Highlights from attending the Simons Workshop on Transformers as a Computational Model

Breandan Considine





"Be guided by beauty. I really mean that. Pretty much everything I've done has had an aesthetic component, at least to me. Now you might think 'well, building a company that's trading bonds, what's so aesthetic about that?' But, what's aesthetic about it is doing it right. Getting the right kind of people, and approaching the problem, and doing it right ... it's a beautiful thing to do something right."

—James Harris Simons (1938–2024)

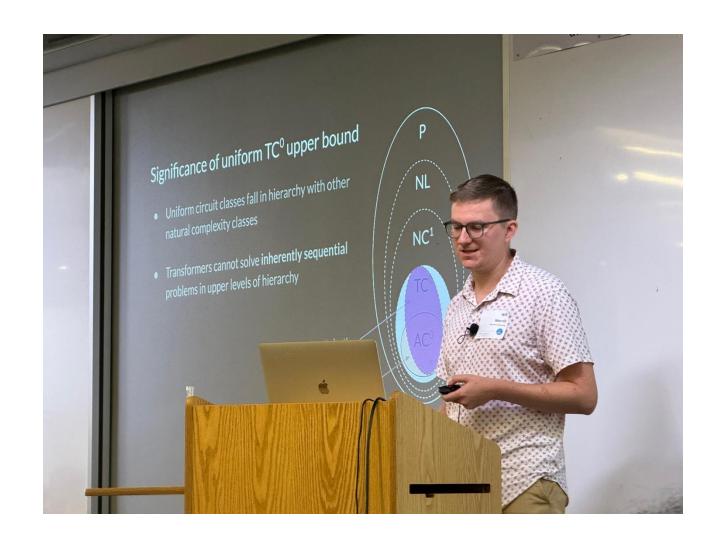
Three overall themes

- Formal language theory
 - Logical expressivity
 - Circuit complexity
 - Algebraic decomposition
- Mechanistic interpretability
 - RASP programs
 - Training dynamics
- Scaling up inference time compute
 - Recurrence and SSMs
 - Search and planning
 - Generator verifier gap



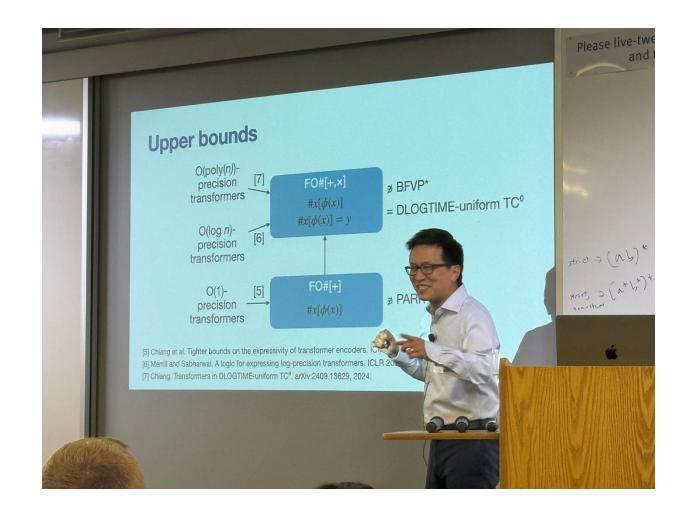
Circuit complexity (Merrill)

- Fixed precision circuits
- Can be studied as logical gates
- Transformer layers = circuit depth
- Computational parallelism vs. sequentiality



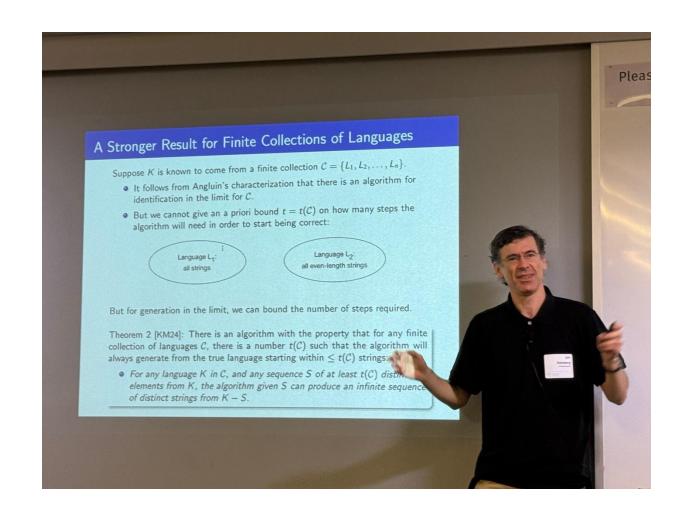
Logical expressivity (Chiang)

