10-301/601: Introduction to Machine Learning Lecture 20: Markov Decision Processes

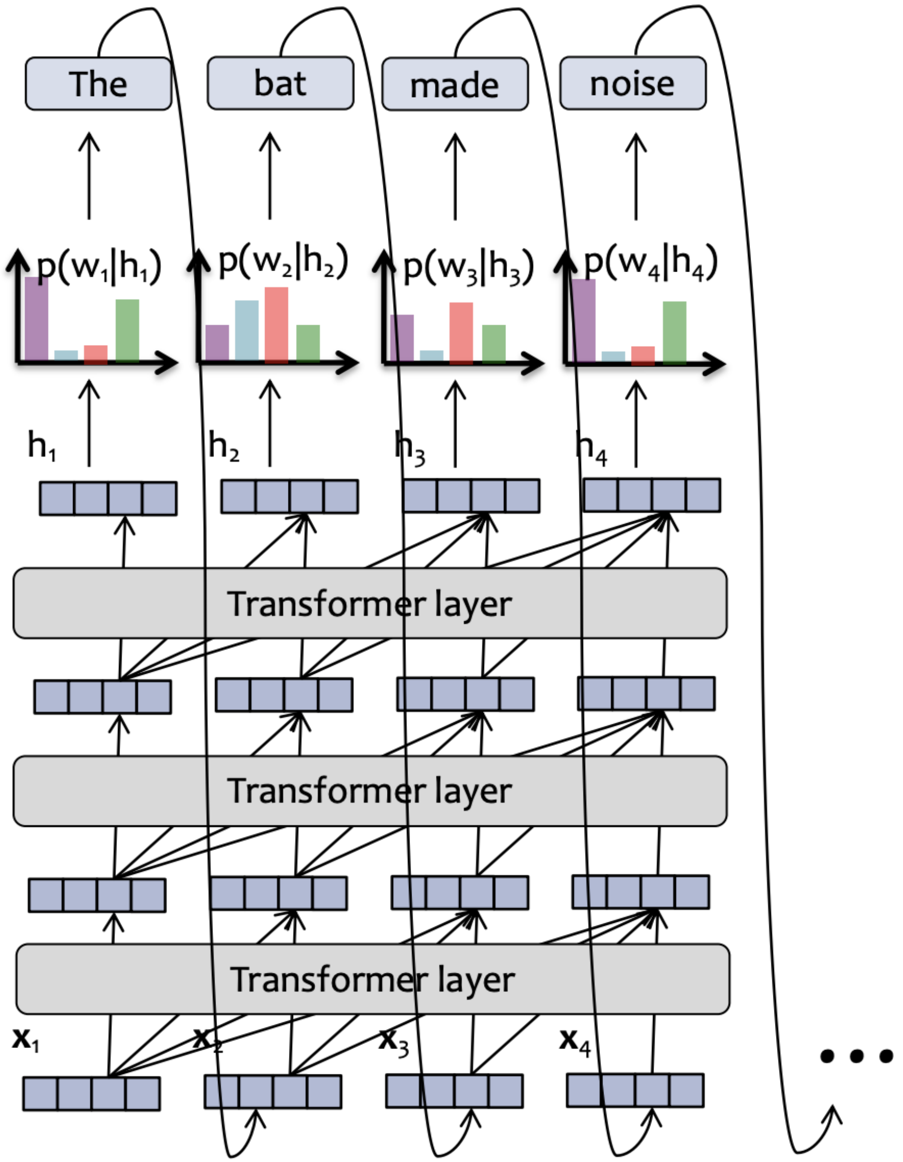
Matt Gormley & Henry Chai

11/6/24

Front Matter

- Announcements
  - Exam 2 on 11/7 (tomorrow!)
    - Please review the seating chart on Piazza and make sure you have a seat / know where you're going
  - HW7 to be released 11/7, due 11/17 at 11:59 PM
    - Please be mindful of your grace day usage (see the course syllabus for the policy)
    - If you have not used PyTorch before, I ***strongly*** encourage you to go to recitation on Friday (11/8)

Recall: Transformers



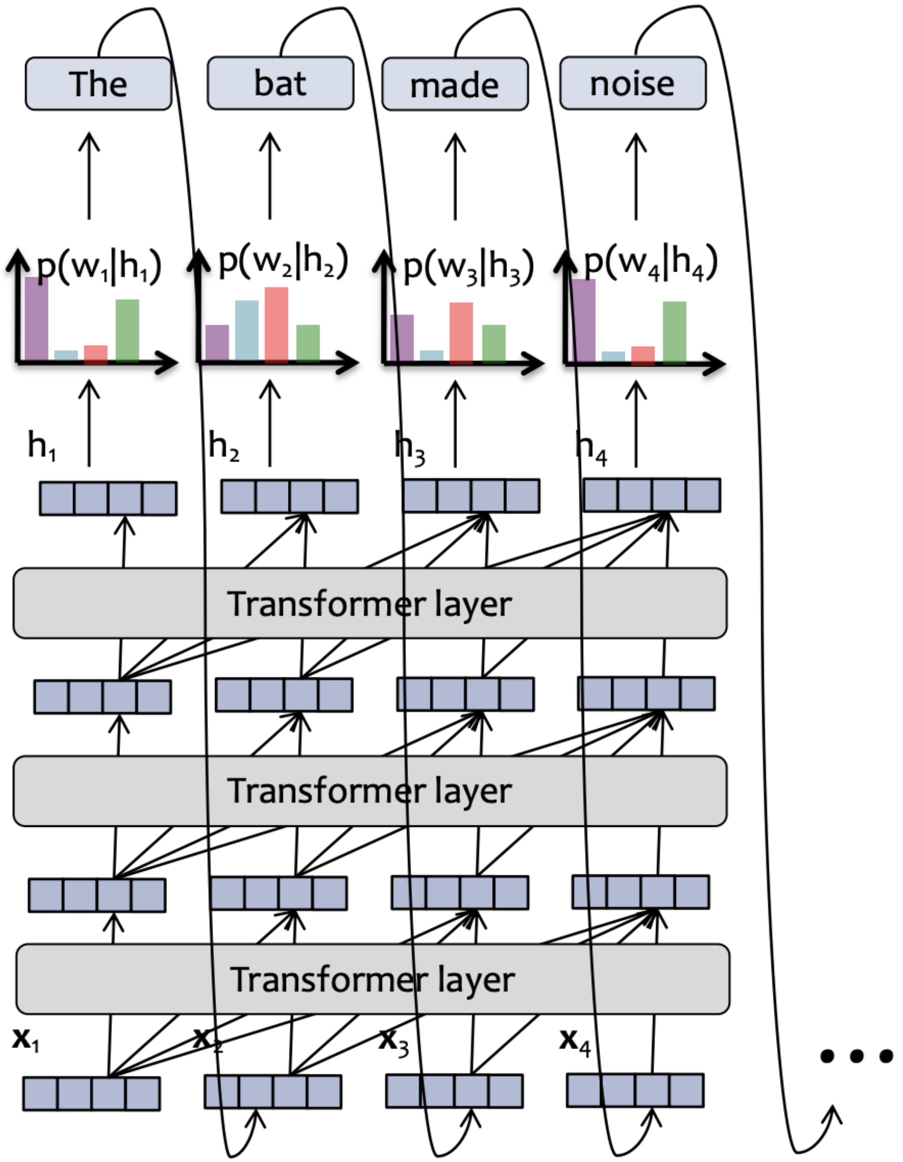
Each layer of a Transformer LM consists of several **sublayers:**

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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Recall: Mini-batch Stochastic Gradient Descent…

- Input: $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right\}_{n=1}^{N}, \eta_{MB}^{(0)}, B$

1. Initialize all weights $W_{(0)}^{(1)}, \ldots, W_{(0)}^{(L)}$ to small, random numbers 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*,
   $$G^{(l)} = \frac{1}{B} \sum_{b=1}^{B} \nabla_{W^{(l)}} \ell^{(b)} \left(W_{(t)}^{(1)}, \ldots, W_{(t)}^{(L)}\right) \ \forall \ l$$
   c. Update $W^{(l)}$: $W_{t+1}^{(l)} \leftarrow W_{t}^{(l)} - \eta_{MB}^{(0)} G^{(l)} \ \forall \ l$
   d. Increment t: $t \leftarrow t + 1$

- Output: $W_{t}^{(1)}, \ldots, W_{t}^{(L)}$

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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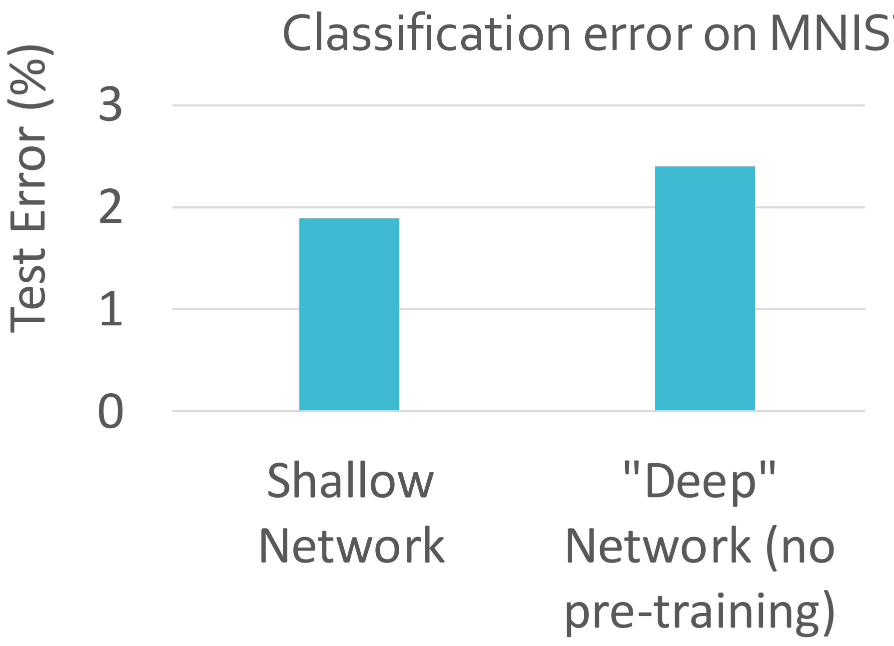
Traditional Supervised Learning

- 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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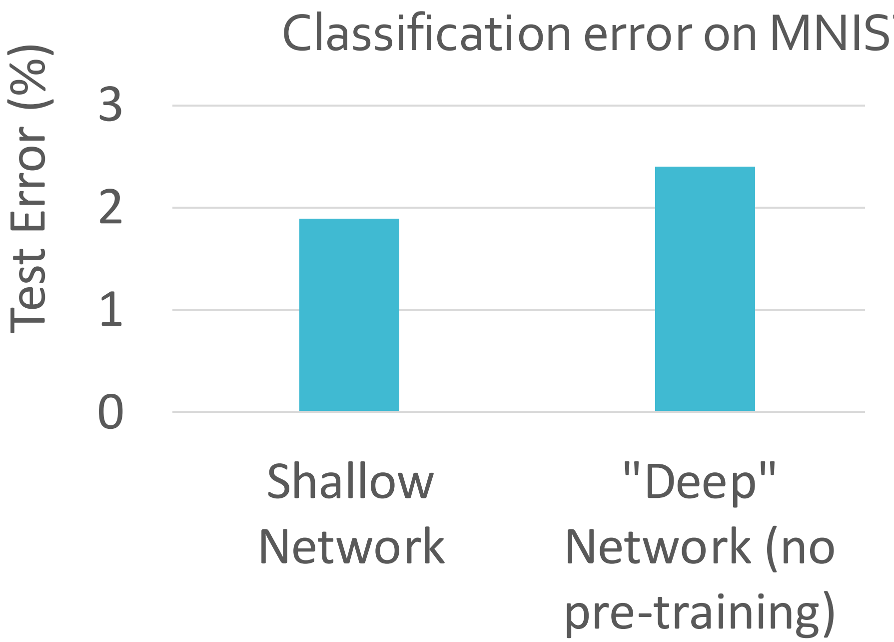
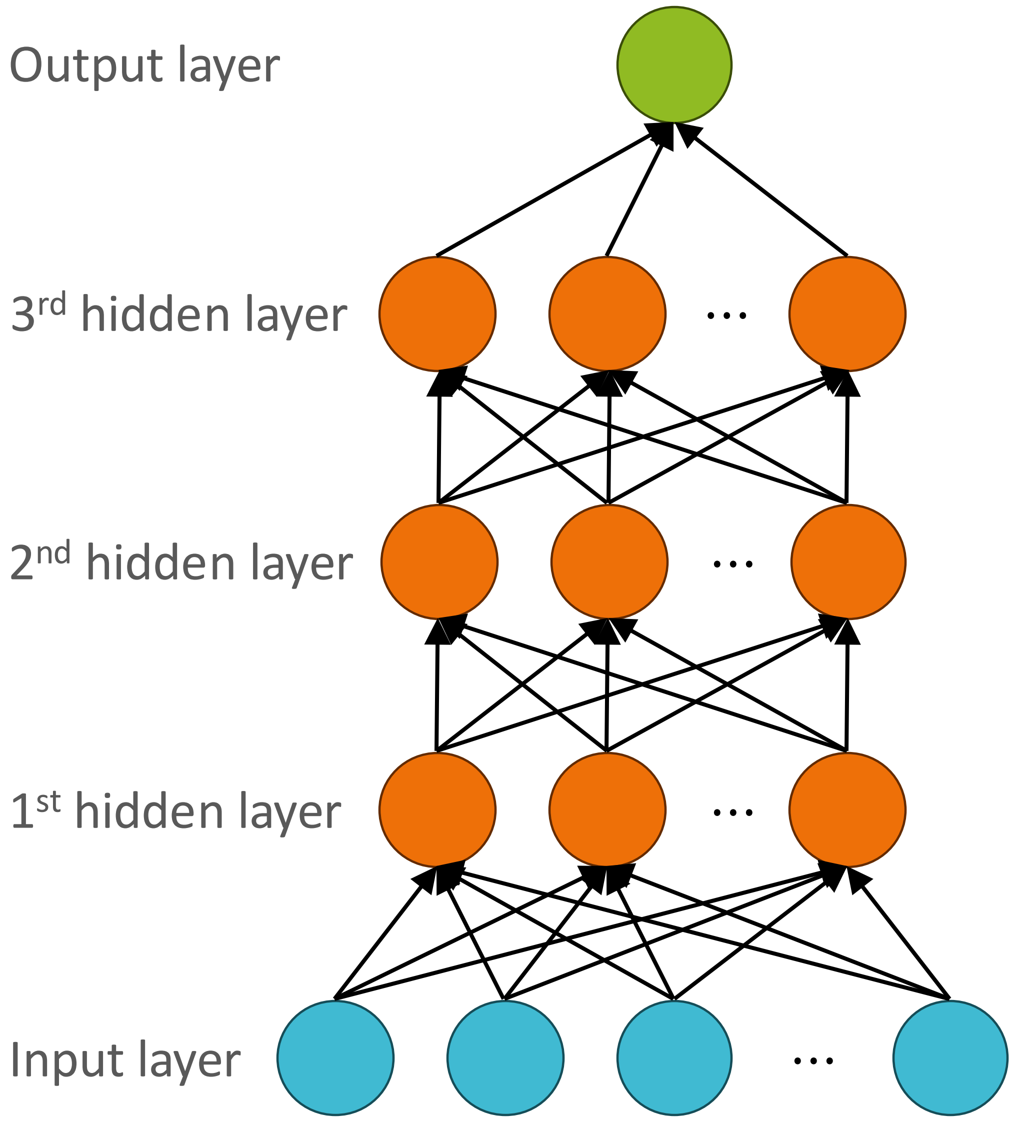


