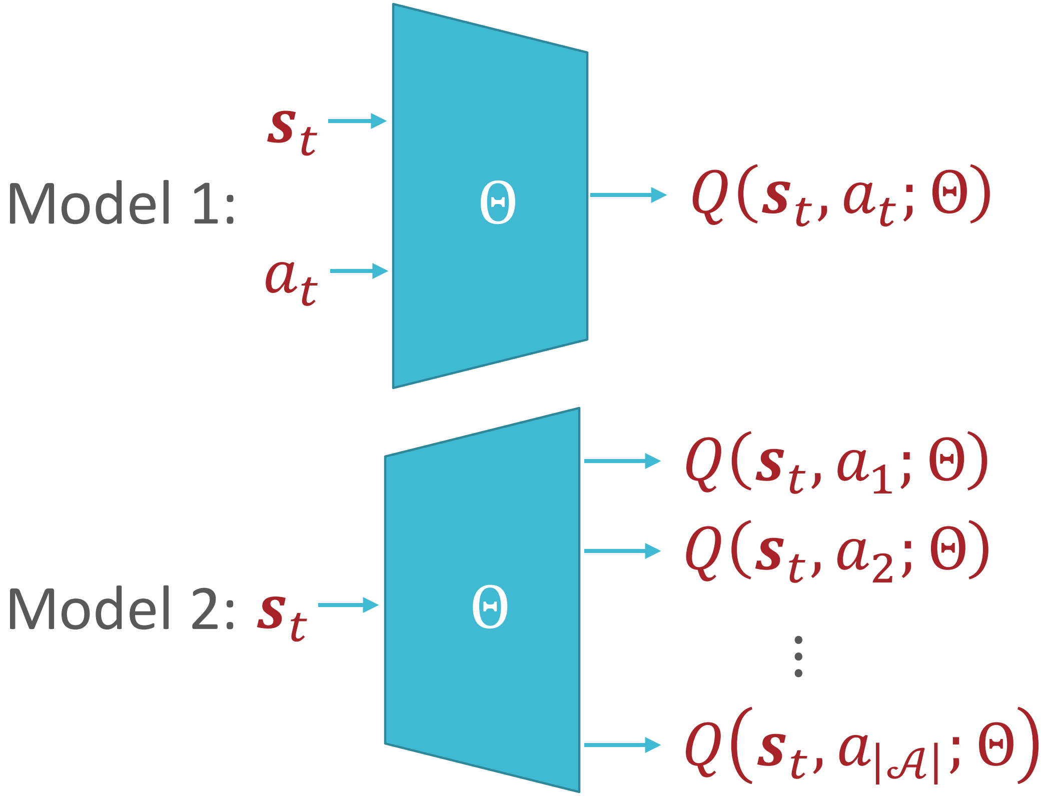
supervised learning   reward model

- 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?