- Starts with linear logic
- Permits fine-grained control over resources
- Can be used to study transformer model expressivity
- Many fruitful connections with PL theory



Language generation in the limit (Kleinberg)

- Identifying the grammar for a language is not possible (Gold)
- But generating strings from the language is possible!
- Very elegant proof technique



Learning to reason with LLMs (Brown)

- Starts with his work designing poker bots
- (Re?)discovered the importance of planning
- Generator-verifier gap
- Cue O1, OpenAl's newest LLM with SoTA reasoning capabilities



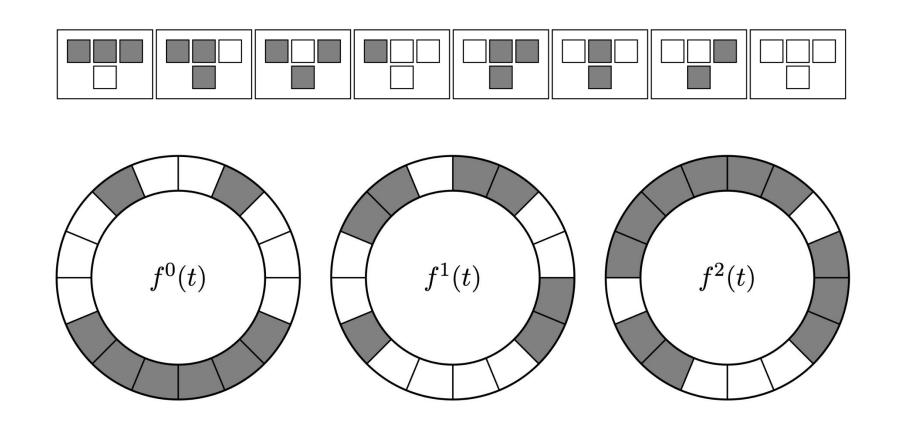
State space models (Gu)

- Combines attention with SSM layers
- S4, Mamba, H3 models
- Gives model variable time to "think"

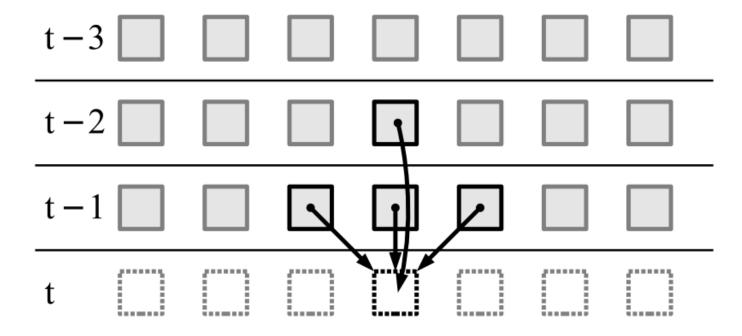
$$x'(t) = \mathbf{A}x(t) + \mathbf{B}u(t)$$
$$y(t) = \mathbf{C}x(t) + \mathbf{D}u(t)$$



Consider the first-order discrete dynamical system



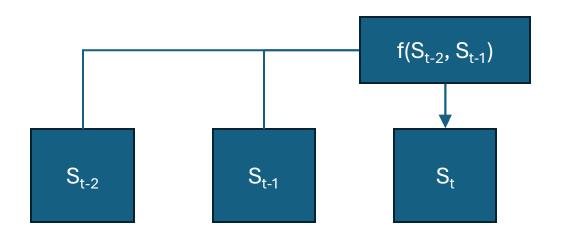
Now consider a second-order dynamical system



A very natural question to ask is the following:
 How do we represent a non-Markovian dynamical system in a Markovian way?

