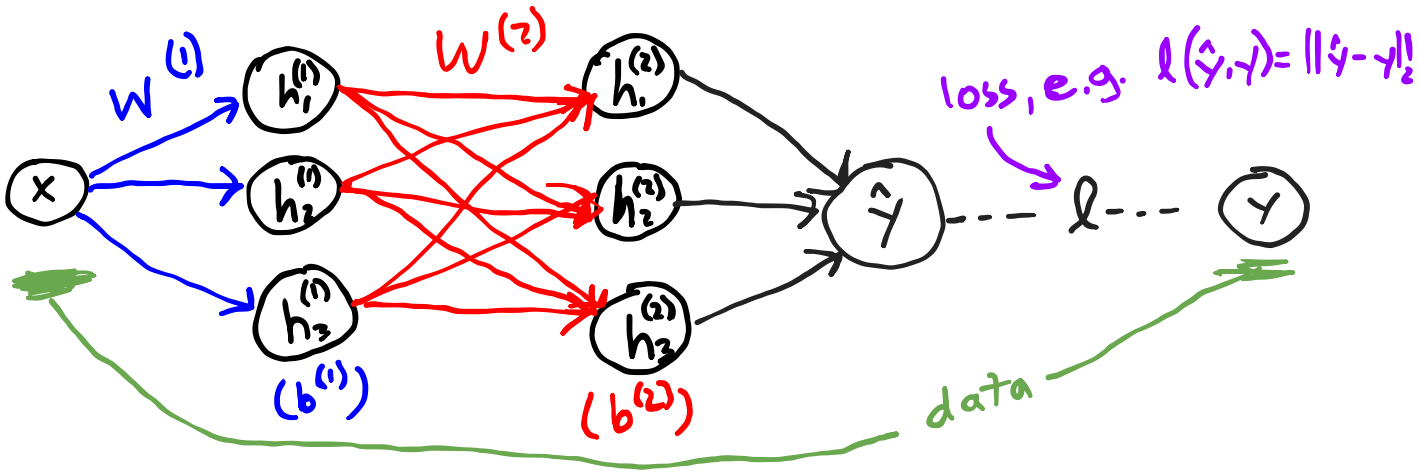
# Neural Network Architectures for Sequential Inputs

# Review from DMU: Neural Networks




$$\theta^* = \arg\min_{\theta} \sum_{(x,y)\in\mathcal{D}} l(f_\theta(x), y)$$

Stochastic Gradient Descent: $\theta \leftarrow \theta - \alpha \nabla_\theta l(f_\theta(x), y)$

**Multi-Layered Perceptron (MLP)**

$$h_i(x) = \sigma(W_i x + b_i)$$

$$\hat{y} = h_3(h_2(h_1(x)))$$

("misnomer" because original perceptron used step function)

AI = Neural Nets

Neural Nets are just another function approximator

# Review: Why sequences are needed

In an MDP, for any $k \geq 0$:

$$P(r_{t+k} \mid \pi, s_t, a_{t-1}, s_{t-1}, \ldots) = P(r_{t+k} \mid \pi, s_t),$$

so there is always an optimal policy based on the state.

In a POMDP, there is no systematic way to simplify

$$P(r_{t+k} \mid \pi, o_t, a_{t-1}, o_{t-1}, \ldots),$$

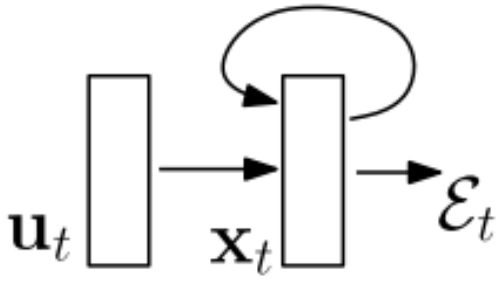
so an optimal policy may depend on the entire action-observation history.

A big MLP that takes the entire sequence in generally has too many parameters (and cannot handle variable length input)

# Recurrent neural networks

$$\mathbf{x}_t = F(\mathbf{x}_{t-1}, \mathbf{u}_t, \theta)$$

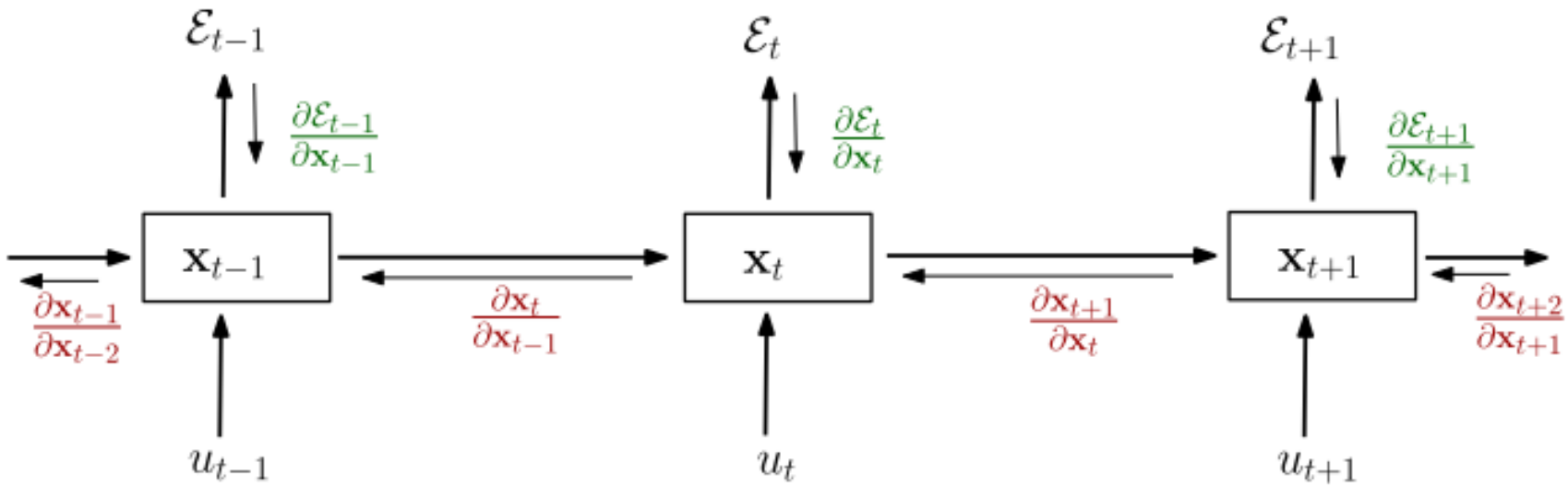
$$\mathbf{x}_t = \mathbf{W}_{rec}\sigma(\mathbf{x}_{t-1}) + \mathbf{W}_{in}\mathbf{u}_t + \mathbf{b}$$




