Initialization Is Critical to Reasoning Ability of Transformer

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Inference example

Try to remember these equations and do test, e.g.,（2，1，24）=?

$$(1,2,21)=27,(1,2,30)=36,(1,2,47)=53,(2,1,15)=21,(2,1,24)=30,(2,1,41)=47$$

$$(3,4,10)=0,(3,4,19)=9,(3,4,34)=24,(3,4,41)=31,(4,3,18)=8,(4,3,27)=17$$

$$(1,3,14)=17,(1,3,18)=21,(1,3,27)=30,(1,3,35)=38,(3,1,9)=12,(3,1,13)=16$$

$$(2,4,16)=9,(2,4,17)=10,(2,4,30)=23,(2,4,38)=31,(4,2,13)=6,(4,2,14)=7$$

$$(1,4,32)=29,(1,4,26)=23,(1,4,13)=10,(1,4,6)=3,(4,1,32)=29,(4,1,26)=23$$

$$(2,3,22)=21,(2,3,17)=16,(2,3,28)=27,(2,3,12)=11,(3,2,22)=21,(3,2,17)=16$$

$$\vdots$$

Inference example

$$(1,2,x) = x+6$$
$$(2,1,x) = x+6$$
$$(1,3,x) = x+3$$
$$(3,1,x) = x+3$$
$$(1,4,x) = x-3$$
$$(4,1,x) = x-3$$
$$(3,2,x) = x-1$$
$$(2,2,x) = x-1$$
$$(4,2,x) = x-9$$
$$(2,4,x) = x-9$$
$$(3,4,x) = x+6$$
$$(4,3,x) = x+6$$
$$(1,1,x) = x+10$$
$$(2,2,x) = x+2$$
$$(3,3,x) = x-4$$
$$(4,4,x) = x-16$$

$$(1,2,21) = 27, \quad (2,1,29) = 35$$
$$(2,1,50) = 56, \quad (1,2,31) = 37$$
$$(1,3,16) = 19, \quad (3,1,16) = 19$$
$$(1,4,67) = 64, \quad (4,1,99) = 96$$
$$(3,2,60) = 59, \quad (2,3,50) = 49$$
$$(4,2,48) = 39, \quad (2,4,33) = 24$$
$$(3,4,77) = 83, \quad (4,3,90) = 96$$
$$(1,1,58) = 68, \quad (1,1,51) = 61$$
$$(2,2,46) = 48, \quad (2,2,35) = 37$$
$$(3,3,36) = 32, \quad (3,3,29) = 25$$
$$(4,4,88) = 54, \quad (4,4,46) = 30$$

$$\vdots$$

Inference example

$$
\begin{aligned}
(1,2,x) &= (2,1,x) = x+6 \\
(1,3,x) &= (3,1,x) = x+3 \\
(1,4,x) &= (4,1,x) = x-3 \\
(3,2,x) &= (2,2,x) = x-1 \\
(4,2,x) &= (2,4,x) = x-9 \\
(3,4,x) &= (4,3,x) = x+6 \\
(1,1,x) &= x+10 \\
(2,2,x) &= x+2 \\
(3,3,x) &= x-4 \\
(4,4,x) &= x-16
\end{aligned}
$$

$$
\begin{aligned}
(1,2,x) &= x+6 \\
(2,1,x) &= x+6 \\
(1,3,x) &= x+3 \\
(3,1,x) &= x+3 \\
(1,4,x) &= x-3 \\
(4,1,x) &= x-3 \\
(3,2,x) &= x-1 \\
(2,2,x) &= x-1 \\
(4,2,x) &= x-9 \\
(2,4,x) &= x-9 \\
(3,4,x) &= x+6 \\
(4,3,x) &= x+6 \\
(1,1,x) &= x+10 \\
(2,2,x) &= x+2 \\
(3,3,x) &= x-4 \\
(4,4,x) &= x-16
\end{aligned}
$$

$$
\begin{aligned}
(1,2,21) &= 27, & (2,1,29) &= 35 \\
(2,1,50) &= 56, & (1,2,31) &= 37 \\
(1,3,16) &= 19, & (3,1,16) &= 19 \\
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(3,3,36) &= 32, & (3,3,29) &= 25 \\
(4,4,88) &= 54, & (4,4,46) &= 30
\end{aligned}
$$

$$\vdots$$

Inference example

$$f_1(x) = x + 5$$
$$f_2(x) = x + 1$$
$$f_3(x) = x - 2$$
$$f_4(x) = x - 8$$

$$(1,2,x) = (2,1,x) = x + 6$$
$$(1,3,x) = (3,1,x) = x + 3$$
$$(1,4,x) = (4,1,x) = x - 3$$
$$(3,2,x) = (2,2,x) = x - 1$$
$$(4,2,x) = (2,4,x) = x - 9$$
$$(3,4,x) = (4,3,x) = x + 6$$
$$(1,1,x) = x + 10$$
$$(2,2,x) = x + 2$$
$$(3,3,x) = x - 4$$
$$(4,4,x) = x - 16$$

$$(1,2,x) = x + 6$$
$$(2,1,x) = x + 6$$
$$(1,3,x) = x + 3$$
$$(3,1,x) = x + 3$$
$$(1,4,x) = x - 3$$
$$(4,1,x) = x - 3$$
$$(3,2,x) = x - 1$$
$$(2,2,x) = x - 1$$
$$(4,2,x) = x - 9$$
$$(2,4,x) = x - 9$$
$$(3,4,x) = x + 6$$
$$(4,3,x) = x + 6$$
$$(1,1,x) = x + 10$$
$$(2,2,x) = x + 2$$
$$(3,3,x) = x - 4$$
$$(4,4,x) = x - 16$$

$$(1,2,21) = 27, \quad (2,1,29) = 35$$
$$(2,1,50) = 56, \quad (1,2,31) = 37$$
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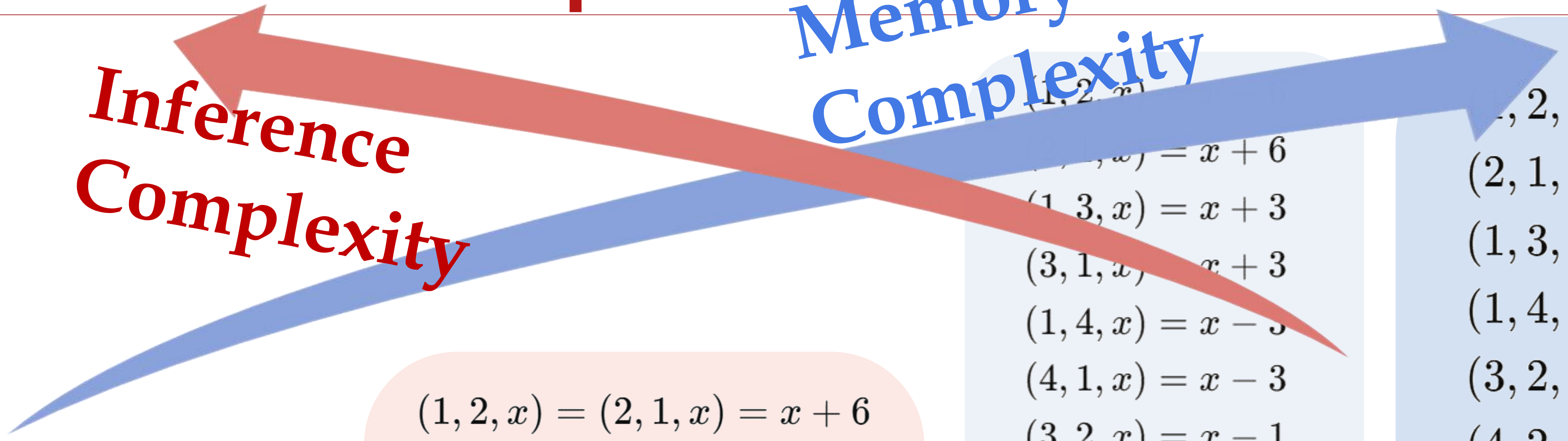
$$(4,4,88) = 54, \quad (4,4,46) = 30$$
$$\vdots$$