- Represent states using some feature vector $\boldsymbol{s}_t \in \mathbb{R}^M$
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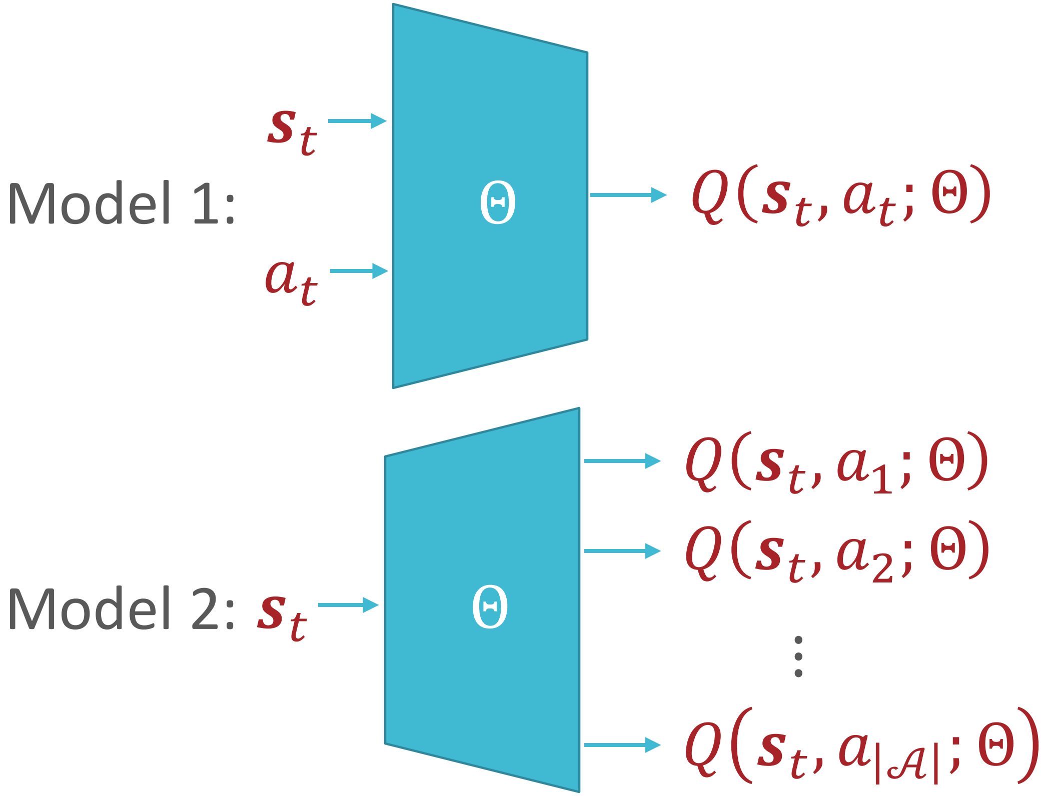
- Define a *differentiable* function that approximates Q

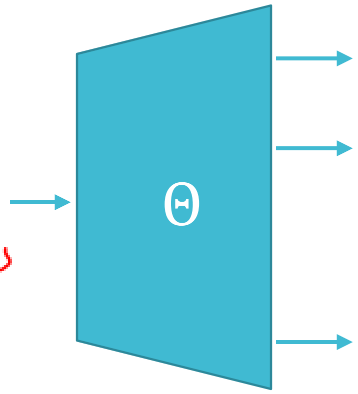


Parametrized Stochastic Policies

- 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: $\boldsymbol{s}_t$



$$p(a_1 | \boldsymbol{s}_t; \Theta) \coloneqq \pi_\Theta(a_1 | \boldsymbol{s}_t)$$

$$p(a_2 | \boldsymbol{s}_t; \Theta) \coloneqq \pi_\Theta(a_2 | \boldsymbol{s}_t)$$

$$\vdots$$

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

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

- 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 specifies a stochastic policy π_Θ
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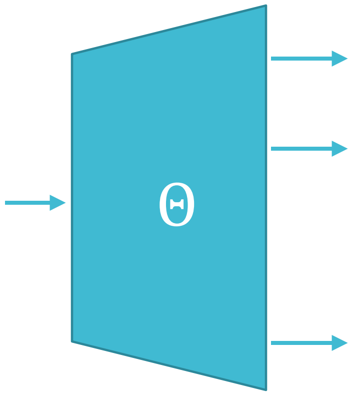
$$\ell(\Theta) = -\mathbb{E}_{\pi_\Theta}\left[\mathbb{E}_{p(s'|s,a)}\left[\sum_{t=0}^{\infty} \gamma^t r_t\right]\right]$$

Model: $\boldsymbol{s}_t$



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

Trajectories

- A *trajectory* $\mathrm{T} = \{\boldsymbol{s}_0, a_0, \boldsymbol{s}_1, a_1, \dots, \boldsymbol{s}_T\}$ 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

$$p_\Theta(\mathrm{T}) = p(\{\boldsymbol{s}_0, a_0, \boldsymbol{s}_1, a_1, \dots, \boldsymbol{s}_T\})$$
$$= p(\boldsymbol{s}_0) \prod_{t=0}^{T-1} p(s_{t+1} | s_t, a_t)\, \pi_\Theta(a_t | \boldsymbol{s}_t)$$

