Exposing Attention Glitches with Flip-Flop Language Modeling

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Occasional errors of language models

(“hallucination”)

GPT-4o: $S = \left(\frac{1}{2} \times 0\right) + \left(\frac{1}{2} \times \frac{1}{2}\right) + (0 \times \frac{1}{2}) = 0.$

This work: one explanation of occasional errors, exposed using a naïve task.

(attention glitches) (flip-flop)

- Revealing inherent limitations of attention.
- Mitigations & next steps?

How Transformers perform sequential reasoning?

background

↘

Capabilities?

Transformer is capable to solve a broad class of reasoning problems.

How to formalize?

today's focus

↙

Limitations?

Transformer struggles to find an optimal solution in practice.

Formalizing sequential reasoning

```
    1
× (-1)
× (-1)
   ×1
   …
```

arithmetic

[Nogueira et al. 21, Jelassi et al. 23]

Bobo is a dog.

A dog is a mammal.

Is Bobo a mammal?

deduction

[Wei et al. 22, Saparov et al. 22]

```
x = 1
for _ in range(10):
  x = x**2 + 1
print(x)
```

program

[Wang et al. 22, Nijkamp et al. 22]

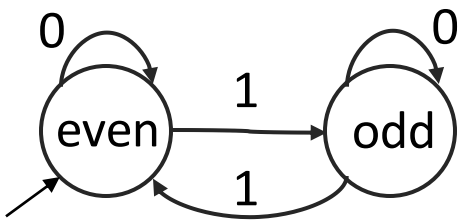
→ Sequential state transitions

Formalizing sequential reasoning

arithmetic

$$1 = (-1)^0,$$
$$-1 = (-1)^1,$$

for the exponents:



aka. **parity counter**

$Q = \{\text{even}, \text{odd}\}$
$\Sigma = \{0, 1\}$

Finite-state automata

$$\mathcal{A} = (Q, \Sigma, \delta)$$

states **inputs** **transitions**

$$q_t = \delta(q_{t-1}, \sigma_t)$$

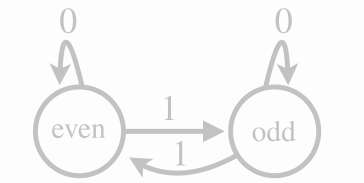
1 state transition
↔ 1 reasoning step

Transformer can simulate automata

$$\mathcal{A} = (Q, \Sigma, \delta),$$
$$q_t = \delta(q_{t-1}, \sigma_t).$$

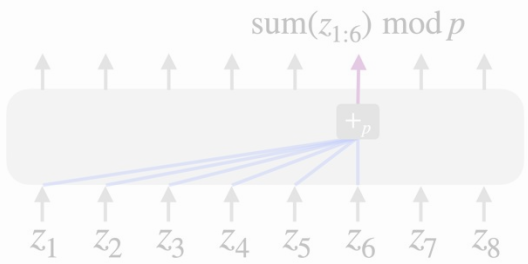
Krohn-Rhodes: (a subset of) $\mathcal{A}$ can be *decomposed* into 2 **base factors**:

- Each factor representable by 1 Transformer layer.

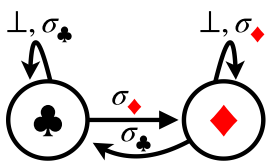


$\delta(q, \sigma) = q + \sigma \bmod p$

mod counter

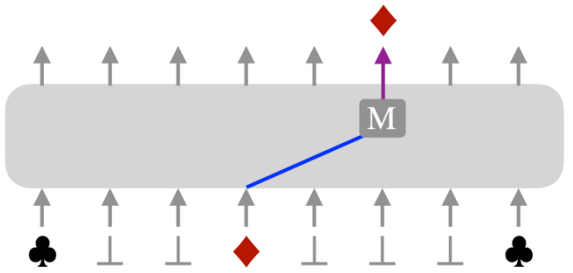


uniform attention



$\delta(q, \sigma) = \sigma,$
$\delta(q, \perp) = q.$

memory unit



sparse attention

Focus of today

How Transformers perform sequential reasoning?

Capabilities?

Transformer is capable to solve
a broad class of reasoning problems.

~ *simulating automata*
(two “base units”)

Limitations?

Transformer struggles to find
an optimal solution in practice.

… even for the base unit.

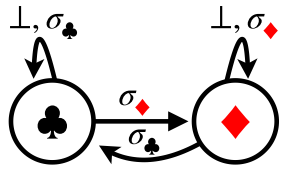
A simple(st) language based on the memory unit

Recall: one (of the 2) *base factor* of automata decomposition.

"flip-flop"

1-bit memory unit

$Q = \{0,1\}, \Sigma = \{\sigma_0, \sigma_1, \perp\}$



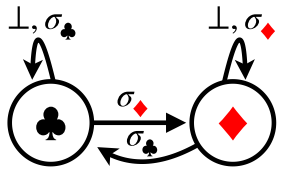
Flip-Flop Language (FFL): sequences of instruction-value pairs.

- 3 instructions: `w` (write), `i` (ignore) , `r` (read).
- 2 values: {0, 1} – ***Constraint***: the value for `r` must be the same as the last `w`.

Why Flip-Flop?

1-bit memory unit

$Q = \{0,1\}, \Sigma = \{\sigma_0, \sigma_1, \perp\}$



Flip-Flop Language (FFL)

`w 1 i 0 r 1 w 0 i 1 r 1`

1. An atomic unit embedded in many reasoning tasks (e.g. automata).

- **`ignore`**: Irrelevant context / distractors
  [Shi et al. 23]

```
Alice put the keys
on the table.
Bob came in later.
….
Bob left and took
the keys from ___ .
```

- **`write`**: Updated code semantics
  [Miceli-Barone et al. 23]

```
def f():
  sum = len
  . . .
  x = [1,2,3]
  . . .
  assert(sum(x))==3
```

Why Flip-Flop?

1-bit memory unit

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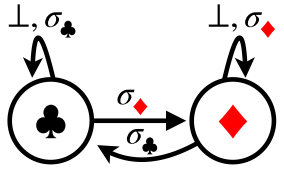
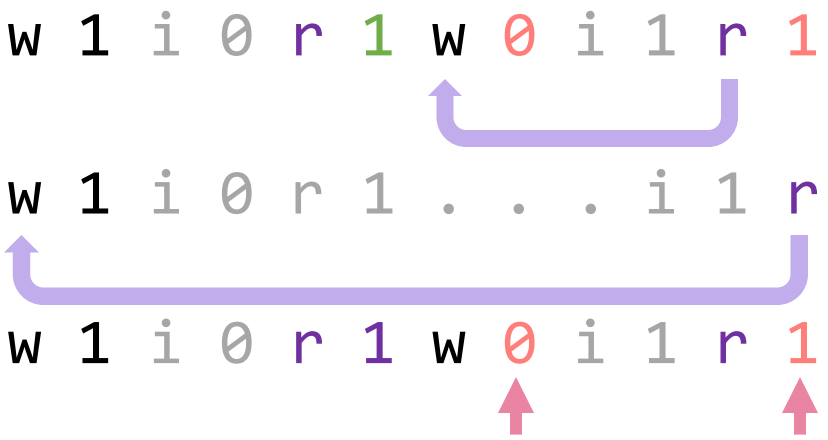


Flip-Flop Language (FFL)

w 1 i 0 r 1 w 0 i 1 r 1

1. An atomic unit embedded in many reasoning tasks (e.g. automata).

- Induction head [Olsson et al. 22]
- Long-range dependency [Tay et al. 20]
- Closed-domain hallucination [Dziri et al. 22, OpenAI 23]



Why Flip-Flop?

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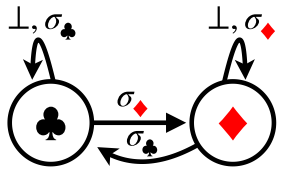


Flip-Flop Language (FFL)

`w 1 i 0 r 1 w 0 i 1 r 1`

2. The cleanest, interesting setting of failure, compared to prior work:

- Less interesting: *fixed attention patterns*. e.g. Parity [Hahn 20, Barak 22], FIRST [Chiang & Cholak 22]
- More complicated:
  - Formal languages [Bhattamishra 20, Yao 21, van der Poel 23].
  - Algorithmic reasoning [Nogueira 21, Anil 22, Zhang 22, Dziri 23, Zhang 23].
  - Code [Chen 21, Miceli-Barone 23], math [Cobbe 21, Lu 22, Shi 23].
  - Natural languages: QA [Rogers 21], long-range tasks [Tay 20], multi-step reasoning [Saparov 22].

Flip-Flop Language Modeling (FFLM)

Flip-Flop Language (FFL): instruction-value pairs; `r` recalls the most recent `w`.

Task: supervise & evaluate only on the values following `r`.

- Deterministic task; training signals not "drawn" by irrelevant tokens.

Data distribution: FFL(p_i), where p_i can vary across train/test.

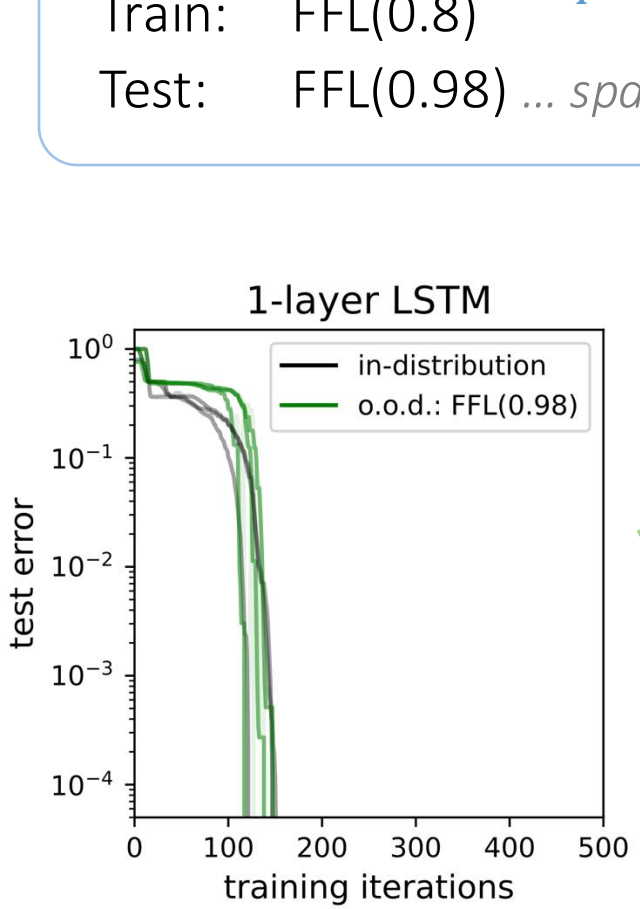
- $p_w = p_r = (1 - p_i)/2$, $p_0 = p_1 = 0.5$. Fix length $T = 512$.