- Idea: if shallow networks are easier to train, let's just decompose our deep network into a series of shallow networks!

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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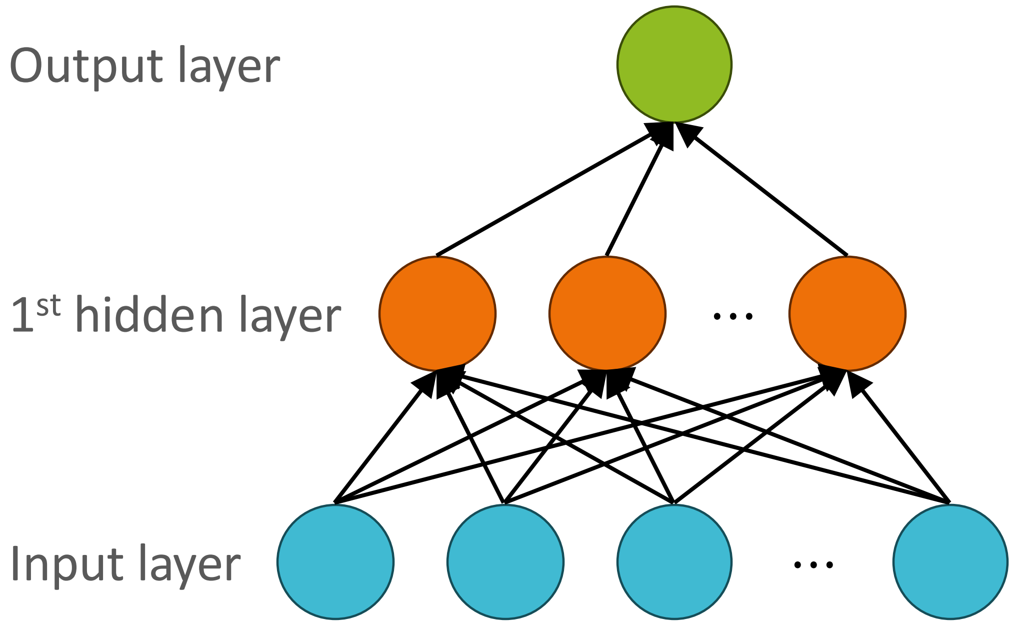

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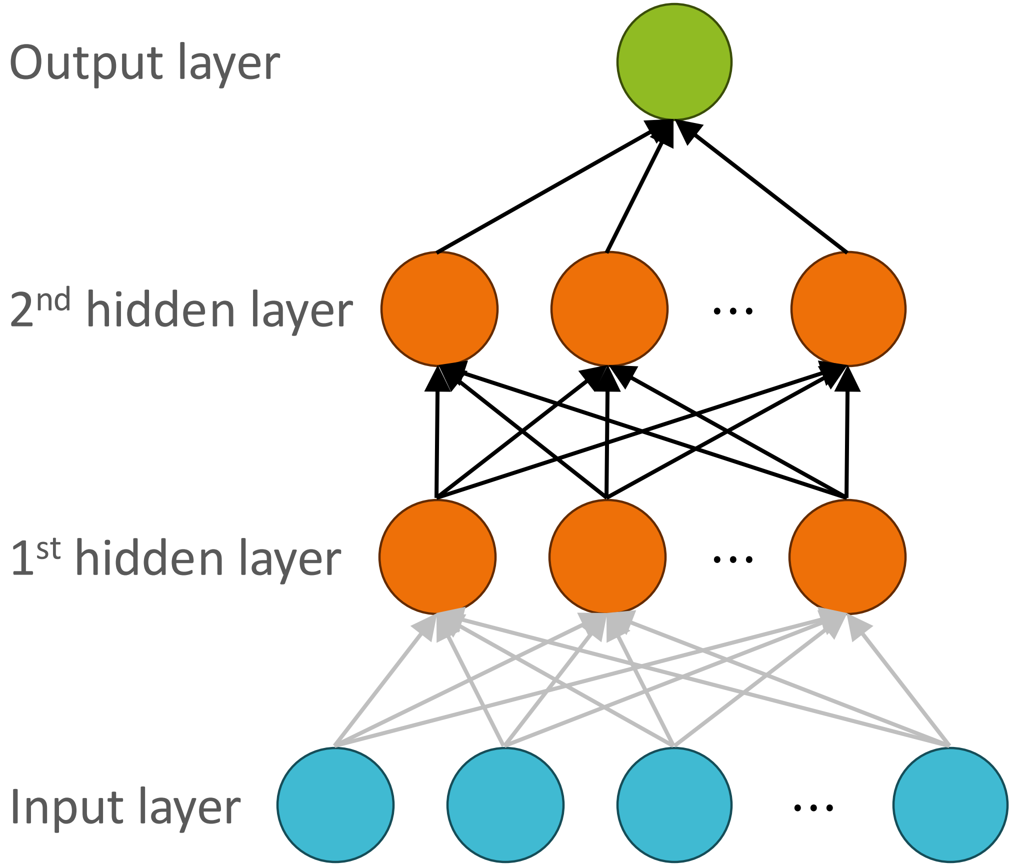

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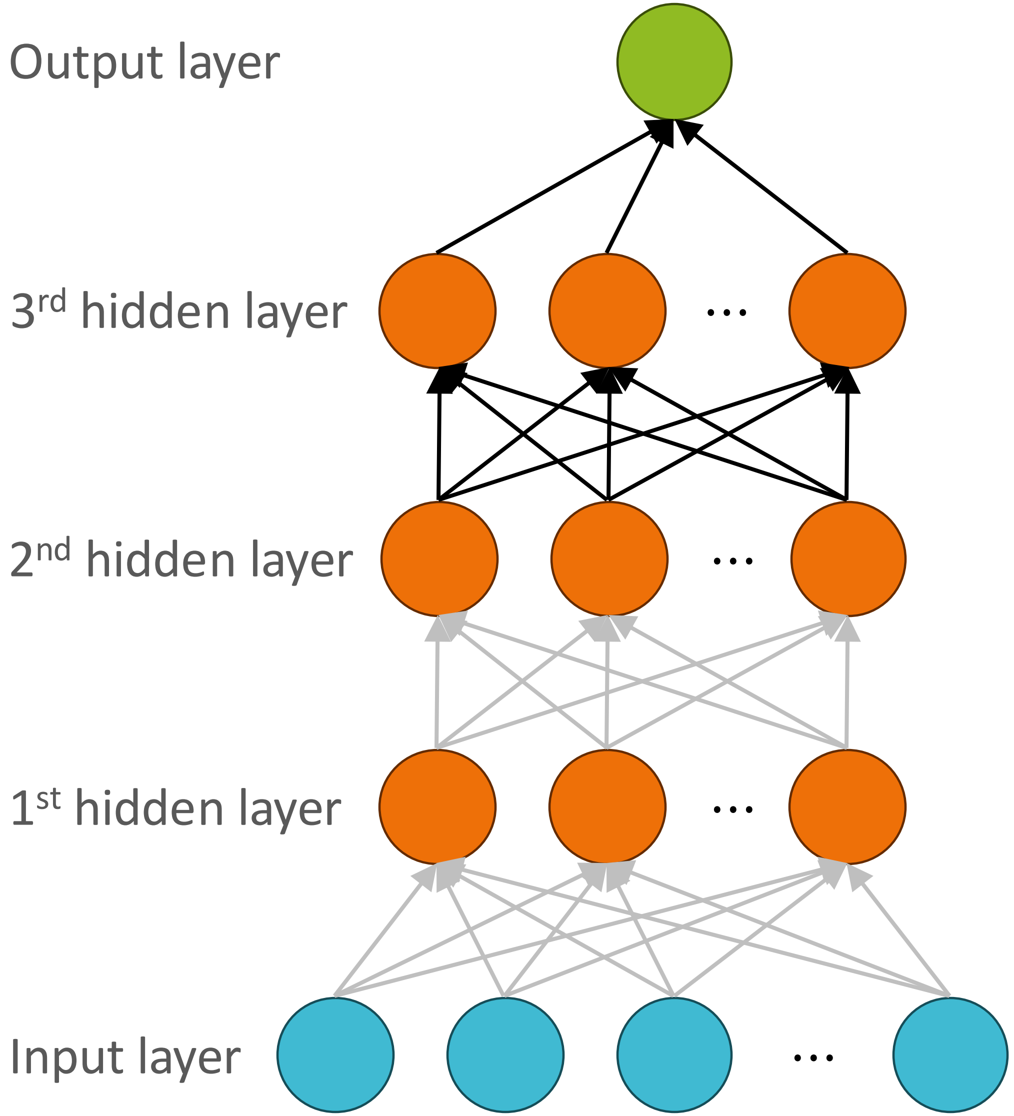

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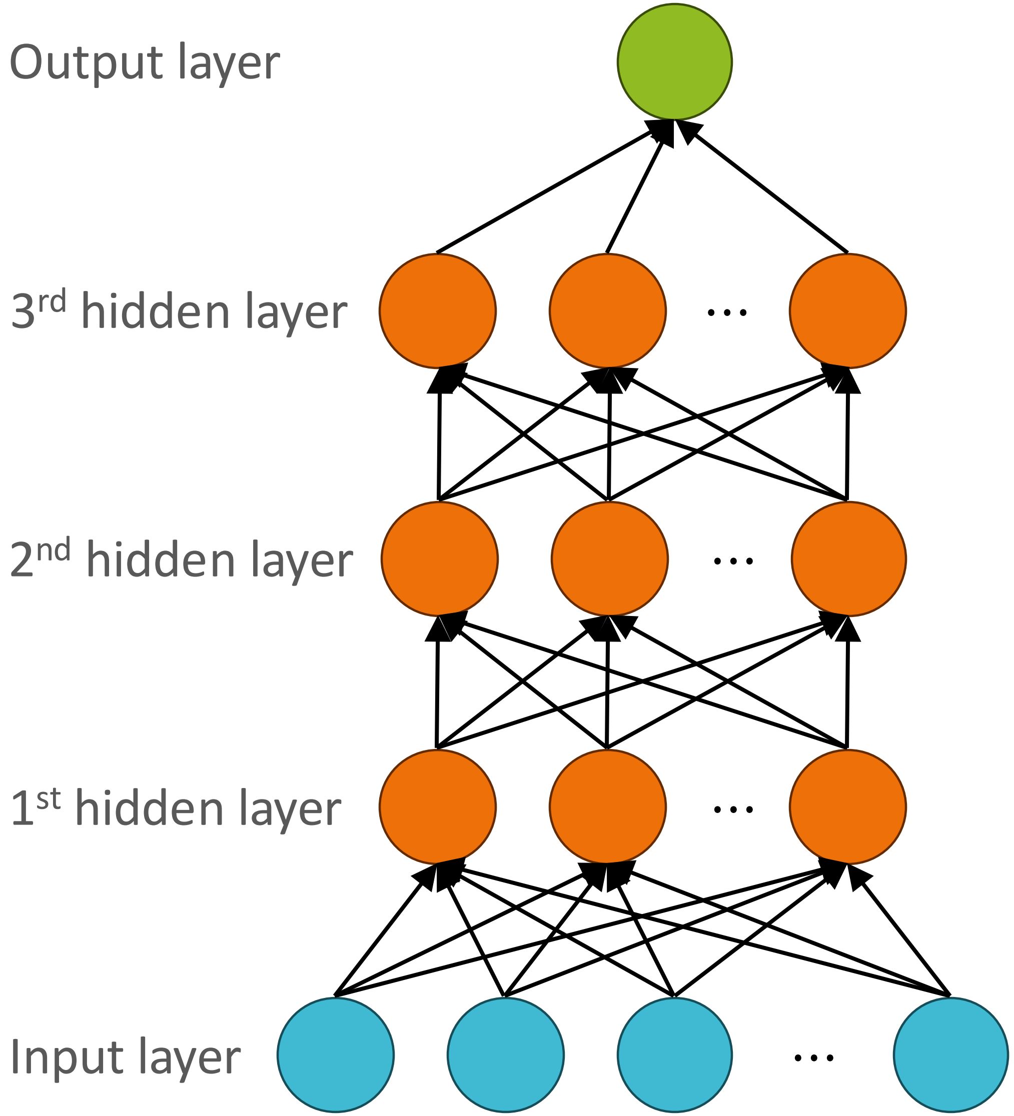
Fine-tuning (Bengio et al., 2006)