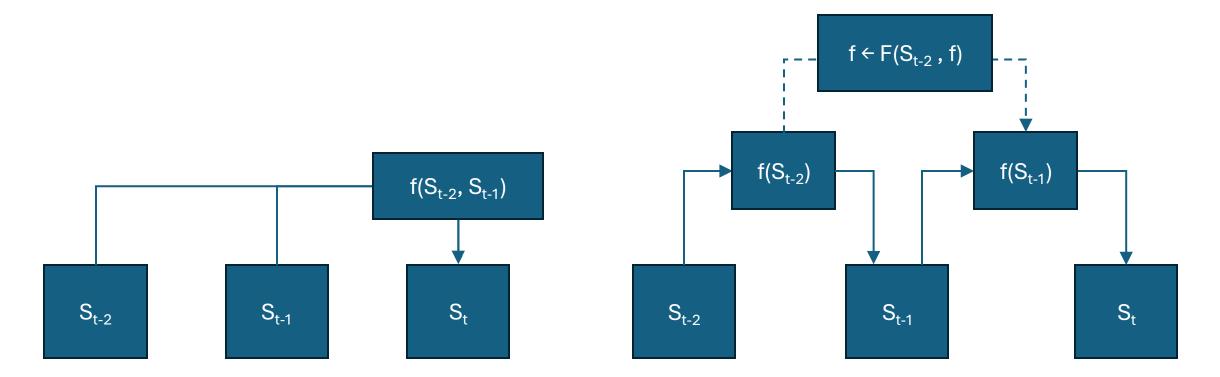
- A very natural question to ask is the following:
 How do we represent a non-Markovian dynamical system in a Markovian way?
- Using the state-space representation!
- Transforms higher-order dependence into a set of 1st-order (i.e., Markovian) differential equations

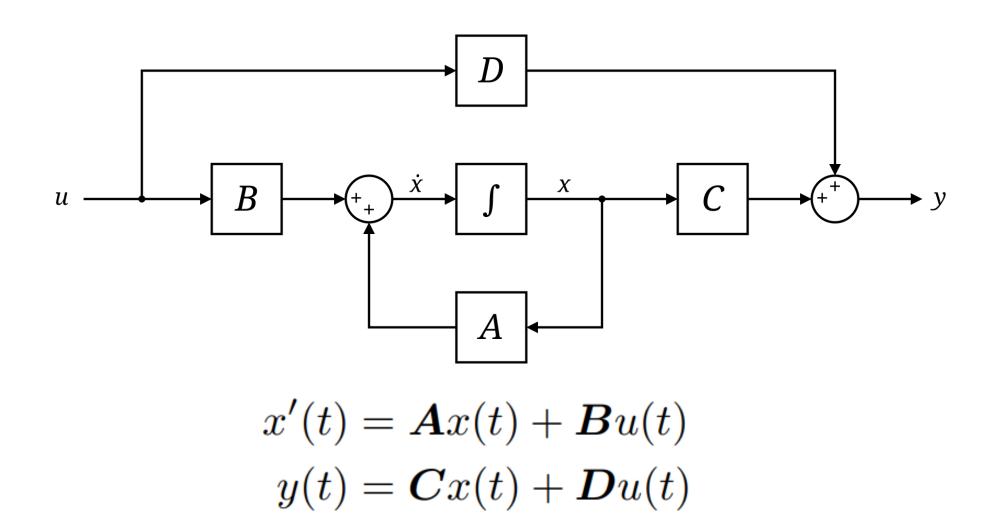
We can take a second-order differential equation...



We can take a second-order differential equation...

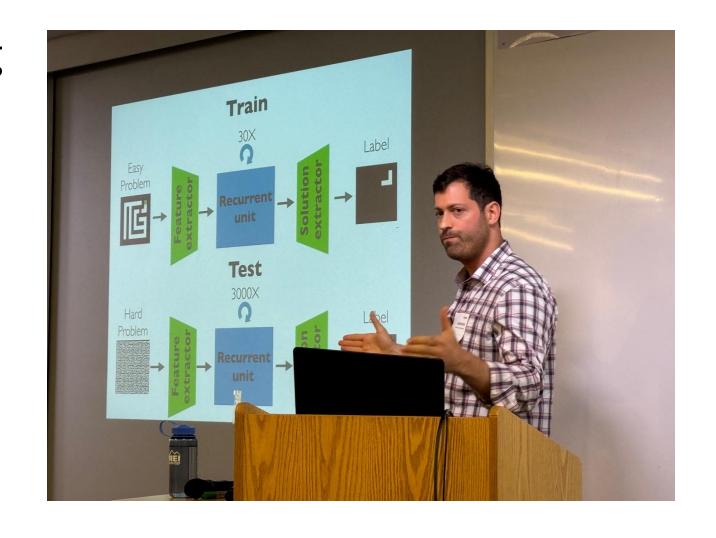
...and make it stateful with an evolving transition function.