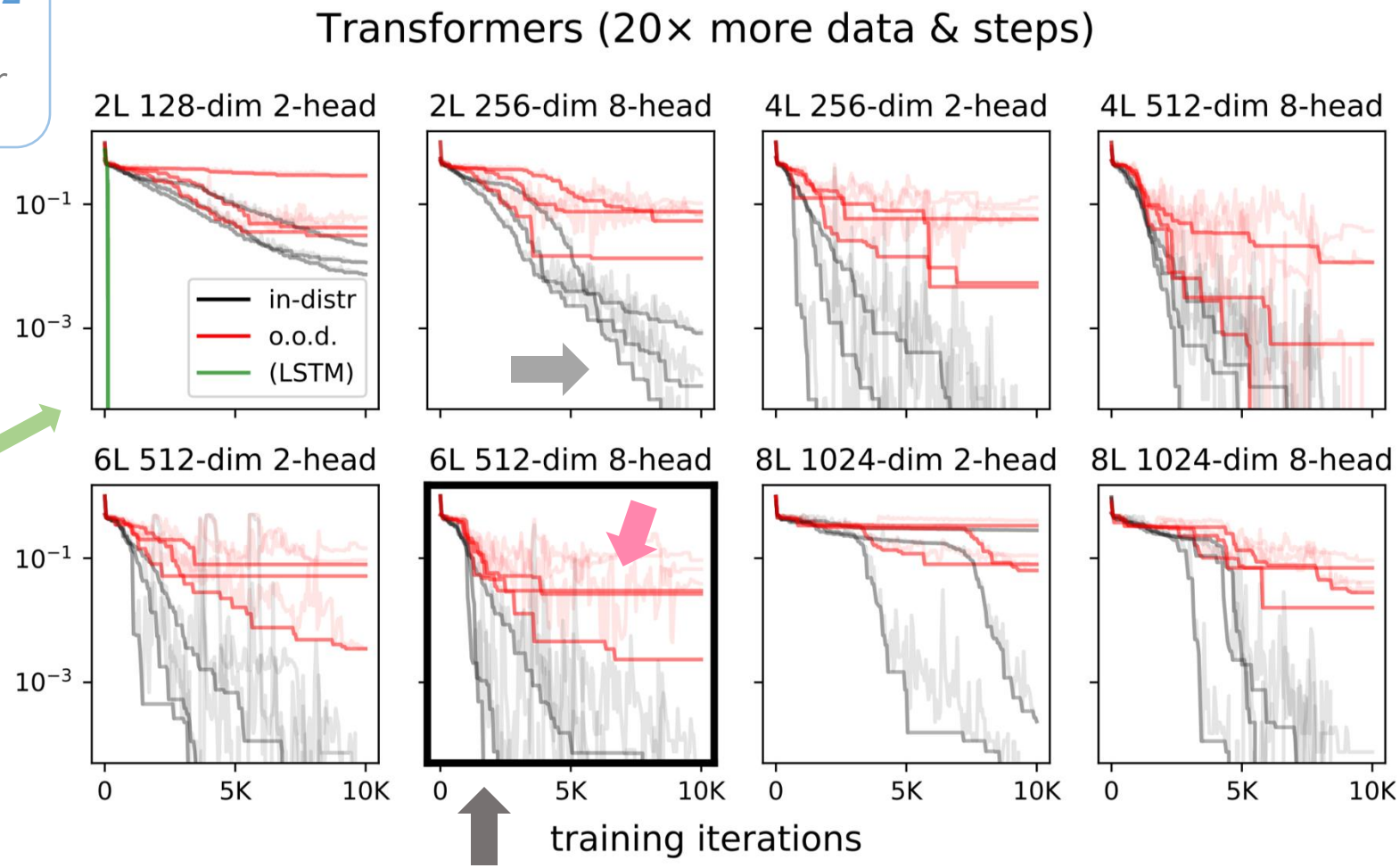
FFLM Results

Train: FFL(0.8)
Test: FFL(0.98) … *sparser*

$T = 512$

Attention glitches





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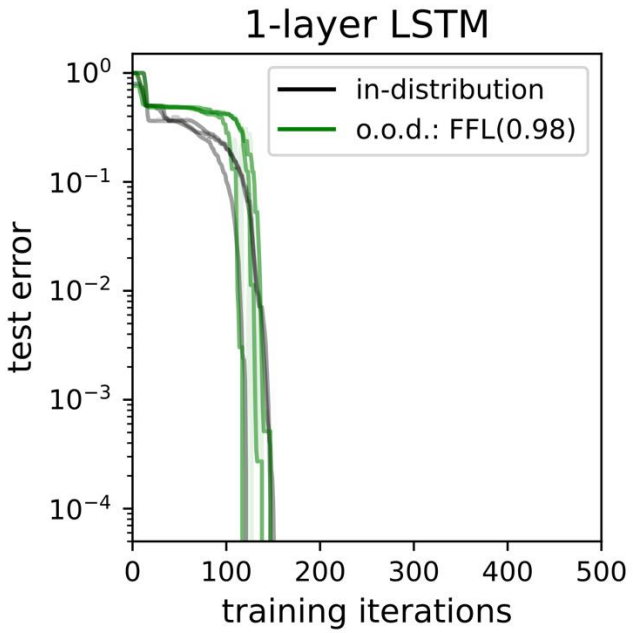
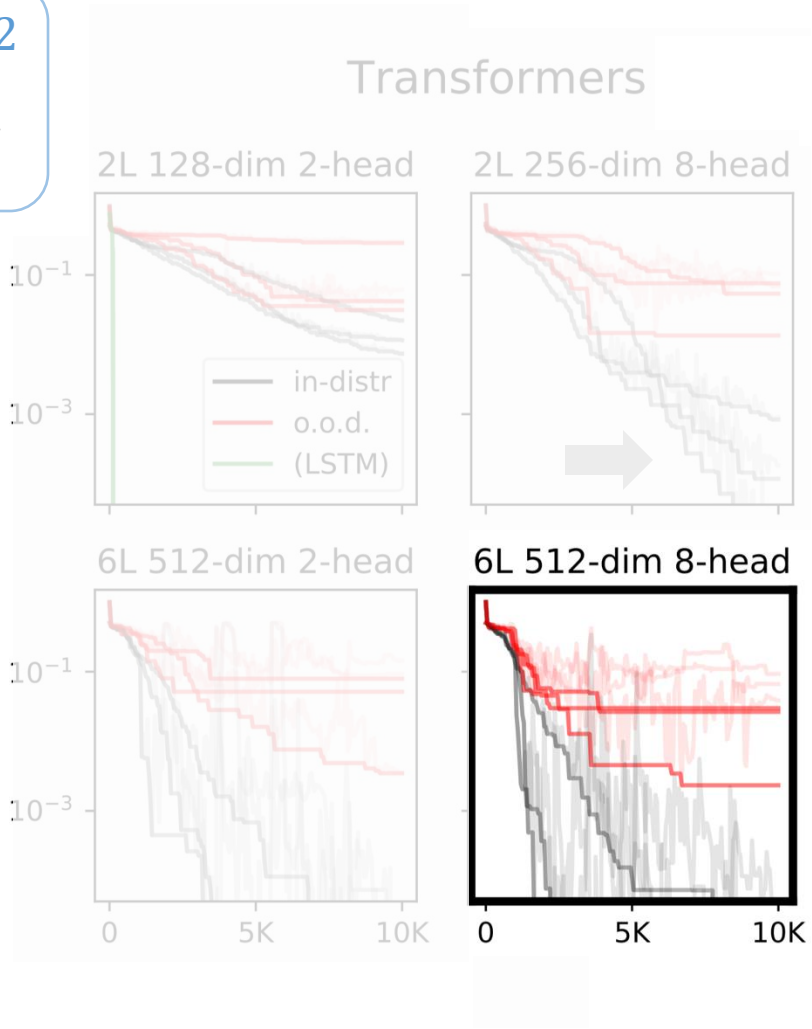
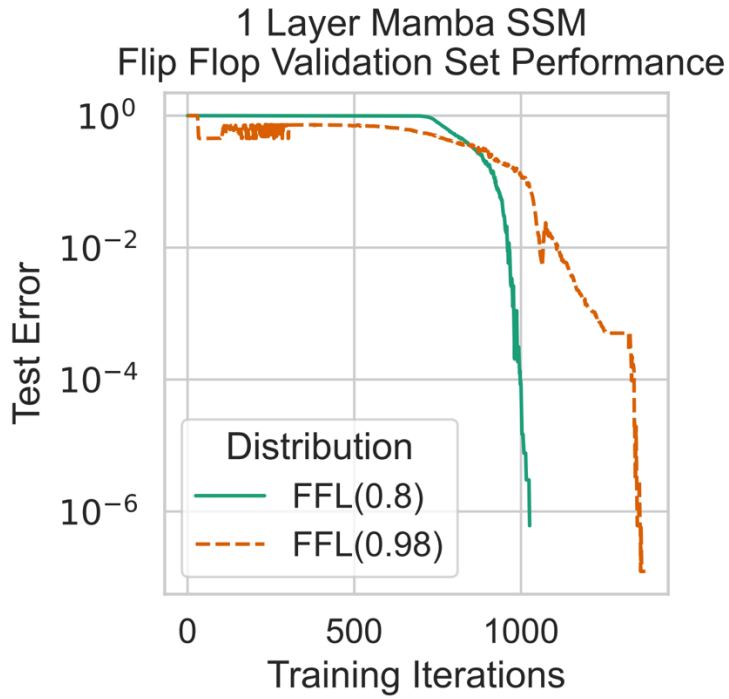




State-Space Models (SSMs)?



[Sarrof et al. 24]

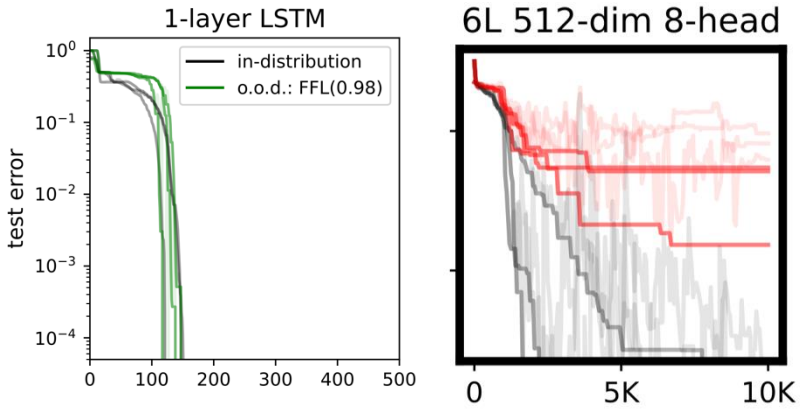
Attention Glitches

$\text{FFL}(p_i)$: $p_w = p_r = (1 - p_i)/2.$

Def: *imperfect hard retrieval*.

- Transformers exhibit a long tail of errors.
- 1-layer LSTMs extrapolate *perfectly*.

Even proprietary models are not robust.



User: Hi, let's play a game. There are 3 instructions: "write", "read", and "ignore".

. . .
For example, ...

Now, please answer the following sequence: …

GPT 4o: ~50% acc
1, 0, 0, 1, 1, 0, 0, 1, 1, 0

GPT o1: ~90% acc

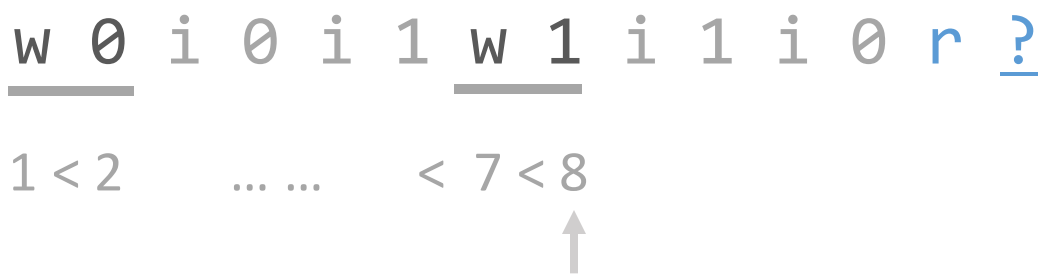
(based on 10 trials)

Cause of attention glitches?

FFL(p_i): $p_w = p_r = (1 - p_i)/2$.

Not due to representation power.

- Solvable with ***2-layer 1-head*** . → see also: induction head [Bietti et al. 23, Sanford et al. 24]
  - 1st layer: locate `w`'s and the associated values.
  - 2nd layer: tie-break using position encoding.



Cause of attention glitches?

FFL(p_i): $p_w = p_r = (1 - p_i)/2$.

Not due to representation power: *2-layer 1-head* suffices (Bietti et al. 23, Sanford et al. 24).

2 potential causes, each related to 1 type of OOD error.

Diluted soft attention: caused by more items (e.g. *denser* `w`) in the softmax.

$$a_{\max} = \frac{\exp(z_{\max})}{\underbrace{\exp(z_1)+\cdots+\exp(z_t)}_{\text{to be ignored}}+\exp(z_{max})}$$

- Also identified in prior work [Hahn 20, Chiang & Cholak 22].
- Possible mitigation: Switching to hard attention.

Cause of attention glitches?

FFL(p_i): $p_w = p_r = (1 - p_i)/2$.

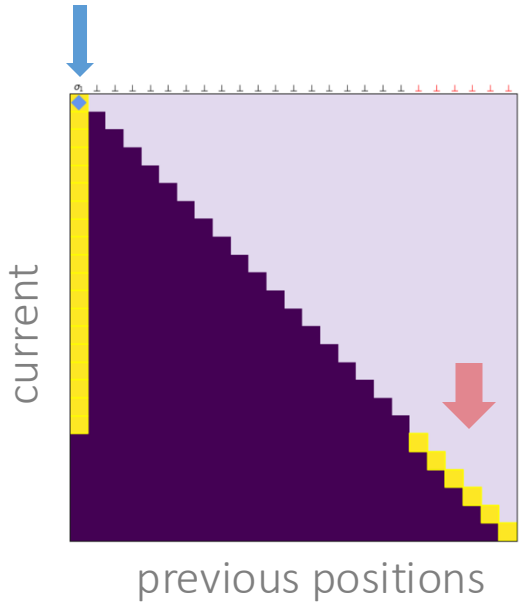
Not due to representation power: *2-layer 1-head* suffices (Bietti et al. 23, Sanford et al. 24).