Input: $u_t$

State/Output: $x_t$

Cost: $\mathcal{E}_t$




Images: Pascanu 2013

# Problem: Vanishing/exploding gradients

$$\frac{\partial \mathcal{E}}{\partial \theta} = \sum_{1 \leq t \leq T} \frac{\partial \mathcal{E}_t}{\partial \theta}$$

$$\mathbf{x}_t = \mathbf{W}_{rec}\sigma(\mathbf{x}_{t-1}) + \mathbf{W}_{in}\mathbf{u}_t + \mathbf{b}$$

$$\frac{\partial \mathcal{E}_t}{\partial \theta} = \sum_{1 \leq k \leq t} \left( \frac{\partial \mathcal{E}_t}{\partial \mathbf{x}_t} \frac{\partial \mathbf{x}_t}{\partial \mathbf{x}_k} \frac{\partial^+ \mathbf{x}_k}{\partial \theta} \right)$$

($\frac{\partial^+ x_k}{\partial \theta}$ is partial with $x_{k-1}$ held constant)

$$\frac{\partial \mathbf{x}_t}{\partial \mathbf{x}_k} = \prod_{t \geq i > k} \frac{\partial \mathbf{x}_i}{\partial \mathbf{x}_{i-1}} = \prod_{t \geq i > k} \mathbf{W}_{rec}^T diag(\sigma'(\mathbf{x}_{i-1}))$$

Generally, informally: If $\sigma' \in [0, 1]$ (e.g. sigmoid is in [0, 0.25]), product can become very small, even numerically zero.

Formally, for the linear case ($\sigma = \mathrm{identity}$)

- Largest eigenvalue of $W_{rec}$ < 1: *sufficient* for vanishing
- Largest eigenvalue of $W_{rec}$ > 1: *necessary* for exploding

Important papers:


- Hochreiter, Sepp. Untersuchungen zu dynamischen neuronalen Netzen. Diploma thesis, TU Munich, 1991.)
- Bengio, Yoshua, Patrice Simard, and Paolo Frasconi. "Learning long-term dependencies with gradient descent is difficult." IEEE transactions on neural networks 5.2 (1994) [11k cit.]
- Pascanu, Razvan, Tomas Mikolov, and Yoshua Bengio. "On the difficulty of training recurrent neural networks." International conference on machine learning, 2013. [6.5k cit.]

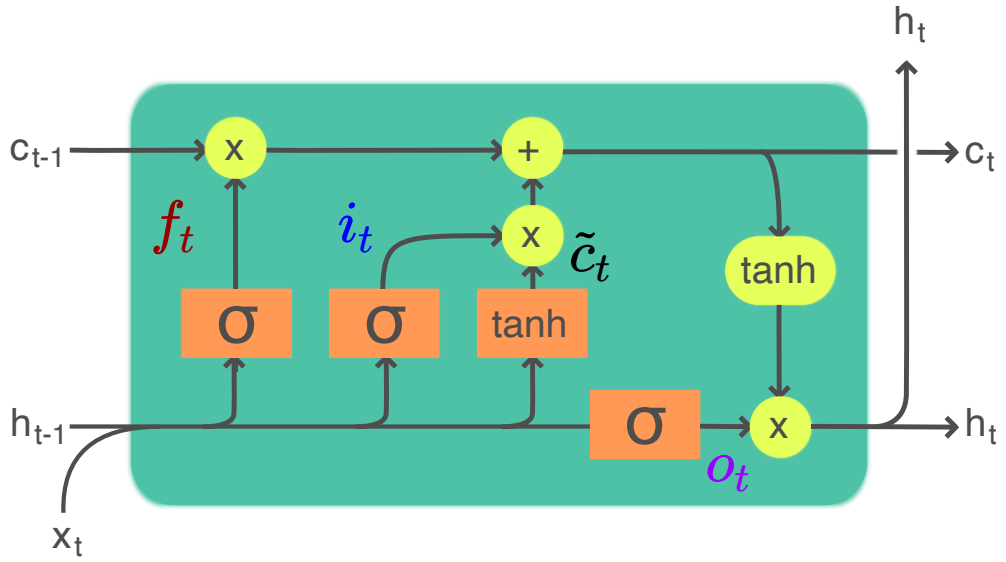
# Long Short Term Memory (LSTM)

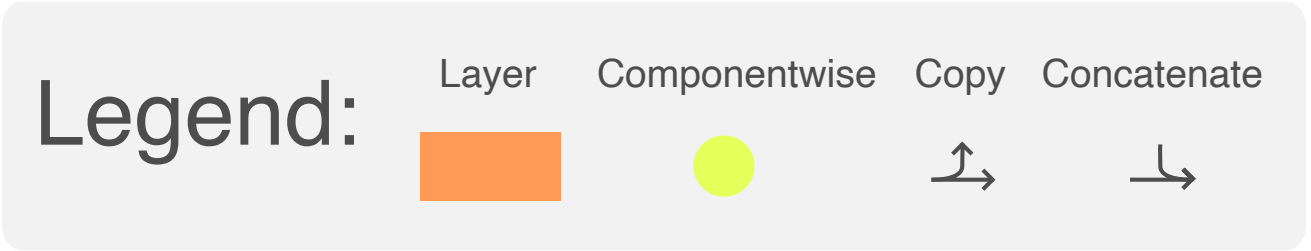
Input: $x_t$

Output: $h_t$

Cell state: $c_t$

$$
\begin{aligned}
f_t &= \sigma_g(W_f x_t + U_f h_{t-1} + b_f) \quad \text{Forget gate} \\
i_t &= \sigma_g(W_i x_t + U_i h_{t-1} + b_i) \quad \text{Input Gate} \\
o_t &= \sigma_g(W_o x_t + U_o h_{t-1} + b_o) \quad \text{Output Gate} \\
\tilde{c}_t &= \sigma_c(W_c x_t + U_c h_{t-1} + b_c) \\
c_t &= f_t \odot c_{t-1} + i_t \odot \tilde{c}_t \\
h_t &= o_t \odot \sigma_h(c_t)
\end{aligned}
$$




By Guillaume Chevalier - File:The_LSTM_Cell.svg, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=109362147

Hochreiter, S. and Schmidhuber, J. (1997). *Long Short-Term Memory*. *1780*, 1735–1780.