Inference example



$$f_1(x) = x + 5$$
$$f_2(x) = x + 1$$
$$f_3(x) = x - 2$$
$$f_4(x) = x - 8$$

$$(1,2,x) = (2,1,x) = x + 6$$
$$(1,3,x) = (3,1,x) = x + 3$$
$$(1,4,x) = (4,1,x) = x - 3$$
$$(3,2,x) = (2,2,x) = x - 1$$
$$(4,2,x) = (2,4,x) = x - 9$$
$$(3,4,x) = (4,3,x) = x + 6$$
$$(1,1,x) = x + 10$$
$$(2,2,x) = x + 2$$
$$(3,3,x) = x - 4$$
$$(4,4,x) = x - 16$$

$$(1,2,x)$$
$$(2,1,x) = x + 6$$
$$(1,3,x) = x + 3$$
$$(3,1,x) = x + 3$$
$$(1,4,x) = x - 3$$
$$(4,1,x) = x - 3$$
$$(3,2,x) = x - 1$$
$$(2,2,x) = x - 1$$
$$(4,2,x) = x - 9$$
$$(2,4,x) = x - 9$$
$$(3,4,x) = x + 6$$
$$(4,3,x) = x + 6$$
$$(1,1,x) = x + 10$$
$$(2,2,x) = x + 2$$
$$(3,3,x) = x - 4$$
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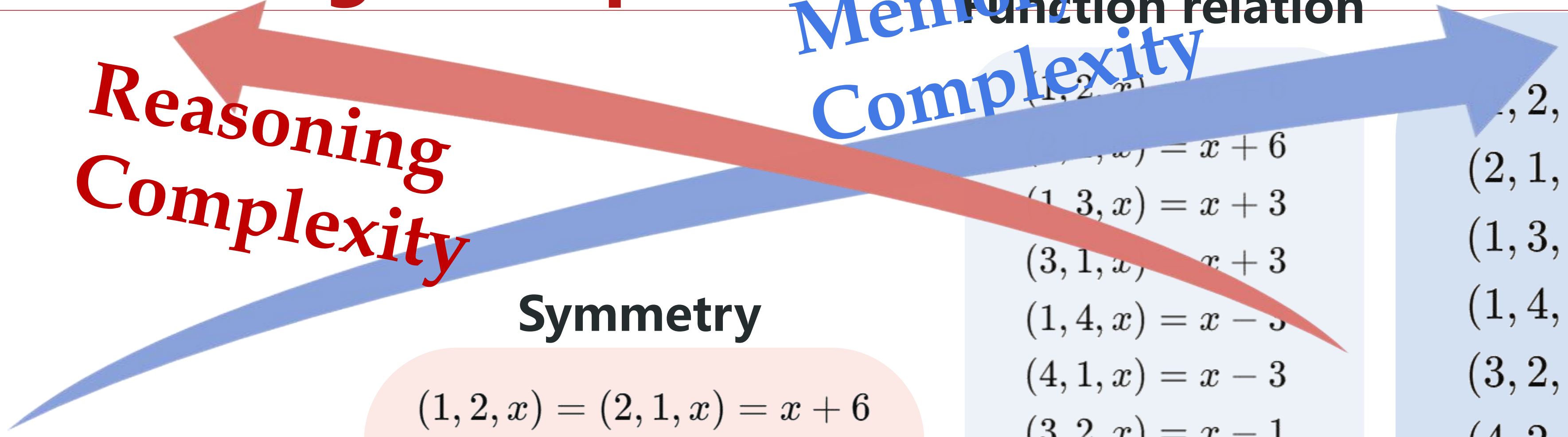
$$(4,4,88) = 54, \quad (4,4,46) = 30$$
$$\vdots$$

Reasoning example

How will LLM do?



Composition

$f_1(x) = x + 5$

$f_2(x) = x + 1$

$f_3(x) = x - 2$

$f_4(x) = x - 8$

Symmetry

$(1, 2, x) = (2, 1, x) = x + 6$

$(1, 3, x) = (3, 1, x) = x + 3$

$(1, 4, x) = (4, 1, x) = x - 3$

$(3, 2, x) = (2, 2, x) = x - 1$

$(4, 2, x) = (2, 4, x) = x - 9$

$(3, 4, x) = (4, 3, x) = x + 6$

$(1, 1, x) = x + 10$

$(2, 2, x) = x + 2$

$(3, 3, x) = x - 4$

$(4, 4, x) = x - 16$

Function relation

$(1, 2, x)$

$) = x + 6$

$(1, 3, x) = x + 3$

$(3, 1, x) = x + 3$

$(1, 4, x) = x - 3$

$(4, 1, x) = x - 3$

$(3, 2, x) = x - 1$

$(2, 2, x) = x - 1$

$(4, 2, x) = x - 9$

$(2, 4, x) = x - 9$

$(3, 4, x) = x + 6$

$(4, 3, x) = x + 6$

$(1, 1, x) = x + 10$

$(2, 2, x) = x + 2$

$(3, 3, x) = x - 4$

$(4, 4, x) = x - 16$

Memorizing

$, 2, 21) = 27, \quad (2, 1, 29) = 35$

$(2, 1, 50) = 56, \quad (1, 2, 31) = 37$

$(1, 3, 16) = 19, \quad (3, 1, 16) = 19$

$(1, 4, 67) = 64, \quad (4, 1, 99) = 96$

$(3, 2, 60) = 59, \quad (2, 3, 50) = 49$

$(4, 2, 48) = 39, \quad (2, 4, 33) = 24$

$(3, 4, 77) = 83, \quad (4, 3, 90) = 96$

$(1, 1, 58) = 68, \quad (1, 1, 51) = 61$

$(2, 2, 46) = 48, \quad (2, 2, 35) = 37$

$(3, 3, 36) = 32, \quad (3, 3, 29) = 25$

$(4, 4, 88) = 54, \quad (4, 4, 46) = 30$

$\vdots$

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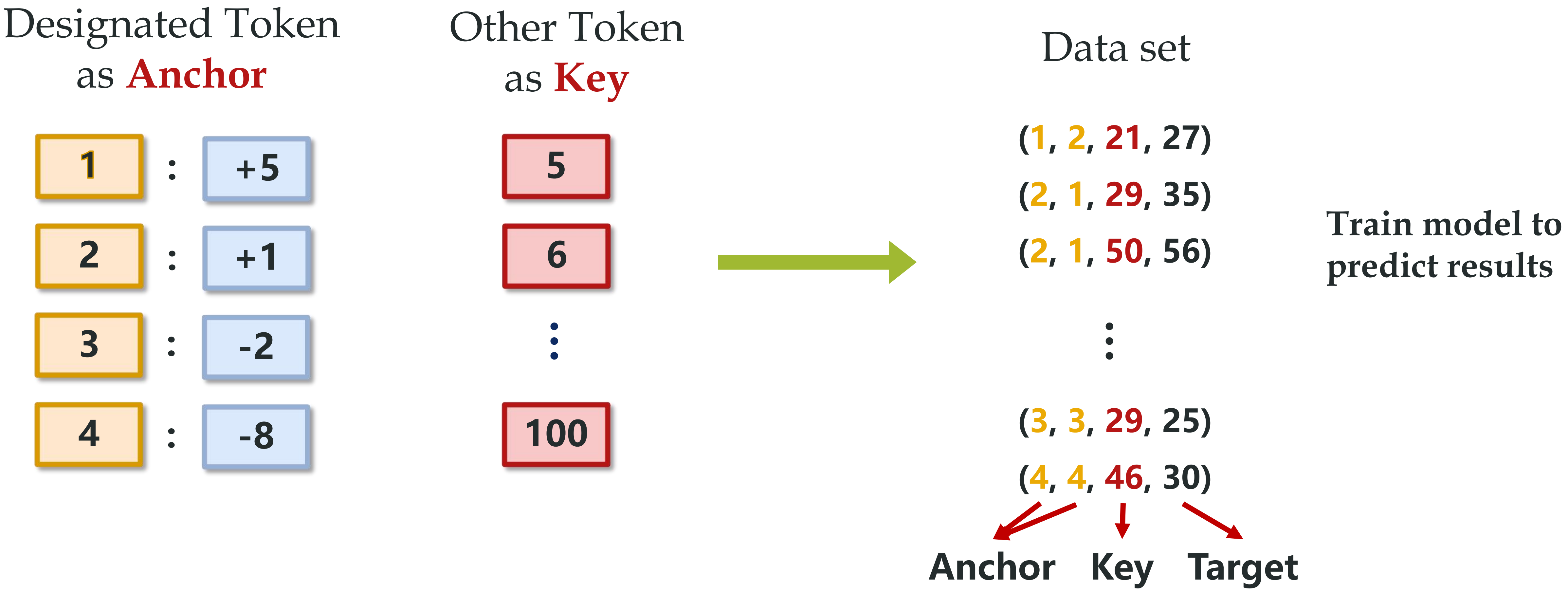
Anchor function



Designated Token as **Anchor**

1 : +5

2 : +1

3 : -2

4 : -8

Other Token as **Key**

5

6

⋮

100

Data set

(1, 2, 21, 27)

(2, 1, 29, 35)

(2, 1, 50, 56)

⋮

(3, 3, 29, 25)

(4, 4, 46, 30)

Anchor Key Target

Train model to predict results

NN to learn Anchor function

Data set

(1, 2, 21, 27)