  - Requires a distribution over initial states $p(\boldsymbol{s}_0)$ e.g., uniform over all states, fixed or deterministic, etc…

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

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

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

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- Insight:

$$\nabla_\Theta p_\Theta(\mathrm{T}) = \frac{p_\Theta(\mathrm{T})}{p_\Theta(\mathrm{T})}\nabla_\Theta p_\Theta(\mathrm{T}) = p_\Theta(\mathrm{T})\boxed{\nabla_\Theta(\log p_\Theta(\mathrm{T}))}$$

$$\log p_\Theta(\mathrm{T}) = \log p(s_0) + \sum_{t=0}^{T-1} \underline{\log p(s_{t+1}|s_t,a_t)} + \log \pi_\Theta(a_t|\boldsymbol{s}_t)$$

$$\underline{\nabla_\Theta(\log p_\Theta(\mathrm{T}))} = \underline{\sum_{t=0}^{T-1} \nabla_\Theta \log \pi_\Theta(a_t|\boldsymbol{s}_t)} \leftarrow$$

No longer depends on $p(s_{t+1}|s_t,a_t)$!

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

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

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

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

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

(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)

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

empirical estimate

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

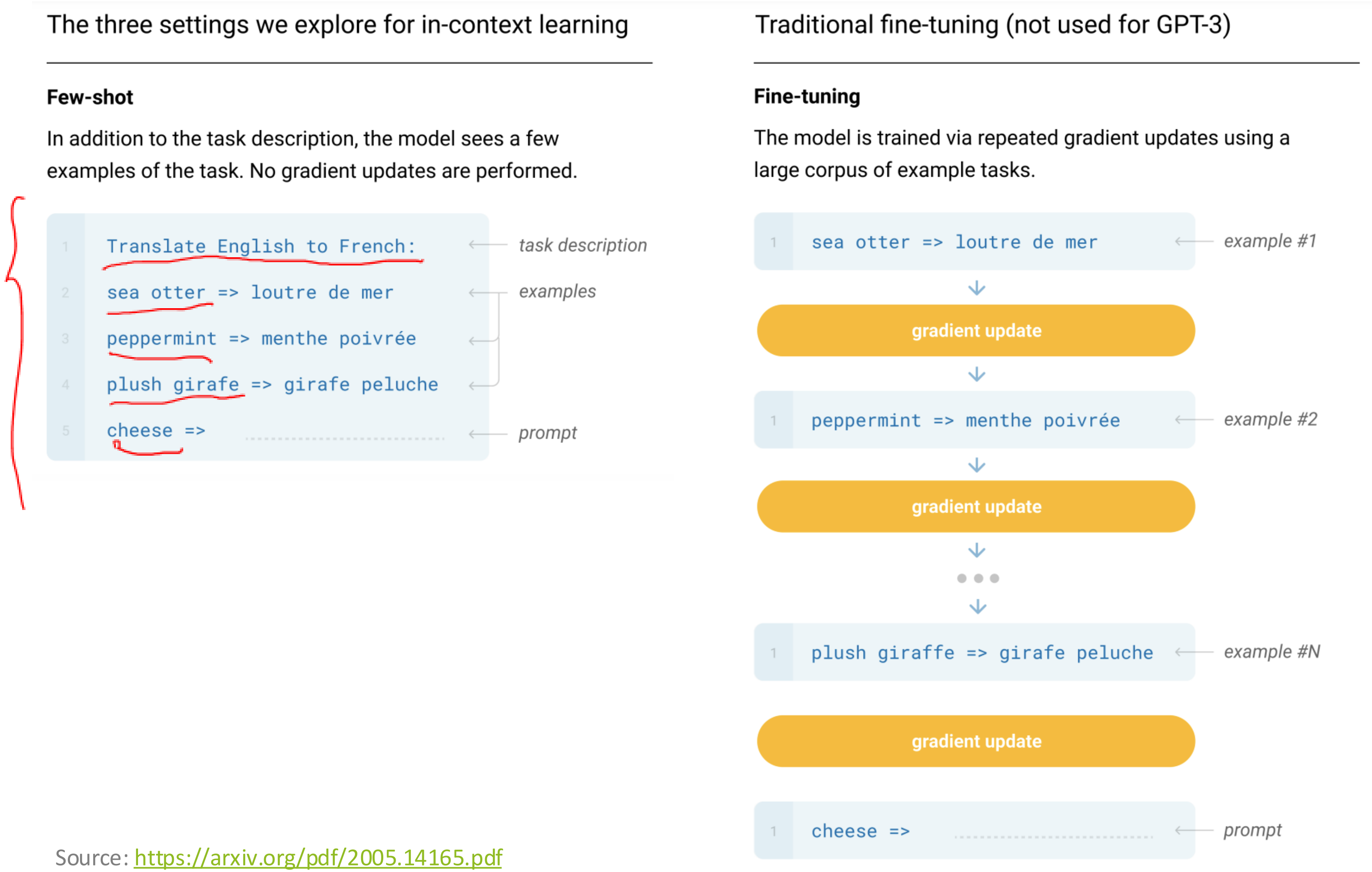
In-context Learning

- 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

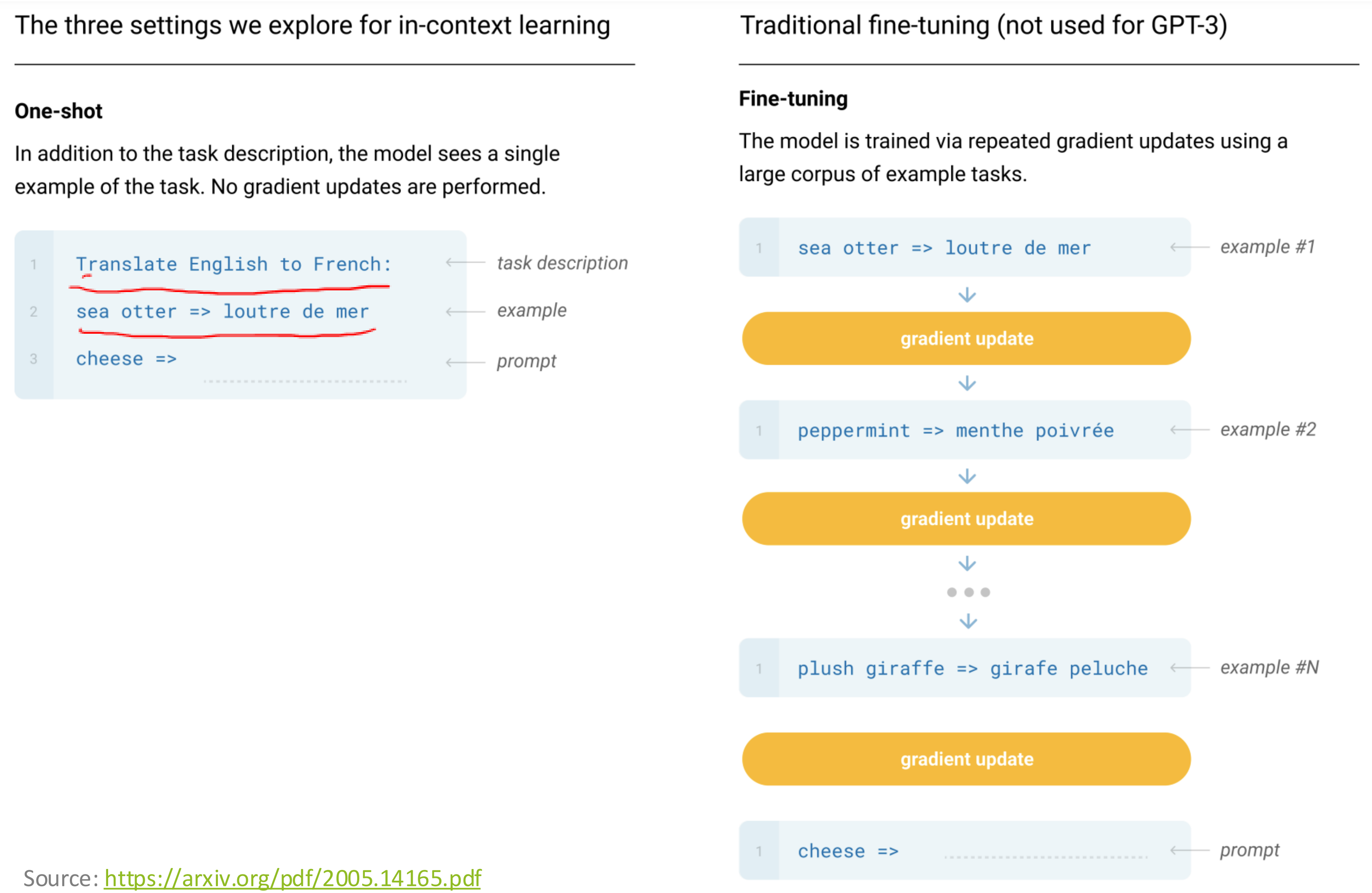
- Idea: leverage the LLM's context window by passing a few examples to the model as input, *without performing any updates to the parameters*



