Building explanation machines for Science

A Neuro-symbolic perspective

André Freitas
Reasoning & Explainable AI (ExplAIn) Lab

IPAM UCLA
(January 2023)

MANCHESTER
1824

The University of Manchester

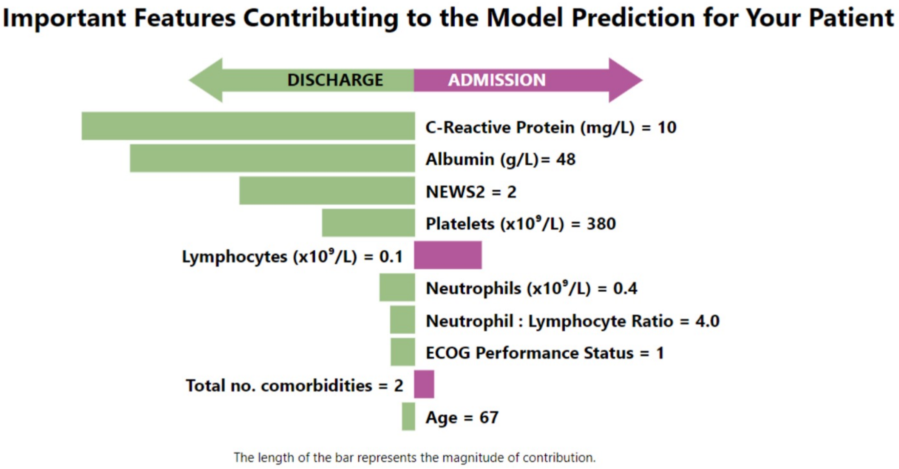
idiap
RESEARCH INSTITUTE

CANCER
RESEARCH
UK

Digital
Experimental
Cancer
Medicine
Team

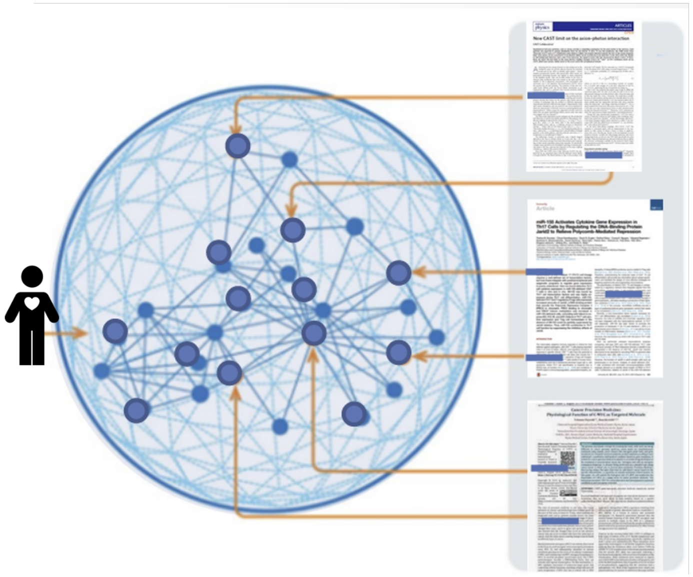
ExplAIn Lab

Three Perspectives on Explanation



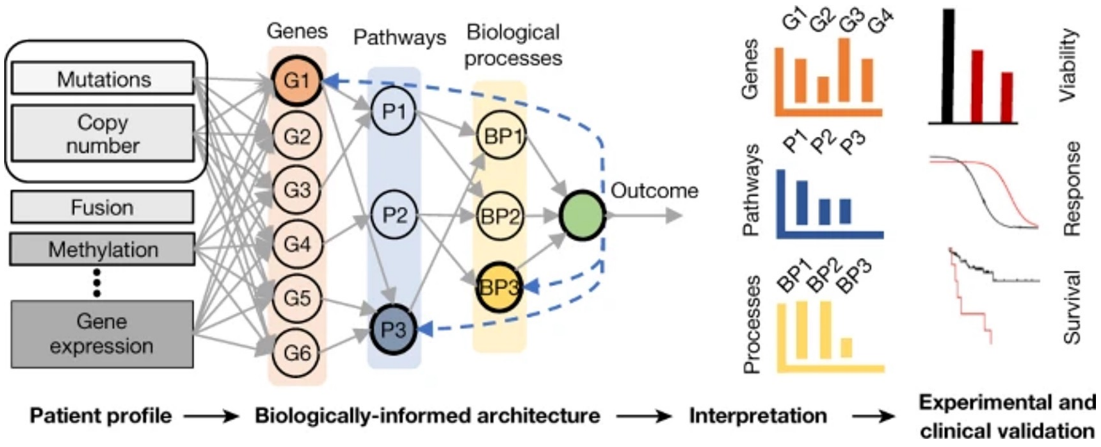
The length of the bar represents the magnitude of contribution.

The score recommends overall to: consider discharge.



Expert-AI Interaction

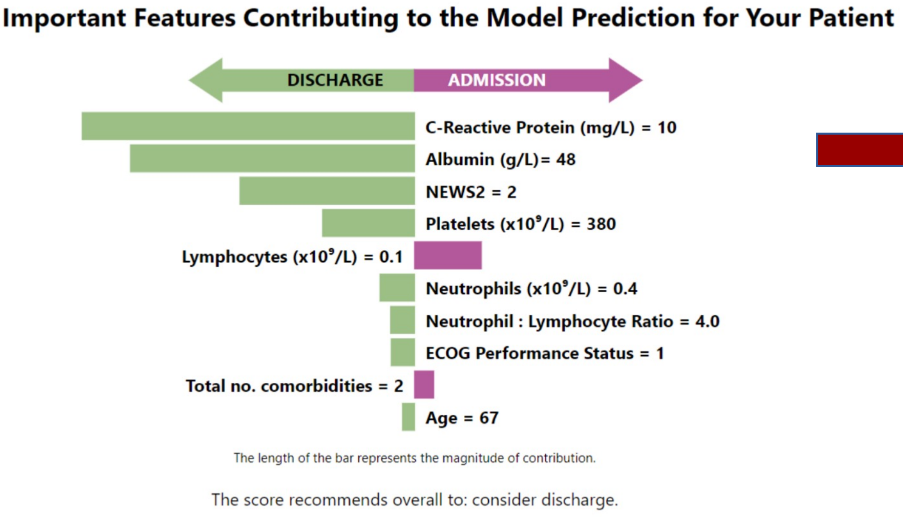
Natural Language Explanations



Prior knowledge & explainability

Elmarakeby et al, Nature (2021)

Three Perspectives on Explanation



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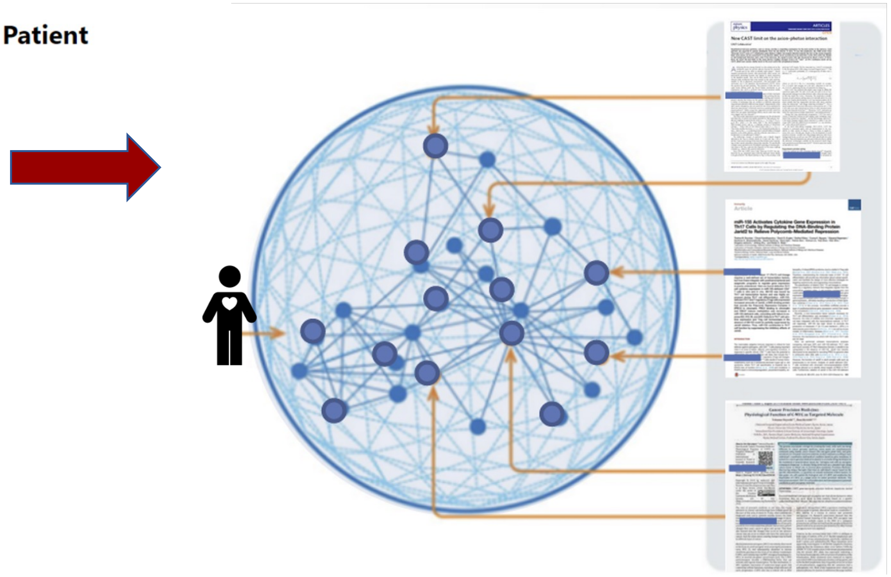
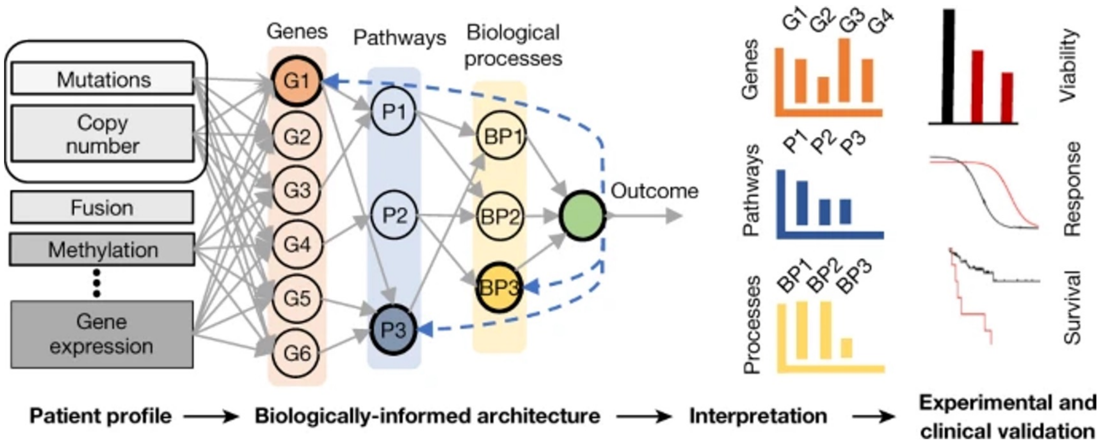


Expert-AI Interaction

Natural Language Explanations



Prior knowledge & explainability

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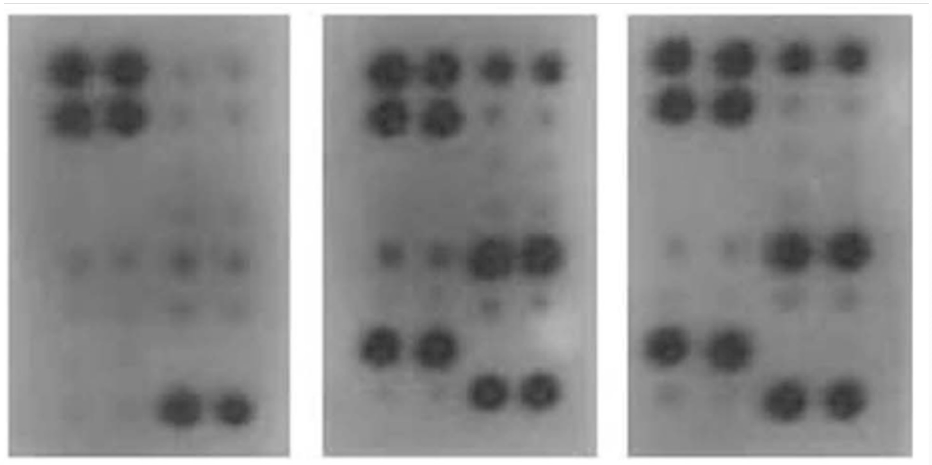
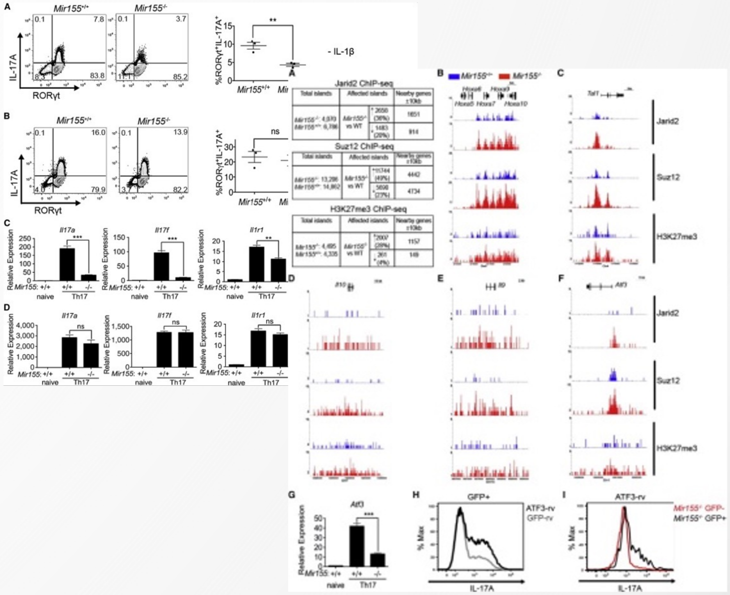
Science, Inference & Language

Experiment /Observations

Analysis





Conclusions

miR-155 Activates Cytokine Gene Expression in Th17 Cells by Regulating the DNA-Binding Protein Jarid2 to Relieve Polycomb-Mediated Repression.

“miR-155 Activates Cytokine Gene Expression in Th17 Cells by Regulating the DNA-Binding Protein Jarid2 to Relieve Polycomb-Mediated Repression.”

	Patients with SARS-Cov-2 confirmed by PCR	Patients without SARS-Cov-2 confirmed by PCR
Median age (IQR)—years	63 (53–72)	60 (49–73)
Male	787/1,309 (60.1%)	90/167 (53.9%)
Race/ethnicity—Hispanic	577/1,268 (45.5%)	62/167 (37.1%)
Race/ethnicity—African American	278/1,268 (21.9%)	46/167 (27.5%)
Race/ethnicity—White	277/1,268 (21.8%)	43/167 (25.7%)
Race/ethnicity—Asian	73/1,268 (5.8%)	5/167 (3.0%)
Race/ethnicity—Other	63/1,268 (5.0%)	11/167 (6.6%)
Obesity (BMI ≥30)	465/1,176 (39.5%)	34/149 (22.8%)[a]
Comorbidities—hypertension	420/1,268 (33.1%)	67/167 (40.1%)
Comorbidities—diabetes	293/1,268 (23.1%)	34/167 (20.4%)
Comorbidities—CKD	167/1,268 (13.2%)	27/167 (16.2%)
…	…	…

Del Valle et al. , *Nature Medicine* (2020)

$$\frac{dx_1(t)}{dt} = x_2\,(t)$$

$$\frac{dx_2(t)}{dt} = ax_1\,(t) - bx_2(t)$$

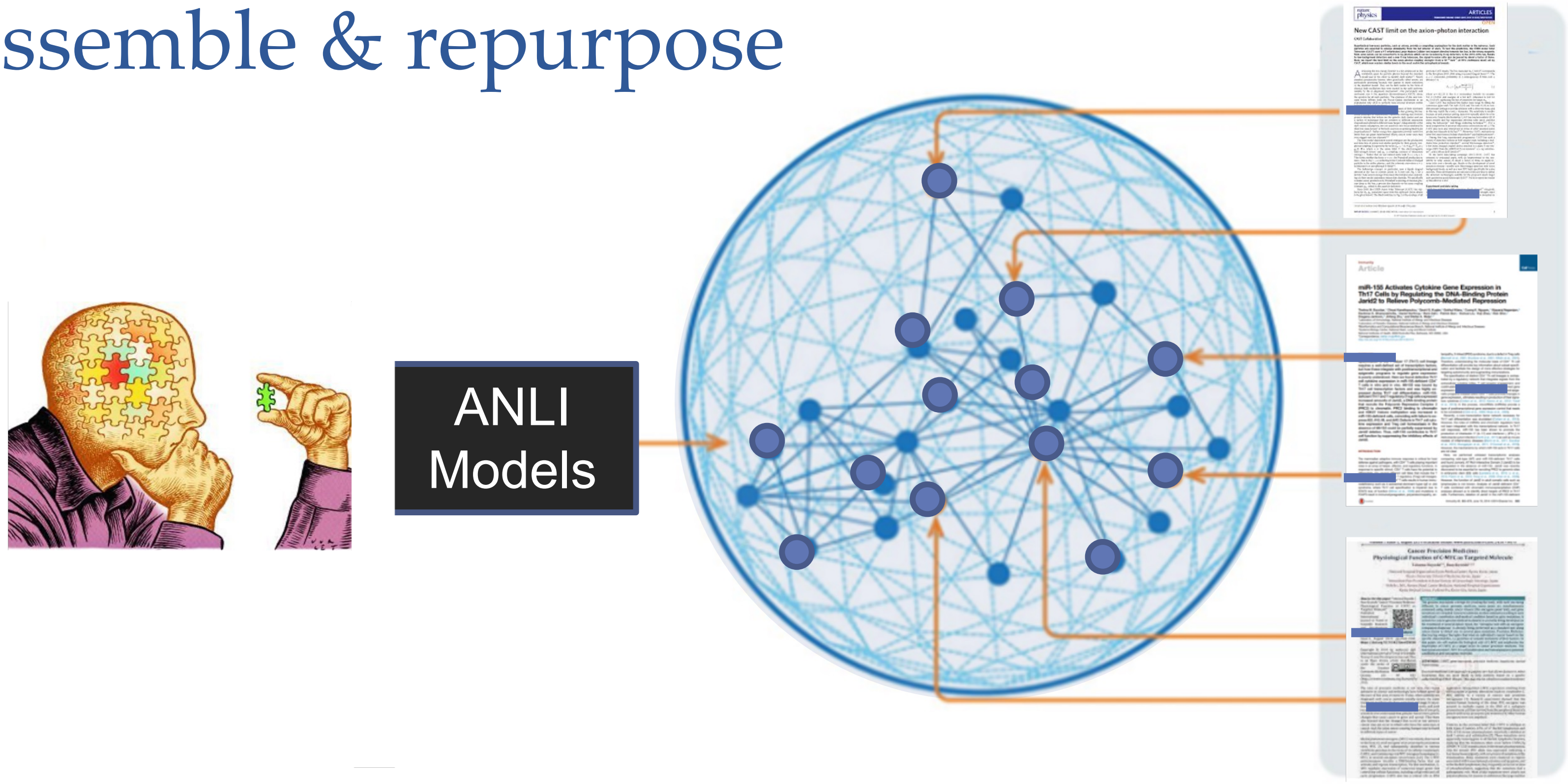
$$\frac{d^2x_1(t)}{dt^2} = \frac{dx_2(t)}{dt}$$

where $x_1(t)$ is the serum concentration of cytokine and its rate of change by $x_2(t)$

Language & Abstraction!

What if we could infer over scientific facts at scale?

Reassemble & repurpose



ANLI Models

nature physics
ARTICLES
New CAST limit on the axion-photon interaction
miR-155 Activates Cytokine Gene Expression in Th17 Cells by Regulating the DNA-Binding Protein Jarid2 to Relieve Polycomb-Mediated Repression
Cancer Precision Medicine:

Hypotheses Questions

Abductive Natural Language Inference (NLI)

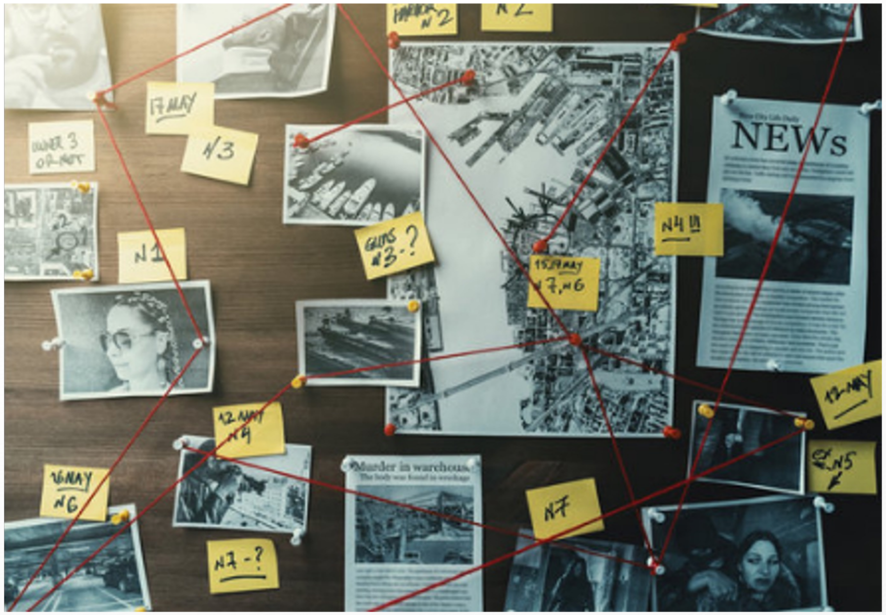
Accumulated Knowledge

Adapted from: https://human-centered.ai/project/explainable-ai-fwf-32554/

Abductive Reasoning

- First introduced by Peirce (1903).
- Inference to the best explanation.
- “Abduction is the mechanism via which we generate hypotheses about what we observe.”
- Dialogues closely with assumed background knowledge.

Veen, Creative leaps in theory: the might of abduction (2021)



Abductive Natural Language Inference (ANLI)

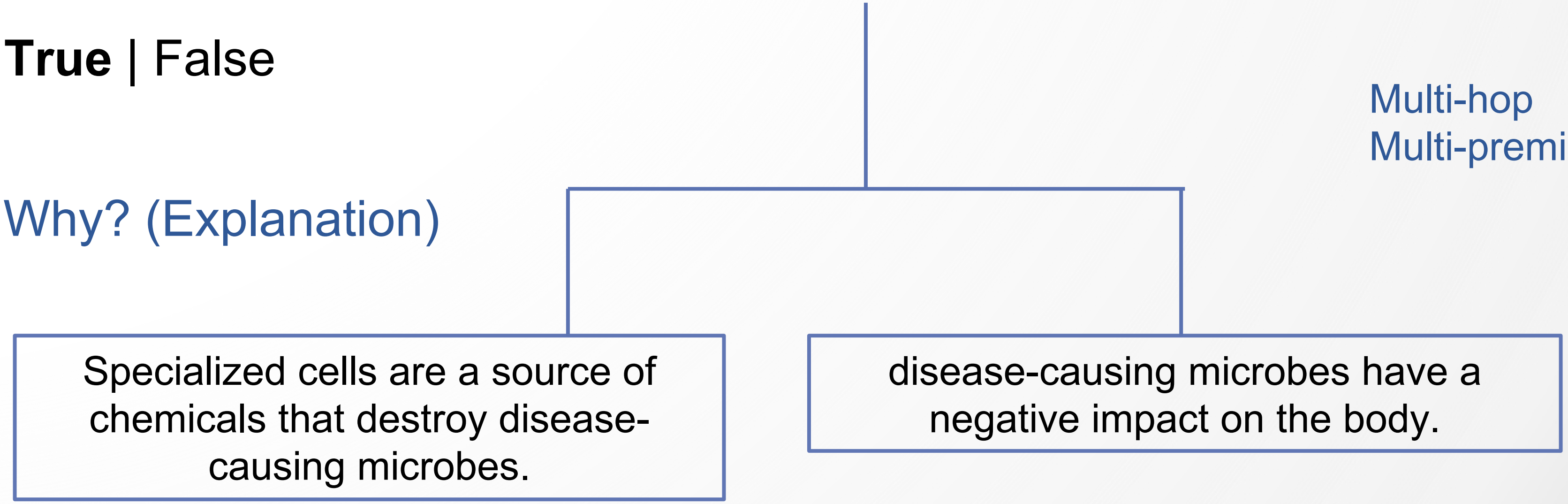
Inference to the best explanation
(facts, evidence)

Claim: Specialized cells protect the human body from disease-causing microbes by producing chemicals that destroy the microbes.

True | False

Multi-hop
Multi-premise

Why? (Explanation)



Specialized cells are a source of chemicals that destroy disease-causing microbes.

disease-causing microbes have a negative impact on the body.

~10.000 facts

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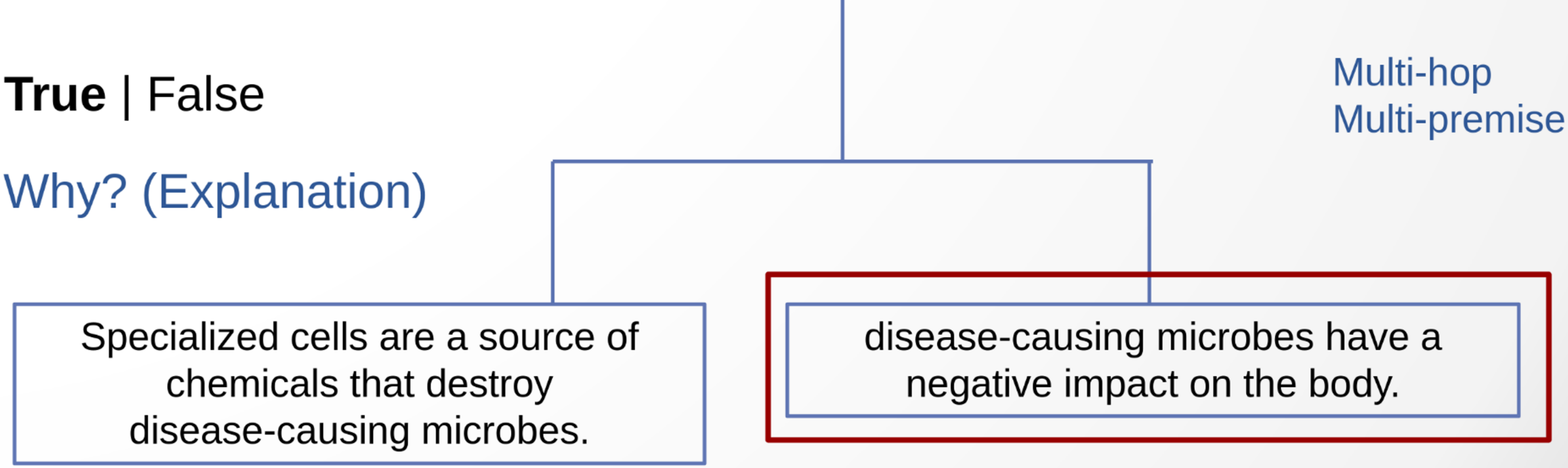

Specialized cells are a source of chemicals that destroy disease-causing microbes.

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Encoding scientific statements

~10.000 facts

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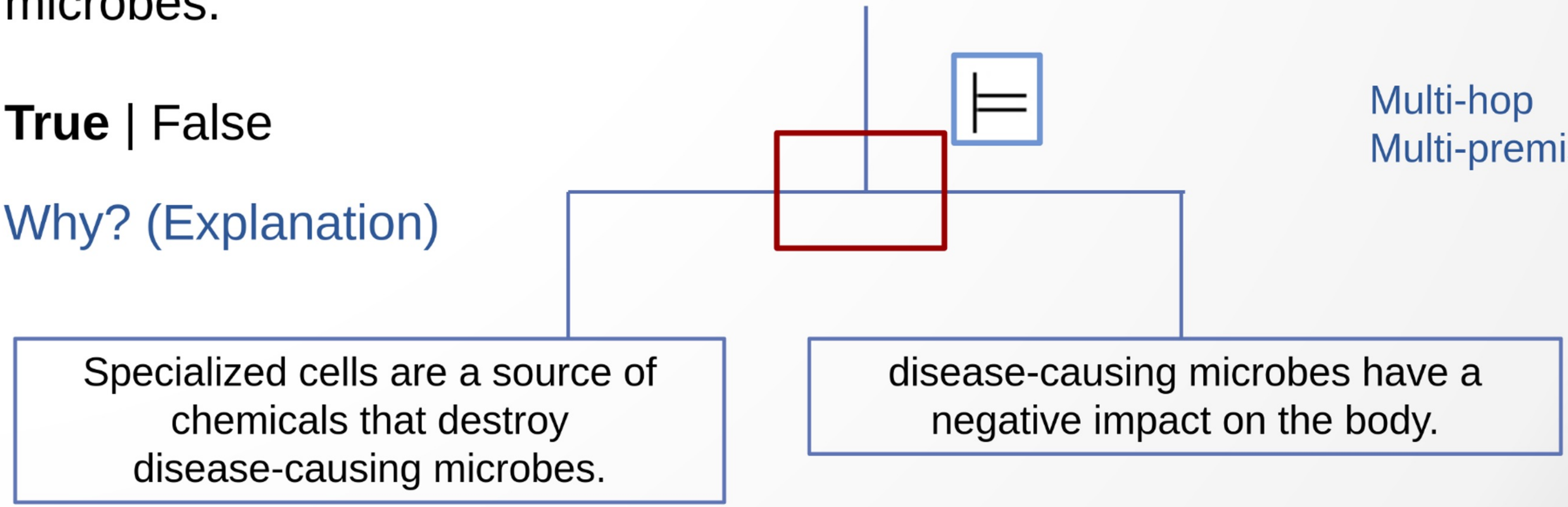


Specialized cells are a source of chemicals that destroy disease-causing microbes.

disease-causing microbes have a negative impact on the body.