(2, 1, 29, 35)

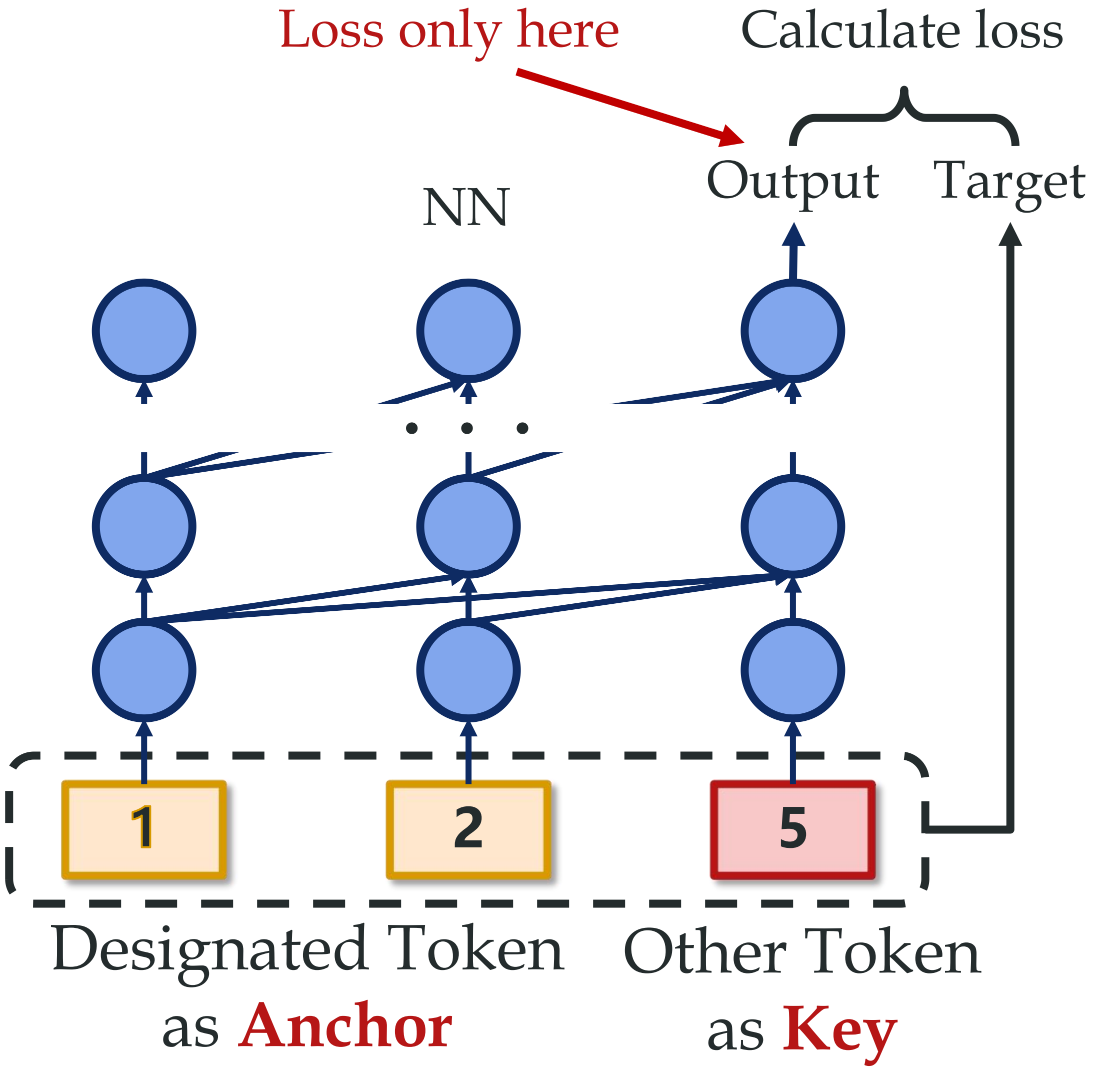
(2, 1, 50, 56)

⋮

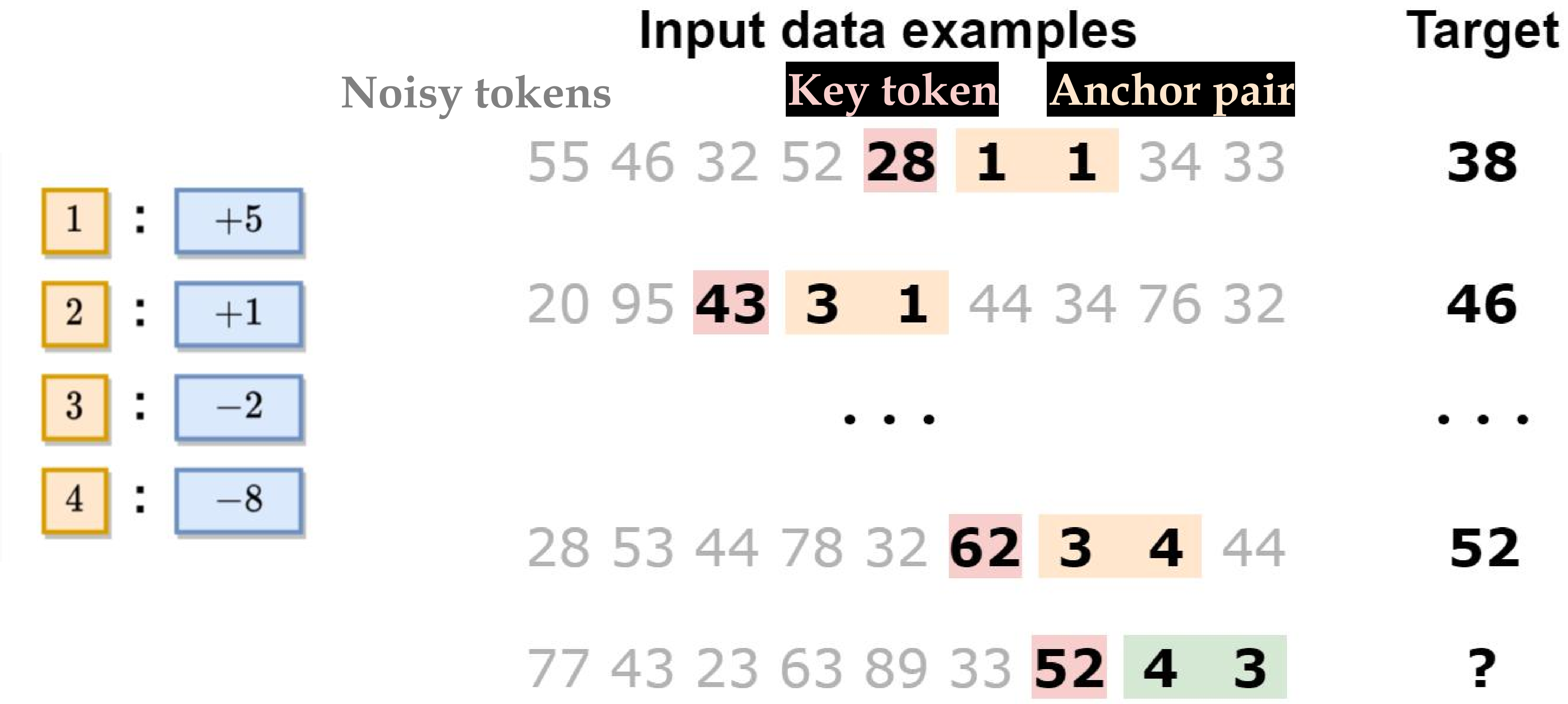
(3, 3, 29, 25)

(4, 4, 46, 30)

Anchor Key Target



Composite Anchor function



1	:	+5
2	:	+1
3	:	−2
4	:	−8

Input data examples	Target
Noisy tokens / Key token / Anchor pair	
55 46 32 52 **28** **1 1** 34 33	**38**
20 95 **43** **3 1** 44 34 76 32	**46**
. . .	. . .
28 53 44 78 32 **62** **3 4** 44	**52**
77 43 23 63 89 33 **52** **4 3**	**?**

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Can it learn [4,3]?