# Gated Recurrent Unit (GRU)

Input: $x_t$

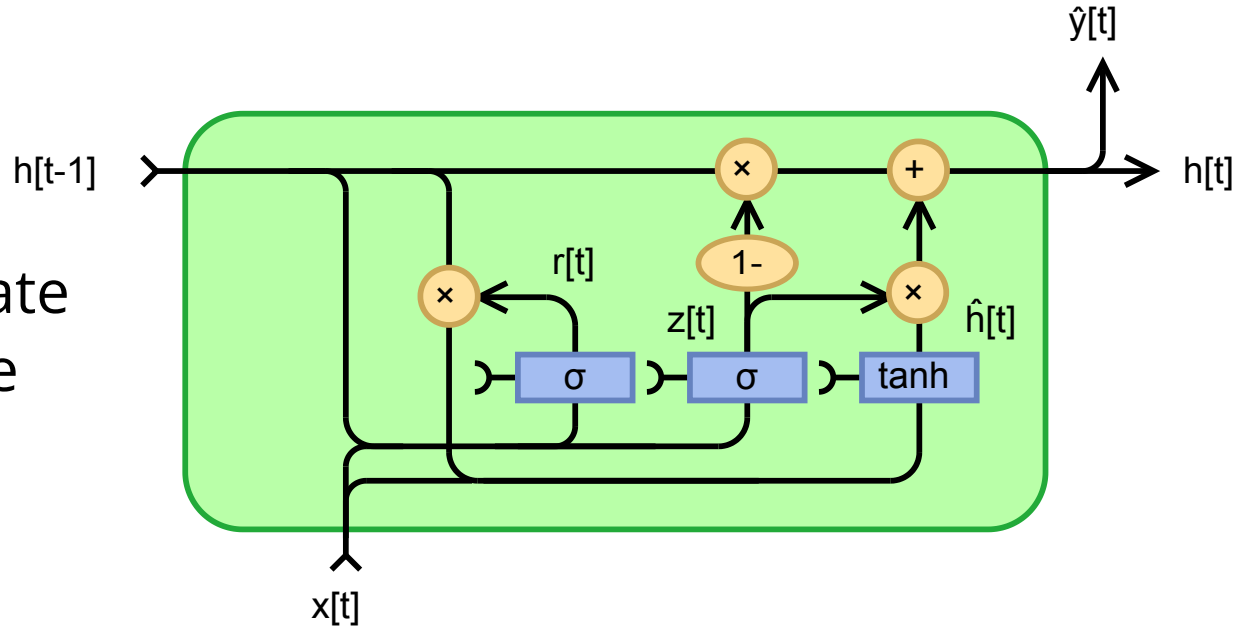
Output: $\hat{y}_t$ ($h_t$)

Recurrent State: $h_t$

$$
\begin{aligned}
z_t &= \sigma(W_z x_t + U_z h_{t-1} + b_z) \\
r_t &= \sigma(W_r x_t + U_r h_{t-1} + b_r) \\
\hat{h}_t &= \phi(W_h x_t + U_h (r_t \odot h_{t-1}) + b_h) \\
h_t &= (1 - z_t) \odot h_{t-1} + z_t \odot \hat{h}_t
\end{aligned}
$$

Update gate

Reset gate



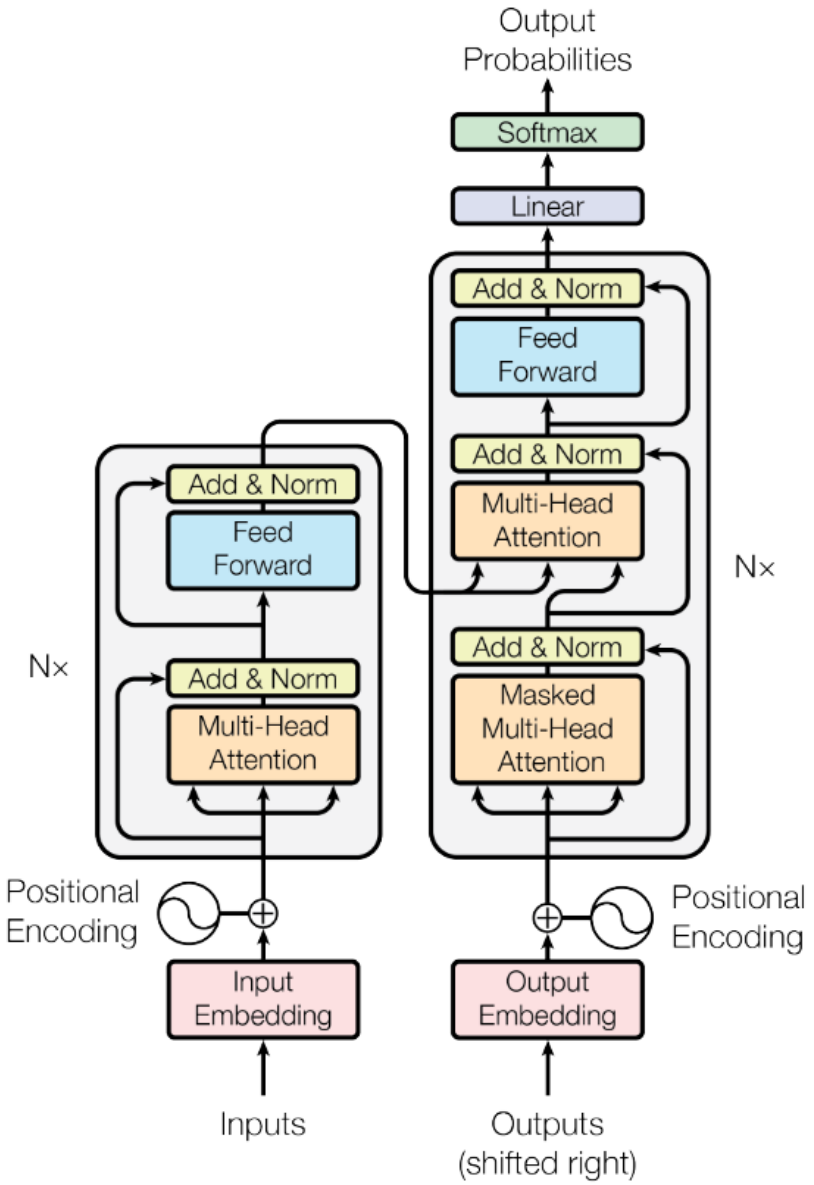

By Jeblad - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=66225938

Fewer parameters than LSTM

$$
\begin{aligned}
f_t &= \sigma_g(W_f x_t + U_f h_{t-1} + b_f) \\
i_t &= \sigma_g(W_i x_t + U_i h_{t-1} + b_i) \\
o_t &= \sigma_g(W_o x_t + U_o h_{t-1} + b_o) \\
\tilde{c}_t &= \sigma_c(W_c x_t + U_c h_{t-1} + b_c)
\end{aligned}
$$