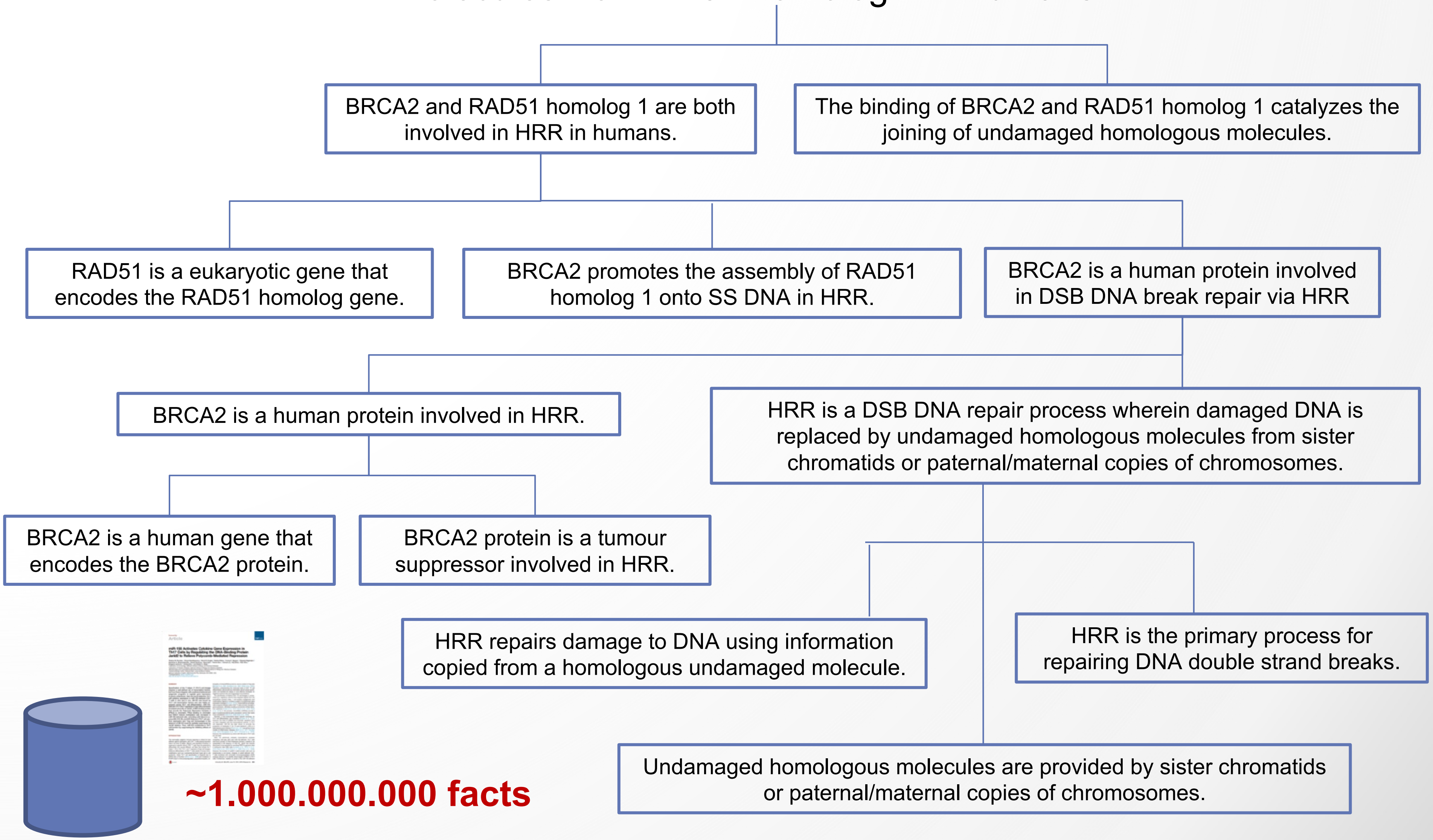
Multi-hop
Multi-premise

Encoding inference relations

~10.000 facts

Expert-level scientific inference & explanation

Claim: BRCA2 promotes the joining of undamaged homologous repair molecules via RAD51 homolog 1 in humans.



BRCA2 and RAD51 homolog 1 are both involved in HRR in humans.

The binding of BRCA2 and RAD51 homolog 1 catalyzes the joining of undamaged homologous molecules.

RAD51 is a eukaryotic gene that encodes the RAD51 homolog gene.

BRCA2 promotes the assembly of RAD51 homolog 1 onto SS DNA in HRR.

BRCA2 is a human protein involved in DSB DNA break repair via HRR

BRCA2 is a human protein involved in HRR.

HRR is a DSB DNA repair process wherein damaged DNA is replaced by undamaged homologous molecules from sister chromatids or paternal/maternal copies of chromosomes.

BRCA2 is a human gene that encodes the BRCA2 protein.

BRCA2 protein is a tumour suppressor involved in HRR.

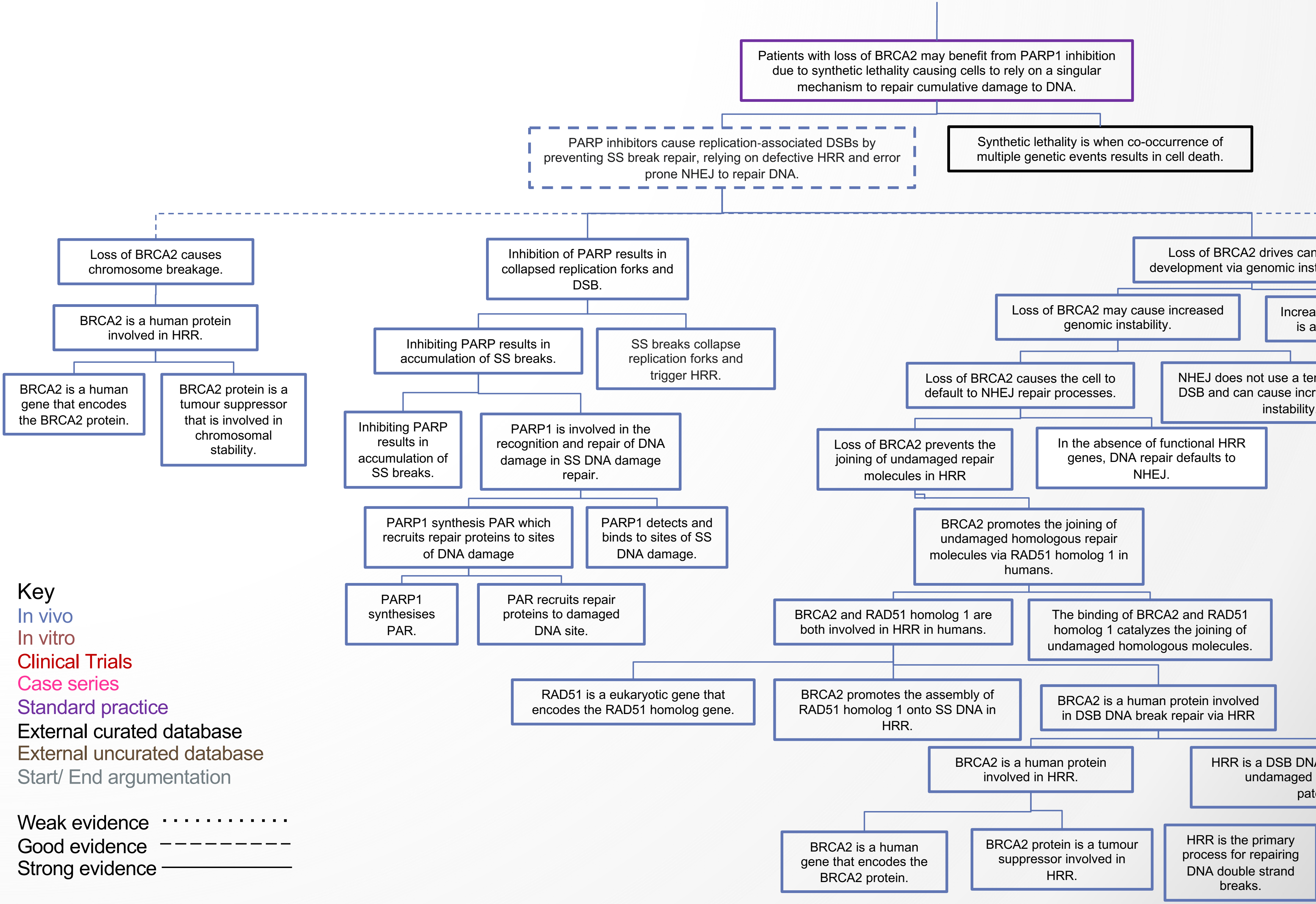
HRR repairs damage to DNA using information copied from a homologous undamaged molecule.

HRR is the primary process for repairing DNA double strand breaks.

Undamaged homologous molecules are provided by sister chromatids or paternal/maternal copies of chromosomes.

~1.000.000.000 facts

Prostate cancer patient with loss of BRCA2 may benefit from PARP1 inhibition



Patients with loss of BRCA2 may benefit from PARP1 inhibition due to synthetic lethality causing cells to rely on a singular mechanism to repair cumulative damage to DNA.

PARP inhibitors cause replication-associated DSBs by preventing SS break repair, relying on defective HRR and error prone NHEJ to repair DNA.

Synthetic lethality is when co-occurrence of multiple genetic events results in cell death.

Loss of BRCA2 causes chromosome breakage.

BRCA2 is a human protein involved in HRR.

BRCA2 is a human gene that encodes the BRCA2 protein.

BRCA2 protein is a tumour suppressor that is involved in chromosomal stability.

Inhibition of PARP results in collapsed replication forks and DSB.

Inhibiting PARP results in accumulation of SS breaks.

SS breaks collapse replication forks and trigger HRR.

Inhibiting PARP results in accumulation of SS breaks.

PARP1 is involved in the recognition and repair of DNA damage in SS DNA damage repair.

PARP1 synthesis PAR which recruits repair proteins to sites of DNA damage

PARP1 detects and binds to sites of SS DNA damage.

PARP1 synthesises PAR.

PAR recruits repair proteins to damaged DNA site.

Loss of BRCA2 drives can development via genomic inst

Loss of BRCA2 may cause increased genomic instability.

Increa is a

Loss of BRCA2 causes the cell to default to NHEJ repair processes.

NHEJ does not use a te DSB and can cause incr instability

Loss of BRCA2 prevents the joining of undamaged repair molecules in HRR

In the absence of functional HRR genes, DNA repair defaults to NHEJ.

BRCA2 promotes the joining of undamaged homologous repair molecules via RAD51 homolog 1 in humans.

BRCA2 and RAD51 homolog 1 are both involved in HRR in humans.

The binding of BRCA2 and RAD51 homolog 1 catalyzes the joining of undamaged homologous molecules.

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BRCA2 protein is a tumour suppressor involved in HRR.

HRR is the primary process for repairing DNA double strand breaks.

Key

In vivo

In vitro

Clinical Trials

Case series

Standard practice

External curated database

External uncurated database

Start/ End argumentation

Weak evidence · · · · · · · · · · · ·

Good evidence – – – – – – – – –

Strong evidence ————————

Patients living in the San Francisco area with ErbB2+ breast cancer, a body weight > 60 kg, and a history of treatment with Cyclophosphamide in the last year, are eligible for this clinical trial.

⊨

Clinical Trial Report - Eligibility Criteria

Inclusion criteria

- Patients with a history of chemotherapy treatment within the last 24 months.
- Age ≥ 60 years
- HER2-positive T1 histologically confirmed invasive carcinoma of the breast.
- Body weight > 110 lbs
- Patients be California residents

Exclusion criteria

- Pregnant women

The Neural Perspective: Language Models

- Probability distributions over strings of text.

The students opened their …
The students opened their books
(predicted)

S = The students opened their books

P(S) = P(The) x P(students | The) x P(opened | The students) x P(their | The students opened) x P(books | The students opened their)

Neural Language Models

output distribution

$$\hat{\boldsymbol{y}} = \mathrm{softmax}(\boldsymbol{U}\boldsymbol{h} + \boldsymbol{b}_2) \in \mathbb{R}^{|V|}$$

hidden layer

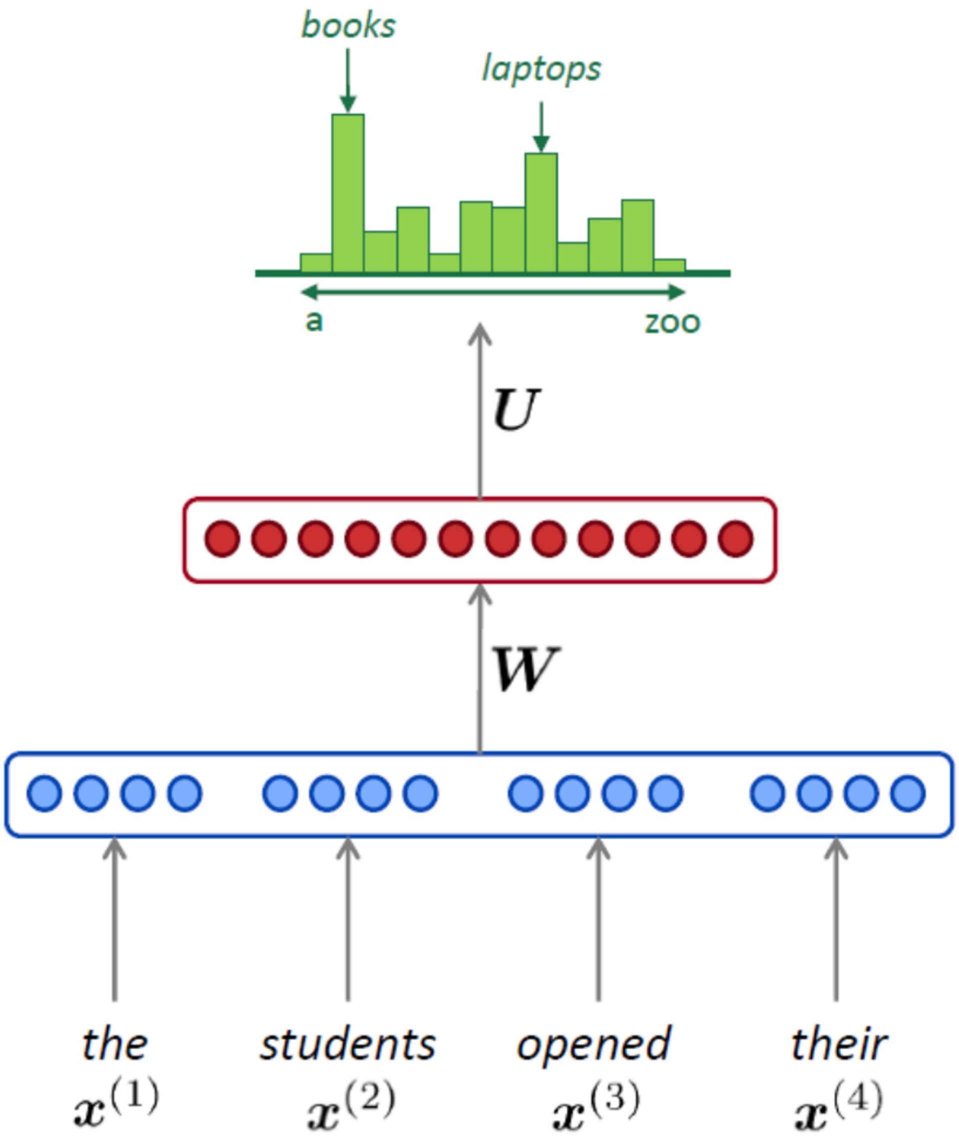
$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{e} + \boldsymbol{b}_1)$$

concatenated word embeddings

$$\boldsymbol{e} = [\boldsymbol{e}^{(1)}; \boldsymbol{e}^{(2)}; \boldsymbol{e}^{(3)}; \boldsymbol{e}^{(4)}]$$

words / one-hot vectors

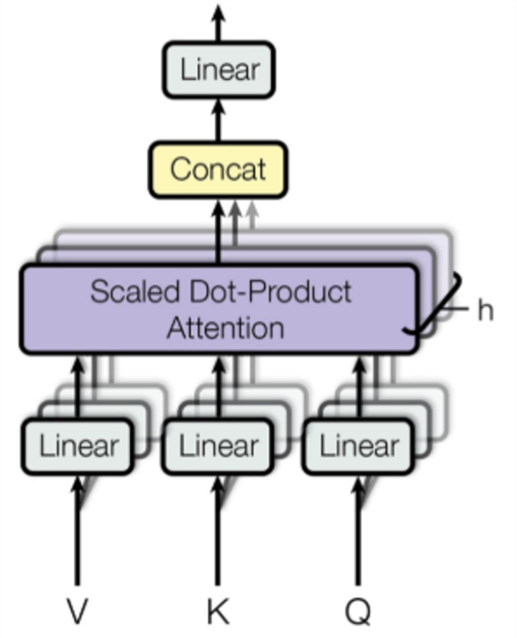
$$\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \boldsymbol{x}^{(3)}, \boldsymbol{x}^{(4)}$$

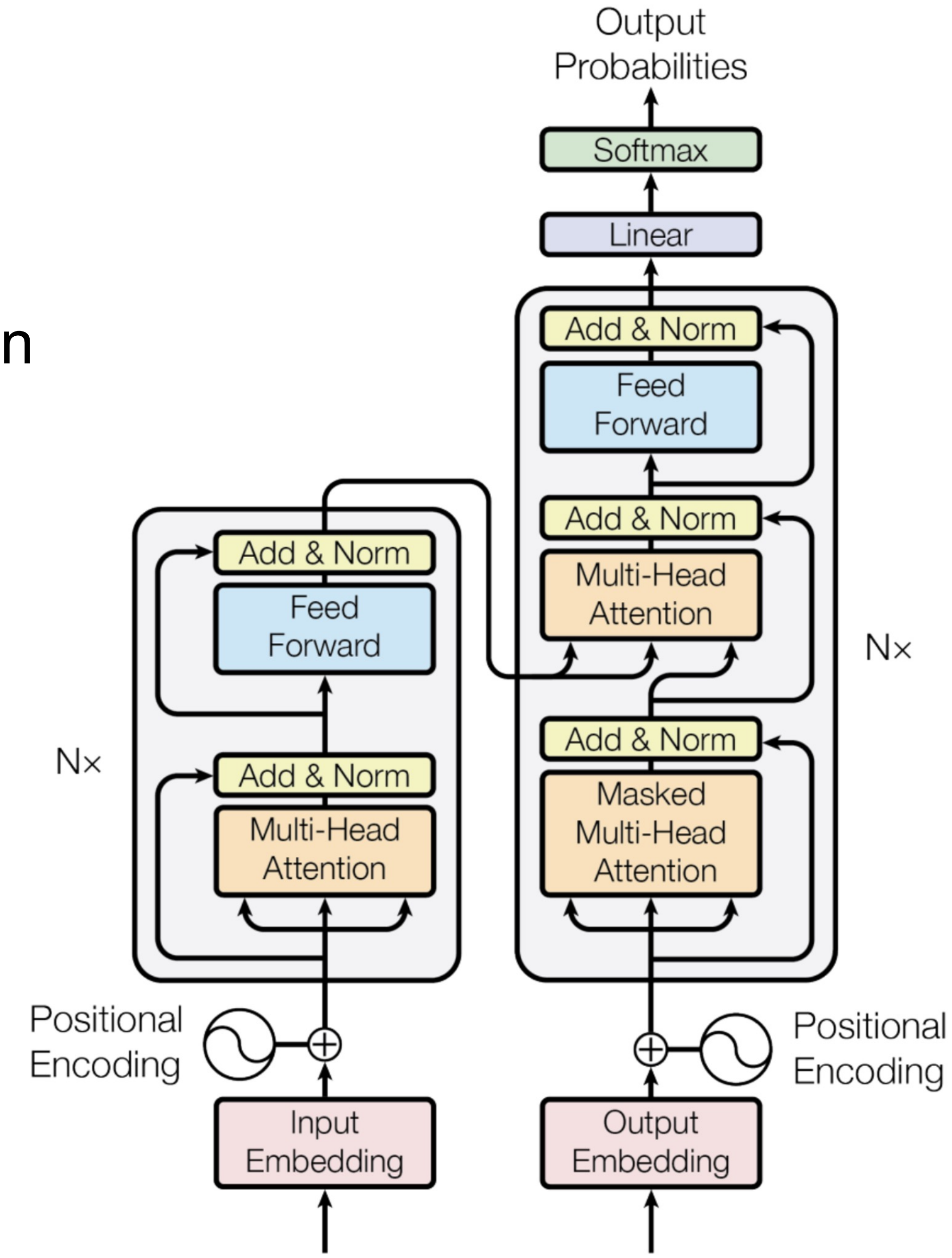


Kapronczay, Towards Data Science (2021)

Transformers

1. Positional Encodings
2. (Multi-head) Self-Attention

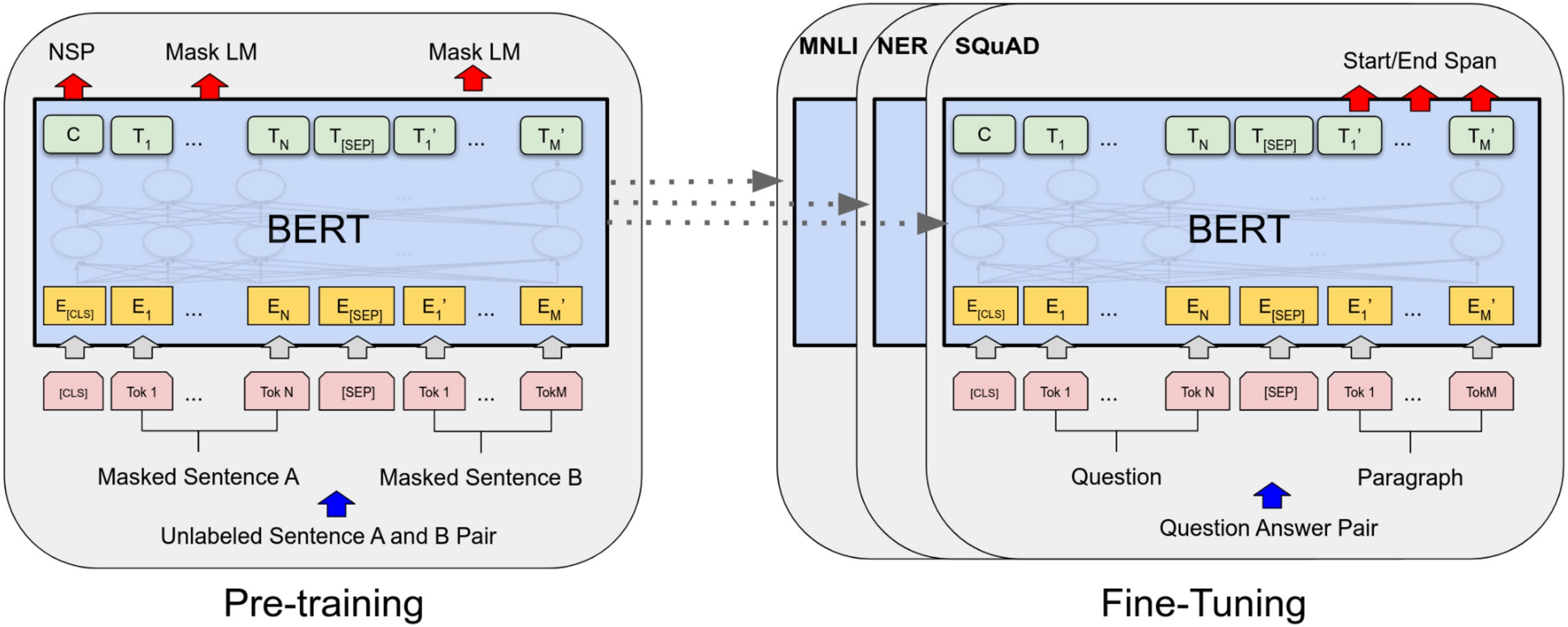




Vaswani et al, NeurIPS (2017)

BERT: Bidirectional Encoder Representations from Transformers

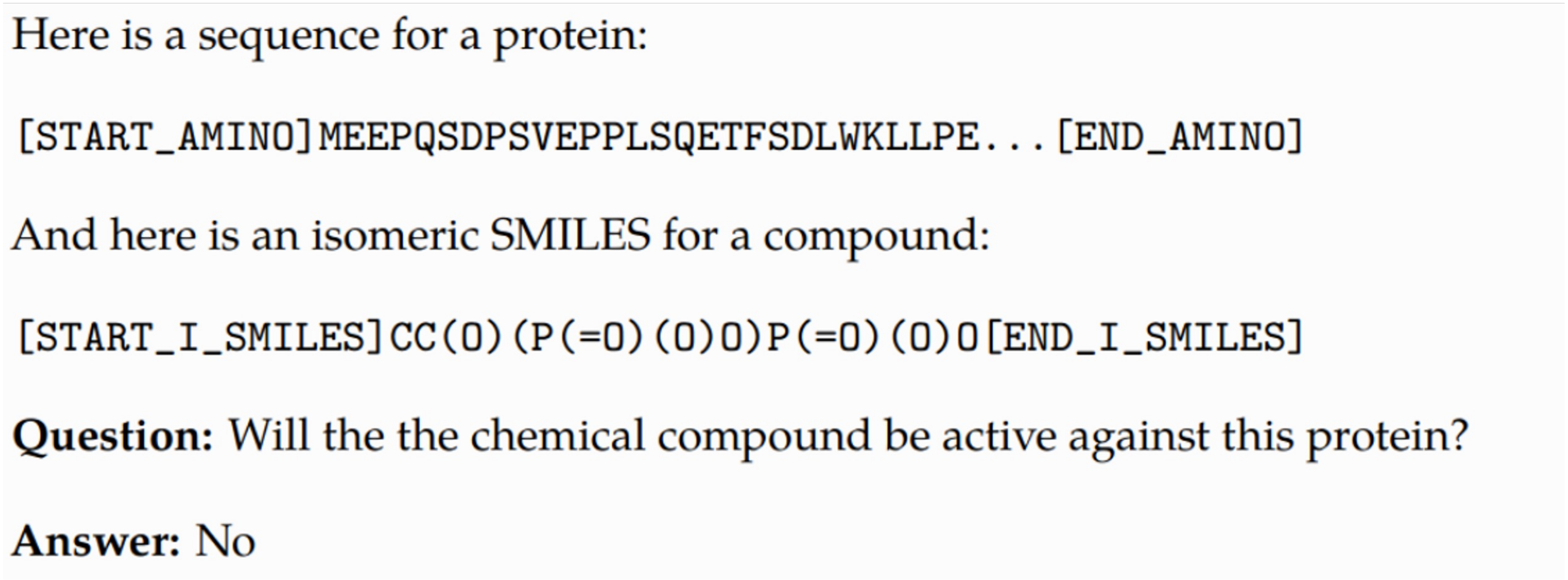
Self-attention allows a a model to assign a meaning to a term in a complex context.



$\vec{S}$

Devlin, Chang, Lee, Toutanova, CoRR (2018)

Trust me, I am a Language Model.



Here is a sequence for a protein:

`[START_AMINO]MEEPQSDPSVEPPLSQETFSDLWKLLPE...[END_AMINO]`

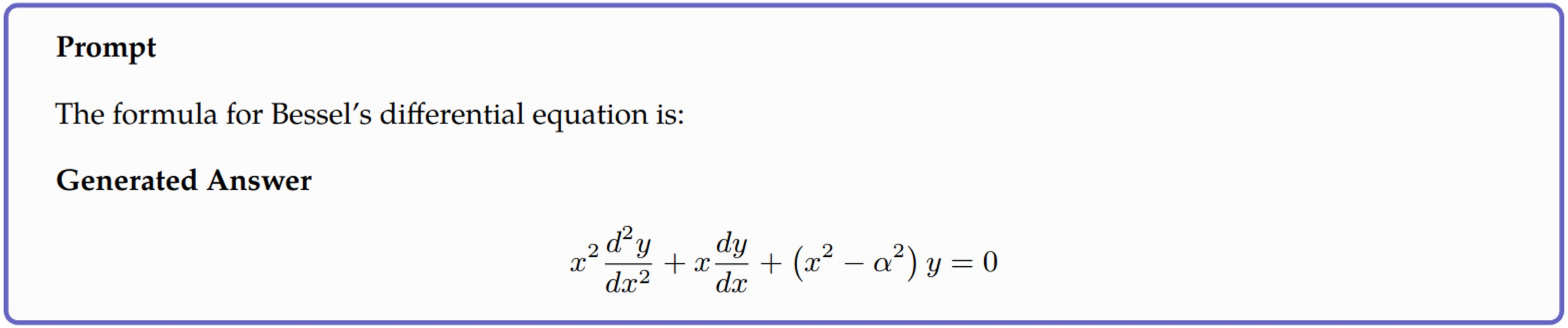
And here is an isomeric SMILES for a compound:

`[START_I_SMILES]CC(O)(P(=O)(O)O)P(=O)(O)O[END_I_SMILES]`

Question: Will the the chemical compound be active against this protein?

Answer: No

Trust me, I am a Language Model.