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 example~~s~~ to the model as input, *without performing any updates to the parameters*



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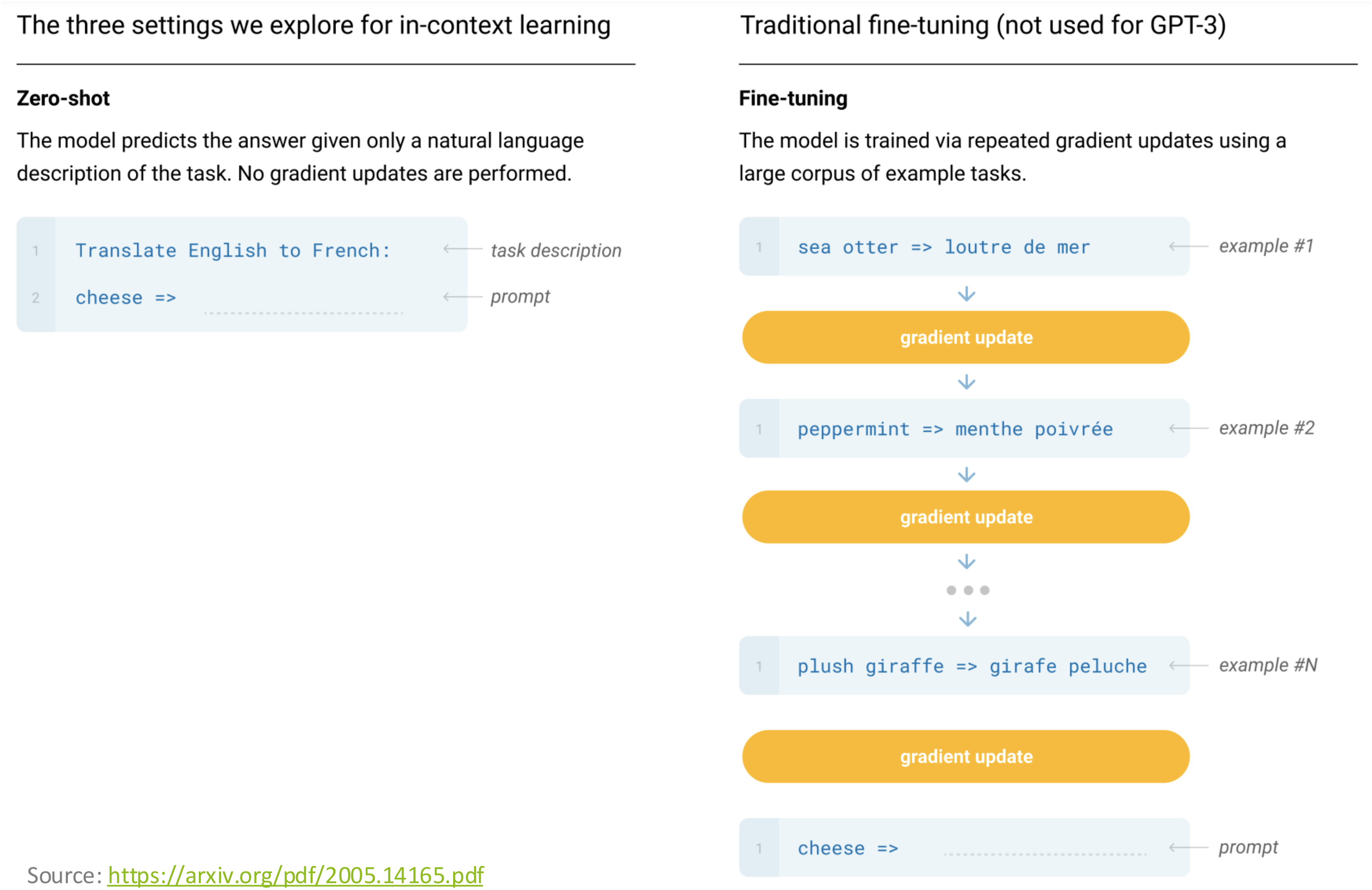
Few-shot, One-shot & Zero-shot (in-context) Learning