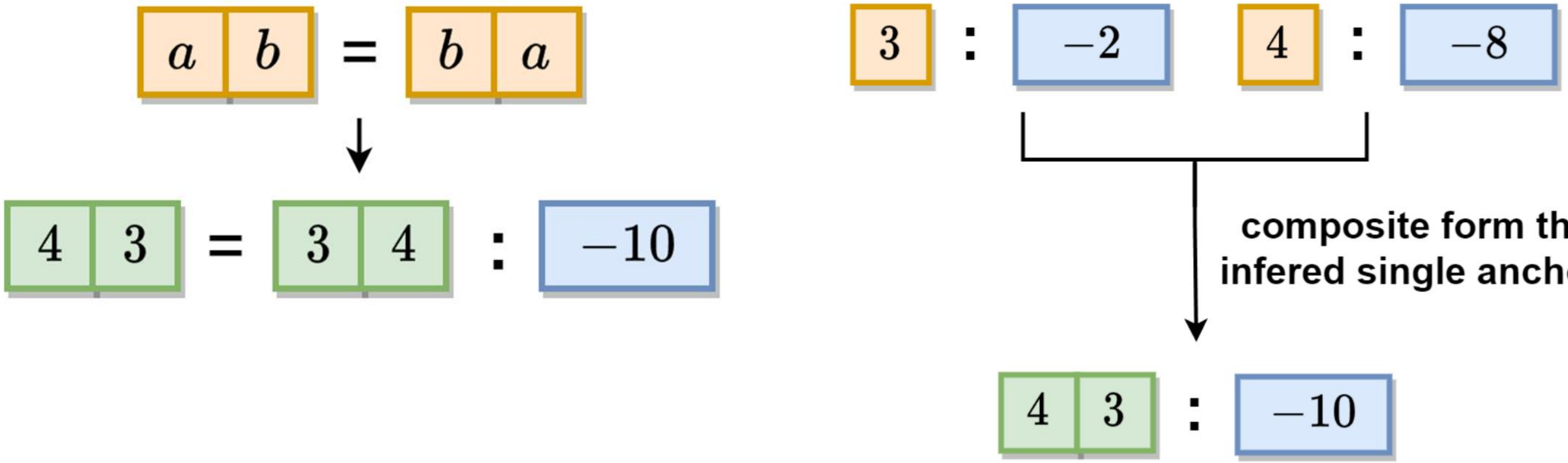
Yes, it can learn [4,3]!

Turn your eyes to preferred answer

Symmetric or Inferential?

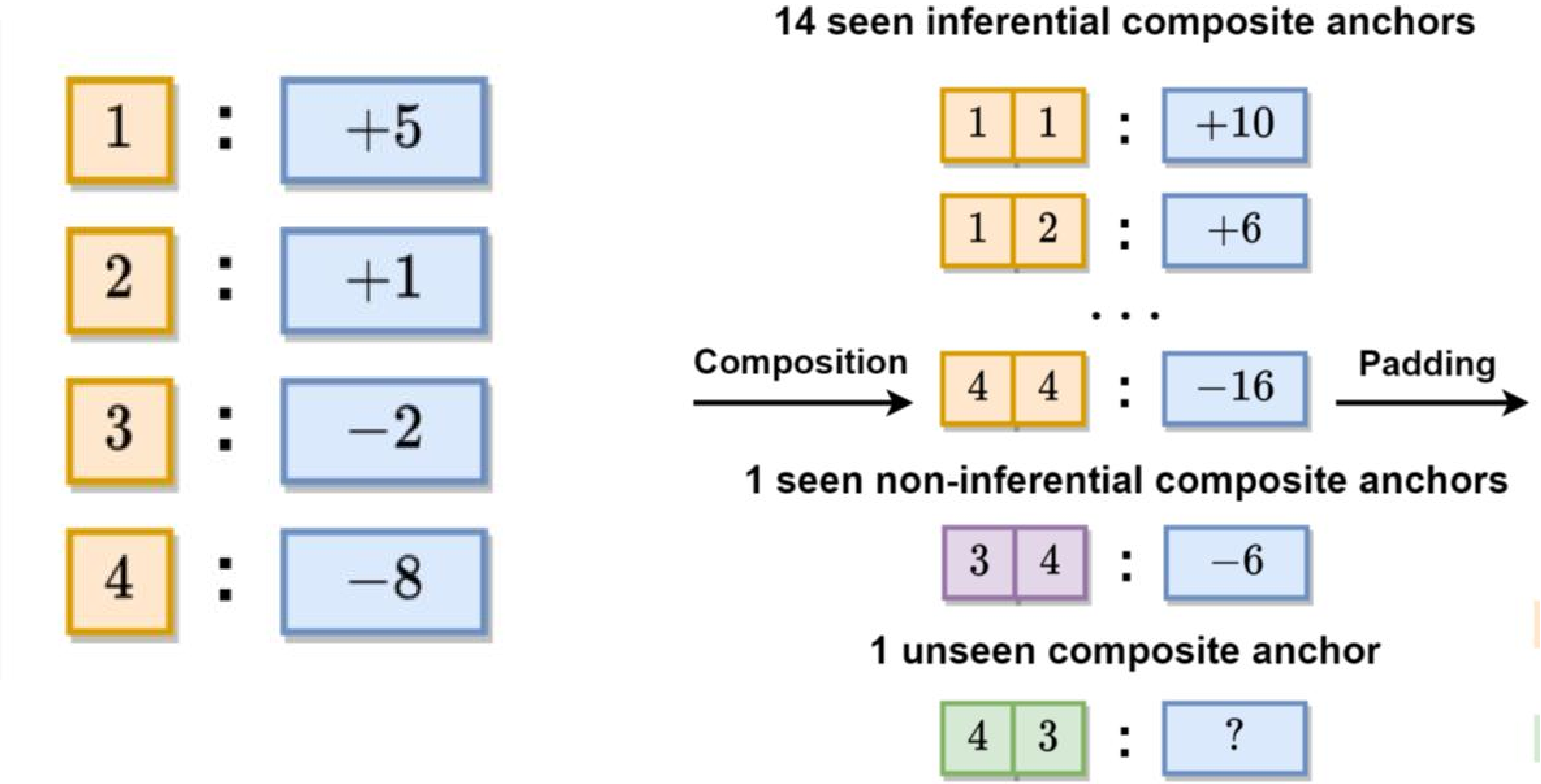
Mechanism 1: learn symmetric structure

Mechanism 2: infer single anchor mappings



composite form the infered single anchors

Composite Anchor function



14 seen inferential composite anchors

Composition

Padding

1 seen non-inferential composite anchors

1 unseen composite anchor

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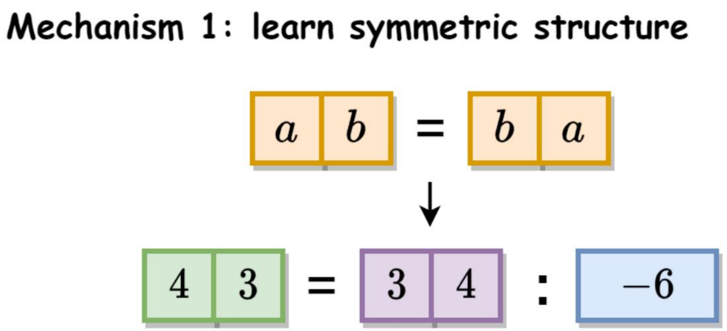
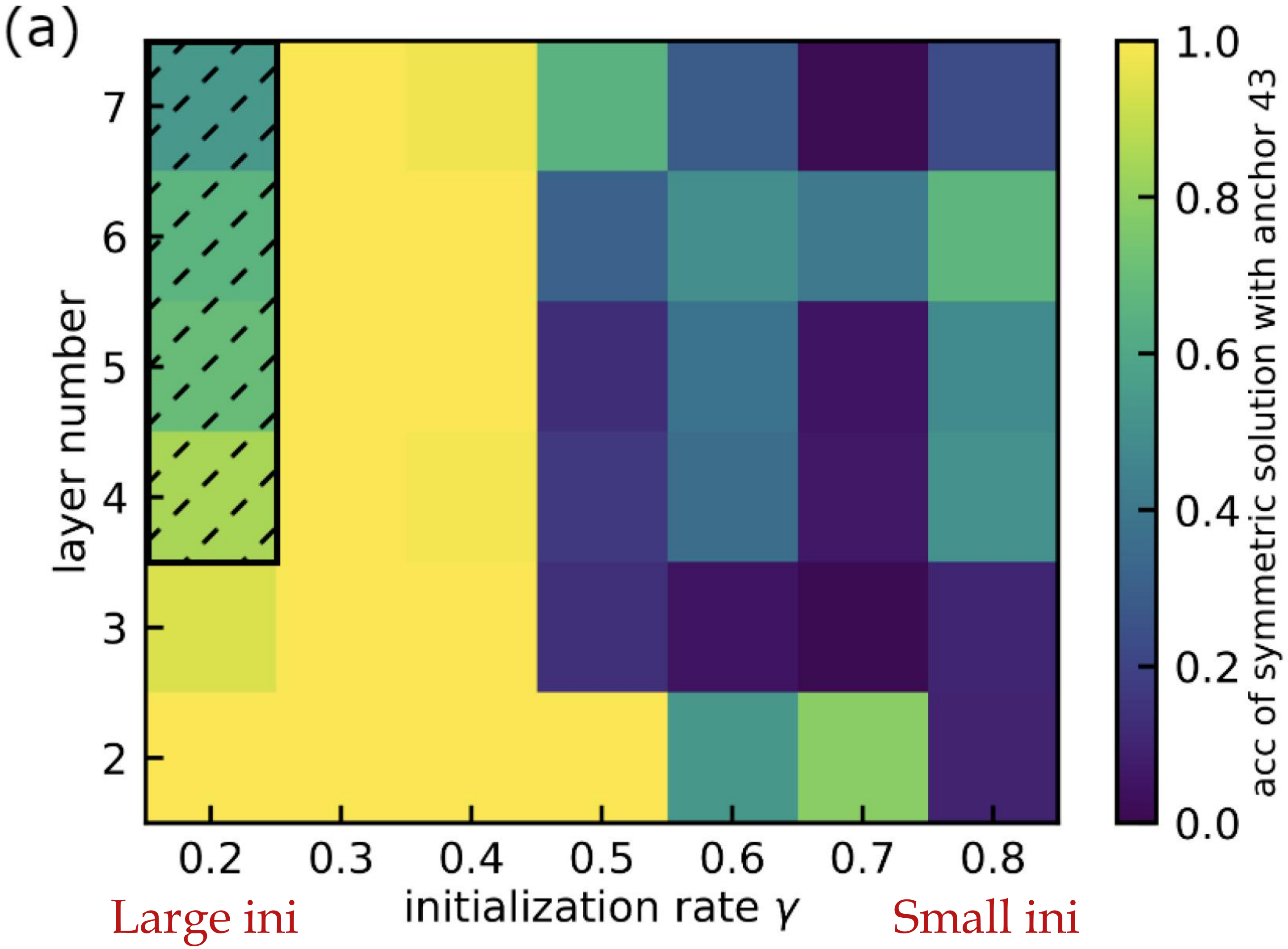
Phase diagram of symmetric solution



