

Large Language Models & Symbolic Structures

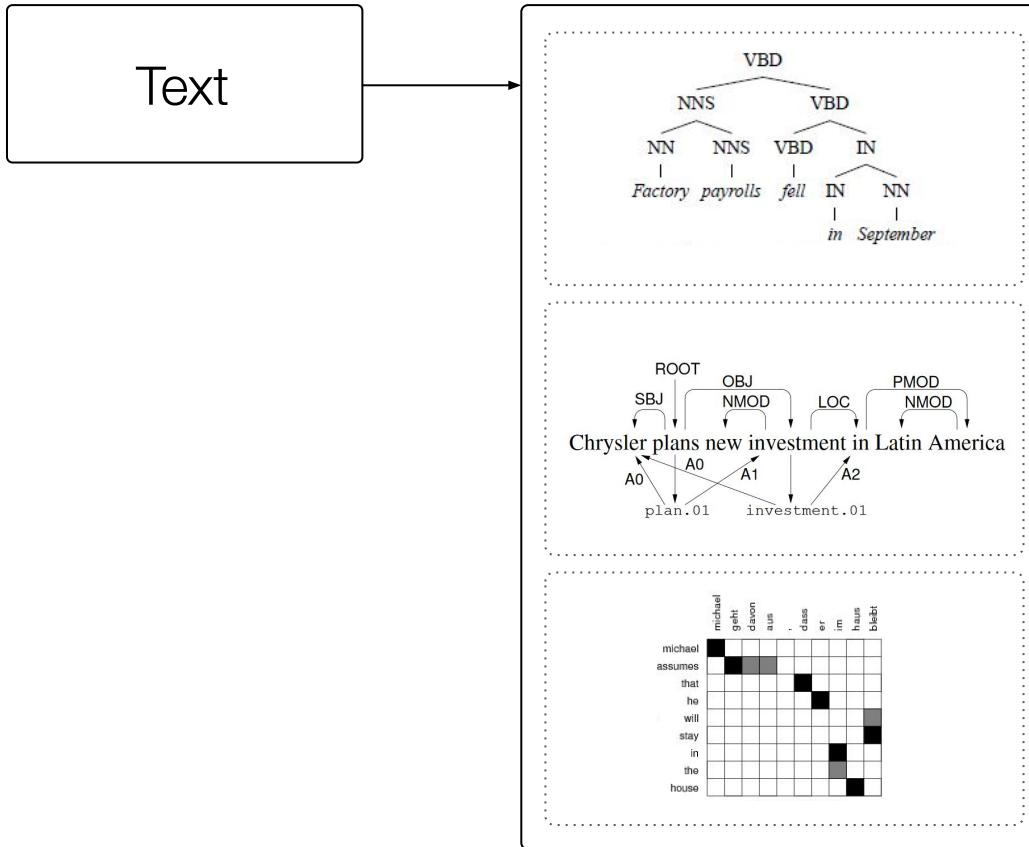
Yoon Kim
MIT

Classic Statistical NLP [1980-2013]

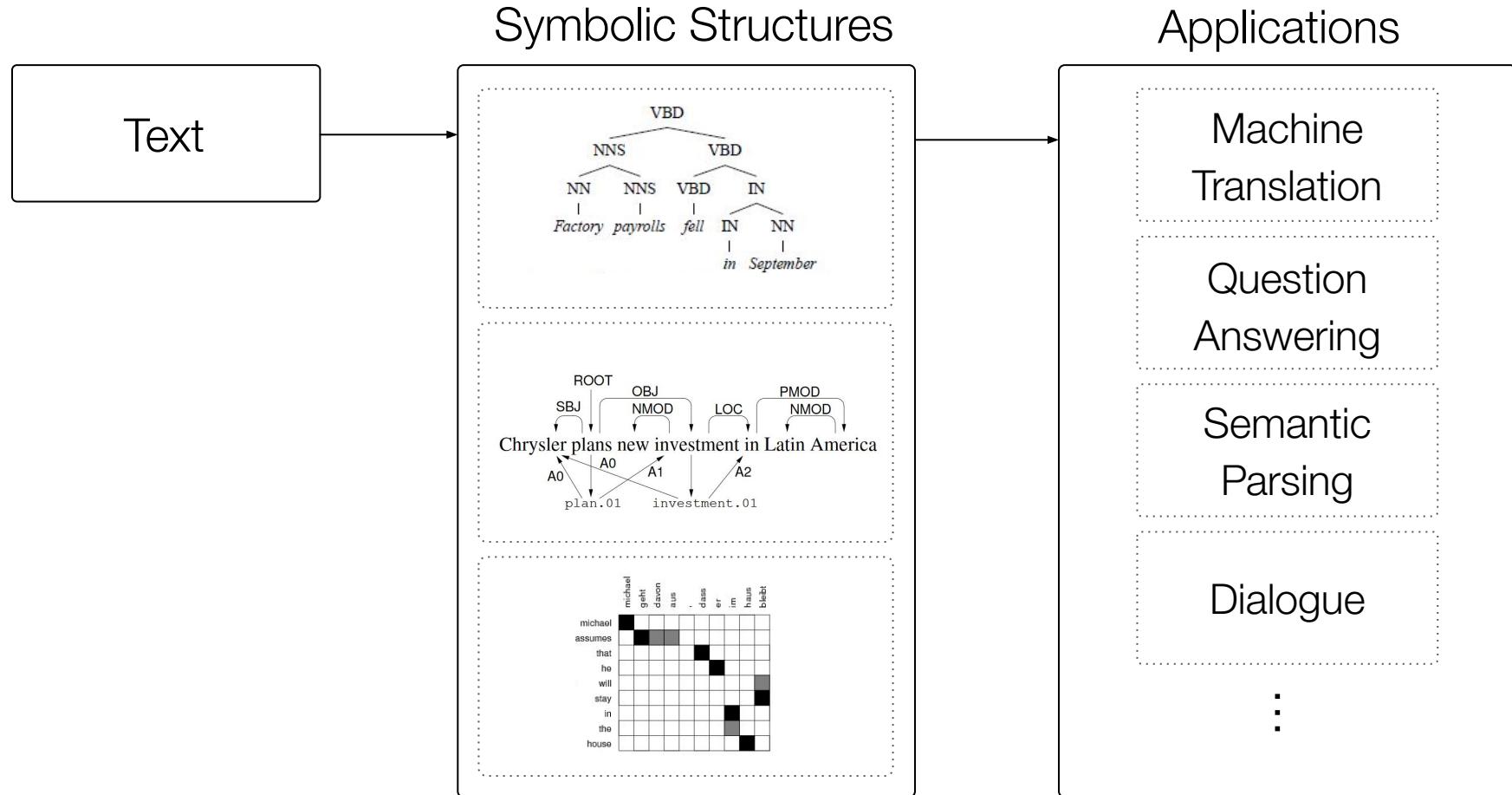
Text

Classic Statistical NLP [1980-2013]

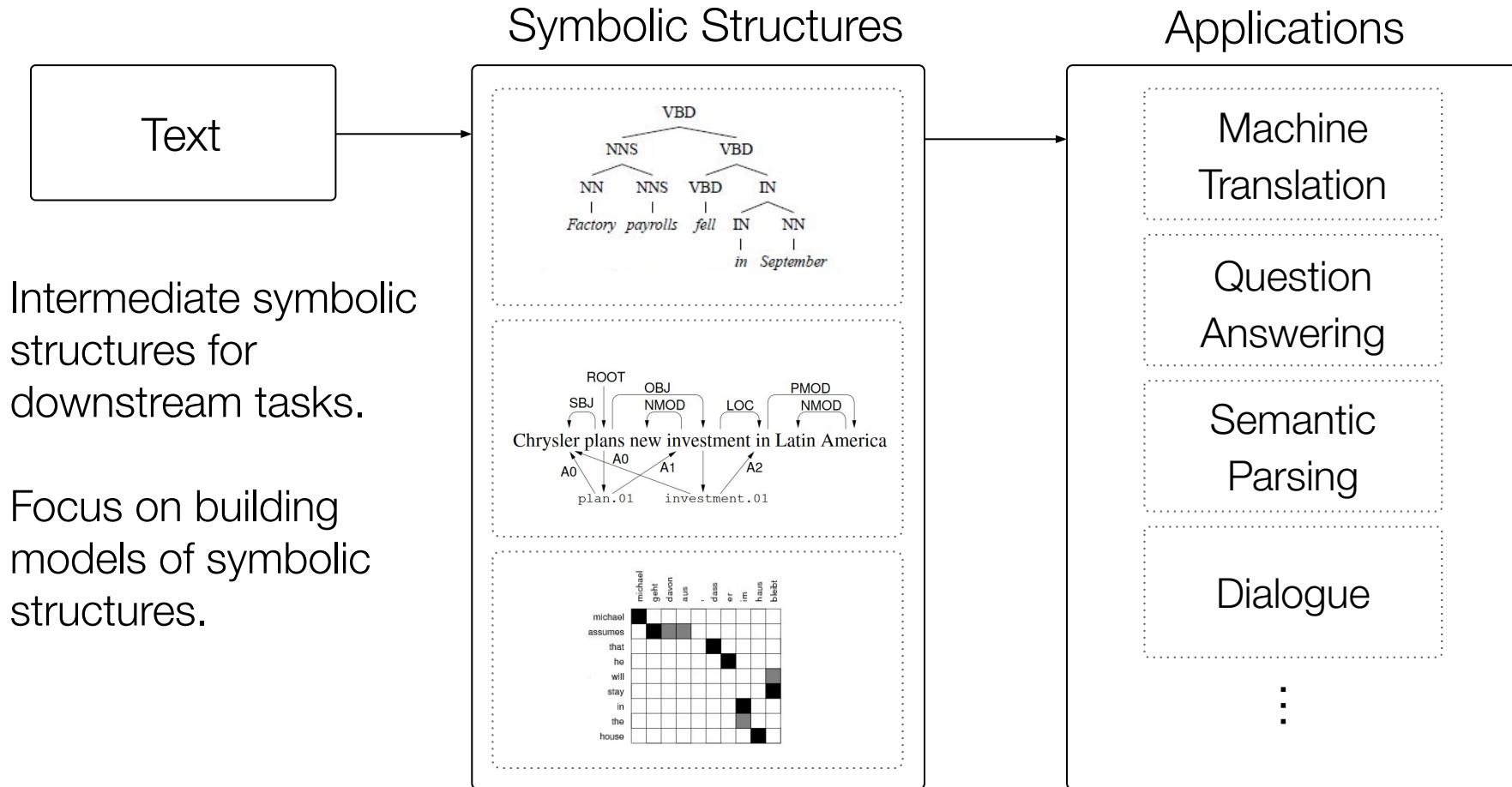
Symbolic Structures



Classic Statistical NLP [1980-2013]



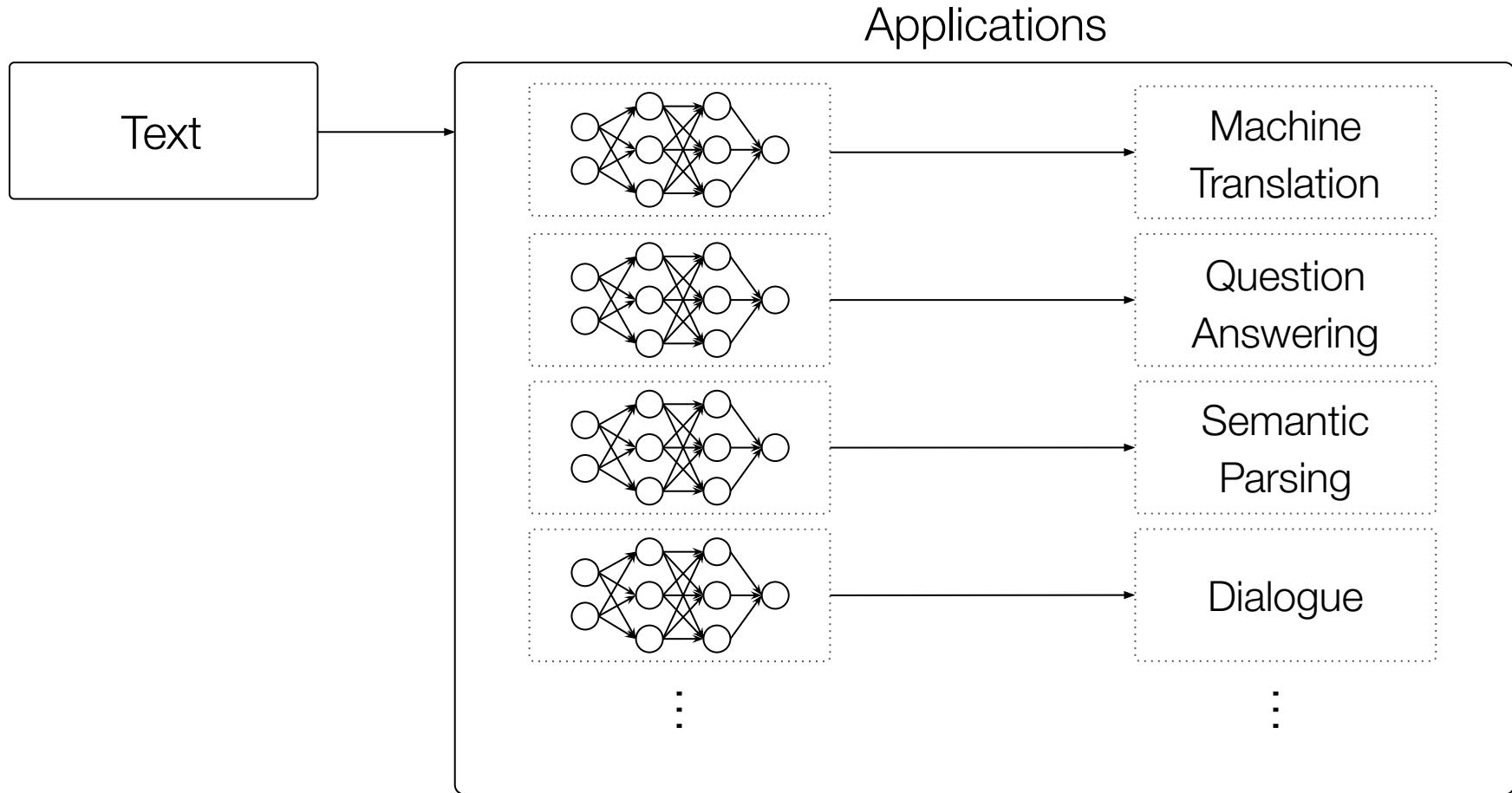
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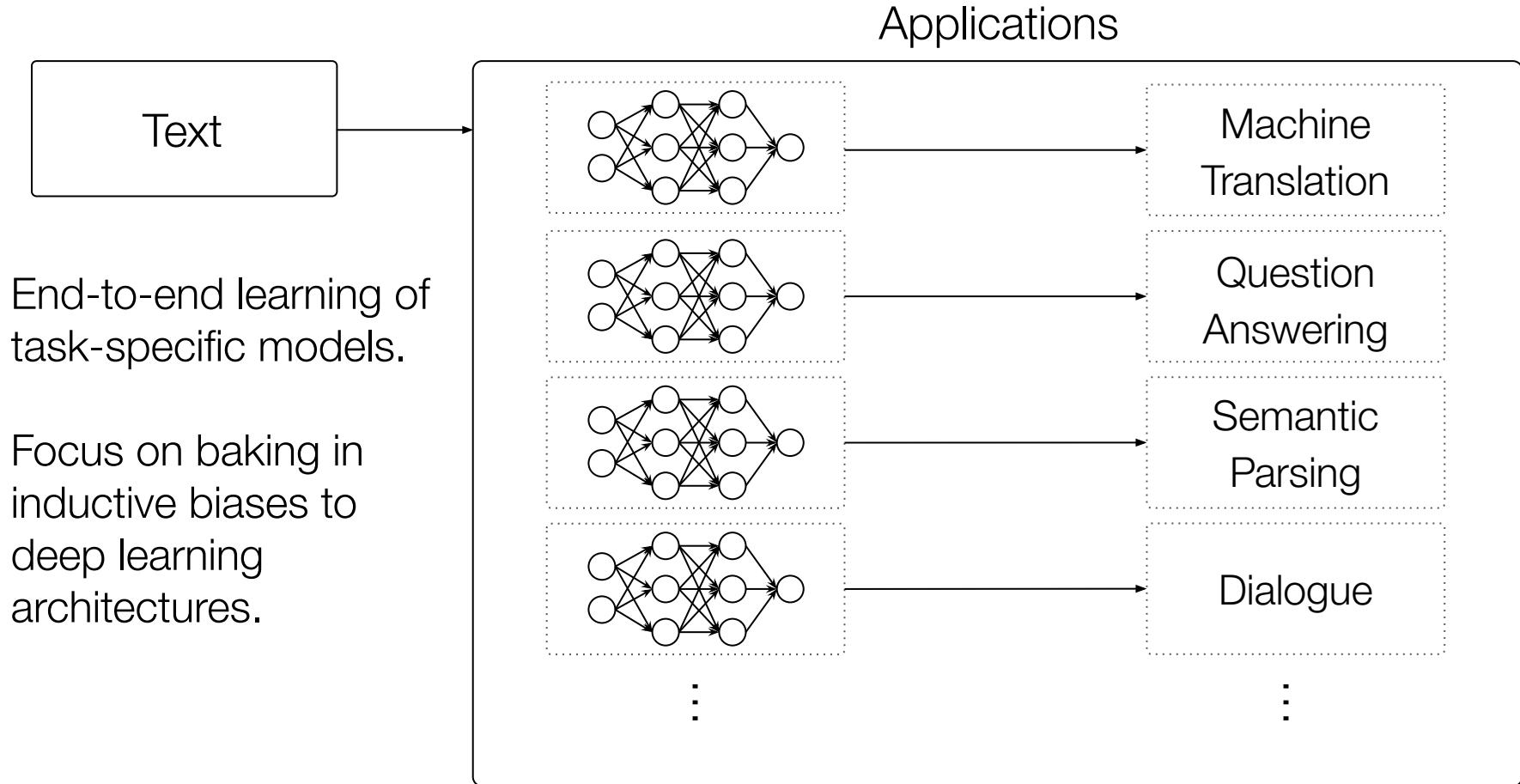
Neural NLP [2013-2018]

Text

Neural NLP [2013-2018]



Neural NLP [2013-2018]

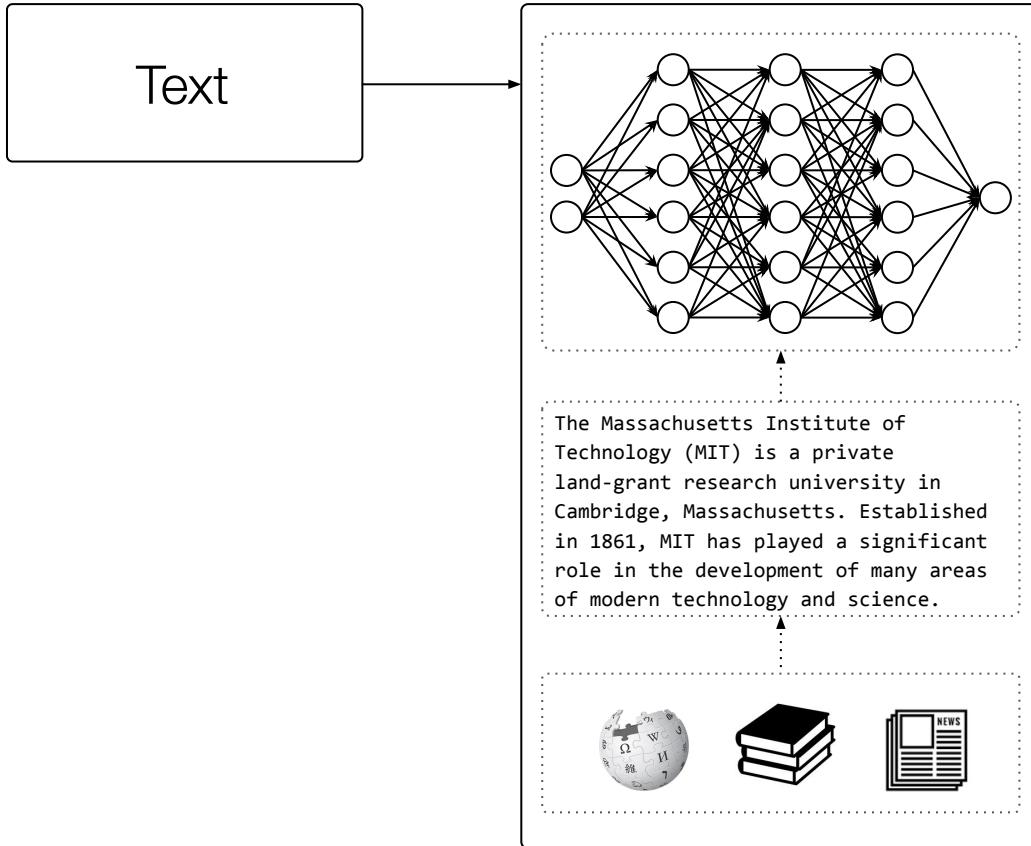


Large Language Models (LLM) [2018-Present]

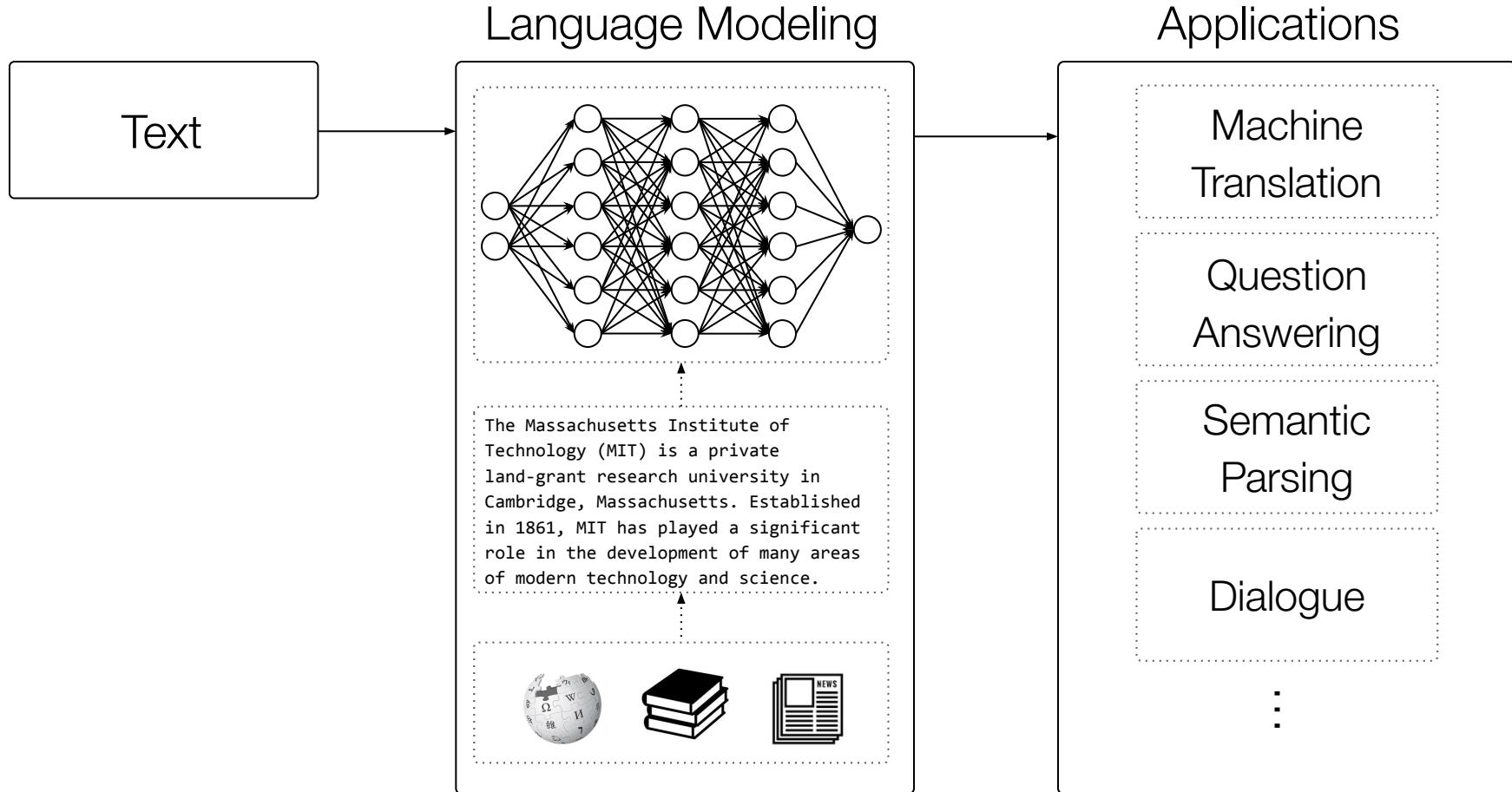
Text

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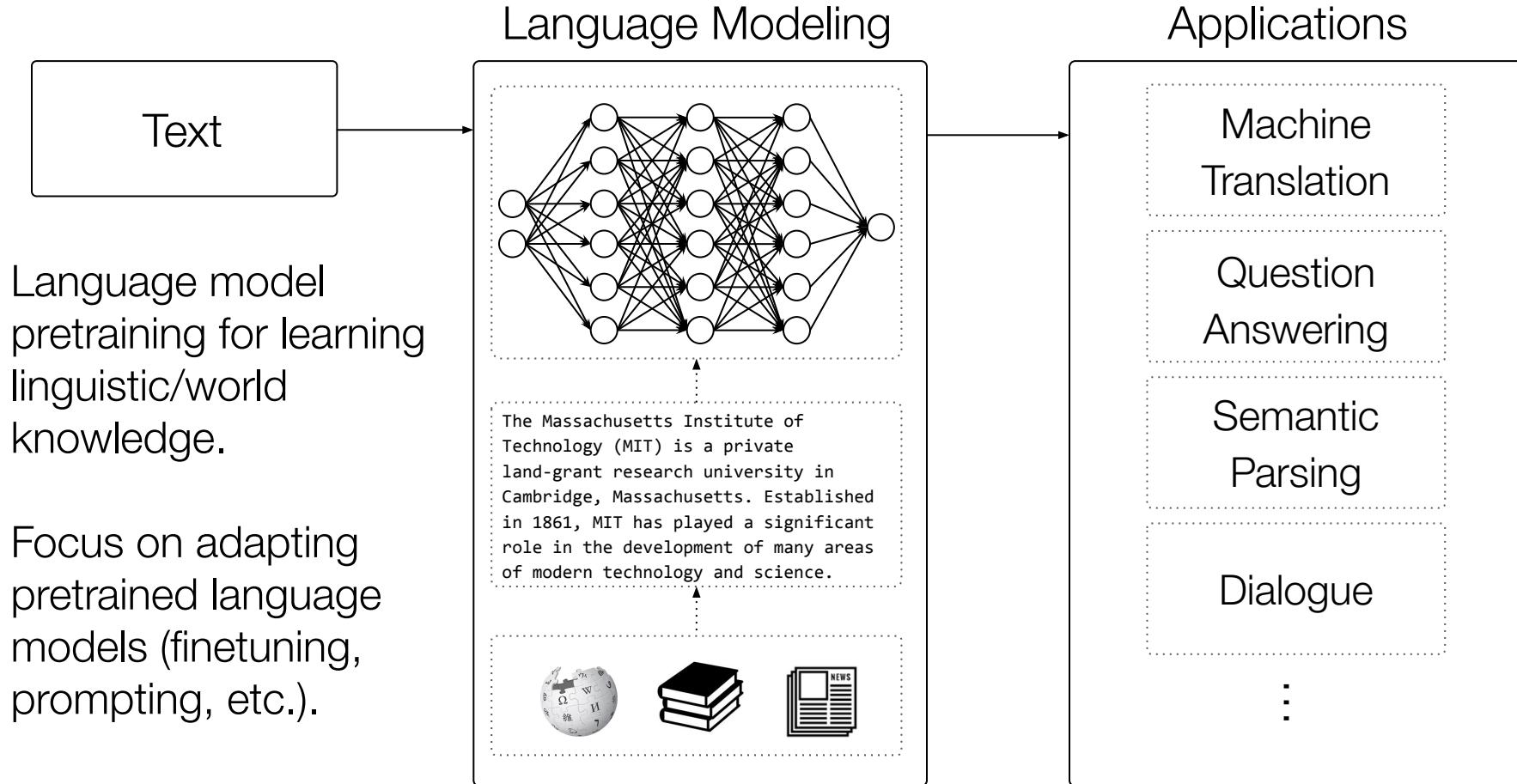
Language Modeling



Large Language Models (LLM) [2018-Present]

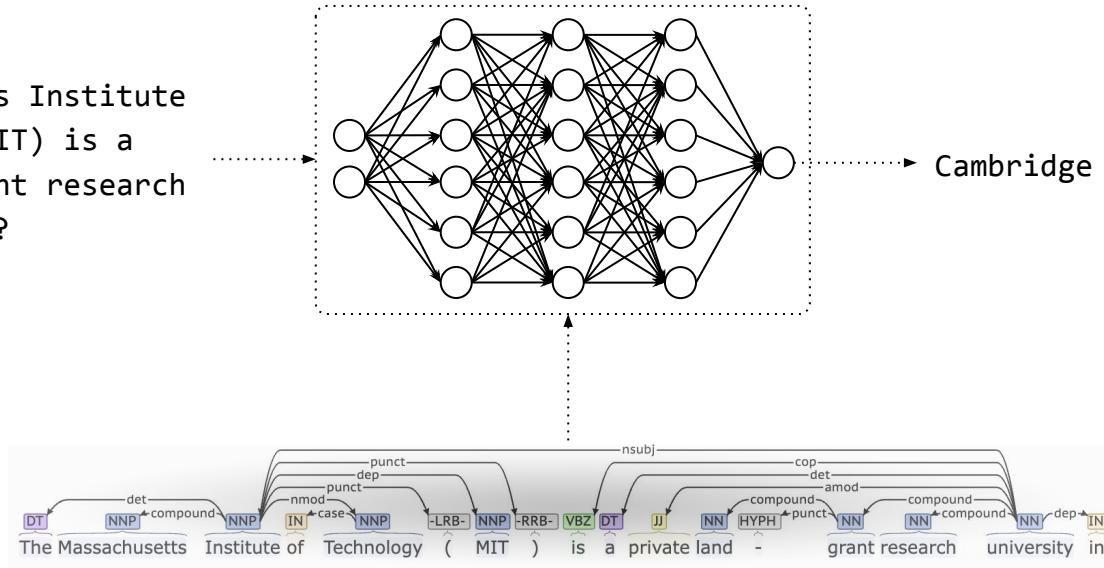


Large Language Models (LLM) [2018-Present]



LLMs & Implicit Structures

The Massachusetts Institute
of Technology (MIT) is a
private land-grant research
university in ???