2 potential causes, each related to 1 type of OOD error.

Diluted soft attention: caused by more items (e.g. *denser* `w`) in the softmax.

Position over content: lead to wrong argmax.
(e.g. *sparser* `w`, length gen)

- "Implicit" length generalization: w-r dist can increase.



Mitigating attention glitches

Data & scaling

- Incorporating OOD data.

  Performance ceiling; a few samples can help.
  e.g. “priming” [Jelassi et al. 23]

- Resource scaling: larger, train for longer.

  Fresh samples → better coverage.

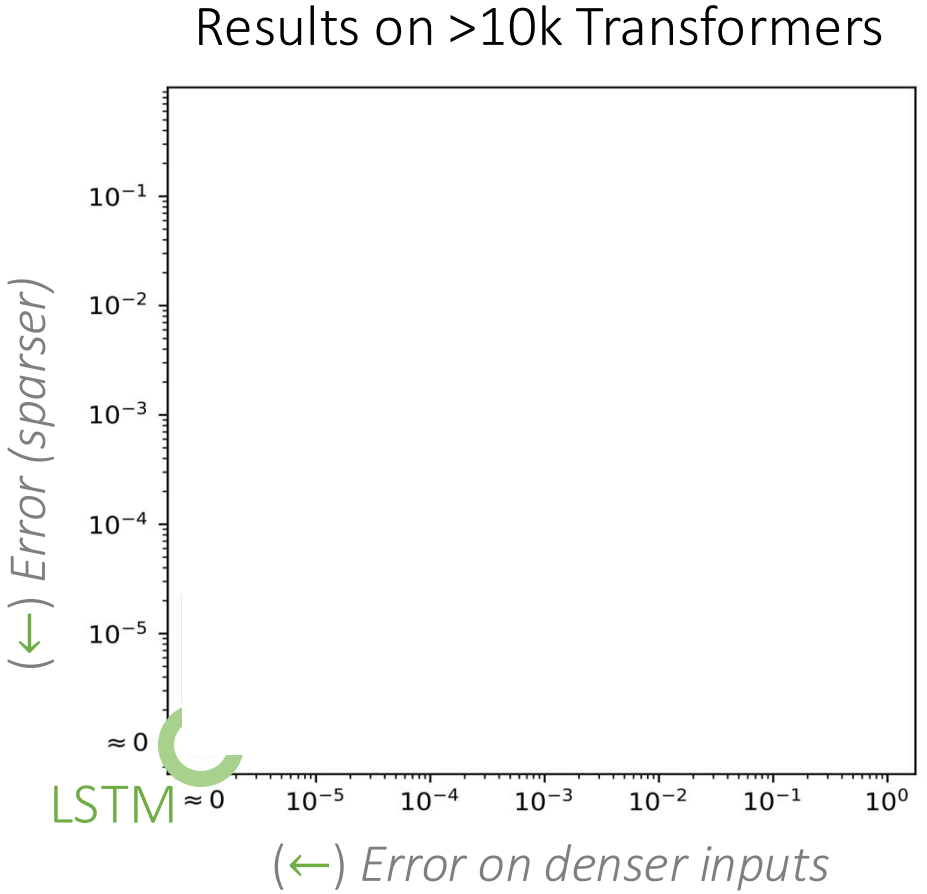
Algorithmic control

- Regularization

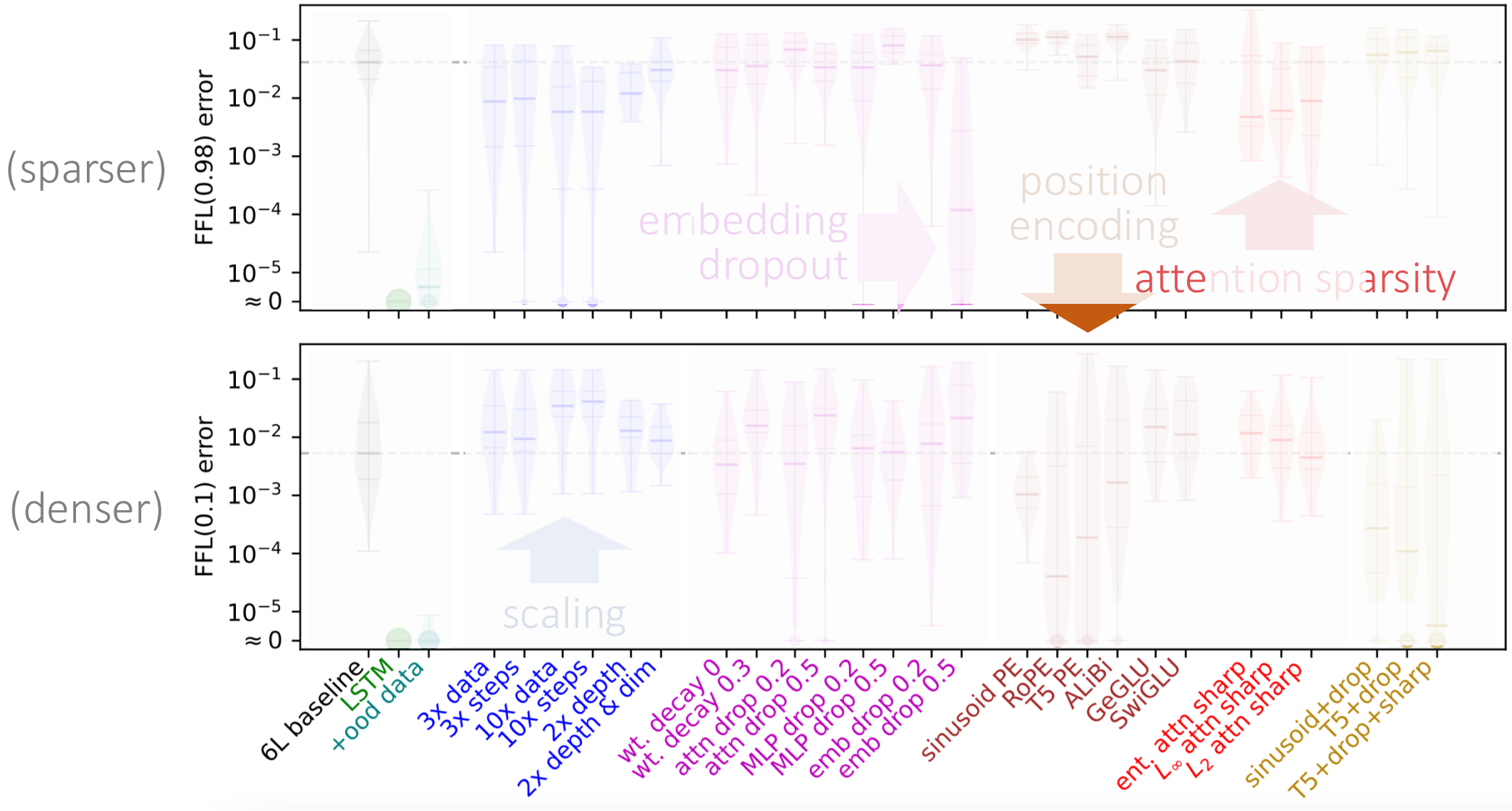
  weight decay, dropout, attention sparsity.

- Architectural choices

  position encoding, activation.



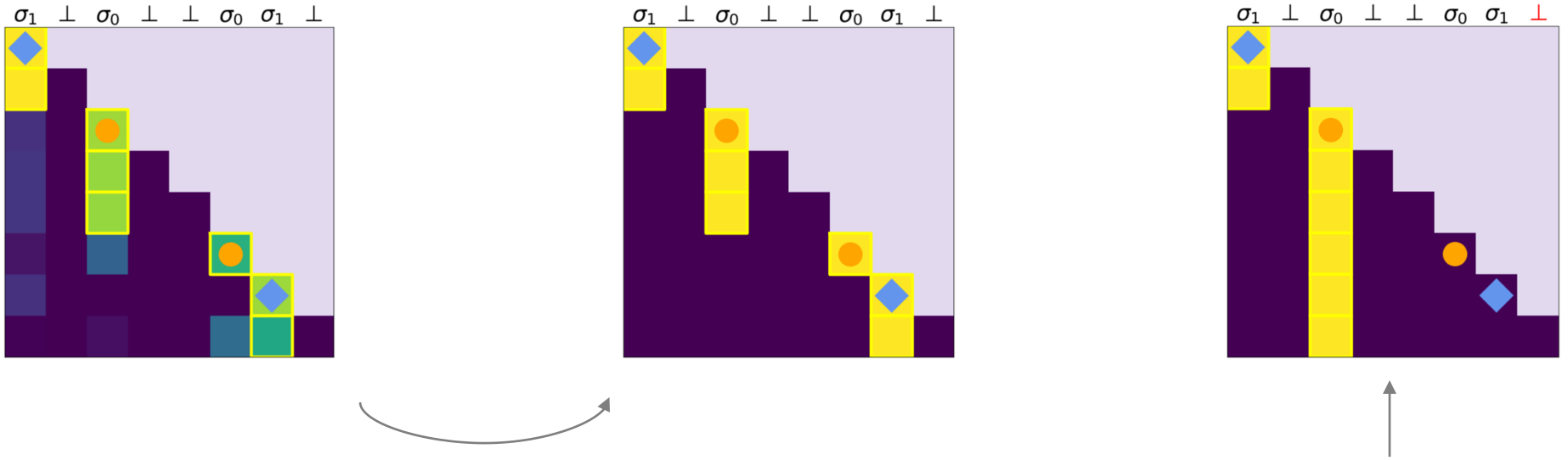
Surprisingly hard to fix: no mitigation helps with *both*



Zoom-in: attention sparsity regularization

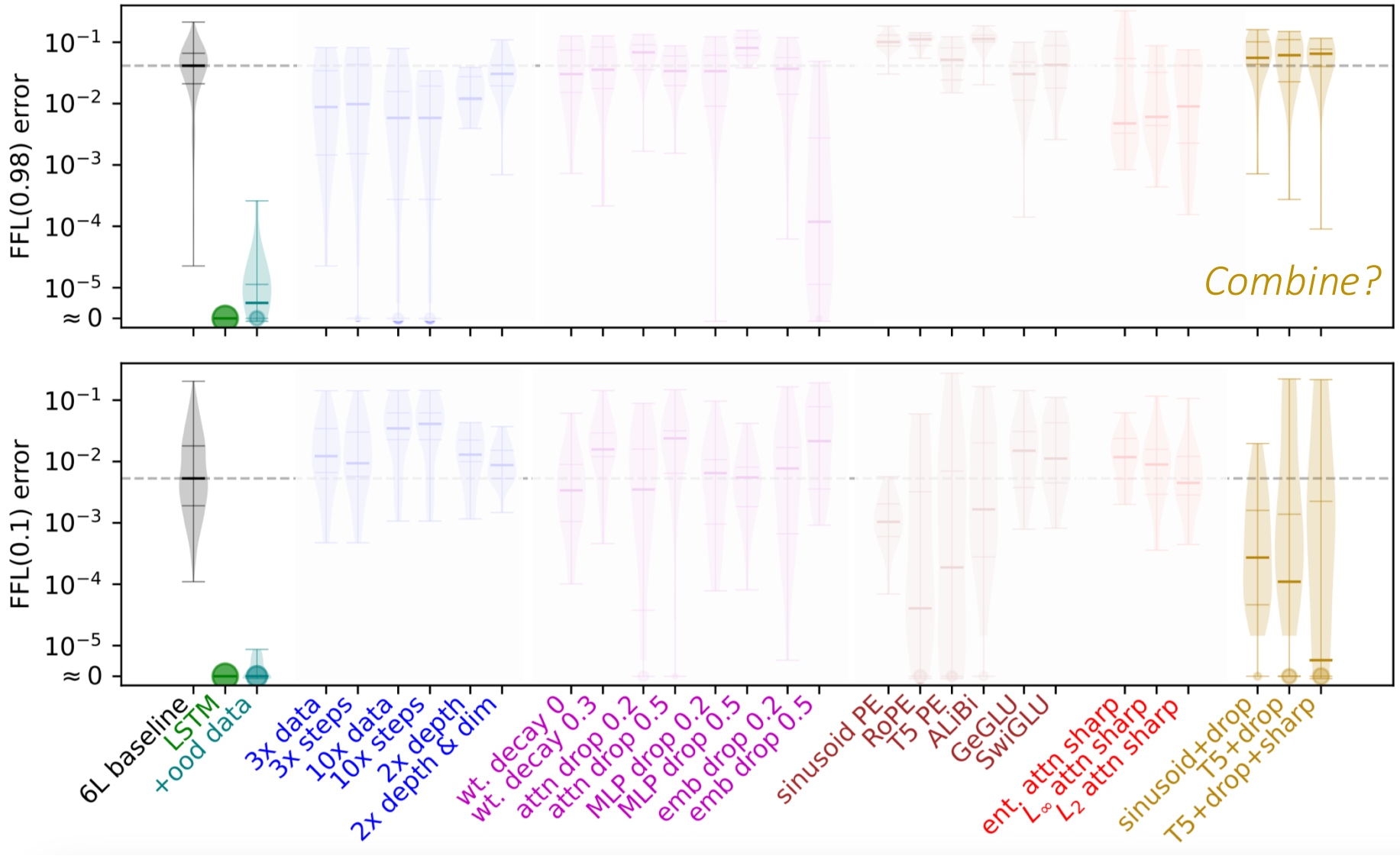
Regularize for sparsity: $\sum_i \alpha_i \log \alpha_i$ (entropy), $-|\alpha|_\infty$ (L_∞), $-|\alpha|_2$ (L_2).