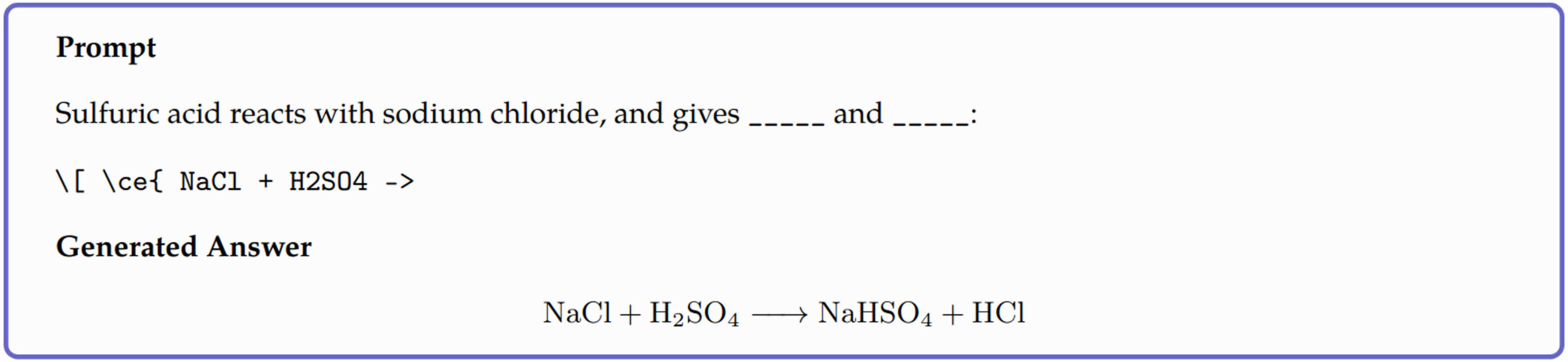


Prompt

The formula for Bessel's differential equation is:

Generated Answer

$$x^2 \frac{d^2 y}{dx^2} + x \frac{dy}{dx} + \left(x^2 - \alpha^2\right) y = 0$$



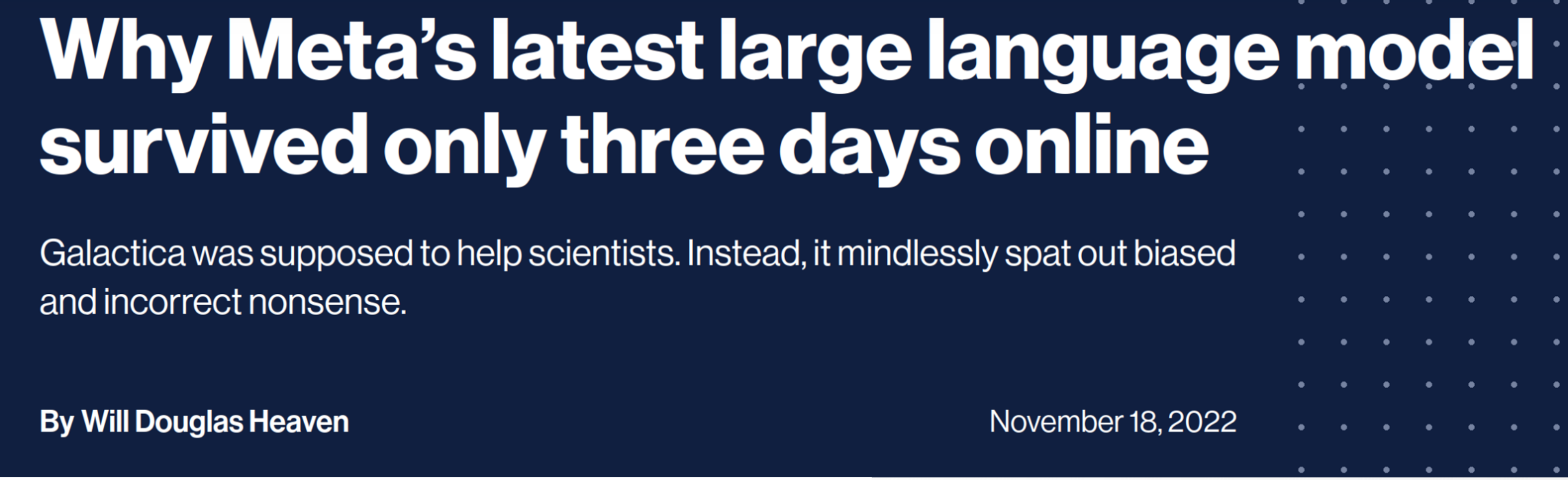
Prompt

Sulfuric acid reacts with sodium chloride, and gives _____ and _____:

```
\[ \ce{ NaCl + H2SO4 ->
```

Generated Answer

$$\mathrm{NaCl} + \mathrm{H_2SO_4} \longrightarrow \mathrm{NaHSO_4} + \mathrm{HCl}$$

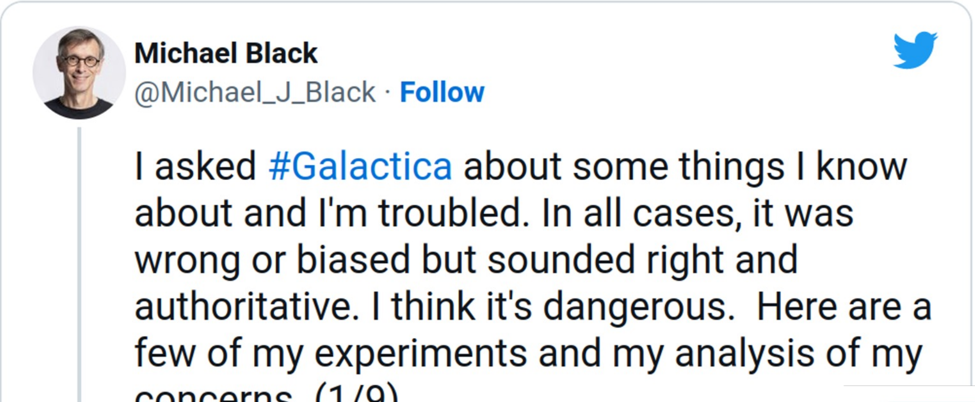


Why Meta's latest large language model survived only three days online

Galactica was supposed to help scientists. Instead, it mindlessly spat out biased and incorrect nonsense.

By Will Douglas Heaven

November 18, 2022

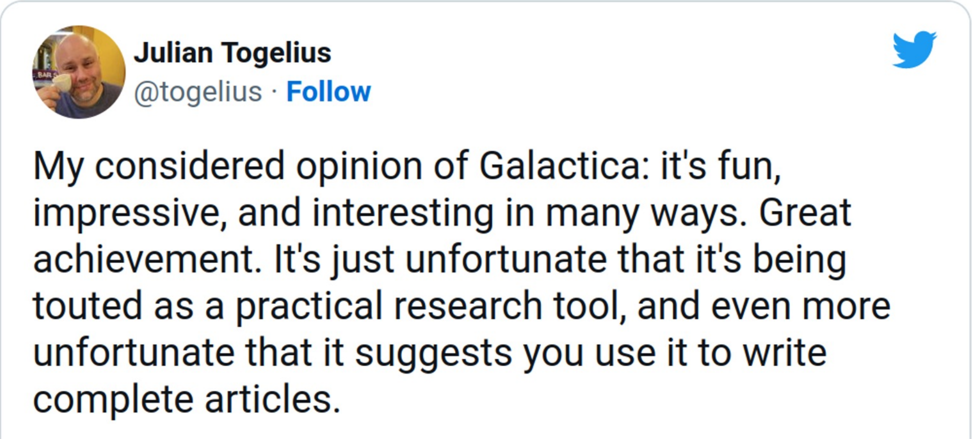


Michael Black
@Michael_J_Black · Follow

I asked #Galactica about some things I know about and I'm troubled. In all cases, it was wrong or biased but sounded right and authoritative. I think it's dangerous. Here are a few of my experiments and my analysis of my concerns. (1/9)

7:47 AM · Nov 17, 2022

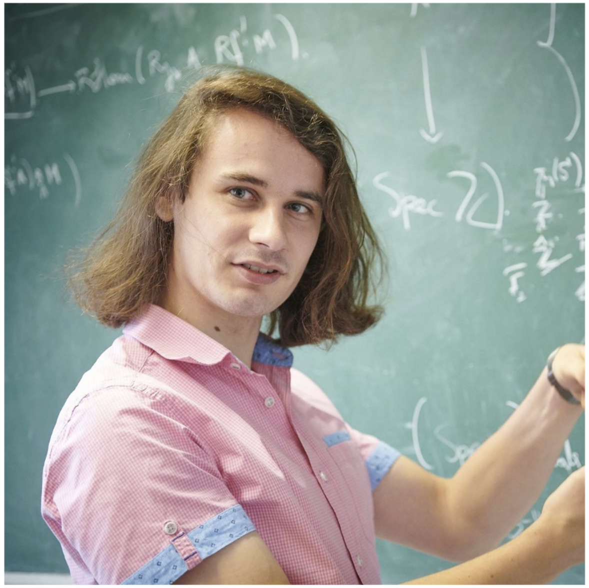
Ouch!



Julian Togelius
@togelius · Follow

My considered opinion of Galactica: it's fun, impressive, and interesting in many ways. Great achievement. It's just unfortunate that it's being touted as a practical research tool, and even more unfortunate that it suggests you use it to write complete articles.

The Liquid Tensor Experiment



LEAN

THEOREM PROVER

Why do I want a formalization?

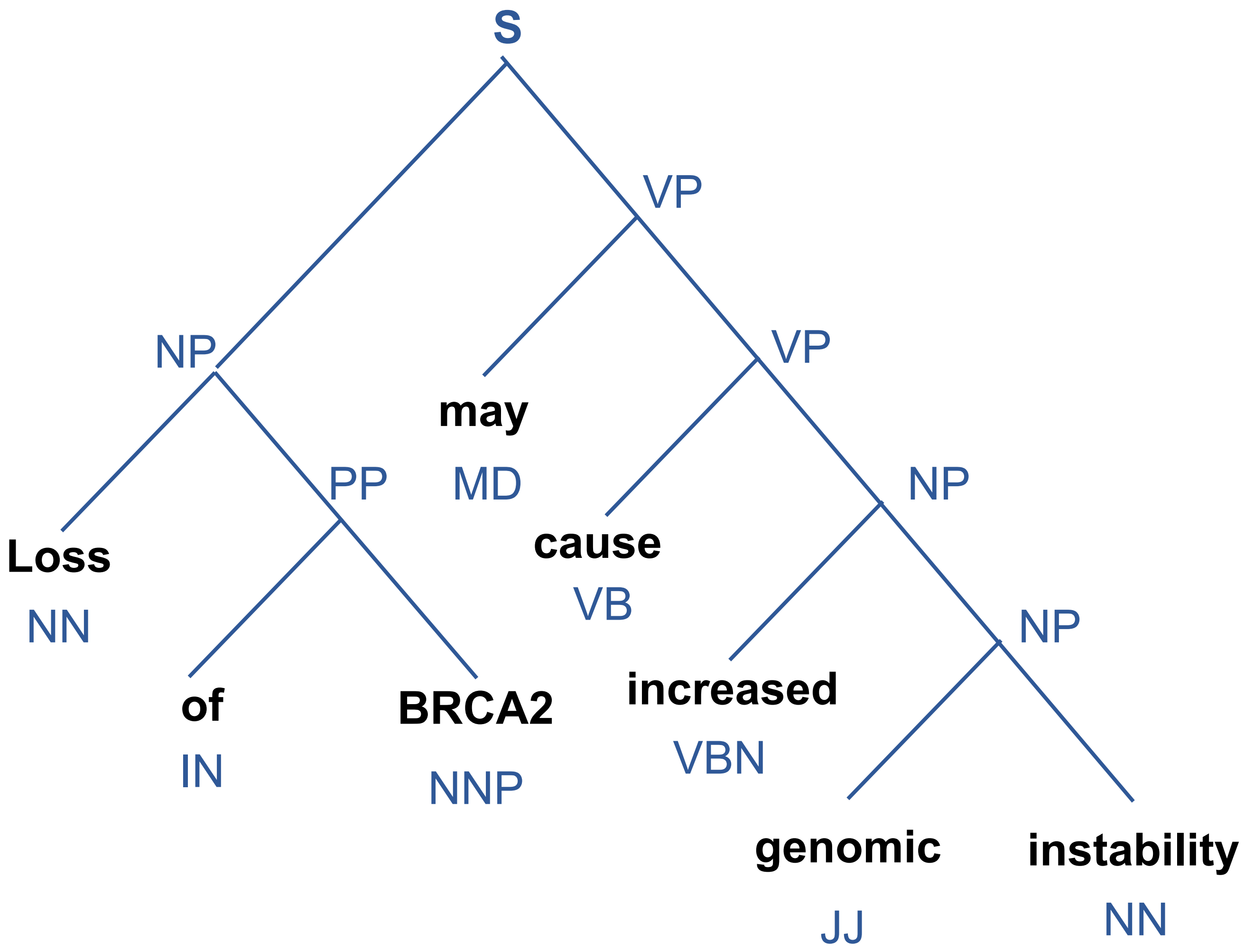
— “with this theorem, the hope that the condensed formalism can be fruitfully applied to real functional analysis stands or falls. I think the theorem is of utmost foundational importance, **so being 99.9% sure is not enough**.”

Verifiability

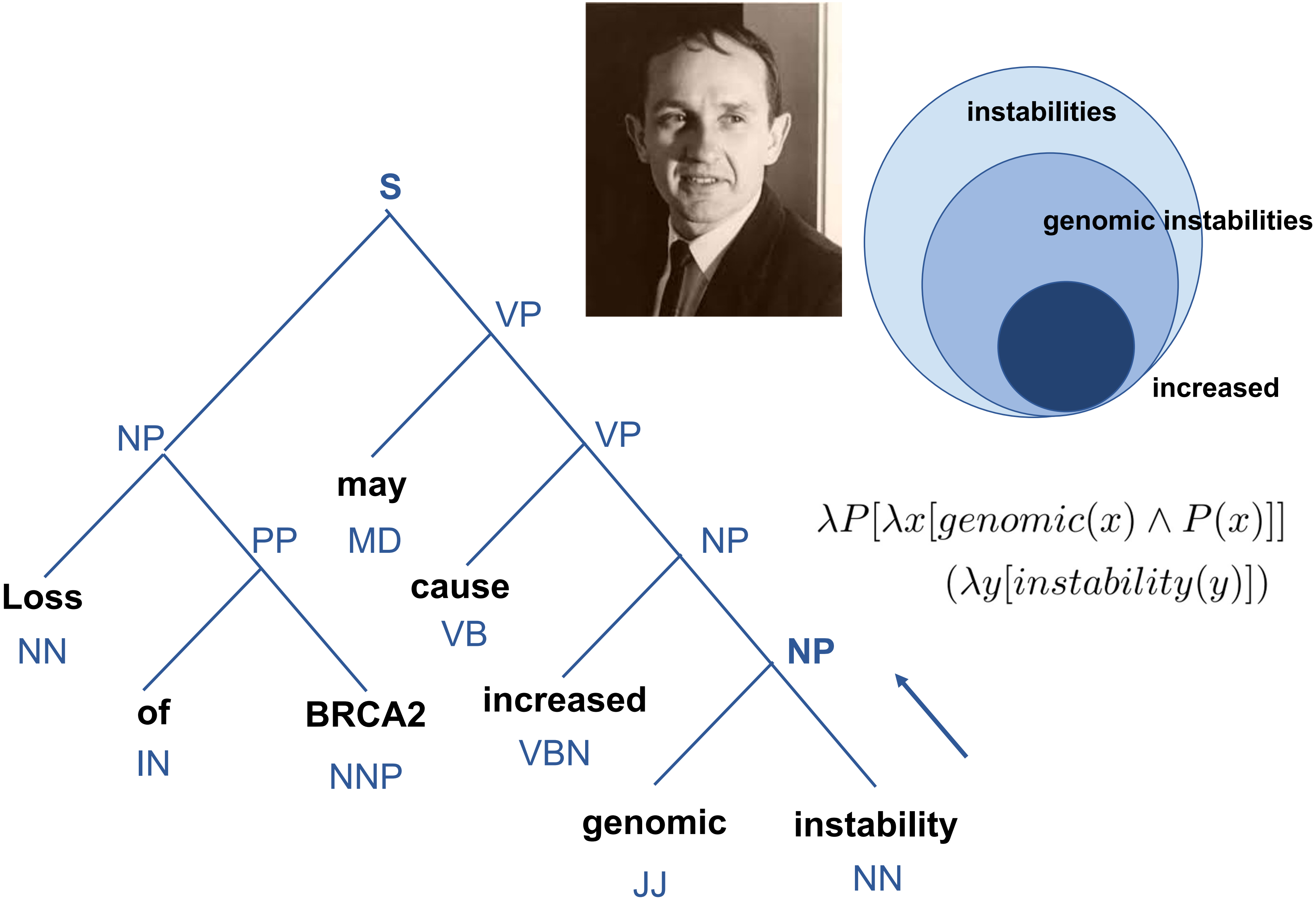
https://xenaproject.wordpress.com/2020/12/05/liquid-tensor-experiment/

The Formal Perspective

Loss of BRCA2 may cause increased genomic instability.



The Formal Perspective



$$\lambda P[\lambda x[genomic(x) \wedge P(x)]]$$
$$(\lambda y[instability(y)])$$

Scientific inference

Scientific discourse

- Step-wise explicit (verbalised) inference.
- Formal, verifiable argument & explanation.
- Preserving the positive aspects of LLMs.
- Improving control.

Large Language Models (LLMs)

Formal

Neuro

Neuro-symbolic

Symbolic

Scientific inference

Scientific discourse

- Step-wise explicit (verbalised) inference.
- Formal, verifiable argument & explanation.
- Preserving the positive aspects of LLMs.
- Improving control.

$$\Gamma \vDash \Phi$$

$$\Gamma \text{ semantically entails } \Phi$$

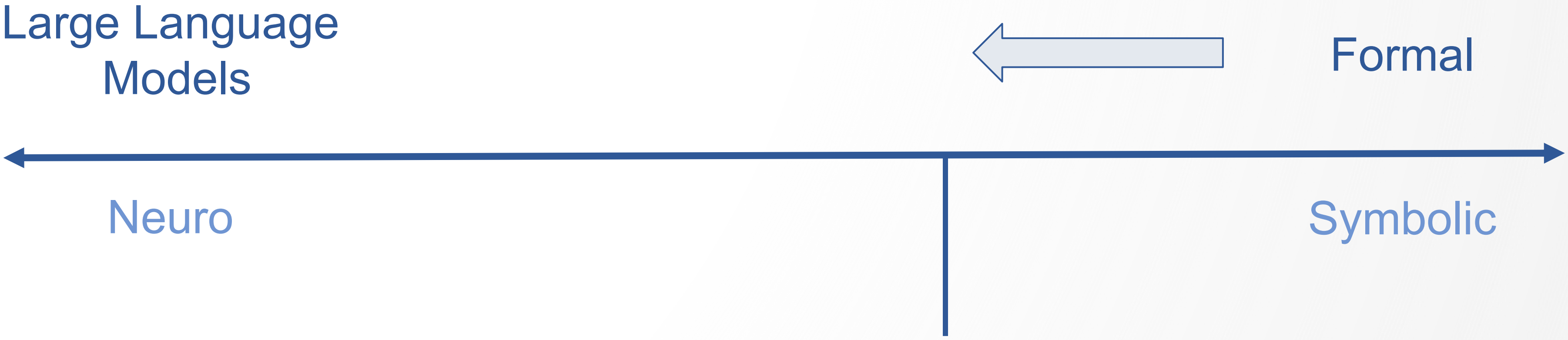
$$\Gamma \vdash \Phi \qquad \boxed{\vdash}$$

- interpretability
- control (inference guarantees)

$$\Gamma \text{ proves } \Phi$$

Encoding scientific statements

Semantic Role Labeling

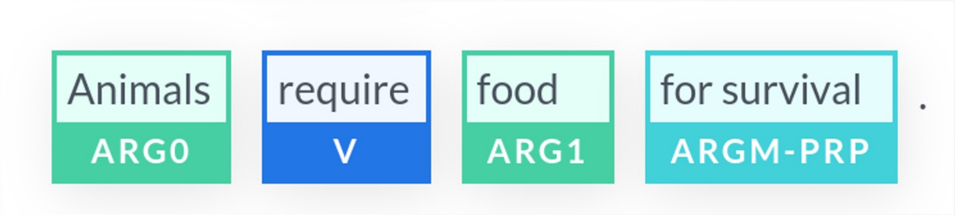


Large Language Models

Formal

Neuro

Symbolic

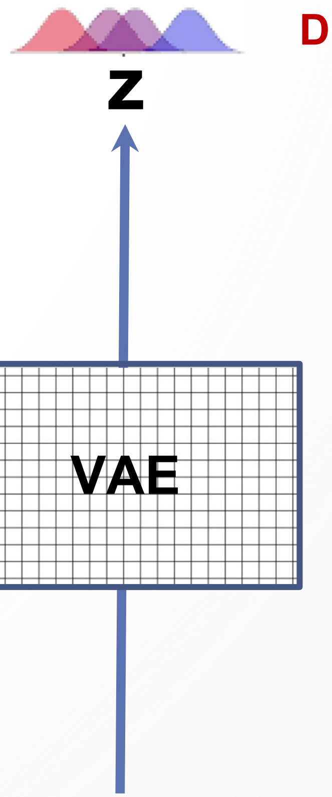


Animals	require	food	for survival	.
ARG0	V	ARG1	ARGM-PRP	

- Lightweight representation (a little semantics goes a long way).
- Robust parsers.
- Expressive semantic roles.

ARGM-DIR	Directionals. E.g. all waves transmit energy **from one place to another**
ARGM-PNC	Purpose. E.g. many animals blend in with their environment **to not be seen by predators**
ARGM-CAU	Cause. E.g. cold environments sometimes are white in color **from being covered in snow**
ARGM-PRP	Purpose. E.g. a pot is made of metal **for cooking**
ARGM-EXT	Extent. E.g. as the amount of oxygen exposed to a fire increases the fire will burn **longer**
ARGM-LOC	Location. E.g. a solute can be dissolved **in a solvent** when they are combined
ARGM-MNR	Manner. E.g. fast means **quickly**
ARGM-MOD	Modal verbs. E.g. atom **can** not be divided into smaller substances
ARGM-DIS	Discourse. E.g. if something required by an organism is depleted **then** that organism must replenish that something
ARGM-GOL	Goal. E.g. We flew **to Chicago**
ARGM-NEG	Negation. E.g. cactus wrens building nests in cholla cacti does **not** harm the cholla cacti
ARGM-ADV	Adverbials
ARGM-PRD	Markers of secondary predication. E.g.
ARGM-TMP	Temporals. E.g. a predator **usually** kills its prey to eat it
O	Empty tag.
V	Verb.
ARG0	Agent or Causer. E.g. **rabbits** eat plants
ARG1	Patient or Theme. E.g. rabbits eat **plants**
ARG2	indirect object / beneficiary / instrument / attribute / end state. E.g. animals are **organisms**
ARG3	start point / beneficiary / instrument / attribute. E.g. sleeping bags are designed **to keep people warm**
ARG4	end point. E.g. when water falls from the sky that

Generative Models



Disentanglement

(Loss of BRCA2) **causes** (the cell) to default to (NHEJ repair processes).

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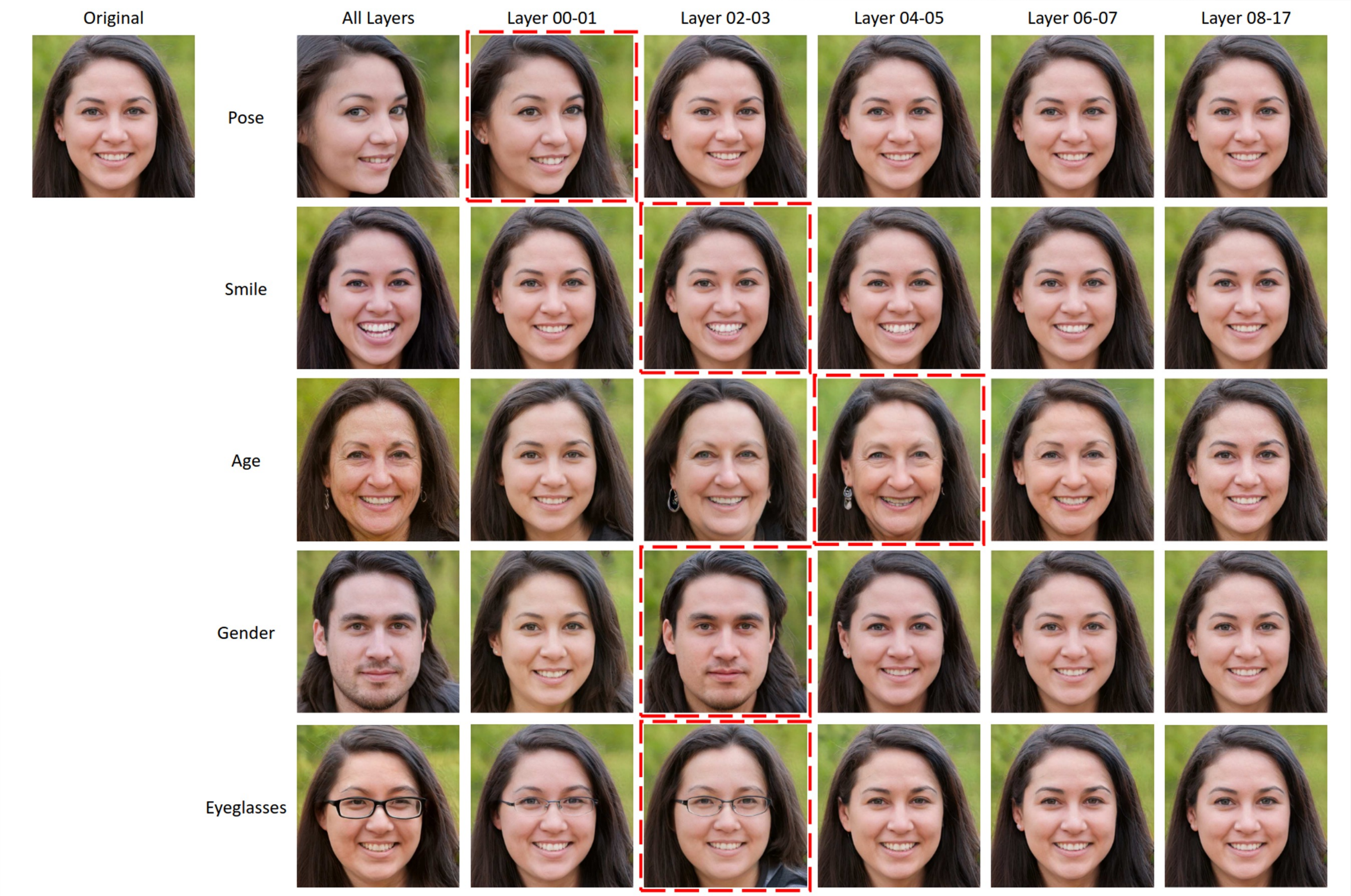
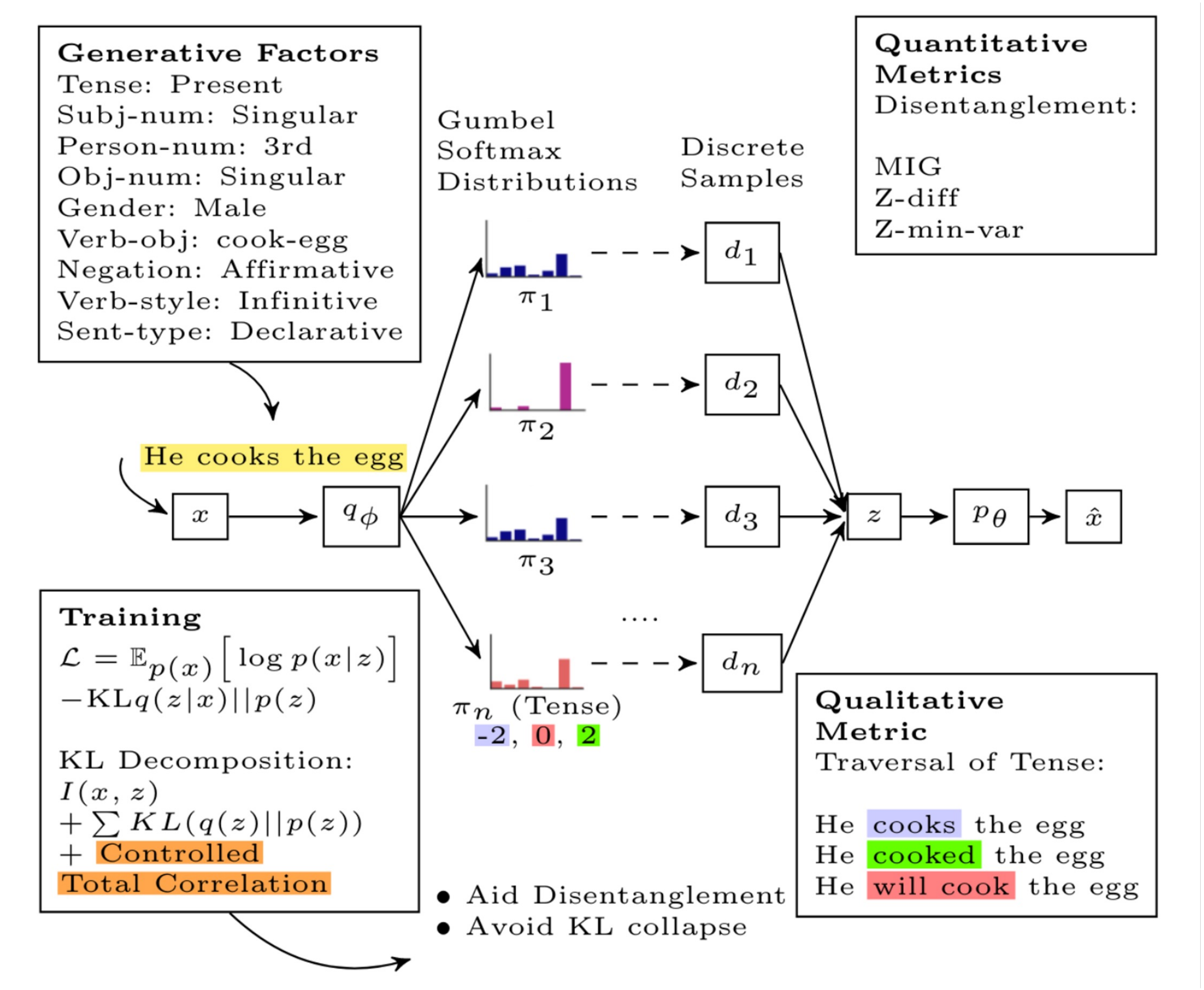
Integrating Syntactic and Semantic Structure into the latent space