The language modeling (next-word prediction) objective forces the LLM to *implicitly* encode useful structure/knowledge.

LLMs & *Explicit* Structures?

Is language modeling “all you need”?

$$\arg \max_{\theta} P_{\theta}(\mathbf{x}_t | \mathbf{x}_{<t})$$

LLMs & *Explicit* Structures?

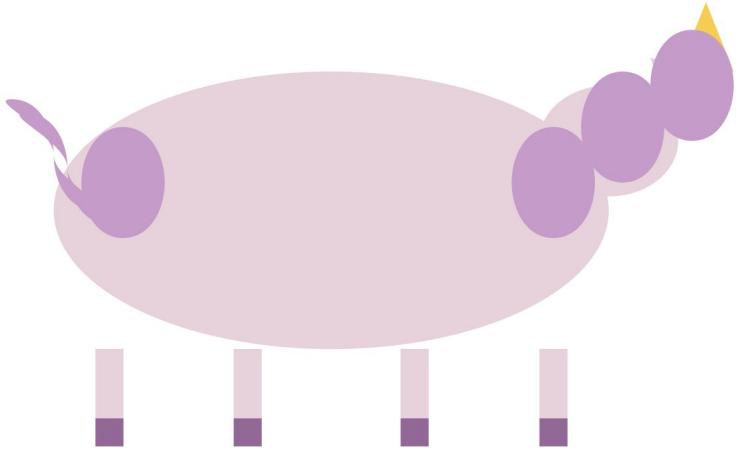
Is language modeling “all you need”?

$$\arg \max_{\theta} P_{\theta}(\mathbf{x}_t | \mathbf{x}_{<t})$$

Maybe...

Prompt: Draw a unicorn in TiKZ.

GPT-4: [Produces L^AT_EX compiling to following picture.]



[Bubeck et al. '23]

LLMs & *Explicit* Structures?

Is language modeling “all you need”?

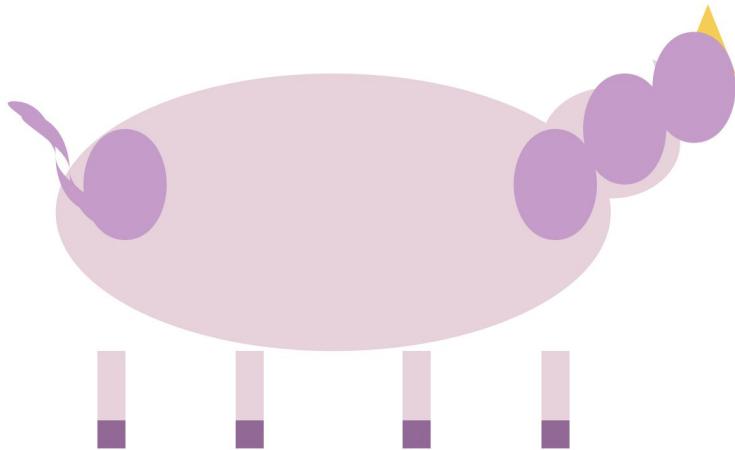
$$\arg \max_{\theta} P_{\theta}(\mathbf{x}_t | \mathbf{x}_{<t})$$

Maybe...

What role (if any) can explicit symbolic structures play in the era of LLMs?

Prompt: Draw a unicorn in TiKZ.

GPT-4: [Produces L^AT_EX compiling to following picture.]

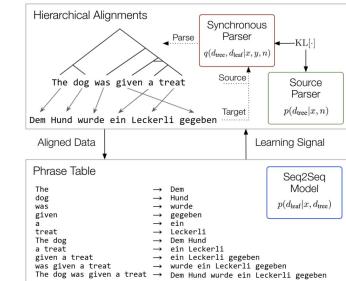


[Bubeck et al. '23]

Symbolic Structures for Controlling & Augmenting LLMs

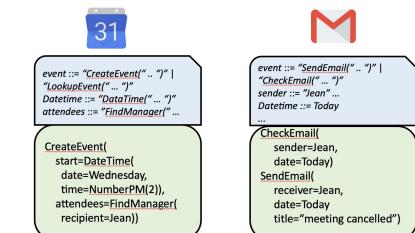
Hierarchical Phrase-based Sequence-to-Sequence Learning

Bailin Wang, Ivan Titov, Jacob Andreas, Yoon Kim
EMNLP '22



Grammar Prompting for DSL Generation with Large Language Models

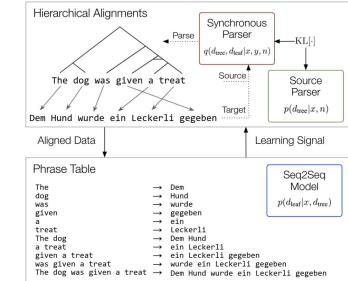
Bailin Wang, Zi Wang, Rif A. Saurous, Xuezhi Wang, Yuan Cao, Yoon Kim
NeurIPS '23



Symbolic Structures for Controlling & Augmenting LLMs

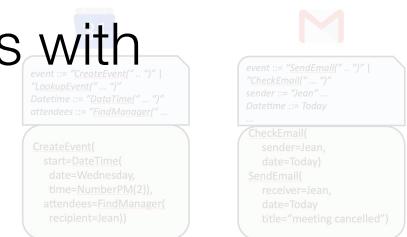
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TL;DR. Combine latent symbolic structures with pretrained LMs for machine translation.

Bailin Wang, Zi Wang, Rif A. Saurous, Xuezhi Wang, Yuan Cao, Yoon Kim
Ongoing work



Encoder-Decoder “Language Model” Pretraining

Unaligned multilingual text

It is a far, far better thing that I do, than I
have ever done; it is a far, far better rest that
I go to than I have ever known.

The Massachusetts Institute of Technology (MIT)
is a private land-grant research university in
Cambridge, Massachusetts.

보스턴과 찰스 강 하나를 사이에 두고 있으며, 실제로
처음에는 보스턴에 위치하였으나 학교가 너무 커져 신규
부지가 필요해져서 1916년 찰스 강변을 메운 현재의
부지에 신축하고 이동하였다

दिल्ली, आधिकारिक तौर पर राष्ट्रीय राजधानी क्षेत्र दिल्ली
भारत की राजधानी और एक केंद्र-शासित प्रदेश है। इसमें नई
दिल्ली सम्मिलित है जो भारत की राजधानी है। दिल्ली राजधानी
होने के नाते केंद्र सरकार की तीनों इकाइयों
⋮

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⋮

Create synthetic input-output pairs

<EN> The Massachusetts [MASK] (MIT)
is a [MASK] research university in
[MASK].

Input

<EN> Institute of Technology [/s]
private land-grand [/s]
Cambridge, Massachusetts [/s]

Output

Encoder-Decoder “Language Model” Pretraining

Unaligned multilingual text

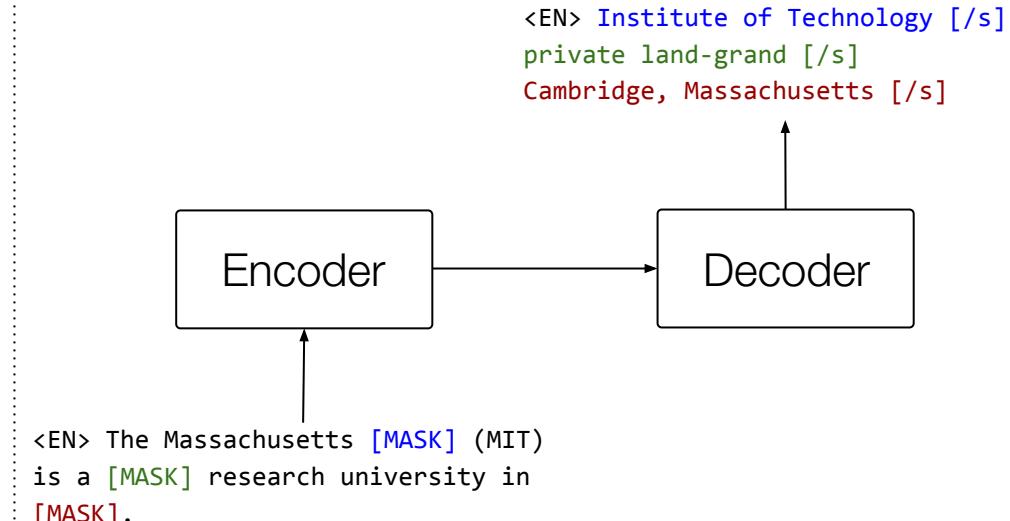
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दिल्ली, आधिकारिक तौर पर राष्ट्रीय राजधानी क्षेत्र दिल्ली भारत की राजधानी और एक केंद्र-शासित प्रदेश है। इसमें नई दिल्ली सम्मिलित है जो भारत की राजधानी है। दिल्ली राजधानी होने के नाते केंद्र सरकार की तीनों इकाइयों
⋮

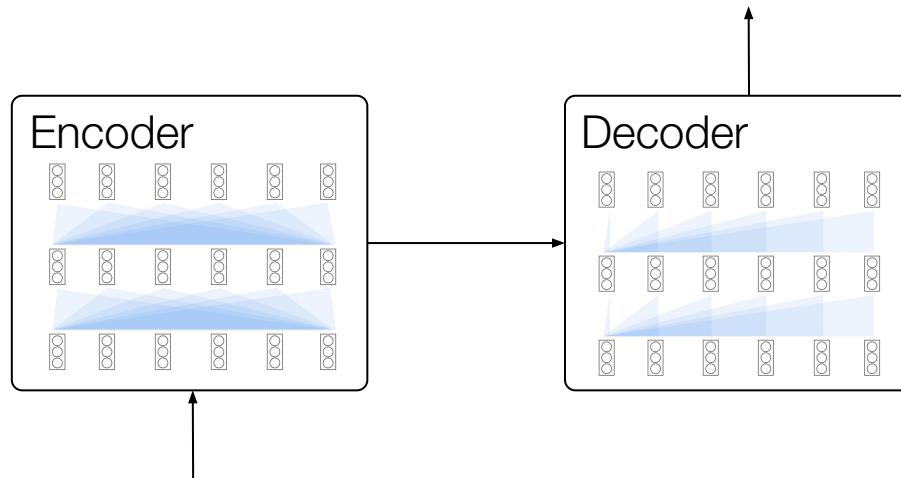
Pretrain as a denoising autoencoder



“Language Model” Pretraining for Machine Translation

Transfer learning: After pretraining, finetune on (smaller) set of aligned sentences

◀KO▶ 대규모 언어 모델을 정확하게 제어하기 위한
메커니즘을 개발해야 할 긴급한 필요성이 있습니다.



◀EN▶ There is a pressing need to develop
mechanisms for precisely controlling large
language models.

[Lewis et al. '19, Raffel et al. '19, Liu et al. '20, Xue et al. '20]

Hasn't GPT-{3, 3.5, 4} made finetuning obsolete?

	German ⇒ English	Romanian ⇒ English	Chinese ⇒ English
Google NMT	45.0	50.1	31.7
GPT-4	43.7	45.0	24.7

Pretrain-then-finetuning paradigm still performant and cost-effective!

Classic Hierarchical Phrase-based MT

Classic Hierarchical Phrase-based MT

Source (English)

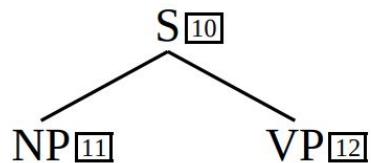
S₁₀

Target (Japanese)

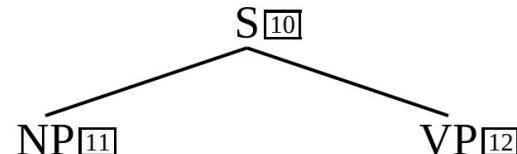
S₁₀

Classic Hierarchical Phrase-based MT

Source (English)



Target (Japanese)

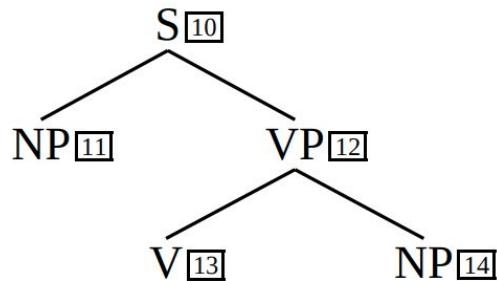


$$S \rightarrow \langle NP_{\overline{1}} VP_{\overline{2}}, NP_{\overline{1}} VP_{\overline{2}} \rangle$$

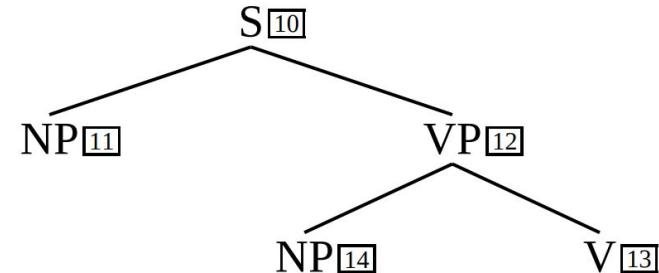
Synchronous context-free
grammar rules

Classic Hierarchical Phrase-based MT

Source (English)



Target (Japanese)



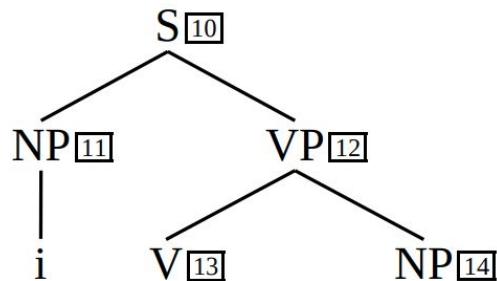
Synchronous context-free
grammar rules

$$S \rightarrow \langle NP_1 \; VP_2, \; NP_1 \; VP_2 \rangle$$

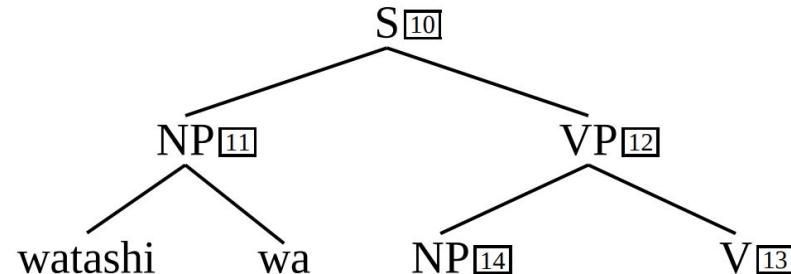
$$VP \rightarrow \langle V_1 \; NP_2, \; NP_2 \; V_1 \rangle$$

Classic Hierarchical Phrase-based MT

Source (English)



Target (Japanese)



Synchronous context-free
grammar rules

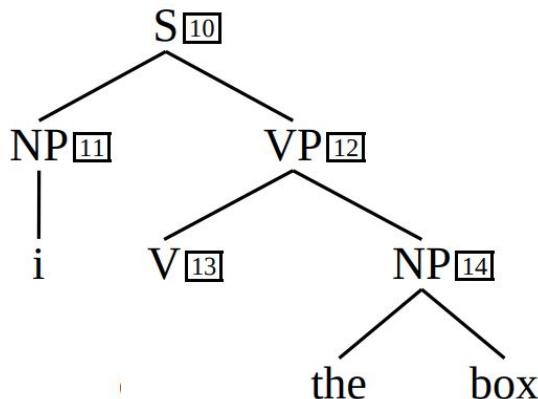
$$S \rightarrow \langle NP_1 \; VP_2, NP_1 \; VP_2 \rangle$$

$$VP \rightarrow \langle V_1 \; NP_2, NP_2 \; V_1 \rangle$$

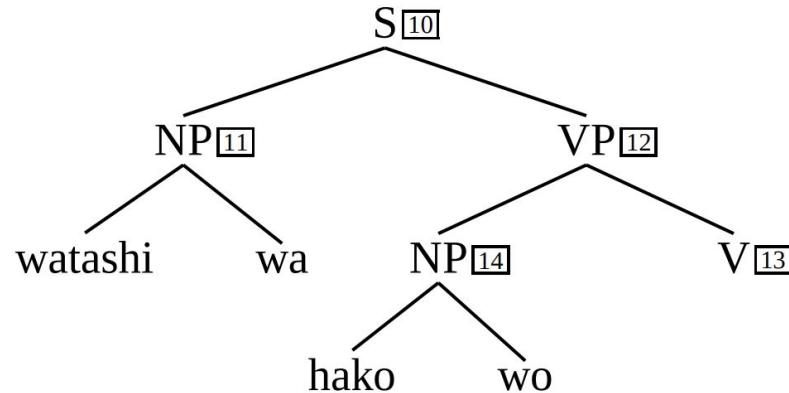
$$NP \rightarrow \langle i, watashi \; wa \rangle$$

Classic Hierarchical Phrase-based MT

Source (English)



Target (Japanese)



Synchronous context-free
grammar rules

$$S \rightarrow \langle NP_1 \; VP_2, NP_1 \; VP_2 \rangle$$

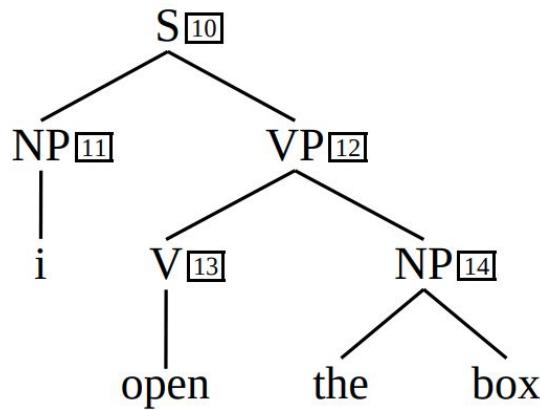
$$VP \rightarrow \langle V_1 \; NP_2, NP_2 \; V_1 \rangle$$

$$NP \rightarrow \langle i, watashi \; wa \rangle$$

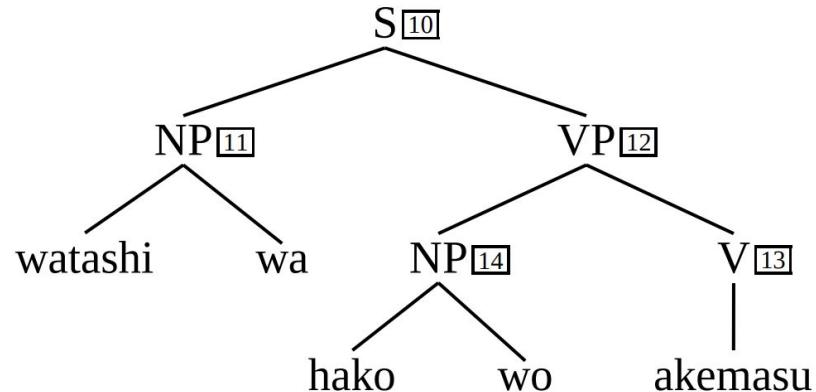
$$NP \rightarrow \langle \text{the box}, hako \; wo \rangle$$

Classic Hierarchical Phrase-based MT

Source (English)



Target (Japanese)

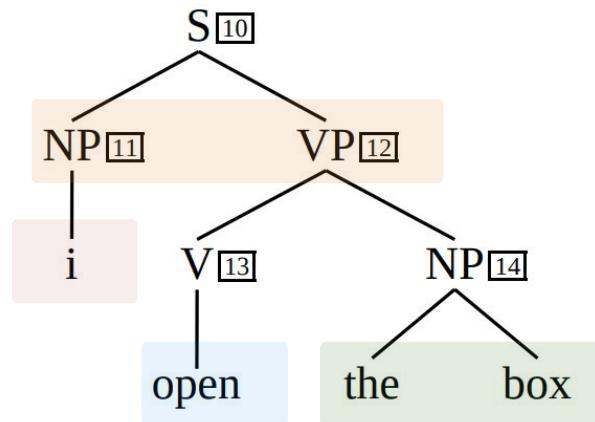


Synchronous context-free
grammar rules

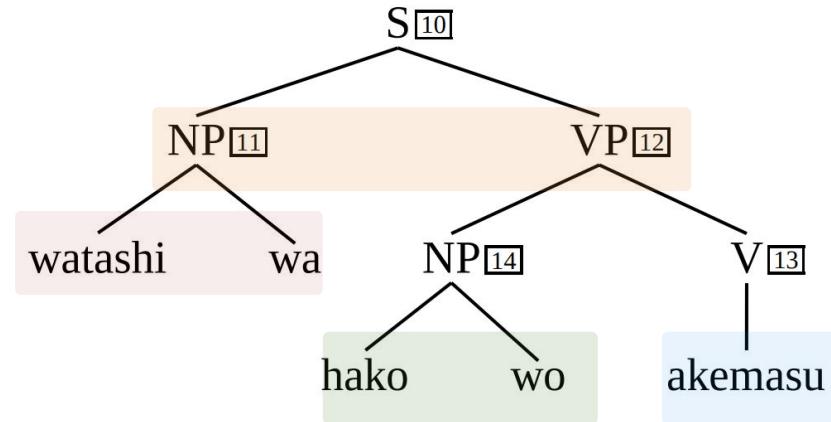
- $S \rightarrow \langle NP_1 \; VP_2, NP_1 \; VP_2 \rangle$
- $VP \rightarrow \langle V_1 \; NP_2, NP_2 \; V_1 \rangle$
- $NP \rightarrow \langle i, watashi \; wa \rangle$
- $NP \rightarrow \langle \text{the box}, hako \; wo \rangle$
- $V \rightarrow \langle \text{open}, akemasu \rangle$

Classic Hierarchical Phrase-based MT

Source (English)



Target (Japanese)

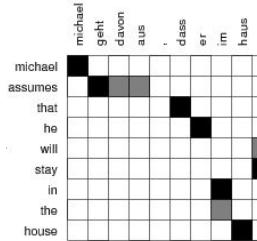


Synchronous context-free
grammar rules

- $S \rightarrow \langle NP_1 \; VP_2, NP_1 \; VP_2 \rangle$
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Classic Hierarchical Phrase-based MT

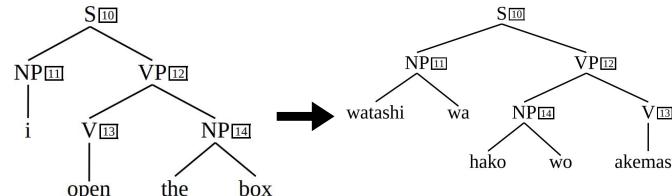
Extract phrase alignments
from parallel sentences



Induce synchronous
grammar rules and weights

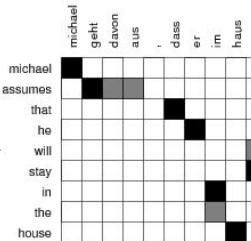
$$\begin{array}{ll} S \rightarrow \langle NP_1 VP_2, NP_1 VP_2 \rangle & s_1 \\ VP \rightarrow \langle V_1 NP_2, NP_2 V_1 \rangle & s_2 \\ NP \rightarrow \langle i, watashi\ wa \rangle & s_3 \\ NP \rightarrow \langle \text{the box}, hako\ wo \rangle & s_4 \\ V \rightarrow \langle \text{open}, akemasu \rangle & s_5 \end{array}$$

Translation as
(monolingual) parsing



Classic Hierarchical Phrase-based MT

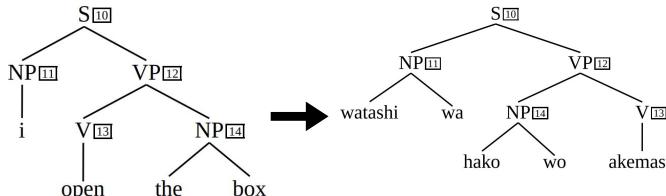
Extract phrase alignments
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Induce synchronous
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$$\begin{aligned} S &\rightarrow \langle NP_1 VP_2, NP_1 VP_2 \rangle & s_1 \\ VP &\rightarrow \langle V_1 NP_2, NP_2 V_1 \rangle & s_2 \\ NP &\rightarrow \langle i, watashi wa \rangle & s_3 \\ NP &\rightarrow \langle \text{the box}, hako wo \rangle & s_4 \\ V &\rightarrow \langle \text{open}, akemasu \rangle & s_5 \end{aligned}$$

Translation as
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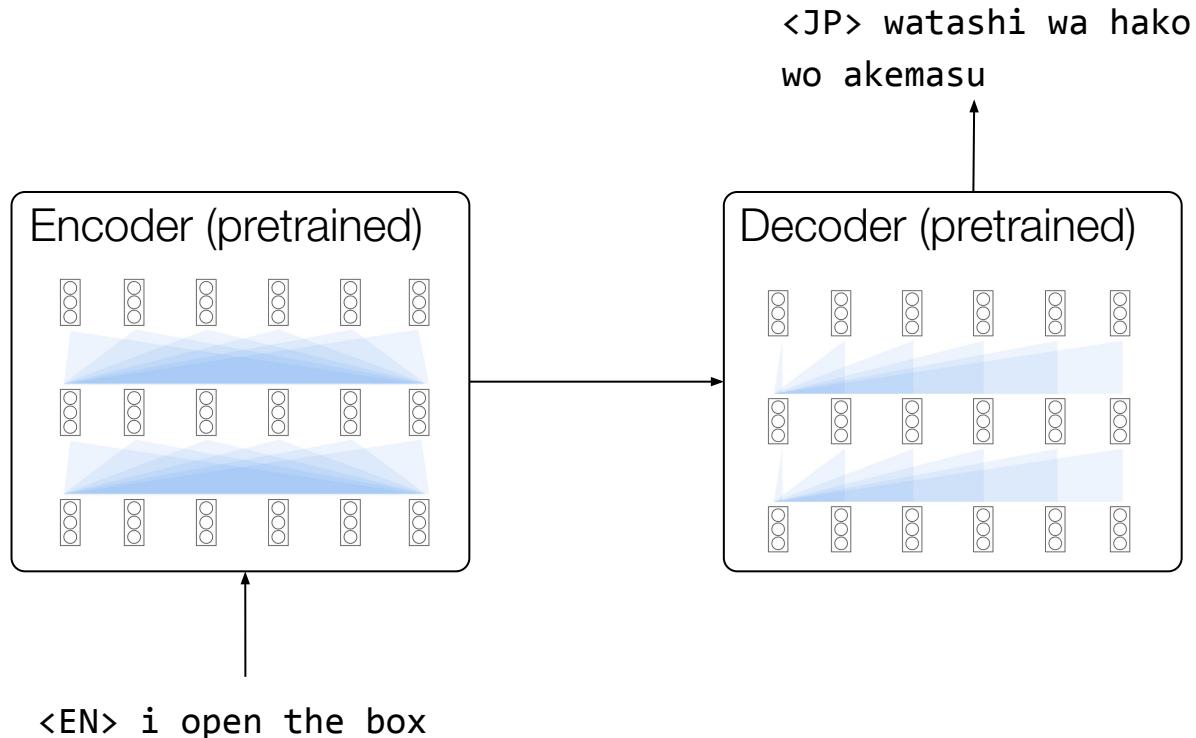


✗ Error propagation due
to “pipelining”.

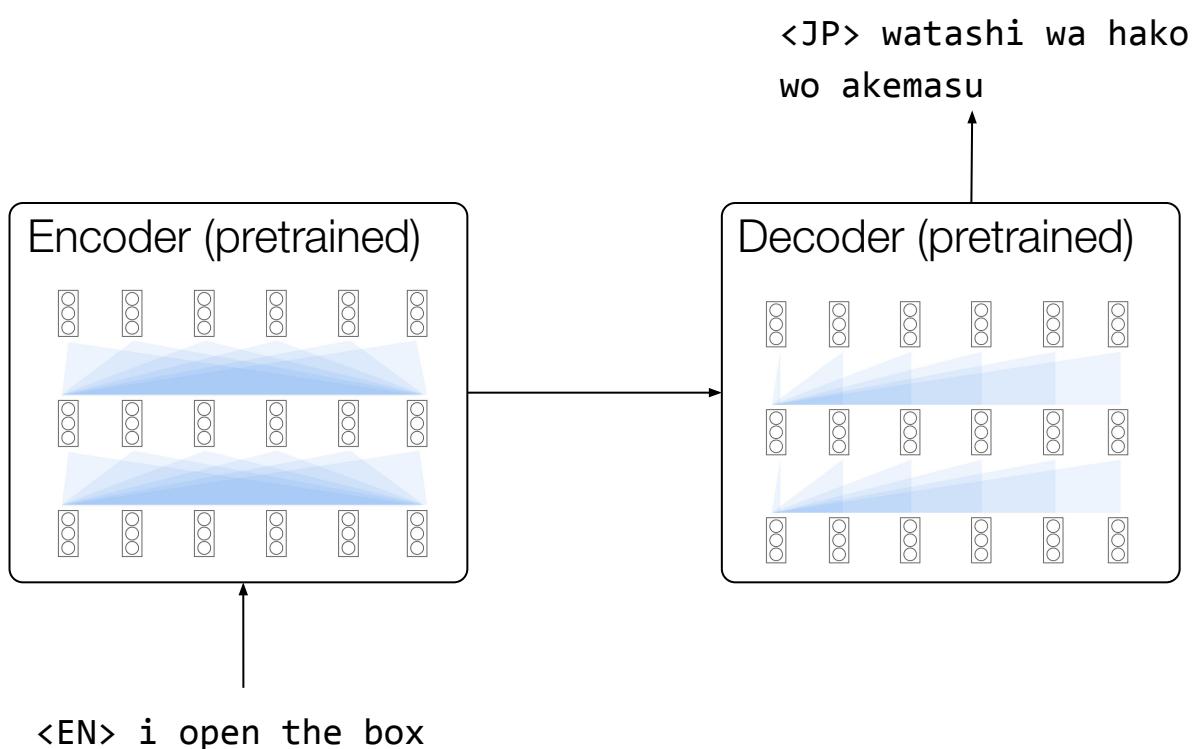
✗ Inflexible model due to
(too) strong
assumptions.

✗ Cannot (directly) be
applied on top of
pretrained LMs.