Initialization~$N\left(0,\frac{1}{d_{in}^{\gamma}}\right)$



▨ bad generalization on seen anchors (test accuracy < 90%)

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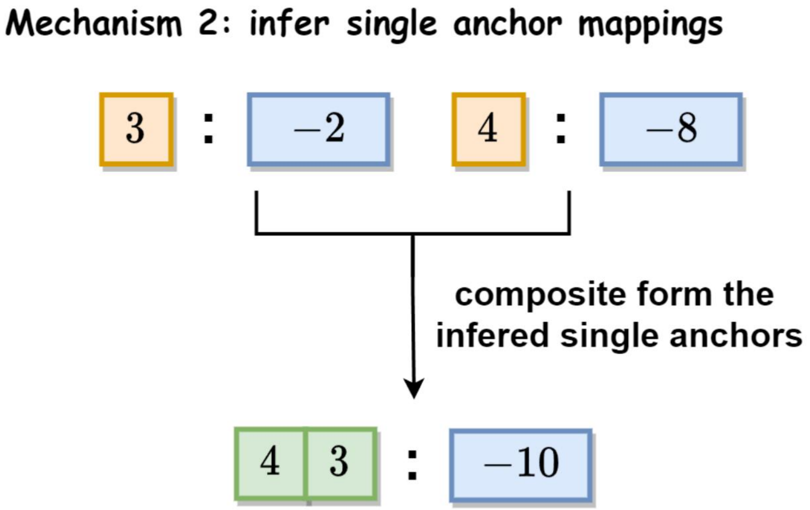
Phase diagram of inferential solution



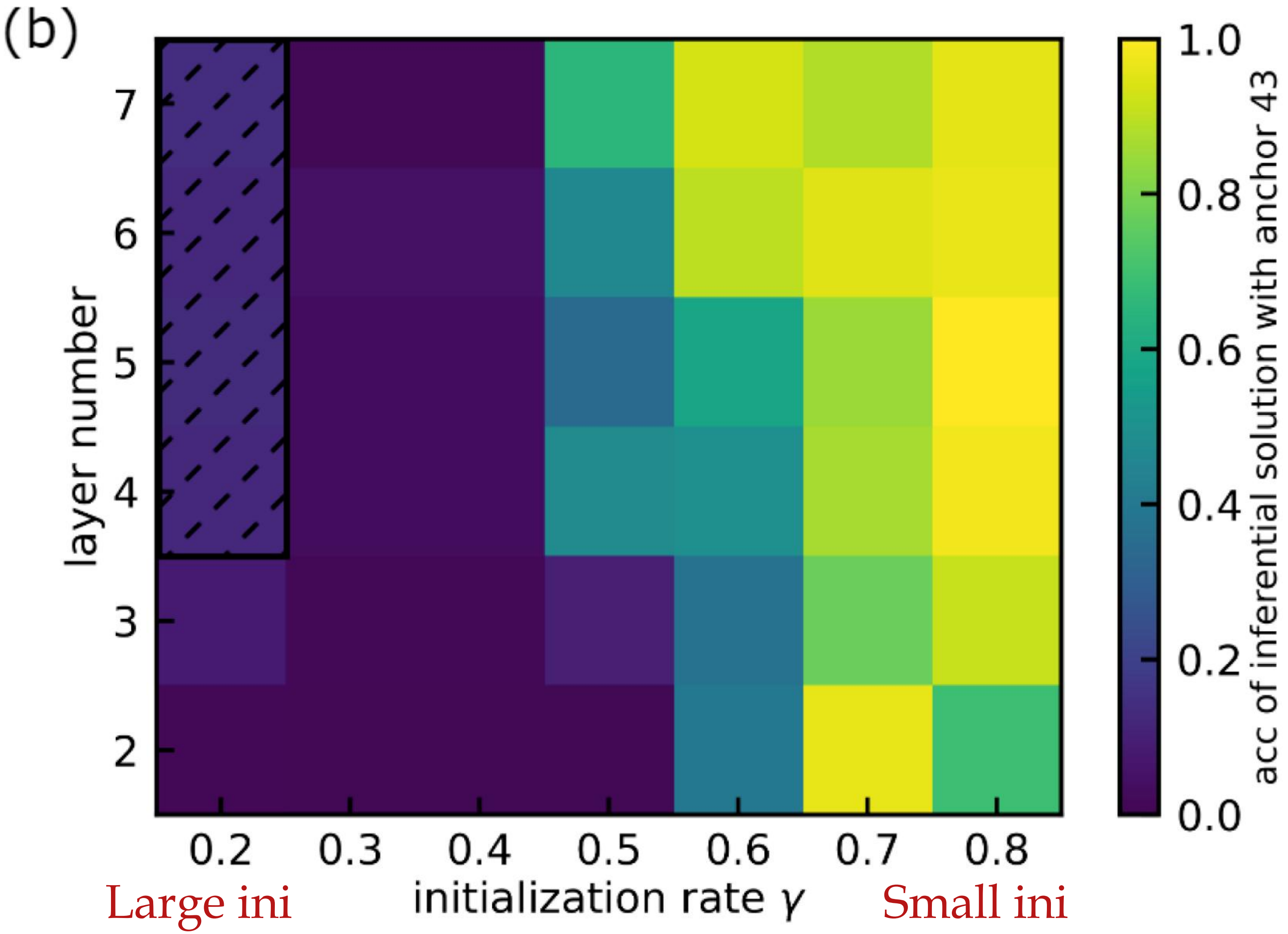
Mechanism 2: infer single anchor mappings

3 : -2 4 : -8

composite form the infered single anchors

4 3 : -10

$$\text{Initialization} \sim N\left(0, \frac{1}{d_{in}^{\gamma}}\right)$$



▨ bad generalization on seen anchors (test accuracy < 90%)

