Efficient Neuro-symbolic Learning of Constraints and Criteria from Sudoku to new functional molecules


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Inductive and deductive reasoning

- From observations (solutions) we construct a theory ($F = m\gamma$)
- We then use the theory to make predictions and design objects
- Until the theory is proven to be incorrect

Sudoku grid with solution

Protein structure with its sequence

The theory is written as a pairwise Graphical Model (a Cost Function Network)

Human reasoning and scientific discovery

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1	**2**	6	4	3	7	9	5	8
8	9	5	**6**	**2**	1	4	7	**3**
3	**7**	**4**	9	**8**	5	1	2	6
4	5	7	1	9	**3**	8	6	**2**
9	**8**	3	2	**4**	6	5	**1**	7
6	1	2	**5**	7	8	3	9	4
2	6	9	3	**1**	4	**7**	**8**	5
5	4	8	7	6	**9**	2	3	1
7	3	1	8	5	2	6	**4**	9

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Reminder

- A set X of variables — n variables
- Variable x_i has domain D_i — max. size d
- a set of cost functions — $c_{ij} : D_i \times D_j \to \mathbb{R}^+ \cup \{\infty\}$

Variables and parameters/costs

- The cost $C(t)$ of an assignment t is the sum of all cost functions on t
- The cost is linear in the parameters (costs in CF tables)
- It defines a probability distribution: $P(t) \propto \exp(-C(t))$ Markov Random Fields

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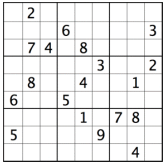
Structured output prediction (SOP) with a CFN model



ω

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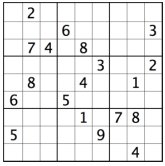

ω ⟶ Neural net

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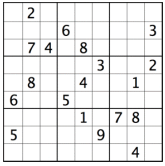

ω ⟶ Neural net ⟶ CFN $P(X|\omega)$

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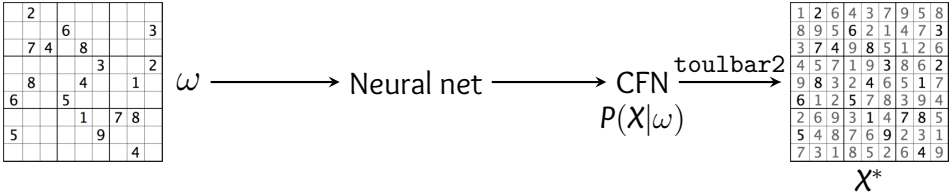

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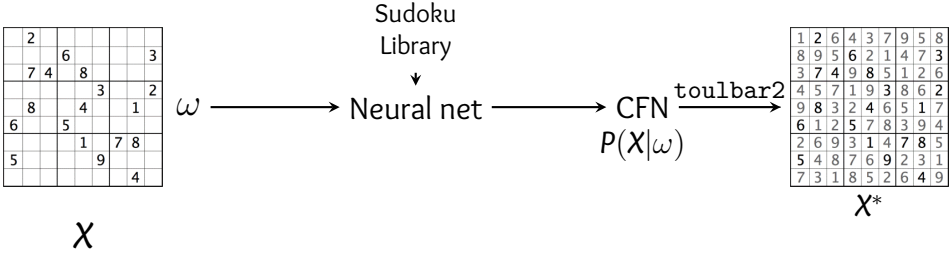

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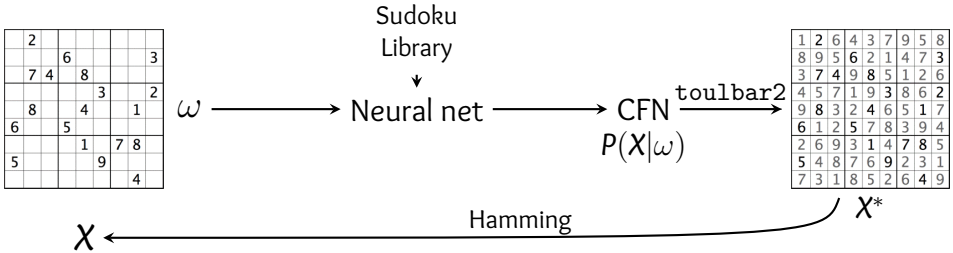

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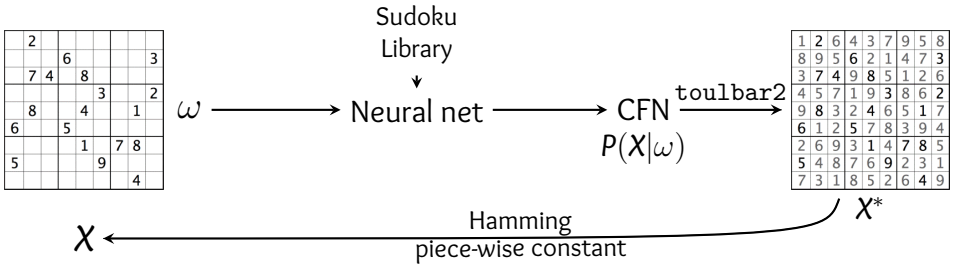