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



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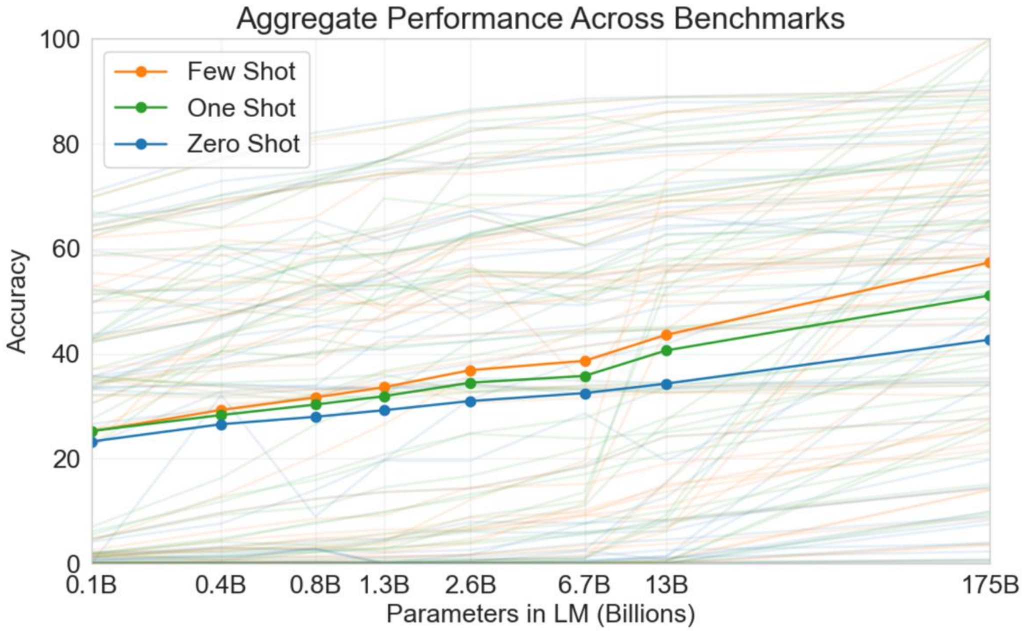

- Key Takeaway: LLMs can perform well on novel tasks without having to fine-tune the model, sometimes even with just one or zero labelled training data points!

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