Generative Models



InterFaceGAN: Interpreting the Disentangled Face Representation Learned by GANs

Syntactic Disentanglement



Generative Factors
Tense: Present
Subj-num: Singular
Person-num: 3rd
Obj-num: Singular
Gender: Male
Verb-obj: cook-egg
Negation: Affirmative
Verb-style: Infinitive
Sent-type: Declarative

Quantitative Metrics
Disentanglement:

MIG
Z-diff
Z-min-var

Training

$$\mathcal{L} = \mathbb{E}_{p(x)}\left[\log p(x|z)\right] - \mathrm{KL}q(z|x)||p(z)$$

KL Decomposition:
$I(x, z)$
$+ \sum KL(q(z)||p(z))$
+ Controlled Total Correlation

- Aid Disentanglement
- Avoid KL collapse

Qualitative Metric
Traversal of Tense:

He cooks the egg
He cooked the egg
He will cook the egg

Mercatali & Freitas, EMNLP Findings (2021)

Syntactic Disentanglement

(Loss of BRCA2) **causes** (the cell) to default to (NHEJ repair processes).
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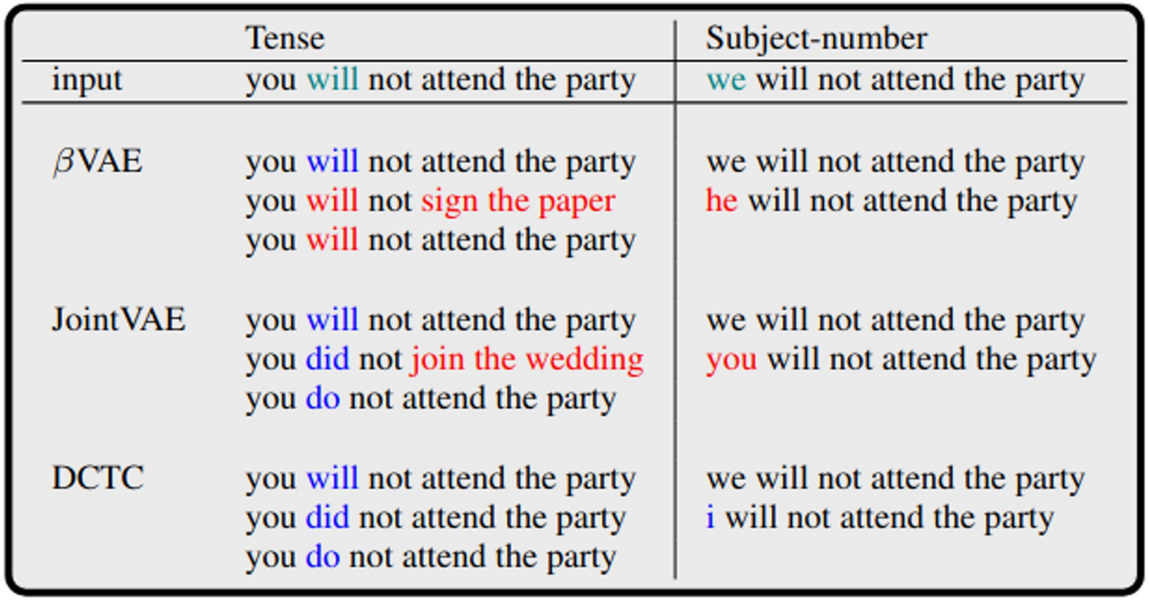
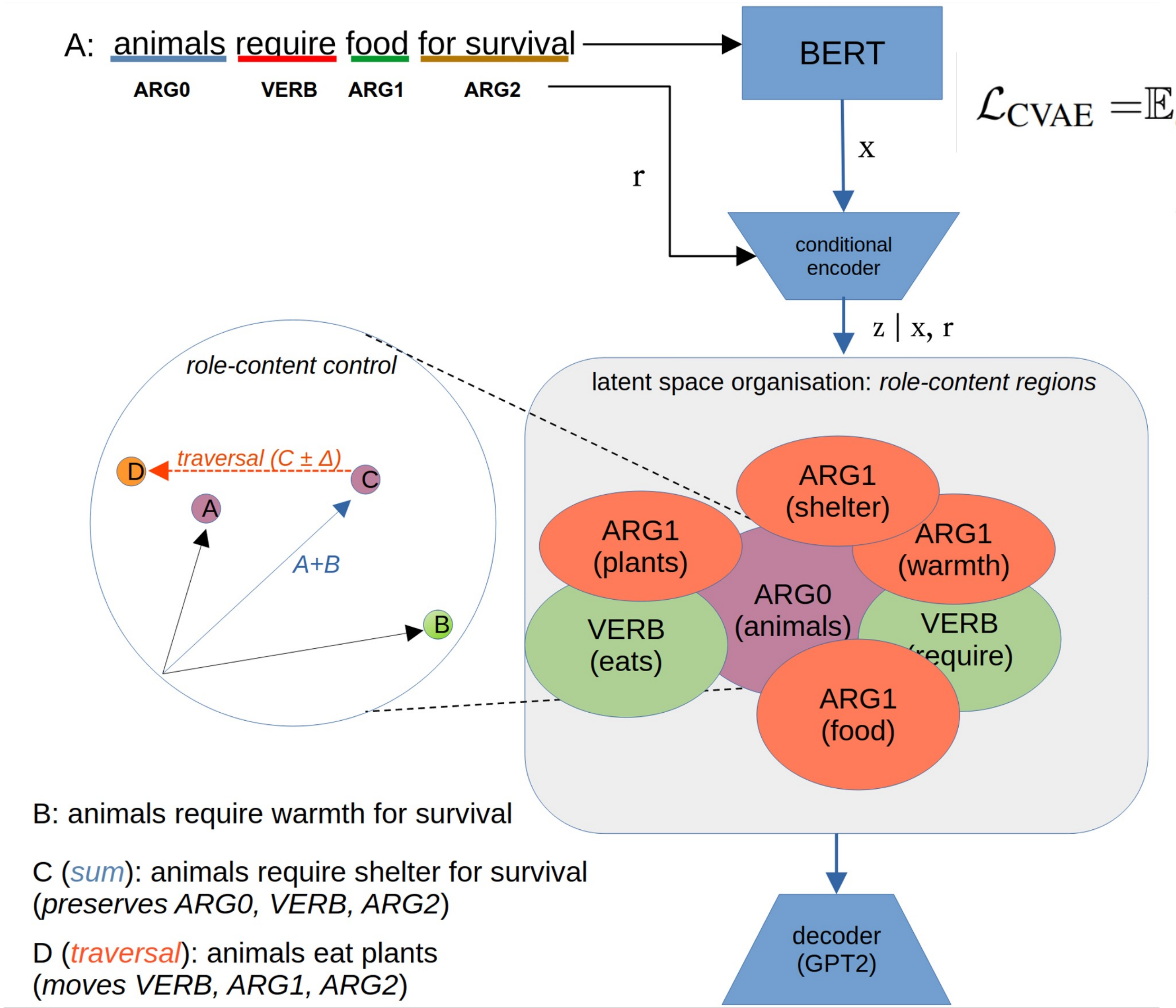


	Tense	Subject-number
input	you will not attend the party	we will not attend the party
βVAE	you will not attend the party	we will not attend the party
	you will not sign the paper	he will not attend the party
	you will not attend the party	
JointVAE	you will not attend the party	we will not attend the party
	you did not join the wedding	you will not attend the party
	you do not attend the party	
DCTC	you will not attend the party	we will not attend the party
	you did not attend the party	i will not attend the party
	you do not attend the party	

Latent traversal

Mercatali & Freitas, EMNLP Findings (2021)

Syntactic-Semantic Disentanglement



B: animals require warmth for survival

C (*sum*): animals require shelter for survival (*preserves ARG0, VERB, ARG2*)

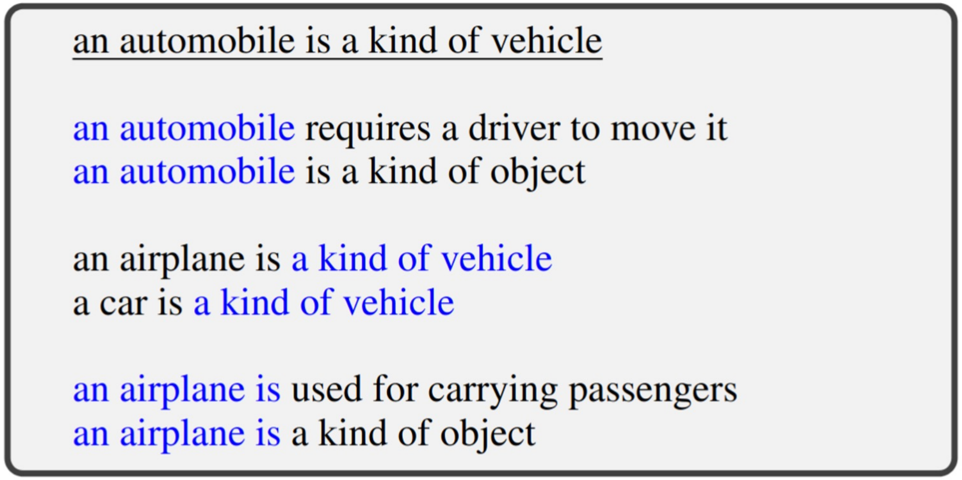
D (*traversal*): animals eat plants (*moves VERB, ARG1, ARG2*)

$$\mathcal{L}_{\text{CVAE}} = \mathbb{E}_{q_\phi(z|r,x)}\Big[\log p_\theta(x|z,r)\Big] - \text{KL}q_\phi(z|x,r)||p(z|r)$$

Extending the Optimus architecture

Zhang, Carvalho, Pratt-Hartmann, Freitas, arXiv:2210.06230 (2022)

Syntactic-Semantic Disentanglement



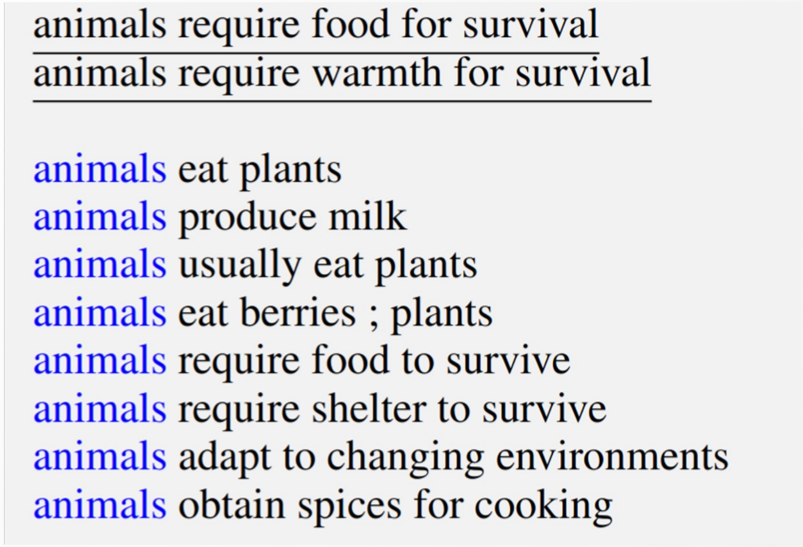
an automobile is a kind of vehicle

an automobile requires a driver to move it
an automobile is a kind of object

an airplane is a kind of vehicle
a car is a kind of vehicle

an airplane is used for carrying passengers
an airplane is a kind of object

Latent traversal



animals require food for survival
animals require warmth for survival

animals eat plants
animals produce milk
animals usually eat plants
animals eat berries ; plants
animals require food to survive
animals require shelter to survive
animals adapt to changing environments
animals obtain spices for cooking

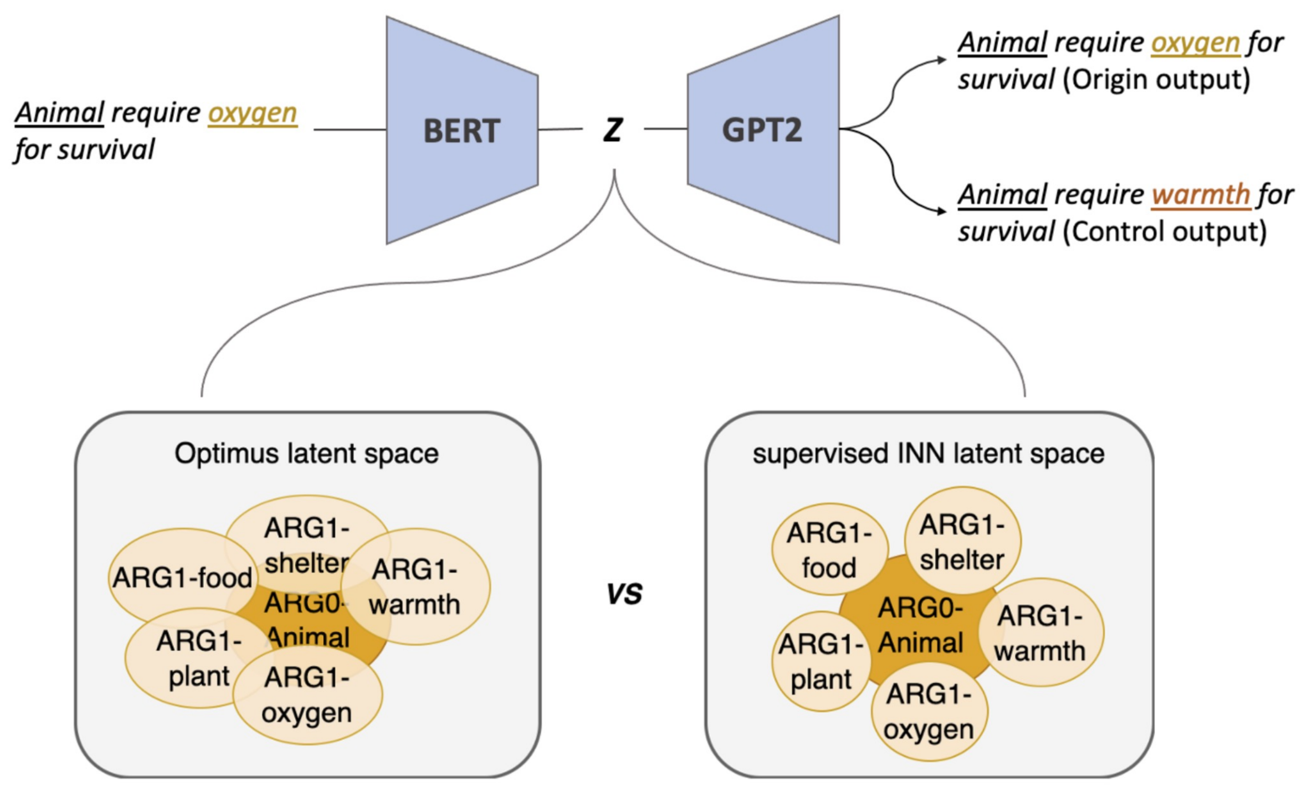
Vector arithmetic (addition)

Zhang, Carvalho, Pratt-Hartmann, Freitas, arXiv:2210.06230 (2022)

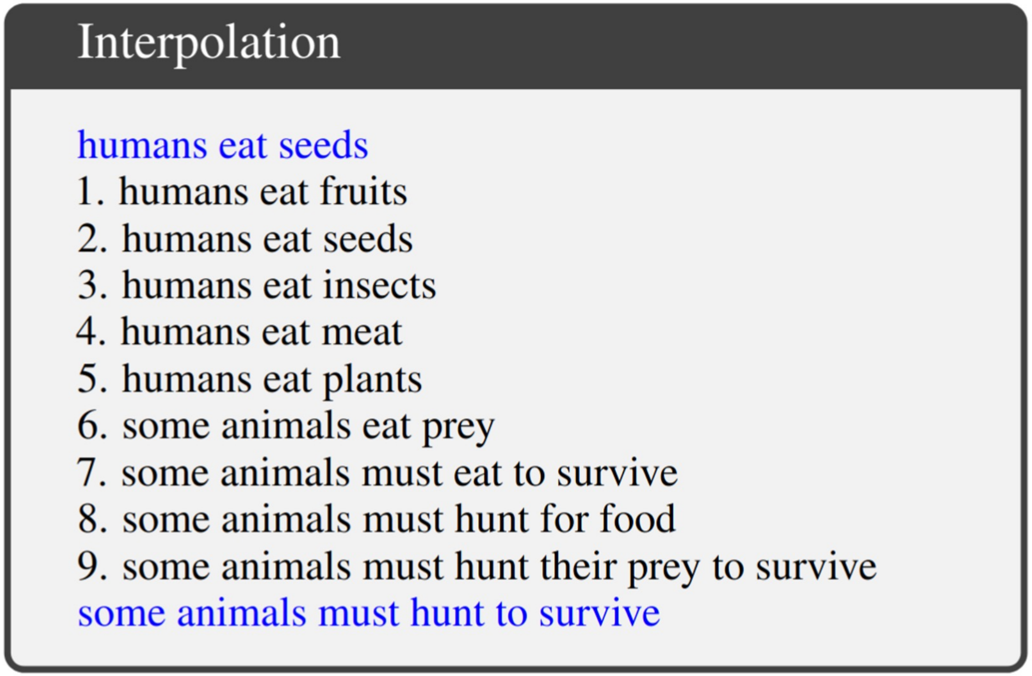
Improving Separability

Adding a flow-based INN component to improve separability

$$\mathcal{L}_{\text{sup}} = -\,\mathbb{E}_{x \sim p_{cluster}(x)} \frac{\left[T(E(x)) - \mu_{cluster}\right]^2}{1-\sigma^2} - \log \left|T'(E(x))\right|$$



Animal require oxygen for survival
BERT
z
GPT2
Animal require oxygen for survival (Origin output)
Animal require warmth for survival (Control output)
Optimus latent space
ARG1-food
ARG1-shelter
ARG1-warmth
ARG0-Animal
ARG1-plant
ARG1-oxygen
vs
supervised INN latent space
ARG1-food
ARG1-shelter
ARG0-Animal
ARG1-warmth
ARG1-plant
ARG1-oxygen

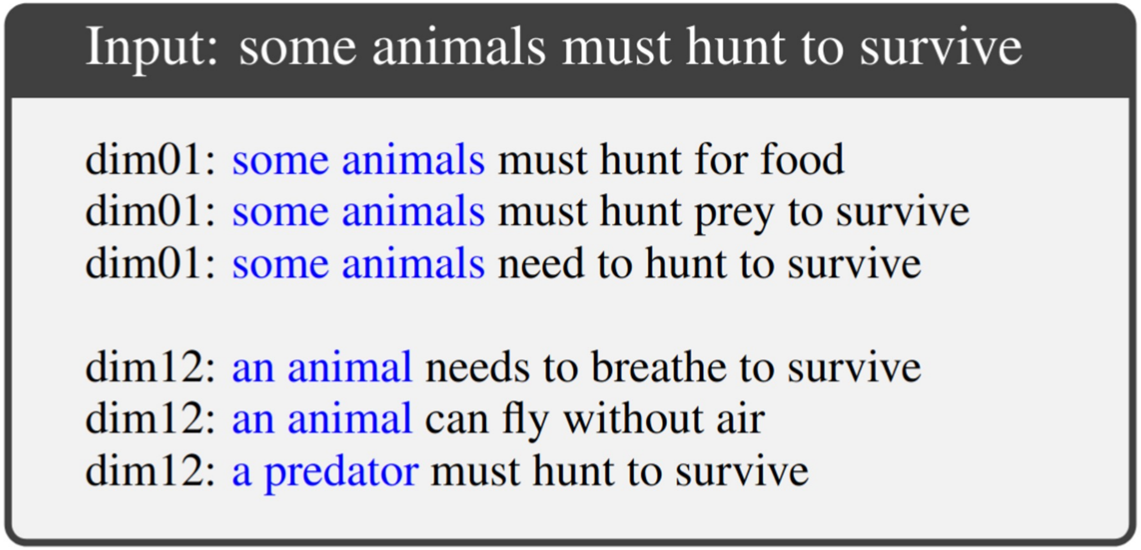


Interpolation

humans eat seeds
1. humans eat fruits
2. humans eat seeds
3. humans eat insects
4. humans eat meat
5. humans eat plants
6. some animals eat prey
7. some animals must eat to survive
8. some animals must hunt for food
9. some animals must hunt their prey to survive
some animals must hunt to survive

Interpolation

Latent traversal

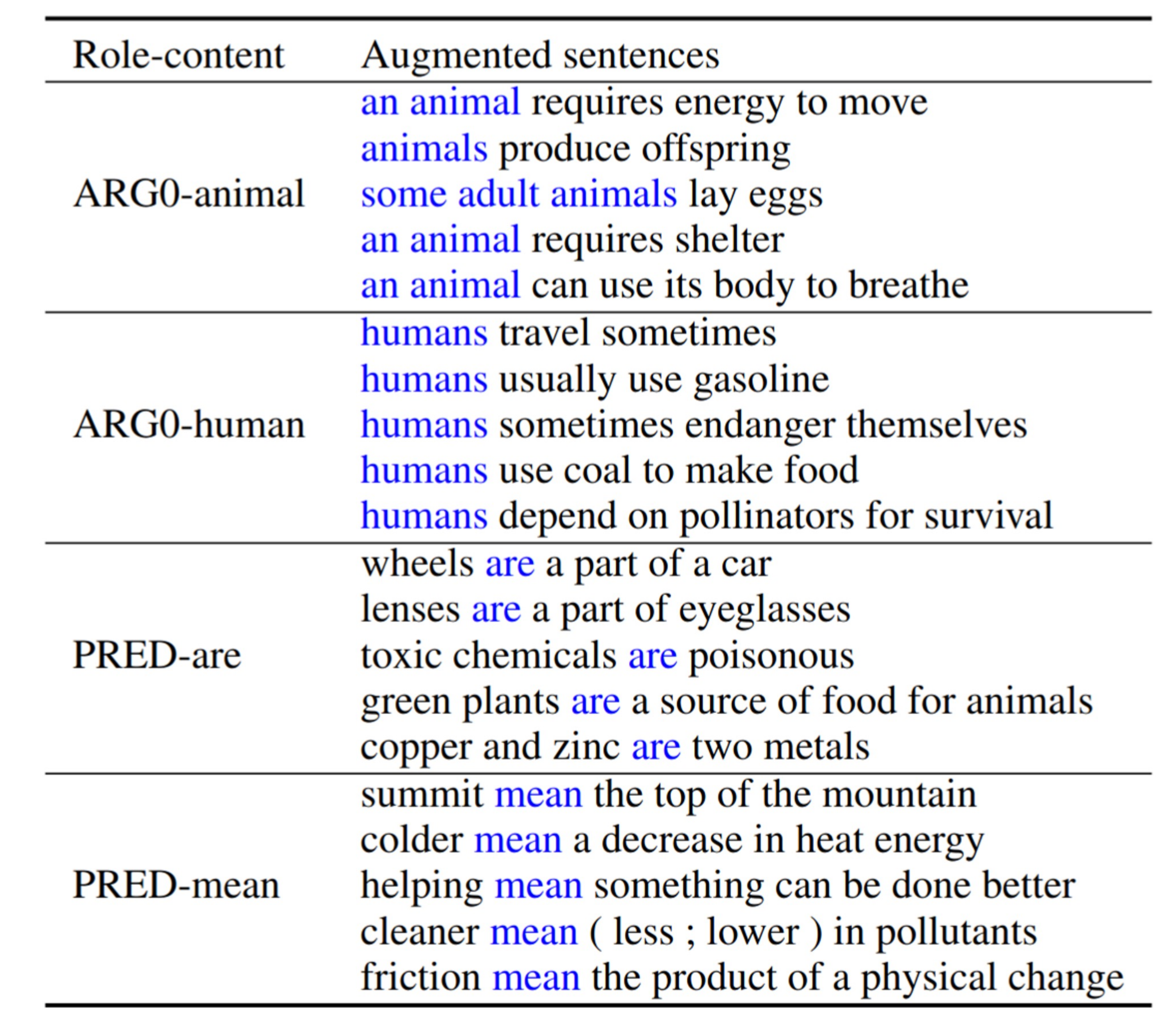


Input: some animals must hunt to survive

dim01: some animals must hunt for food
dim01: some animals must hunt prey to survive
dim01: some animals need to hunt to survive

dim12: an animal needs to breathe to survive
dim12: an animal can fly without air
dim12: a predator must hunt to survive

Data Augmentation



Role-content	Augmented sentences
ARG0-animal	an animal requires energy to move
	animals produce offspring
	some adult animals lay eggs
	an animal requires shelter
	an animal can use its body to breathe
ARG0-human	humans travel sometimes
	humans usually use gasoline
	humans sometimes endanger themselves
	humans use coal to make food
	humans depend on pollinators for survival
PRED-are	wheels are a part of a car
	lenses are a part of eyeglasses
	toxic chemicals are poisonous
	green plants are a source of food for animals
	copper and zinc are two metals
PRED-mean	summit mean the top of the mountain
	colder mean a decrease in heat energy
	helping mean something can be done better
	cleaner mean (less ; lower) in pollutants
	friction mean the product of a physical change

Representing concepts and definitions

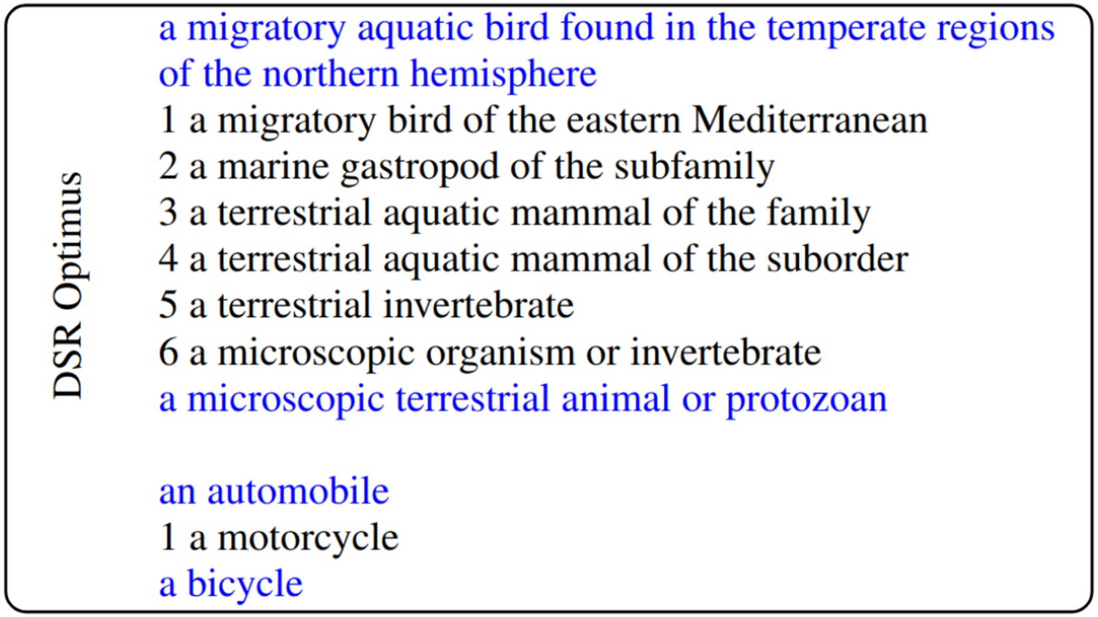
- Essential attributes of a conceptualisation.
- Abundance of NL definitions in scientific discourse.
- Definition RL: Decomposing conceptual components.