Issues

- Gradients either zero or undefined
- Requires to repeatedly solve random NP-hard instances

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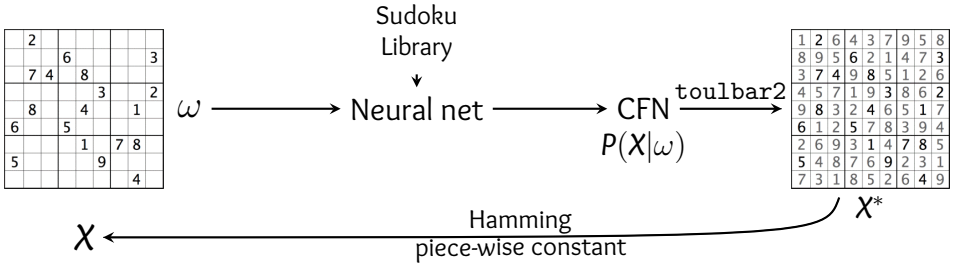

Natural choice: the negative loglikelihood

#P-hard

(Besag 1975)

- Use Besag's pseudo-loglikelihood (1975, efficient)
- Kicks the solver out of the training loop (scalable training)

Besag's Pseudo-Loglikelihood

- The Pseudo-LL masks each variable successively in the solution X (Besag 1975)

$$NLL = -\sum_{x} \log(P(x)) \qquad NPLL = -\sum_{x} \sum_{x_i} \log(P(x_i|x_{-i}))$$

- Nice asymptotic properties — statistically consistent
- The NPLL is a "Fenchel-Young" loss (Defresne, Gambardella, et al. 2026; Blondel et al. 2020)
- Does not work in practice (high costs) (Montanari et al. 2009)

Vanishing gradient issue

- If enough constraints have been learned to force the observed value of X_i in the context of x_{-i}, it becomes impossible to learn other constraints.
- Related to the idempotence of logical information

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Removing vanishing gradients

We ignore a random fraction of the neighbors/functions when computing $P(x_i|x_{-i})$

Easy, hard and extremely hard Sudoku grids

Type	Approach	Acc.	#hints	Train set	Param.	Train time (h)
DL	RRN (Palm et al. 2018)	96.6%	17	180,000	200k	> 50
	Rec. Trans. (Yang et al. 2023)	96.7%	17	180,000	211k	> 50
	Rec. Trans.	76.2–78.2%	17	9,000	-	1.8
	DDPM (Ye et al. 2025)	99.2–100%	33.8	100,000	6M	13.6
	DDPM	0.2%	17	-	-	-
	HRM (G. Wang et al. 2025)	55%	24.8	$1,000 \times 1,001$	27M	>10
Relax+DL	SATNet (P.-W. Wang et al. 2019)	95.1–99.8%	36.2	9,000	600k	2.9
	SATNet	86.1–86.2%	17	-	-	-
CO	(Bessiere et al. 2023)	**100%**	-	200	-	0.01
CO + ML	(Brouard et al. 2020)	**100%**	17	9,000	-	1.5
CO+DL	Hinge (Defresne, Barbe, et al. 2023)	**100%**	17	1,000	180k	>50
	E-PLL (ours)	**100%**	17	**100**	22k	0.05
	E-PLL (HRM dataset)	**100%**	24.8	**10** $\times$ 100	22k	0.04

Learning to play Many-Solutions Sudokus

Sudokus have only one solution (single target for DL)

- Existing DL architectures fail on many-solutions Sudokus (Nandwani et al. 2021)
- Corrected using a Reinforcement learning approach
- Training set with 5 solutions per instance
- Ability to generate additional solutions

Our architecture directly learns how to solve many-solutions Sudokus

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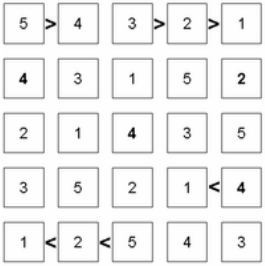
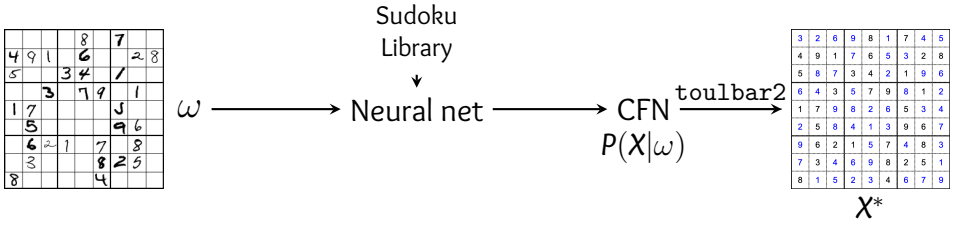
Learning to play Futoshiki