Neural MT with Pretraining

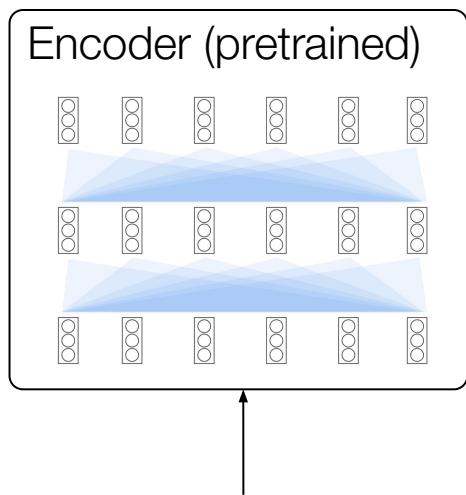


Neural MT with Pretraining



- ✓ End-to-end learning: all phenomena captured implicitly in the hidden layers.

Neural MT with Pretraining



<JP> watashi wa hako
wo akemasu

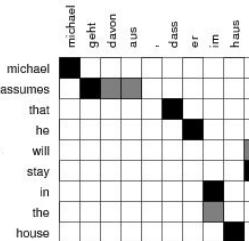
✓ End-to-end learning: all phenomena captured implicitly in the hidden layers.

✗ Too flexible of a model
⇒ data hungry and prone to overfitting.

✗ End-to-end generation
⇒ hard to control/interpret translation process.

Classic Hierarchical Phrase-based MT

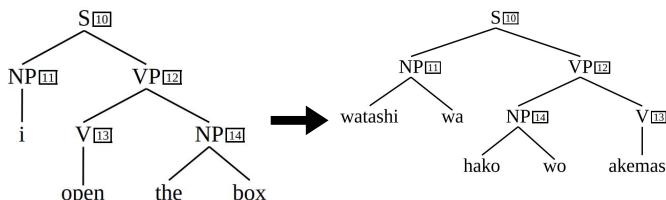
Extract phrase alignments
from parallel sentences



Induce synchronous
grammar rules and weights

$$\begin{aligned} S &\rightarrow \langle NP_1 VP_2, NP_1 VP_2 \rangle & s_1 \\ VP &\rightarrow \langle V_1 NP_2, NP_2 V_1 \rangle & s_2 \\ NP &\rightarrow \langle i, watashi wa \rangle & s_3 \\ NP &\rightarrow \langle \text{the box}, hako wo \rangle & s_4 \\ V &\rightarrow \langle \text{open}, akemasu \rangle & s_5 \end{aligned}$$

Translation as
(monolingual) parsing



✓ Explicit symbolic rules
⇒ controllable &
interpretable generation.

$NP \rightarrow \langle \text{the student}, \text{gakusei-ga} \rangle$

$NP \rightarrow \langle \text{the teacher}, \text{sensei-ga} \rangle$

$V \rightarrow \langle \text{danced}, \text{odotta} \rangle$

$V \rightarrow \langle \text{said}, \text{itta} \rangle$

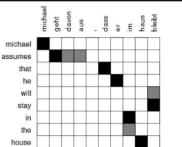
✓ Strong inductive bias for
compositionality.

✓ Data-efficient.

Classic MT + Modern Pretraining?

Can we combine the controllability and the compositional inductive bias of classic methods with the flexibility of pretrained LMs?

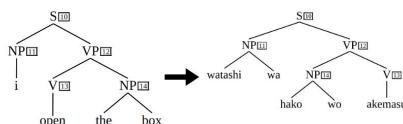
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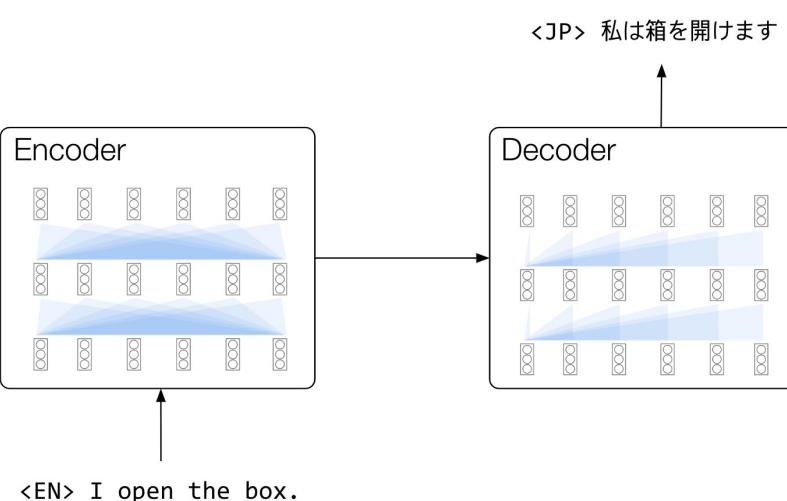
Induce synchronous grammar rules and weights

$S \rightarrow \langle NP \square, VP \square, NP \square, VP \square \rangle$	s_1
$VP \rightarrow \langle V \square, NP \square, NP \square, V \square \rangle$	s_2
$NP \rightarrow \langle i, watashi \ wa \rangle$	s_3
$NP \rightarrow \langle \text{the box}, hako \ wo \rangle$	s_4
$V \rightarrow \langle \text{open}, akemasu \rangle$	s_5

Translation as (monolingual) parsing

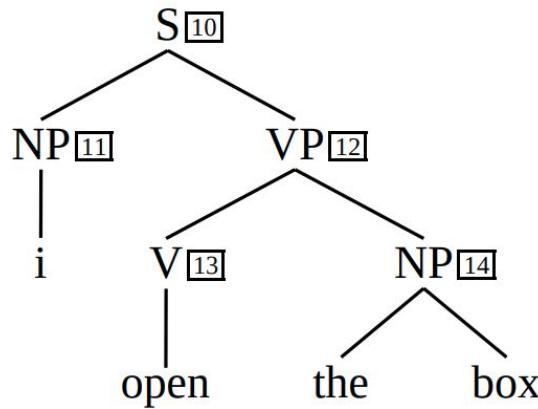


+

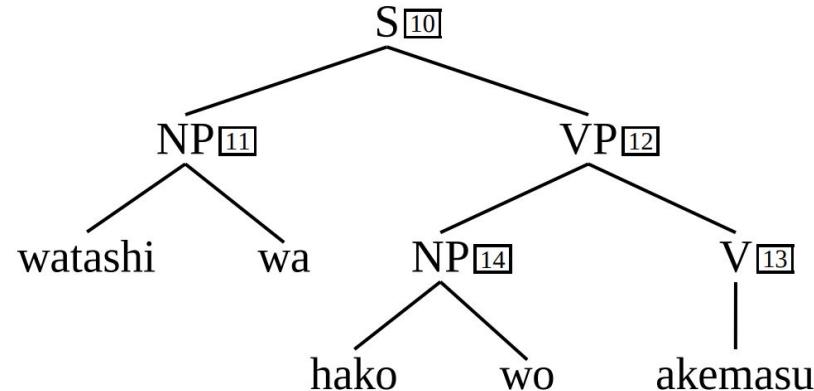


A “Neural” Parameterization of Grammar Rules

Source



Target



Synchronous context-free
grammar rules

$$S \rightarrow \langle NP_1 \; VP_2, NP_1 \; VP_2 \rangle$$

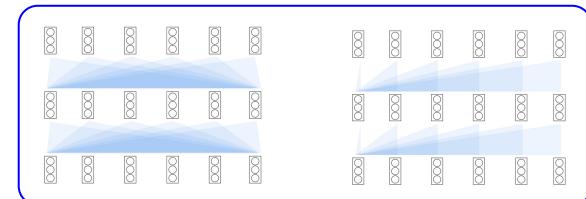
$$VP \rightarrow \langle V_1 \; NP_2, NP_2 \; V_1 \rangle$$

$$NP \rightarrow \langle i, watashi \; wa \rangle$$

$$NP \rightarrow \langle \text{the box}, hako \; wo \rangle$$

$$V \rightarrow \langle \text{open}, akemasu \rangle$$

From a pretrained LM!



A Neural Synchronous Grammar

i open the box

A Neural Synchronous Grammar

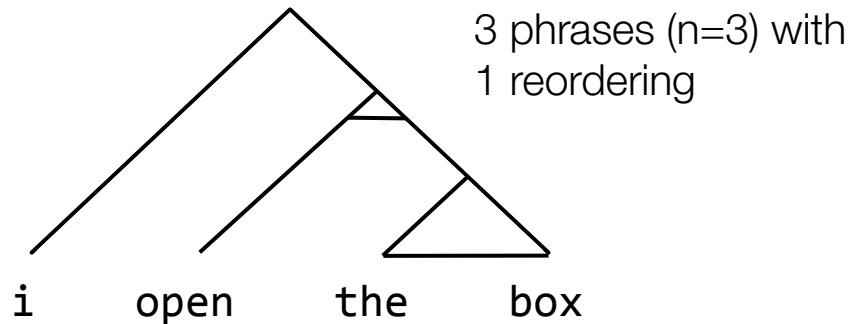
i open the box

$$P_{\text{BTG}}(\mathbf{t} \mid \mathbf{x})$$

Bracketing Transduction Grammar
(BTG) segments and reorders source
sentence.

A Neural Synchronous Grammar

i | the box | open

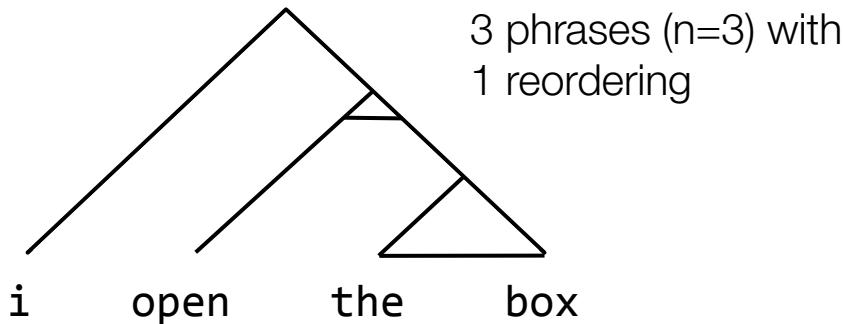


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A Neural Synchronous Grammar

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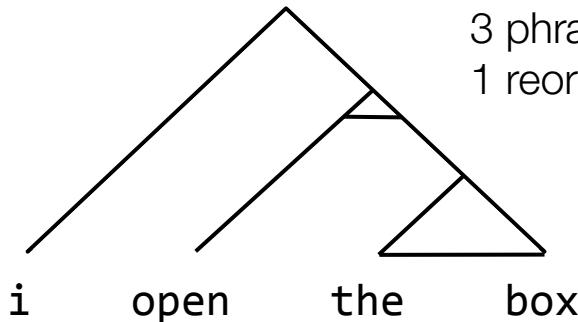
$$P_{\text{BTG}}(\mathbf{t} \mid \mathbf{x}) \propto P_{\text{seg}}(n \mid \mathbf{x}) \prod_{1 \leq i < j \leq |\mathbf{x}|} e_S^\top f(\mathbf{h}_i, \mathbf{h}_j)$$

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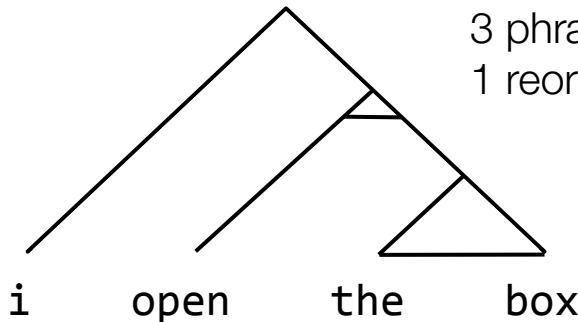
Bracketing Transduction Grammar (BTG) segments and reorders source sentence.

Distribution over number of phrase segments

$$P_{\text{BTG}}(\mathbf{t} \mid \mathbf{x}) \propto P_{\text{seg}}(n \mid \mathbf{x}) \prod_{1 \leq i < j \leq |\mathbf{x}|} e_S^\top f(\mathbf{h}_i, \mathbf{h}_j)$$

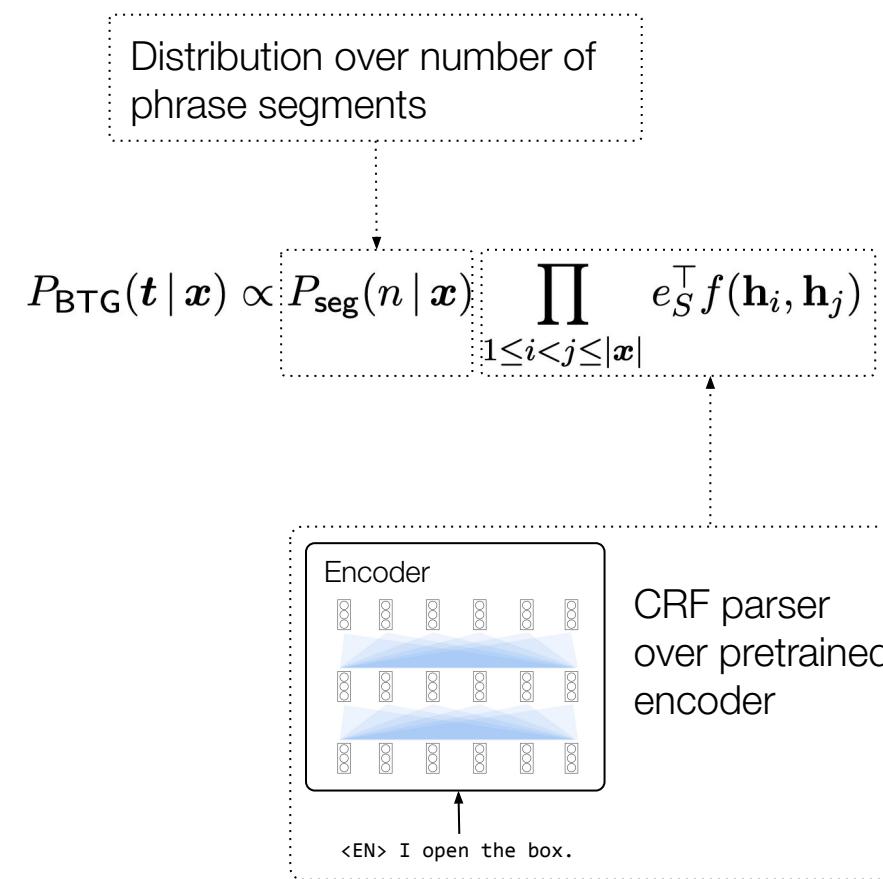
A Neural Synchronous Grammar

i | the box | open



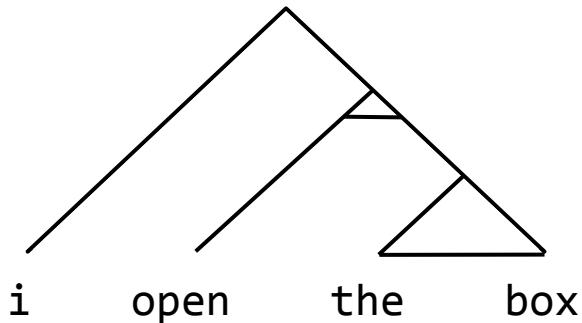
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A Neural Synchronous Grammar

i | the box | open



$$P_{\text{BTG}}(\mathbf{t} \mid \mathbf{x})$$

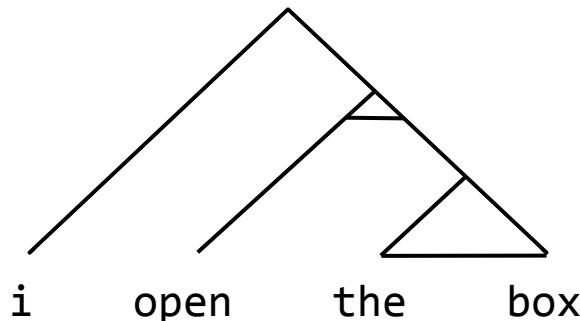
Bracketing Transduction Grammar (BTG) segments and reorders source sentence.

$$P_{\text{seq2seq}}(\mathbf{y} \mid \mathbf{x}, \mathbf{t})$$

Seq2seq model translates segmented source phrases one-by-one.

A Neural Synchronous Grammar

i | the box | open



$$P_{\text{BTG}}(\mathbf{t} \mid \mathbf{x})$$

Bracketing Transduction Grammar (BTG) segments and reorders source sentence.

watashi wa hako wo akemasu

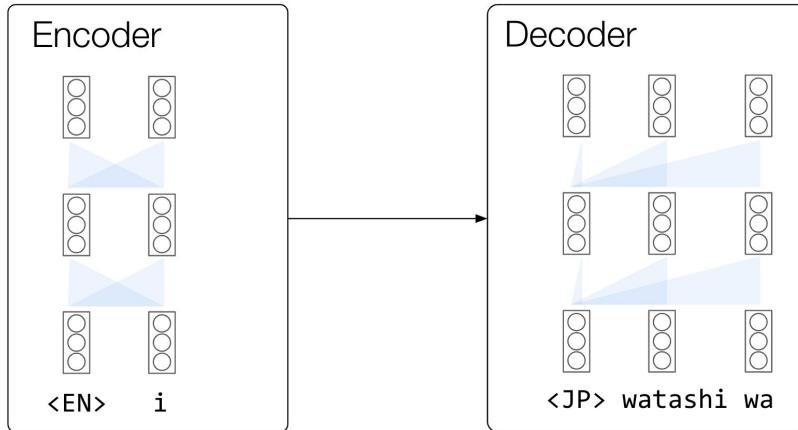
$$P_{\text{seq2seq}}(\mathbf{y} \mid \mathbf{x}, \mathbf{t})$$

Seq2seq model translates segmented source phrases one-by-one.

A Neural Synchronous Grammar

$$P_{\text{seq2seq}}(\mathbf{y} \mid \mathbf{x}, \mathbf{t}) = P_{\text{LM}}(\text{"watashi wa"} \mid \text{"i"}) \times$$

i | the box | open



watashi wa

$$P_{\text{seq2seq}}(\mathbf{y} \mid \mathbf{x}, \mathbf{t})$$

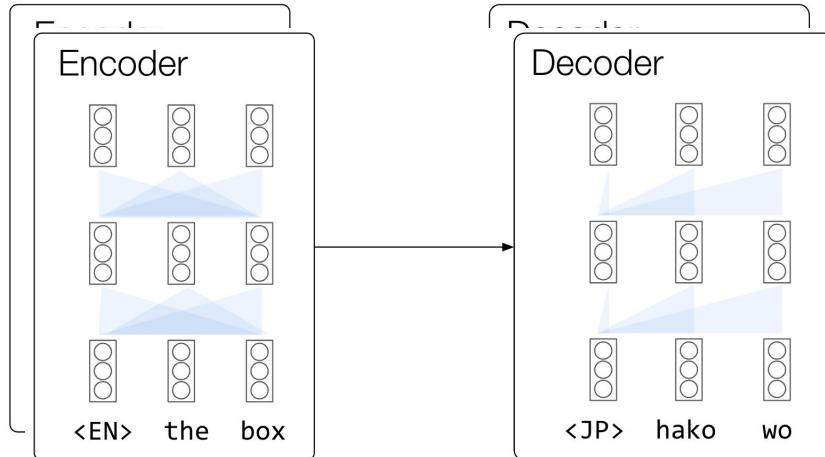
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A Neural Synchronous Grammar

$$P_{\text{seq2seq}}(\mathbf{y} \mid \mathbf{x}, \mathbf{t}) = P_{\text{LM}}(\text{"watashi wa"} \mid \text{"i"}) \times \\ P_{\text{LM}}(\text{"hako wo"} \mid \text{"the box"}) \times$$

i | the box | open



watashi wa hako wo

$$P_{\text{seq2seq}}(\mathbf{y} \mid \mathbf{x}, \mathbf{t})$$

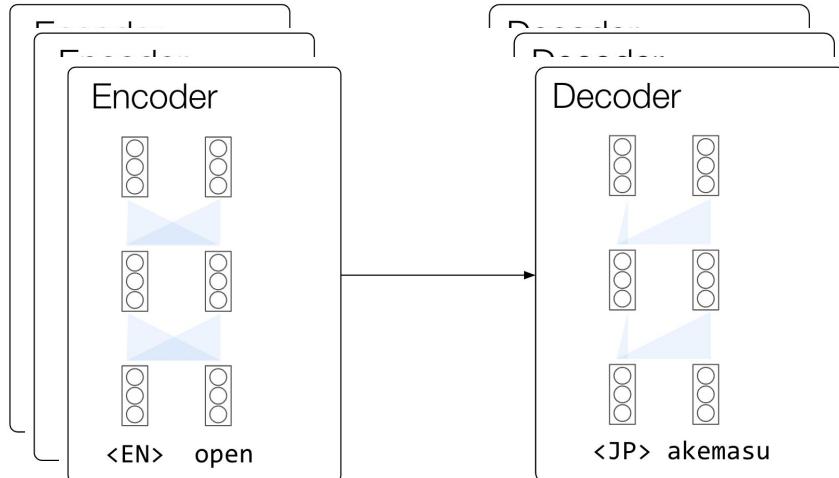
Bracketing Transduction Grammar (BTG) segments and reorders source sentence.

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A Neural Synchronous Grammar

$$P_{\text{seq2seq}}(\mathbf{y} \mid \mathbf{x}, \mathbf{t}) = P_{\text{LM}}(\text{"watashi wa"} \mid \text{"i"}) \times \\ P_{\text{LM}}(\text{"hako wo"} \mid \text{"the box"}) \times \\ P_{\text{LM}}(\text{"akemasu"} \mid \text{"open"}) \times$$

i | the box | open



Bracketing Transduction Grammar
(BTG) segments and reorders source sentence.

watashi wa hako wo akemasu

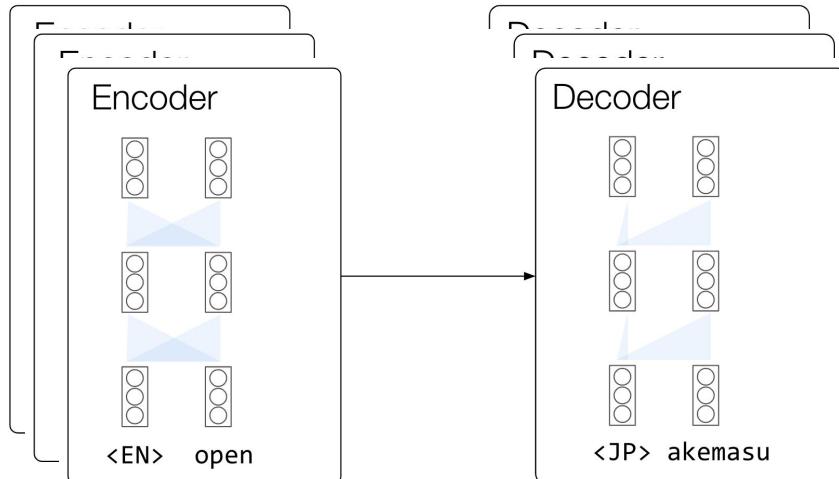
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A Neural Synchronous Grammar

$$P_{\text{seq2seq}}(\mathbf{y} | \mathbf{x}, \mathbf{t}) = P_{\text{LM}}(\text{"watashi wa"} | \text{"i"}) \times \\ P_{\text{LM}}(\text{"hako wo"} | \text{"the box"}) \times \\ P_{\text{LM}}(\text{"akemasu"} | \text{"open"}) \times$$

i | the box | open



Bracketing Transduction Grammar (BTG) segments and reorders source sentence.

Same pretrained LM (which will be finetuned) to translate at all phrase scales.

watashi wa hako wo akemasu

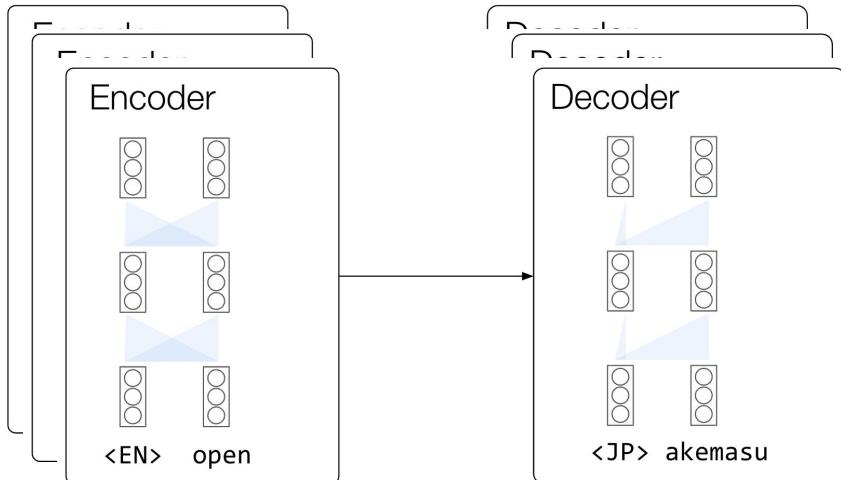
$$P_{\text{seq2seq}}(\mathbf{y} | \mathbf{x}, \mathbf{t})$$

Seq2seq model translates segmented source phrases one-by-one.

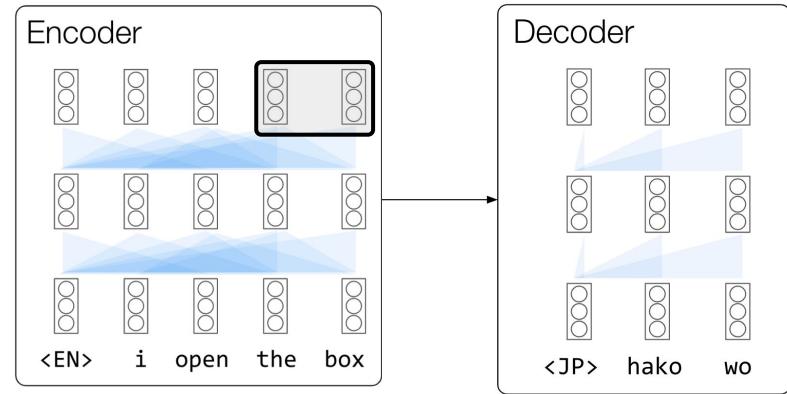
A Neural Synchronous Grammar

$$P_{\text{seq2seq}}(\mathbf{y} \mid \mathbf{x}, \mathbf{t}) = P_{\text{LM}}(\text{"watashi wa"} \mid \text{"i"}) \times \\ P_{\text{LM}}(\text{"hako wo"} \mid \text{"the box"}) \times \\ P_{\text{LM}}(\text{"akemasu"} \mid \text{"open"}) \times$$

i | the box | open



Bracketing Transduction Grammar (BTG) segments and reorders source sentence.

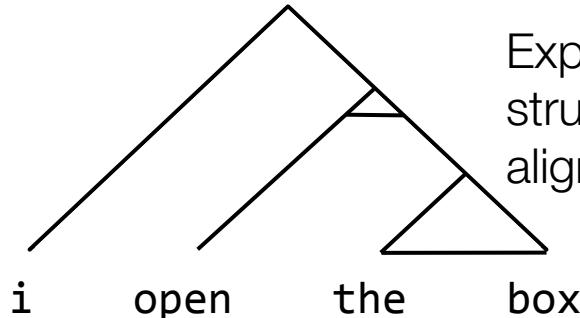


Actually use **contextualized** word representations on the source side.

A Neural Synchronous Grammar

$$P_{\text{seq2seq}}(\mathbf{y} | \mathbf{x}, \mathbf{t}) = P_{\text{LM}}(\text{"watashi wa"} | \text{"i"}) \times \\ P_{\text{LM}}(\text{"hako wo"} | \text{"the box"}) \times \\ P_{\text{LM}}(\text{"akemasu"} | \text{"open"}) \times$$

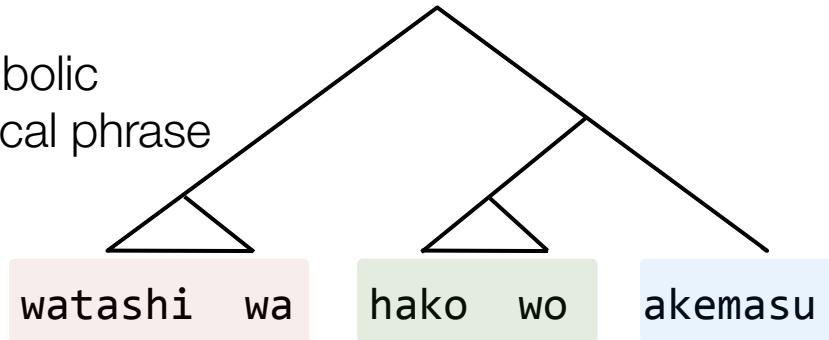
i | the box | open



Explicit use of symbolic structure (hierarchical phrase alignments)!

$$P_{\text{BTG}}(\mathbf{t} | \mathbf{x})$$

Bracketing Transduction Grammar (BTG) segments and reorders source sentence.

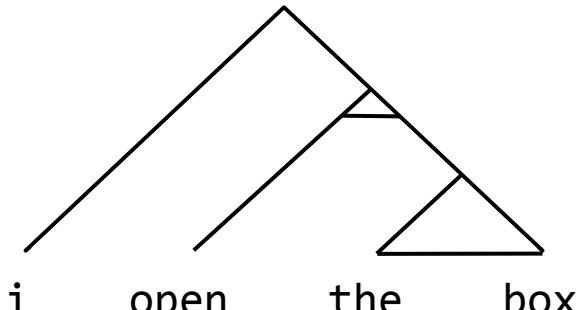


$$P_{\text{seq2seq}}(\mathbf{y} | \mathbf{x}, \mathbf{t})$$

Seq2seq model translates segmented source phrases one-by-one.

A Neural Synchronous Grammar

i | the box | open



$$P_{\text{BTG}}(\mathbf{t} \mid \mathbf{x})$$

Bracketing Transduction Grammar (BTG) segments and reorders source sentence.

Distribution over number of phrase segments

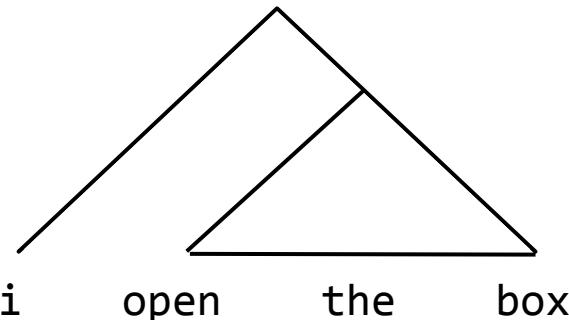
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This example: 3 phrase segments ($n=3$) with 1 reordering.

What if the number of phrase segments is different (e.g., $n=2$)?