DEFINIENDUM **DIFFERENTIA QUALITY** **SUPERTYPE** **DIFFERENTIA-EVENT**

Homologous recombination repair is a DNA repair process that includes the invasion of an undamaged DNA molecule by a damaged molecule of identical or very similar sequence.

Santos, Freitas, Handschuh, AAAI (2018, 2019)

Interpolation

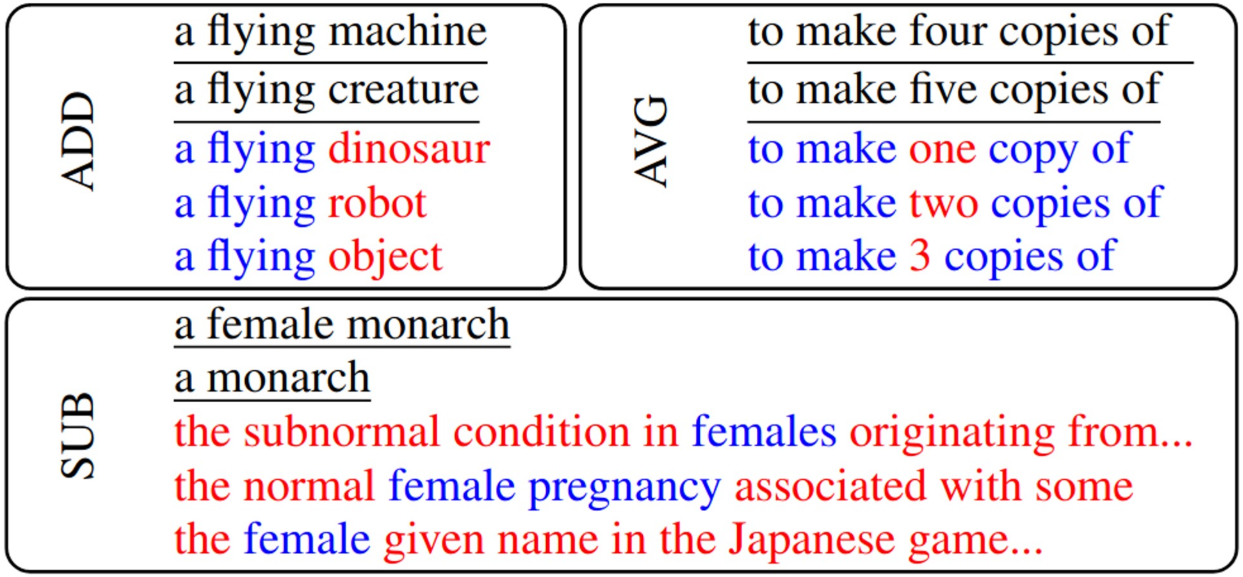


DSR Optimus

a migratory aquatic bird found in the temperate regions of the northern hemisphere
1 a migratory bird of the eastern Mediterranean
2 a marine gastropod of the subfamily
3 a terrestrial aquatic mammal of the family
4 a terrestrial aquatic mammal of the suborder
5 a terrestrial invertebrate
6 a microscopic organism or invertebrate
a microscopic terrestrial animal or protozoan

an automobile
1 a motorcycle
a bicycle

Latent traversal



ADD

a flying machine
a flying creature
a flying dinosaur
a flying robot
a flying object

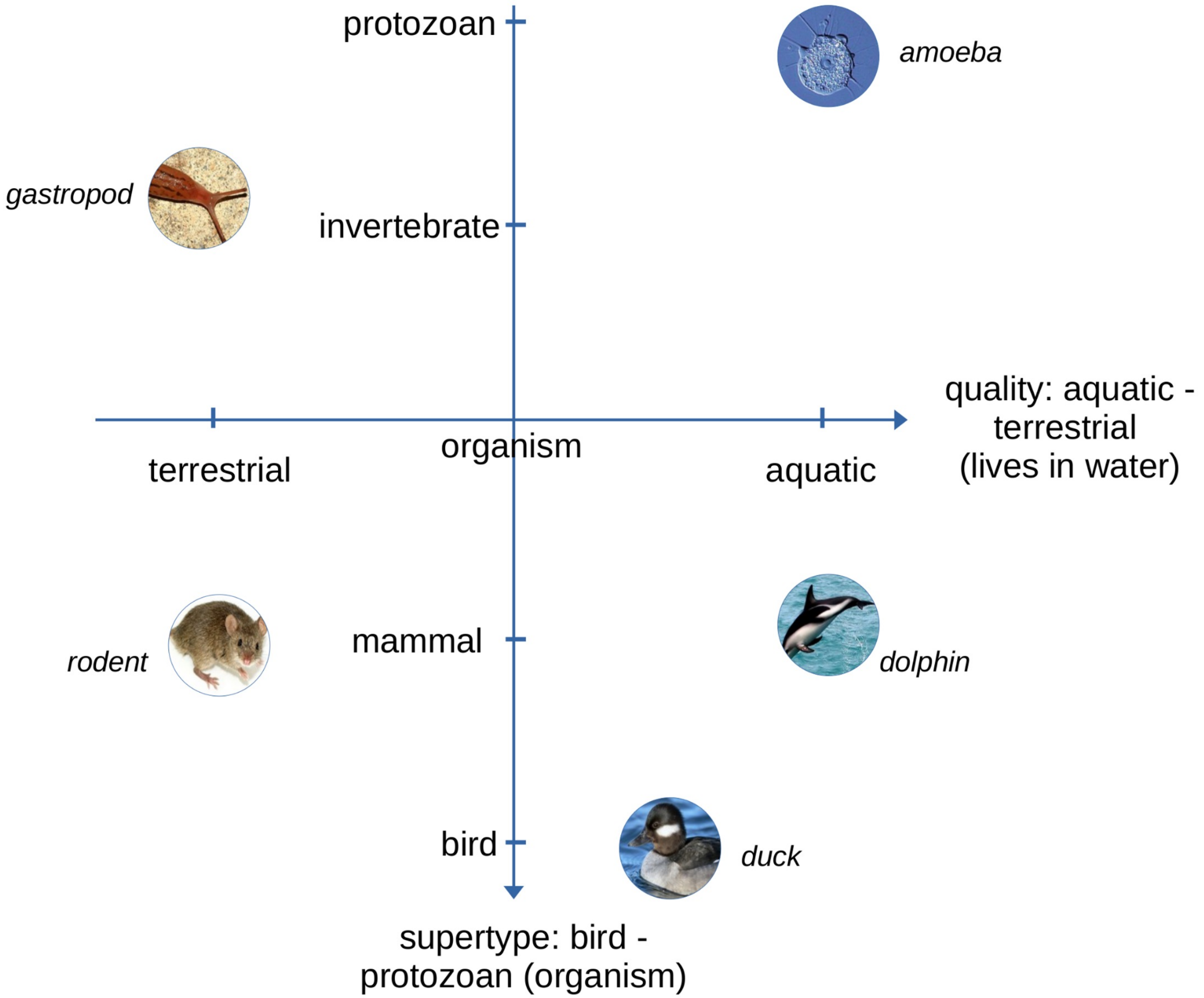
AVG

to make four copies of
to make five copies of
to make one copy of
to make two copies of
to make 3 copies of

SUB

a female monarch
a monarch
the subnormal condition in females originating from...
the normal female pregnancy associated with some
the female given name in the Japanese game...

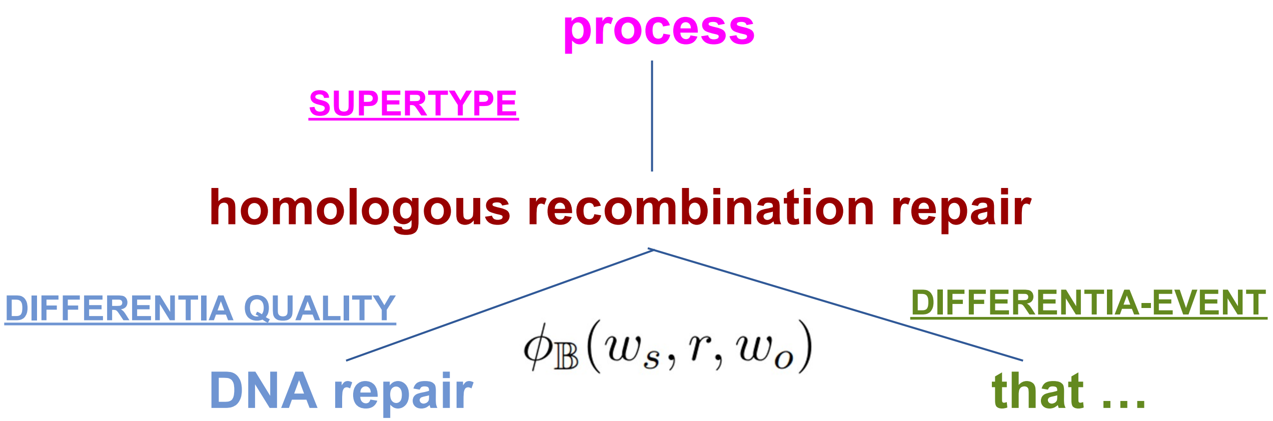
Carvalho, Mercatali, Zhang, Freitas, arXiv:2210.02898 (2022)



Carvalho, Mercatali, Zhang, Freitas, arXiv:2210.02898 (2022)

Multi-relational Hyperbolic Embeddings

Induction of a hierarchical, multi-relational, multi-resolution conceptual representation. Abstracts OOV words.



process

SUPERTYPE

homologous recombination repair

DIFFERENTIA QUALITY

DIFFERENTIA-EVENT

$\phi_{\mathbb{B}}(w_s, r, w_o)$

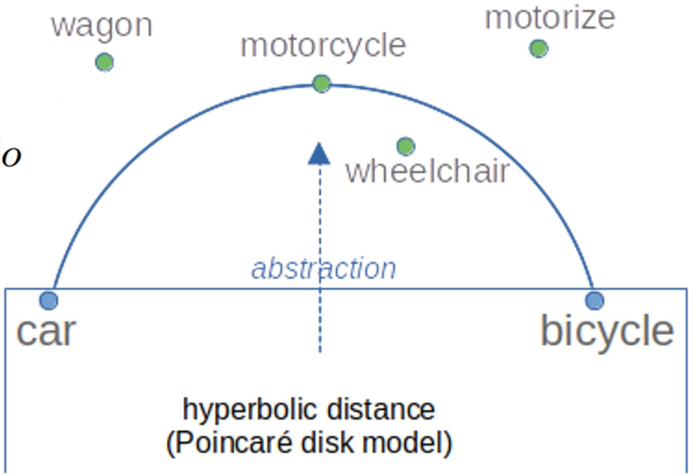
DNA repair

that …

Learn as a link prediction problem via a translational objective function in hyperbolic space.

$$\phi_{\mathbb{B}}(w_s, r, w_o) = -d_{\mathbb{B}}(\mathbf{h}_s^{(r)}, \mathbf{h}_o^{(r)})^2 + b_s + b_o$$

$$d_{\mathbb{B}}(x, y) = \frac{2}{\sqrt{c}} tanh^{-1}(\sqrt{c}\|{-x} \oplus y\|)$$



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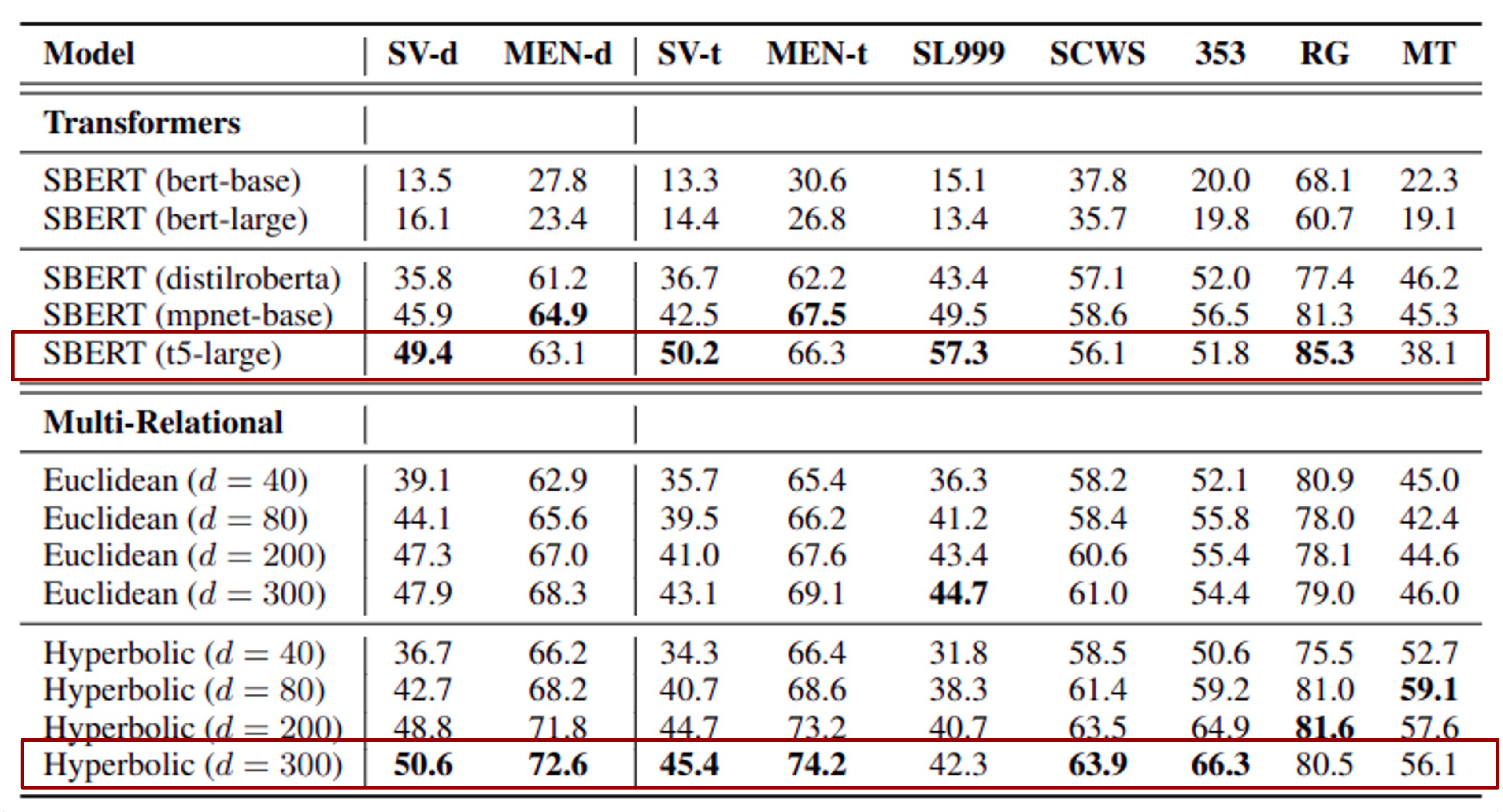
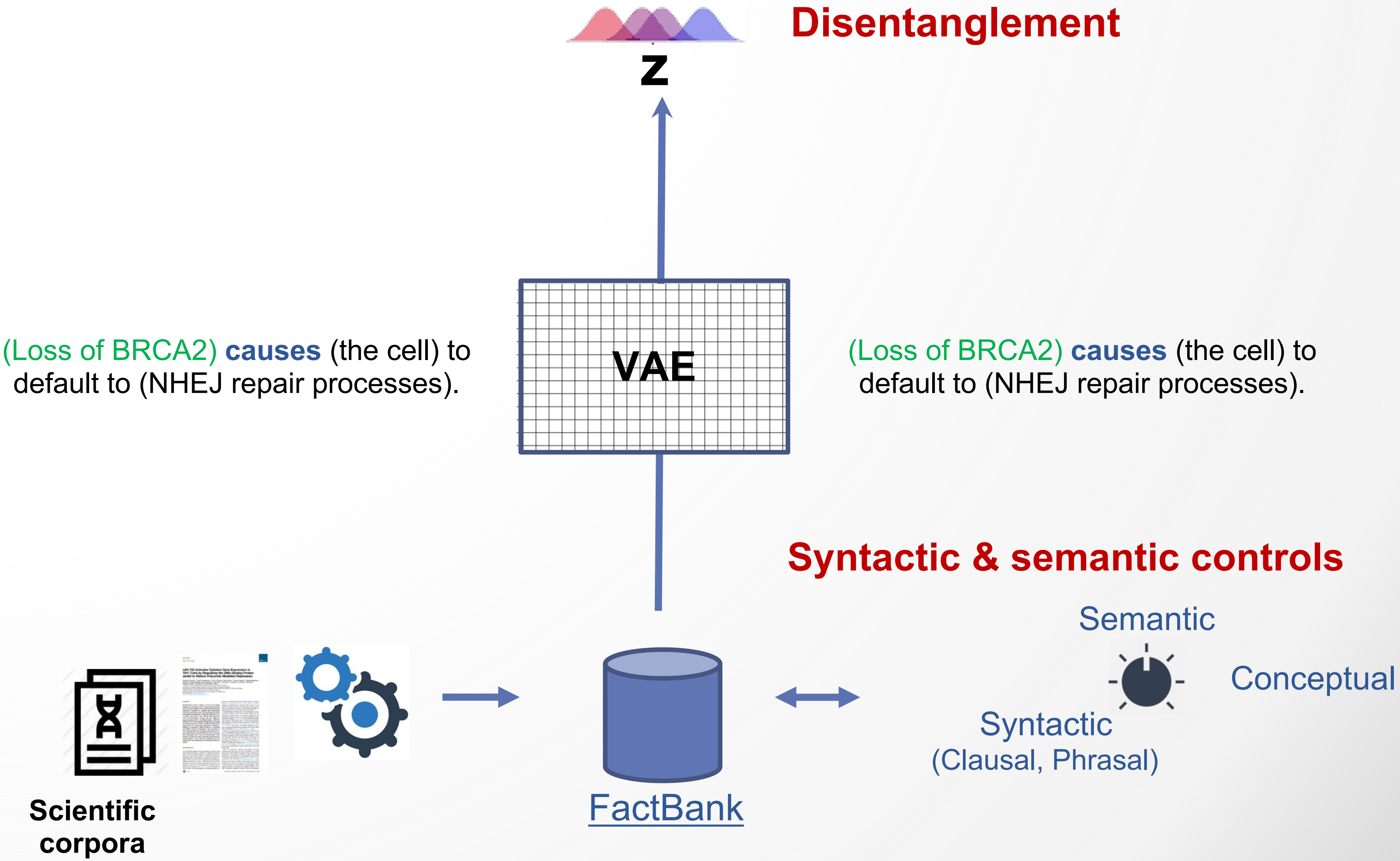


Model	SV-d	MEN-d	SV-t	MEN-t	SL999	SCWS	353	RG	MT
Transformers									
SBERT (bert-base)	13.5	27.8	13.3	30.6	15.1	37.8	20.0	68.1	22.3
SBERT (bert-large)	16.1	23.4	14.4	26.8	13.4	35.7	19.8	60.7	19.1
SBERT (distilroberta)	35.8	61.2	36.7	62.2	43.4	57.1	52.0	77.4	46.2
SBERT (mpnet-base)	45.9	**64.9**	42.5	**67.5**	49.5	58.6	56.5	81.3	45.3
SBERT (t5-large)	**49.4**	63.1	**50.2**	66.3	**57.3**	56.1	51.8	**85.3**	38.1
Multi-Relational									
Euclidean ($d = 40$)	39.1	62.9	35.7	65.4	36.3	58.2	52.1	80.9	45.0
Euclidean ($d = 80$)	44.1	65.6	39.5	66.2	41.2	58.4	55.8	78.0	42.4
Euclidean ($d = 200$)	47.3	67.0	41.0	67.6	43.4	60.6	55.4	78.1	44.6
Euclidean ($d = 300$)	47.9	68.3	43.1	69.1	**44.7**	61.0	54.4	79.0	46.0
Hyperbolic ($d = 40$)	36.7	66.2	34.3	66.4	31.8	58.5	50.6	75.5	52.7
Hyperbolic ($d = 80$)	42.7	68.2	40.7	68.6	38.3	61.4	59.2	81.0	**59.1**
Hyperbolic ($d = 200$)	48.8	71.8	44.7	73.2	40.7	63.5	64.9	**81.6**	57.6
Hyperbolic ($d = 300$)	**50.6**	**72.6**	**45.4**	**74.2**	42.3	**63.9**	**66.3**	80.5	56.1

T5-large: "Colossal Clean Crawled Corpus" (C4): ~750GB.
MR–Hyperbolic: “CPAE Dictionary”: ~19MB.

Sentence-level representation



Disentanglement

z

(Loss of BRCA2) **causes** (the cell) to default to (NHEJ repair processes).

VAE

(Loss of BRCA2) **causes** (the cell) to default to (NHEJ repair processes).

Syntactic & semantic controls

Semantic

Conceptual

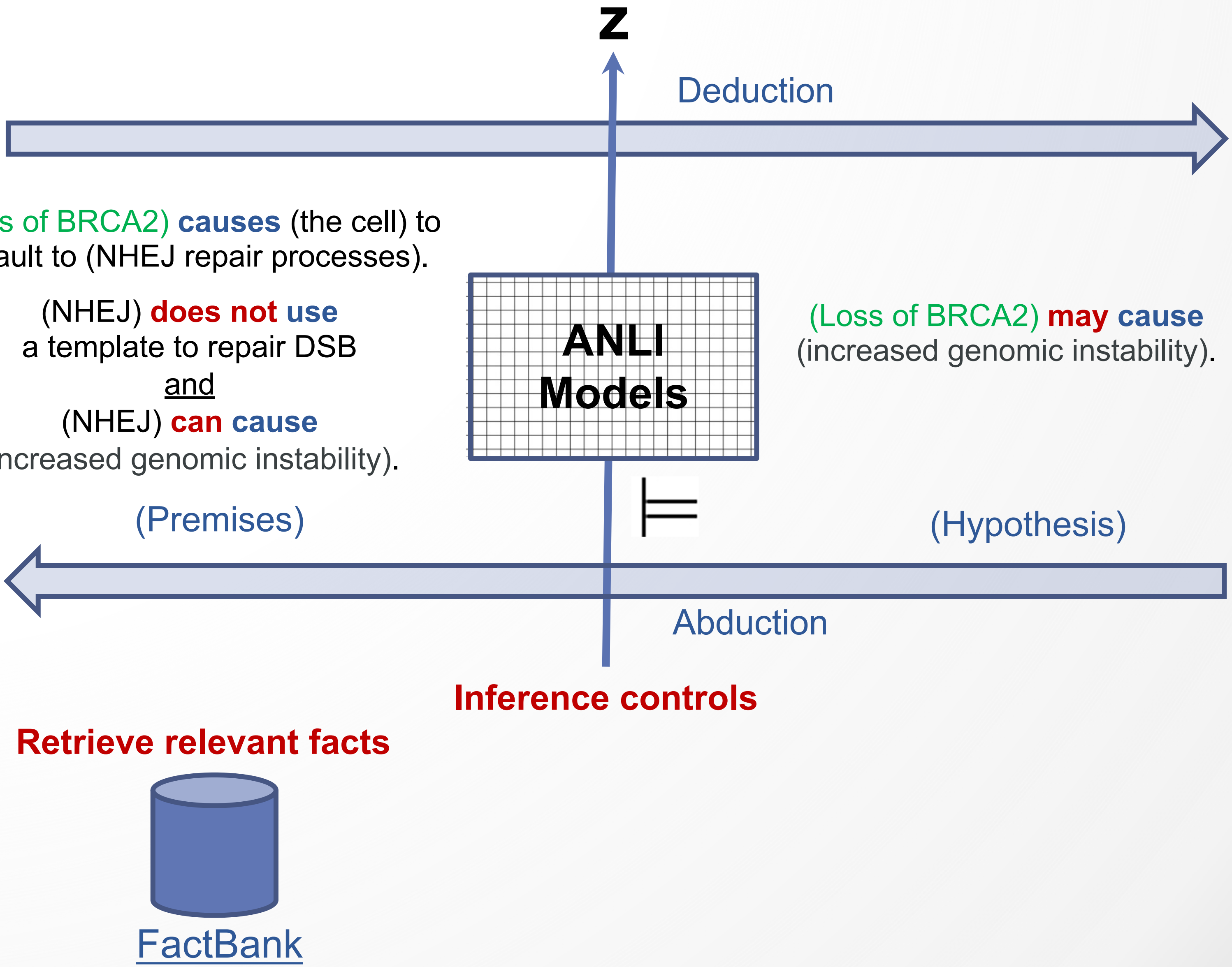
Syntactic
(Clausal, Phrasal)

Scientific corpora

FactBank

Encoding step-wise (multi-hop) inference

Encoding Abductive (Explanatory) Reasoning



z

Deduction

(Loss of BRCA2) **causes** (the cell) to default to (NHEJ repair processes).

(NHEJ) **does not use** a template to repair DSB
and
(NHEJ) **can cause** (increased genomic instability).

ANLI Models

(Loss of BRCA2) **may cause** (increased genomic instability).

$\models$

(Premises)

(Hypothesis)

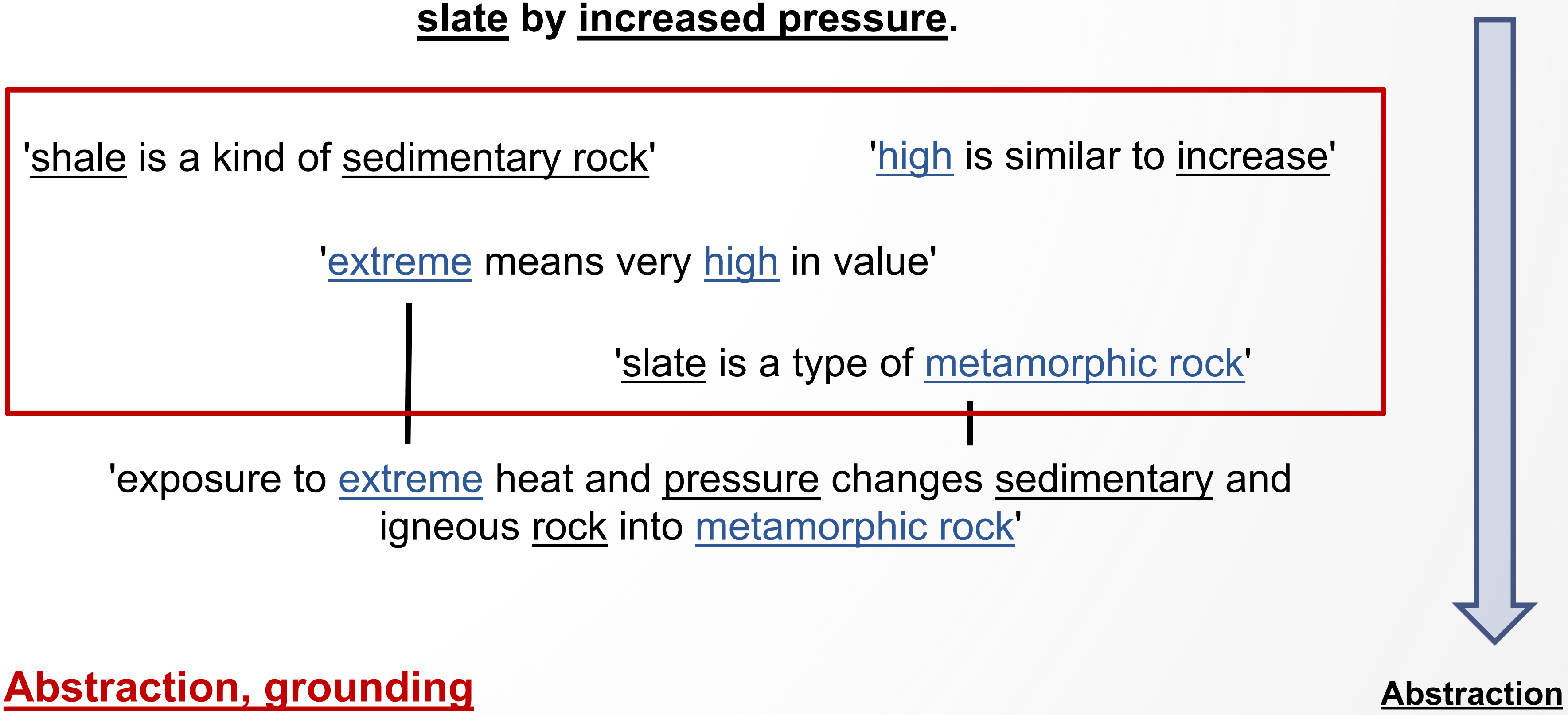
Abduction

Inference controls

Retrieve relevant facts

FactBank

h: Shale is a sedimentary rock that can be metamorphosed into slate by increased pressure.