Cho, Kyunghyun; van Merrienboer, Bart; Bahdanau, DZmitry; Bougares, Fethi; Schwenk, Holger; Bengio, Yoshua (2014). "Learning Phrase Representations using RNN Encoder-Decoder for Statistical Machine Translation". arXiv:1406.1078.

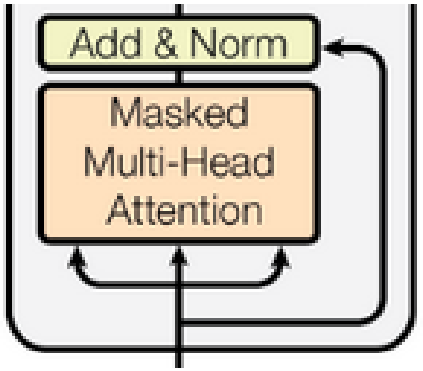
# Transformer Overview




- **Multi-Head Attention**
- Skip Connections
- Embeddings
- Positional Encodings
- Layer Norm

Vaswani, Ashish, et al. "Attention is all you need." Advances in neural information processing systems 30 (2017).
Excellent Blog Post: https://dugas.ch/artificial_curiosity/GPT_architecture.html

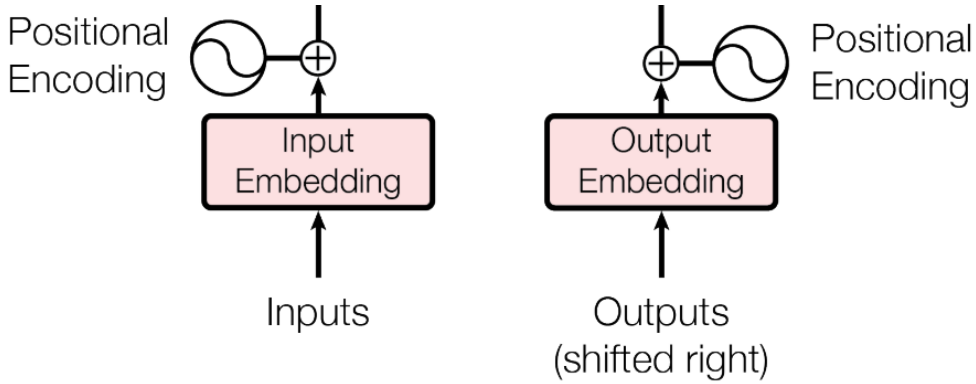
# Skip Connections (Resnets)




# Word (Token) Embeddings

# Positional Encodings

$$PE_{(pos,2i)} = sin(pos/10000^{2i/d_{\text{model}}})$$
$$PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{\text{model}}})$$




# Layer Norm

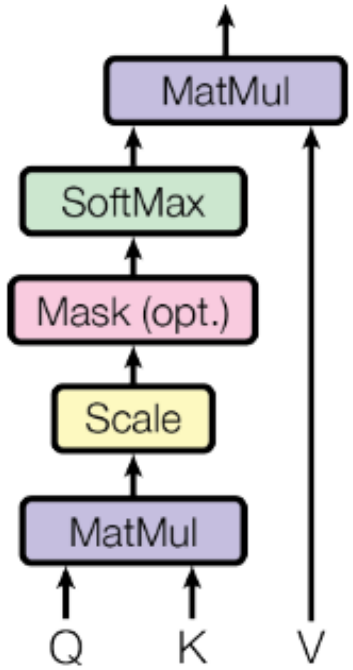
$$\mu_l = \frac{1}{d}\sum_{i=1}^{d} x_i$$

$$\sigma_l^2 = \frac{1}{d}\sum_{i=1}^{d}(x_i - \mu_l)^2$$

$$\hat{x}_i = \frac{x_i - \mu_l}{\sqrt{\sigma_l^2}} \quad \text{or} \quad \hat{x}_i = \frac{x_i - \mu_l}{\sqrt{\sigma_l^2 + \epsilon}}$$

# Attention: Fully differentiable key-value lookup

$$\text{Attention}(Q, K, V) = \text{softmax}(\frac{QK^T}{\sqrt{d_k}})V$$




(missing a transpose between softmax and V???)