Sudoku is easy, only one type of constraint

- Our architecture directly learns how to play Futoshiki
- Includes both difference and inequality constraints
- Perfect solving, expected constraints learned



Learning to play Visual Sudoku



Simultaneously learns to recognize digits and to play the Sudoku

SATNet	Theoretical (no corrections)	Hybrid
63.2 %	74.2%	**94.1** $\pm$ 0.8%

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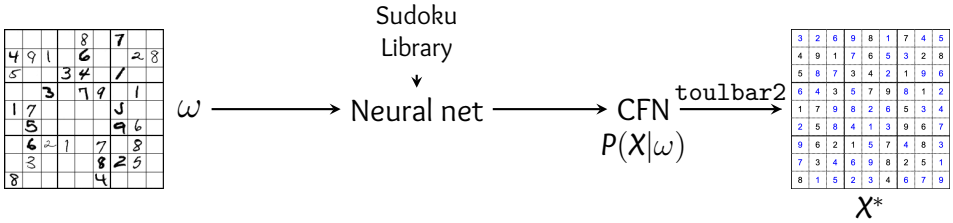

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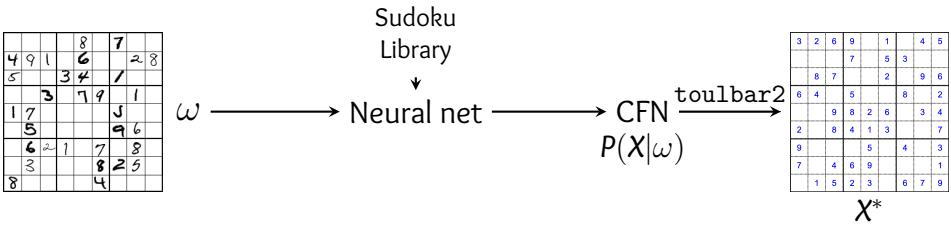
Reading numbers without cheating (grounding)



Grounding issue: a nasty form of data leakage

(Chang et al. 2020)

- The training set contains images and associated decoded digits (hints).
- Solved using a complex architecture (InfoGAN+clustering+Distillation) (Topan et al. 2021)
- E-PLL: missing data, imputation by optimisation
- Much longer training (a few hours)

Existing approaches

Approach	MNIST accuracy	Percep.	Solved	Training (h)
SATNet	0.0 %	0.0 %	0.0 %	-
Rec. Trans (Yang et al. 2023)	99.4%	74.8%	75.6%	5.1
NeSy. Prog. (Li et al. 2023)	99.6–99.7%	90.7–93.1%	92.2–94.4%	4.7
E-PLL (Ours)	98.8%	72.9%	93.4%	3.2

Relation with Decision-focused learning

From DFL to Structured Output Prediction

- Data: pairs $\langle \omega, c \rangle$ where c define the criterion parameters
- Assumes constraints are known
- we can compute a SOP data-set (ω, X^*)
- Aim: minimize regret (difference in real cost of the predicted and optimal solution)

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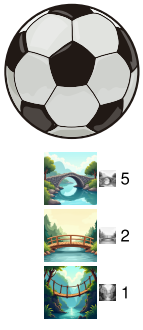
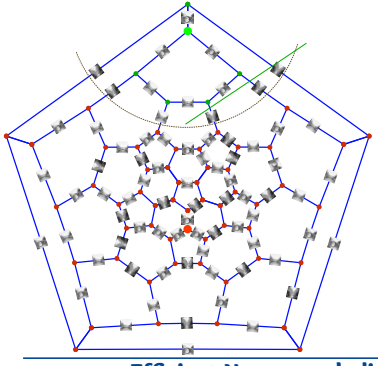
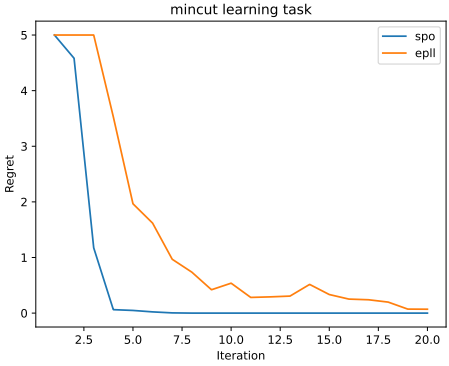
The Min/Max-Cut problems