1-layer 1-head model:



** In general, use caution with attention-based interpretability.* [Wen et al. 23]

Surprisingly hard to fix: no mitigation helps with *both*



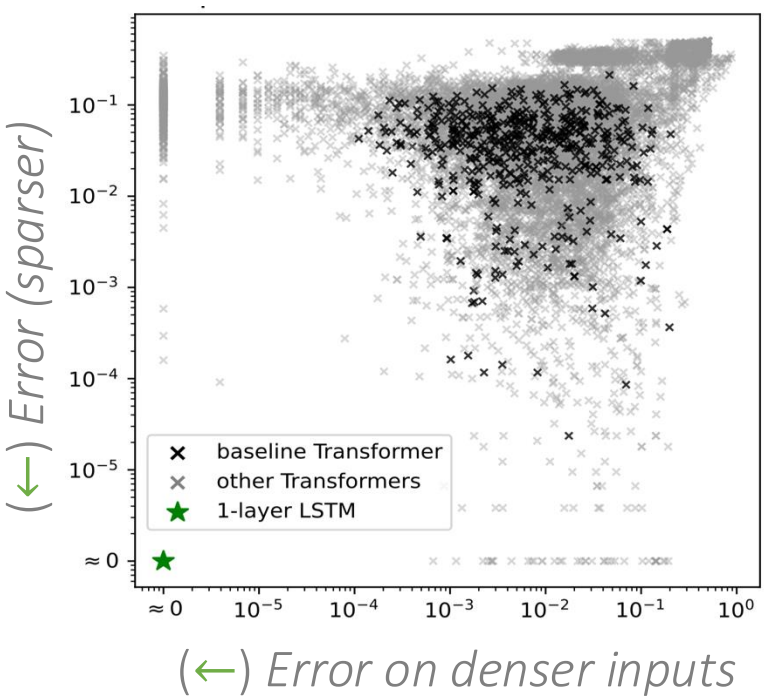
Attention glitches with Flip-flop

One source of Transformer's occasional errors: imperfect hard retrieval.

- What: Transformer's long tail of errors, even on an *extremely simple* task.
  - *Goal: learn as well as LSTM?*
- Why: Two inherent limitations of attention.
  - Imply various errors; hard to mitigate.
- How: Scaling is no panacea. Data matters.
  - *… recurring theme recently.*

Flip-Flop Language (FFL)

`w 1 i 0 r 1 w 0 i 1 r 1`



How Transformers perform sequential reasoning?

Capabilities?

Transformer is capable to solve a broad class of reasoning problems.

- Formalized as simulating automata.
- Parallel solution of $o(\mathbf{length})$ steps.

Limitations?

Transformer struggles to find an optimal solution in practice.

- Occasional errors on the naïve flip-flop.
- Exposing inherent limitations of attention.

Discussion: Towards glitch-free models

Data: collection/selection (“priming”), format, usage (curriculum, repetition).

Architecture: recurrence/hybrid, positional encoding, tokenization.

(RoPE, FIRE, Abacus)

- Different notions of error: average-case (L_2) vs worst-case (L_∞) .
- Do we really need to be stringent?

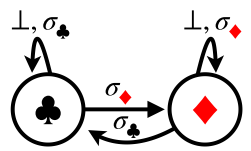
> **Turing** (1947)*: “If a machine is expected to be infallible, it cannot also be intelligent.”*

Still: awareness & caution when there are other priorities (e.g. safety, robustness).

Discussion: Using small-scale “sandboxes”

“Sandbox for the Blackbox”

Sandboxes: minimal, representative abstractions of complex systems.



- Why: formal analyses, rapid iteration; controllable & accessible.

Can be used for…

- Scientific understanding

  e.g. methods, training dynamics, mech interp.

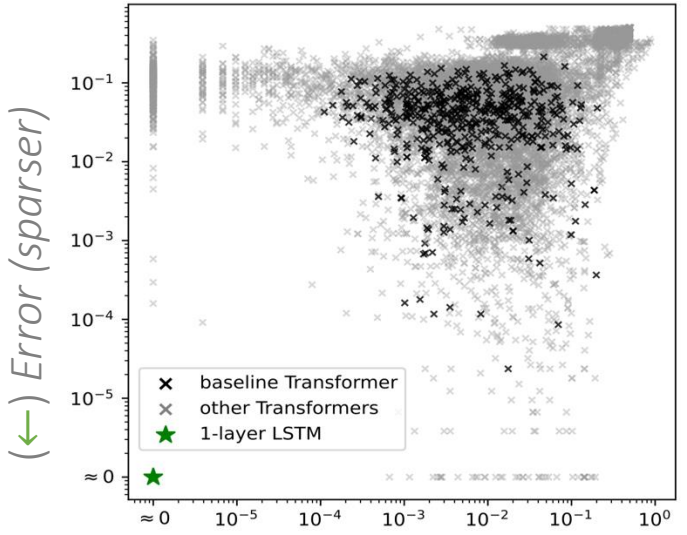
- Evaluation and diagnosis

  e.g. flip-flop, arithmetic, needle-in-a-haystack.

- Efficient algorithmic innovations

  e.g. architecture, training recipe, inference procedure.

Results on 10k Transformers



Discussion: Scaling (up)

Scaling is not a panacea…

- e.g. inverse scaling challenges; environmental/accessibility considerations.

… but it does help.

- Representation: larger models are more expressive.
- Optimization: wider models are more stable to train.
- Favorable properties: generalization; “emergent” abilities *… how to evaluate?*

∴ Be mindful of it when making design choices. (The Bitter Lesson – Sutton 19)

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Thank you! Questions? 

Appendix

Thanks for wanting to know more! ☺

Part I
Transformers learn shortcut to automata

Reasoning as simulating automata

$\mathcal{A} = (Q, \Sigma, \delta)$

states, inputs, transitions

Simulating $\mathcal{A}$: learn a *seq2seq function* for sequences of length T.

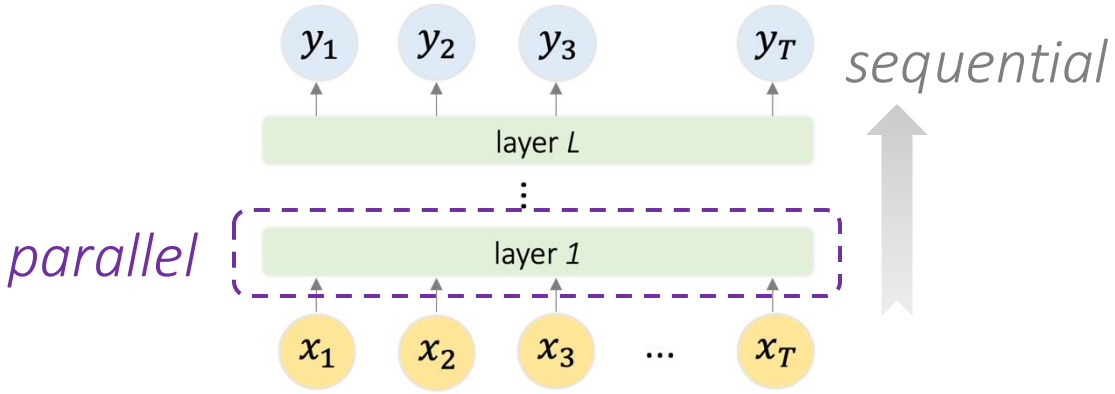
Output: q_1 q_2 $\cdots$ q_T $\subset Q^T$ (states)

Model (Transformer/RNN)

Input: σ_1 σ_2 $\cdots$ σ_T $\subset \Sigma^T$ (alphabet)

Solutions with much fewer sequential steps?

Transformers

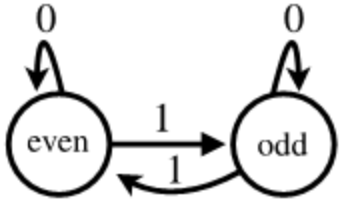


#layers ≪ #positions

Why are $o(T)$-step solutions possible

$\mathcal{A} = (Q, \Sigma, \delta)$

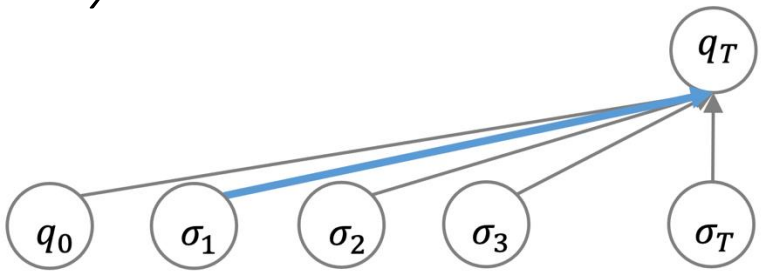
states, inputs, transitions

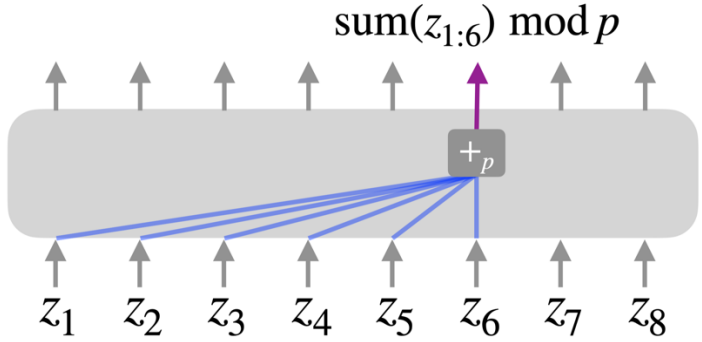
e.g. parity 

… T-step solution: $q_t = \delta(q_{t-1}, \sigma_t), \forall t \in [T]$.

1 step solution: $q_t = (\sum_{\tau \le t} \sigma_\tau) \bmod 2$.

no dependency on T



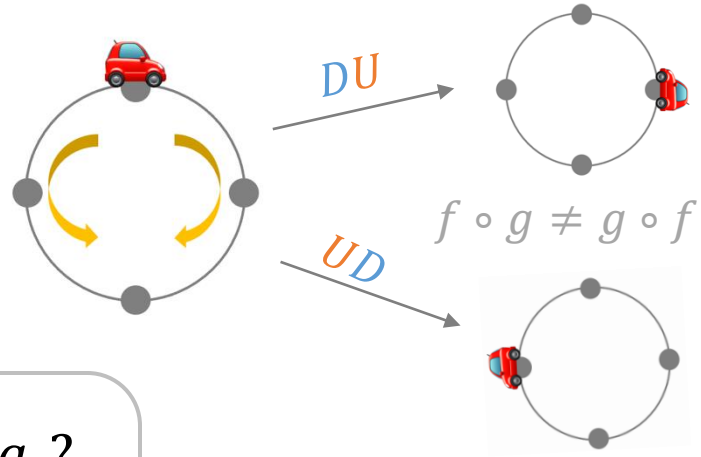


uniform attention

Decomposition: example

$$\mathcal{A} = (Q, \Sigma, \delta), \quad q_t = \delta(q_{t-1}, \sigma_t).$$

$Q = \{$ 🚗 (1), 🚙 (-1) $\} \times \{0,1,2,3\}$, $\Sigma = \{D\,(\text{drive}), U\,(\text{U-turn})\}$.



	q_0	D	D	D	U	D	D	U	U	D $\rightarrow q_t$?
Parity:	1	1	1	1	-1	-1	-1	1	-1	-1 $\rightarrow$ 🚗
Signed sum:	0	1	1	1	0	-1	-1	0	0	-1 $\rightarrow$ 0

$O(1)$ layer each

1. Direction = parity (sum) of U. (parity: {1, -1} $\leftrightarrow$ {0, 1})
2. Position = signed sum mod 4 : sign = parity of U.