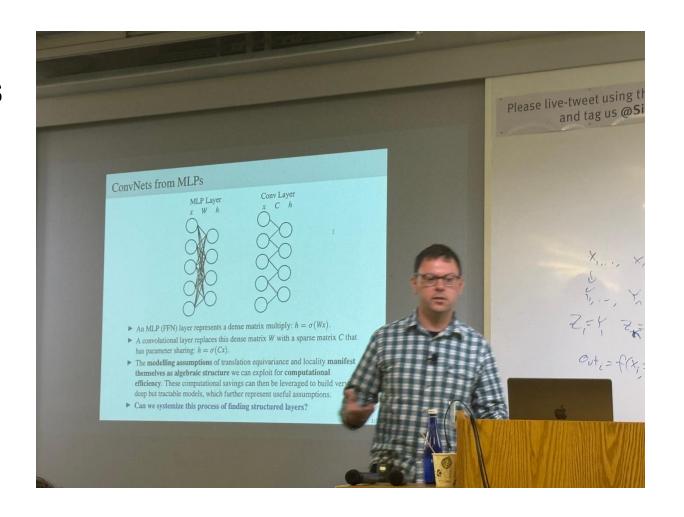
Weak to strong generalization (Goldstein)

- Train on easy reasoning tasks, then evaluate on harder instances of the same task
- Uses recurrent units
- Shows plenty of convincing results on mazes and sudoku

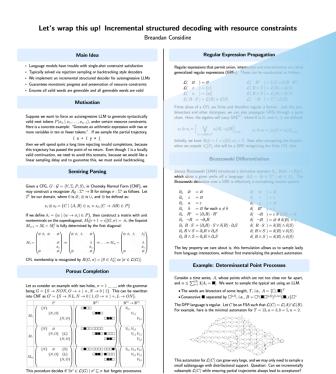


Machine learning is linear algebra (Wilson)

- Inductive biases for pretraining transformers
- Can leverage sparse structure from domain
- Continuous design space of structured matrices and tensors



My poster: Incremental structured decoding



Main Idea

- · Language models have trouble with single-shot constraint satisfaction
- Typically solved via rejection sampling or backtracking style decoders
- We implement an incremental structured decoder for autoregressive LLMs
- Guarantees monotonic progress and preservation of resource constraints
- Ensures all valid words are generable and all generable words are valid

Motivation

Suppose we want to force an autoregressive LLM to generate syntactically valid next tokens $P(x_n \mid x_1, \ldots, x_{n-1})$, under certain resource constraints. Here is a concrete example: "Generate an arithmetic expression with two or more variables in ten or fewer tokens.". If we sample the partial trajectory,

$$(x + (y * \underline{)})$$

then we will spend quite a long time rejecting invalid completions, because this trajectory has passed the point of no return. Even though (is a locally valid continuation, we need to avoid this scenario, because we would like a linear sampling delay and to guarantee this, we must avoid backtracking.

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Let's wrap this up! Incremental structured decoding with resource constraints

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Semiring Parsing

Given a CFG, $G:\mathcal{G}=\langle V,\Sigma,P,S\rangle$, in Chomsky Normal Form (CNF), we may construct a recognizer $R_{\mathcal{G}}:\Sigma^n\to\mathbb{B}$ for strings $\sigma:\Sigma^n$ as follows. Let $2^{\mathcal{V}}$ be our domain, where 0 is \varnothing,\oplus is \cup , and \otimes be defined as:

$$s_1 \otimes s_2 = \{C \mid \langle A,B \rangle \in s_1 \times s_2, (C \to AB) \in P\}$$