'shale is a kind of sedimentary rock'

'high is similar to increase'

'extreme means very high in value'

'slate is a type of metamorphic rock'

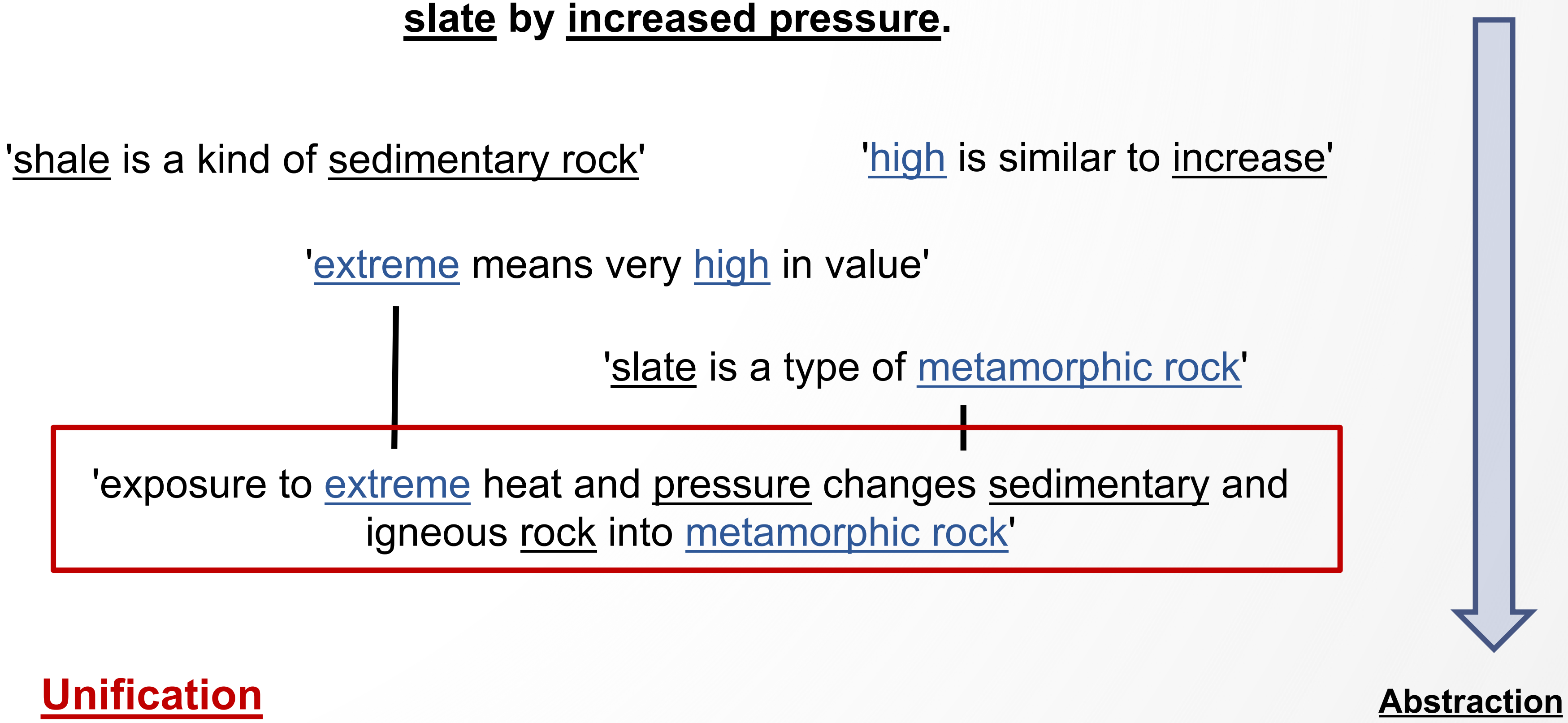
'exposure to extreme heat and pressure changes sedimentary and igneous rock into metamorphic rock'

Abstraction, grounding

Abstraction

Concrete facts tend to share key concepts with the hypotheses and can therefore be effectively retrieved by lexical relevance.

h: Shale is a sedimentary rock that can be metamorphosed into slate by increased pressure.



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'high is similar to increase'

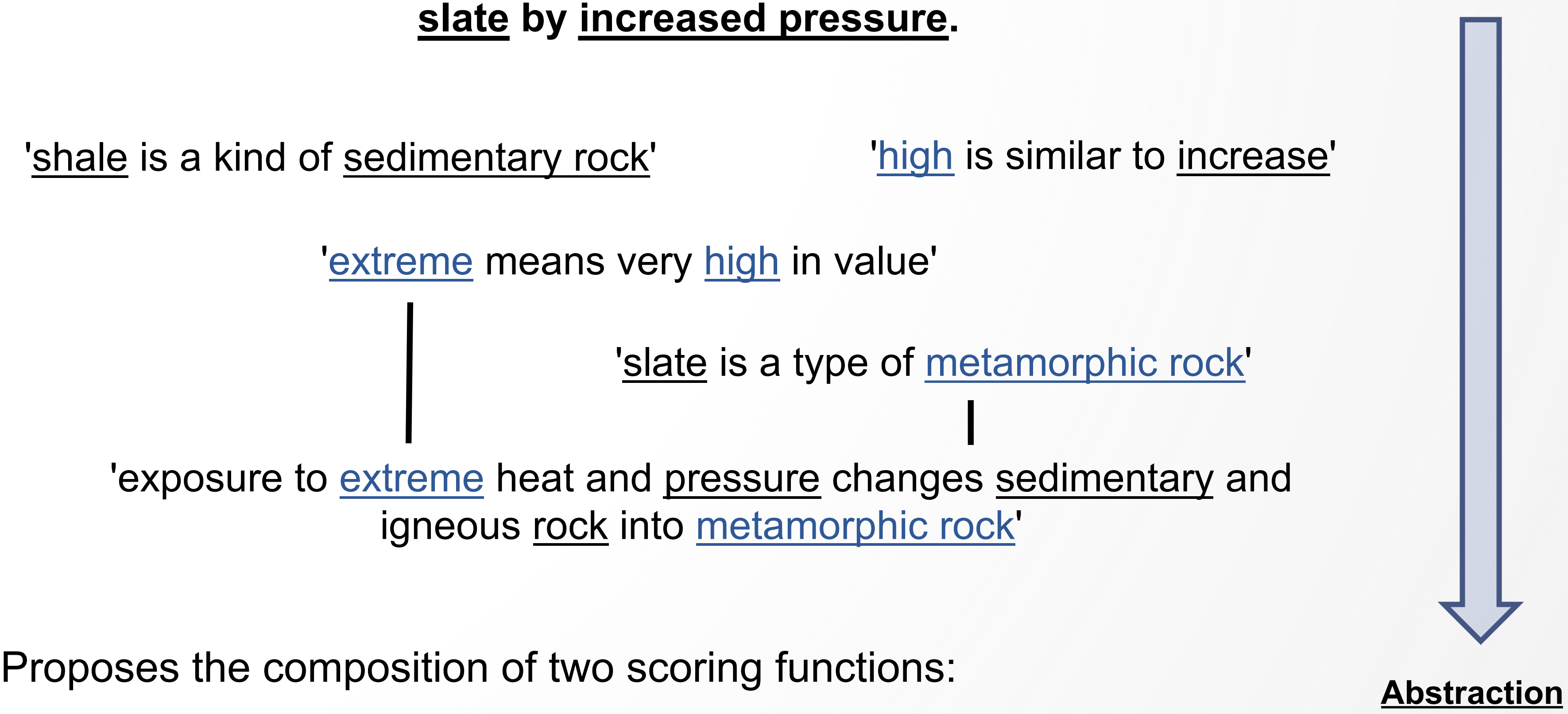
'extreme means very high in value'

'slate is a type of metamorphic rock'

'exposure to extreme heat and pressure changes sedimentary and igneous rock into metamorphic rock'

More uiversal scientific statements tend to be abstract and therefore difficult to rank by means of shared concepts.

h: Shale is a sedimentary rock that can be metamorphosed into slate by increased pressure.



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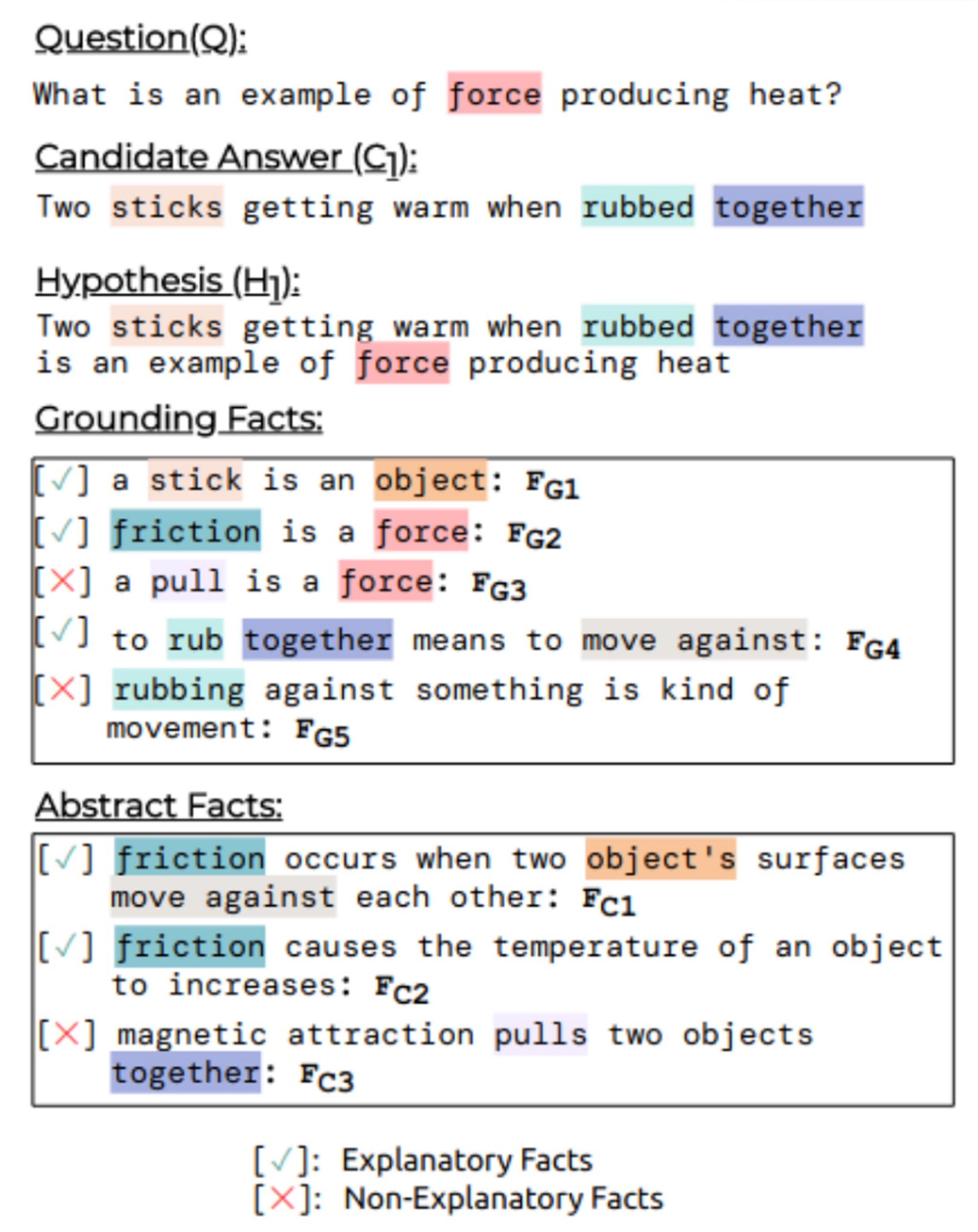
Abstraction

Proposes the composition of two scoring functions:

- A **Relevance Score (RS)** that represents the lexical relevance of a given fact.

- A **Unification Score (US)** that models the explanatory power of a fact according to its frequency in explanations for similar questions

Valentino, Thayaparan, Freitas, EACL (2021)



Question(Q):

What is an example of force producing heat?

Candidate Answer (C_1):

Two sticks getting warm when rubbed together

Hypothesis (H_1):

Two sticks getting warm when rubbed together is an example of force producing heat

Grounding Facts:

[✓] a stick is an object: F_{G1}

[✓] friction is a force: F_{G2}

[✗] a pull is a force: F_{G3}

[✓] to rub together means to move against: F_{G4}

[✗] rubbing against something is kind of movement: F_{G5}

Abstract Facts:

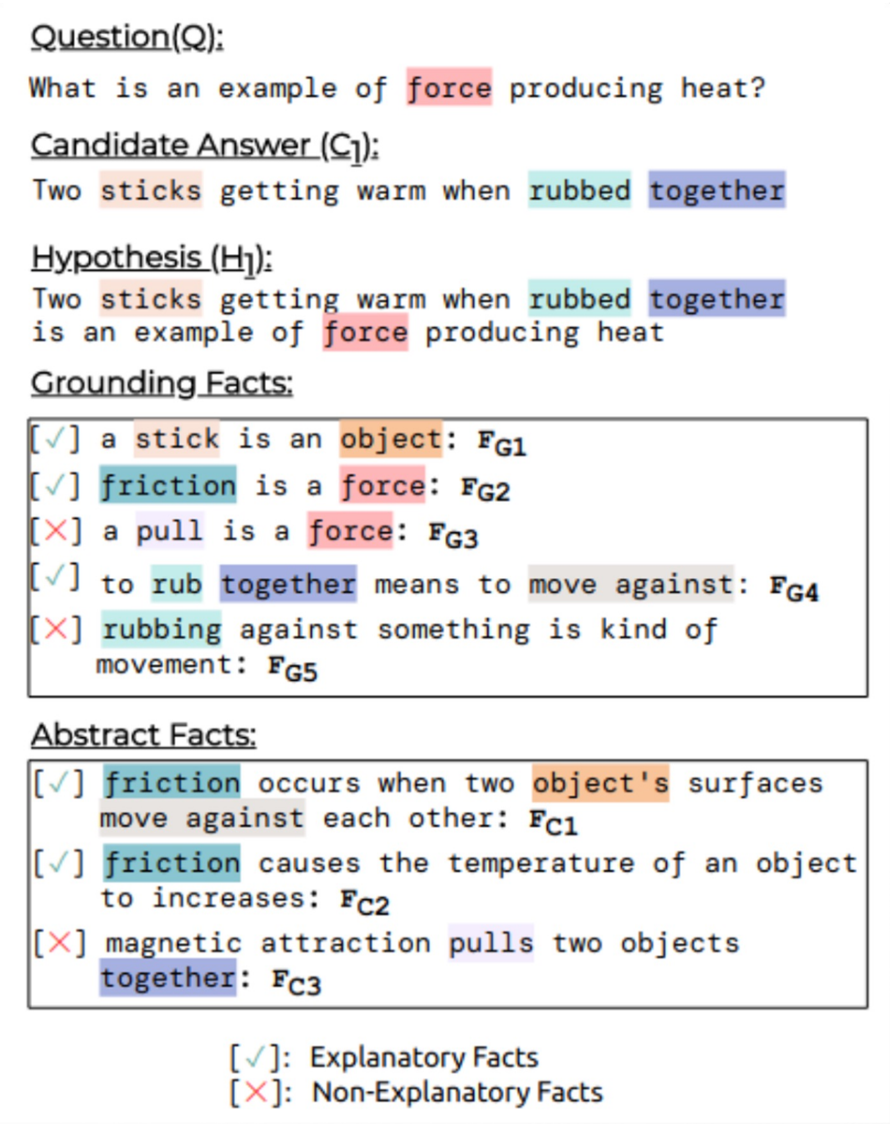
[✓] friction occurs when two object's surfaces move against each other: F_{C1}

[✓] friction causes the temperature of an object to increases: F_{C2}

[✗] magnetic attraction pulls two objects together: F_{C3}

[✓]: Explanatory Facts
[✗]: Non-Explanatory Facts

Thayaparan, Valentino, Freitas, ACL Findings (2021)



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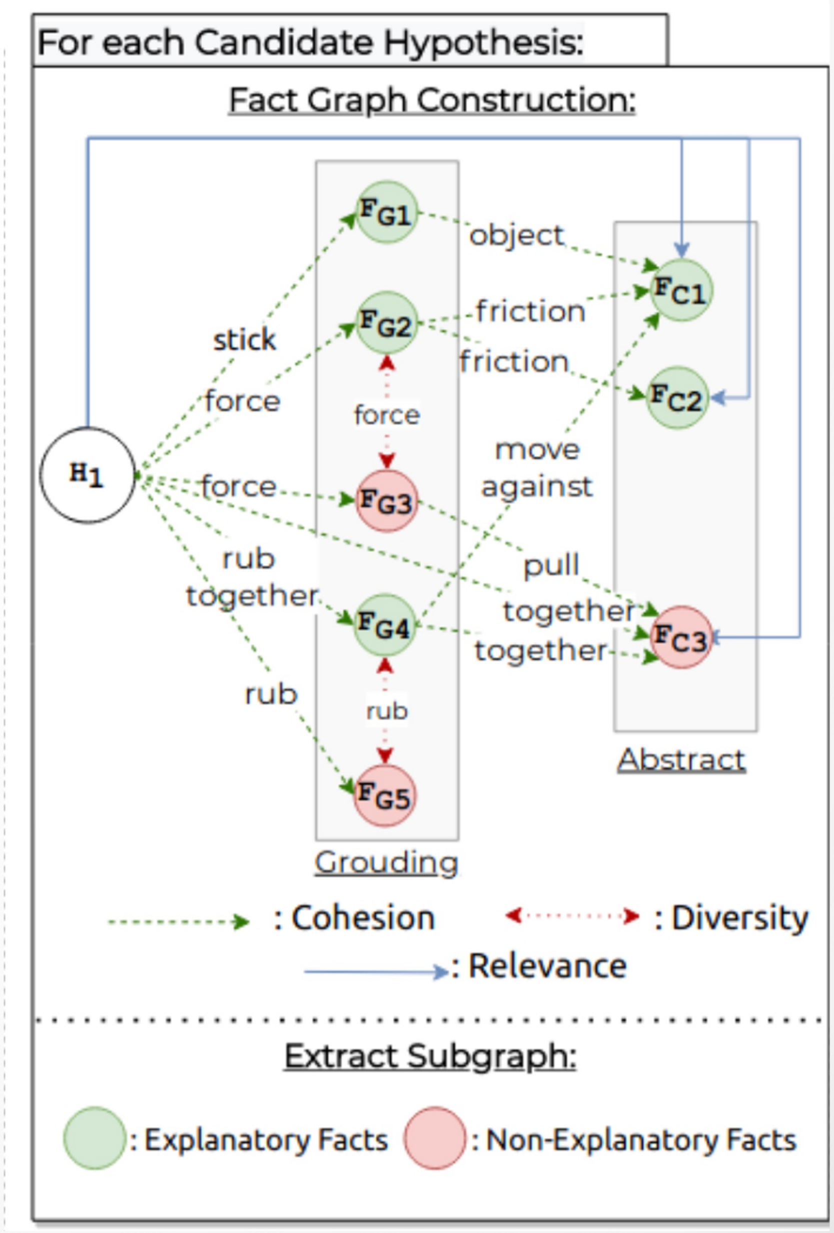


For each Candidate Hypothesis:

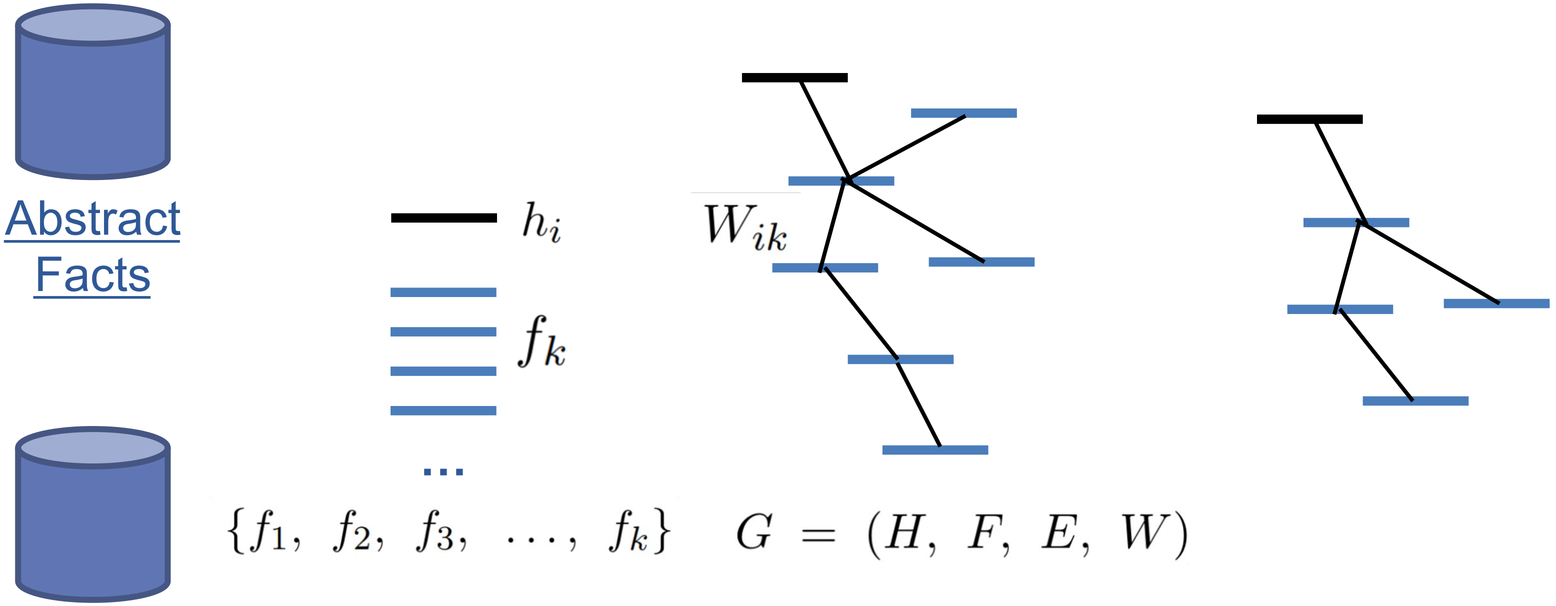
Fact Graph Construction:

- - - - → : Cohesion
← · · · → : Diversity
——→: Relevance

Extract Subgraph:

🟢: Explanatory Facts 🔴: Non-Explanatory Facts

Thayaparan, Valentino, Freitas, ACL Findings (2021)



$\{f_1,\ f_2,\ f_3,\ \ldots,\ f_k\}$ $G = (H,\ F,\ E,\ W)$

Retrieve
relevant facts

Relevance

Construct
a weighted fact graph

Extract subgraph
via ILP optimization

Diversity

$$D(f_j^{h_i}, f_k^{h_i}) = -1 \frac{|t_{h_i}(f_j^{h_i}) \cap t_{h_i}(f_k^{h_i})|}{max(|t_{h_i}(f_j^{h_i})|, |t_{h_i}(f_k^{h_i})|)}$$

Saturation

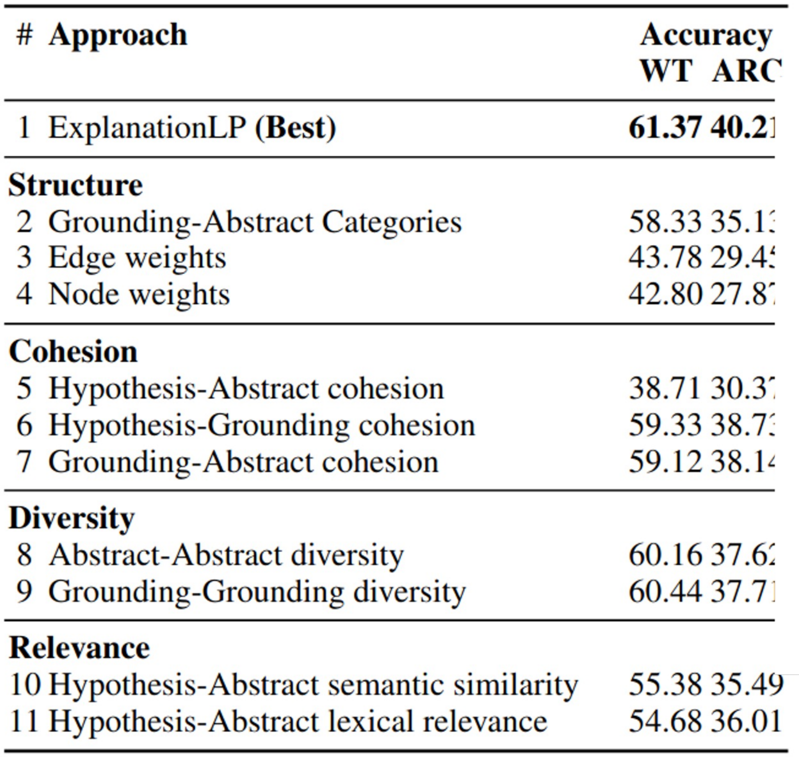
$$C(f_j^{h_i}, f_k^{h_i}) = \frac{|t(f_j^{h_i}) \cap t(f_k^{h_i})|}{max(|t(f_j^{h_i})|, |t(f_k^{h_i})|)}$$

Prior semantic/inference knowledge

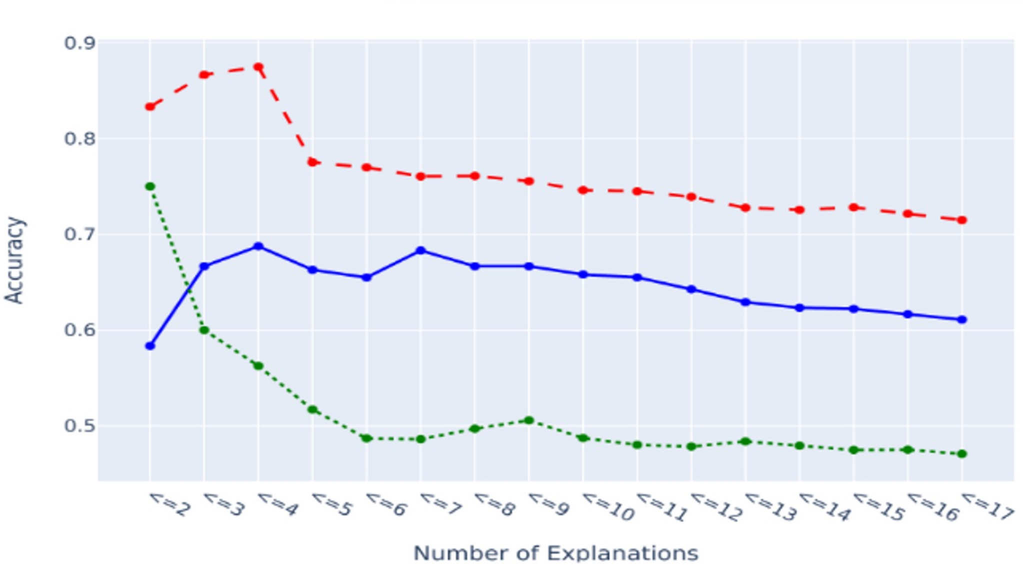
$$\omega_e(v_j, v_k; \theta_1) = \begin{cases} \theta_{gg} D(v_j, v_k) & v_j, v_k \in F_G^{h_i} \\ \theta_{aa} D(v_j, v_k) & v_j, v_k \in F_A^{h_i} \\ \theta_{ga} C(v_j, v_k) & v_j \in F_G^{h_i}, v_k \in F_A^{h_i} \\ \theta_{qg} C(v_j, v_k) & v_j \in F_G^{h_i}, v_k = h_i \\ \theta_{qa} C(v_j, v_k) & v_j \in F_A^{h_i}, v_k = h_i \end{cases}$$

$$\omega_v(v_i^{h_i}; \theta_2) = \begin{cases} \theta_{lr} L(v_j, h_i) + \theta_{ss} S(v_j, h_i) & v_j \in F_A^{h_i} \\ 0 & v_i \in F_G^{h_i} \\ 0 & v_i = h_i \end{cases}$$

Thayaparan, Valentino, Freitas, ACL Findings (2021)



#	Approach	Accuracy WT	Accuracy ARC
1	ExplanationLP **(Best)**	**61.37**	**40.21**
Structure			
2	Grounding-Abstract Categories	58.33	35.13
3	Edge weights	43.78	29.45
4	Node weights	42.80	27.87
Cohesion			
5	Hypothesis-Abstract cohesion	38.71	30.37
6	Hypothesis-Grounding cohesion	59.33	38.73
7	Grounding-Abstract cohesion	59.12	38.14
Diversity			
8	Abstract-Abstract diversity	60.16	37.62
9	Grounding-Grounding diversity	60.44	37.71
Relevance			
10	Hypothesis-Abstract semantic similarity	55.38	35.49
11	Hypothesis-Abstract lexical relevance	54.68	36.01



red: ExplanationLP
blue: BERT$_{\text{Large}}$
green: PathNet

# of parameters:

- BERTBase: 110M parameters
- BERTLarge: 340M parameters
- ExplanationLP: 9 parameters

Thayaparan, Valentino, Freitas, ACL Findings (2021)

Diff-Explainer: End-to-end abductive learning

An end-to-end differentiable framework that incorporates constraints via convex optimization layers into broader transformers-based architectures.