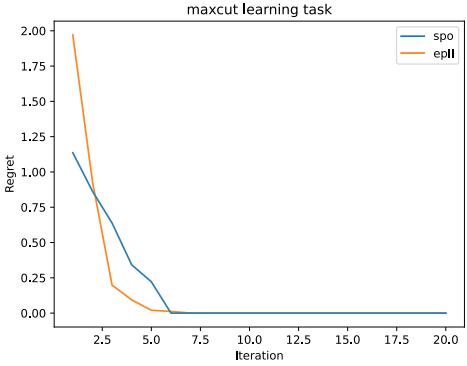
- one Boolean variable per vertex (cut side)
- per-edge difference (Min-Cut) or equality (Max-Cut) function scaled by a predicted scalar $c(\omega)$
- bridge images with Gaussian noise (std-dev 10)



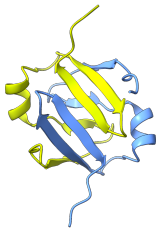


MinCut, MaxCut, Regret and SPO+ (Elmachtoub et al. 2022)





Learning to design proteins: Effie



ω → Neural net → CFN $P(X|\omega)$ → X^*

PDB
170,000 (ω, X)

Design
constraints

toulbar2

Neural architecture

- More complex SE(3)-equivariant neural network
- Relies on Gated MLPs (post-transformer architecture)

(Liu et al. 2021)

Optimizing a complete protein sequence

Full redesign of large proteins in the test set

- Guaranteed `toulbar2` solution expensive
- Using LR-BCD SDP solver instead (Durante et al. 2022)

Outperforms all-atoms XIXth-century physics

- Metric: **Native Sequence Recovery** rate (NSR)

Approach	Rosetta	Effie
NSR	17.9%	32.8%

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Effie vs. the model-free ProteinMPNN

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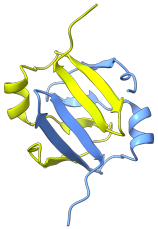
GPT-style



$\omega \longrightarrow$ Autoregressive NN $\longrightarrow X_1, X_2, \ldots$

PDB

$P(X_i|X_{i-1}, \ldots, X_1, \omega)$

Pros and cons

- $P(X_1, \ldots, X_n) = P(X_1)P(X_2|X_1) \cdots P(X_n|X_1, \ldots X_{n-1})$ is a mathematical identity
- But an easily broken one (*e.g.*, low temperature sampling)
- Heuristic score instead of NP-hard solving
- Limited control for design constraints, hard to "reason forward"

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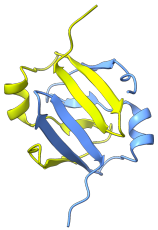

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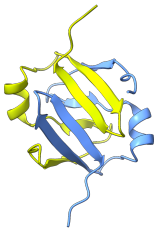

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Predicting SARS-CoV2 variants

Enumerate CoViD variants with a bounded number of mutations

- Uses only the initial March 2020 RBD-ACE2 structure + Effie/toulbar2
- Relies on a global constraint to bound mutations (Ruffini et al. 2021)
- Predicts all the first SARS-CoV2 VoCs ($\alpha, \beta, \gamma, \delta, \kappa, \iota, \lambda$ and μ)
- In a few seconds, on one CPU-thread.

Not achievable by pure autoregressive models (ProteinMPNN).
Previously shown to predict contagious antibody-resistant variants (Colom et al. 2024).

Design of an enzyme organizing platform

Design of an heteromeric hexamer

- Design  and  that self-assemble as  but not as  or 
- Physics+logic: requires bi-level optimization (NP^{NP}-complete) (Vucinic et al. 2020)
- Compare Effie+tb2 (NP-complete) with ProteinMPNN, bi-criteria (Buchet et al. 2024)

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Scoring →	Effie	PMPNN
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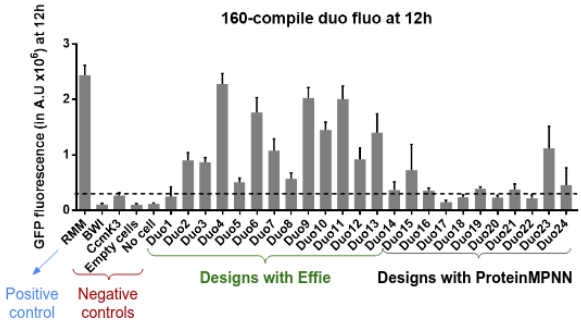

Conclusions

A Neural Net, a GM, and a discrete optimizer in a NeSy autoencoder

- A NeSy Generative AI that benefits from each component
- Neural Network: ideal to extract a representation of $P(X|\omega)$ from raw inputs
- Represented as a GM in a fully explorable and controllable latent layer
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Acknowledgments

AI/toolbar2

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