Transformers can simulate automata in practice

19 automata, across various depths.

- Good in-distribution accuracy.
- Deeper factorization → more layers.
  - Rows ordered by #factorization steps.

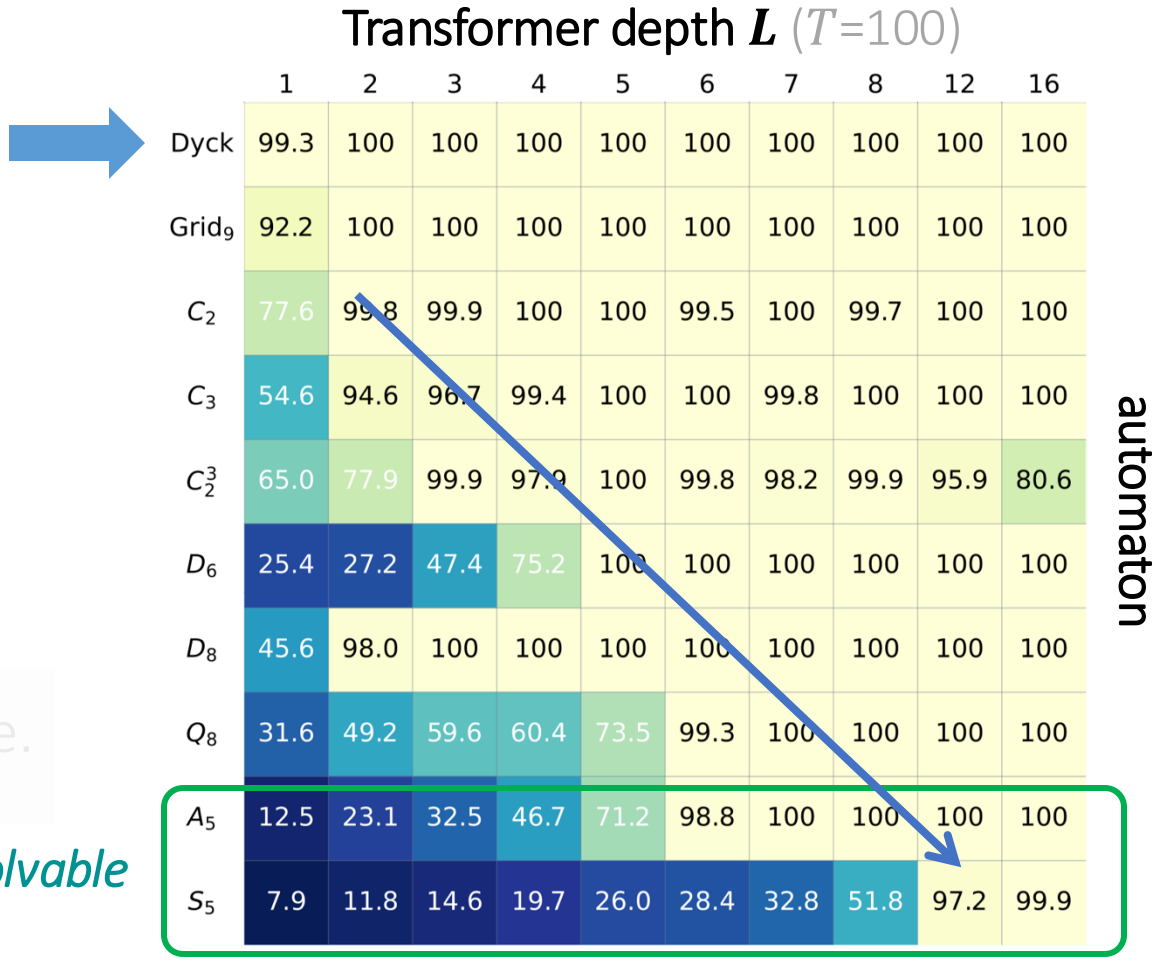
Constructions ≠ empirical solutions

There are multiple constructions.

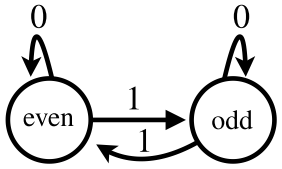
- $O(\log|Q|)$ layers suffice; $O(|Q|^2)$ if solvable.

Infinitely many

non-solvable



OOD Generalization - Parity



$(T = 40)$

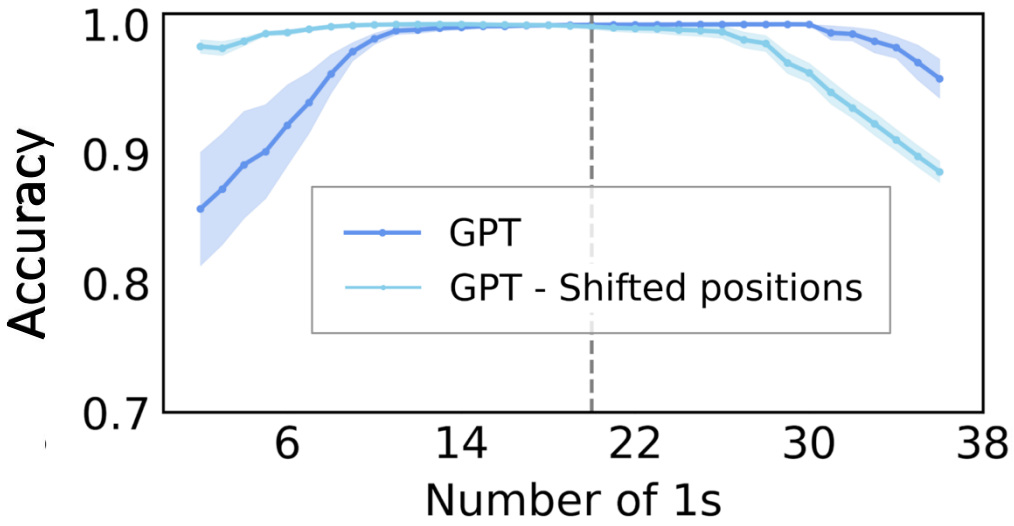
- train: $p(1) = 0.5$
- test: other $p(1)$.

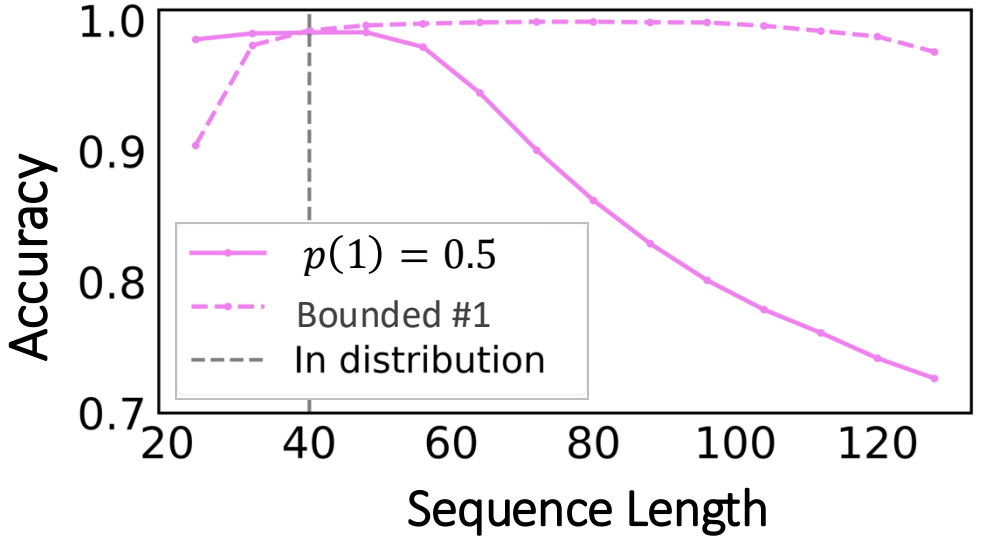
$$q_t = \left(\sum_{i\in[t]} \sigma_i\right) \bmod 2$$

concentrates $\approx 0.5t$

memorized by MLP

→ fail at unseen $\left(\sum_{i\in[t]} \sigma_i\right)$.

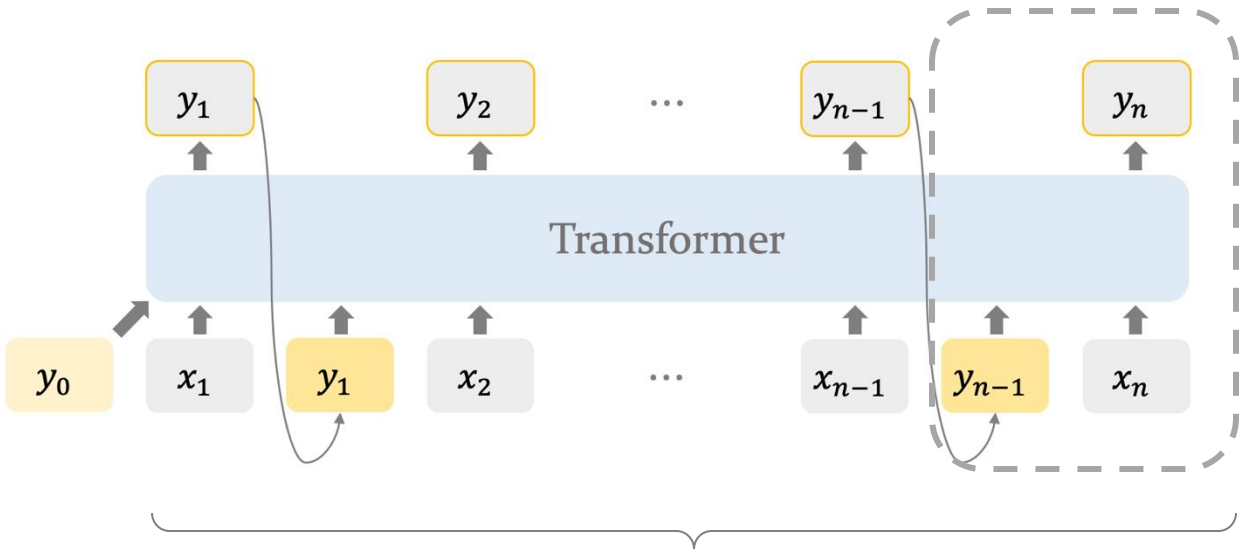




Autoregressive mode of Transformers

Fix to OOD: iterative/autoregressive solutions: use q_{t-1} as inputs.

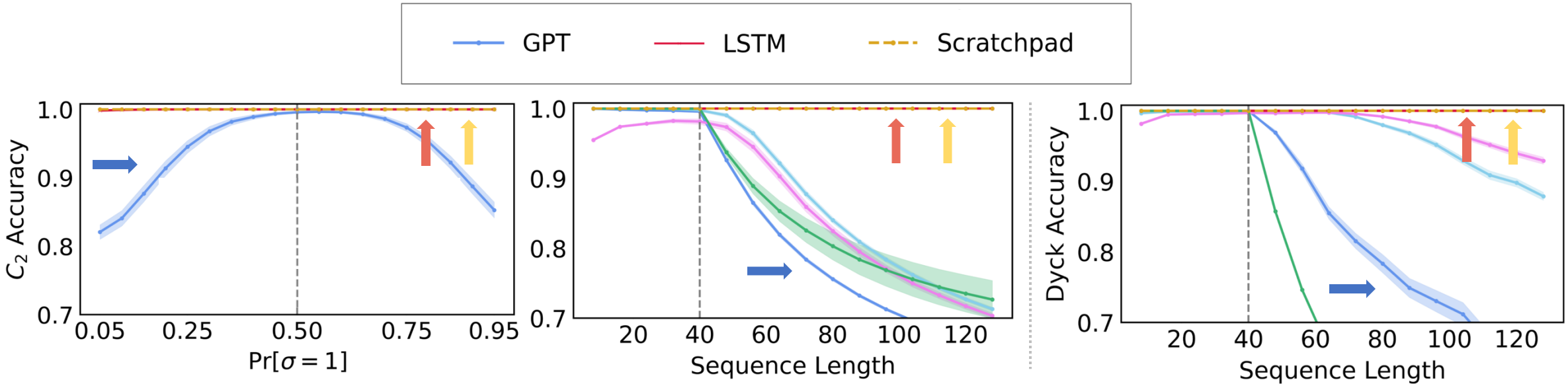
Scratchpad (Nye et al. 21) $q_t = \delta(q_{t-1}, \sigma_t)$



Not shortcut

No longer parallel across positions

Autoregressive mode of Transformers



Transformers generalize, when made autoregressive with scratchpad [Nye et al. 22].