A Neural Synchronous Grammar

i | open the box



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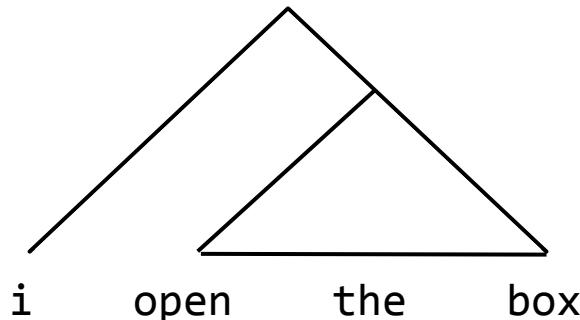
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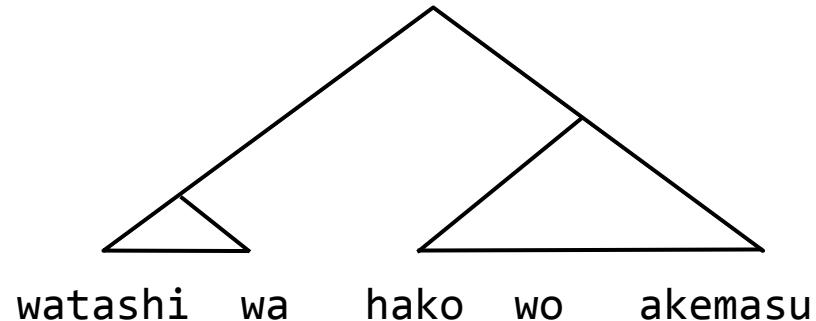
A Neural Synchronous Grammar

i | open the box



$$P_{\text{BTG}}(\mathbf{t} \mid \mathbf{x})$$

$$P_{\text{seq2seq}}(\mathbf{y} \mid \mathbf{x}, \mathbf{t}) = P_{\text{LM}}(\text{"watashi wa" | "i"}) \times \\ P_{\text{LM}}(\text{"hako wo akemasu" | "open the box"})$$



$$P_{\text{seq2seq}}(\mathbf{y} \mid \mathbf{x}, \mathbf{t})$$

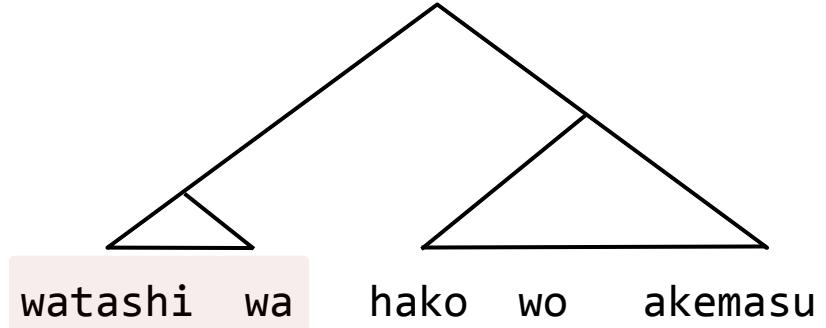
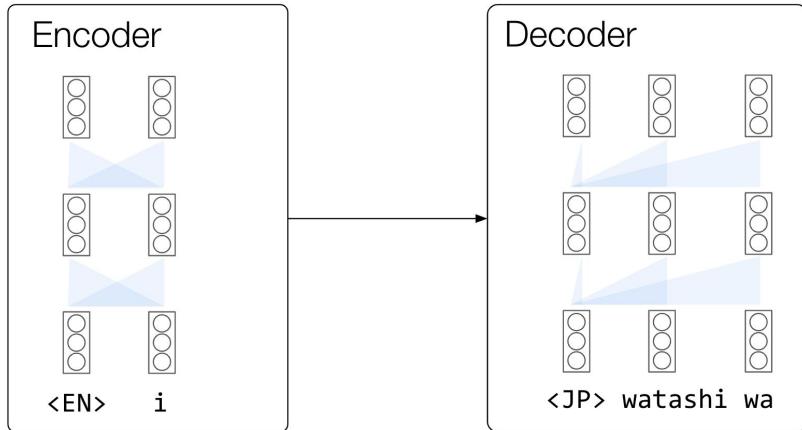
Bracketing Transduction Grammar (BTG) segments and reorders source sentence.

Seq2seq model translates segmented source phrases one-by-one.

A Neural Synchronous Grammar

i | open the box

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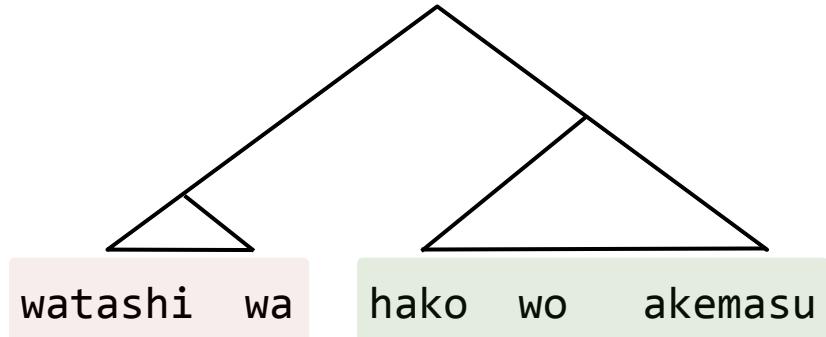
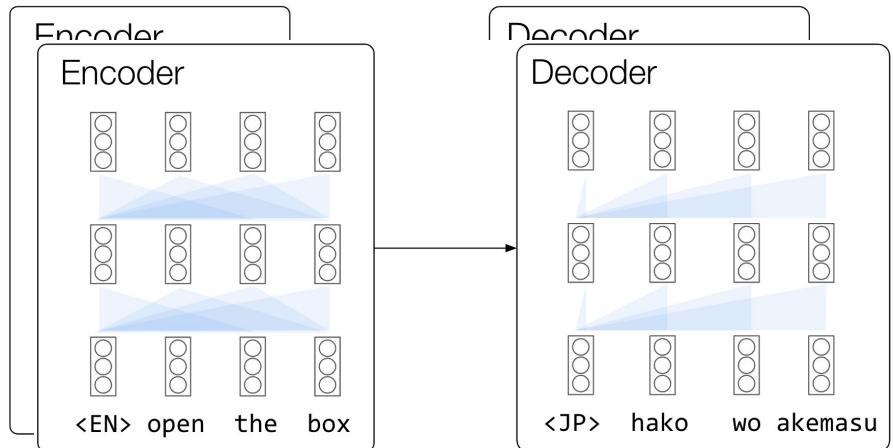
Seq2seq model translates segmented source phrases one-by-one.

A Neural Synchronous Grammar

$$P_{\text{seq2seq}}(\mathbf{y} | \mathbf{x}, \mathbf{t}) = P_{\text{LM}}(\text{"watashi wa"} \mid \text{"i"}) \times$$

$$P_{\text{LM}}(\text{"hako wo akemasu"} \mid \text{"open the box"})$$

i | open the box



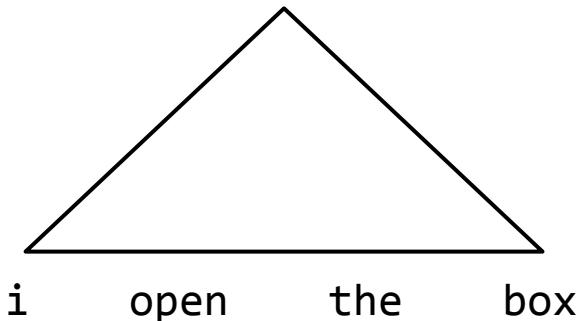
$$P_{\text{seq2seq}}(\mathbf{y} | \mathbf{x}, \mathbf{t})$$

Pretrained LM has to (learn) to capture reorderings in this case!

Seq2seq model translates segmented source phrases one-by-one.

A Neural Synchronous Grammar

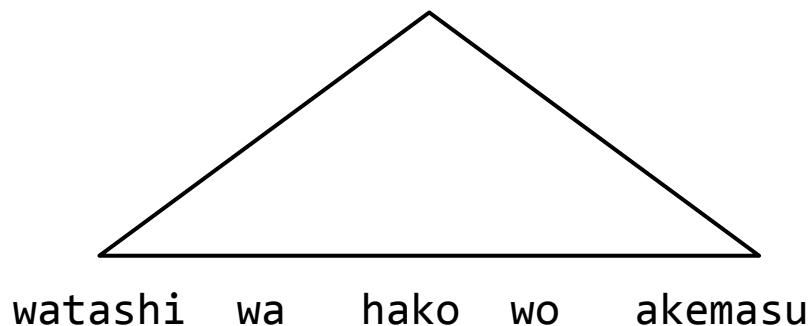
i open the box



$$P_{\text{BTG}}(\mathbf{t} \mid \mathbf{x})$$

$$P_{\text{seq2seq}}(\mathbf{y} \mid \mathbf{x}, \mathbf{t}) =$$

$P_{\text{LM}}(\text{"watashiwa hako wo akemasu"} \mid \text{"i open the box"})$



$$P_{\text{seq2seq}}(\mathbf{y} \mid \mathbf{x}, \mathbf{t})$$

Bracketing Transduction Grammar (BTG) segments and reorders source sentence.

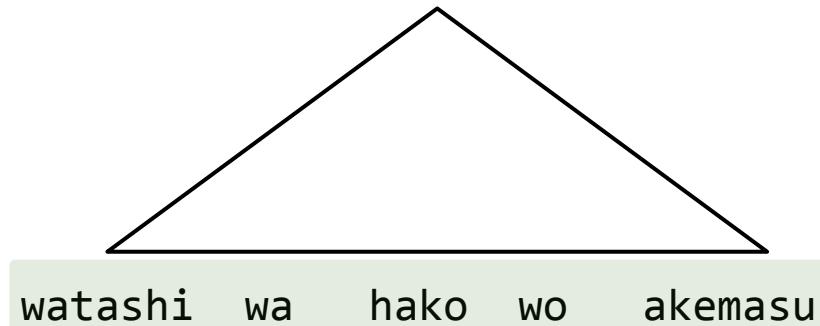
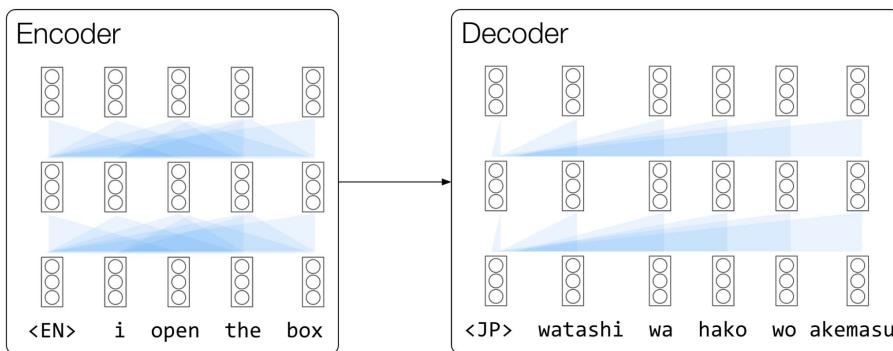
Seq2seq model translates segmented source phrases one-by-one.

A Neural Synchronous Grammar

$$P_{\text{seq2seq}}(\mathbf{y} | \mathbf{x}, \mathbf{t}) =$$

i open the box

$P_{\text{LM}}(\text{"watashiwa hako wo akemasu"} | \text{"i open the box"})$



$$P_{\text{seq2seq}}(\mathbf{y} | \mathbf{x}, \mathbf{t})$$

The setting with $n=1$ reduces to standard neural MT finetuning with pretrained LMs!

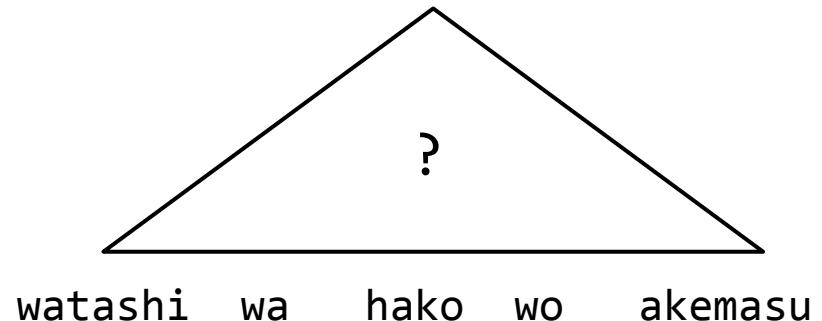
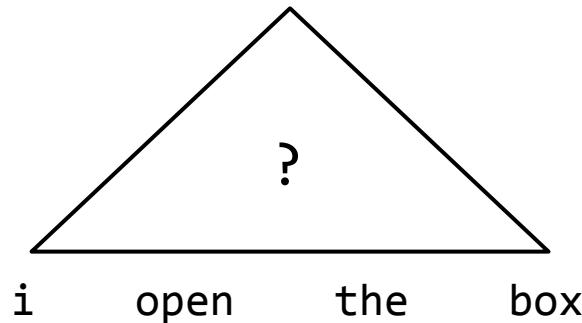
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LM-based Neural Synchronous Grammar

Synchronous grammar whose rule probabilities are given by a pretrained LM.

LM-based Neural Synchronous Grammar

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All we have are source/target sentences.

No ground-truth structure \Rightarrow treat the hierarchical phrase alignments as latent variables.

LM-based Neural Synchronous Grammar

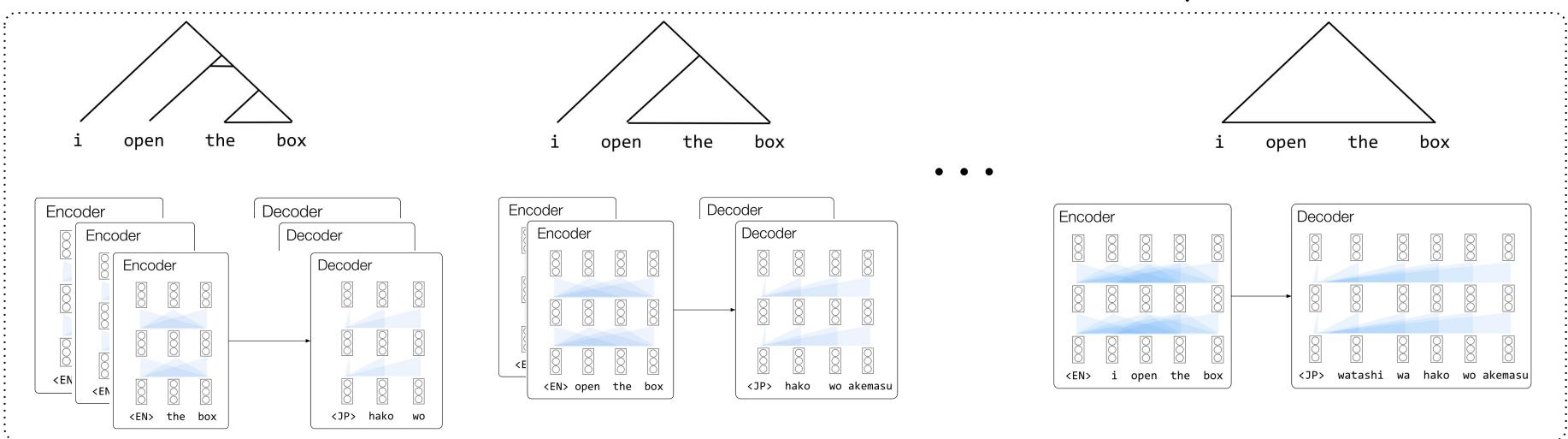
Synchronous grammar whose rule probabilities are given by a pretrained LM.

Learning/Finetuning: $\log P(\mathbf{y} \mid \mathbf{x}) = \log \left(\sum_{\mathbf{t} \in \mathcal{T}(\mathbf{x})} P_{\text{BTG}}(\mathbf{t} \mid \mathbf{x}) P_{\text{seq2seq}}(\mathbf{y} \mid \mathbf{x}, \mathbf{t}) \right)$

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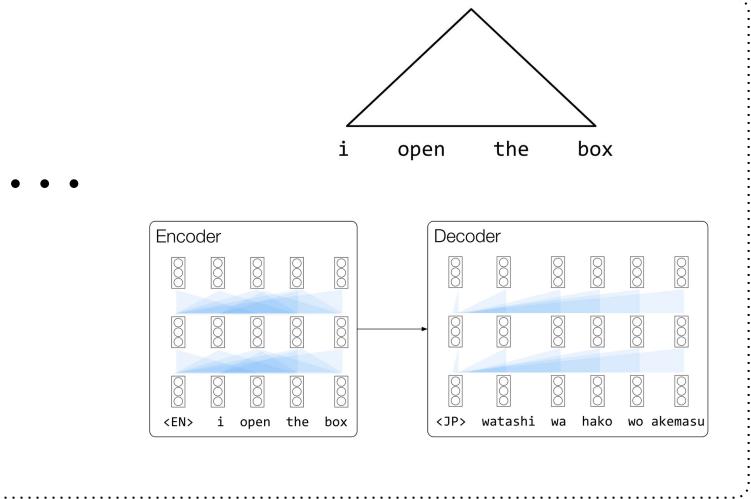
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Marginalization is tractable in theory but requires a $\mathcal{O}(L^7)$ dynamic program, where $L = \min\{|\mathbf{x}|, |\mathbf{y}|\}$

⇒ Variational inference to perform approximate inference in $\mathcal{O}(L^3)$



Learning

The dog was given a treat

Source

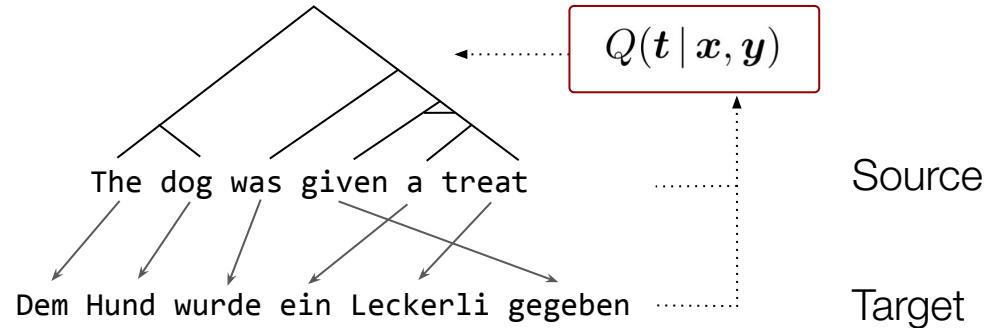
Dem Hund wurde ein Leckerli gegeben

Target

Learning

$Q(t | x, y)$: Variational Synchronous Parser. CRF over pretrained encoder/decoder representations.

ϕ



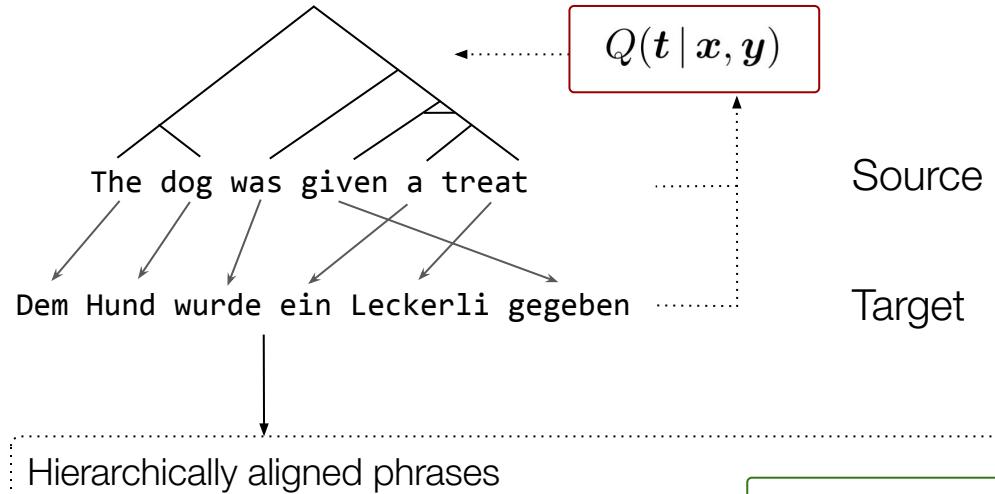
Learning

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$P_{\text{seq2seq}}(y | x, t)$: Seq2seq model initialized with pretrained encoder/decoder. Finetuned on sampled source phrases.

ϕ

θ



Hierarchically aligned phrases

The	→ Dem
dog	→ Hund
was	→ wurde
given	→ gegeben
a	→ ein
treat	→ Leckerli
The dog	→ Dem Hund
a treat	→ ein Leckerli
given a treat	→ ein Leckerli gegeben
was given a treat	→ wurde ein Leckerli gegeben
The dog was given a treat	→ Dem Hund wurde ein Leckerli gegeben

Learning

$Q(t | x, y)$: Variational Synchronous Parser. CRF over pretrained encoder/decoder representations.

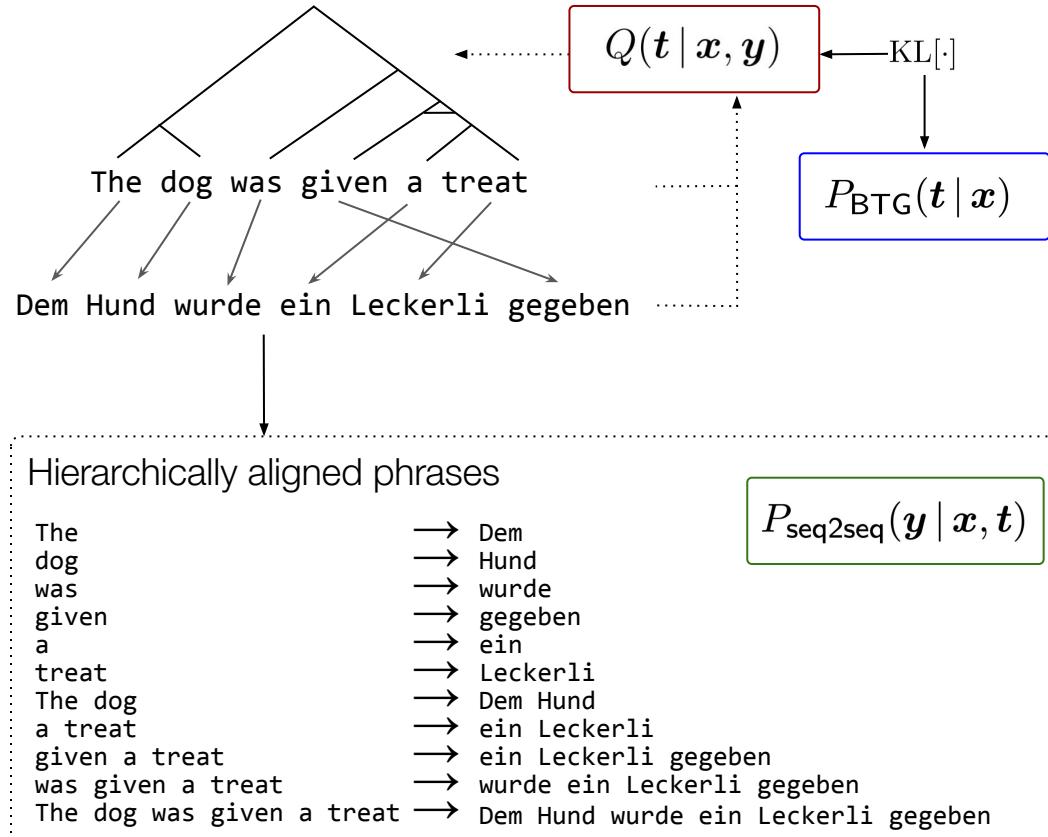
ϕ

$P_{\text{seq2seq}}(y | x, t)$: Seq2seq model initialized with pretrained encoder/decoder. Finetuned on sampled source phrases.

θ

$P_{\text{BTG}}(t | x)$: “Prior” BTG parser. CRF over pretrained encoder/decoder representations.

π



Learning

$Q(t | x, y)$: Variational Synchronous Parser. CRF over pretrained encoder/decoder representations.

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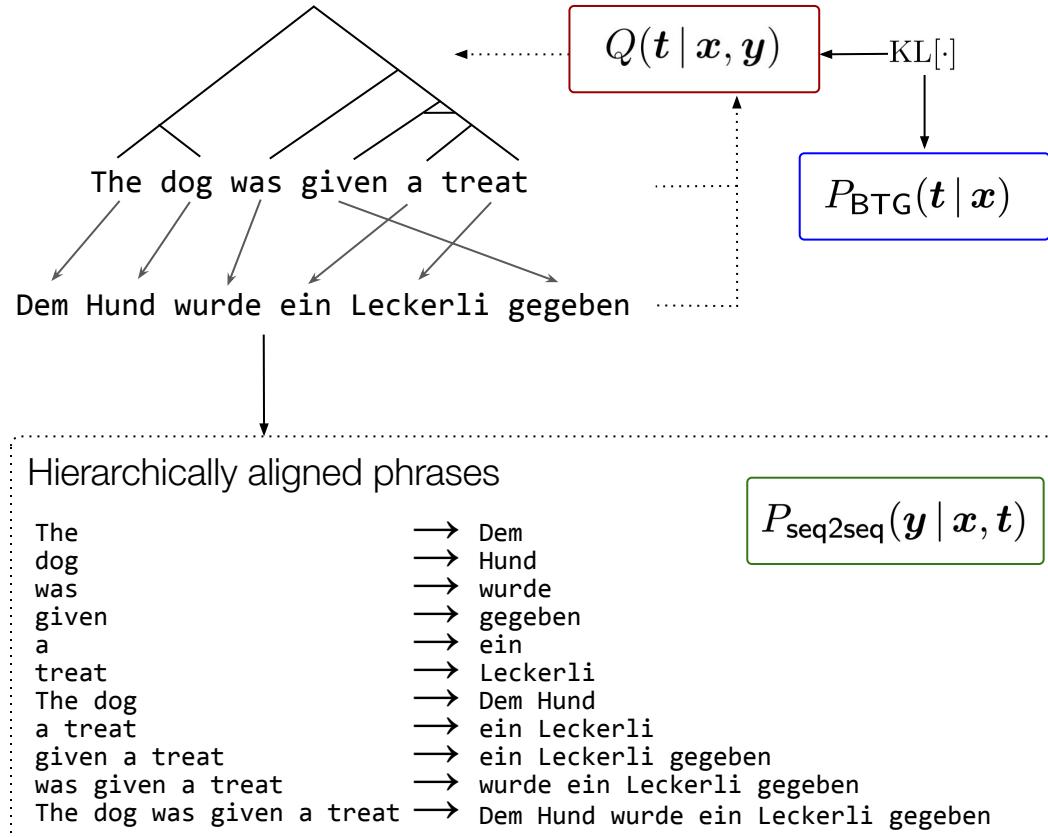
$P_{\text{BTG}}(t | x)$: “Prior” BTG parser. CRF over pretrained encoder/decoder representations.

$$\max_{\theta, \phi, \pi} \mathbb{E}_{Q(t | x, y; \phi)} [\log P_{\text{seq2seq}}(y | x, t; \theta)] - \text{KL}[Q(t | x, y; \phi) \| P_{\text{BTG}}(t | x; \pi)]$$

ϕ

θ

π



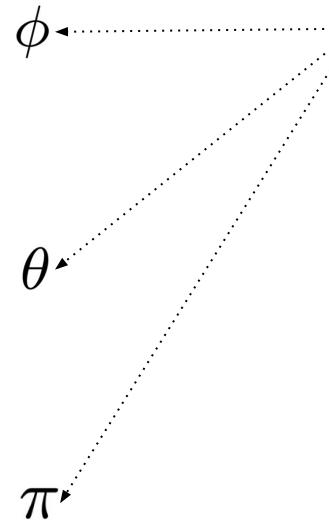
Learning

$Q(\mathbf{t} | \mathbf{x}, \mathbf{y})$: Variational Synchronous Parser. CRF over pretrained encoder/decoder representations.

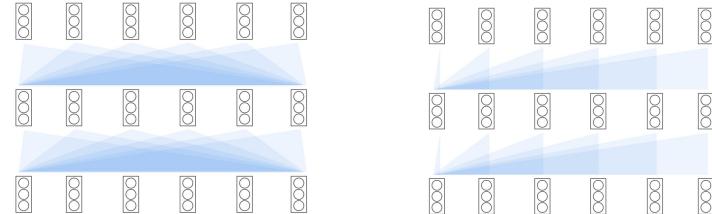
$P_{\text{seq2seq}}(\mathbf{y} | \mathbf{x}, \mathbf{t})$: Seq2seq model initialized with pretrained encoder/decoder. Finetuned on sampled source phrases.

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$$\max_{\theta, \phi, \pi} \mathbb{E}_{Q(\mathbf{t} | \mathbf{x}, \mathbf{y}; \phi)} [\log P_{\text{seq2seq}}(\mathbf{y} | \mathbf{x}, \mathbf{t}; \theta)] - \text{KL}[Q(\mathbf{t} | \mathbf{x}, \mathbf{y}; \phi) \| P_{\text{BTG}}(\mathbf{t} | \mathbf{x}; \pi)]$$



Pretrained Encoder-Decoder



Encoder-decoder parameter-sharing across all three models.

Encoder-decoder initialized (and finetuned) from the same backbone LM (mBART/mT5).

(Comparatively) Few additional parameters on top of the shared model.

Inference: Neural Grammar + Single-segment Decoding

Mode 1: Discard $P_{\text{BTG}}(\mathbf{t} \mid \mathbf{x})$ and decode with one segment (n=1)

Inference: Neural Grammar + Single-segment Decoding

Mode 1: Discard $P_{\text{BTG}}(\mathbf{t} \mid \mathbf{x})$ and decode with one segment ($n=1$)

$$\arg \max_{\mathbf{y} \in \mathcal{Y}} P_{\text{seq2seq}}(\mathbf{y} \mid \mathbf{x}, \mathbf{t} = \begin{array}{c} \text{open} \\ \text{i} \quad \text{the} \quad \text{box} \end{array})$$

$$= \arg \max_{\mathbf{y} \in \mathcal{Y}} P_{\text{LM}}(\mathbf{y} \mid \mathbf{x})$$

Inference: Neural Grammar + Single-segment Decoding

Mode 1: Discard $P_{\text{BTG}}(\mathbf{t} \mid \mathbf{x})$ and decode with one segment ($n=1$)

$$\begin{aligned} \arg \max_{\mathbf{y} \in \mathcal{Y}} P_{\text{seq2seq}}(\mathbf{y} \mid \mathbf{x}, \mathbf{t} = & \begin{array}{c} \text{open} \\ \text{i} \quad \text{the} \quad \text{box} \end{array}) \\ = \arg \max_{\mathbf{y} \in \mathcal{Y}} P_{\text{LM}}(\mathbf{y} \mid \mathbf{x}) \end{aligned}$$

Reduces to regular beam search in neural MT \Rightarrow Fast inference.