# Attention: Fully differentiable key-value lookup

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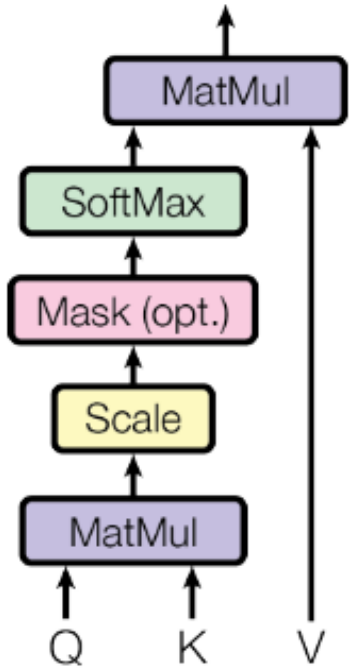
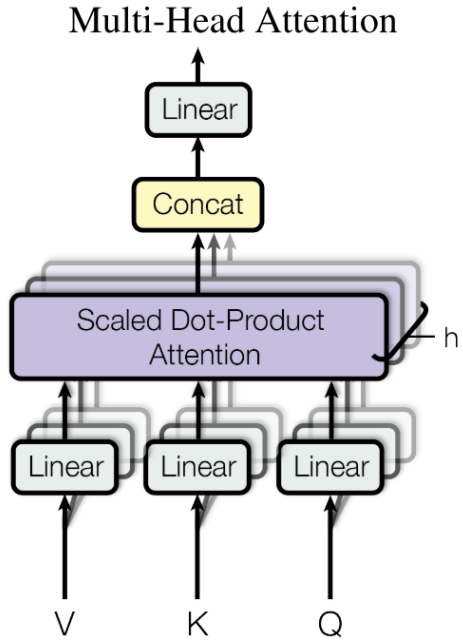
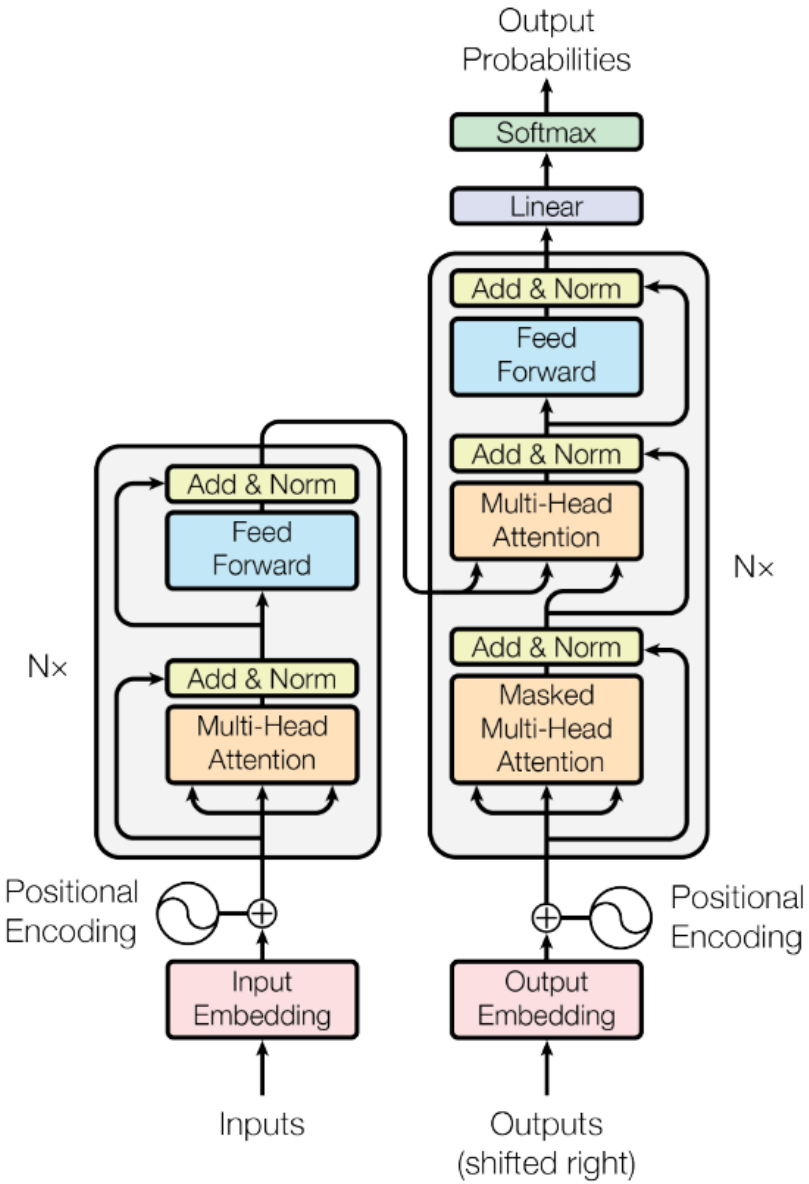



$$\text{MultiHead}(Q, K, V) = \text{Concat}(\text{head}_1, ..., \text{head}_\text{h})W^O$$
$$\text{where head}_\text{i} = \text{Attention}(QW_i^Q, KW_i^K, VW_i^V)$$




missing a transpose between softmax and V???

# Transformers: Putting it all together



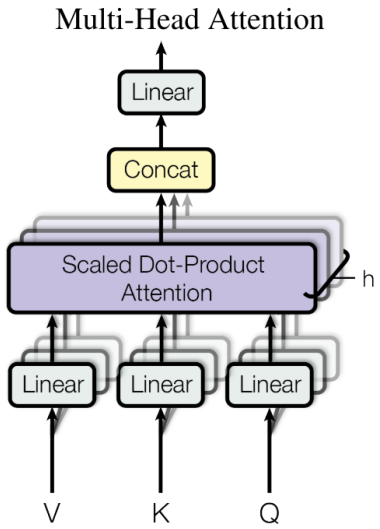




Table 1: Maximum path lengths, per-layer complexity and minimum number of sequential operations for different layer types. $n$ is the sequence length, $d$ is the representation dimension, $k$ is the kernel size of convolutions and $r$ the size of the neighborhood in restricted self-attention.

| Layer Type | Complexity per Layer | Sequential Operations | Maximum Path Length |
|---|---|---|---|
| Self-Attention | $O(n^2 \cdot d)$ | $O(1)$ | $O(1)$ |
| Recurrent | $O(n \cdot d^2)$ | $O(n)$ | $O(n)$ |
| Convolutional | $O(k \cdot n \cdot d^2)$ | $O(1)$ | $O(log_k(n))$ |
| Self-Attention (restricted) | $O(r \cdot n \cdot d)$ | $O(1)$ | $O(n/r)$ |

# GPT-3

Brown, T. B., Mann, B., Ryder, N., Subbiah, M., Kaplan, J., Dhariwal, P., Neelakantan, A., Shyam, P., Sastry, G., Askell, A., Agarwal, S., Herbert-Voss, A., Krueger, G., Henighan, T., Child, R., Ramesh, A., Ziegler, D. M., Wu, J., Winter, C., … Amodei, D. (2020). Language models are few-shot learners. *Advances in Neural Information Processing Systems*, *2020-December*.