→ Open: *Can we learn shortcuts that generalize?*

Training with limited supervision

Less ideal setups?

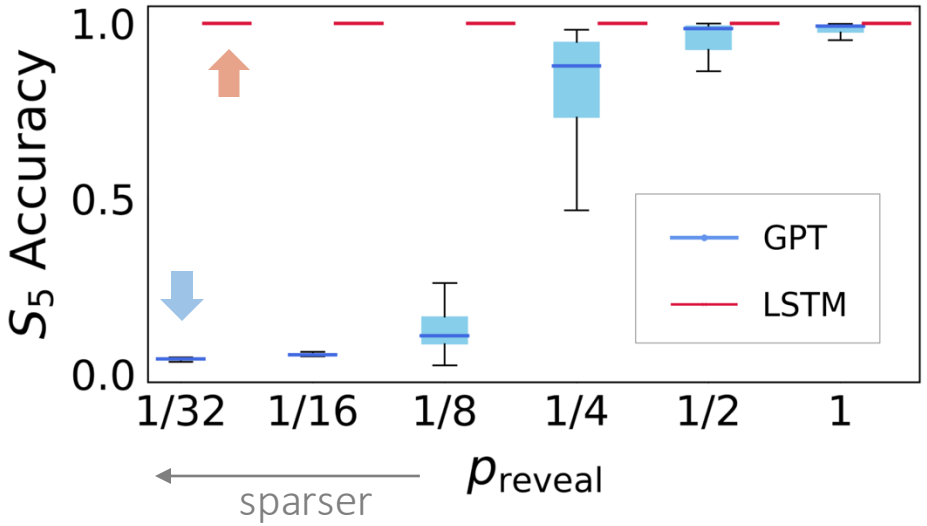
Indirect supervision

train & test on a function of q_t.

$\text{Dyck}_{4,8}$	Grid_9	S_5	C_4	D_8
stack top	$\mathbb{1}_{\text{boundary}}$	$\pi_{1:t}(1)$	$\mathbb{1}_{0 \bmod 4}$	location
100.0	99.8	99.8	99.7	99.8

Incomplete supervision

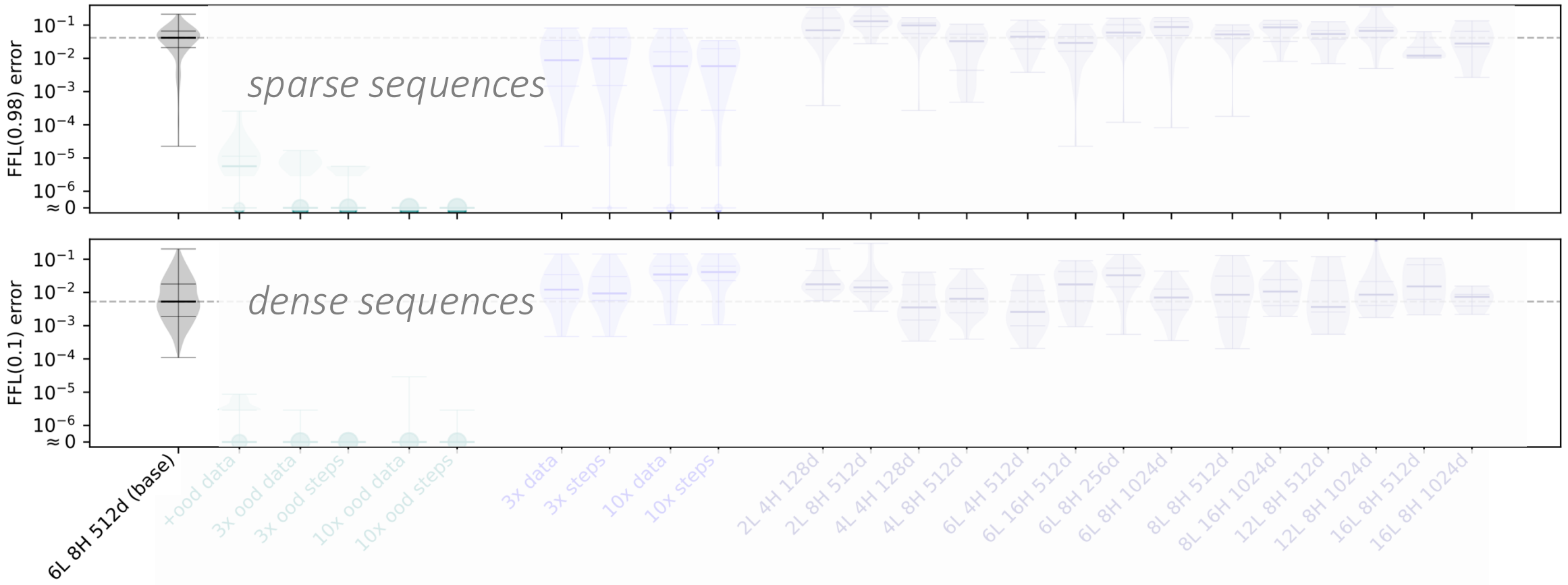
q_t is revealed w.p. $p_{\text{reveal}} \in [0,1]$.



LSTM is always 100% → Open: *How to improve Transformer training?*

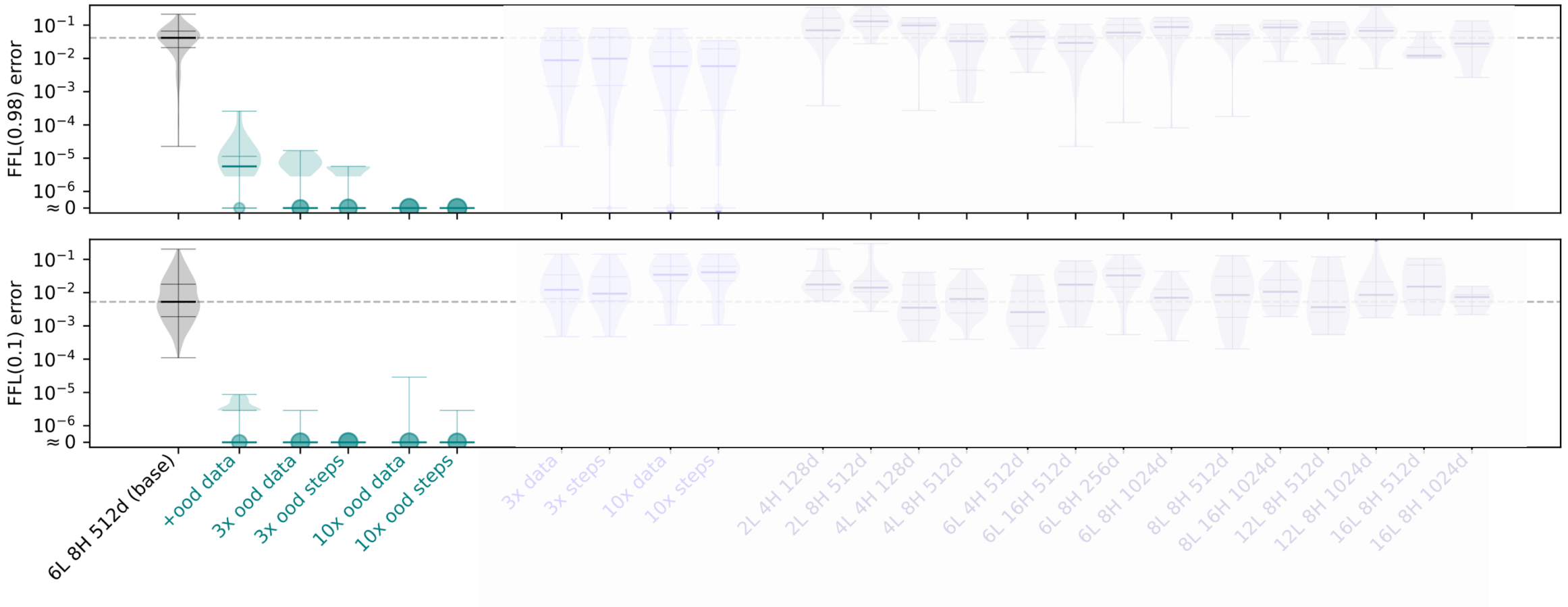
Part II
Exposing attention glitches with FFLM

Mitigations



Mitigations – Data

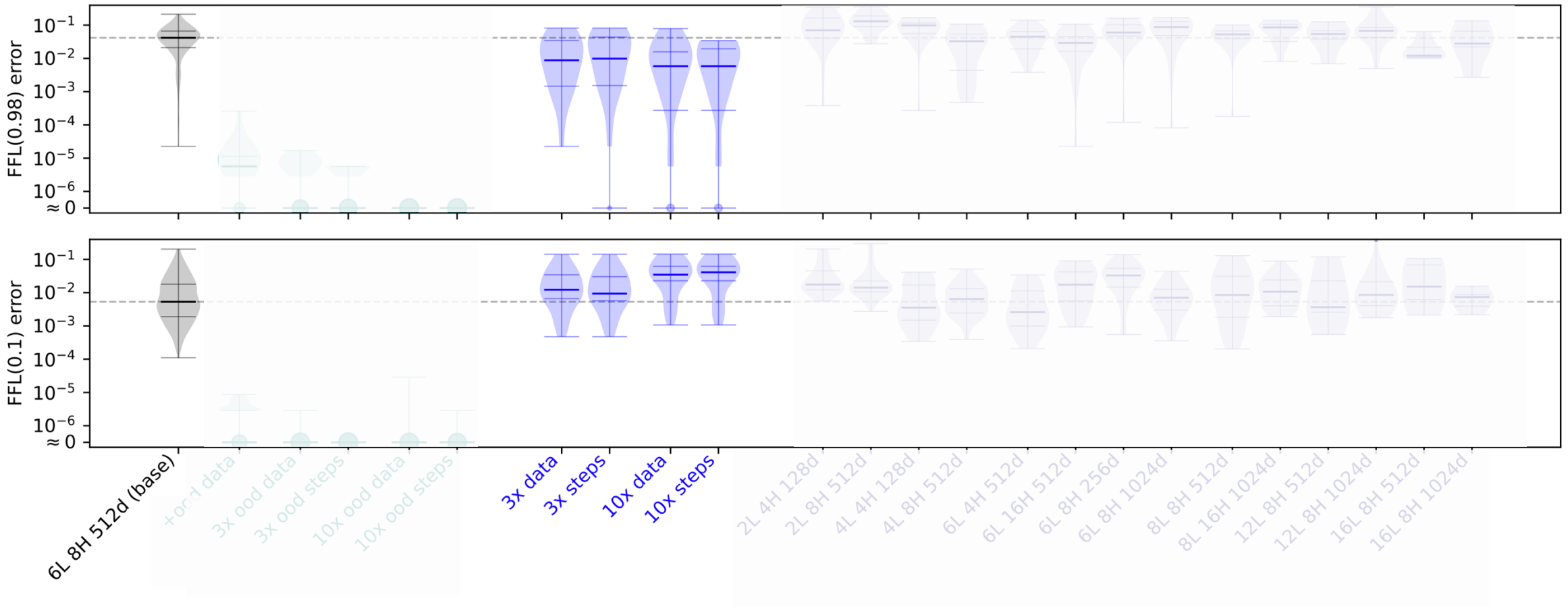
(R4) Incorporating OOD data works the best, by far.