- 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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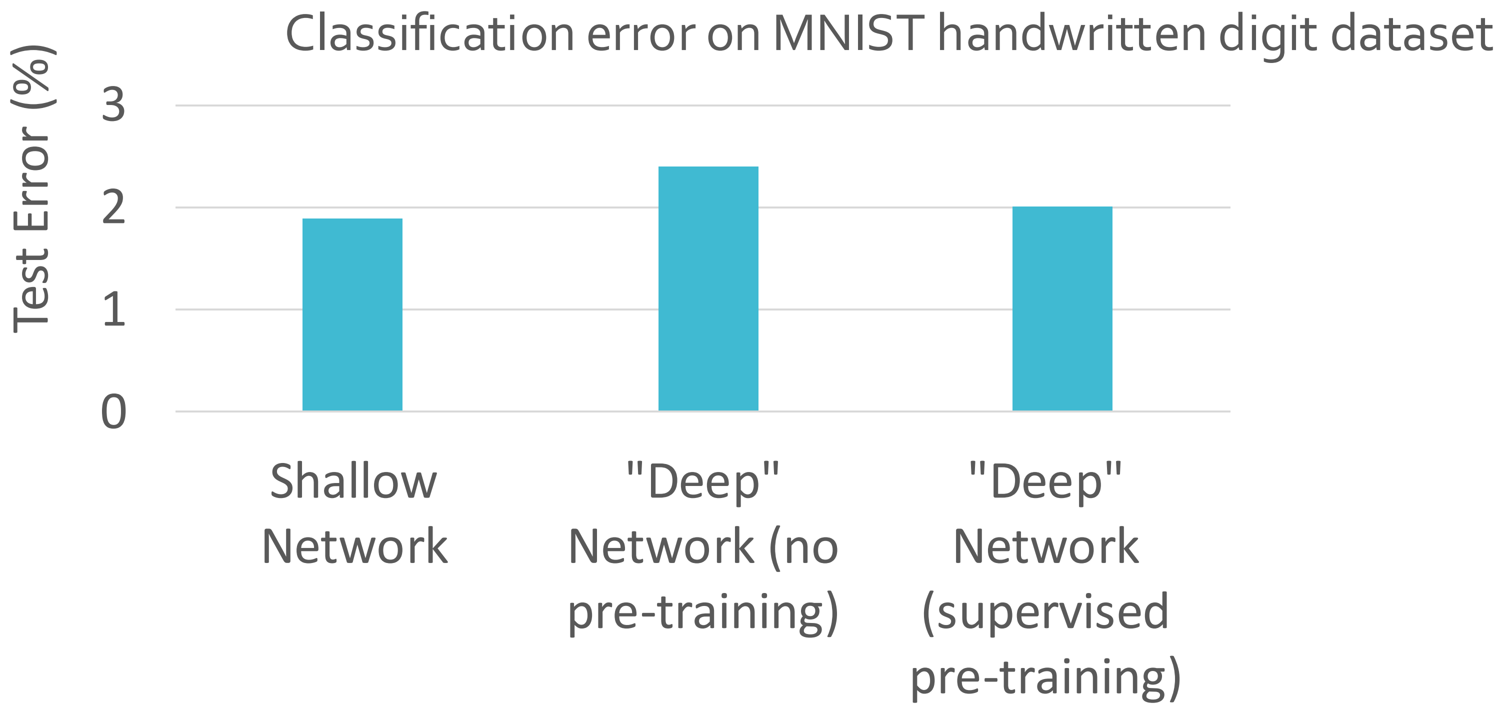
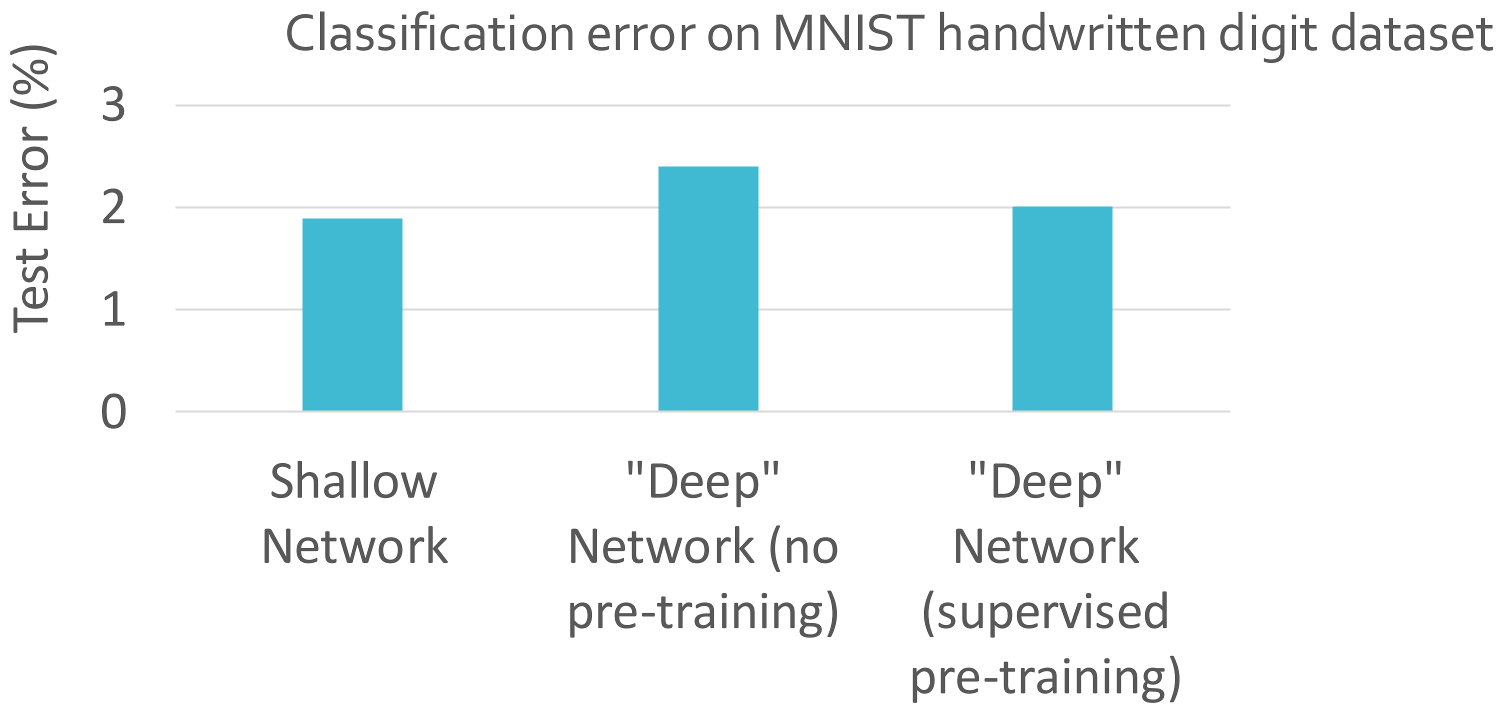


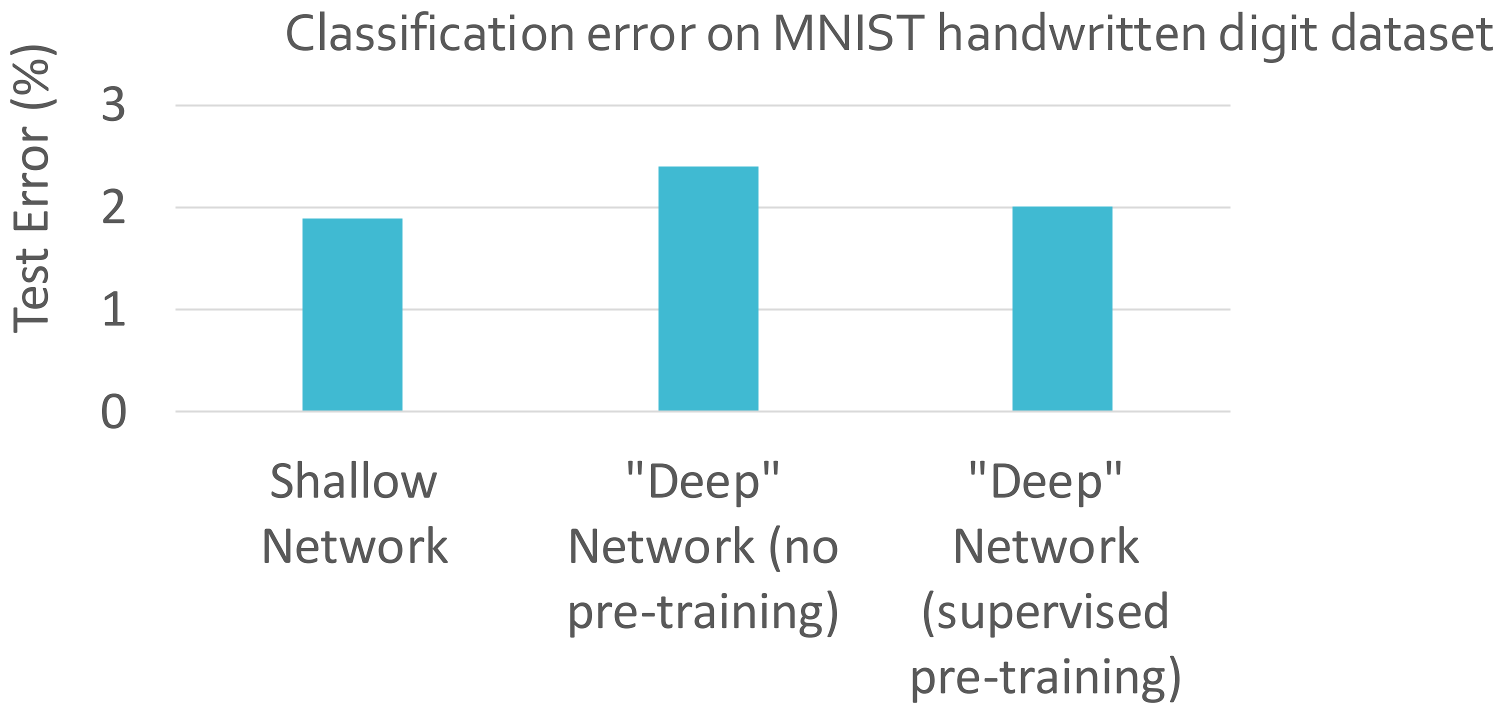
Supervised Pre-training (Bengio et al., 2006)