Differentiable convex optimization (DCX) layers (Agrawal et al., 2019) provide a way to encode constraints as part of a deep neural network.

Problem: ILP formulation is non-convex and cannot be incorporated into a differentiable convex optimization layer.

Solution:

- Approximate ILP with convex optimization constraints.
- Semi-Definite programming (SDP) is non-linear but convex and has shown to efficiently approximate combinatorial problems.

Specifically, we incorporate a differentiable convex optimization layer with Sentence-Transformers (STrans).

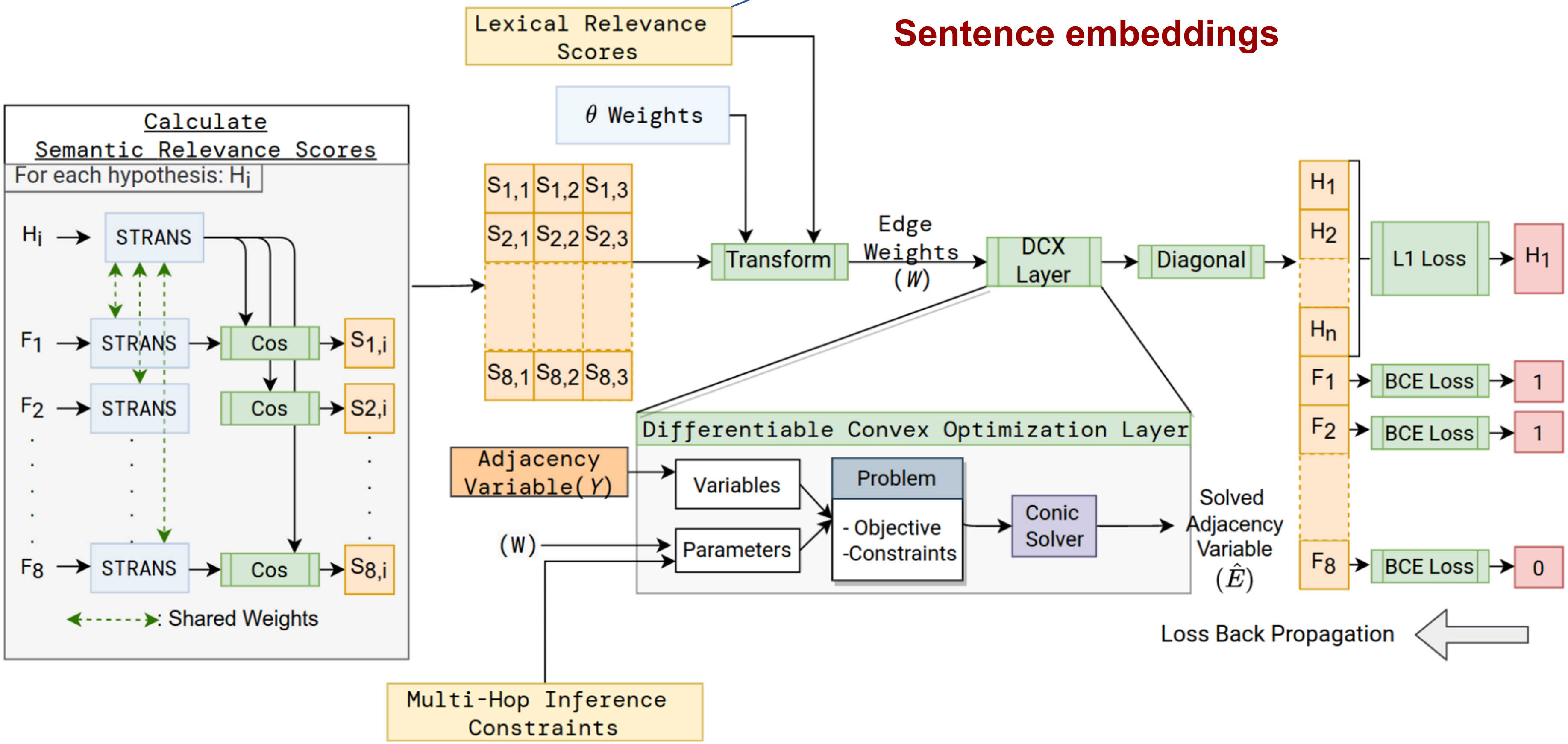
Thayaparan, Valentino, Ferreira, Rozanova, Freitas, TACL (2022)

Programmable abductive NLI Solver

Relevance

$$s_{ij} = S(\vec{h_i}, \vec{f_j}) = \frac{\vec{h_i} \cdot \vec{f_j}}{\|\vec{h_i}\| \|\vec{f_j}\|}$$

Sentence embeddings



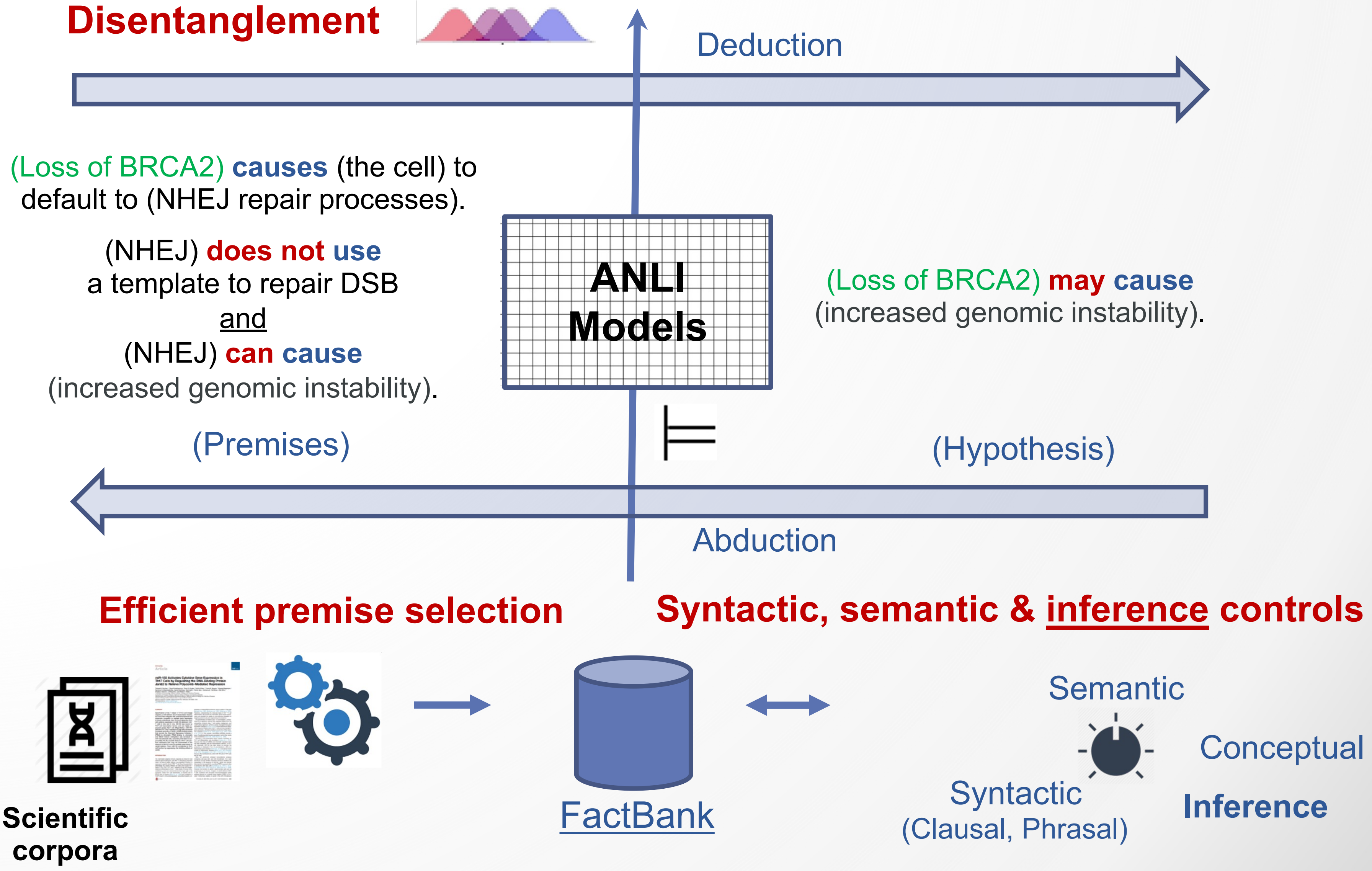
Saturation

$$l_{ij} = L(h_i, f_j) = \frac{|trm(h_i) \cap trm(f_j)|}{max(|trm(h_i)|, |trm(f_j)|)}$$

$$W_{ij} = [\theta^s_1, \theta^s_2, \ldots, \theta^s_n] \cdot [s^{\mathcal{D}_1}_{ij}, s^{\mathcal{D}_2}_{ij}, \ldots, s^{\mathcal{D}_n}_{ij}] + [\theta^l_1, \theta^l_2, \ldots, \theta^l_n] \cdot [l^{\mathcal{D}_1}_{ij}, l^{\mathcal{D}_2}_{ij}, \ldots, l^{\mathcal{D}_n}_{ij}]$$

Prior semantic/inference knowledge

Exploiting the structure of scientific explanations for multi-hop inference design



Disentanglement

Deduction

(Loss of BRCA2) **causes** (the cell) to default to (NHEJ repair processes).

(NHEJ) **does not use** a template to repair DSB

and

(NHEJ) **can cause** (increased genomic instability).

ANLI Models

(Loss of BRCA2) **may cause** (increased genomic instability).

⊨

(Premises)

(Hypothesis)

Abduction

Efficient premise selection

Syntactic, semantic & inference controls

Scientific corpora

FactBank

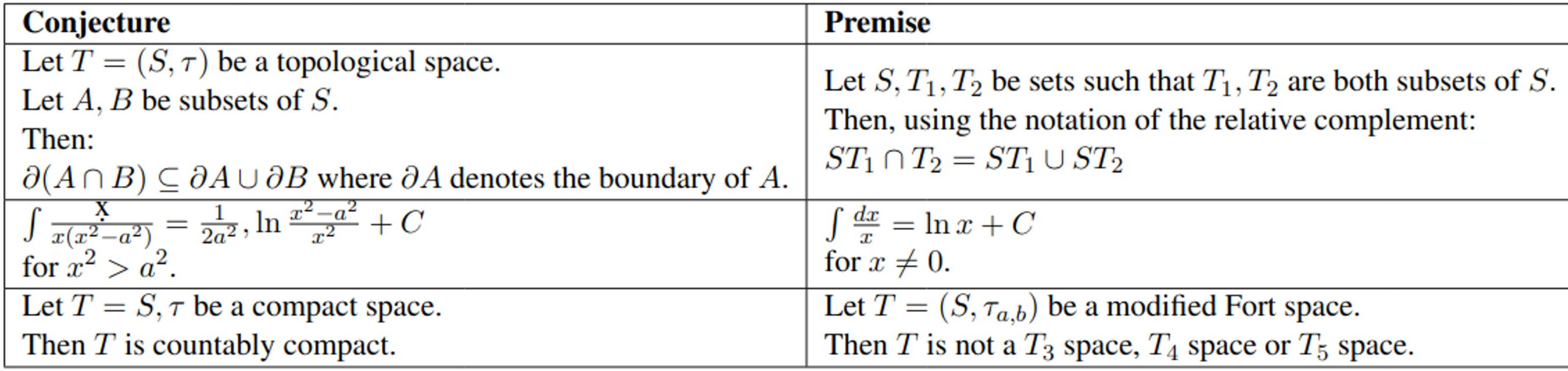
Semantic

Conceptual

Syntactic (Clausal, Phrasal)

Inference

Encoding abstract, mathematical inference



Conjecture	Premise
Let $T = (S, \tau)$ be a topological space. Let A, B be subsets of S. Then: $\partial(A \cap B) \subseteq \partial A \cup \partial B$ where ∂A denotes the boundary of A.	Let S, T_1, T_2 be sets such that T_1, T_2 are both subsets of S. Then, using the notation of the relative complement: $ST_1 \cap T_2 = ST_1 \cup ST_2$
$\int \frac{\text{X}}{x(x^2-a^2)} = \frac{1}{2a^2}, \ln \frac{x^2-a^2}{x^2} + C$ for $x^2 > a^2$.	$\int \frac{dx}{x} = \ln x + C$ for $x \neq 0$.
Let $T = S, \tau$ be a compact space. Then T is countably compact.	Let $T = (S, \tau_{a,b})$ be a modified Fort space. Then T is not a T_3 space, T_4 space or T_5 space.

STAR: Cross-modal STAtement Representation for selecting relevant mathematical premises

Ferreira & Freitas, EACL (2021)

To be or not to be an Integer? Encoding Variables for Mathematical Text

Ferreira et al., EACL (2021)

Abstract statement representation

Similarity-based equational inference in physics

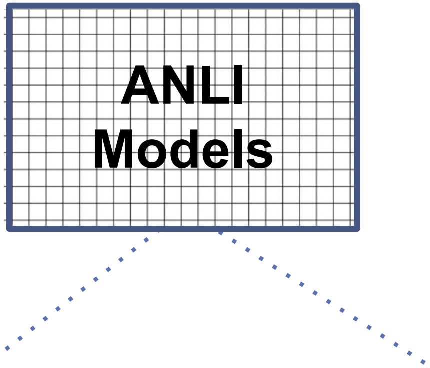
Meadows & Freitas, PRR (2021)

Premise Selection in Natural Language Mathematical Texts

Ferreira & Freitas, ACL (2020)

Multi-hop mathematical inference

Interventional, causal and granular evaluation of semantic and inference properties



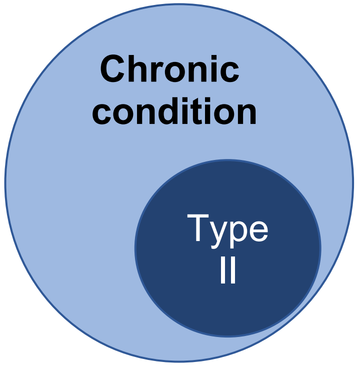
ANLI Models

Is reasoning really happening? (**quantifying causal effect)**
Are the semantic features present in the representations? (**probing**)
Do models reveal behavioural consistency? (**metamorphic testing**)

Inferences should follow **logical regularities** based on **abstract semantic features**.

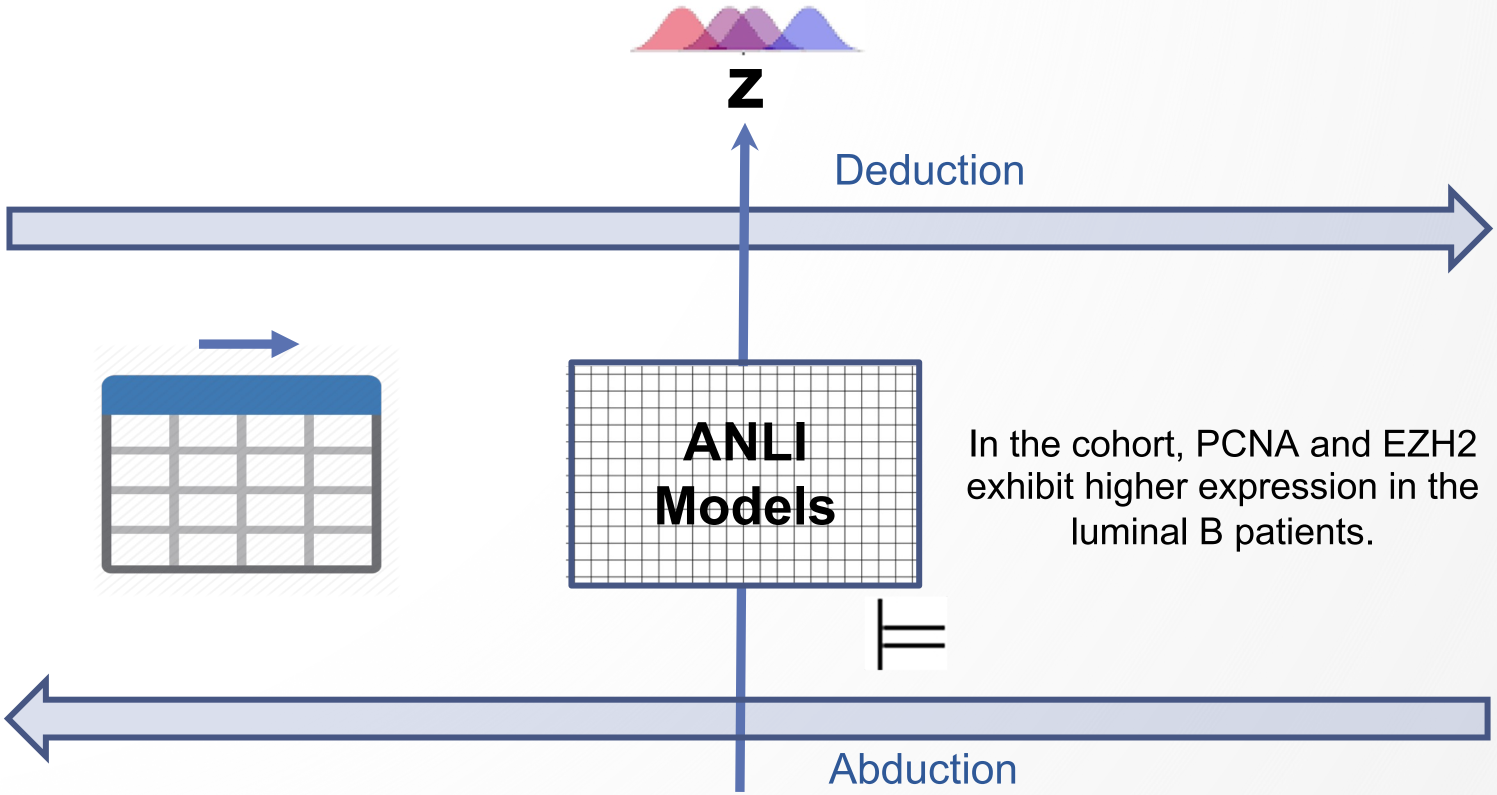
"The patient does not have a **chronic condition**" $\models$ "The patient does not have **type II Diabetes** "

conceptual relations $\subseteq$ monotonicity



Manino et al. ACL Findings (2022)
Rozanova et al. BlackBoxNLP@EMNLP (2022)
Rozanova et al., NALOMA (2021)

Encoding inferences over table evidence



z

Deduction

ANLI Models

In the cohort, PCNA and EZH2 exhibit higher expression in the luminal B patients.

$\models$

Abduction

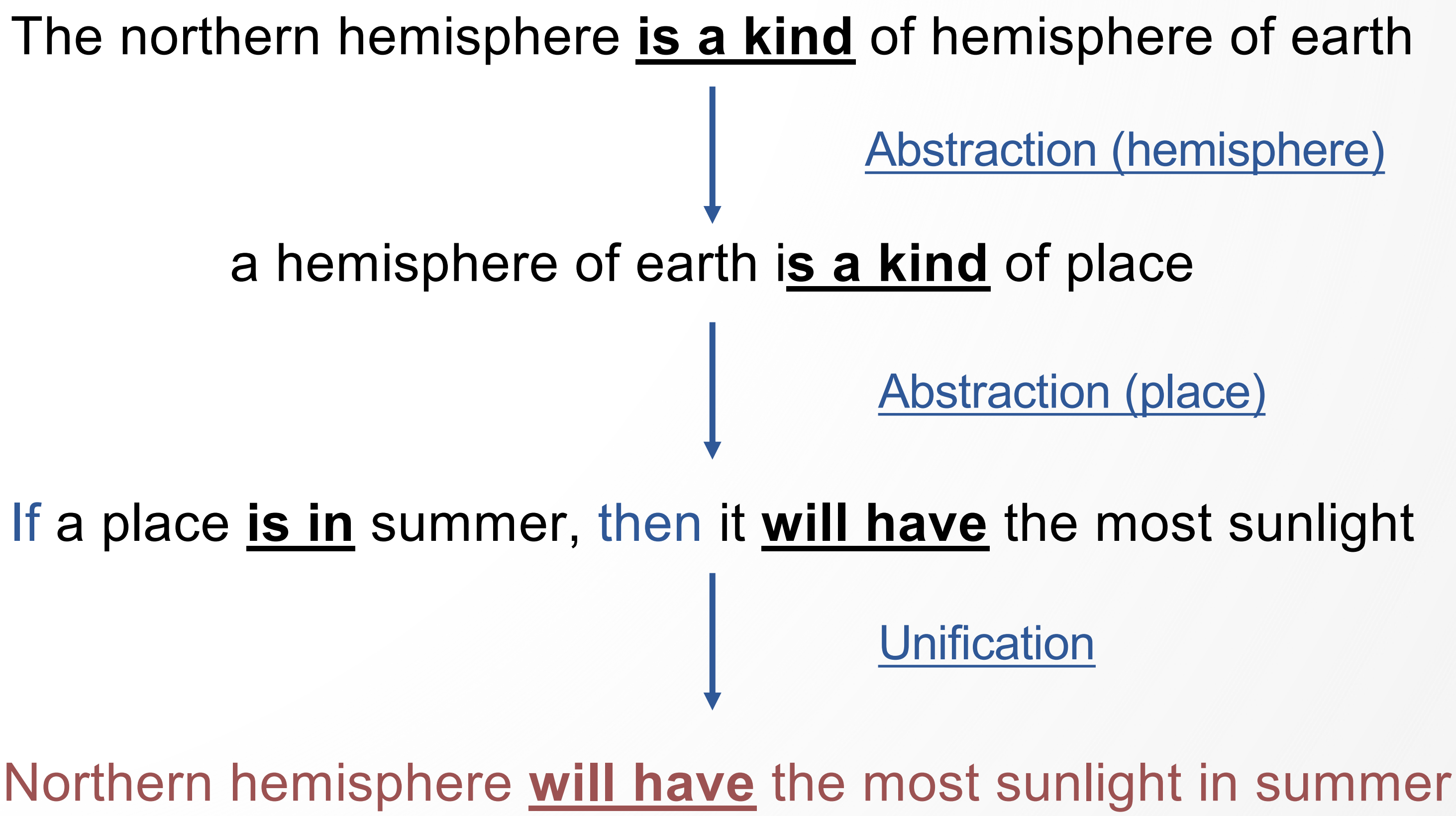
Badaro, Saeed, Papotti, TACL (2023)

Take away

Building natural language explanation machines for science (key neuro-symbolic strategies)

- Granular, controlled, neuro-symbolic inference.
- Integrating and controlling LLMs properties.
- **Sentence-level encoding strategies:**
  - Exploit disentanglement with semantic priors.
  - Use robust lightweight semantic representations.
  - Organise your semantic space.
  - Use specialised strategies for concepts and abstract statements.
- **Inference-level encoding strategies:**
  - Exploit the structure of scientific explanations.
  - Integrate inference priors as constraints.
  - Use differentiable convex layers for end-to-end training.
- **Evaluation of true inference properties:**
  - Determine true reasoning performance by using causal, interventional methods.
  - Probe your model for key properties.
  - Apply systematic behavioural testing.

Thank you



The northern hemisphere **is a kind** of hemisphere of earth

Abstraction (hemisphere)

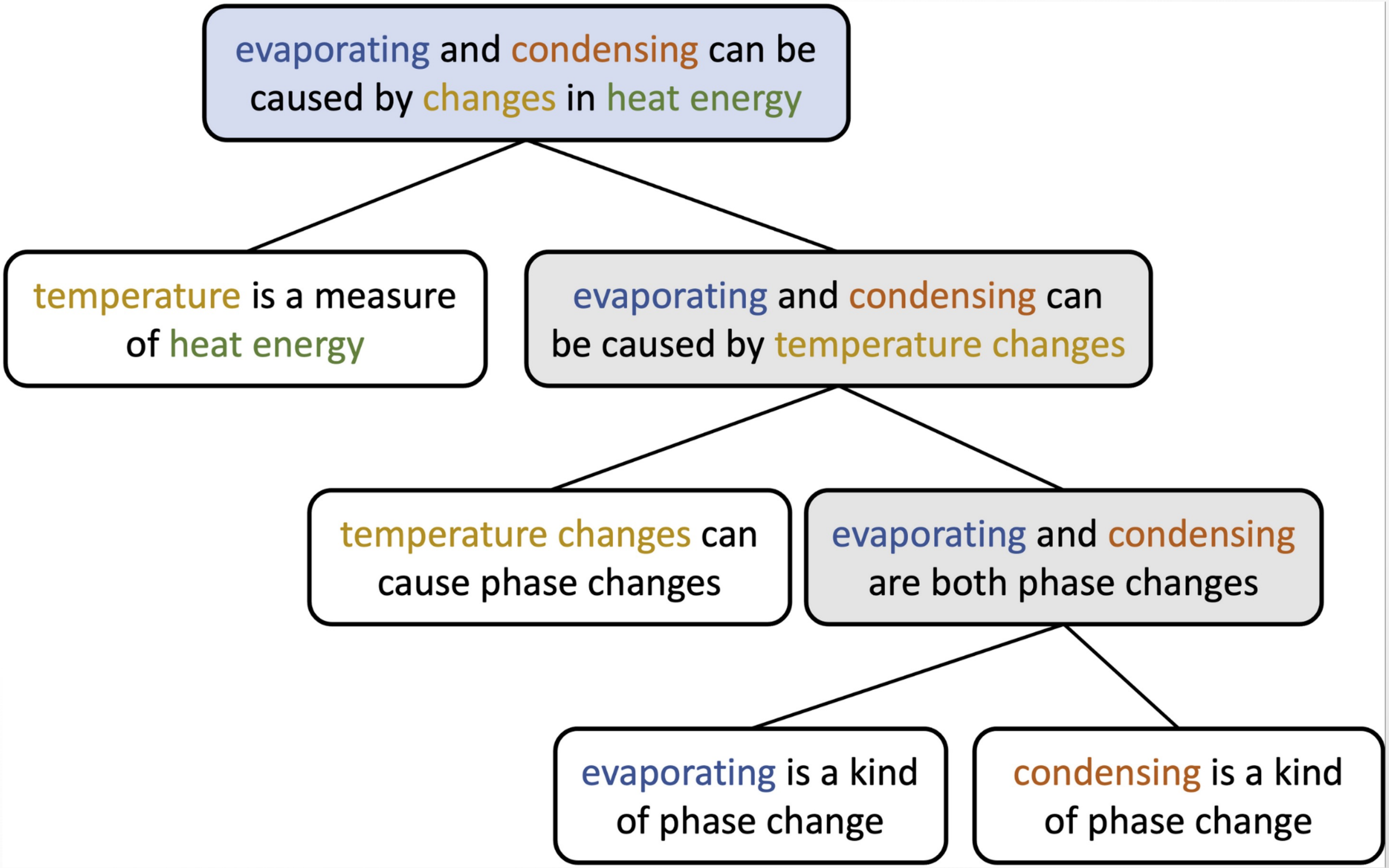
a hemisphere of earth i**s a kind** of place

Abstraction (place)

If a place **is in** summer, then it **will have** the most sunlight

Unification

Northern hemisphere **will have** the most sunlight in summer



evaporating and condensing can be caused by changes in heat energy

temperature is a measure of heat energy

evaporating and condensing can be caused by temperature changes

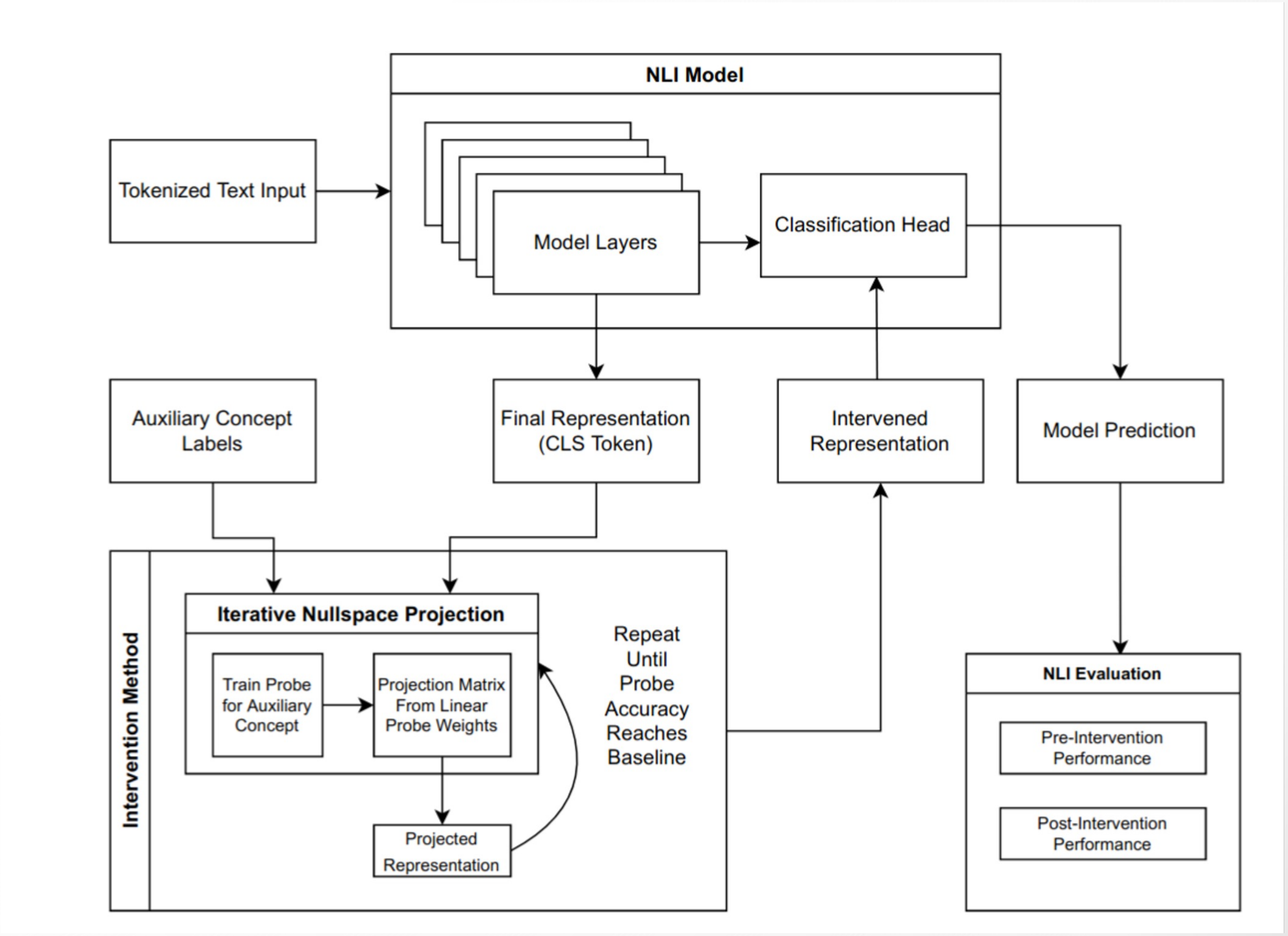
temperature changes can cause phase changes

evaporating and condensing are both phase changes

evaporating is a kind of phase change

condensing is a kind of phase change

Granular evaluation


NLI Model
Tokenized Text Input
Model Layers
Classification Head
Auxiliary Concept Labels
Final Representation (CLS Token)
Intervened Representation
Model Prediction
Intervention Method
Iterative Nullspace Projection
Train Probe for Auxiliary Concept
Projection Matrix From Linear Probe Weights
Projected Representation
Repeat Until Probe Accuracy Reaches Baseline
NLI Evaluation
Pre-Intervention Performance
Post-Intervention Performance

Ferreira et al., ACL Demo (2021)

Does My Representation Capture X? Probe-Ably

https://github.com/ai-systems/Probe-Ably

Question: A group of students are studying bean plants. All of the following traits are affected by changes in the environment except . . .