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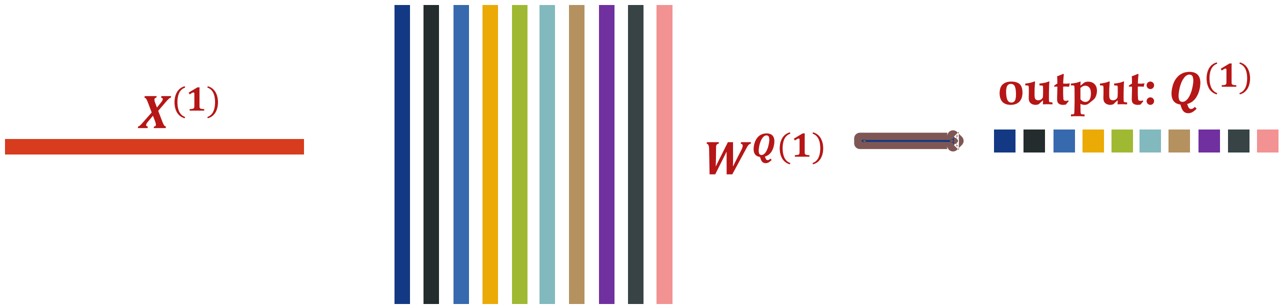
Condensation of $W^{Q(1)}$ by column

$$Q^{(l)} = X^{(l)} W^{Q(l)}$$



$X^{(1)}$

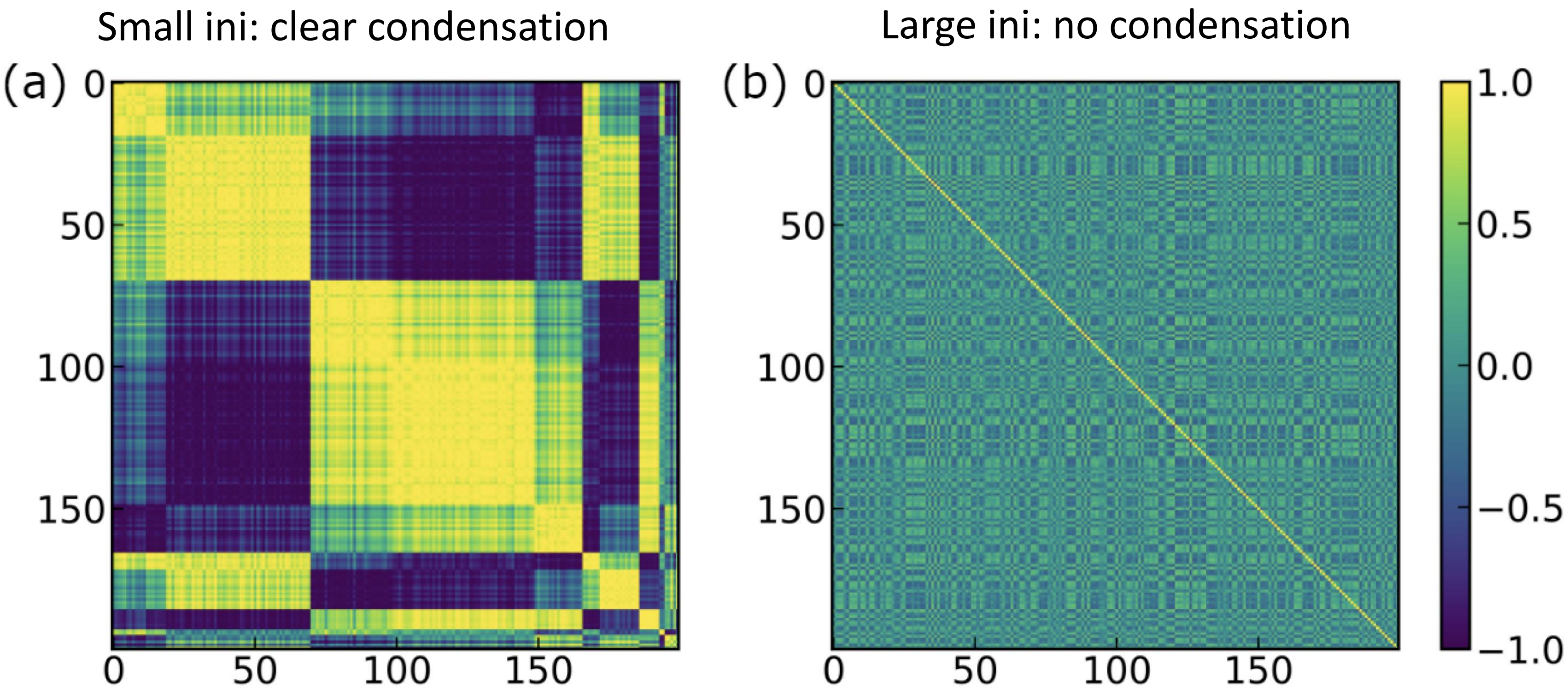
$W^{Q(1)}$

output: $Q^{(1)}$

Cosine Similarity b/w

Columns of $W^{Q(1)}$

Input weight of Q neurons



Small ini: clear condensation

Large ini: no condensation

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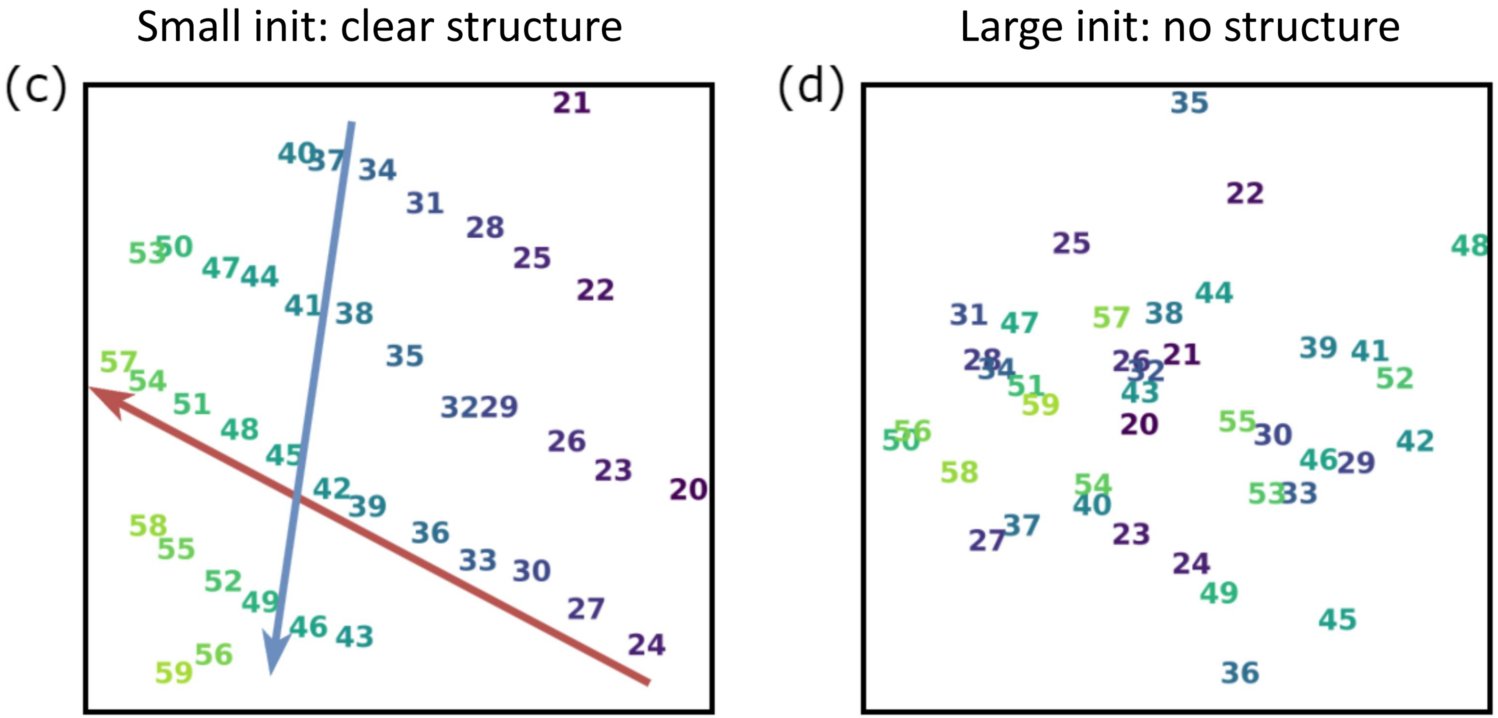
Structural Features of the Word Embedding

T-SNE

$$f_a(x) = \begin{cases} x+5, \; if \; a \; = 1 \\ x+1, \; if \; a \; = 2 \\ x-2, \; if \; a \; = 3 \\ x-8, \; if \; a \; = 4 \end{cases}$$