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



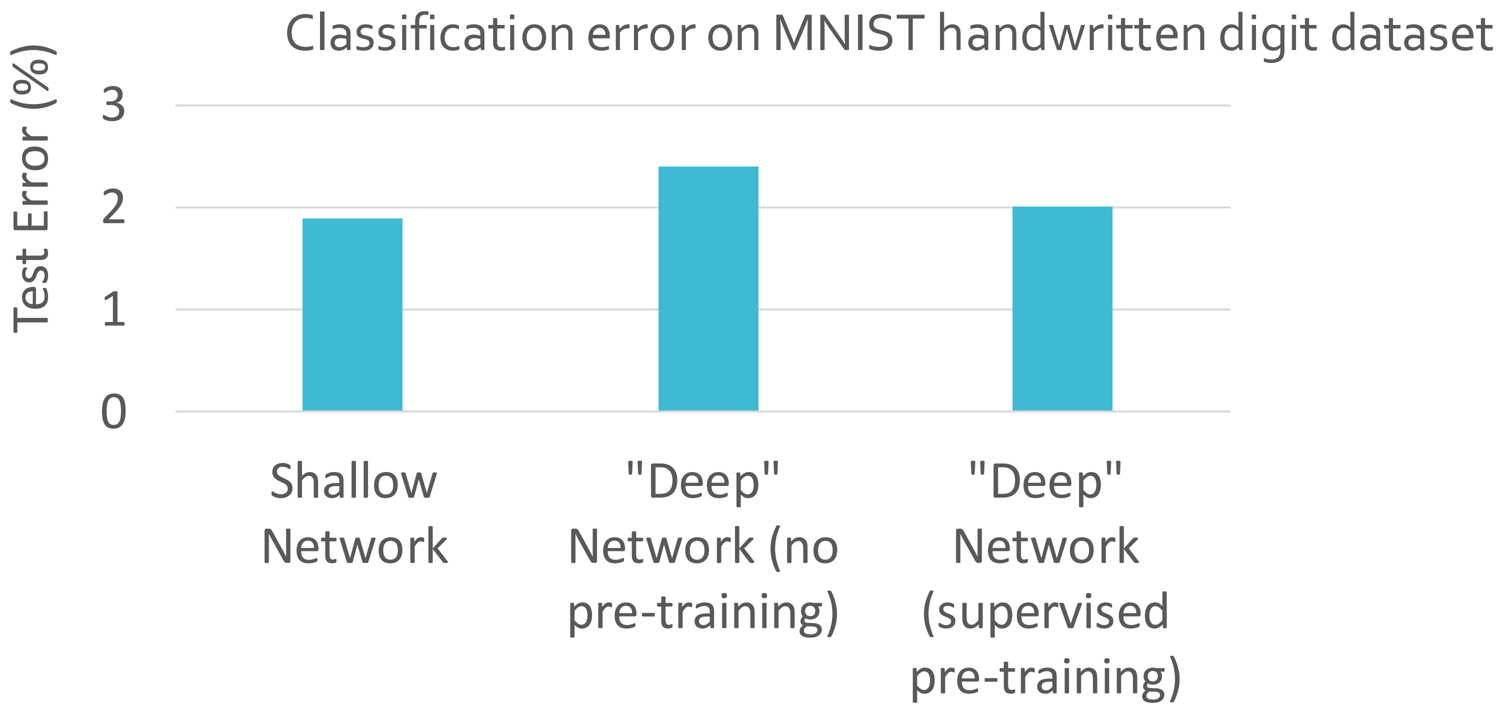
Is this the only thing we could do with the training data?

- 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)

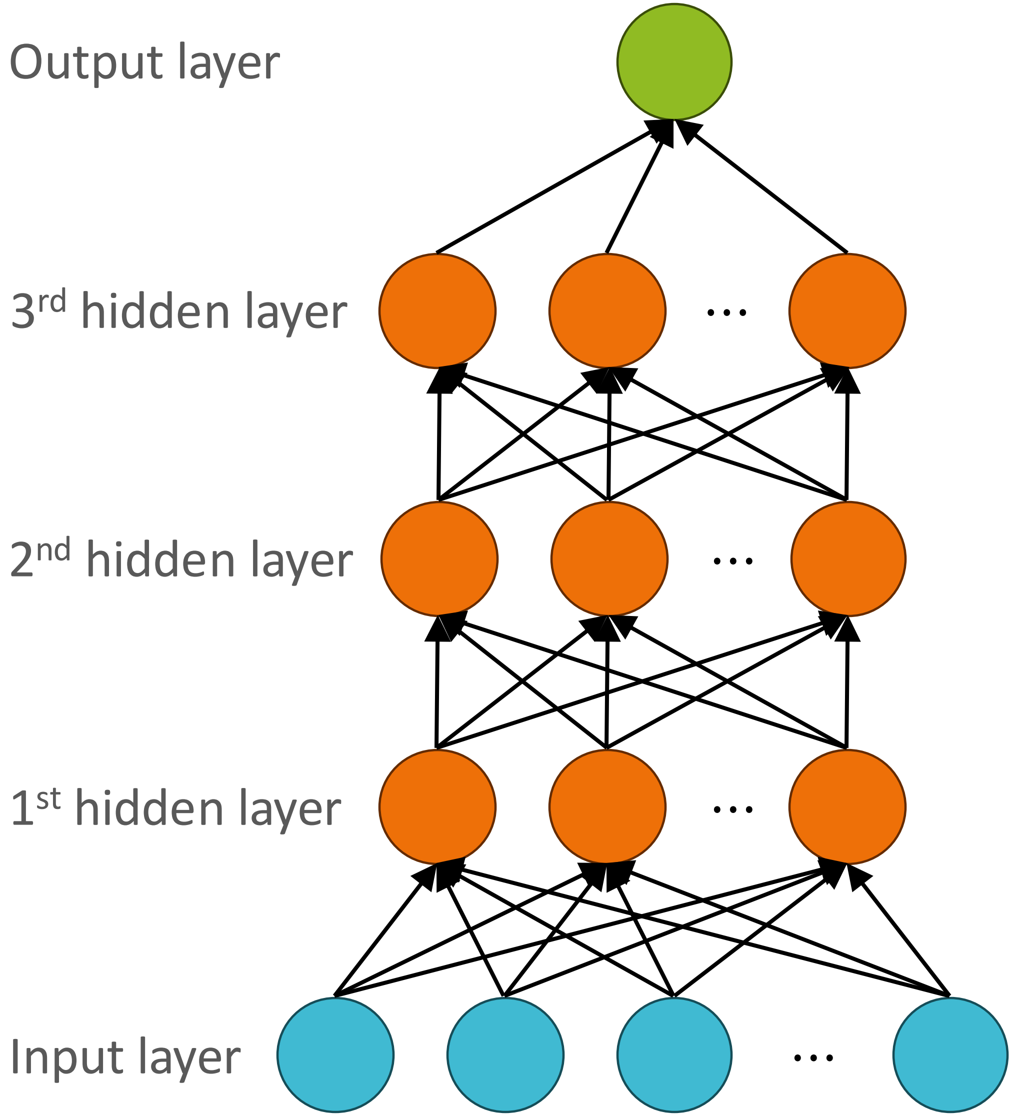
- Train each layer of the network iteratively using the training dataset *to learn useful representations*
- Idea: a good representation is one preserves a lot of information and could be used to recreate the inputs



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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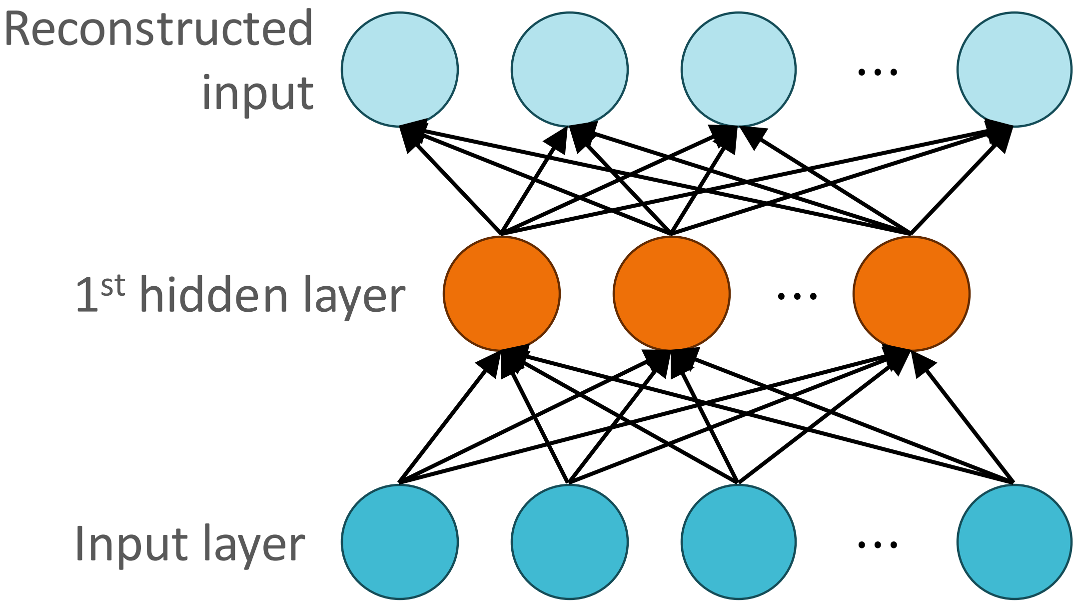
- This architecture/ objective defines an *autoencoder*



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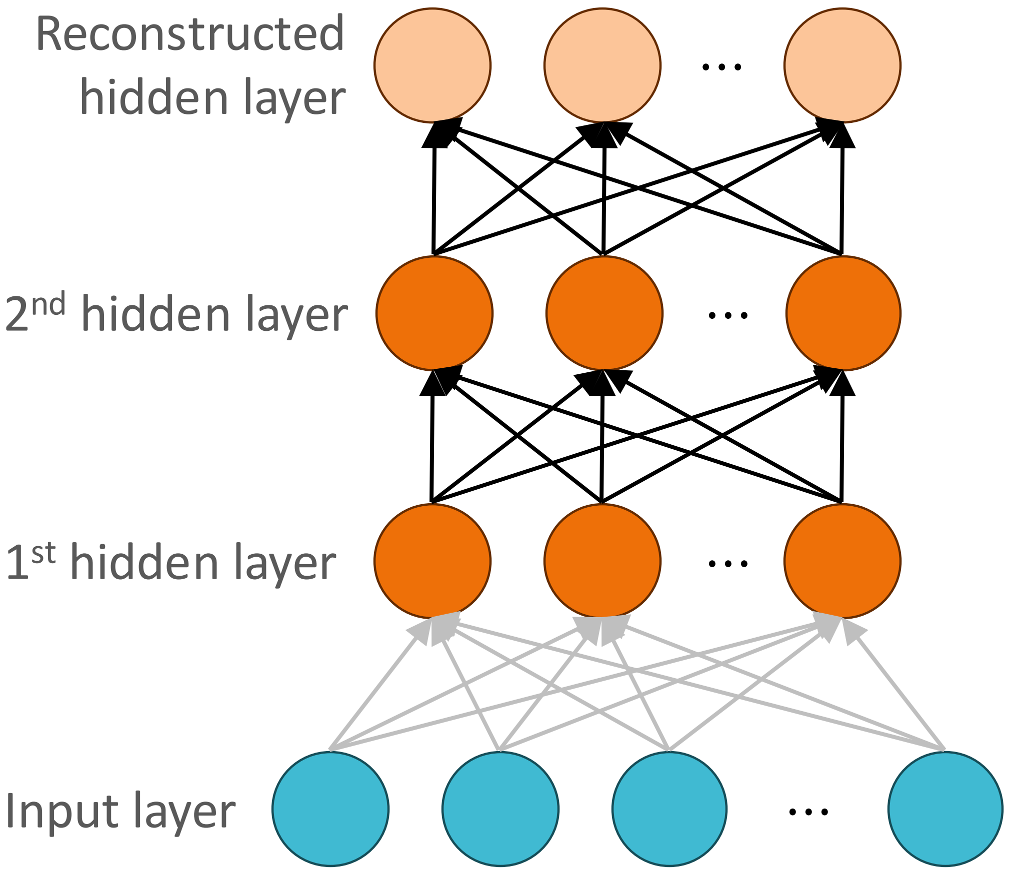

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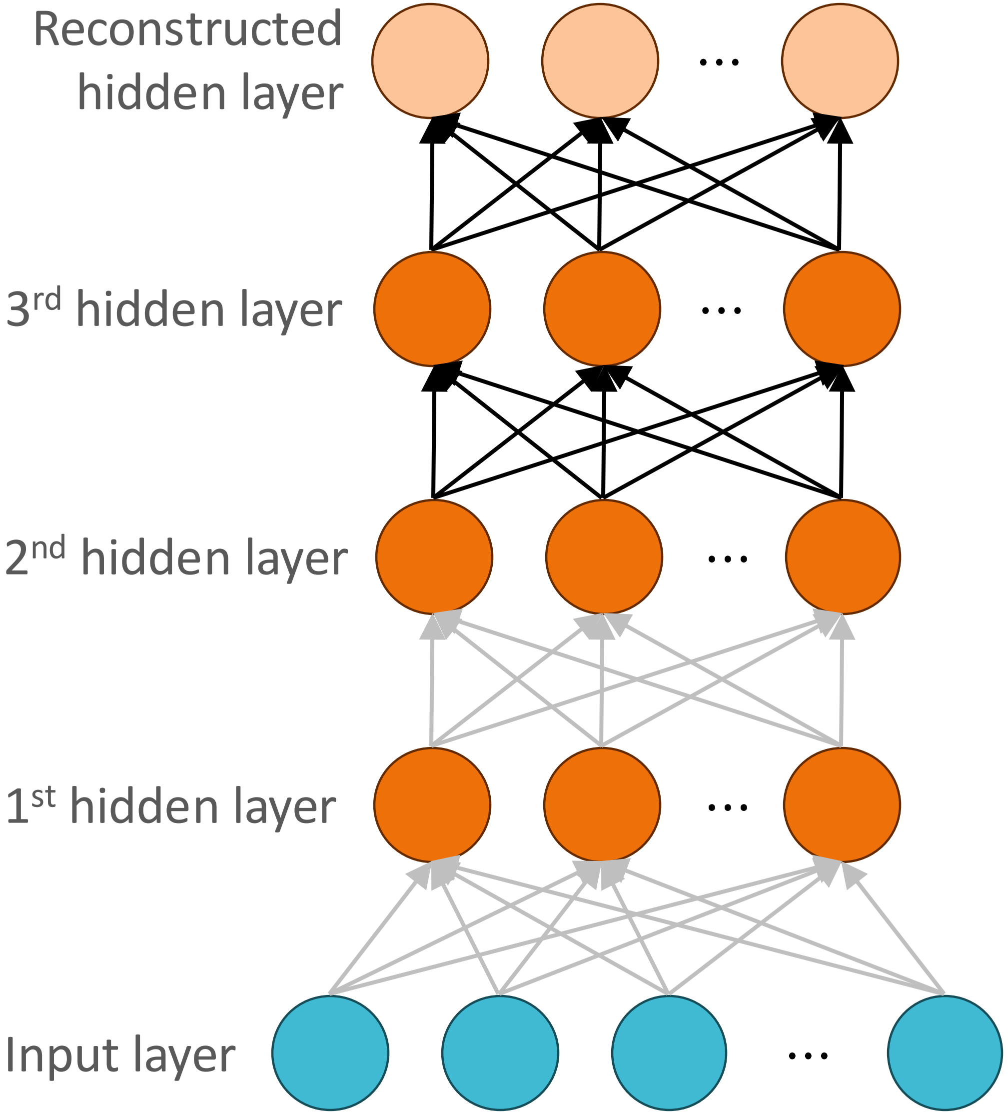