| Dataset | Quantity (tokens) | Weight in training mix | Epochs elapsed when training for 300B tokens |
|---|---|---|---|
| Common Crawl (filtered) | 410 billion | 60% | 0.44 |
| WebText2 | 19 billion | 22% | 2.9 |
| Books1 | 12 billion | 8% | 1.9 |
| Books2 | 55 billion | 8% | 0.43 |
| Wikipedia | 3 billion | 3% | 3.4 |

| Model Name | $n_{\text{params}}$ | $n_{\text{layers}}$ | $d_{\text{model}}$ | $n_{\text{heads}}$ | $d_{\text{head}}$ | Batch Size | Learning Rate |
|---|---|---|---|---|---|---|---|
| GPT-3 Small | 125M | 12 | 768 | 12 | 64 | 0.5M | $6.0 \times 10^{-4}$ |
| GPT-3 Medium | 350M | 24 | 1024 | 16 | 64 | 0.5M | $3.0 \times 10^{-4}$ |
| GPT-3 Large | 760M | 24 | 1536 | 16 | 96 | 0.5M | $2.5 \times 10^{-4}$ |
| GPT-3 XL | 1.3B | 24 | 2048 | 24 | 128 | 1M | $2.0 \times 10^{-4}$ |
| GPT-3 2.7B | 2.7B | 32 | 2560 | 32 | 80 | 1M | $1.6 \times 10^{-4}$ |
| GPT-3 6.7B | 6.7B | 32 | 4096 | 32 | 128 | 2M | $1.2 \times 10^{-4}$ |
| GPT-3 13B | 13.0B | 40 | 5140 | 40 | 128 | 2M | $1.0 \times 10^{-4}$ |
| GPT-3 175B or "GPT-3" | 175.0B | 96 | 12288 | 96 | 128 | 3.2M | $0.6 \times 10^{-4}$ |

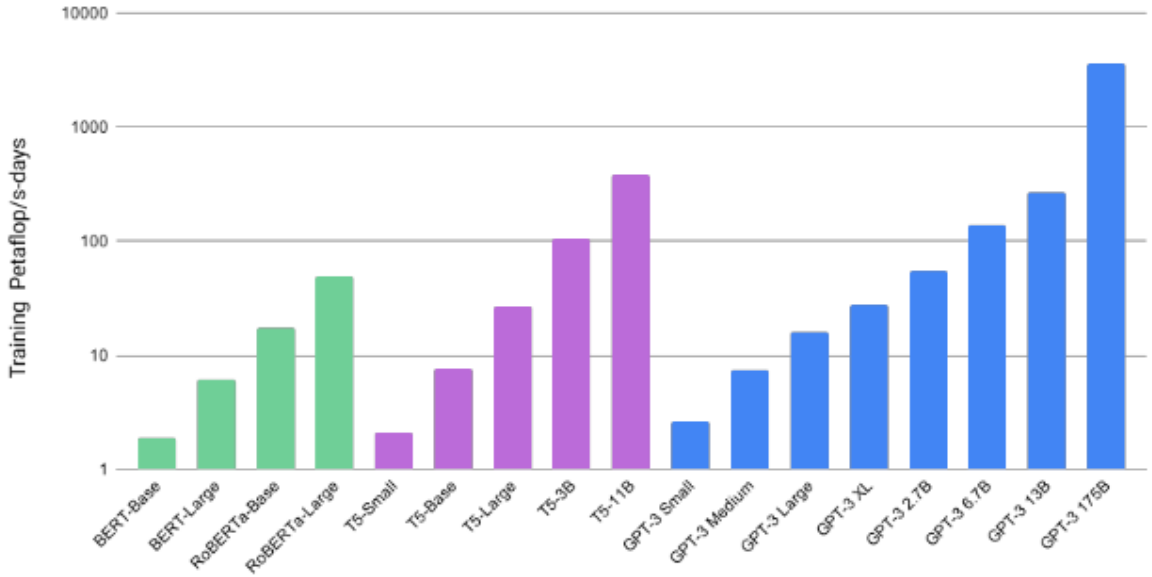


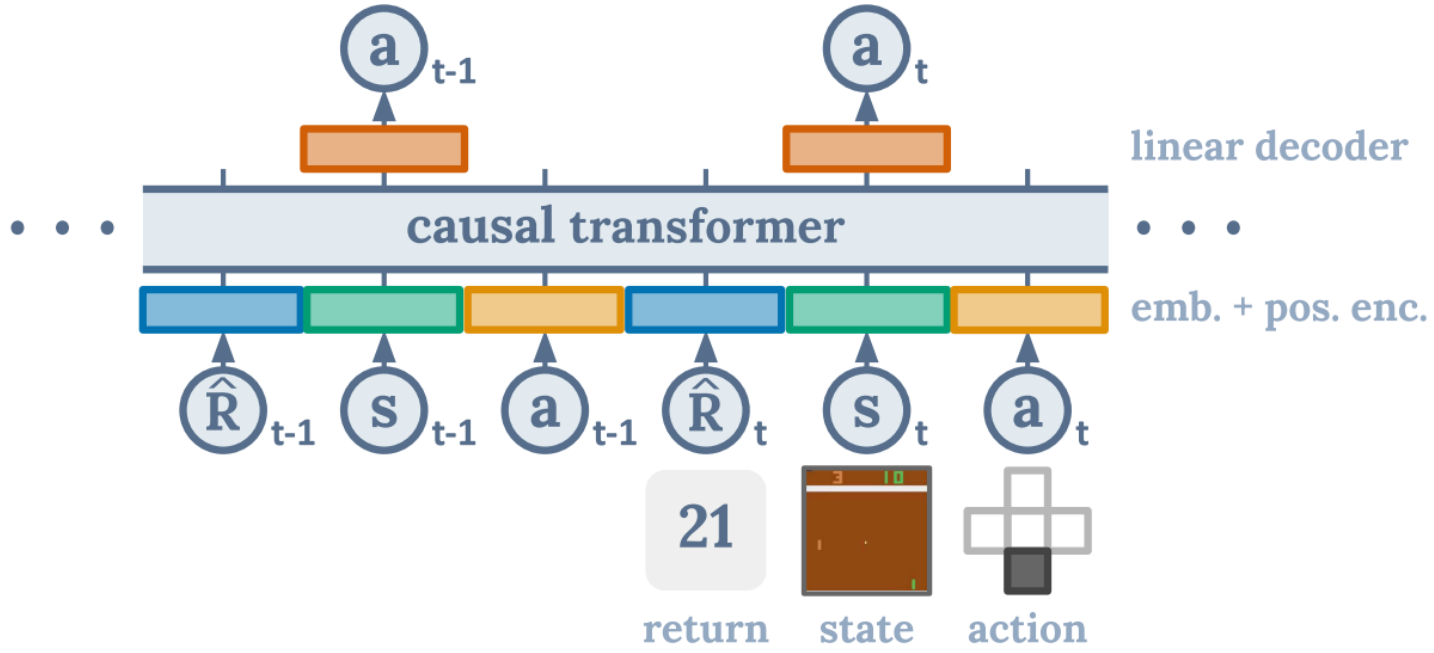

**Figure 2.2: Total compute used during training**. Based on the analysis in Scaling Laws For Neural Language Models [KMH+20] we train much larger models on many fewer tokens than is typical. As a consequence, although GPT-3 3B is almost 10x larger than RoBERTa-Large (355M params), both models took roughly 50 petaflop/s-days of compute during pre-training. Methodology for these calculations can be found in Appendix D.