Mitigations – Scaling

More data/iterations

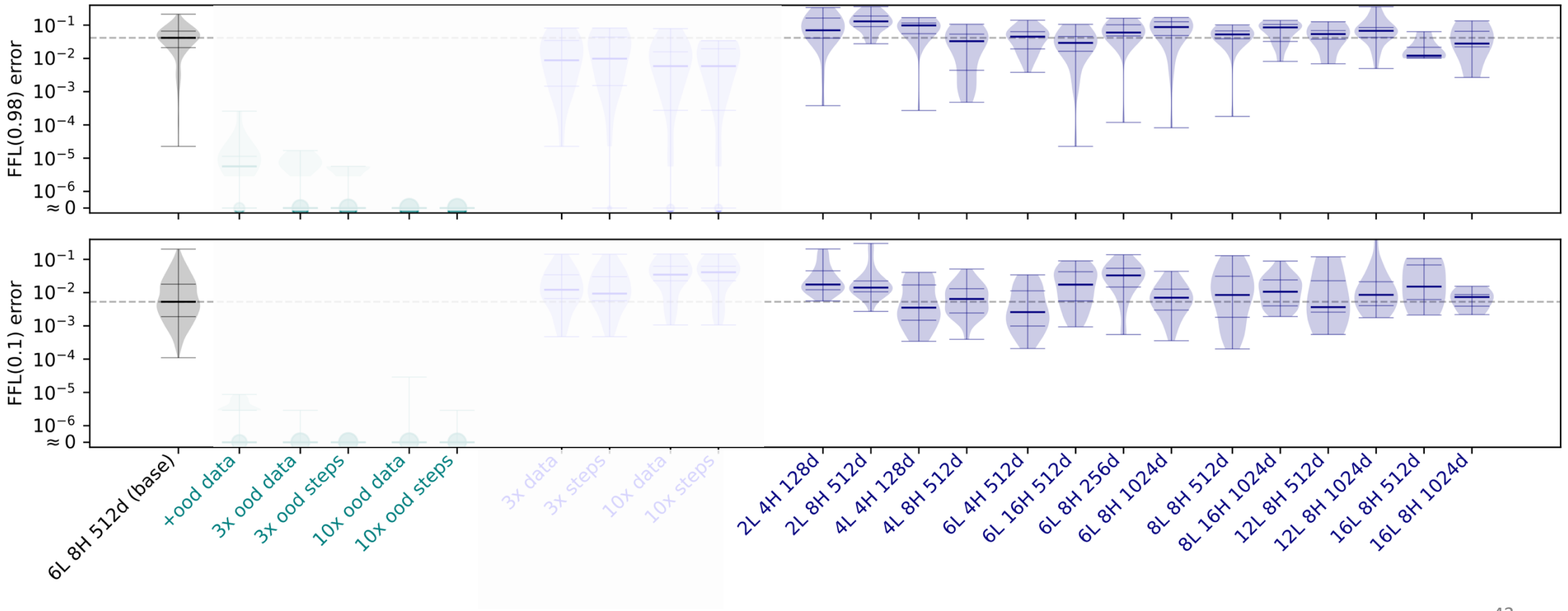
(R5) Resource scaling helps, but there's a **dense-sparse trade-off**.



Mitigations – Scaling

Larger models

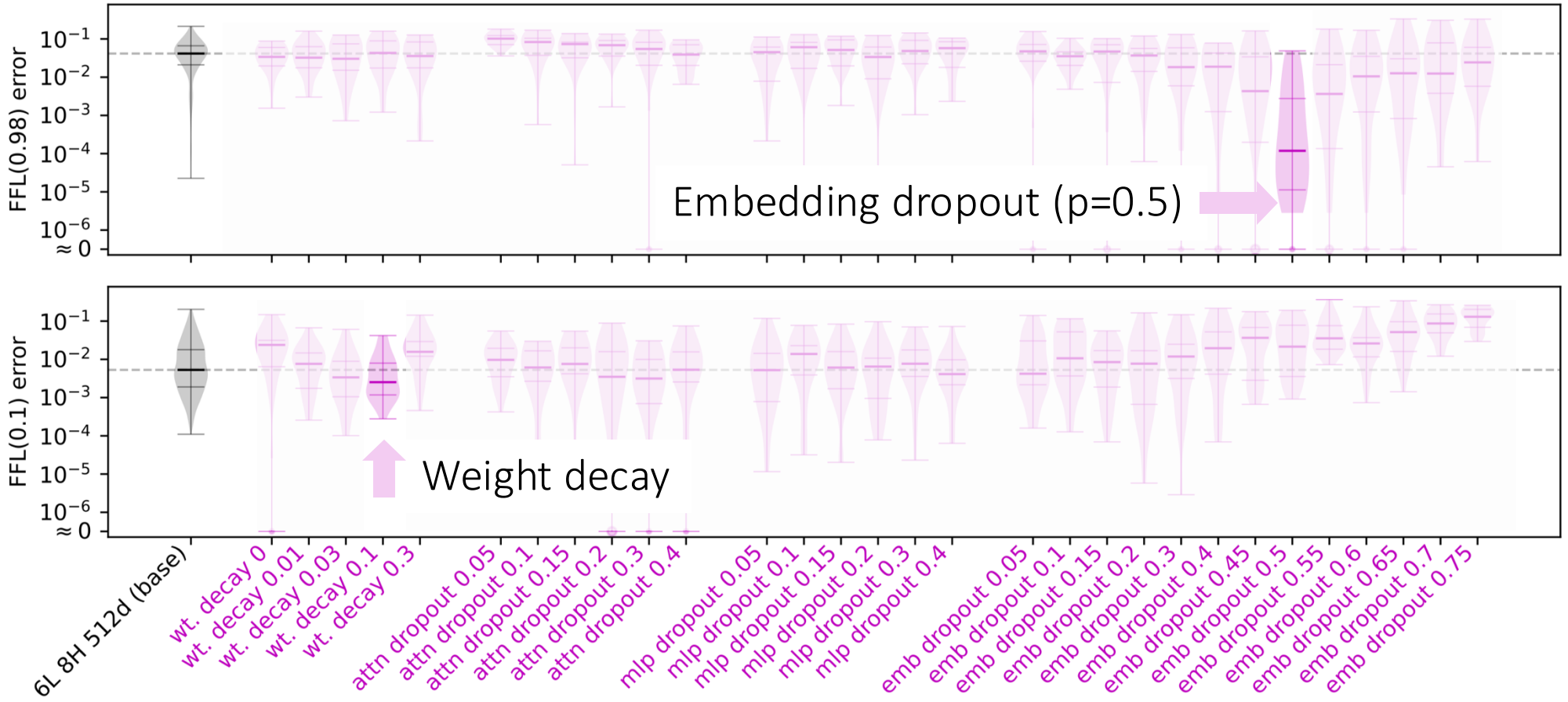
(R5) Resource scaling helps, but there's a **dense-sparse trade-off**.



Mitigations – Regularization

- Weight decay
- Dropout (attention, MLP, embedding)

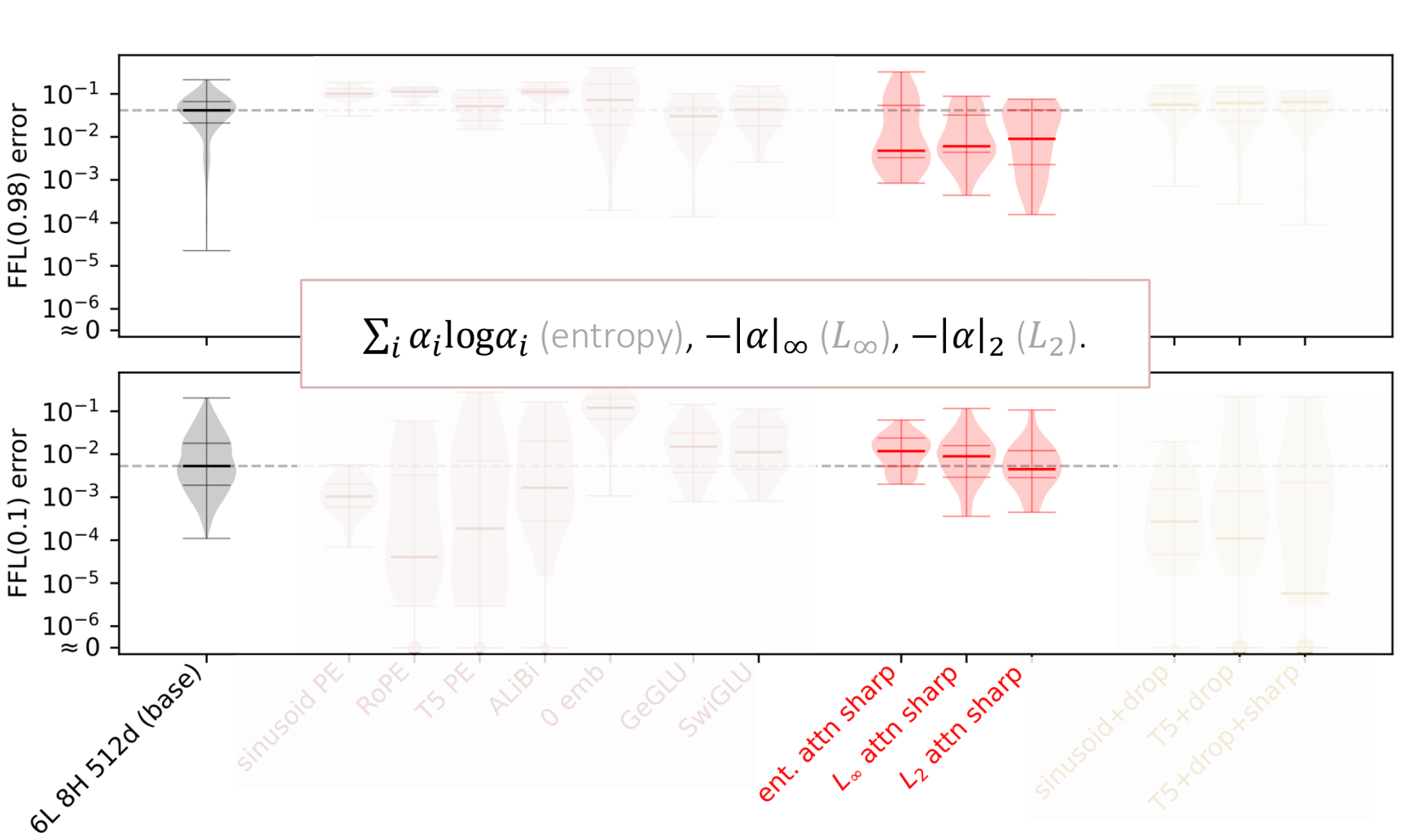
(R6) Standard regularizations have various influences.

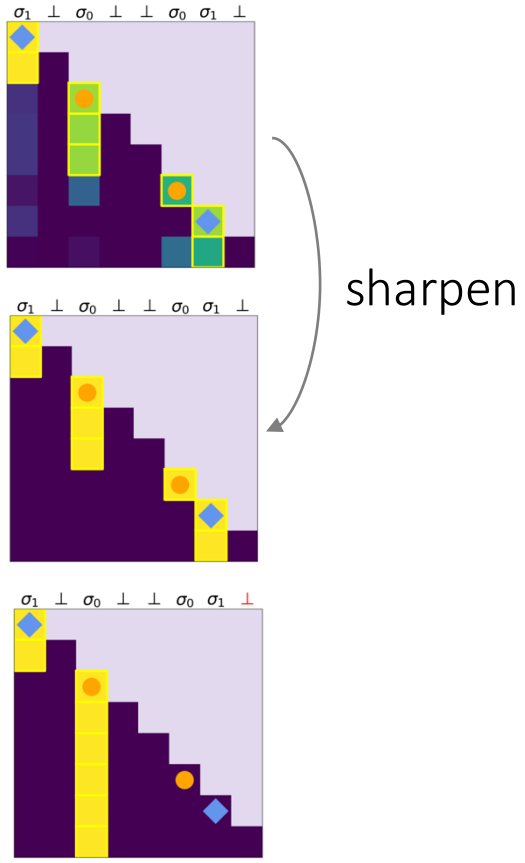


Mitigations – Regularization

Attention-sharpening regularization

(R6) Standard regularizations have various influences.