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Fine-tuning (Bengio et al., 2006)

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

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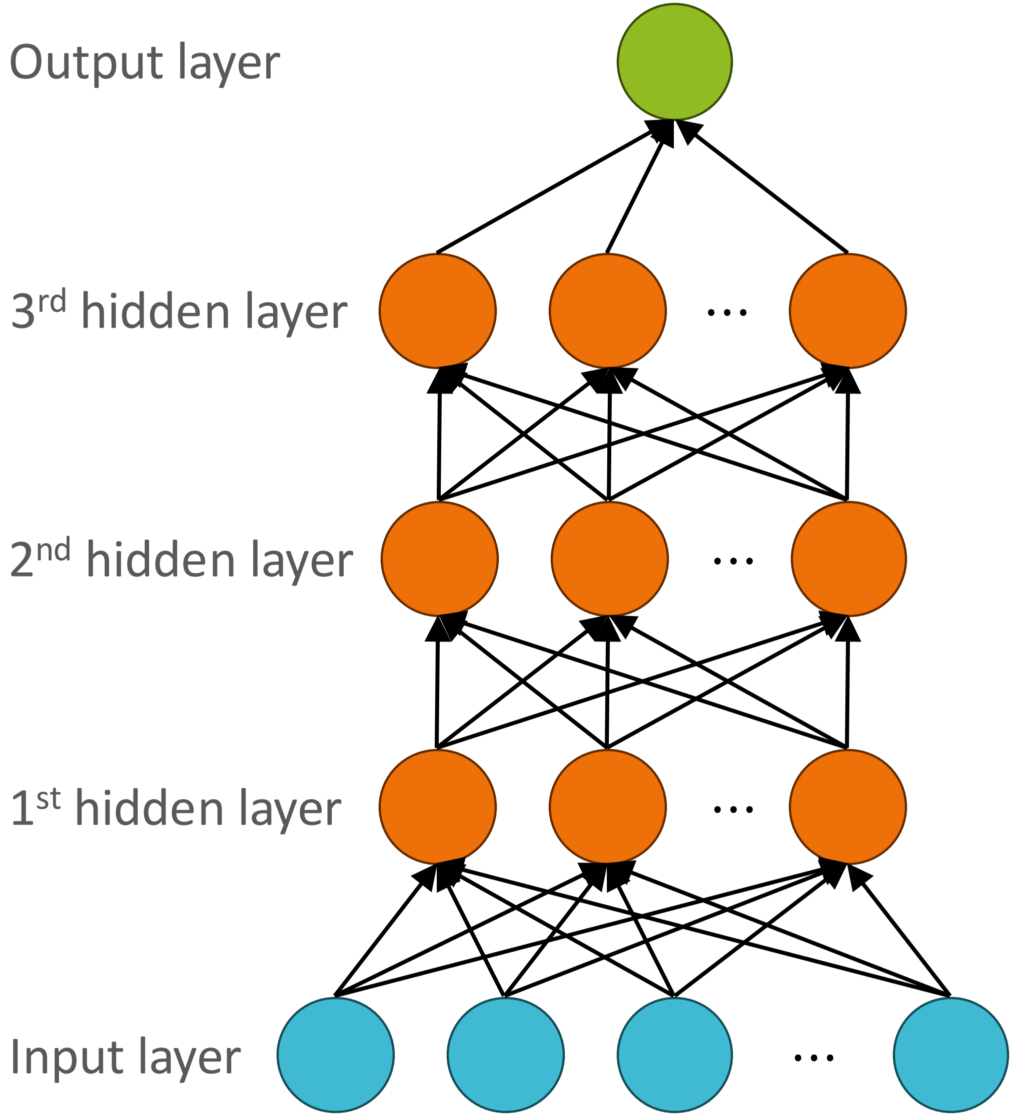
- When fine-tuning, we're effectively swapping out the last layer and fitting all the weights to the training dataset



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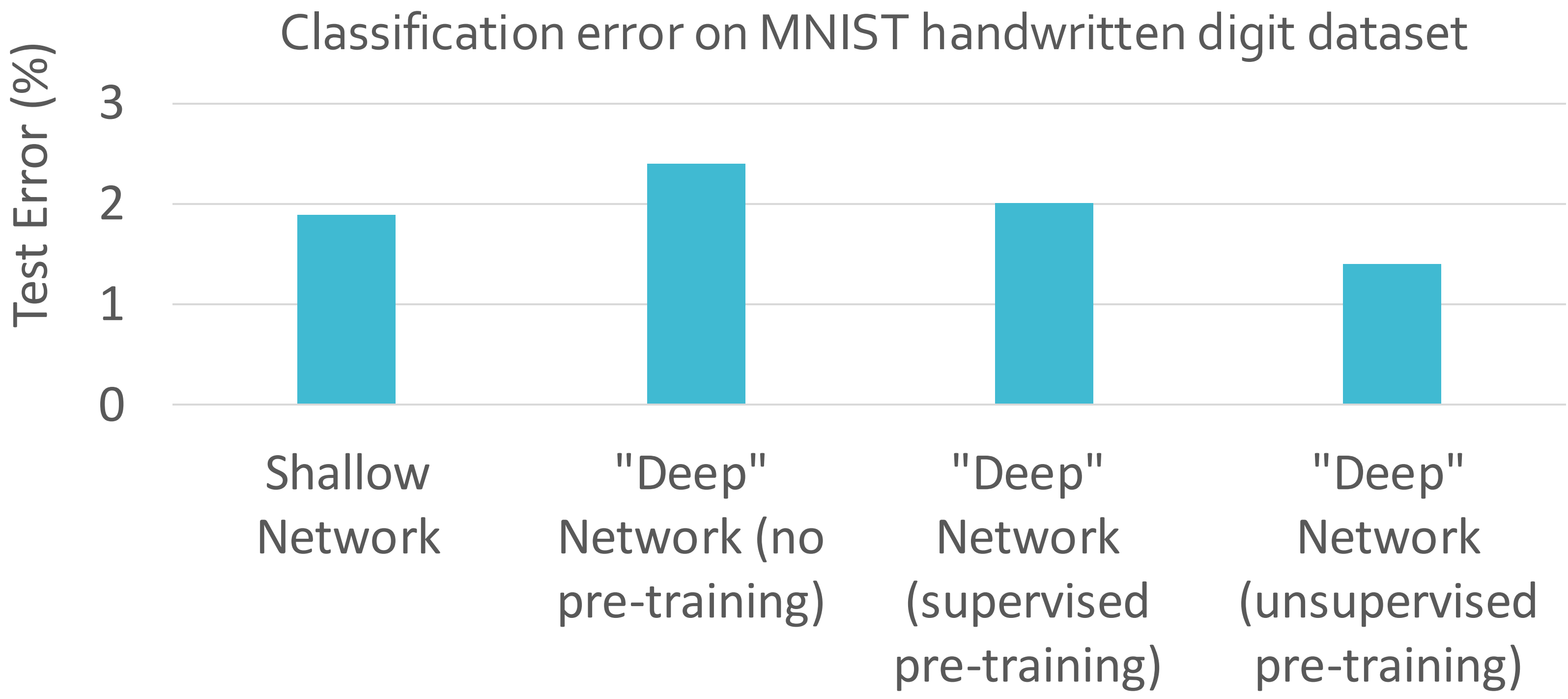

Another dose of Reality

- 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
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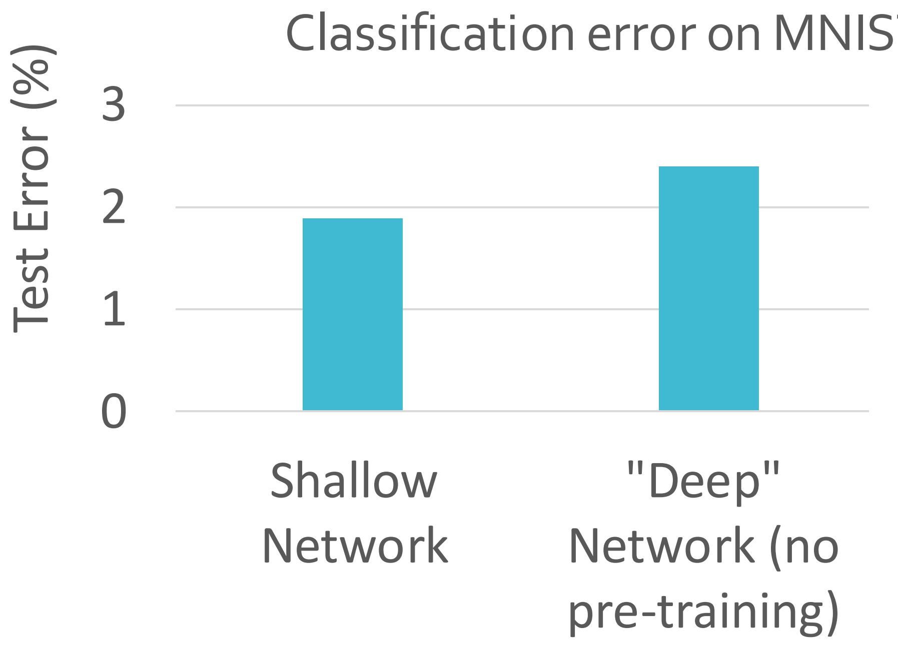

- Problem: what if you don't even have enough data to train a single layer/fine-tune the pre-trained network?

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- Surprise, surprise: it overfits and your test error is super high
- 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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- Key observation: you can pre-train on basically any labelled or unlabelled dataset!
  - 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 have a tiny labelled dataset to train with
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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?