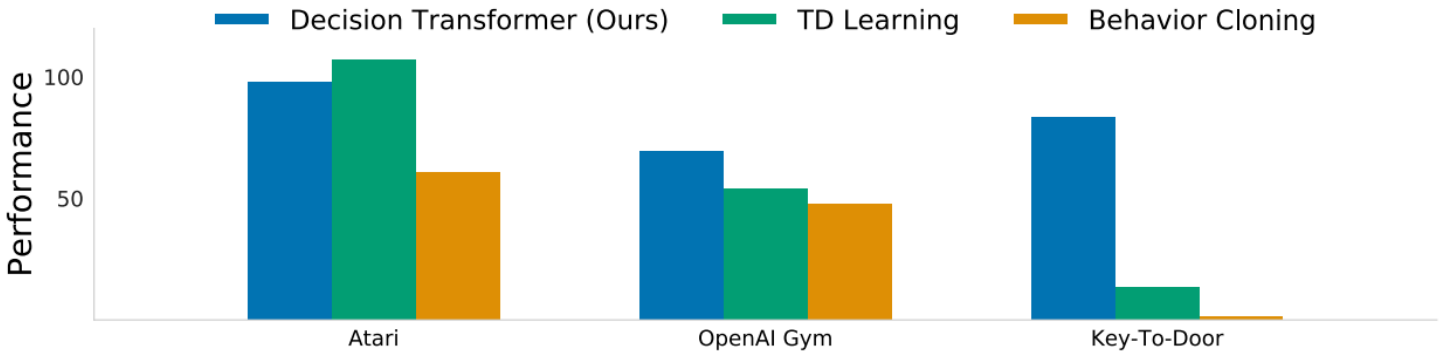
To do a "farduddle" means to jump up and down really fast. An example of a sentence that uses the word farduddle is:

**One day when I was playing tag with my little sister, she got really excited and she started doing these crazy farduddles.**

# Decision Transformer

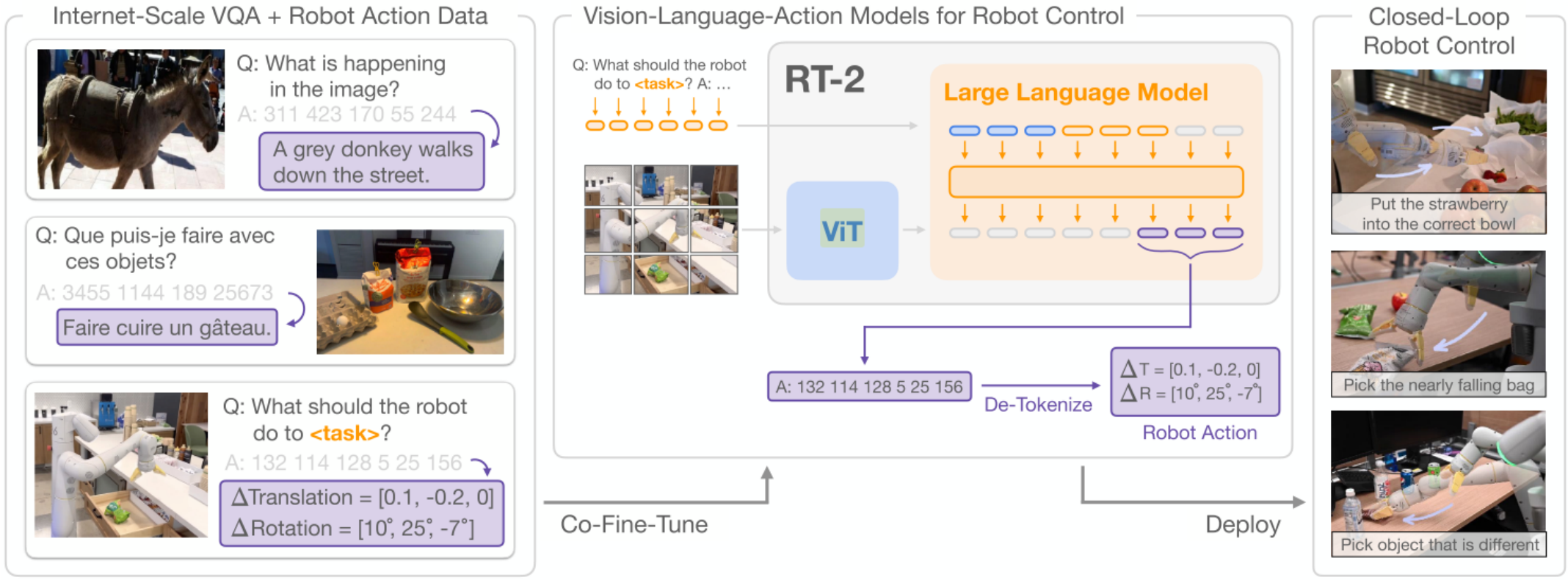
Chen, L., Lu, K., Rajeswaran, A., Lee, K., Grover, A., Laskin, M., Abbeel, P., Srinivas, A., & Mordatch, I. (2021). Decision Transformer: Reinforcement Learning via Sequence Modeling. *Advances in Neural Information Processing Systems*, *18*, 15084–15097.