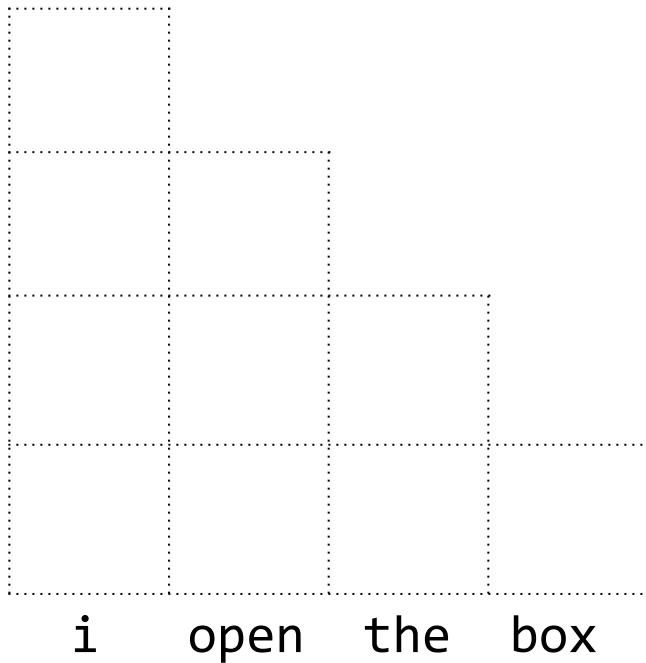
Use latent symbolic structures to softly guide (overly) flexible neural networks.

Inference: Neural Grammar + CKY Decoding

Mode 2: Jointly parse and translate. $\arg \max_{t,y} P_{\text{BTG}}(t | x) P_{\text{seq2seq}}(y | x, t)$

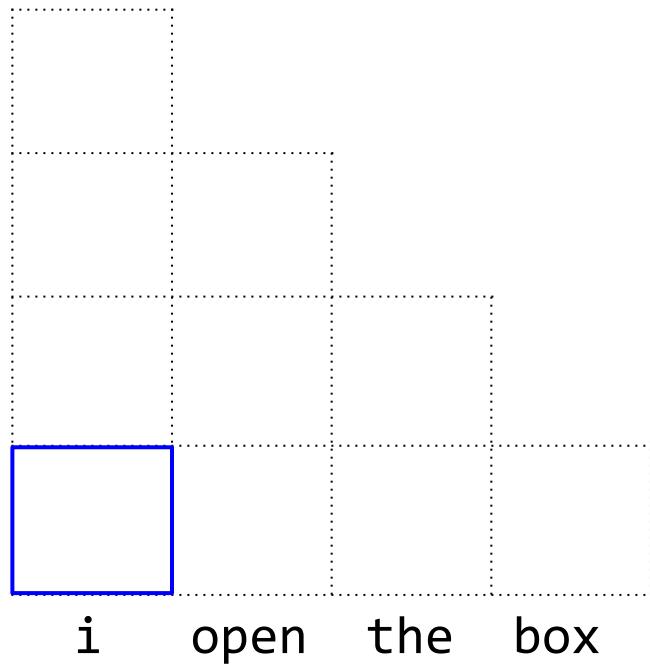
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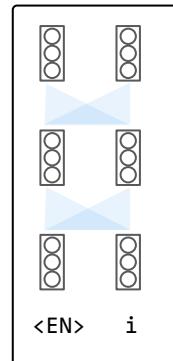


Inference: Neural Grammar + CKY Decoding

Mode 2: Jointly parse and translate. $\arg \max_{t,y} P_{\text{BTG}}(t | x) P_{\text{seq2seq}}(y | x, t)$



Encoder



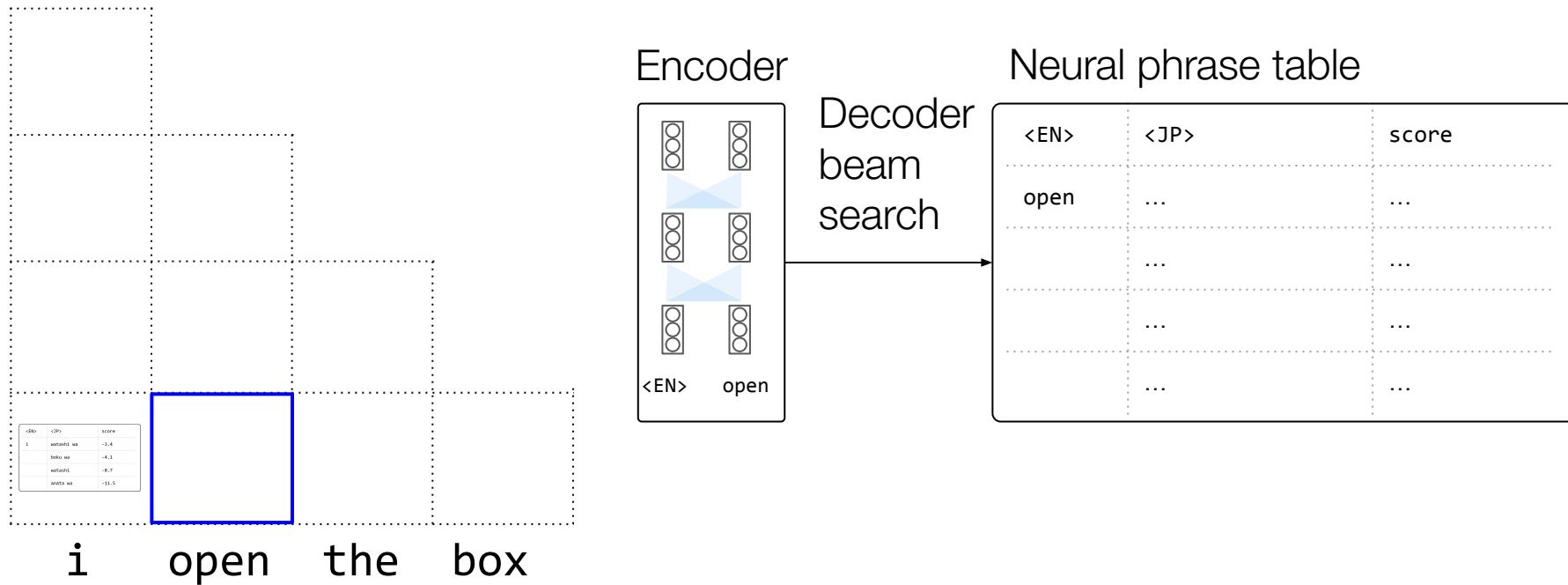
Decoder
beam
search

Neural phrase table

<EN>	<JP>	score
i	watashi wa	-3.4
	boku wa	-4.1
	watashi	-8.7
	anata wa	-11.5

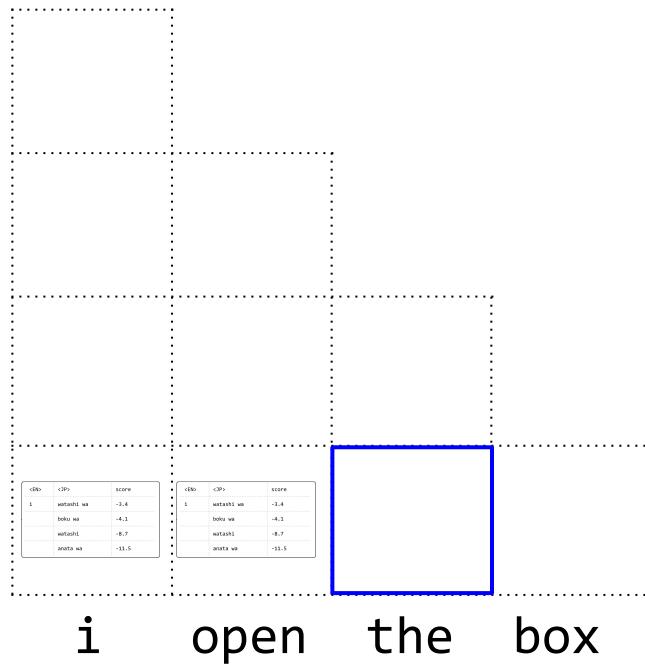
Inference: Neural Grammar + CKY Decoding

Mode 2: Jointly parse and translate. $\arg \max_{t,y} P_{\text{BTG}}(t | x) P_{\text{seq2seq}}(y | x, t)$

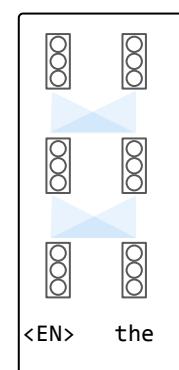


Inference: Neural Grammar + CKY Decoding

Mode 2: Jointly parse and translate. $\arg \max_{t,y} P_{\text{BTG}}(t | x) P_{\text{seq2seq}}(y | x, t)$



Encoder



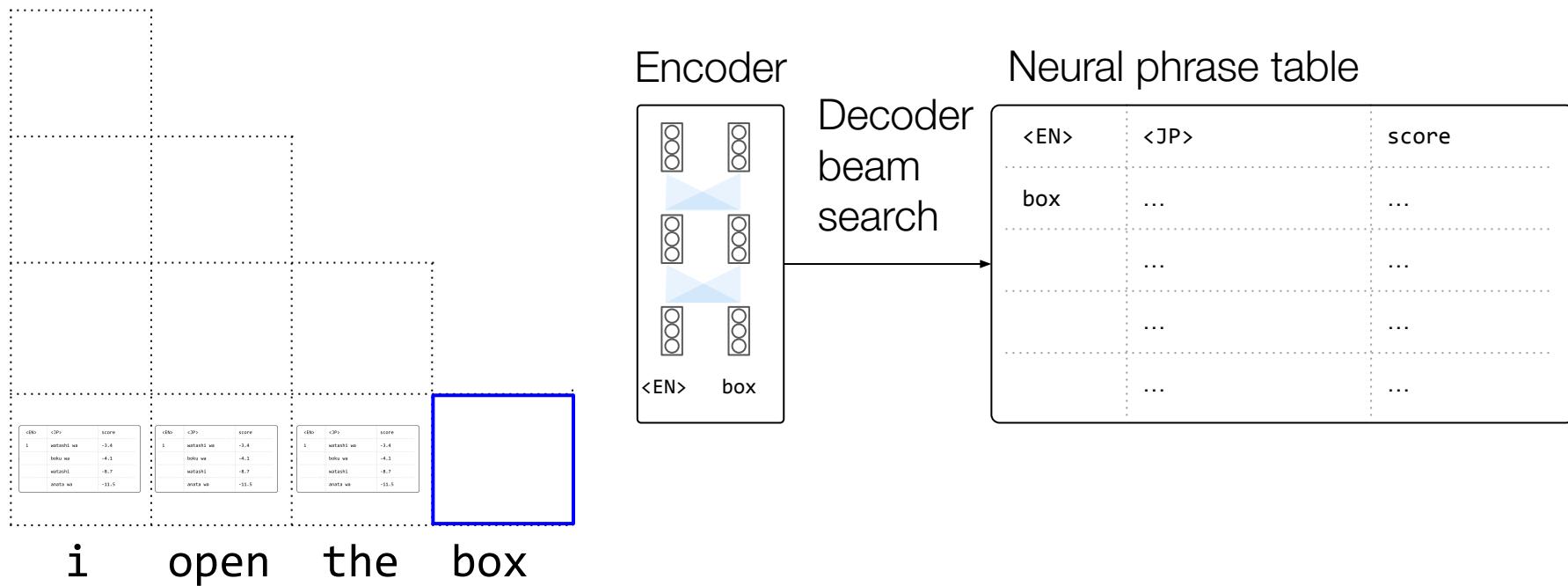
Decoder
beam
search

Neural phrase table

<EN>	<JP>	score
the
...
...
...

Inference: Neural Grammar + CKY Decoding

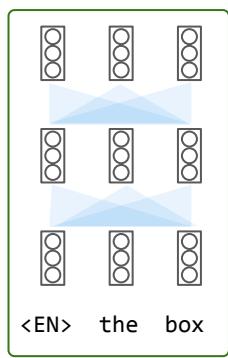
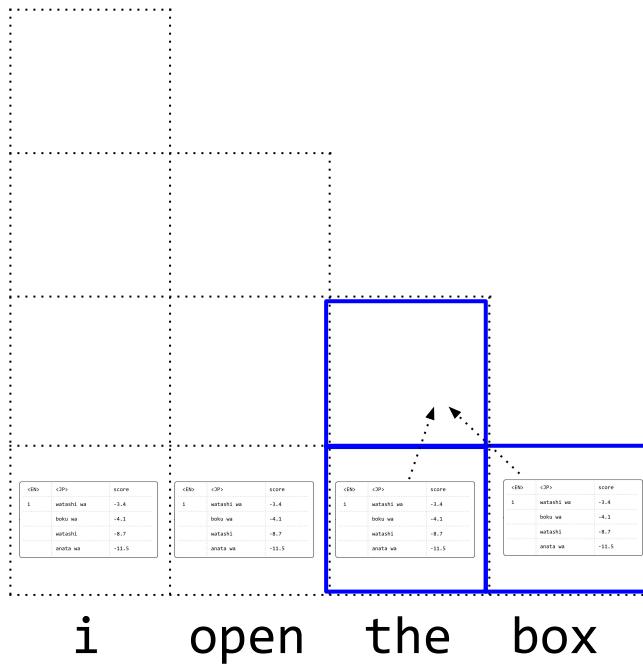
Mode 2: Jointly parse and translate. $\arg \max_{t,y} P_{\text{BTG}}(t | x) P_{\text{seq2seq}}(y | x, t)$



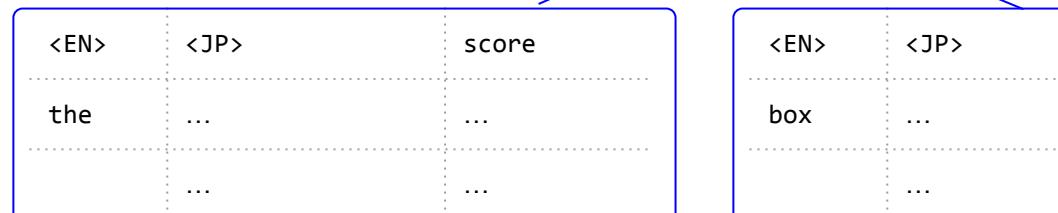
Inference: Neural Grammar + CKY Decoding

Mode 2: Jointly parse and translate.

phrase-level translation score +
merging children score



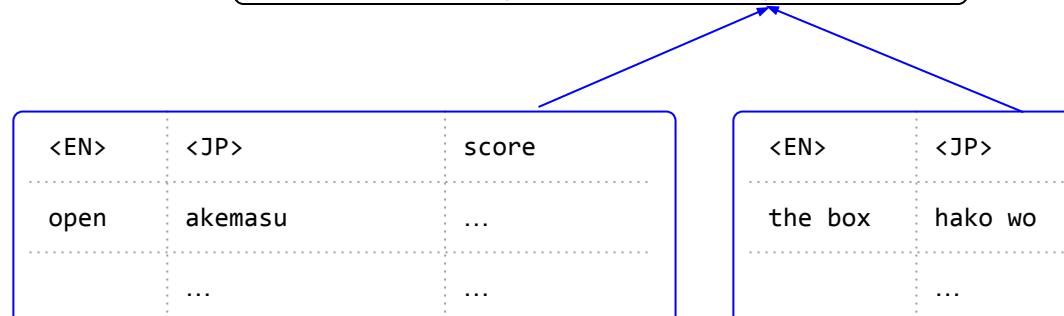
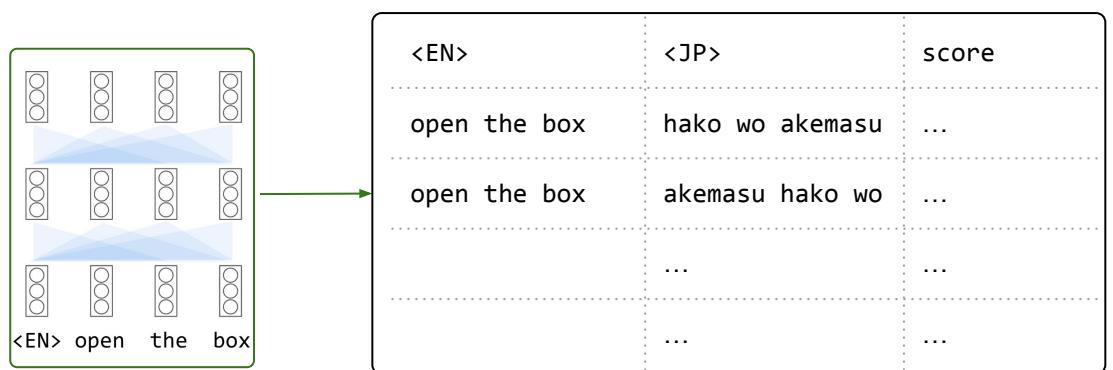
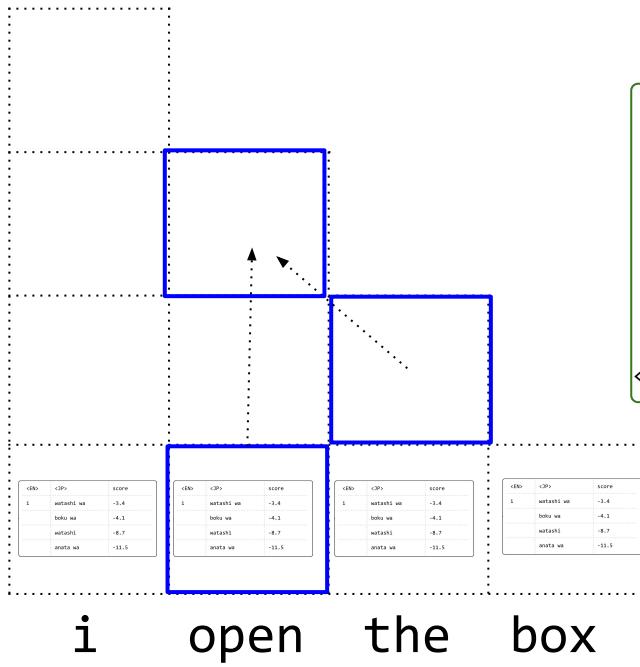
<EN>	<JP>	score
the box	hako wo	...
...
...
...



Inference: Neural Grammar + CKY Decoding

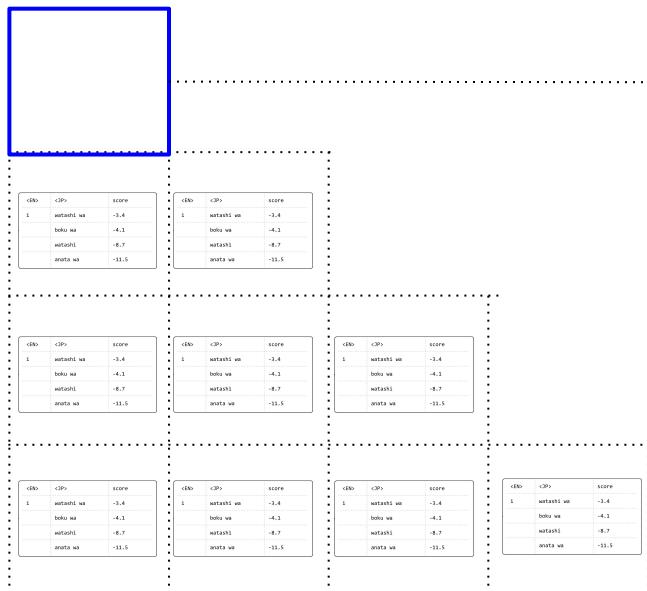
Mode 2: Jointly parse and translate.

phrase-level translation score +
merging children score +
phrase inversion score

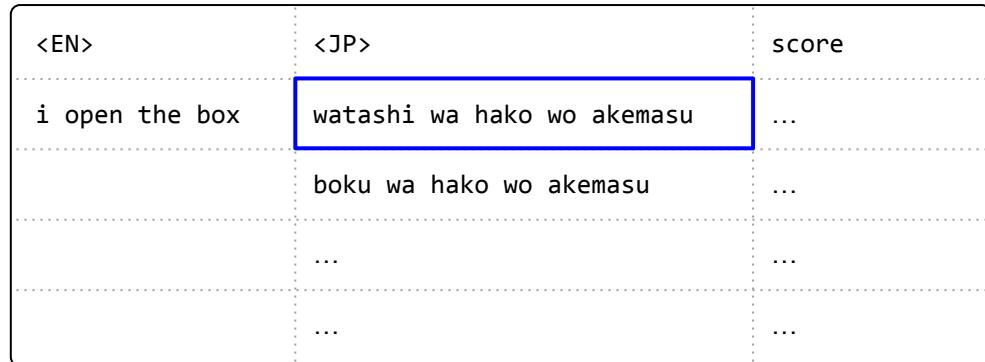


Inference: Neural Grammar + CKY Decoding

Mode 2: Jointly parse and translate. $\arg \max_{t,y} P_{\text{BTG}}(t|x) P_{\text{seq2seq}}(y|x, t)$



i open the box

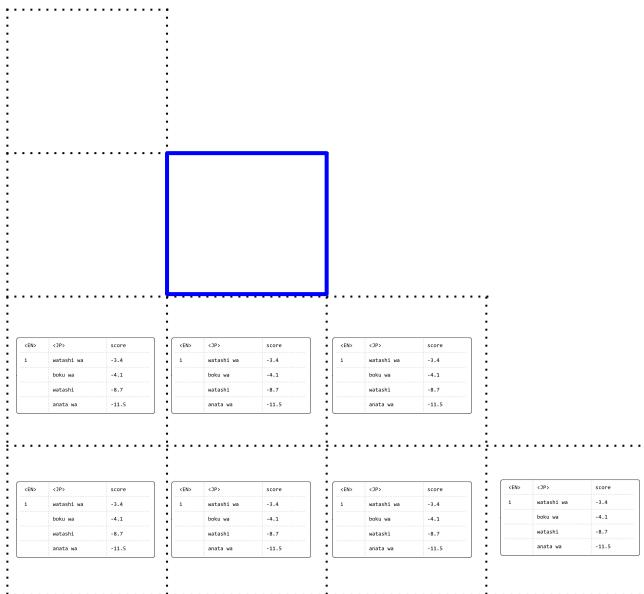


CKY-style bottom up dynamic
programming + beam search from LM.

"Cube-pruned" CKY [Huang and Chiang '05]

Inference: Neural Grammar + CKY Decoding

Mode 2: Jointly parse and translate. $\arg \max_{t,y} P_{\text{BTG}}(t | x) P_{\text{seq2seq}}(y | x, t)$



<EN>	<JP>	score
walking on air	kuuchuu o aruite imasu	-4.2
	kuuchuu o aruite iru	-6.5
...

Inference: Neural Grammar + CKY Decoding

Mode 2: Jointly parse and translate. $\arg \max_{t,y} P_{\text{BTG}}(t | x) P_{\text{seq2seq}}(y | x, t)$

CKY			
	cP _i	cP _j	score
1	watashi wa	-3.4	
	boku wa	-4.2	
	watashi	-8.7	
	arita wa	-11.5	

CKY			
	cP _i	cP _j	score
1	watashi wa	-3.4	
	boku wa	-4.2	
	watashi	-8.7	
	arita wa	-11.5	

CKY			
	cP _i	cP _j	score
1	watashi wa	-3.4	
	boku wa	-4.2	
	watashi	-8.7	
	arita wa	-11.5	

i'm walking on

English

i'm walking on air



<EN>

walking on air

<JP>

kuuchuu o aruite imasu

score

-4.2

kuuchuu o aruite iru

-6.5

YO

Translate to Japanese in romaji:

i'm walking on air



watashi wa kuuchuu wo aruite iru

Open in Google Translate • Feedback

Inference: Neural Grammar + CKY Decoding

Mode 2: Jointly parse and translate. $\arg \max_{t,y} P_{\text{BTG}}(t | x) P_{\text{seq2seq}}(y | x, t)$

CKY			
	cP _i	cP _j	score
1	watashi wa	-3.4	
boku wa	-4.2		
watashi	-8.7		
arata wa	-11.5		

CKY			
	cP _i	cP _j	score
1	watashi wa	-3.4	
boku wa	-4.2		
watashi	-8.7		
arata wa	-11.5		

CKY			
	cP _i	cP _j	score
1	watashi wa	-3.4	
boku wa	-4.2		
watashi	-8.7		
arata wa	-11.5		

i'm walking on

English

i'm walking on air



<EN>

walking on air

<JP>

kuuchuu o aruite imasu

score

-4.2

kuuchuu o aruite iru

-6.5

YO

Translate to Japanese in romaji:

i'm walking on air

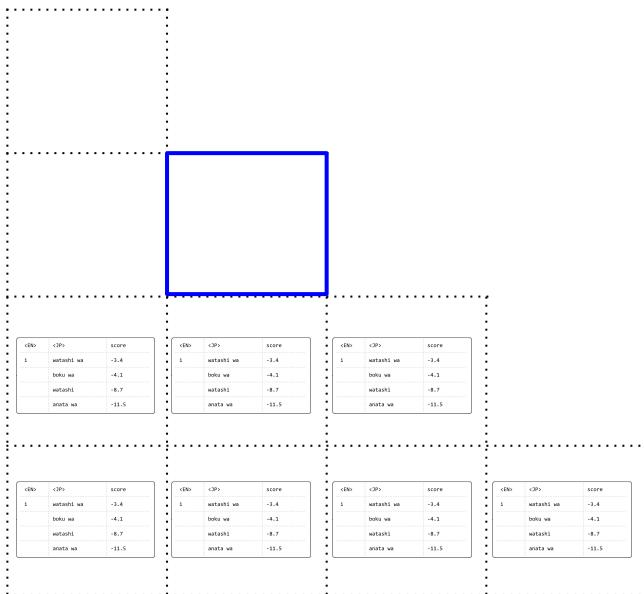


watashi wa kuuchuu wo aruite iru

Open in Google Translate • Feedback

Inference: Neural Grammar + CKY Decoding

Mode 2: Jointly parse and translate. $\arg \max_{t,y} P_{\text{BTG}}(t | x) P_{\text{seq2seq}}(y | x, t)$



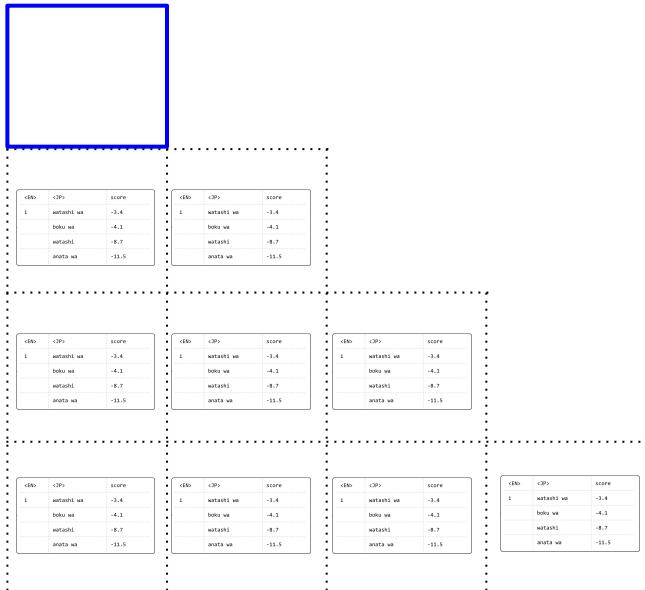
i'm walking on air

<EN>	<JP>	score
walking on air	totemo wakuwaku shiteimasu	0
	kuuchuu o aruite imasu	-4.2
	kuuchuu o aruite iru	-6.5

$$P(\text{"totemo wakuwaku shiteimasu"} | \text{"walking on air"}) = 1$$

Inference: Neural Grammar + CKY Decoding

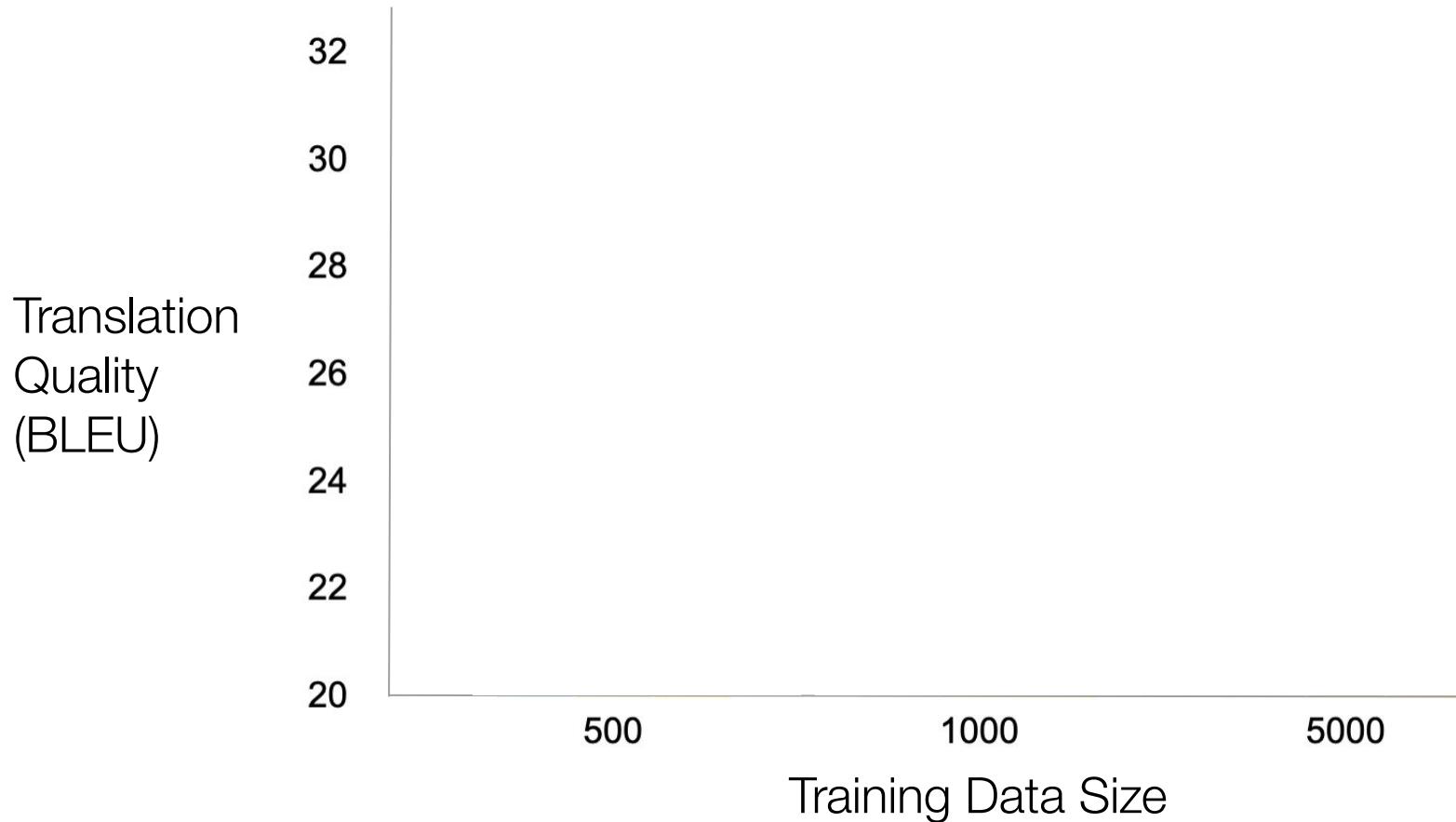
Mode 2: Jointly parse and translate. $\arg \max_{t,y} P_{\text{BTG}}(t|x) P_{\text{seq2seq}}(y|x, t)$