If we define $\hat{\sigma}_r = \{w \mid (w \to \sigma_r) \in P\}$, then construct a matrix with unit nonterminals on the superdiagonal, $M_0[r+1=c](G,\sigma) = \hat{\sigma}_r$ the fixpoint $M_{t+1} = M_t + M_t^2$ is fully determined by the first diagonal:

CFL membership is recognized by $R(G, \sigma) = [S \in \Lambda^*] \Leftrightarrow [\sigma \in \mathcal{L}(G)]$

Porous Completion

being $G = \{S \rightarrow NON, O \rightarrow 1\} \times N \rightarrow 0 \mid 1\}$. This can be received in the CMF and $C \in S \rightarrow ML, N \rightarrow 0 \mid 1\}$. The CMF is the CMF and $C \in S \rightarrow ML, N \rightarrow 0 \mid 1, O \rightarrow 1 \mid +, L \rightarrow ON$, the CMF is (S, O) = (S, O)

Regular Expression Propagation

Regular expressions that permit union, intersection and concatenation are called

$$\begin{array}{lll} \mathcal{L}(&\varnothing&)=\varnothing& & \mathcal{L}(&R^*-)=\{\varepsilon\}\cup\mathcal{L}(R\cdot R^*\\ \mathcal{L}(&\varepsilon&)=\{\varepsilon\}& & \mathcal{L}(R\vee S)=\mathcal{L}(R)\cup\mathcal{L}(S)\\ \mathcal{L}(&a&)=\{a\}& & \mathcal{L}(R\wedge S)=\mathcal{L}(R)\cap\mathcal{L}(S)\\ \mathcal{L}(R\cdot S)=\mathcal{L}(R)\times\mathcal{L}(S)& & \mathcal{L}(&\neg R)=\Sigma^*\setminus\mathcal{L}(R) \end{array}$$

Finite slices of a CFL are finite and therefore regular a fortiori. Just like sets bitvectors and other datatypes, we can also propagate GREs through a parschart. Here, the algebra will carry $\mathsf{GRE}^{|V|}$, where 0 is \varnothing , and \oplus , \otimes are defined

$$s_1 \otimes s_2 = \Big[\bigvee_{(v \rightarrow AB) \in P} s_1[A] \cdot s_2[B] \Big]_{v \in V} \qquad \quad s_1 \oplus s_2 = \big[s_1[v] \vee s_2[v] \big]_{v \in V}$$

Initially, we have $M_0[r+1=c](G,\sigma)=\Sigma$. Now after computing the fixpoint, when we unpack $\Lambda^*_{-}[S]$, this will be a GRE recognizing the finite CFL slice.

Brzozowski Differentiation

Janusz Brzozowski (1964) introduced a derivative operator $\partial_a: \operatorname{ReG} \to \operatorname{ReG}$, which slices a given prefix off a language: $\partial_a L = \{b \in \Sigma^* \mid ab \in L\}$. The Brzozowski derivative over a GRE is effectively a normalizing rewrite system:

<i>a.</i>	α	= Ø	$\delta(\varnothing) = \varnothing$	
∂_a	ε	= Ø	$\delta(-\varepsilon) = \varepsilon$	
∂_a	a	$= \varepsilon$	$\delta(-a-)=\varnothing$	
∂_a	ь	$= \varnothing$ for each $a \neq b$	$\delta(-R^*-) = \varepsilon$	
∂_a	R^*	$= (\partial_x R) \cdot R^*$	$\delta(\neg R) = \varepsilon \text{ if } \delta(R) = \varnothing$	
∂_a	$\neg R$	$= \neg \partial_a R$	$\delta(\neg R) = \emptyset \text{ if } \delta(R) = \varepsilon$	
$\partial_a I$	$R \cdot S$	$= (\partial_a R) \cdot S \vee \delta(R) \cdot \partial_a S$	$\delta(R \cdot S) = \delta(R) \wedge \delta(S)$	
$\partial_a E$	V S	$I = \partial_a R \vee \partial_a S$	$\delta(R \vee S) = \delta(R) \vee \delta(S)$	