Candidate answers: [A] leaf color [B] seed type [C] bean production [D] plant height

Explanation

(i) The type of seed of a plant is an inherited characteristic;

(ii) Inherited characteristics are the opposite of acquired characteristics;

(iii) An organism’s environment affects that organism’s acquired characteristics;

(iv) A plant is a kind of organism;

(v) A bean plant is a kind of plant;

(vi) Trait is synonymous with characteristic.

Explanation

(i) The type of seed of a plant is an inherited characteristic;

$$\forall xy(\text{plant}(x) \wedge \text{seedType}(y, x) \rightarrow \text{characteristic}(y, x) \wedge \text{inherited}(y))$$

(ii) Inherited characteristics are the opposite of acquired characteristics;

$$\forall xy(\text{characteristic}(x, y) \wedge \text{inherited}(x) \rightarrow \neg\text{acquired}(x))$$

(iii) An organism’s environment affects that organism’s acquired characteristics;

$$\forall xyw(\text{organism}(x) \wedge \text{environment}(y, x) \wedge \text{characteristic}(w, x) \wedge \text{acquired}(w) \rightarrow$$

$$\rightarrow \exists e(\text{affect}(e) \wedge \text{agent}(e, y) \wedge \text{patient}(e, w))$$

(iv) A plant is a kind of organism;

$$\forall x(\text{plant}(x) \rightarrow \text{organism}(x))$$

(v) A bean plant is a kind of plant;

$$\forall x(\text{beanPlant}(x) \rightarrow \text{plant}(x))$$

(vi) Trait is synonymous with characteristic.

$$\forall xy(\text{trait}(x, y) \leftrightarrow \text{characteristic}(x, y))$$

$$\forall xy(\mathrm{plant}(x) \land \mathrm{seedType}(y, x) \rightarrow \mathrm{characteristic}(y, x) \land \mathrm{inherited}(y))$$

$$\forall xy(\mathrm{characteristic}(x, y) \land \mathrm{inherited}(x) \rightarrow \neg \mathrm{acquired}(x))$$

KB Φ

$$\forall xyw(\mathrm{organism}(x) \land \mathrm{environment}(y, x) \land \mathrm{characteristic}(w, x) \land \mathrm{acquired}(w) \rightarrow$$
$$\rightarrow \exists e(\mathrm{affect}(e) \land \mathrm{agent}(e, y) \land \mathrm{patient}(e, w))$$

$$\forall x(\mathrm{plant}(x) \rightarrow \mathrm{organism}(x))$$

$$\forall x(\mathrm{beanPlant}(x) \rightarrow \mathrm{plant}(x))$$

$$\forall xy(\mathrm{trait}(x, y) \leftrightarrow \mathrm{characteristic}(x, y))$$

$\Phi \vDash \psi$?

Question: find a characteristic of plants not affected by those plants’ environments. That is, we are asked for a **P** making the schematic formula **true**.

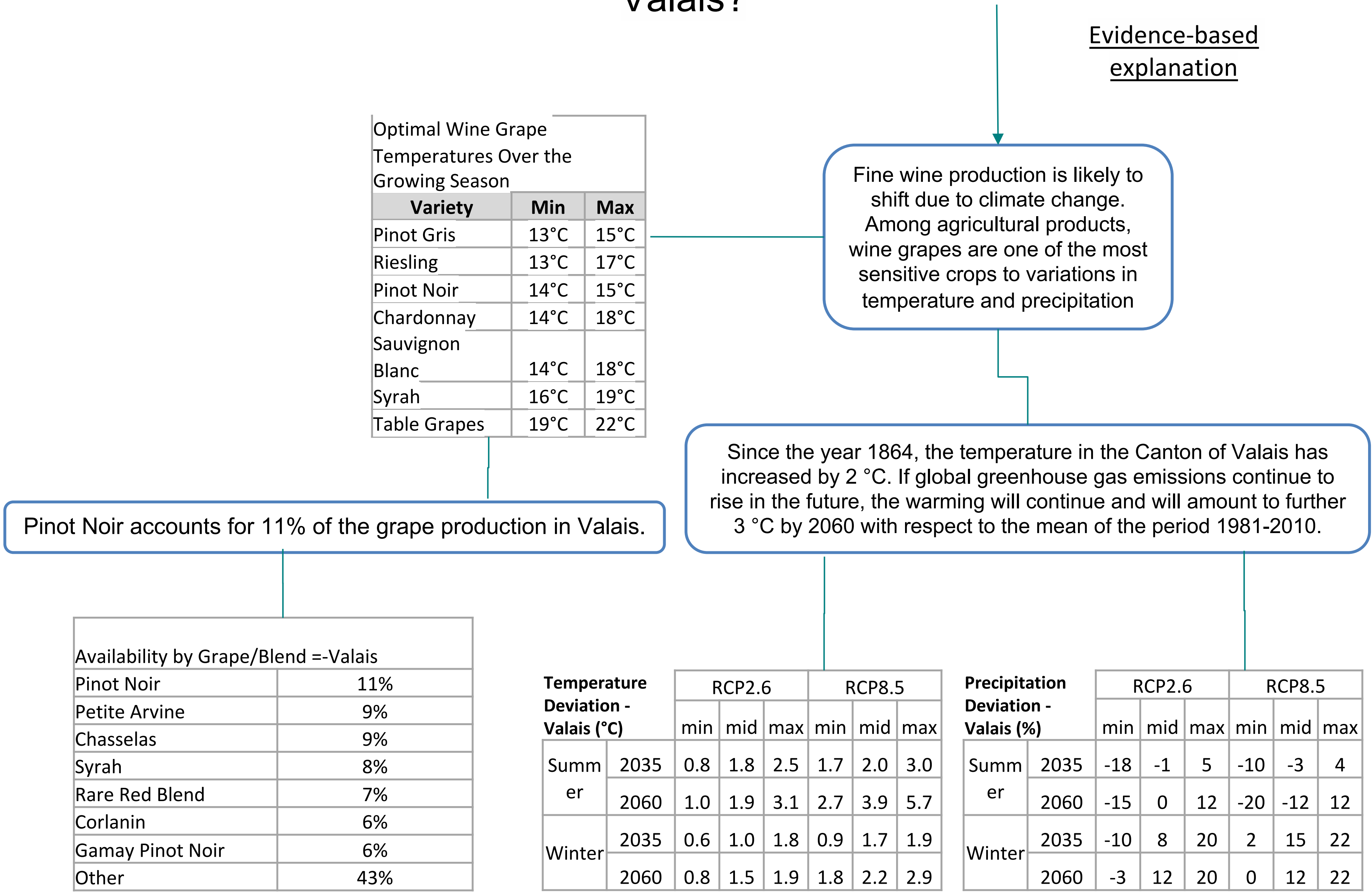
ψ

$$\forall xyzwe(\mathrm{beanPlant}(x) \land \mathrm{environment}(y, x) \land \mathrm{changeIn}(z, y) \land \mathrm{trait}(w, x) \land \mathrm{affect}(e) \land \mathrm{agent}(e, z) \land \mathbf{P} \rightarrow \neg \mathrm{patient}(e, w))$$

P: seedType(w, x)

Valentino, Pratt-Hartmann, Freitas, IWCS (2021)

Question: How a 1 degree rise in temperature will affect the grape harvest in Valais?



Evidence-based explanation

Fine wine production is likely to shift due to climate change. Among agricultural products, wine grapes are one of the most sensitive crops to variations in temperature and precipitation

Since the year 1864, the temperature in the Canton of Valais has increased by 2 °C. If global greenhouse gas emissions continue to rise in the future, the warming will continue and will amount to further 3 °C by 2060 with respect to the mean of the period 1981-2010.

Pinot Noir accounts for 11% of the grape production in Valais.

Optimal Wine Grape Temperatures Over the Growing Season

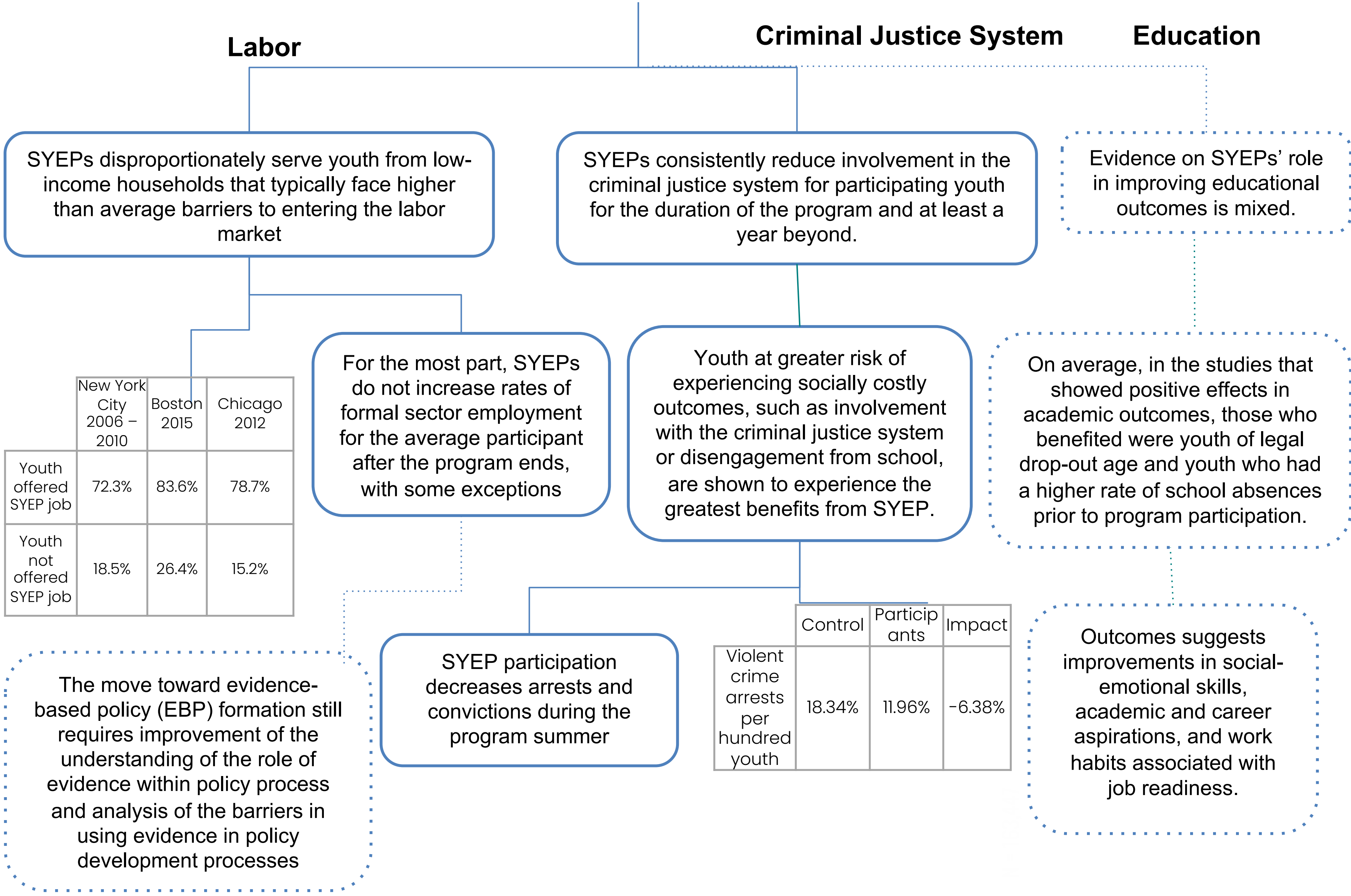
Variety	Min	Max
Pinot Gris	13°C	15°C
Riesling	13°C	17°C
Pinot Noir	14°C	15°C
Chardonnay	14°C	18°C
Sauvignon Blanc	14°C	18°C
Syrah	16°C	19°C
Table Grapes	19°C	22°C

Availability by Grape/Blend =-Valais	
Pinot Noir	11%
Petite Arvine	9%
Chasselas	9%
Syrah	8%
Rare Red Blend	7%
Corlanin	6%
Gamay Pinot Noir	6%
Other	43%

Temperature Deviation - Valais (°C)		RCP2.6			RCP8.5		
		min	mid	max	min	mid	max
Summer	2035	0.8	1.8	2.5	1.7	2.0	3.0
	2060	1.0	1.9	3.1	2.7	3.9	5.7
Winter	2035	0.6	1.0	1.8	0.9	1.7	1.9
	2060	0.8	1.5	1.9	1.8	2.2	2.9

Precipitation Deviation - Valais (%)		RCP2.6			RCP8.5		
		min	mid	max	min	mid	max
Summer	2035	-18	-1	5	-10	-3	4
	2060	-15	0	12	-20	-12	12
Winter	2035	-10	8	20	2	15	22
	2060	-3	12	20	0	12	22

Claim: US Summer Youth Employment programs can be replicated in Central Europe to help low income youth overcome barriers to accessing jobs.



Labor

Criminal Justice System

Education

SYEPs disproportionately serve youth from low-income households that typically face higher than average barriers to entering the labor market

SYEPs consistently reduce involvement in the criminal justice system for participating youth for the duration of the program and at least a year beyond.

Evidence on SYEPs' role in improving educational outcomes is mixed.

	New York City 2006 – 2010	Boston 2015	Chicago 2012
Youth offered SYEP job	72.3%	83.6%	78.7%
Youth not offered SYEP job	18.5%	26.4%	15.2%

For the most part, SYEPs do not increase rates of formal sector employment for the average participant after the program ends, with some exceptions

Youth at greater risk of experiencing socially costly outcomes, such as involvement with the criminal justice system or disengagement from school, are shown to experience the greatest benefits from SYEP.

On average, in the studies that showed positive effects in academic outcomes, those who benefited were youth of legal drop-out age and youth who had a higher rate of school absences prior to program participation.

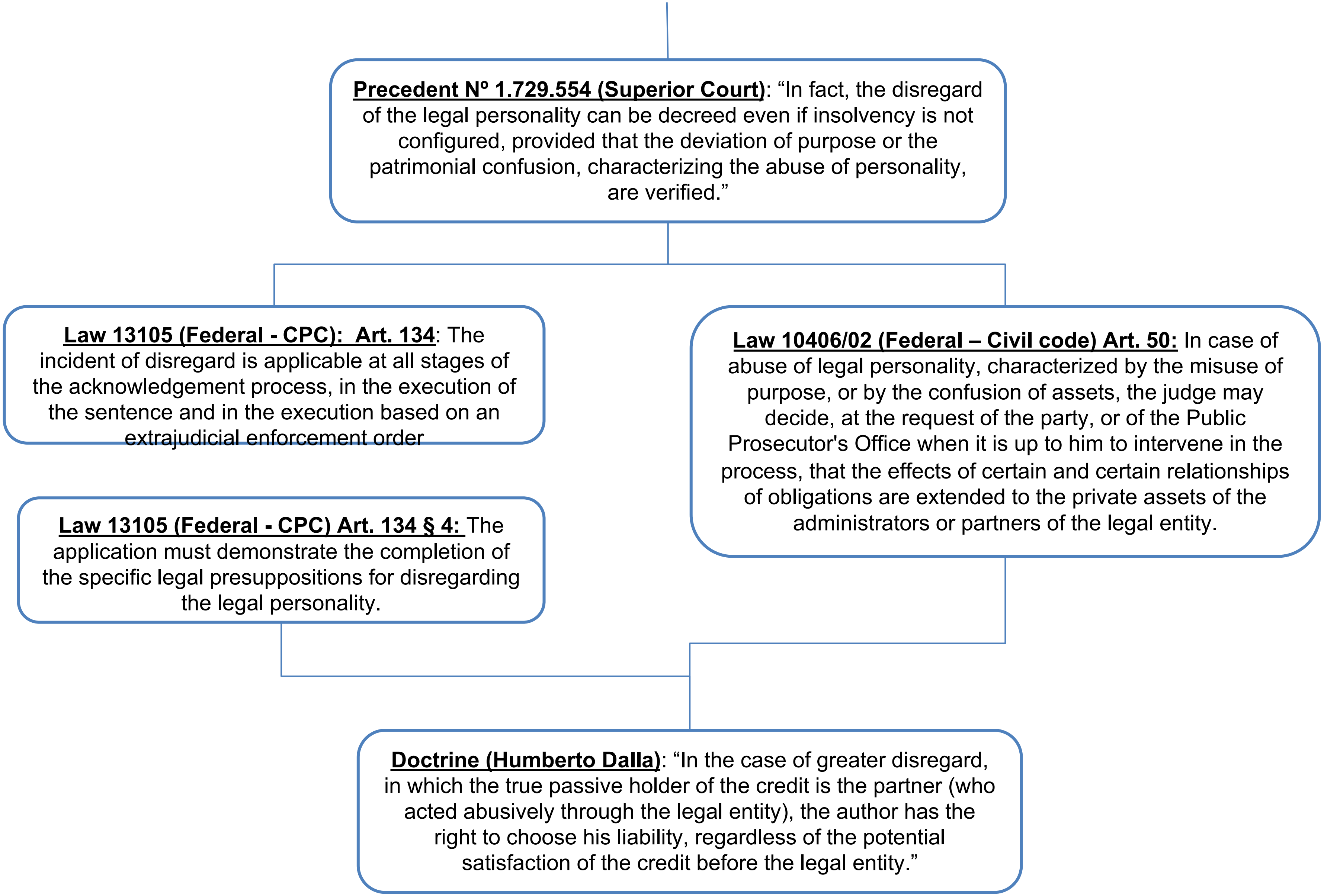
The move toward evidence-based policy (EBP) formation still requires improvement of the understanding of the role of evidence within policy process and analysis of the barriers in using evidence in policy development processes

SYEP participation decreases arrests and convictions during the program summer

	Control	Participants	Impact
Violent crime arrests per hundred youth	18.34%	11.96%	-6.38%

Outcomes suggests improvements in social-emotional skills, academic and career aspirations, and work habits associated with job readiness.

Claim: it is not necessary to prove the absence of the debtor's assets to obtain the disregard of legal personality.



Precedent Nº 1.729.554 (Superior Court): “In fact, the disregard of the legal personality can be decreed even if insolvency is not configured, provided that the deviation of purpose or the patrimonial confusion, characterizing the abuse of personality, are verified.”

Law 13105 (Federal - CPC): Art. 134: The incident of disregard is applicable at all stages of the acknowledgement process, in the execution of the sentence and in the execution based on an extrajudicial enforcement order

Law 10406/02 (Federal – Civil code) Art. 50: In case of abuse of legal personality, characterized by the misuse of purpose, or by the confusion of assets, the judge may decide, at the request of the party, or of the Public Prosecutor's Office when it is up to him to intervene in the process, that the effects of certain and certain relationships of obligations are extended to the private assets of the administrators or partners of the legal entity.

Law 13105 (Federal - CPC) Art. 134 § 4: The application must demonstrate the completion of the specific legal presuppositions for disregarding the legal personality.

Doctrine (Humberto Dalla): “In the case of greater disregard, in which the true passive holder of the credit is the partner (who acted abusively through the legal entity), the author has the right to choose his liability, regardless of the potential satisfaction of the credit before the legal entity.”

Complex Sentence Representation

- Clausal-Phrasal Disembedding (CPD).
- Minimal, localised, self-contained propositions.

“Programmed death-ligand 1 (PD-L1) also known as cluster of differentiation 274 (CD274) or B7 homolog 1 (B7-H1) is a protein that in humans is encoded by the CD274 gene.”

Core: PD-L1 is encoded by the CD274 gene.
Context: This is in humans.

PD-L1 is also known as cluster of differentiation 274.
PD-L1 is also known as B7-H1.
PD-L1 is a protein.

Programmed death-ligand 1 has abbreviation PD-L1.
Cluster of differentiation 274 has abbreviation CD274.
B7 homolog 1 has abbreviation B7-H1.

Niklaus, Cetto, Freitas, Handschuh ACL (2019)

Complex Sentence Representation

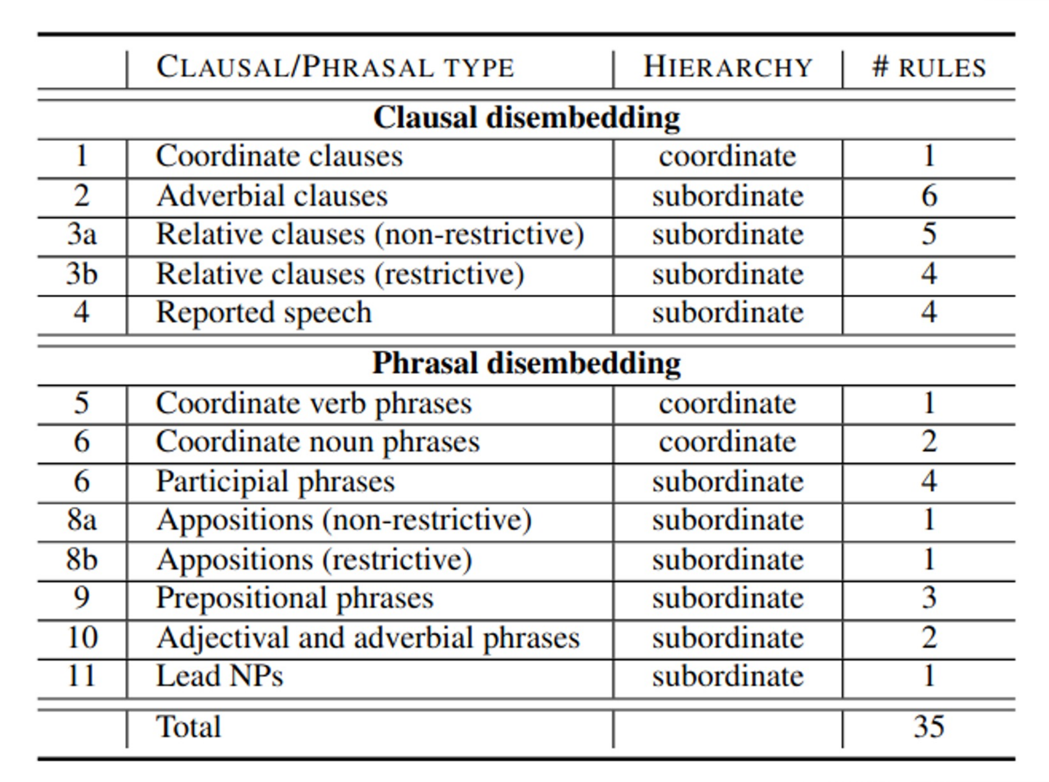
“Programmed death-ligand 1 (PD-L1) also known as cluster of differentiation 274 (CD274) or B7 homolog 1 (B7-H1) is a protein that in humans is encoded by the CD274 gene.”

Core: is encoded by(e, PD-L1, the CD274 gene).
Context: in(e, humans).

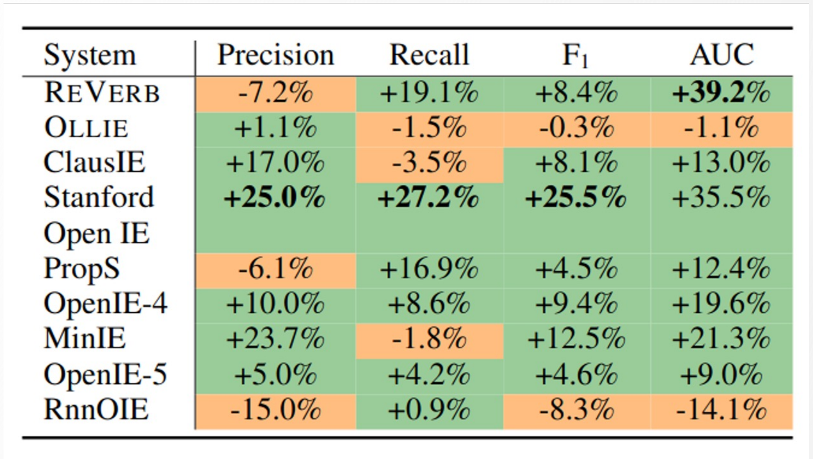
is also known as(PD-L1, cluster of differentiation 274).
is also known as(PD-L1, B7-H1).
is a(PD-L1, protein).

has abbreviation(Programmed death-ligand 1, PD-L1).
has abbreviation(Cluster of differentiation 274, CD274).
has abbreviation(B7 homolog 1, B7-H1).

Complex Sentence Representation



	CLAUSAL/PHRASAL TYPE	HIERARCHY	# RULES
	Clausal disembedding		
1	Coordinate clauses	coordinate	1
2	Adverbial clauses	subordinate	6
3a	Relative clauses (non-restrictive)	subordinate	5
3b	Relative clauses (restrictive)	subordinate	4
4	Reported speech	subordinate	4
	Phrasal disembedding		
5	Coordinate verb phrases	coordinate	1
6	Coordinate noun phrases	coordinate	2
6	Participial phrases	subordinate	4
8a	Appositions (non-restrictive)	subordinate	1
8b	Appositions (restrictive)	subordinate	1
9	Prepositional phrases	subordinate	3
10	Adjectival and adverbial phrases	subordinate	2
11	Lead NPs	subordinate	1
	Total		35



System	Precision	Recall	F_1	AUC
REVERB	-7.2%	+19.1%	+8.4%	**+39.2%**
OLLIE	+1.1%	-1.5%	-0.3%	-1.1%
ClausIE	+17.0%	-3.5%	+8.1%	+13.0%
Stanford Open IE	**+25.0%**	**+27.2%**	**+25.5%**	+35.5%
PropS	-6.1%	+16.9%	+4.5%	+12.4%
OpenIE-4	+10.0%	+8.6%	+9.4%	+19.6%
MinIE	+23.7%	-1.8%	+12.5%	+21.3%
OpenIE-5	+5.0%	+4.2%	+4.6%	+9.0%
RnnOIE	-15.0%	+0.9%	-8.3%	-14.1%

Niklaus, Cetto, Freitas, Handschuh ACL (2019)