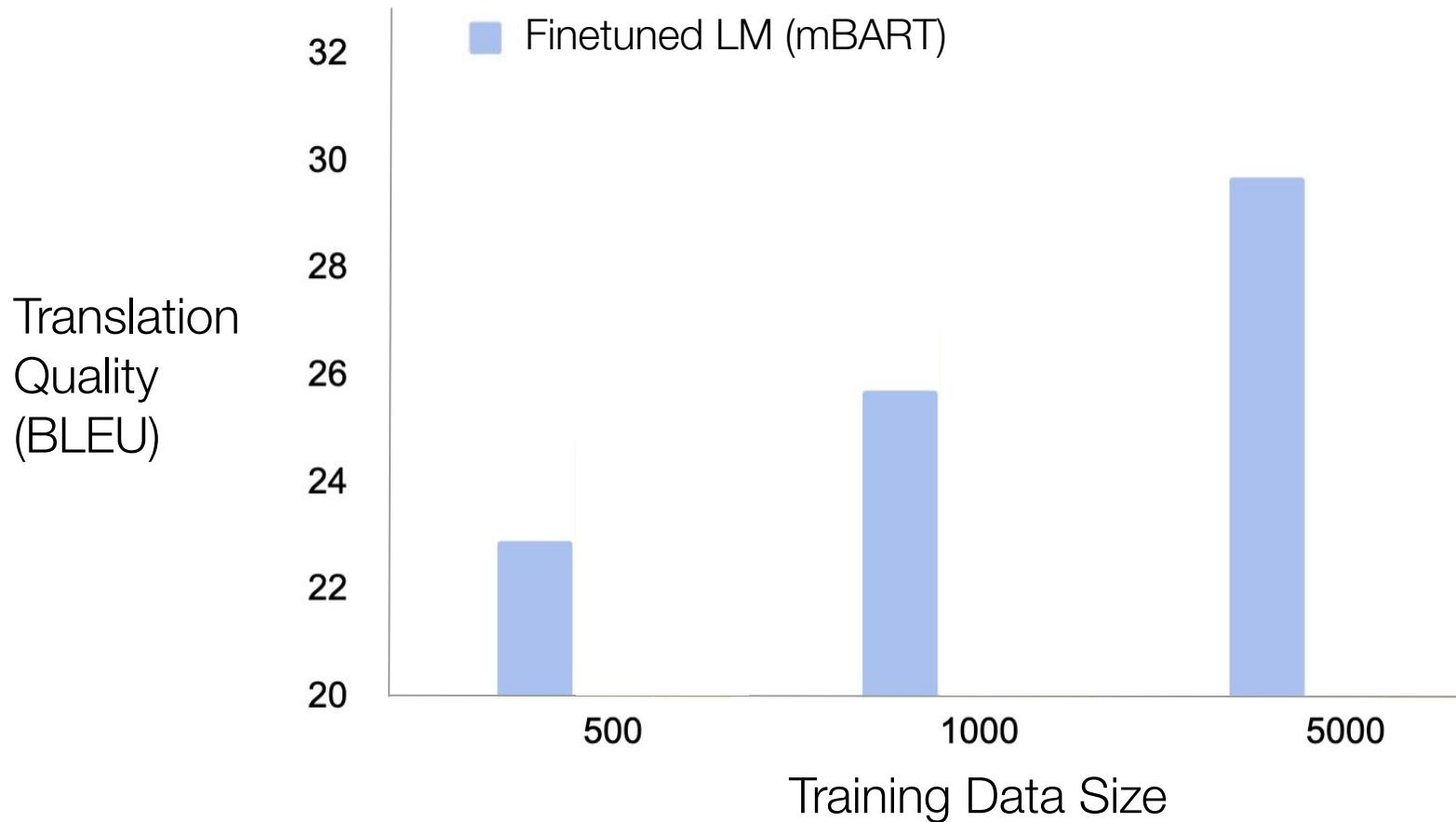
More expensive than single-segment decoding, but can incorporate new translation rules during inference for idioms & transliterations.

i'm walking on air

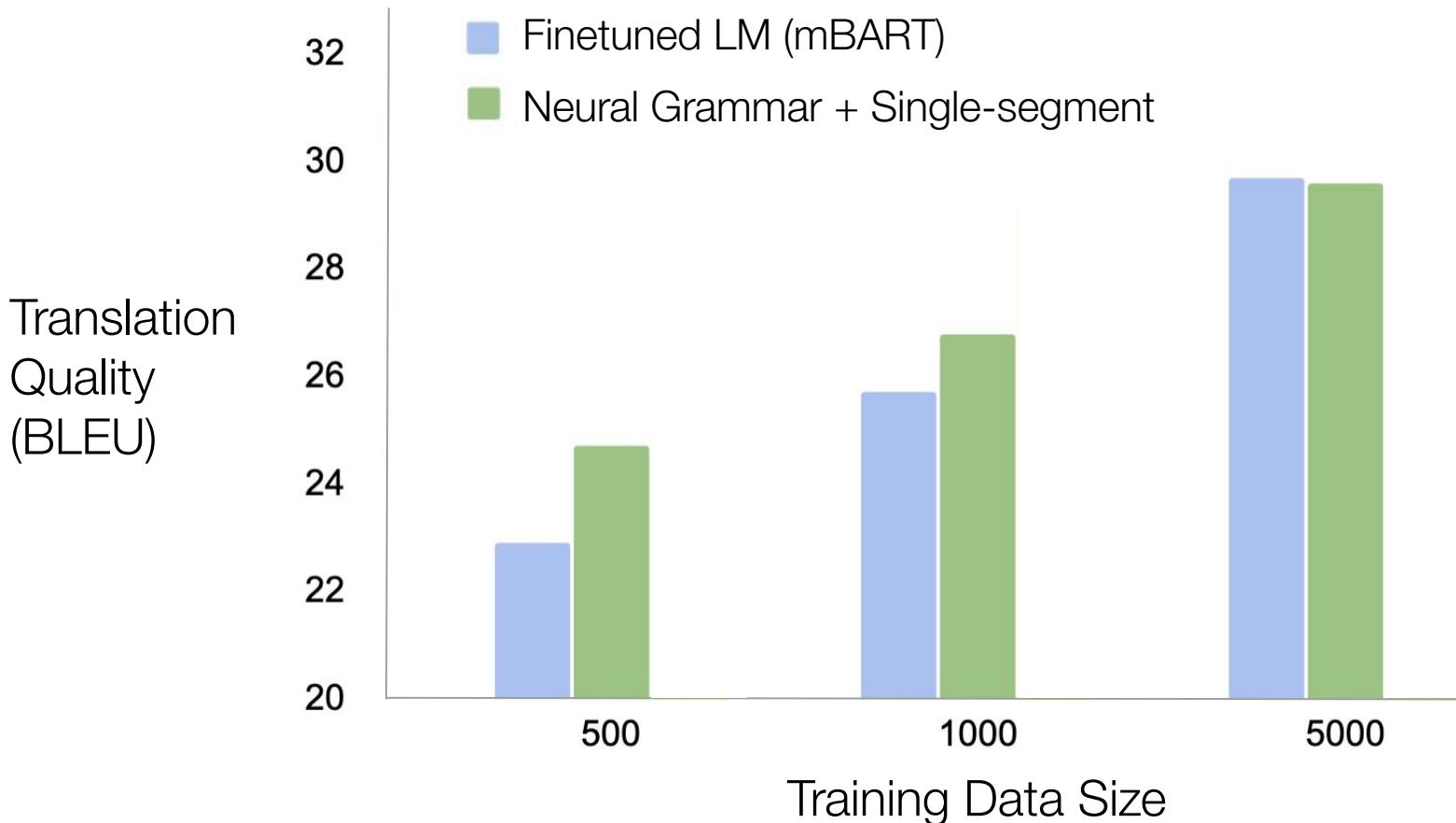
Results: German → English



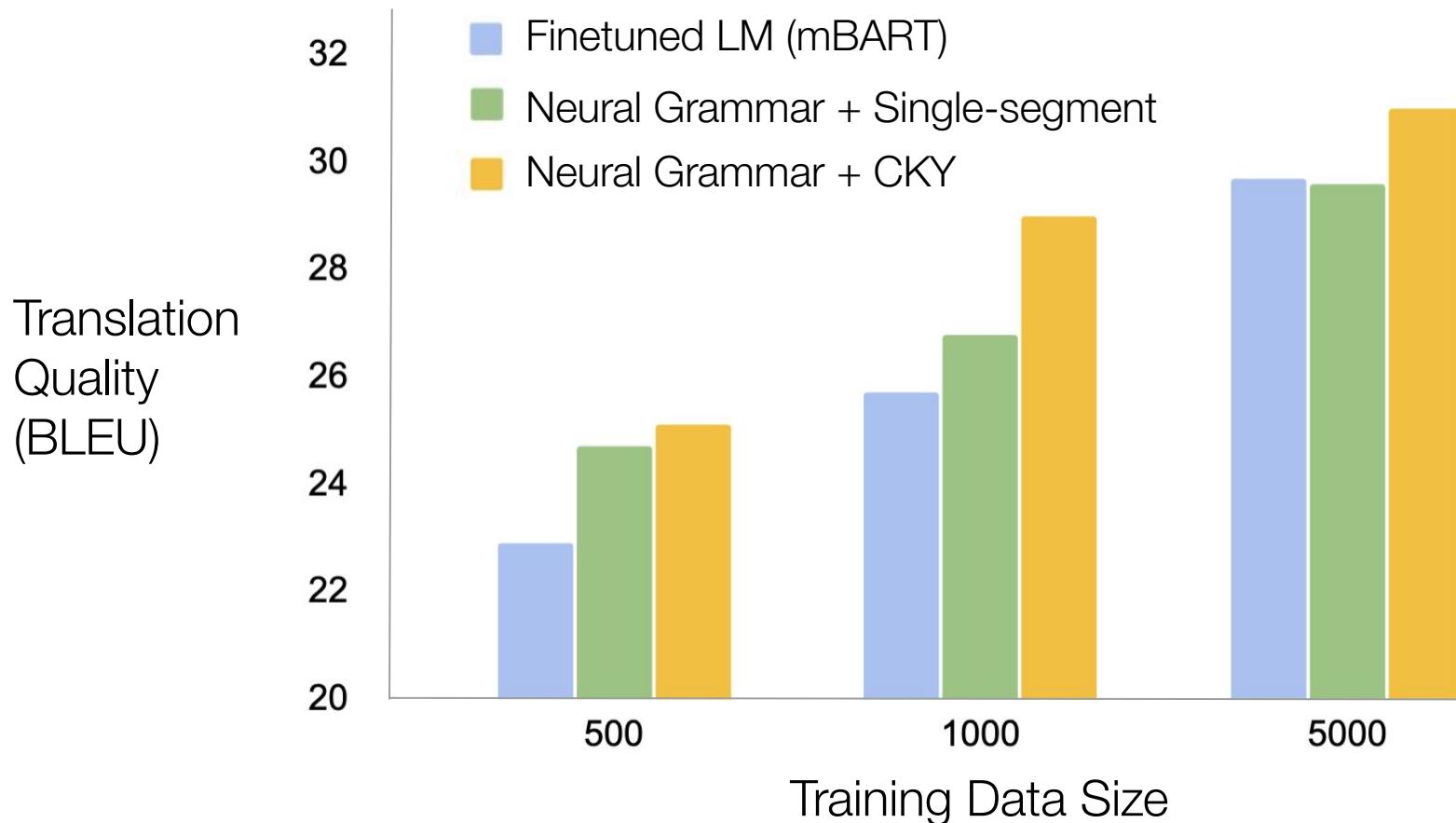
Results: German → English



Results: German → English



Results: German → English



Results: German → English

Input: Er hat das Unternehmen *von Grund auf* aufgebaut

New translation rule: *von Grund auf* → *from scratch*

Original Prediction: He built the company from the ground up

New Prediction: He built the company from scratch

Reference: He built the company from scratch

Google Translate: He built the company from the ground up

Input: Die europäische Krise *schließt den Kreis*

New translation rule: *schließt den Kreis* → *is coming full circle*

Original Prediction: The euro crisis closes the loop

New Prediction: The European crisis is coming full circle

Reference: The European crisis is coming full circle

Google Translate: The European crisis closes the circle

Input: Die ARD strahlte gestern um 20:15 "Aus dem Nichts" aus

New translation rule: "Aus dem Nichts" → "In the Fade", 20:15 → 8.15 pm

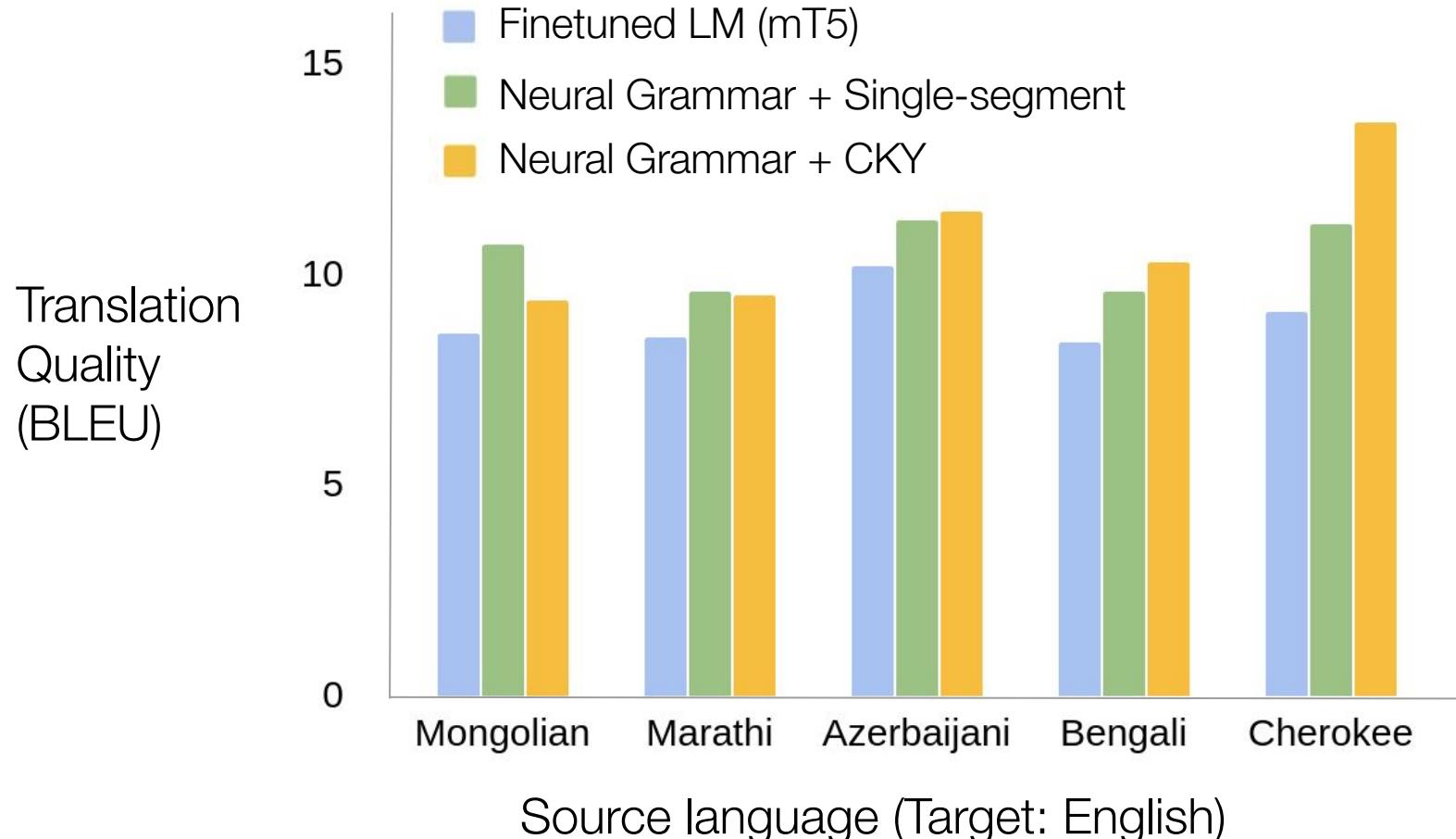
Original Prediction: The ARD aired yesterday at 20:15 "Out of Nowhere"

New Prediction: The ARD aired yesterday 8.15 pm "In the Fade"

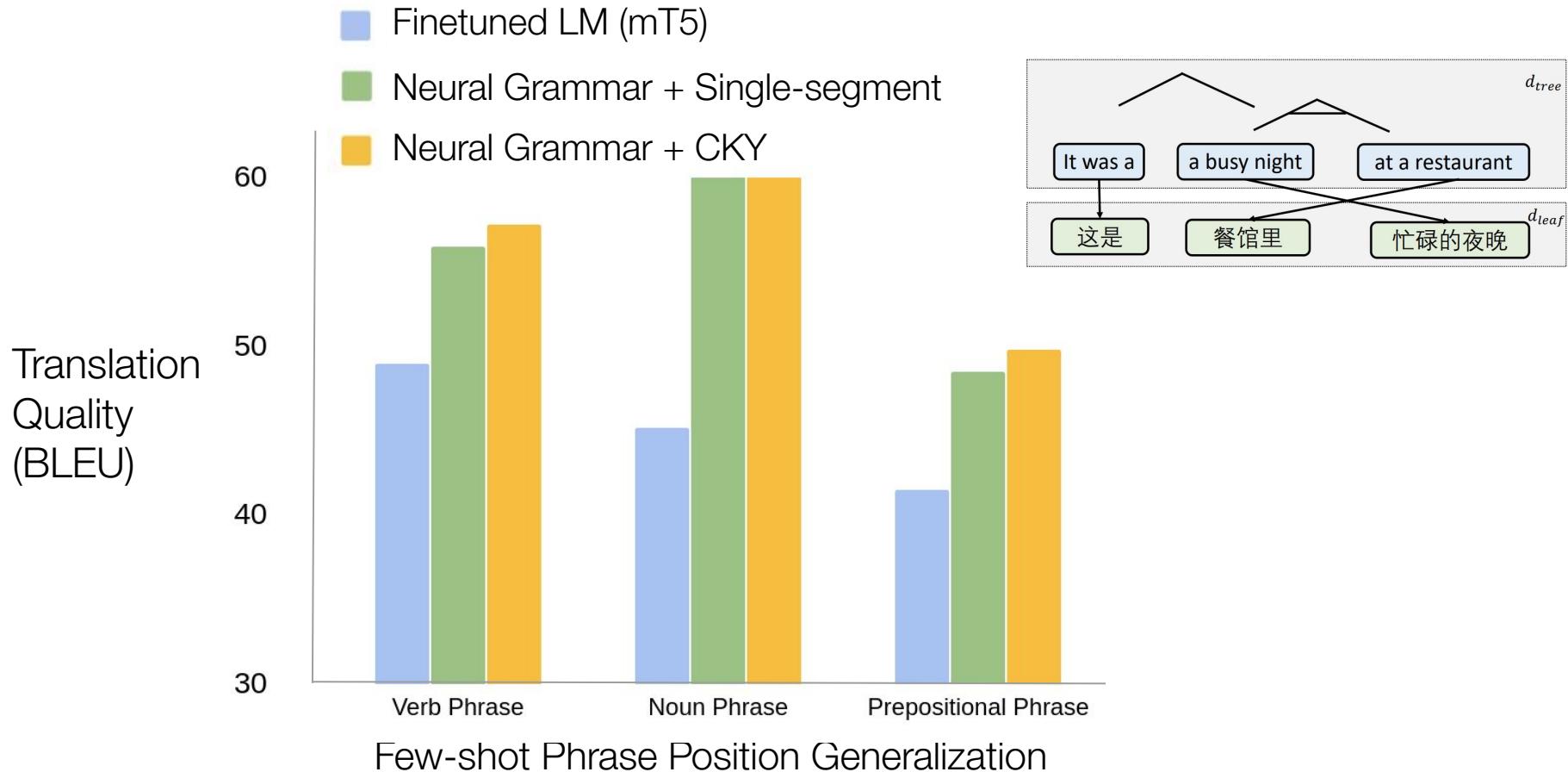
Reference: ARD broadcast "In the Fade" yesterday at 8.15 pm

Google Translate: Yesterday at 8:15 p.m., ARD broadcast "Out of Nowhere".

Results: Low Resource MT



Results: “Compositional” MT on English→Chinese



Summary

Latent symbolic structures (hierarchical phrase alignments) can be used in conjunction with pretrained LMs.

Neural grammar can incorporate “hard” translation rules during inference.

Still requires finetuning the pretrained model... what if we can't?

Translate the following sentence to English:
Pada dasarnya, hal tersebut terbagi ke dalam dua kategori: Anda bekerja sambil mengadakan perjalanan atau mencoba mencoba atau membatasi pengeluaran Anda. Artikel ini berfokus pada hal yang terakhir.

In this context, the word "sambil" means "while"; the word "membatasi" means "limiting", "restrict", "limit".

The full translation to English is: *Basically, they fall into two categories: Either work while you travel or try and limit your expenses. This article is focused on the latter.*

Translate the following sentence to English:
Ia melakukan pembuatan bel pintu dengan teknologi WiFi, katanya.

In this context, the word "pembuatan" means "creation"; the word "bel" means "buzzer", "bell"; the word "pintu" means "door", "doors".

The full translation to English is:

“Dictionary Prompting” [Ghazvininejad et al. '23]

Symbolic Structures for Controlling & Augmenting LLMs

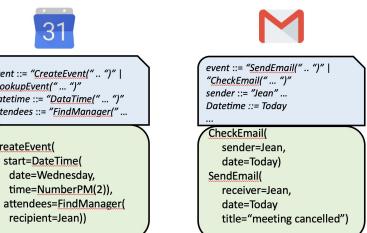
TL;DR. Use grammars within in-context learning to improve generation of strings in a “structured” language (DSL).

Bailin Wang, Zi Wang, Rif A. Saurous, Xuezhi Wang, Yuan Cao, Yoon Kim
EMNLP '22

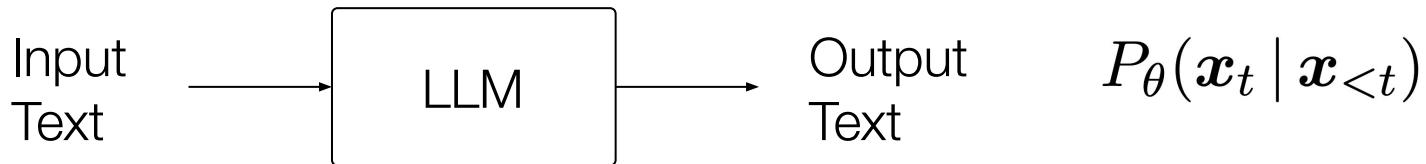


Grammar Prompting for DSL generation with Large Language Models

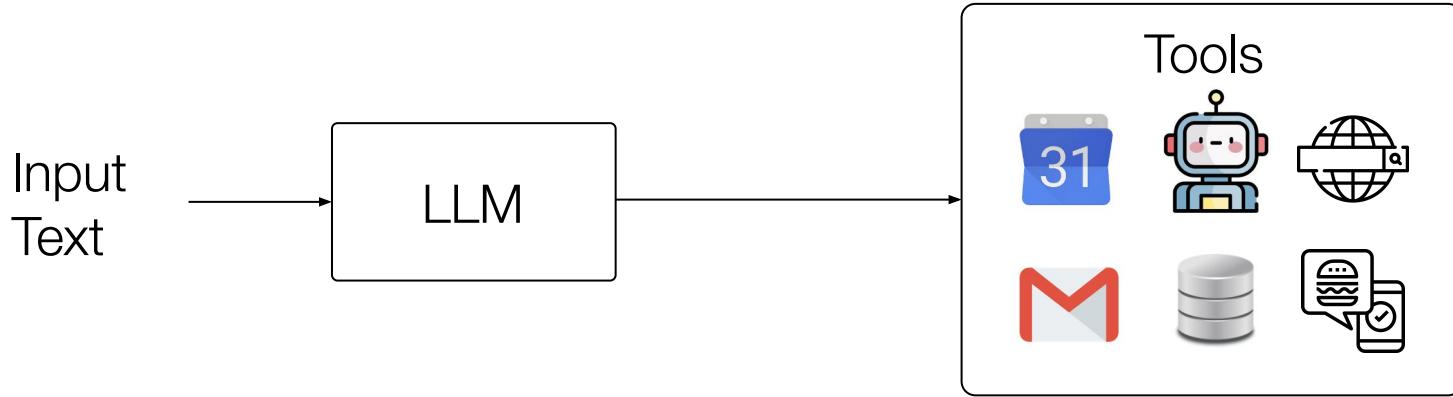
Bailin Wang, Zi Wang, Rif A. Saurous, Xuezhi Wang, Yuan Cao, Yoon Kim
NeurIPS '23



LLMs & The External World



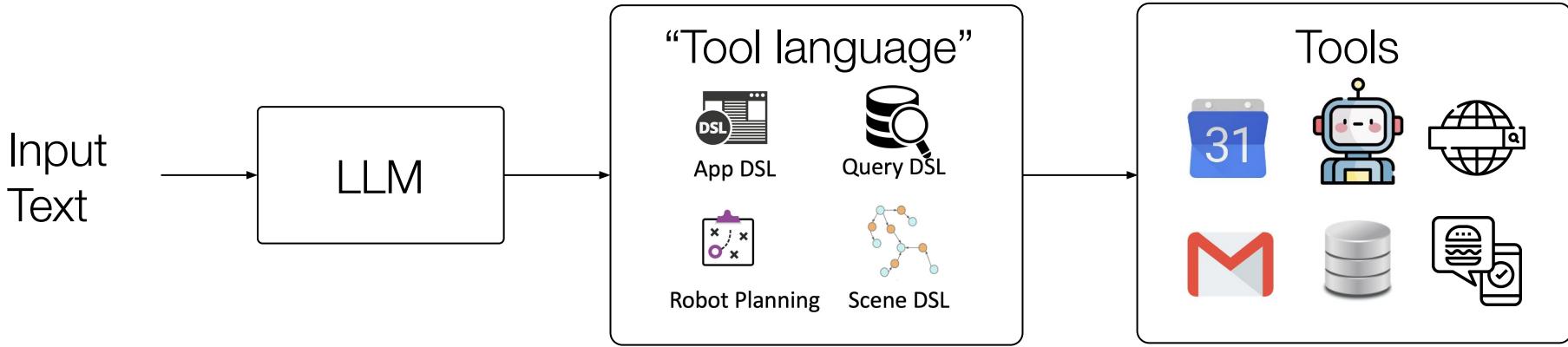
LLMs & The External World



How can we get LLMs to

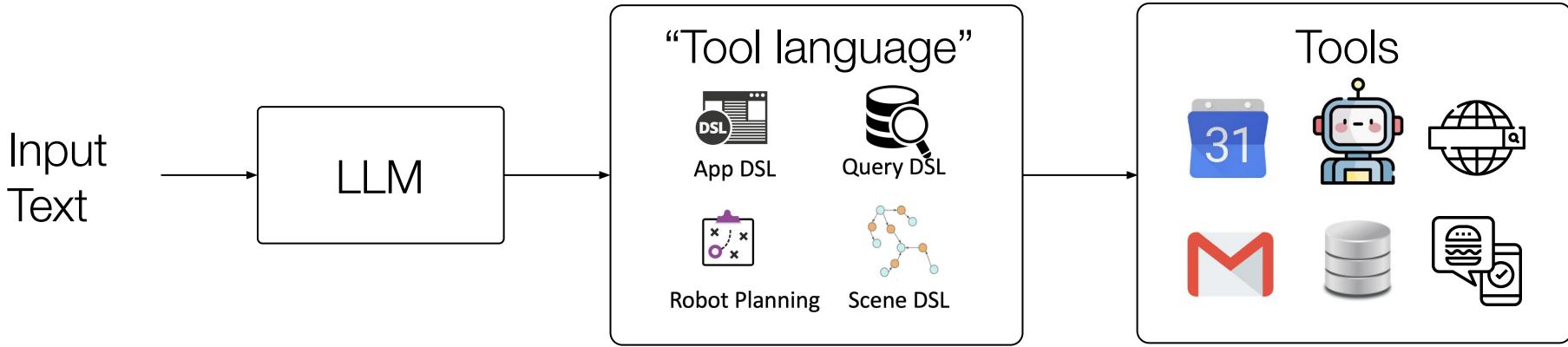
book appointments?
send emails?
search?
affect the external world?

LLMs & Tools



... through domain-specific tool languages (DSL)!