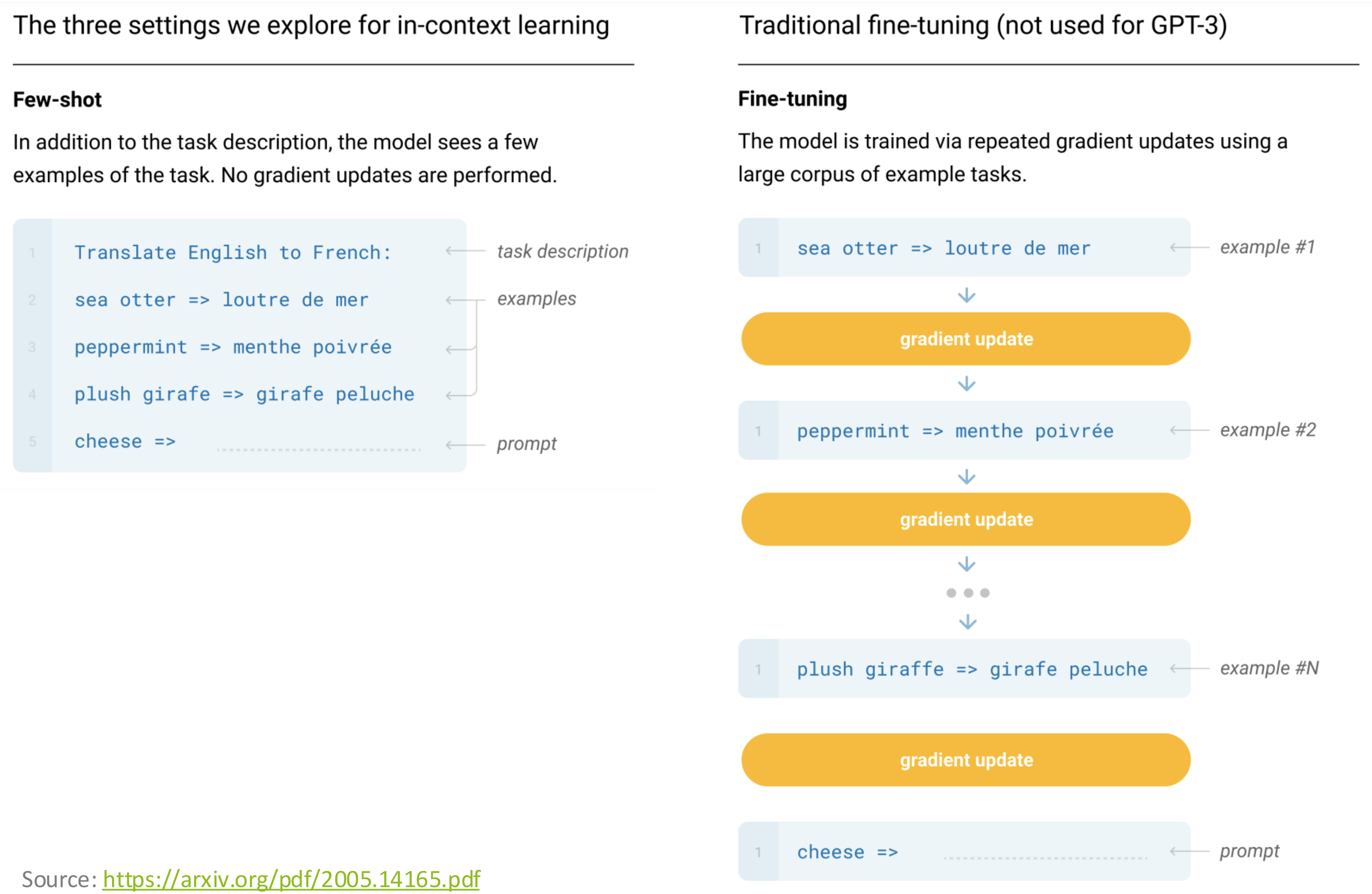
In-context Learning

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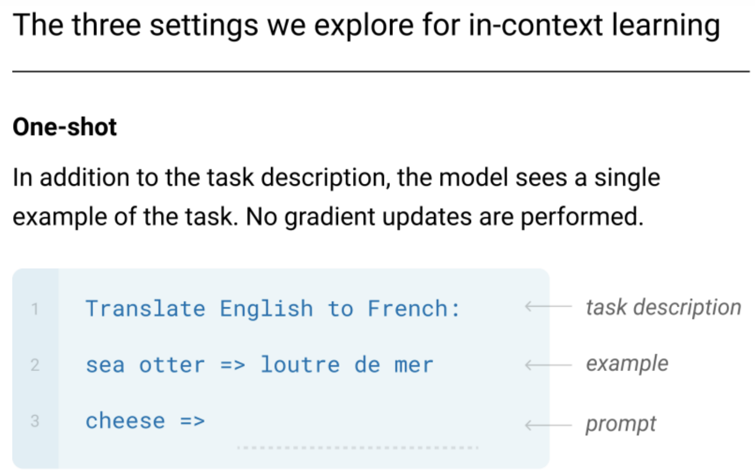
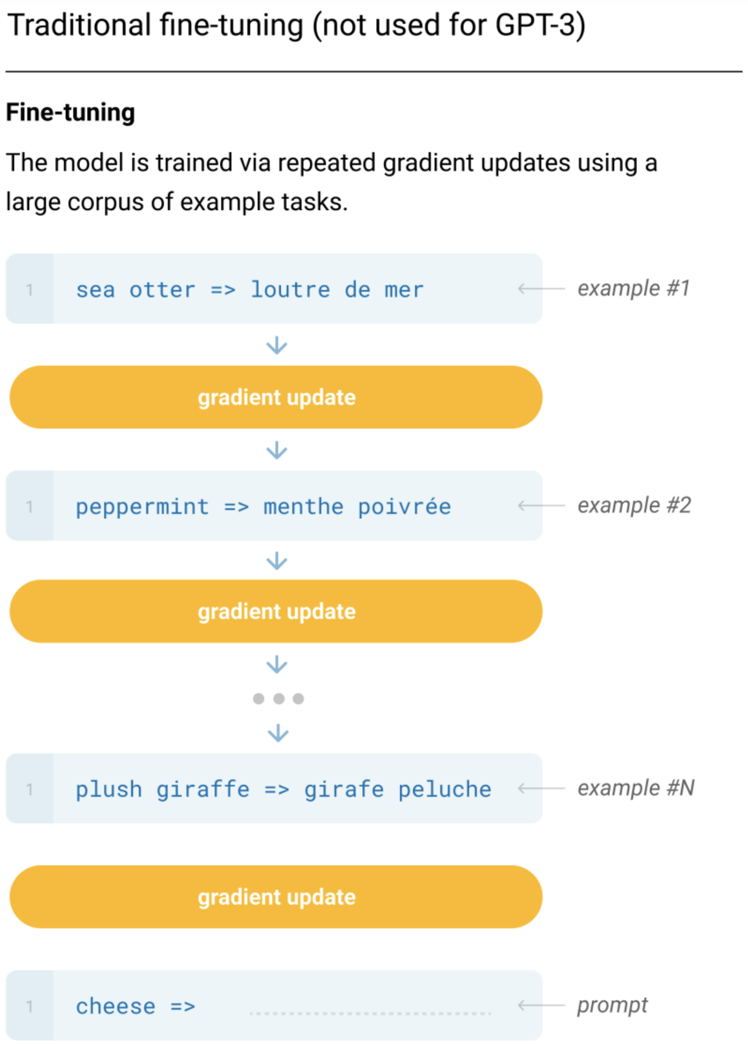
Few-shot, One-shot & Zero-shot (in-context) Learning

- Idea: leverage the LLM's context window by passing ~~a~~ ~~few~~ one examples 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

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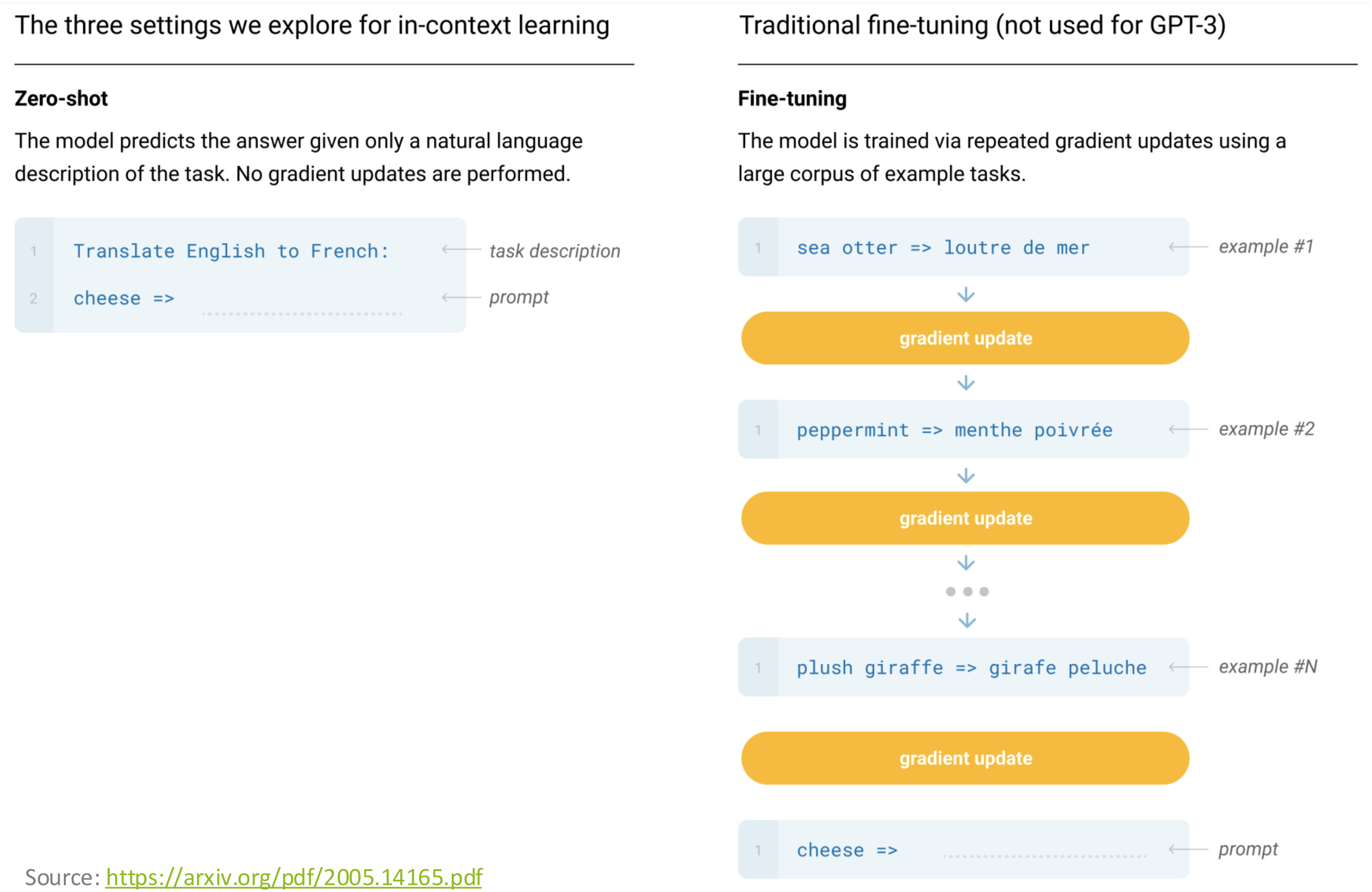

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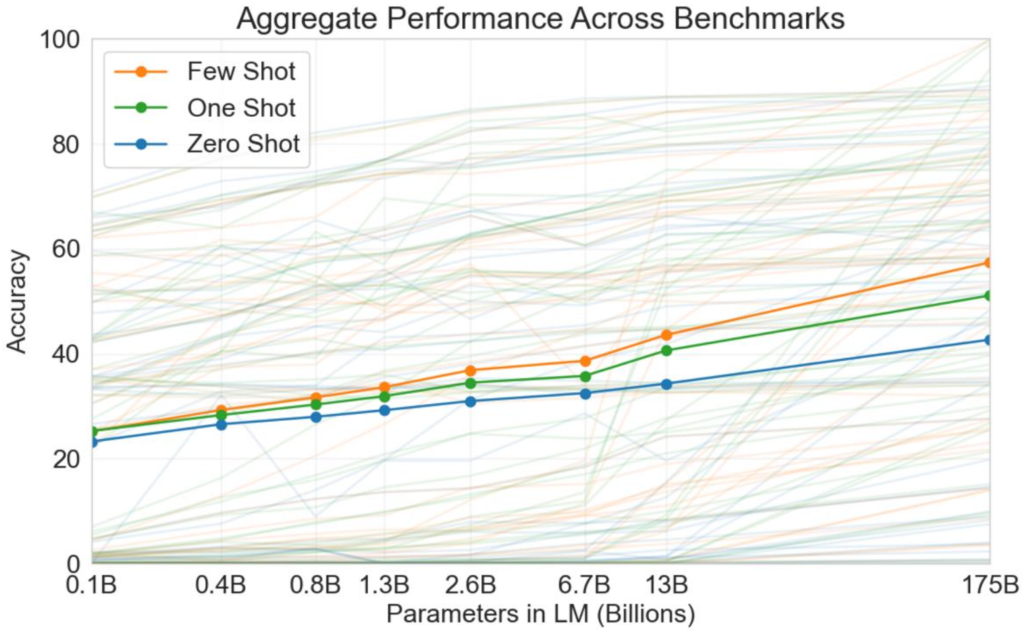