Small init: clear structure

Large init: no structure

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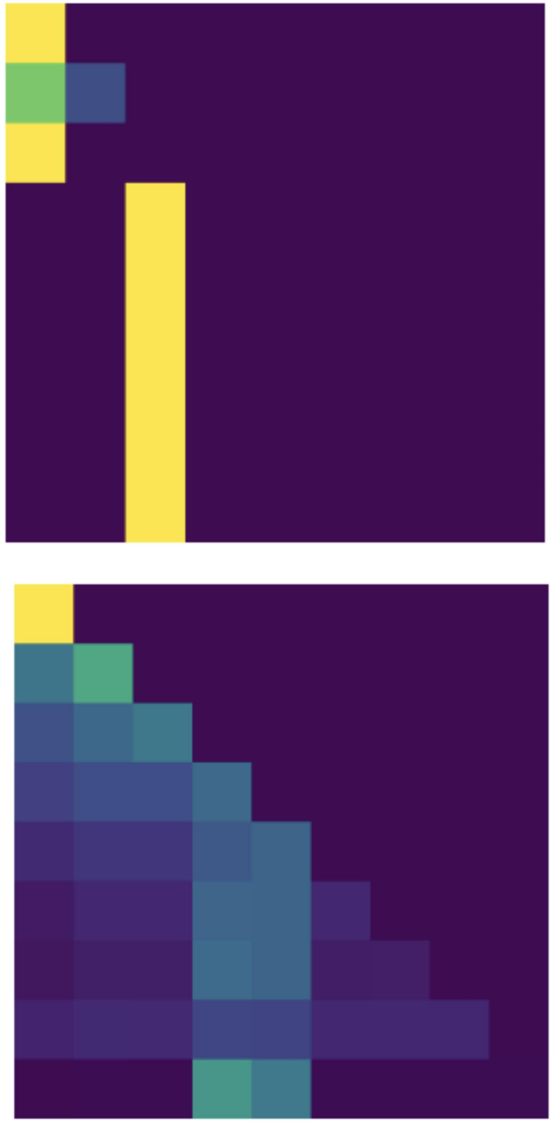
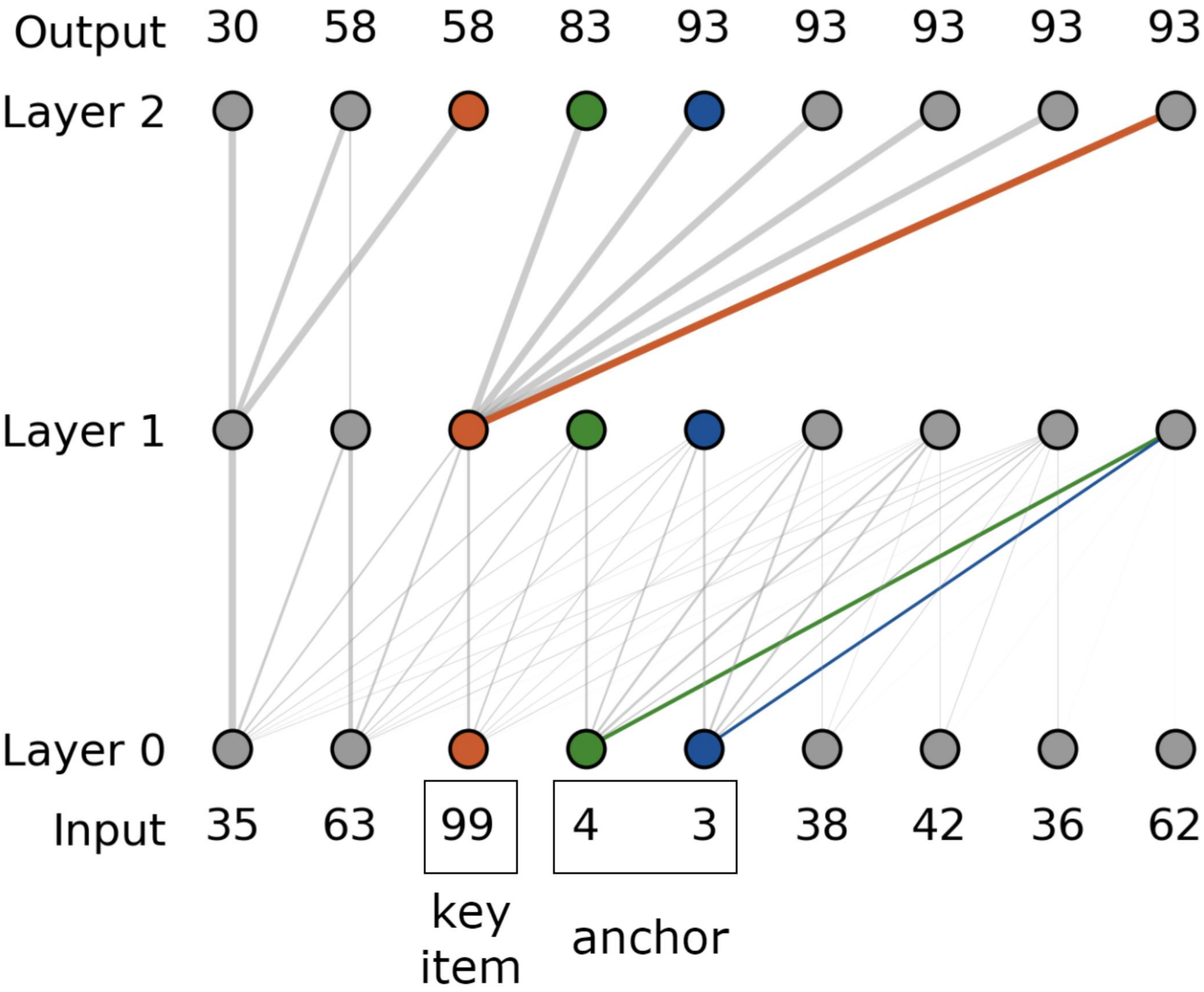
Symmetric solution




Output 30 58 58 83 93 93 93 93 93
Layer 2
Layer 1
Layer 0
Input 35 63 99 4 3 38 42 36 62
key item
anchor

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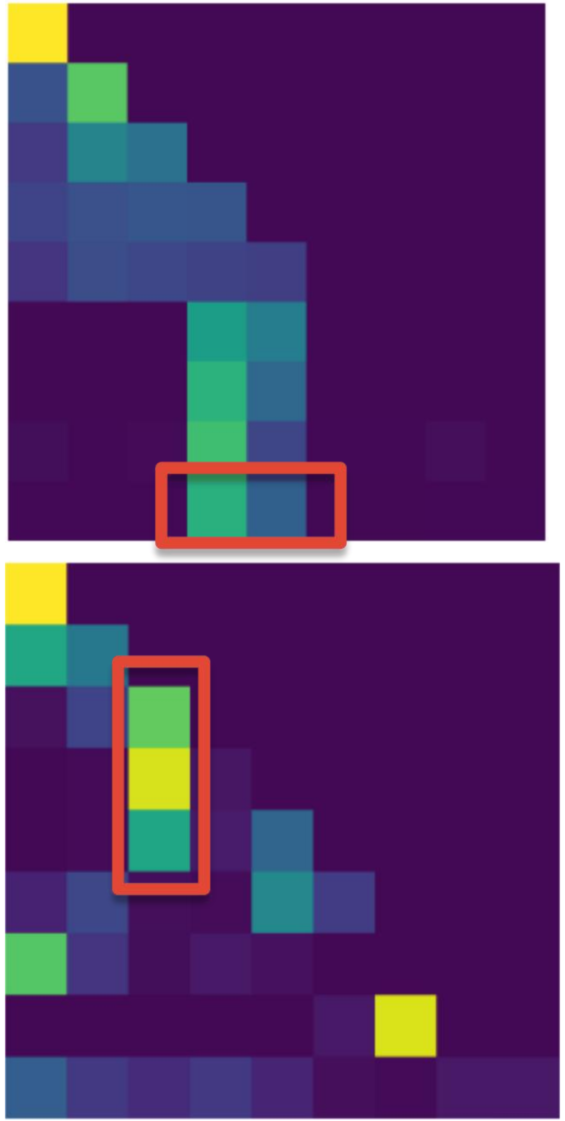
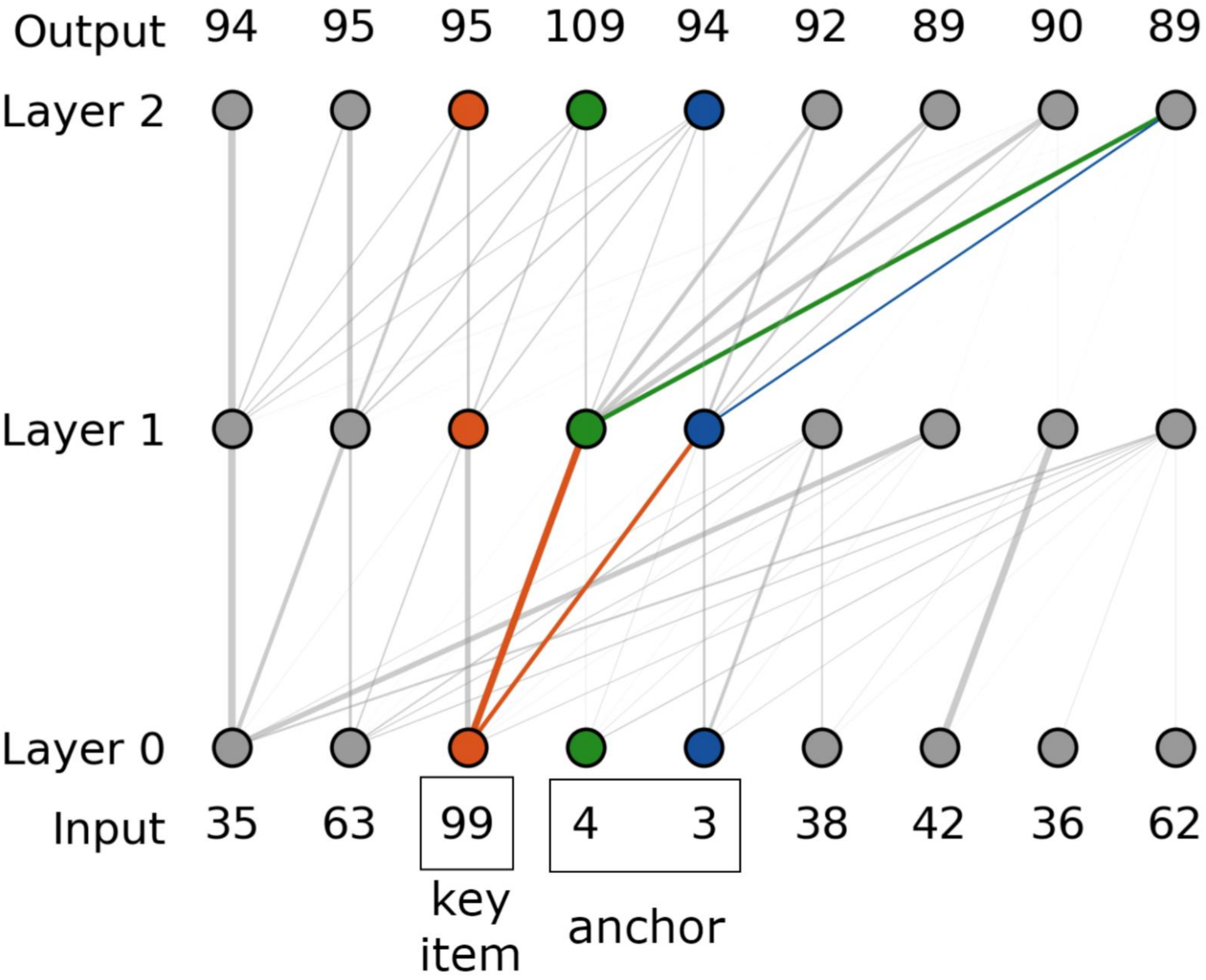
Inferential solution