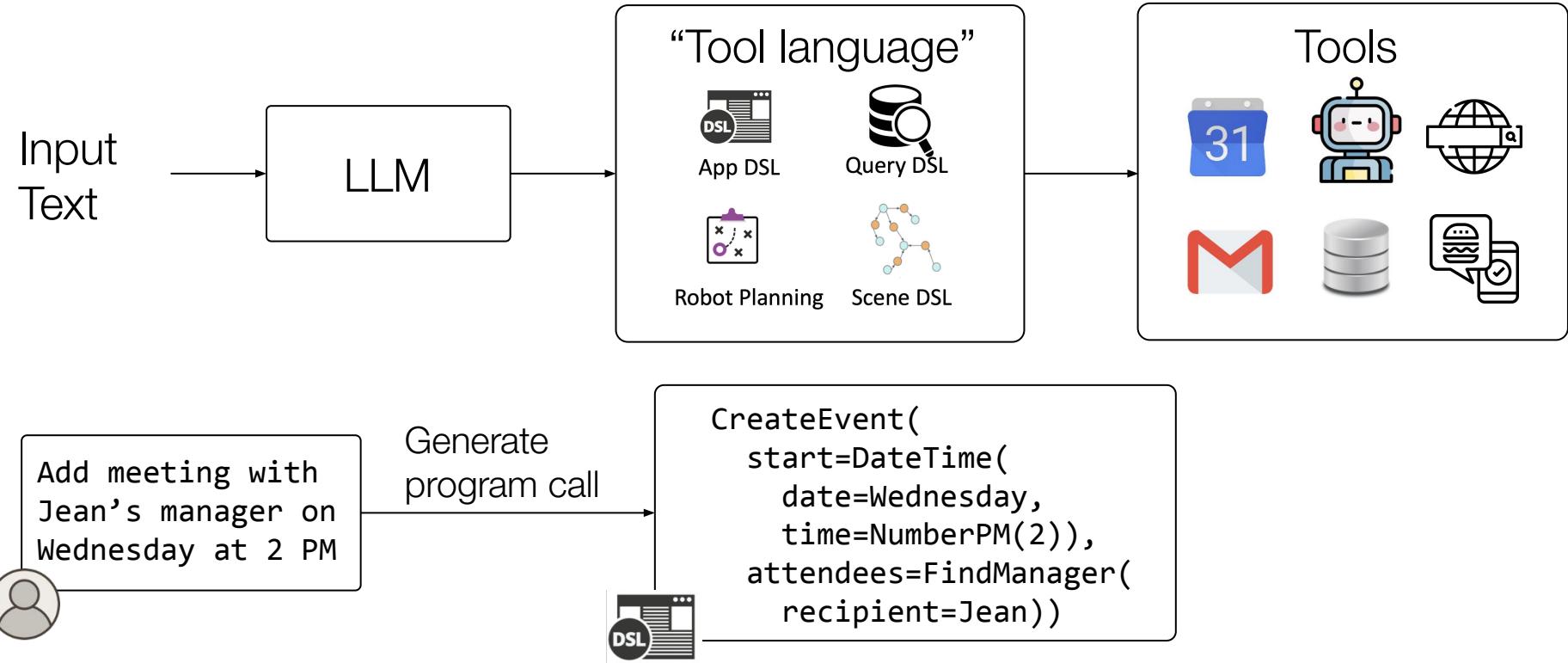
LLMs & Tools



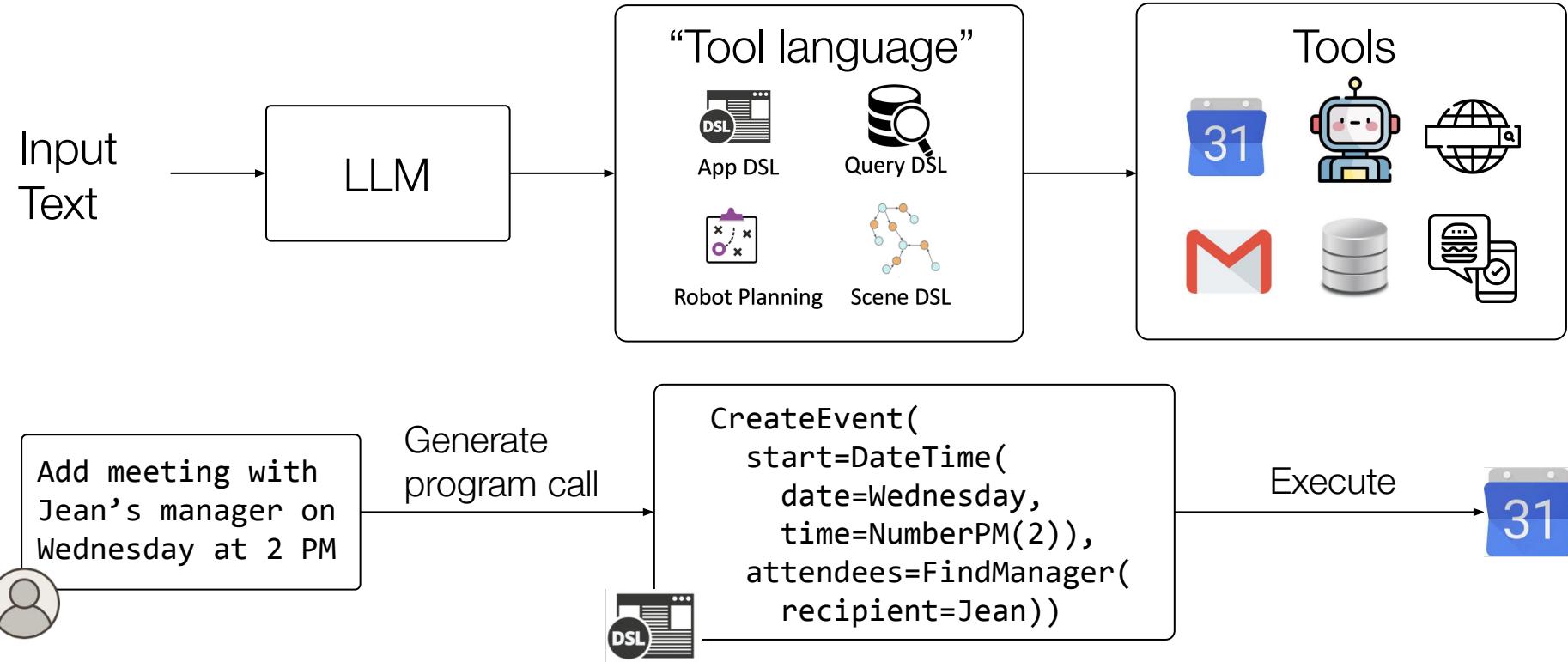
Add meeting with
Jean's manager on
Wednesday at 2 PM



LLMs & Tools



LLMs & Tools



LLMs & Tools

ChatGPT plugins

We've implemented initial support for plugins in ChatGPT. Plugins are tools designed specifically for language models with safety as a core principle, and help ChatGPT access up-to-date information, run computations, or use third-party services.

 Expedia Bring your trip plans to life—get there, stay there, find things to see and do.	 FiscalNote Provides and enables access to select market-leading, real-time data sets for legal, political, and regulatory data and information.	 Instacart Order from your favorite local grocery stores.
 KAYAK Search for flights, stays and rental cars. Get recommendations for all the places you can go within your budget.	 Klarna Shopping Search and compare prices from thousands of online shops.	 Milo Family AI Giving parents superpowers to turn the manic to magic, 20 minutes each day. Ask: Hey Milo, what's magic today?
 OpenTable Search for restaurants available for booking dining experiences.	 Shop Search for millions of products from the world's greatest brands.	 Speak Learn how to say anything in another language with Speak, your AI-powered language tutor.
 Wolfram Access computation, math, curated knowledge & real-time data through Wolfram Alpha and Wolfram Language.	 Zapier Interact with over 5,000+ apps like Google Sheets, Trello, Gmail, HubSpot, Salesforce, and more.	

LLMs & Tools



how do this year's oscar winners compare to recently released movies for box office sales?

Finished browsing

Searched: "2023 Oscar winners box office sales compared to recently released movies"
Clicked on: Oscars 2023: Everything Everywhere All at Once Domi...
Reading content

Searched: "recently released movies box office sales"
Clicked on: Domestic Box Office For Mar 16, 2023 - Box Office Mojo
Reading content
Finished browsing

The 2023 Oscar winner for Best Picture, "Everything Everywhere All at Once," earned \$100 million at the box office¹. Recently released movies such as "Scream VI" have grossed \$58,529,284 in its first seven days². While "Scream VI" has had a strong start at the box office, it's worth noting that "Everything Everywhere All at Once" has had a longer run in theaters to accumulate its \$100 million in box office sales.

Search



What is the integral of $x^2 \cos(2x)$?

Used Wolfram

The integral of $x^2 \cos(2x)$ with respect to x is:

$$\frac{x \cos(2x)}{2} + \frac{(-1 + 2x^2) \sin(2x)}{4} + C$$

where C is the constant of integration.

Math

```
find_restaurant(  
    type=vegan  
    location=San Francisco,  
    time=Saturday)
```



Looking to eat vegan food in San Francisco this weekend. Could you get me one great restaurant suggestion for Saturday and a simple recipe for Sunday (just the ingredients)? Please calculate the calories for the recipe using WolframAlpha. Finally order the ingredients on Instacart.

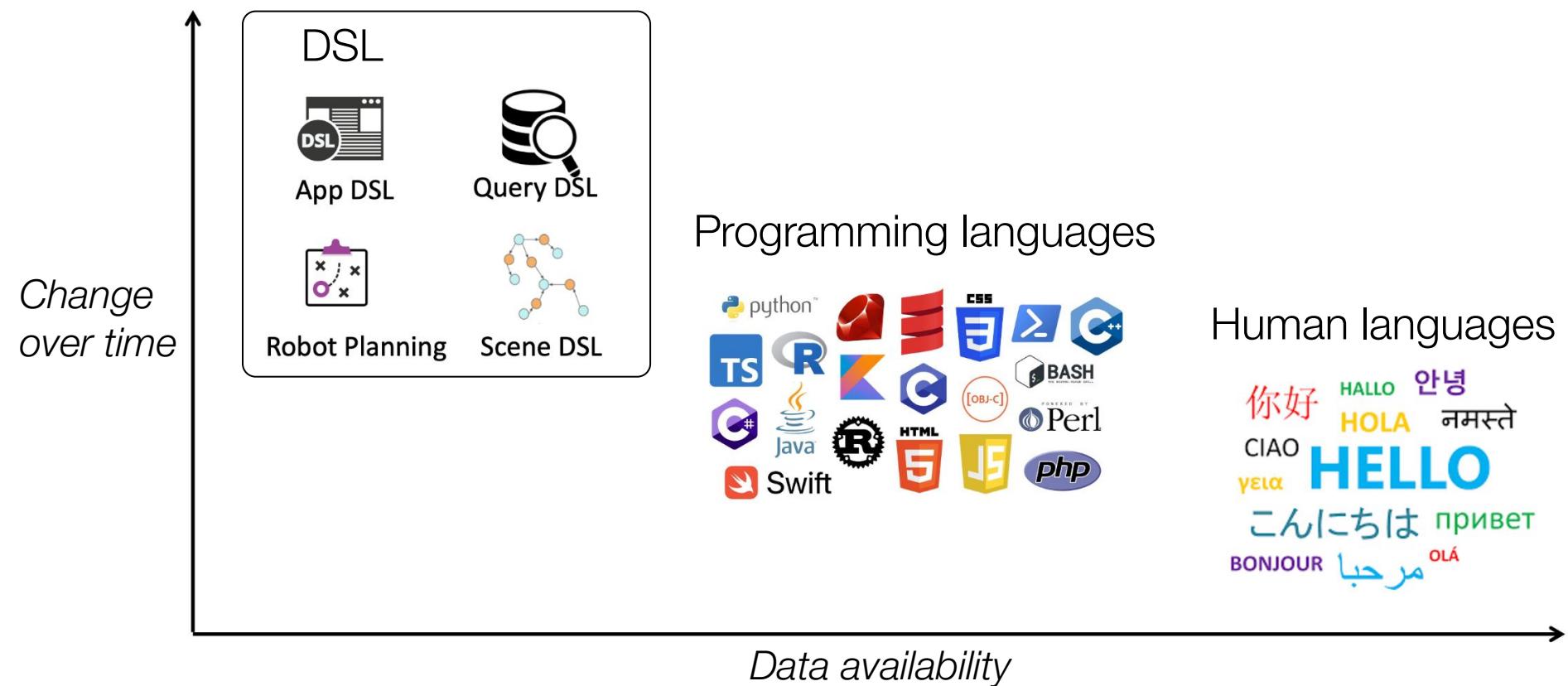
Used OpenTable

I found a great vegan restaurant in San Francisco for you to try on Saturday: [Greens Restaurant](#). You can make a reservation for your desired time through the provided link.

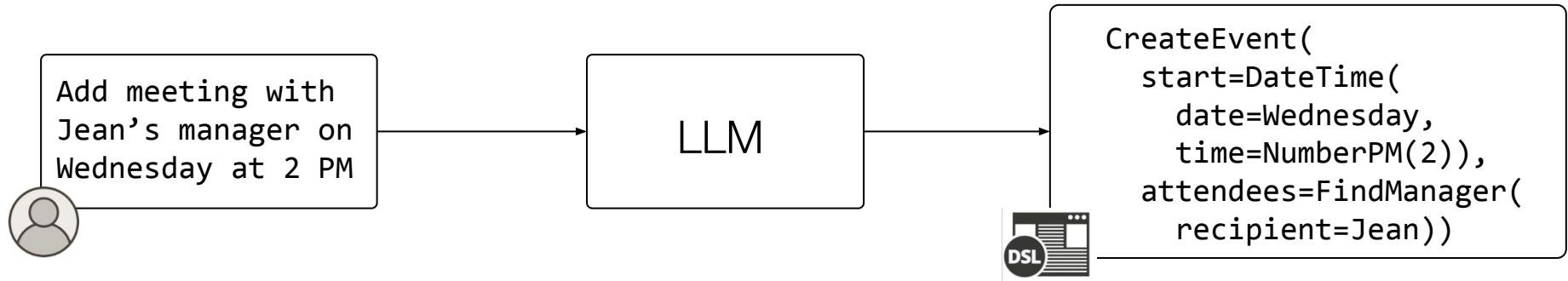
Restaurant reservation

[OpenAI]

LLMs & DSL: Challenges



LLMs for Generating DSL (Semantic Parsing)



LLMs for Generating DSL (Semantic Parsing)

“In-context”
demonstrations
(from training)



What time on Tuesday is my planning meeting?

```
start(findEvent(EventSpec( name='planning',
    start=DateTimeSpec(weekday=tuesday))))
```

Can you remind me to go to the airport tomorrow morning at 8am?

```
createCommitEventWrapper(
    createPreflightEventWrapper(
        EventBuilder(subject='go to the airport',
            start=dateAtTime( date=tomorrow(),
                time=numberAM(8)))))
```

Add meeting with Jean's manager on Wednesday at 2 PM

} Input 1
} Output 1
} Input 2
} Output 2

LLMs for Generating DSL (Semantic Parsing)

“In-context”
demonstrations
(from training)



What time on Tuesday is my planning meeting?

```
start(findEvent(EventSpec( name='planning',  
    start=DateTimeSpec(weekday=tuesday))))
```

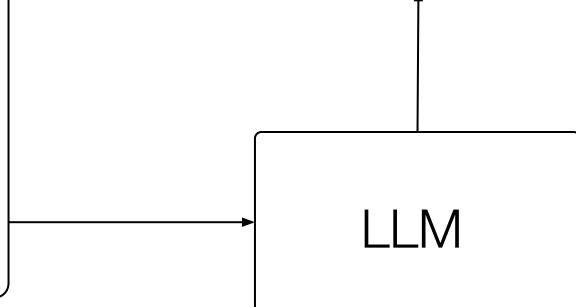
Can you remind me to go to the airport tomorrow morning at 8am?

```
createCommitEventWrapper(  
    createPreflightEventWrapper(  
        EventBuilder(subject='go to the airport',  
            start=dateAtTime( date=tomorrow(),  
                time=numberAM(8))))
```

⋮

Add meeting with Jean’s manager on Wednesday at 2 PM

```
CreateEvent(start=DateTime(  
    date=Wednesday,  
    time=NumberPM(2)),  
    attendees=FindManager(  
        recipient=Jean))
```



LLMs for Generating DSL (Semantic Parsing)

“In-context”
demonstrations
(from training)



What time on Tuesday is my planning meeting?

```
start(findEvent(EventSpec( name='planning',  
    start=DateTimeSpec(weekday=tuesday))))
```

Can you remind me to go to the airport tomorrow morning at 8am?

```
createCommitEventWrapper(  
    createPreflightEventWrapper(  
        EventBuilder(subject='go to the airport',  
            start=dateAtTime( date=tomorrow(),  
                time=numberAM(8))))
```

Add meeting with Jean’s manager on Wednesday at 2 PM

Where do these outputs come from?

```
CreateEvent(start=DateTime(  
    date=Wednesday,  
    time=NumberPM(2)),  
    attendees=FindManager(  
        recipient=Jean))
```



DSL for a Scheduling Assistant

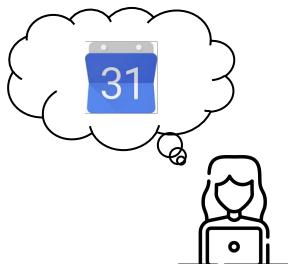


Domain expert

DSL for a Scheduling Assistant

```
call ::= event | "(Yield org)" | "(Yield (size org))" | "(Yield event)" | "(Yield weather)" |  
    "(Yield (> (size event) number))" | "(do datetime call)" | "(do call call)" | "(do org call)"  
  
event ::= "(CreateCommitEventWrapper (CreatePreflightEventWrapper event_constraint))" |  
    "(FindEventWrapperWithDefaults event_constraint)" |  
    "(QueryEventResponse.results (FindEventWrapperWithDefaults event_constraint))" | "(singleton event)" |  
    "(FindNumNextEvent event_constraint number)" | "(FindLastEvent event_constraint)" |  
    "(Execute (refer (^Dynamic ActionIntensionConstraint)))" |  
    "(Execute (refer (extensionConstraint (^Event EmptyStructConstraint))))" |  
    "^(Event) EmptyStructConstraint"  
  
event_constraint ::= "(&" event_constraint event_constraint ")" | "(Event.subject_? (?=" string ))" | "(Event.subject_? (?~=" string ))" |  
    "(Event.start_?" datetime_constraint ")" | "(Event.end_?" datetime_constraint ")" |  
    "(Event.location_?" location_constraint ")" | "(Event.duration_?" duration_constraint ")" |  
    "(Event.showAs_?" status_constraint ")" | "(Event.attendees_?" attendee_constraint ")" |  
    "(EventAllDayForDateRange event_constraint date_range )" | "(EventAllDayOnDate event_constraint date )"
```

⋮



Domain expert

DSL Grammar

DSL for a Scheduling Assistant

```

call ::= event | "(Yield" org ")" | "(Yield (size" org "))" | "(Yield" event )" | "(Yield" weather ")" | "(Yield (> (size" event ") number ))" | "(do" datetime call ")" | "(do" call call ")" | "(do" org call ")"
event ::= "(CreateCommitEventWrapper (CreatePreflightEventWrapper event_constraint))" |
        "(FindEventWrapperWithDefaults event_constraint)" |
        "(QueryEventResponse.results (FindEventWrapperWithDefaults event_constraint))" | "(singleton" event ")" |
        "(FindNumNextEvent event_constraint number )" | "(FindLastEvent event_constraint)" |
        "(Execute (refer (^(Dynamic) ActionIntensionConstraint)))" |
        "(Execute (refer (extensionConstraint (^(Event) EmptyStructConstraint))))" |
        "^(Event) EmptyStructConstraint"
event_constraint ::= "&" event_constraint event_constraint" | "(Event.subject_?" (?=" string ))" | "(Event.subject_?" (?~=" string ))" |
                    "(Event.start_?" datetime_constraint )" | "(Event.end_?" datetime_constraint )" |
                    "(Event.location_?" location_constraint )" | "(Event.duration_?" duration_constraint )" |
                    "(Event.showAs_?" status_constraint )" | "(Event.attendees_?" attendee_constraint ")" |
                    "(EventAllDayForDateRange" event_constraint date_range ")" | "(EventAllDayOnDate" event_constraint date ")"

```

Invite my boss and his team to
a party tomorrow

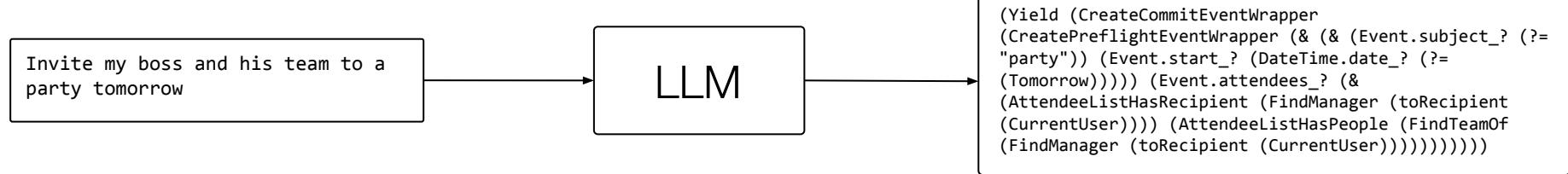
```
(Yield (CreateCommitEventWrapper (CreatePreflightEventWrapper (&
(& (Event.subject_? (=? "party")) (Event.start_?
(DateTime.date_? (=? (Tomorrow)))))) (Event.attendees_? (&
(AttendeeListHasRecipient (FindManager (toRecipient
(CurrentUser)))) (AttendeeListHasPeople (FindTeamOf (FindManager
(toRecipient (CurrentUser)))))))))))
```

DSL for a Scheduling Assistant

```
call ::= event | "(Yield" org ")" | "(Yield (size" org "))" | "(Yield" event ")" | "(Yield" weather ")" |  
    "(Yield (> (size" event ") number ))" | "(do" datetime call ")" | "(do" call call ")" | "(do" org call ")"  
  
event ::= "(CreateCommitEventWrapper (CreatePreflightEventWrapper" event_constraint "))" |  
    "(FindEventWrapperWithDefaults" event_constraint ")" |  
    "(QueryEventResponse.results (FindEventWrapperWithDefaults" event_constraint "))" | "(singleton" event ")" |  
    "(FindNumNextEvent" event_constraint number ")" | "(FindLastEvent" event_constraint ")" |  
    "(Execute (refer (^Dynamic) ActionIntensionConstraint)))" |  
    "(Execute (refer (extensionConstraint (^(Event) EmptyStructConstraint))))" |  
    "^(Event) EmptyStructConstraint"  
  
event_constraint ::= "(&" event_constraint event_constraint ")" | "(Event.subject_? (=?= string ))" | "(Event.subject_? (?=~ string ))" |  
    "(Event.start_?" datetime_constraint ")" | "(Event.end_?" datetime_constraint ")" |  
    "(Event.location_?" location_constraint ")" | "(Event.duration_?" duration_constraint ")" |  
    "(Event.showAs_?" status_constraint ")" | "(Event.attendees_?" attendee_constraint ")" |  
    "(EventAllDayForDateRange" event_constraint date_range ")" | "(EventAllDayOnDate" event_constraint date ")"  
  
    :
```

How can we enable LLMs to use the expert knowledge embedded within the symbolic structure/rules of the DSL?

LLMs & Grammars



LLMs & Grammars

Full DSL grammar

```
call ::= event | "(Yield" org ")" | "(Yield (size" org "))" | "(Yield" event ")" | "(Yield" weather ")" |  
    "(Yield (> (size" event ") number))" | "(do" datetime call ")" | "(do" call call ")" | "(do" org call ")"  
event ::= "(CreateCommitEventWrapper (CreatePreflightEventWrapper" event_constraint "))" |  
    "(FindEventWrapperWithDefaults" event_constraint ")" |  
    "(QueryEventResponse.results (FindEventWrapperWithDefaults" event_constraint "))" | "(singleton" event ")" |  
    "(FindNumNextEvent" event_constraint number ")" | "(FindLastEvent" event_constraint ")" |  
    "(Execute (refer (^Dynamic) ActionIntensionConstraint))" |  
    "(Execute (refer (extensionConstraint (^Event) EmptyStructConstraint)))" |  
    "^(^Event) EmptyStructConstraint"  
event_constraint ::= "(&" event_constraint event_constraint ")" | "(Event.subject_? (=?= string ))" | "(Event.subject_? (?=~ string ))" |  
    "(Event.start_?" datetime_constraint ")" | "(Event.end_?" datetime_constraint ")" |  
    "(Event.location_?" location_constraint ")" | "(Event.duration_?" duration_constraint ")" |  
    "(Event.showAs_?" status_constraint ")" | "(Event.attendees_?" attendee_constraint ")" |  
    "(EventAllDayForDateRange" event_constraint date_range ")" | "(EventAllDayOnDate" event_constraint date ")"  
    ...
```

Minimal grammar
for generating the
output program

```
call ::= "(Yield" event ")"  
event ::= "(CreateCommitEventWrapper (CreatePreflightEventWrapper"  
    event_constraint ))"  
event_constraint ::= "(&" event_constraint event_constraint ")" |  
    "(Event.subject_? (=?= string ))" | "(Event.start_?" datetime_constraint "  
    ")" | "(Event.attendees_?"  
    attendee_constraint ")"  
string ::= "\"party\""  
datetime_constraint ::= "(DateTime.date_?" datetime_constraint ")"  
    | "(? OP datetime ")"  
OP ::= "=" datetime ::= date  
    ...
```

Invite my boss and his team to a
party tomorrow

LLM

```
(Yield (CreateCommitEventWrapper  
    (CreatePreflightEventWrapper (& (& (Event.subject_? (=?= "party")) (Event.start_? (DateTime.date_? (=?= (Tomorrow)))) (Event.attendees_? (& (AttendeeListHasRecipient (FindManager (toRecipient (CurrentUser)))) (AttendeeListHasPeople (FindTeamOf (FindManager (toRecipient (CurrentUser)))))))))))
```

LLMs & Grammars

Full DSL grammar

```
call ::= event | "(Yield" org ")" | "(Yield (size" org "))" | "(Yield" event ")" | "(Yield" weather ")" |  
    "(Yield (> (size" event ")" number ))" | "(do" datetime call ")" | "(do" call call ")" | "(do" org call ")"  
event ::= "(CreateCommitEventWrapper (CreatePreflightEventWrapper" event_constraint ))" |  
    "(FindEventWrapperWithDefaults" event_constraint ")" |  
    "(QueryEventResponse.results (FindEventWrapperWithDefaults" event_constraint ))" | "(singleton" event ")" |  
    "(FindNumNextEvent" event_constraint number ")" | "(FindLastEvent" event_constraint ")" |  
    "(Execute (refer (^Dynamic) ActionIntensionConstraint))" |  
    "(Execute (refer (extensionConstraint (^Event) EmptyStructConstraint)))" |  
    "^(^Event) EmptyStructConstraint"  
event_constraint ::= "(&" event_constraint event_constraint ")" | "(Event.subject_? (?:= string ))" | "(Event.subject_? (?:~=" string ))" |  
    "(Event.start_?" datetime_constraint ")" | "(Event.end_?" datetime_constraint ")" |  
    "(Event.location_?" location_constraint ")" | "(Event.duration_?" duration_constraint ")" |  
    "(Event.showAs_?" status_constraint ")" | "(Event.attendees_?" attendee_constraint ")" |  
    "(EventAllDayForDateRange" event_constraint date_range ")" | "(EventAllDayOnDate" event_constraint date ")"  
    ...
```

```
(Yield (CreateCommitEventWrapper  
    (CreatePreflightEventWrapper (& (& (Event.subject_? (?:=  
        "party")) (Event.start_? (DateTime.date_? (?:=  
            (Tomorrow)))) (Event.attendees_? (&  
                (AttendeeListHasRecipient (FindManager (toRecipient  
                    (CurrentUser)))) (AttendeeListHasPeople (FindTeamOf  
                        (FindManager (toRecipient (CurrentUser)))))))))))
```

Parsing!

```
call ::= "(Yield" event ")"  
event ::= "(CreateCommitEventWrapper (CreatePreflightEventWrapper"  
    event_constraint ))"  
event_constraint ::= "(&" event_constraint event_constraint ")" |  
    "(Event.subject_? (?:= string ))" | "(Event.start_?" datetime_constraint ")" |  
    "(Event.attendees_?" attendee_constraint ")"  
string ::= "\\"party\\\""  
datetime_constraint ::= "(DateTime.date_?" datetime_constraint ")"  
    | "(? OP datetime ")"  
OP ::= "=" datetime ::= date  
    ...
```

Training output program

Minimal grammar for generating
output program

Standard Prompting with LLMs

“In-context”
demonstrations
(from training)

What time on Tuesday is my planning meeting?