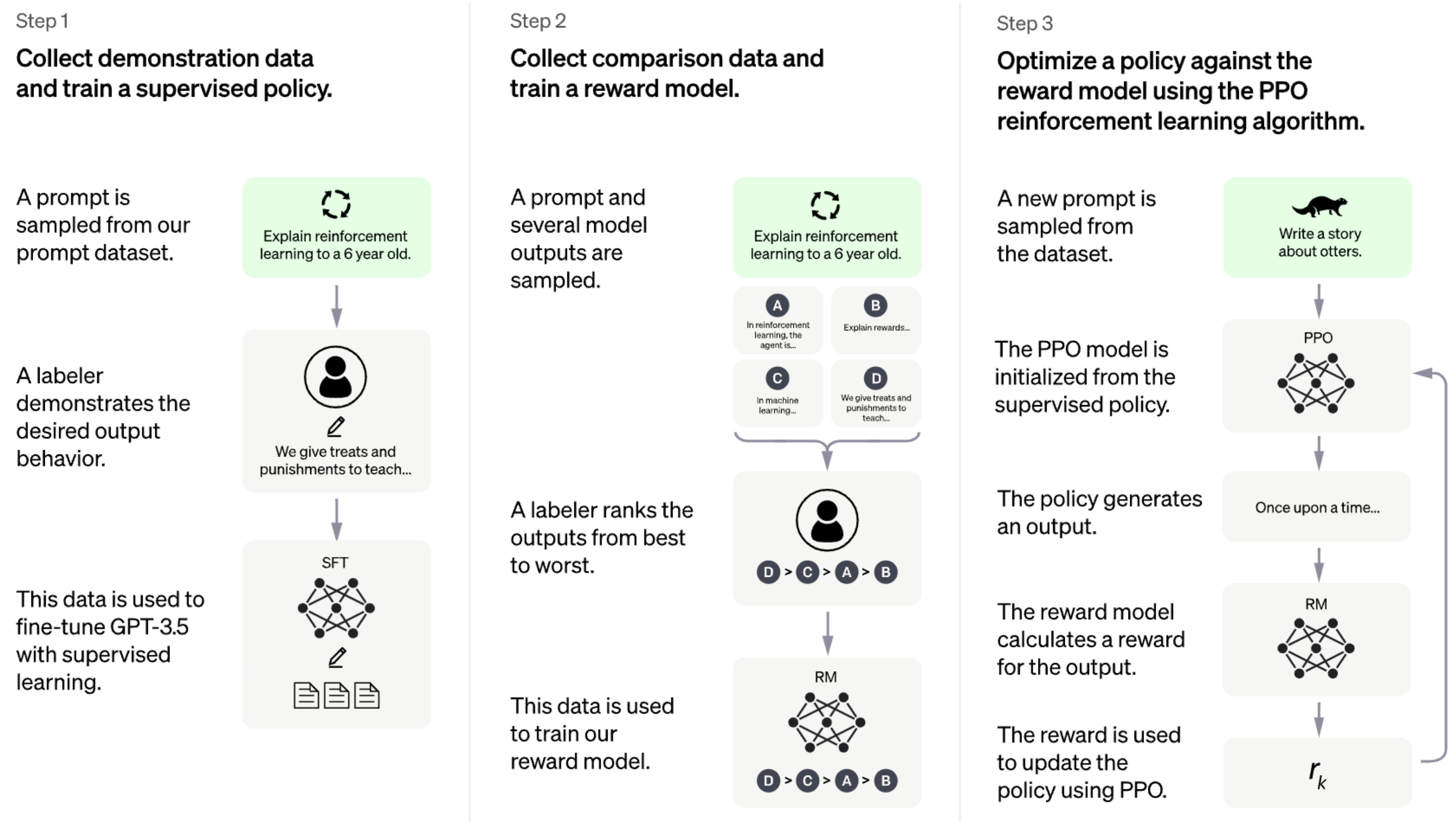
- Key Takeaway: LLMs can perform well on novel tasks without having to fine-tune the model, sometimes even with just one or zero labelled training data points!

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!

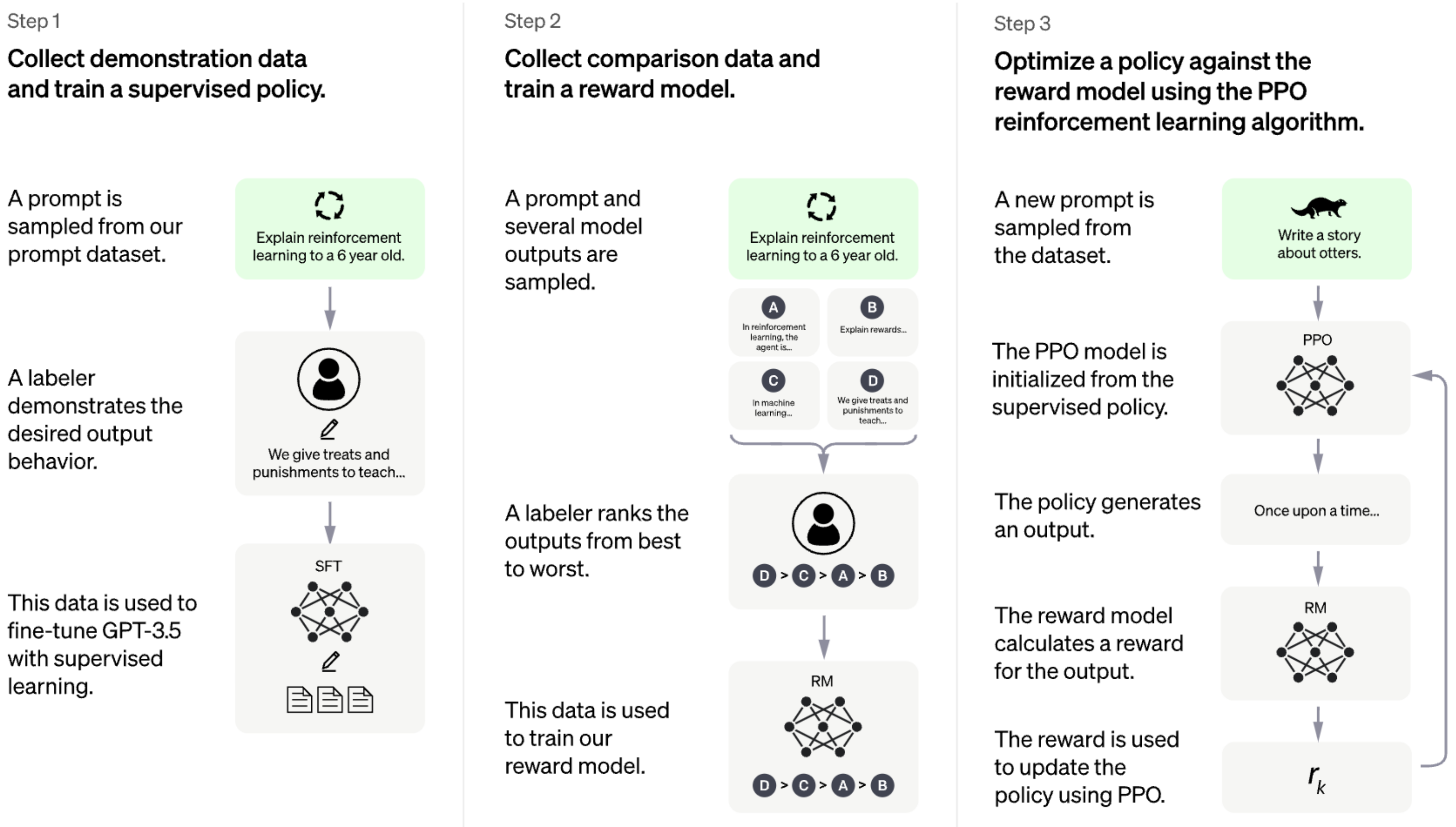
Reinforcement Learning from Human Feedback (RLHF)



- 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"?



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Learning Paradigms

- Supervised learning - $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right\}_{n=1}^{N}$
  - Regression - $y^{(n)} \in \mathbb{R}$
  - Classification - $y^{(n)} \in \{1, \ldots, C\}$
- Reinforcement learning - $\mathcal{D} = \left\{\left(\boldsymbol{s}^{(n)}, \boldsymbol{a}^{(n)}, r^{(n)}\right)\right\}_{n=1}^{N}$

Source: https://techobserver.net/2019/06/argo-ai-self-driving-car-research-center/

Source: https://www.wired.com/2012/02/high-speed-trading/

Reinforcement Learning: Examples

Source: https://www.cnet.com/news/boston-dynamics-robot-dog-spot-finally-goes-on-sale-for-74500/

Source: https://twitter.com/alphagomovie

Reinforcement Learning: Problem Formulation

- State space, $\mathcal{S}$
- Action space, $\mathcal{A}$
- Reward function
  - Stochastic, $p(r \mid s, a)$
  - Deterministic, $R: \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$
- Transition function
  - Stochastic, $p(s' \mid s, a)$
  - Deterministic, $\delta: \mathcal{S} \times \mathcal{A} \rightarrow \mathcal{S}$

Reinforcement Learning: Problem Formulation

- Policy, $\pi : \mathcal{S} \rightarrow \mathcal{A}$
  - Specifies an action to take in *every* state
- Value function, $V^{\pi} \colon \mathcal{S} \rightarrow \mathbb{R}$
  - Measures the expected total payoff of starting in some state s and executing policy π, i.e., in every state, taking the action that π returns

Toy Example

- $\mathcal{S}$ = all empty squares in the grid
- $\mathcal{A}$ = {up, down, left, right}
- Deterministic transitions
- Rewards of +1 and -1 for entering the labelled squares
- Terminate after receiving either reward

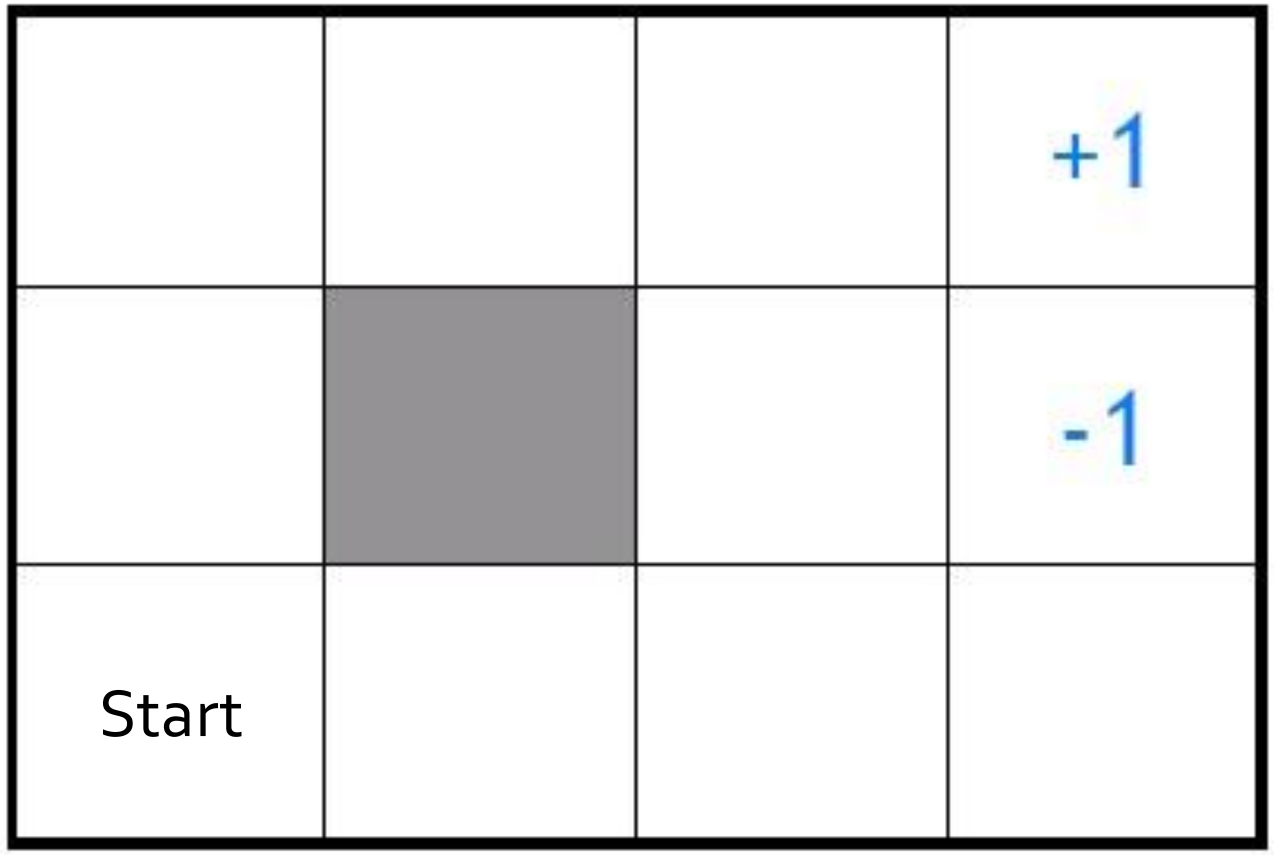

Figure courtesy of Eric Xing

Toy Example: Policy

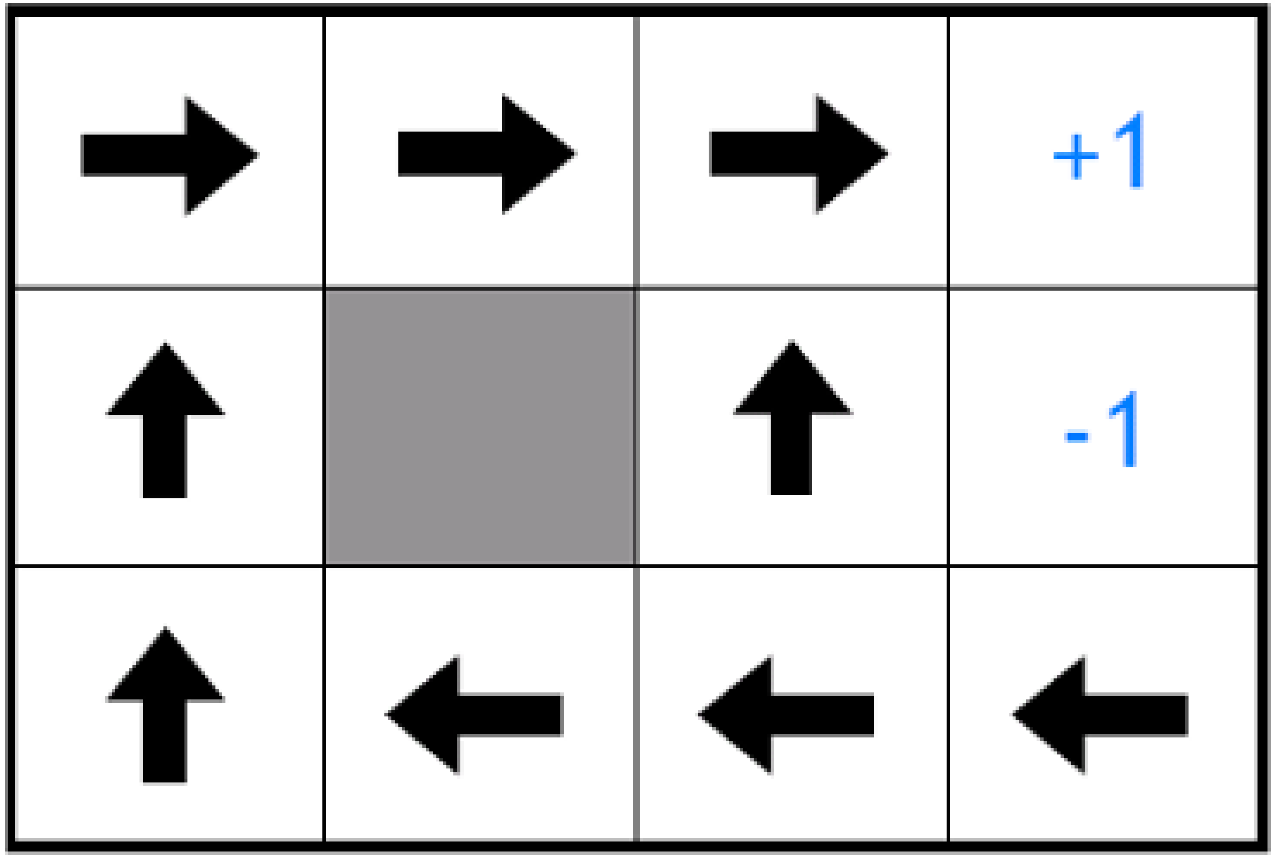

Figure courtesy of Eric Xing

Poll Question 1:

Is this policy optimal?