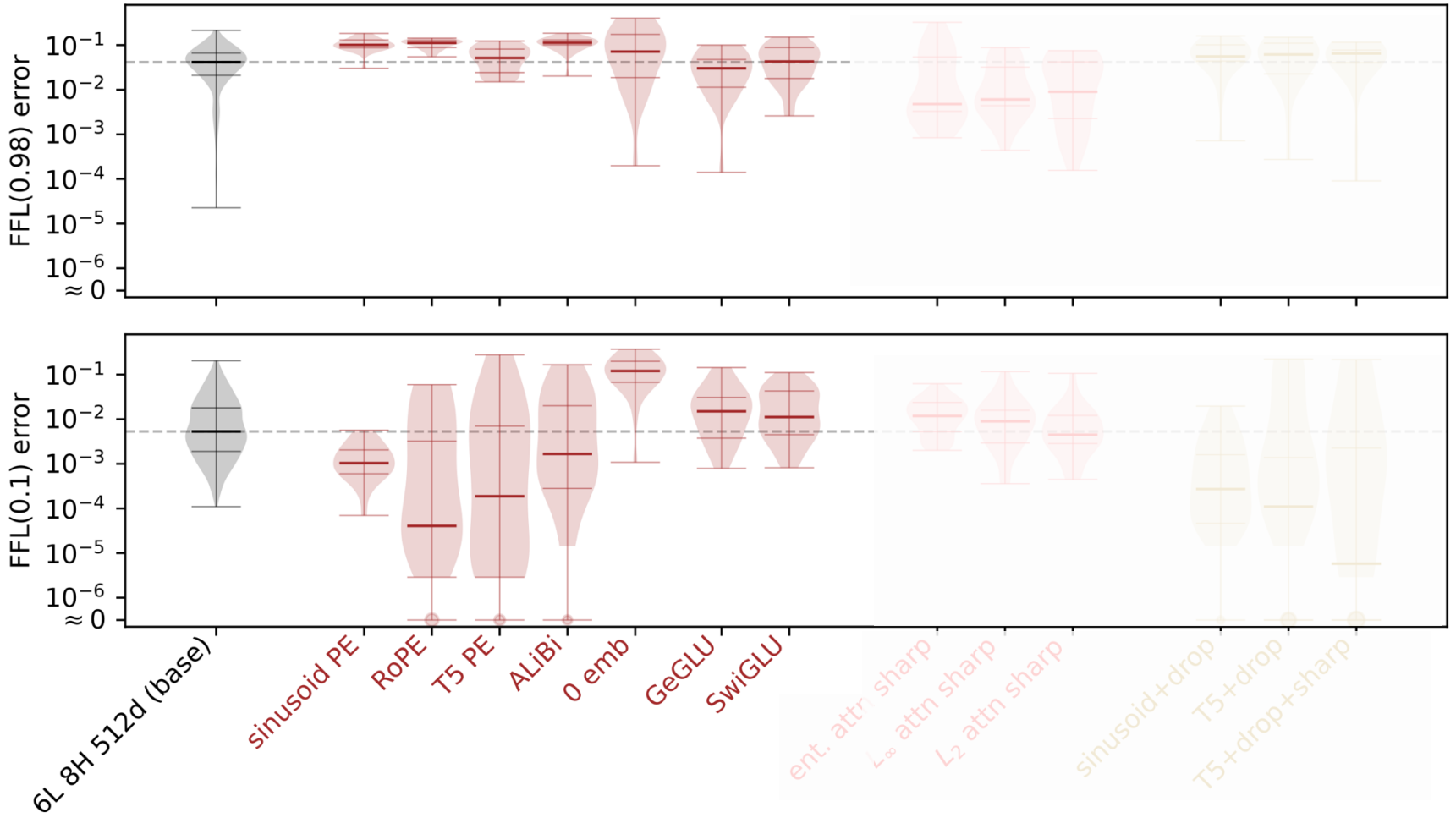




Mitigations – Architectural details

- Positional encoding
- Activation function

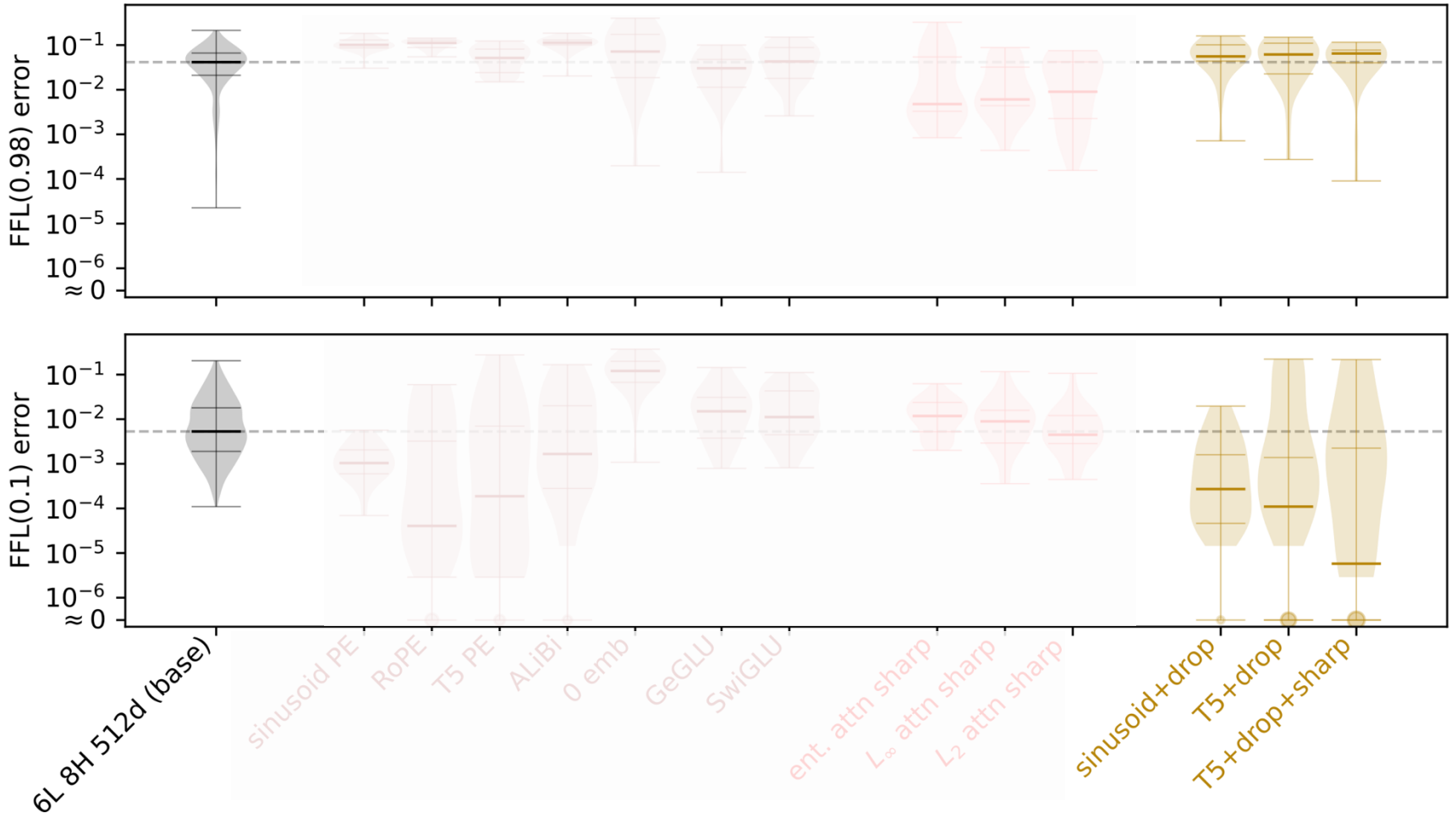
(R6) Standard regularizations have various influences.



Mitigations – Combination?

Combining multiple indirect controls

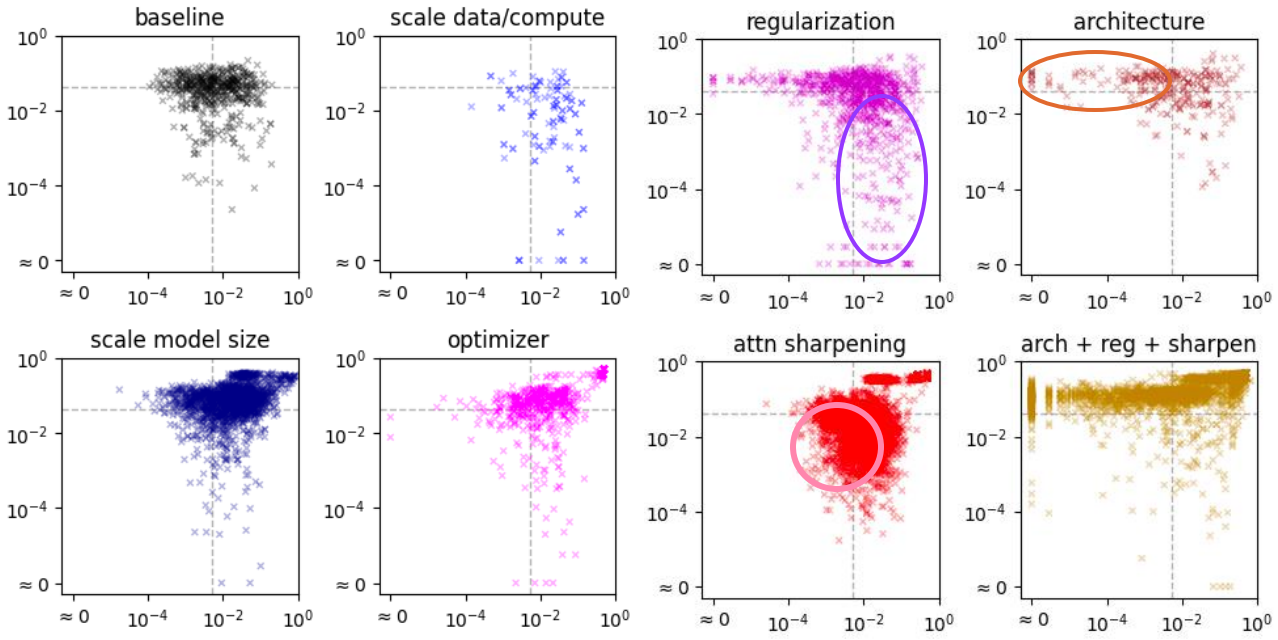
(R6) Standard regularizations have various influences.

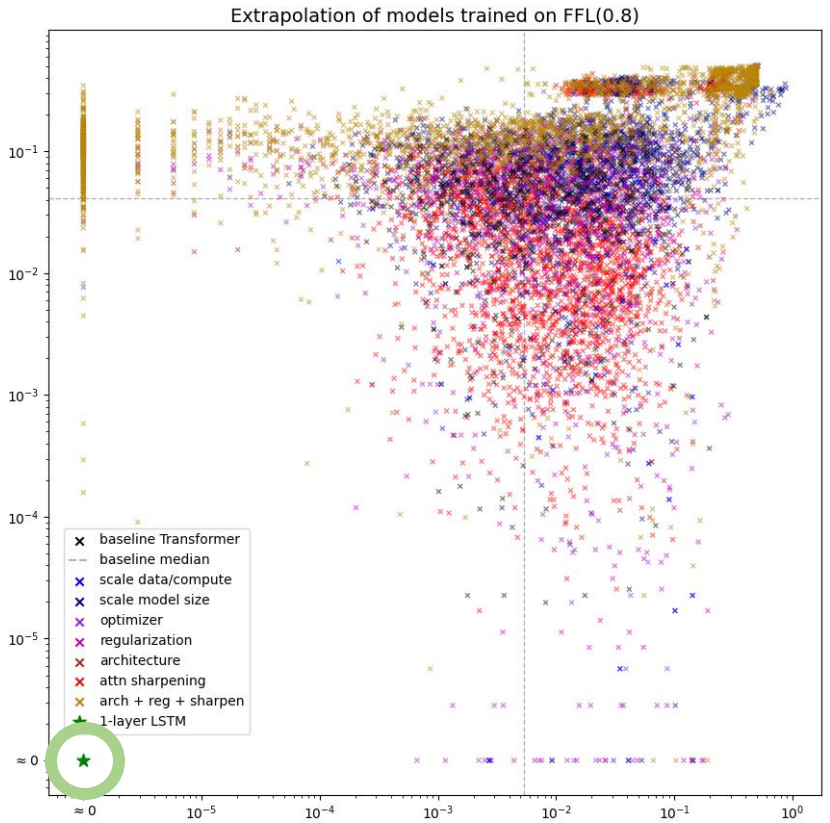


Trade-off: 2 types of OOD errors

Dense vs sparse: seldom improve both.

dense = x-axis, sparse = y-axis.





LSTM