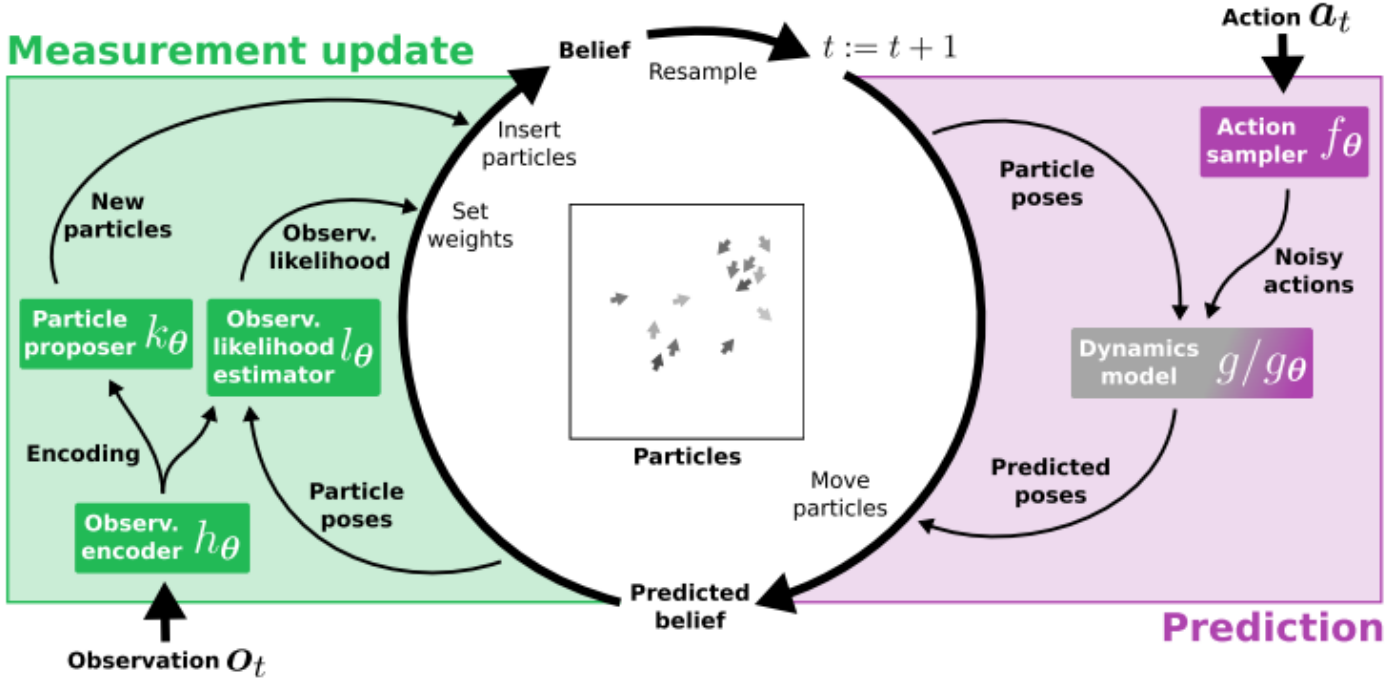



# Robot Transformer

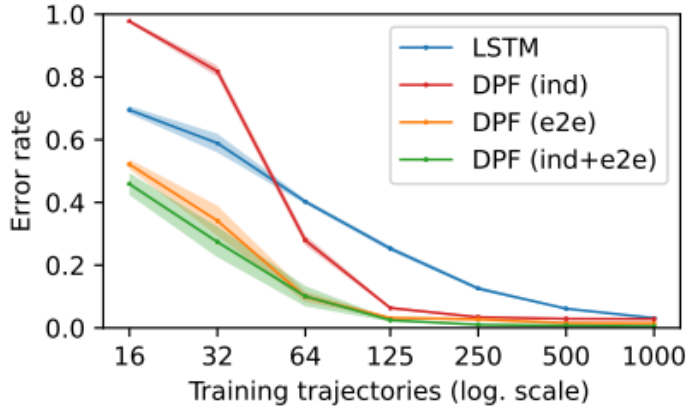
Brohan, A., Brown, N., Carbajal, J., Chebotar, Y., Chen, X., Choromanski, K., Ding, T., Driess, D., Dubey, A., Finn, C., Florence, P., Fu, C., Arenas, M. G., Gopalakrishnan, K., Han, K., Hausman, K., Herzog, A., Hsu, J., Ichter, B., … Zitkovich, B. (2023). *RT-2: Vision-Language-Action Models Transfer Web Knowledge to Robotic Control*. *July*. http://arxiv.org/abs/2307.15818



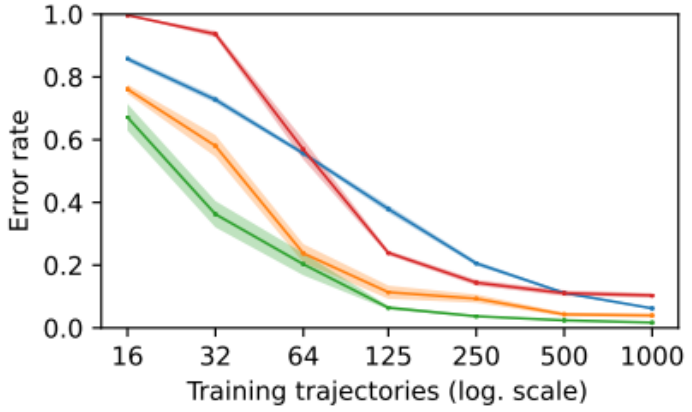

# Differentiable Particle Filters



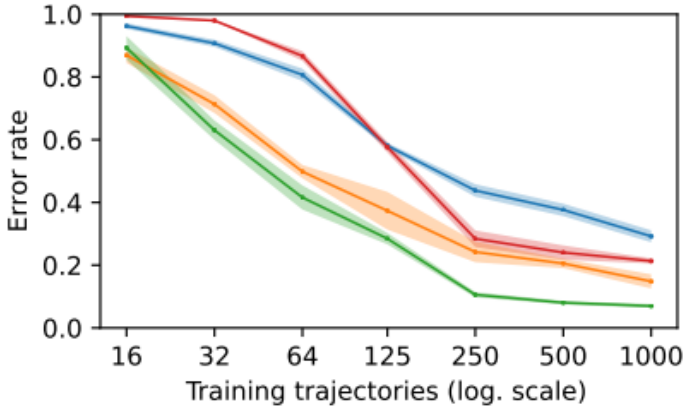

Jonschkowski, R., Rastogi, D., & Brock, O. (2018, June). Differentiable Particle Filters: End-to-End Learning with Algorithmic Priors. *Proceedings of Robotics: Science and Systems*. https://doi.org/10.15607/RSS.2018.XIV.001




(a) Maze 1 (10x5)




(b) Maze 2 (15x9)




(c) Maze 3 (20x13)

# My Thoughts

- Transformers work really well for interpreting structured data that is communicated in a time series (Language is a way of serializing ideas)
- State estimation is NOT usually the hardest part of a POMDP, so just use filtering if you have a decent model (?)
- Use an algorithmic prior when you are learning.
- In tasks where you have to interpret language, transformers are probably the way to go.