A. Yes

B. TOXIC

C. No

Poll Question 2:

Justify your answer to the previous question

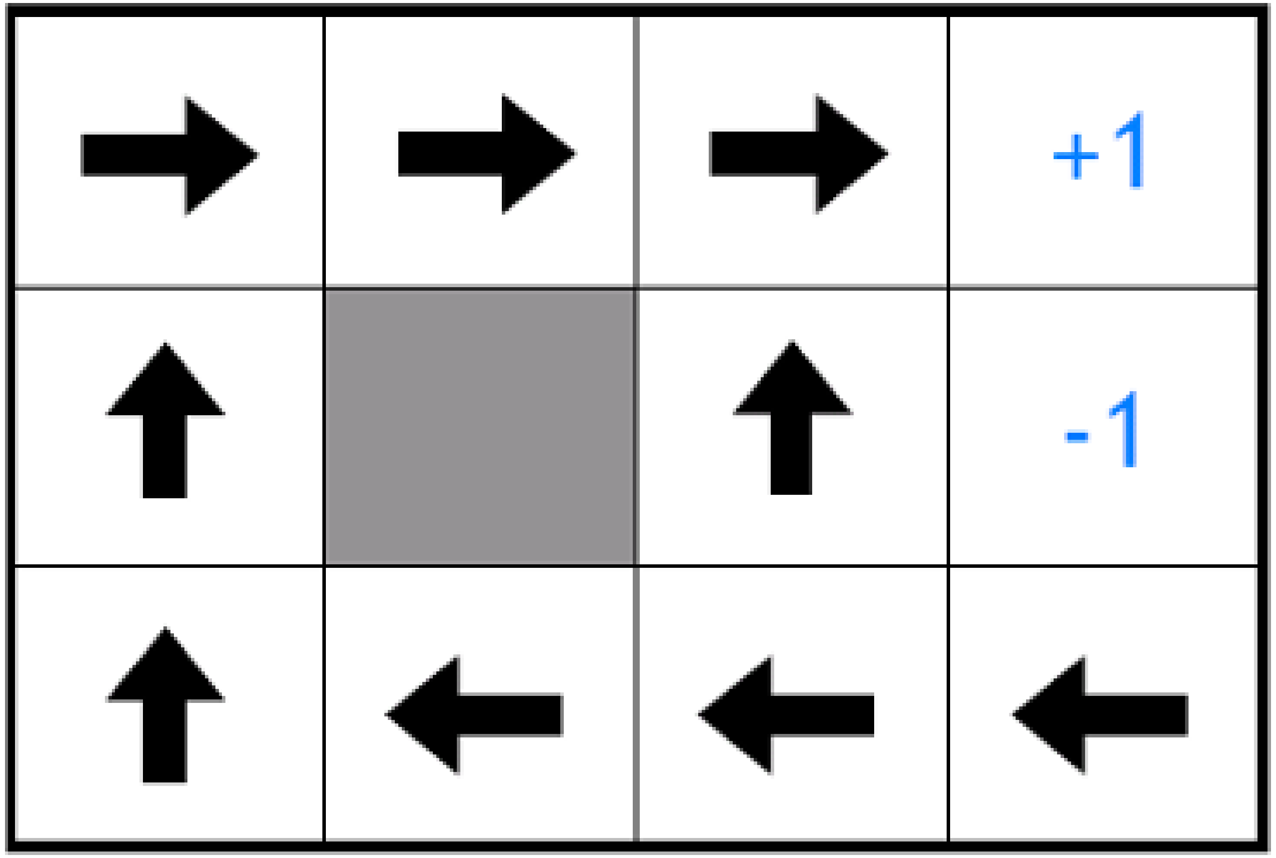

Figure courtesy of Eric Xing

Toy Example

Optimal policy given a reward of -2 per step

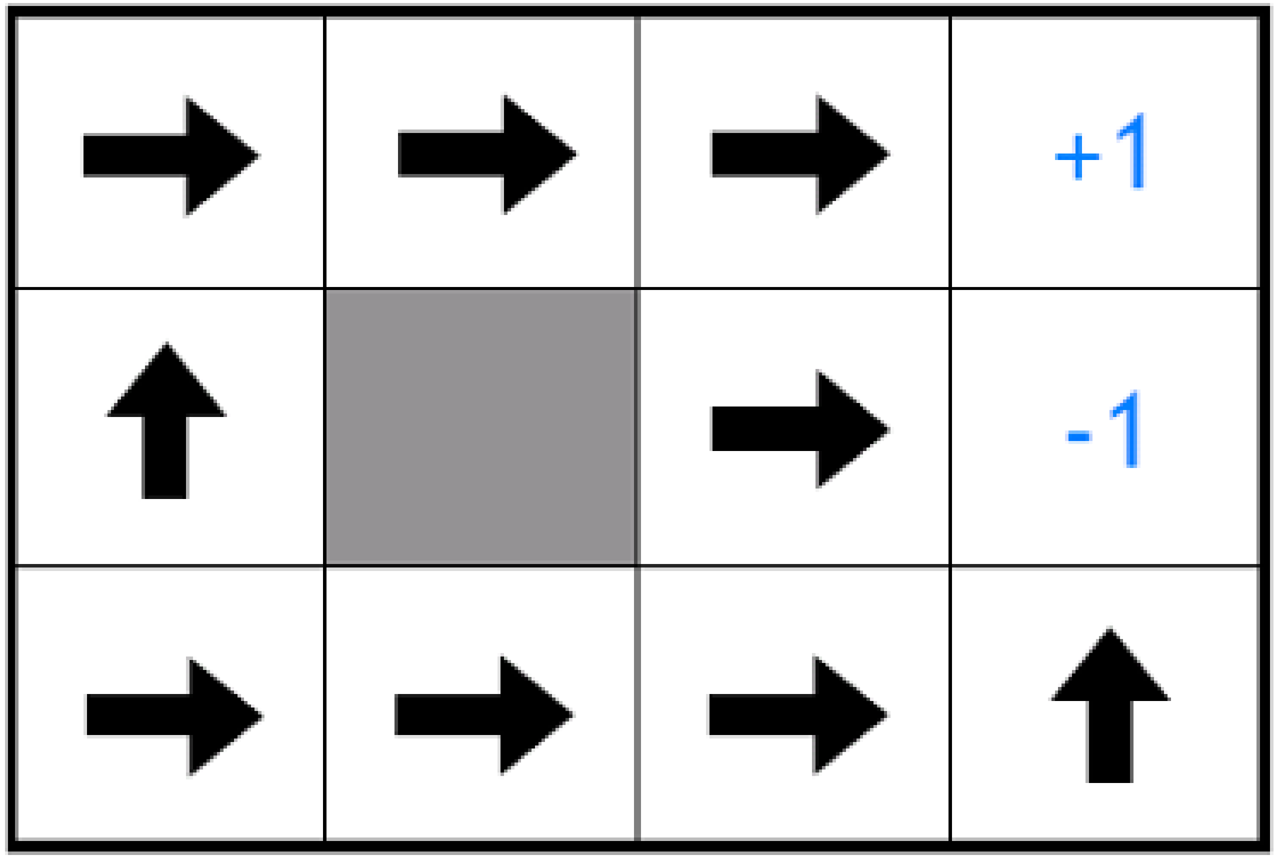

Figure courtesy of Eric Xing

Toy Example

Optimal policy given a reward of -0.1 per step

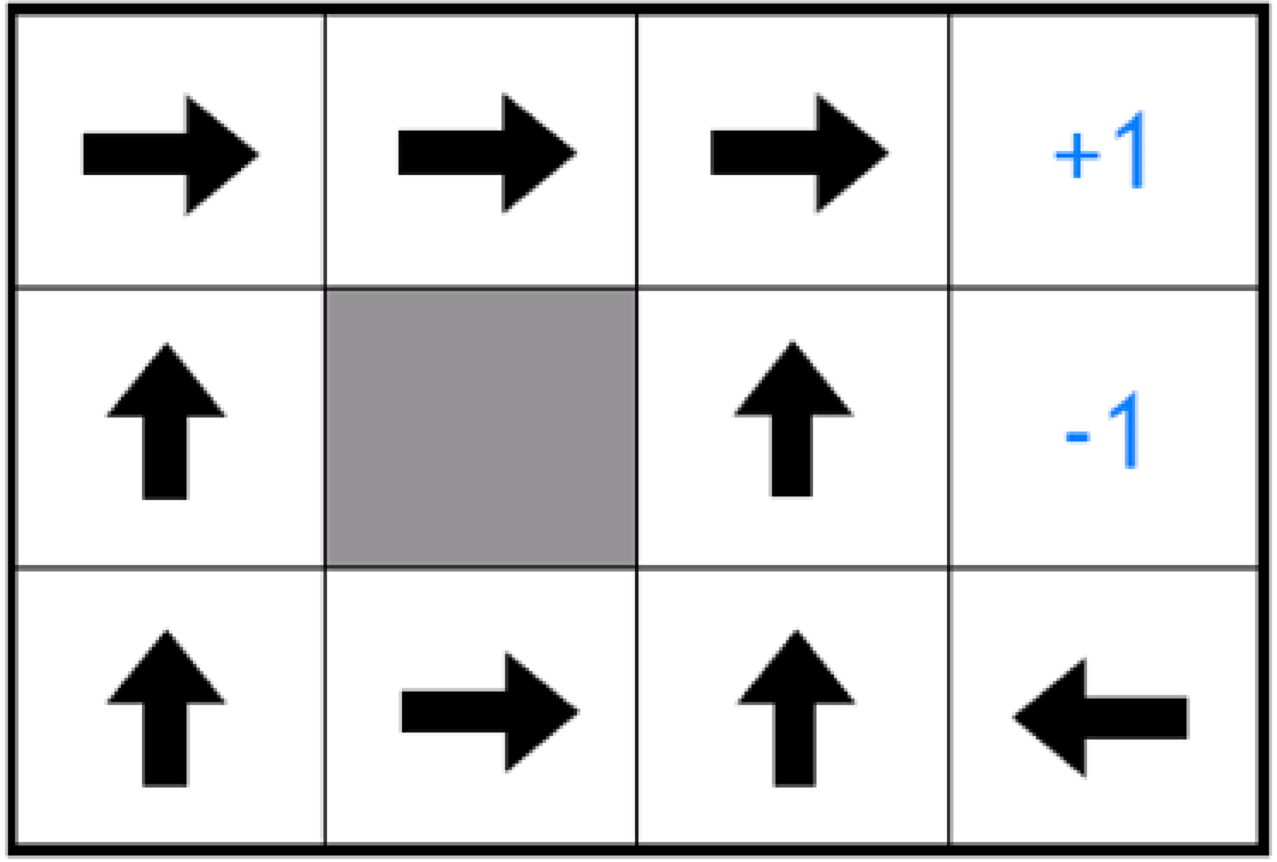

Figure courtesy of Eric Xing

Markov Decision Process (MDP)

- Assume the following model for our data:

1. Start in some initial state s_0
2. For time step t:
   1. Agent observes state s_t
   2. Agent takes action $a_t = \pi(s_t)$
   3. Agent receives reward $r_t \sim p(r \mid s_t, a_t)$
   4. Agent transitions to state $s_{t+1} \sim p(s' \mid s_t, a_t)$
3. Total reward is $\sum_{t=0}^{\infty} \gamma^t r_t$

- MDPs make the *Markov assumption*: the reward and next state only depend on the current state and action.