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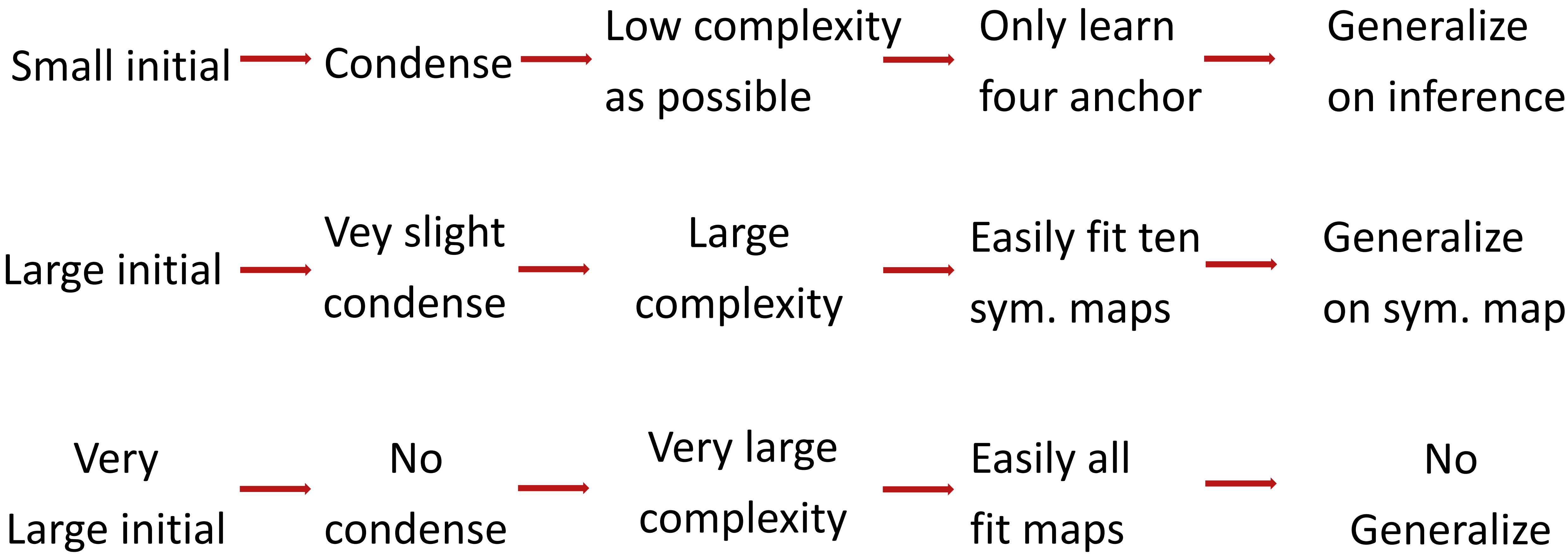
Mechanisms underlying initialization effect



Small initial → Condense → Low complexity as possible → Only learn four anchor → Generalize on inference

Large initial → Vey slight condense → Large complexity → Easily fit ten sym. maps → Generalize on sym. map

Very Large initial → No condense → Very large complexity → Easily all fit maps → No Generalize

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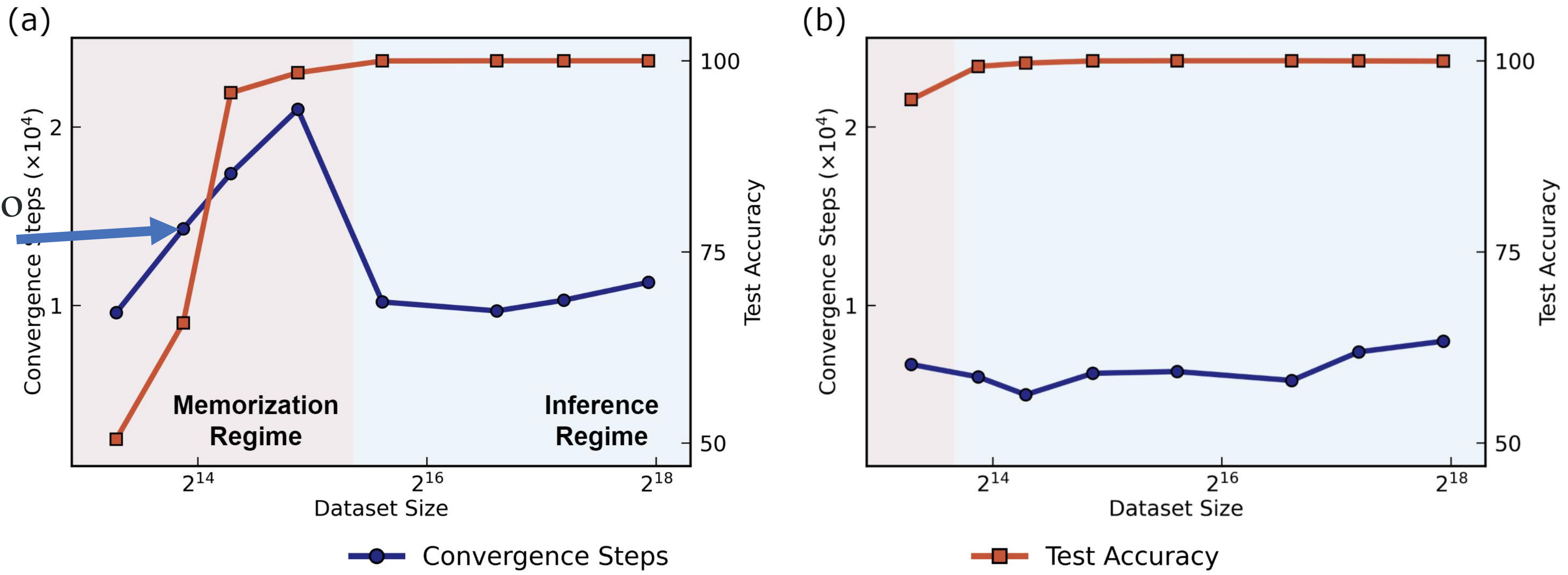
Other realistic reasoning dataset

Large initial → Large complexity → Memorization to inference

Small initial → Low complexity as possible → Inference



More data, more steps to memorize

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