The key property we care about is, this formulation allows us to sample lazily

Example: Determinantal Point Processes

Consider a time series, A_i whose points which are not too close nor far apart and $n \le \sum_{i=1}^{|A|} \mathbf{1}[A_i = \mathbf{m}]$. We want to sample the typical set using an LLM. • The words are bitvectors of some length, T_i i.e., $A = \{\Box, \mathbf{m}\}^T$

• Consecutive \blacksquare separated by $\Box^{(a,b)}$, i.e., $B = \Box^*(\blacksquare)^{(a,b)}|^{b,\infty}|\{\blacksquare,\epsilon\}\Box^*$ The DPP language is regular. Let C be an FSA such that $\mathcal{L}(C) = \mathcal{L}(A) \cap \mathcal{L}(B)$. For example, here is the minimal automaton for T=13, a=3, b=5, n=2.



This automaton for $\mathcal{L}(C)$ can grow very large, and we may only need to sample small sublanguage with distributional support. Question: Can we incrementally $\mathcal{L}(C)$









Regular Expression Propagation

Regular expressions that permit union, intersection and concatenation are called generalized regular expressions (GREs). These can be constructed as follows:

$$\begin{array}{lll} \mathcal{L}(&\varnothing &) = \varnothing & & \mathcal{L}(&R^* &) = \{\varepsilon\} \cup \mathcal{L}(R \cdot R^*) \\ \mathcal{L}(&\varepsilon &) = \{\varepsilon\} & & \mathcal{L}(R \vee S) = \mathcal{L}(R) \cup \mathcal{L}(S) \\ \mathcal{L}(&a &) = \{a\} & & \mathcal{L}(R \wedge S) = \mathcal{L}(R) \cap \mathcal{L}(S) \\ \mathcal{L}(&R \cdot S) = \mathcal{L}(R) \times \mathcal{L}(S) & & \mathcal{L}(&\neg R) = \Sigma^* \setminus \mathcal{L}(R) \end{array}$$

Finite slices of a CFL are finite and therefore regular a fortiori. Just like sets, bitvectors and other datatypes, we can also propagate GREs through a parse chart. Here, the algebra will carry $GRE^{|V|}$, where 0 is \varnothing , and \oplus , \otimes are defined:

$$s_1 \otimes s_2 = \Big[igvee_{(v o AB) \in P} s_1[A] \cdot s_2[B]\Big]_{v \in V} \qquad \quad s_1 \oplus s_2 = ig[s_1[v] ee s_2[v]ig]_{v \in V}$$

Initially, we have $M_0[r+1=c](G,\sigma)=\Sigma$. Now after computing the fixpoint, when we unpack $\Lambda_{\sigma}^*[S]$, this will be a GRE recognizing the finite CFL slice.

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Let's wrap this up! Incremental structured decoding with resource constraints Breandan Considine

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- Language models have trouble with single-shot constraint satisfaction
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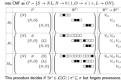
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If we define $\dot{\sigma}_r = \{w \mid (w \to \sigma_r) \in P\}$, then construct a matrix with unit



Porous Completion

being $G=\{S\to NON,O\to+|\times,N\to0\mid 1\}$. This can be rewritten into CNF as $G'=\{S\to NL,N\to0\mid 1,O\to\times\mid+,L\to ON\}$.



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$\partial_e \varepsilon = \varnothing$	$\delta(-\varepsilon) = \varepsilon$
$\partial_a a = \varepsilon$	$\delta(-a^-) = \varnothing$
$\partial_a b = \varnothing \text{ for each } a \neq b$	$\delta(-R^*-) = \varepsilon$
$\partial_a R^* = (\partial_x R) \cdot R^*$	$\delta(\neg R) = \varepsilon \text{ if } \delta(R) = \varnothing$
$\partial_e \neg R = \neg \partial_e R$	$\delta(\neg R) = \emptyset \text{ if } \delta(R) = \varepsilon$
$\partial_a R \cdot S = (\partial_a R) \cdot S \vee \delta(R) \cdot \delta$	$\partial_{a}S$ $\delta(R \cdot S) = \delta(R) \wedge \delta(S)$
$\partial_a R \vee S = \partial_a R \vee \partial_a S$	$\delta(R \vee S) = \delta(R) \vee \delta(S)$
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The key property we care about is, this formulation allows us to sample lazily from language intersections, without first materializing the product automaton.