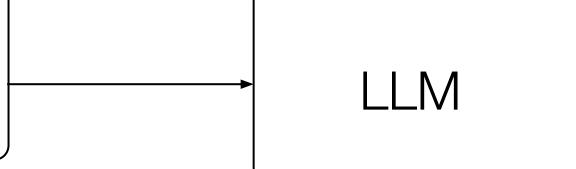
```
start(findEvent(EventSpec( name='planning',  
    start=DateTimeSpec(weekday=tuesday))))
```

Can you remind me to go to the airport tomorrow morning at 8am?

```
createCommitEventWrapper(  
    createPreflightEventWrapper(  
        EventBuilder(subject='go to the airport',  
        start=dateAtTime( date=tomorrow(),  
        time=numberAM(8))))
```

⋮

Add meeting with Jean's manager on Wednesday at 2 PM



Grammar Prompting for LLMs

“In-context”
demonstrations
(from training)



What time on Tuesday is my planning meeting?

```
call ::= "(Yield" query ")"
query ::= "start(" & event & )" ...
```

```
start(findEvent(EventSpec( name='planning',
    start=DateTimeSpec(weekday=tuesday))))
```

Can you remind me to go to the airport
tomorrow morning at 8am?

```
call ::= "(Yield" event ")"
event ::= "createCommitEventWrapper("constraint")" ...
```

```
createCommitEventWrapper(
    createPreflightEventWrapper(
        EventBuilder(subject='go to the airport',
            start=dateAtTime( date=tomorrow(),
                time=numberAM(8))))
```

⋮

Add meeting with Jean's manager on
Wednesday at 2 PM

} Input example

} Minimal DSL grammar

} Output example

LLM

Grammar Prompting for LLMs

“In-context”
demonstrations
(from training)

What time on Tuesday is my planning meeting?

```
call ::= "(Yield" query ")"
query ::= "start(" & event & ")" ...
```

```
start(findEvent(EventSpec( name='planning',
    start=DateTimeSpec(weekday=tuesday))))
```

Can you remind me to go to the airport
tomorrow morning at 8am?

```
call ::= "(Yield" event ")"
event ::= "createCommitEventWrapper("constraint")" ...
```

```
createCommitEventWrapper(
    createPreflightEventWrapper(
        EventBuilder(subject='go to the airport',
            start=dateAtTime( date=tomorrow(),
                time=numberAM(8)))))
```

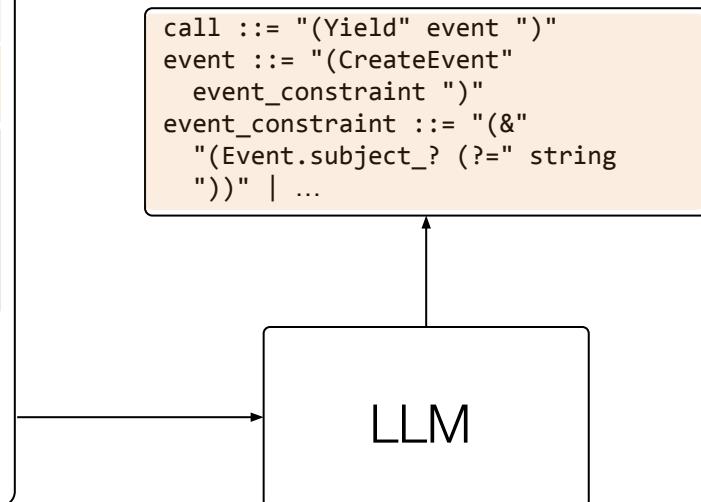
⋮

Add meeting with Jean's manager on
Wednesday at 2 PM



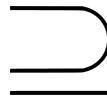
```
call ::= "(Yield" event ")"
event ::= "(CreateEvent"
    event_constraint)"
event_constraint ::= "(&
    "Event.subject_? (=?" string
    "))" | ...
```

LLM



Grammar Prompting for LLMs

```
call ::= event | "(Yield" org ")" | "(Yield (size" org "))" | "(Yield" event ")" | "(Yield" weather ")" |  
    "(Yield (> (size" event ")" number ))" | "(do" datetime call ")" | "(do" call call ")" | "(do" org call ")"  
  
event ::= "(CreateCommitEventWrapper (CreatePreflightEventWrapper" event_constraint ")" |  
    "(FindEventWrapperWithDefaults" event_constraint ")" |  
    "(QueryEventResponse.results (FindEventWrapperWithDefaults" event_constraint ")" | "(singleton" event ")" |  
        "(FindNumNextEvent" event_constraint number ")" | "(FindLastEvent" event_constraint ")" |  
        "(Execute (refer (^Dynamic) ActionIntensionConstraint))" |  
        "(Execute (refer (extensionConstraint (^Event) EmptyStructConstraint))))" |  
        "^(^Event) EmptyStructConstraint"  
  
event_constraint ::= "(&" event_constraint event_constraint ")" | "(Event.subject_? (=? string ))" | "(Event.subject_? (?=~ string ))" |  
    "(Event.start_?" datetime_constraint ")" | "(Event.end_?" datetime_constraint ")" |  
    "(Event.location_?" location_constraint ")" | "(Event.duration_?" duration_constraint ")" |  
    "(Event.showAs_?" status_constraint ")" | "(Event.attendees_?" attendee_constraint ")" |  
    "(EventAllDayForDateRange" event_constraint date_range ")" | "(EventAllDayOnDate" event_constraint date ")"  
    :  
:
```



```
call ::= "(Yield" event ")"  
event ::= "(CreateEvent"  
    event_constraint ")"  
event_constraint ::= "(&"  
    "(Event.subject_? (=? string  
    ))" | ...
```



Add meeting with Jean's manager on
Wednesday at 2 PM

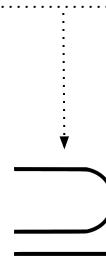
LLM

Grammar Prompting for LLMs

Constrain the minimal grammar output to be a subset of the full DSL grammar

$$P(x_t | \mathbf{x}_{<t}) \propto P_{\text{LLM}}(x_t | \mathbf{x}_{<t}) \times \mathbb{1}\{\mathbf{x}_t \mathbf{x}_{<t} \text{ is a valid rule in the DSL grammar}\}$$

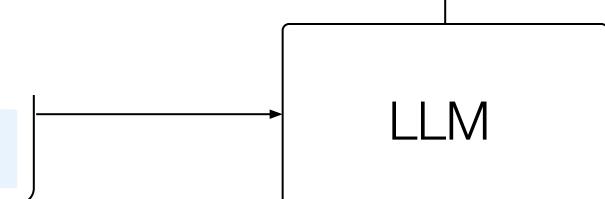
```
call ::= event | "(Yield" org ")" | "(Yield (size" org "))" | "(Yield" event ")" | "(Yield" weather ")" |  
    "(Yield (> (size" event ")" number ))" | "(do" datetime call ")" | "(do" call call ")" | "(do" org call ")"  
  
event ::= "(CreateCommitEventWrapper (CreatePreflightEventWrapper" event_constraint ))" |  
    "(FindEventWrapperWithDefaults" event_constraint ")" |  
    "(QueryEventResponse.results (FindEventWrapperWithDefaults" event_constraint ))" | "(singleton" event ")" |  
    "(FindNumNextEvent" event_constraint number ")" | "(FindLastEvent" event_constraint ")" |  
    "(Execute (refer (^Dynamic) ActionIntensionConstraint))" |  
    "(Execute (refer (extensionConstraint (^Event) EmptyStructConstraint))))" |  
    "(\^Event) EmptyStructConstraint"  
  
event_constraint ::= "(&" event_constraint event_constraint ")" | "(Event.subject_? (=? string ))" | "(Event.subject_? (?=~ string ))" |  
    "(Event.start_?" datetime_constraint ")" | "(Event.end_?" datetime_constraint ")" |  
    "(Event.location_?" location_constraint ")" | "(Event.duration_?" duration_constraint ")" |  
    "(Event.showAs_?" status_constraint ")" | "(Event.attendees_?" attendee_constraint ")" |  
    "(EventAllDayForDateRange" event_constraint date_range ")" | "(EventAllDayOnDate" event_constraint date ")"  
    :  
    :
```



```
call ::= "(Yield" event ")"  
event ::= "(CreateEvent"  
    event_constraint ")"  
event_constraint ::= "(&"  
    "(\^Event.subject_? (=? string  
    ))" | ...
```



Add meeting with Jean's manager on
Wednesday at 2 PM



Grammar Prompting for LLMs

“In-context”
demonstrations
(from training)



What time on Tuesday is my planning meeting?

```
call ::= "(Yield" query ")"
query ::= "start(" & event & ")" ...
```

```
start(findEvent(EventSpec( name='planning',
    start=DateTimeSpec(weekday=tuesday))))
```

Can you remind me to go to the airport
tomorrow morning at 8am?

```
call ::= "(Yield" event ")"
event ::= "createCommitEventWrapper("constraint")" ...
```

```
createCommitEventWrapper(
    createPreflightEventWrapper(
        EventBuilder(subject='go to the airport',
            start=dateAtTime( date=tomorrow(),
                time=numberAM(8)))))
```

⋮

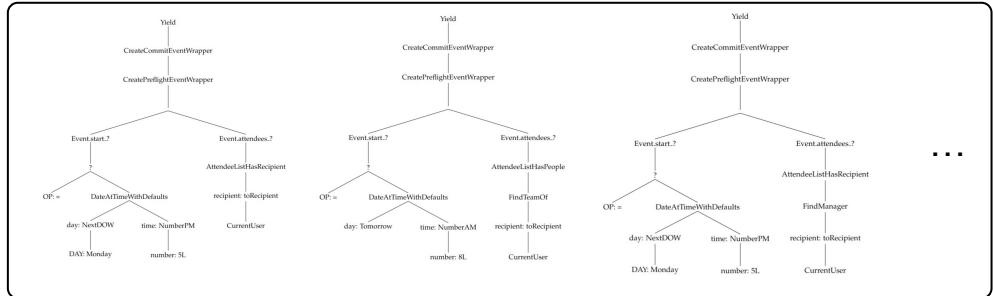
Add meeting with Jean's manager on
Wednesday at 2 PM

```
CreateEvent(start=DateTime(
    date=Wednesday,
    time=NumberPM(2)),
    attendees=FindManager(
        recipient=Jean))
```

```
call ::= "(Yield" event ")"
event ::= "(CreateEvent"
    event_constraint)"
event_constraint ::= "(&
    "(Event.subject_? (=?" string
    ))" | ...
```

LLM

Grammar Prompting for LLMs



Set of valid strings under the minimal grammar



```
CreateEvent(start=DateTime(  
    date=Wednesday,  
    time=NumberPM(2)),  
    attendees=FindManager(  
        recipient=Jean))
```

```
call ::= "(Yield" event ")"  
event ::= "(CreateEvent"  
    event_constraint ")"  
event_constraint ::= "("&  
    "(Event.subject_? (?=" string  

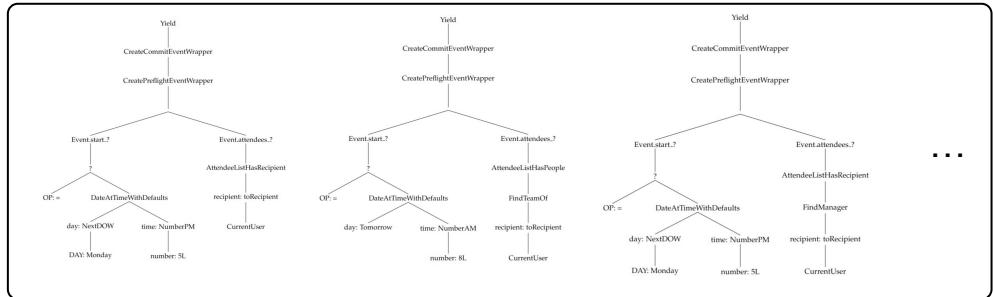
```

LLM



Add meeting with Jean's manager on Wednesday at 2 PM

Grammar Prompting for LLMs



Set of valid strings under the minimal grammar



$$P(x_t | \mathbf{x}_{<t}) \propto P_{\text{LLM}}(x_t | \mathbf{x}_{<t}) \times$$

$\mathbb{1}\{\mathbf{x}_t \mathbf{x}_{<t} \text{ is licensed by conditional DSL grammar}\}$

Minimal grammar → Earley parser → Left-to-right parsing

```
CreateEvent(start=DateTime(  
    date=Wednesday,  
    time=NumberPM(2)),  
    attendees=FindManager(  
        recipient=Jean))
```

```
call ::= "(Yield" event ")"  
event ::= "(CreateEvent"  
    event_constraint ")"  
event_constraint ::= "("&  
    "(Event.subject_? (?=" string  
    "))" | ...
```



Add meeting with Jean's manager on
Wednesday at 2 PM

LLM

Constrained Decoding

Actual algorithm:

- 1) Decode from LM
- 2) Check with Earley parser
- 3) Continue from earliest point of failure

Algorithm 1 Earley-based Constrained Generation

Input: Test input x , predicted grammar \hat{G}

Output: Program $y \in L(\hat{G})$

```
1:  $t \leftarrow 0, \hat{y}^{(0)} \leftarrow \epsilon$       ▷ initialize to empty string
2: while True do
3:    $t \leftarrow t + 1$       ▷ unconstrained greedy decoding
4:    $\bar{y} \leftarrow \text{decode} \left( P_{\text{LLM}}(\cdot | x, \hat{G}, \hat{y}^{(t-1)}, \dots) \right)$ 
5:    $\hat{y}^{(t)} \leftarrow \hat{y}^{(t-1)} \cdot \bar{y}$           ▷ concatenation
6:   if  $\hat{y}^{(t)} \in L(\hat{G})$  then    ▷ try parsing with  $\hat{G}$ 
7:     return  $\hat{y}^{(t)}$           ▷ return if successful
8:   else           ▷ if parsing fails, need to correct
9:      $y_{\text{prefix}}, \Sigma[y_{\text{prefix}}] \leftarrow \text{EarleyParse}(\hat{y}^{(t)}, \hat{G})$ 
10:     $w^* \leftarrow \arg \max_{w \in \Sigma[y_{\text{prefix}}]} P_{\text{LLM}}(w | y_{\text{prefix}}, \dots)$ 
11:     $\hat{y}^{(t)} \leftarrow y_{\text{prefix}} \cdot w^*$ 
12:   end if
13: end while
```

Constraining LLM Outputs

“Language” licensed by minimal DSL grammar

```
call ::= "(Yield" event ")"
event ::= "(CreateCommitEventWrapper (CreatePreflightEventWrapper"
    "event_constraint))"
event_constraint ::= "(&" event_constraint event_constraint ")" |
    "(Event.subject_? (=? string ))" | "(Event.start_?" datetime_constraint ")" |
    "(Event.attendees_?" attendee_constraint)"
string ::= "'party''"
datetime_constraint ::= "(DateTime.date_?" datetime_constraint ")" |
    "(?> OP datetime )"
OP ::= "=" datetime ::= date
:
:
```

Language licensed by full DSL grammar

```
call ::= event | "(Yield" org ")" | "(Yield (size" org "))" | "(Yield" event ")" | "(Yield" weather ")" |
    "(Yield (> (size" event ")" number ))" | "(do" datetime call ")" | "(do" call call ")" | "(do" org call ")"
event ::= "(CreateCommitEventWrapper (CreatePreflightEventWrapper" event_constraint }}"
    | "(FindEventWrapperWithDefaults" event_constraint ")"
    | "(QueryEventResponse.results (FindEventWrapperWithDefaults" event_constraint "))" | "(singleton" event ")"
    | "(FindNextEvent" event_constraint ")"
    | "(execute (refer extensionConstraint ((Event EmptyStructConstraint))))" |
    "(execute (refer extensionConstraint ((Event EmptyStructConstraint))))" |
    "(^<(Event) EmptyStructConstraint)" |
    :
event_constraint ::= "(&" event_constraint event_constraint ")" |
    "(Event.subject_? (=? string ))" | "(Event.subject_? (=?= string ))" |
    "(Event.start_?" datetime_constraint ")" | "(Event.end_?" datetime_constraint ")" |
    "(Event.location_?" location_constraint ")" | "(Event.duration_?" duration_constraint ")" |
    "(Event.showAs_?" status_constraint ")" | "(Event.attendees_?" attendee_constraint )" |
    "(EventAllDayForDateRange" event_constraint date_range ")" | "(EventAllDayOnDate" event_constraint date ")" |
    :
:
```

All strings

你好 HALLO 안녕
CIAO HOLA नमस्ते
yeala HELLO こんにちは привет
BONJOUR مرحبا OLÁ



Why should this work?

LLMs may have been exposed to enough BNF grammar examples (and their derivations) during pretraining.

LLM as a metalanguage learner!



The image shows the cover of the book "Formal Languages and Compilation" (Third Edition) by Stefano Crespi Reghizzi, Luca Breveglieri, and Angelo Morzenti, published by Springer. The cover features a large yellow arrow graphic on the right side.

README.md

bnf

CI passing coverage 97% crates.io v0.5.0 downloads 11k license MIT

A library for parsing Backus–Naur form context-free grammars.

What does a parsable BNF grammar look like?

The following grammar from the [Wikipedia page on Backus–Naur form](#) exemplifies a compatible grammar. (*Note: parser allows for an optional ';' to indicate the end of a production)

```
<postal-address> ::= <name-part> <street-address> <zip-part>
<name-part> ::= <personal-part> <last-name> <opt-suffix-part> <EOL>
| <personal-part> <name-part>
<personal-part> ::= <initial> "." | <first-name>
<street-address> ::= <house-num> <street-name> <opt-apt-num> <EOL>
<zip-part> ::= <town-name> "," <state-code> <ZIP-code> <EOL>
<opt-suffix-part> ::= "Sr." | "Jr." | <roman-numeral> | ""
<opt-apt-num> ::= <apt-num> | ""
```

Results on Semantic Parsing

	SMCalflow	Overnight	GeoQuery
Regular Prompting	46.4%	54.7%	81.5%

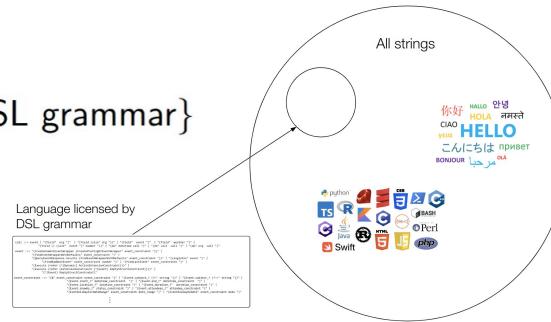
GeoQuery	 Which rivers run through the states bordering Texas?	answer(traverse(next_to(stateid('texas'))))
	31  Which meeting has the earliest end time?	(call listValue (call superlative (call getProperty (call singleton en.meeting) (string !type)) (string min) (call ensureNumericProperty (string end_time))))

Results on Semantic Parsing

	SMCalflow	Overnight	GeoQuery
Regular Prompting	46.4%	54.7%	81.5%
Regular Prompting + Constrained Decoding	49.2%	54.7%	81.8%

$$P(x_t | \mathbf{x}_{<t}) \propto P_{\text{LLM}}(x_t | \mathbf{x}_{<t}) \times \\ \mathbb{1}\{\mathbf{x}_t \mathbf{x}_{<t} \text{ is licensed by unconditional DSL grammar}\}$$

(Guarantee syntactic validity)



Results on Semantic Parsing

	SMCalflow	Overnight	GeoQuery
Regular Prompting	46.4%	54.7%	81.5%
Regular Prompting + Constrained Decoding	49.2%	54.7%	81.8%
Linearized Tree Prompting	50.0%	56.4%	77.5%

Original output: (attendee_? FindManager(Jean))

Linearized tree output: [constraint "(attendee_?" [attendee "FindManager(" [attendee "Jean" ")] ")"]")]

Results on Semantic Parsing

	SMCalflow	Overnight	GeoQuery
Regular Prompting	46.4%	54.7%	81.5%
Regular Prompting + Constrained Decoding	49.2%	54.7%	81.8%
Linearized Tree Prompting	50.0%	56.4%	77.5%
Grammar Prompting + Constrained Decoding	52.4%	60.9%	88.9%

Results on Semantic Parsing

	SMCalflow	Overnight	GeoQuery
Regular Prompting	46.4%	54.7%	81.5%
Regular Prompting + Constrained Decoding	49.2%	54.7%	81.8%
Linearized Tree Prompting	50.0%	56.4%	77.5%
Grammar Prompting + Constrained Decoding	52.4%	60.9%	88.9%
Grammar Prompting + Oracle Grammar	83.6%	96.5%	96.8%

More results (different LMs, retrieval-based prompting, etc.) in the paper.

Controlling LLM Outputs with New Rules

“Cancel the Wednesday 5pm meeting with
the marketing team in New York and
reschedule it to Thursday 2pm”



Domain expert

Controlling LLM Outputs with New Rules

```
call ::= event | "(Yield" org ")" | "(Yield (size" org "))" | "(Yield" event ")" | "(Yield" weather ")" |  
    "(Yield (> (size" event ") number ))" | "(do" datetime call ")" | "(do" call call ")" | "(do" org call ")"  
  
event ::= "(CreateCommitEventWrapper (CreatePreflightEventWrapper" event_constraint "))" |  
    "(FindEventWrapperWithDefaults" event_constraint ")" |  
    "(QueryEventResponse.results (FindEventWrapperWithDefaults" event_constraint "))" | "(singleton" event ")" |  
    "(FindNumNextEvent" event_constraint number ")" | "(FindLastEvent" event_constraint ")" |  
    "(Execute (refer (^Dynamic) ActionIntensionConstraint)))" |  
    "(Execute (refer (extensionConstraint (^Event) EmptyStructConstraint))))" |  
    "^(Event) EmptyStructConstraint)" | "(Execute (CancelEvent" event_constraint " event ))"  
  
event_constraint ::= "(&" event_constraint event_constraint ")" | "(Event.subject_? (=?= string ))" | "(Event.subject_? (?=~ string ))" |  
    "(Event.start_?" datetime_constraint ")" | "(Event.end_?" datetime_constraint ")" |  
    "(Event.location_?" location_constraint ")" | "(Event.duration_?" duration_constraint ")" |  
    "(Event.showAs_?" status_constraint ")" | "(Event.attendees_?" attendee_constraint ")" |  
    "(EventAllDayForDateRange" event_constraint date_range ")" | "(EventAllDayOnDate" event_constraint date ")"  
    :  
    :
```

“Cancel the Wednesday 5pm meeting with
the marketing team in New York and
reschedule it to Thursday 2pm”



Domain expert

Add function: **CancelEvent**
Add organization: **Marketing**
Add location: **New York**

Controlling LLM Outputs with New Rules

Full DSL with new rules

```
river ::= "shortest(" river ")" | "longest(" river ")"
city ::= "smallest(" city ")" | "largest(" city ")" |
       "major(" state ")"
num ::= "population(" city ")" ...
```

what state has the largest city ?

```
query ::= "answer(" answer_type ")"
answer_type ::= state
state ::= "state(" state ")" | "loc_1(" city ")"
city ::= "largest(" city ")" | ALL_CITY
ALL_CITY ::= "city(all)"
```

```
answer(state(loc_1(largest(city(all)))))
```

what is the capital of the state with the longest river ?

```
query ::= "answer(" answer_type ")"
answer_type ::= city
city ::= "capital(" city ")" | "loc_2(" state ")"
state ::= "state(" state ")" | "loc_1(" river ")"
river ::= "longest(" river ")" | ALL_RIVER
ALL_RIVER ::= "river(all)"
```

```
answer(capital(loc_2(state(loc_1(longest(river(all)))))))
```

:

what is the smallest city in CA ?



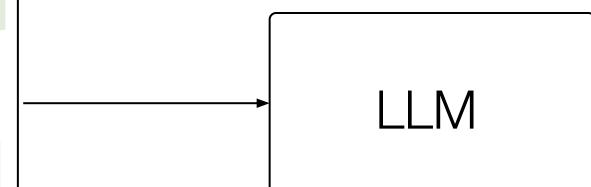
Example 1

} Input

Example 2

} Instance-specific DSL grammar

} Output



Controlling LLM Outputs with New Rules

GeoQuery	New Rules	Compositional Gen.
LLM	63.3%	77.1%
LLM + Instance-level DSL grammar	90.8%	86.6%

New rules: holding out "smallest", "shortest", "most", "highest", "sum", "population_1", "count", "major"

Compositional generalization: Unseen combinations (e.g., test combines "length" and "longest" but training never uses them in combination).

Grammar Prompting for Molecule Generation

SMILES Grammar

```
smiles: atom (chain | branch)*

chain: (bond? (atom | ring_closure))+

branch: "(" bond? smiles+ ")"

atom: organic_symbol | aromatic_symbol | atom_spec
    | wildcard | group_symbol

bond: "-" | "=" | "#" | "$" | ":" | "/" | "\\" | "."

atom_spec: "[" isotope? ("se" | "as" | aromatic_symbol
    | element_symbol | wildcard) chiral_class? h_count? ...

organic_symbol: "Br" | "Cl" | "N" | "O" | "P" | "S"
    | "F" | "I" | "B" | "C"

aromatic_symbol: "b" | "c" | "n" | "o" | "p" | "s"

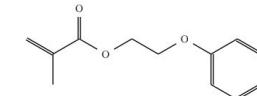
group_symbol.2: "C=CC(=O)O" | "C=CC(O)=O" | "C(=C)C(=O)O"
    | "C(=C)C(O)=O" | "OC(=O)C=C" | "O=C(O)C=C" | ...
    :
```

Specialized SMILES Grammar for Molecule Generation

G[y]:

smiles	::=	atom chain branch chain chain atom chain
atom	::=	organic_symbol
organic_symbol	::=	"C" "N" "O"
chain	::=	atom ring_closure bond atom bond atom
		bond atom ring_closure atom
		atom bond atom bond atom
		bond atom bond atom
ring_closure	::=	"1"
bond	::=	"="
branch	::=	"(" smiles ")"

y: CC(=C)C(=O)OCCOC1 = CC = CC = C1



Grammar Prompting for Molecule Generation

SMILES Grammar

```
smiles: atom (chain | branch)*

chain: (bond? (atom | ring_closure))+

branch: "(" bond? smiles+ ")"

atom: organic_symbol | aromatic_symbol | atom_spec
    | wildcard | group_symbol

bond: "-" | "=" | "#" | "$" | ":" | "/" | "\\" | "."

atom_spec: "[" isotope? ("se" | "as" | aromatic_symbol
    | element_symbol | wildcard) chiral_class? h_count? ...

organic_symbol: "Br" | "Cl" | "N" | "O" | "P" | "S"
    | "F" | "I" | "B" | "C"

aromatic_symbol: "b" | "c" | "n" | "o" | "p" | "s"

group_symbol.2: "C=CC(=O)O" | "C=CC(O)=O" | "C(=C)C(=O)O"
    | "C(=C)C(O)=O" | "OC(=O)C=C" | "O=C(O)C=C" | ...

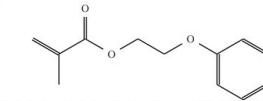
:
:
```

Specialized SMILES Grammar for Molecule Generation

G[y]:

smiles	::=	atom chain branch chain chain atom chain
atom	::=	organic_symbol
organic_symbol	::=	"C" "N" "O"
chain	::=	atom ring_closure bond atom bond atom
		bond atom ring_closure atom
		atom bond atom bond atom
		bond atom bond atom
ring_closure	::=	"1"
bond	::=	"="
branch	::=	"(" smiles ")"

y: CC(= C)C(= O)OCCOC1 = CC = CC = C1



Generating Chain Extenders	Validity	Diversity	Retrosynthesis Score
Graph Grammar [Guo et al. '22]	1.0	0.86	0.73
Standard Prompting	0.60	0.89	0.73
Grammar Prompting	0.96	0.90	0.87

Grammar Prompting for Planning

Specialized Action Grammar for PDDL Planning



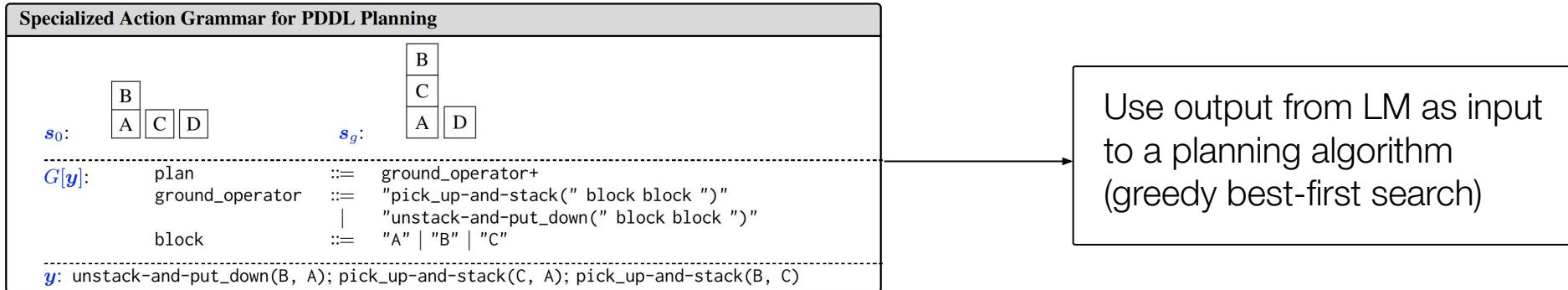
$G[y]:$

```
plan           ::= ground_operator+
ground_operator ::= "pick_up-and-stack(" block block ")"
                  |
                  "unstack-and-put_down(" block block ")"
block          ::= "A" | "B" | "C"
```

$y:$ unstack-and-put_down(B, A); pick_up-and-stack(C, A); pick_up-and-stack(B, C)

Use output from LM as input
to a planning algorithm
(greedy best-first search)

Grammar Prompting for Planning

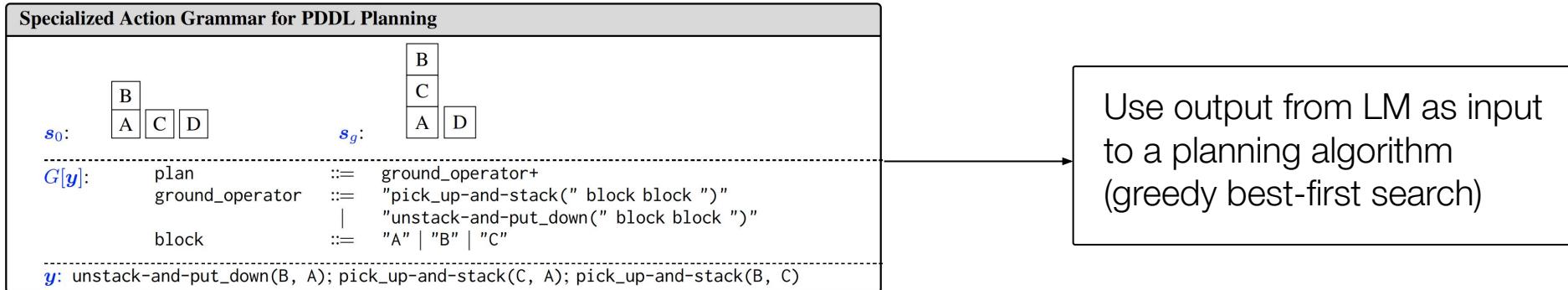


LLM + Planning	Success Rate	Success Rate
No LLM-based Pruning	100%	40%
Standard Prompting	100%	40%
Grammar Prompting	100%	40%

“Easy”

“Hard”

Grammar Prompting for Planning



“Easy”

“Hard”

LLM + Planning	Success Rate	Nodes Created	Nodes Expanded	Success Rate	Nodes Created	Nodes Expanded
No LLM-based Pruning	100%	360	188	40%	18407	3870
Standard Prompting	100%	348	180	40%	17597	4039
Grammar Prompting	100%	251	124	40%	15033	3641

Summary

Including instance-specific grammars as intermediate variables improves DSL generation with LLMs.

What other type of structured representations (metalanguages) can LLMs make use of?

LLM Prompt

You are an expert programmer, and you need to write a program for the given natural language query. First, you should write a grammar that contains all the necessary BNF rules. Then, you should write programs that conform to your predicted rules.

(optional) G : [BEGIN RULES] ... [END RULES]

$x^{(1)}$: find the meeting on Wednesday with Bob and Carol

$G[y^{(1)}]$:

event	$::=$	"QueryEvent(" constraint ")"
constraint	$::=$	"(&" constraint constraint ")"
	$ $	"(start_?" date ")"
	$ $	"(attendee_?" attendee attendee ")"
date	$::=$	"Wednesday"
attendee	$::=$	"Bob" "Carol"

$y^{(1)}$: QueryEvent(& (start_? Wednesday)(attendee_? Bob Carol))

x : Add meeting with Jean's manager on Wednesday at 3PM

LLM Output

\hat{G} :

event	$::=$	"CreateEvent(" constraint ")"
constraint	$::=$	"(&" constraint constraint ")"
	$ $	"(start_?" date time ")"
	$ $	"(attendee_?" attendee ")"
date	$::=$	"Wednesday"
time	$::=$	"NumberPM(3)"
attendee	$::=$	"FindManager(" attendee ")" "Jean"

\hat{y} : CreateEvent(& (start_? Wednesday NumberPM(3))(attendee_? FindManager(Jean)))

Maybe language modeling will be all you need eventually.
Meanwhile, symbolic structures can still help!

Thanks!

