

Structural Causal Models, Abstraction, and Learning

Fabio Massimo Zennaro

University of Bergen

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1 Structural Causal Modelling

2 Causal Abstraction

3 Abstraction Learning

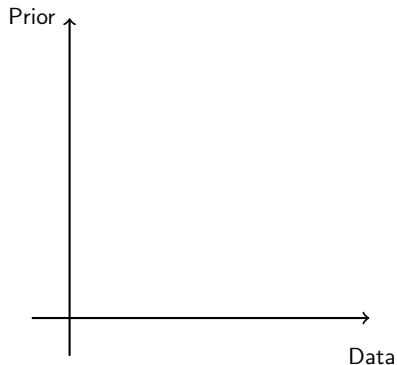
4 Current Developments

1. Structural Causal Modelling

Modelling

Assume we want to model a *system*.

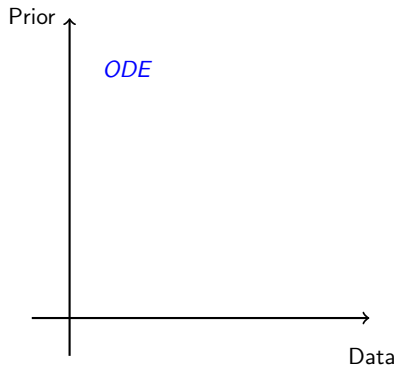
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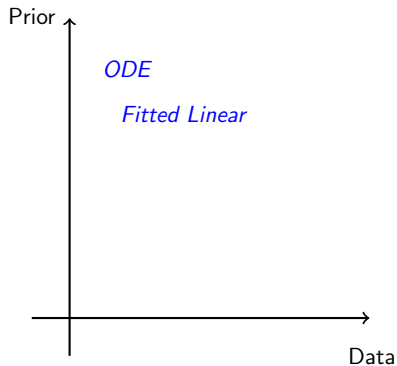
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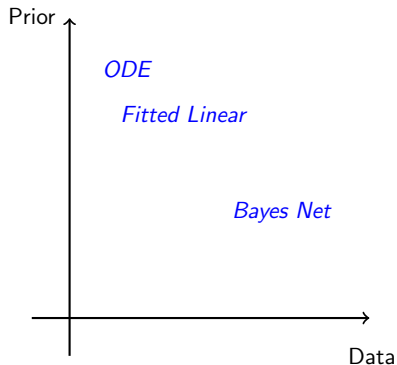
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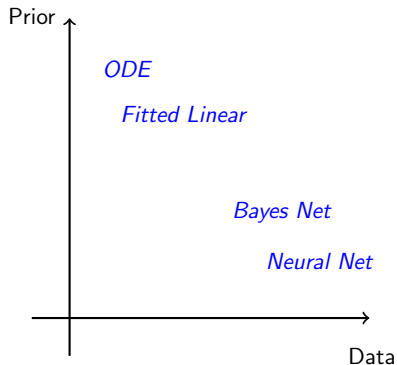
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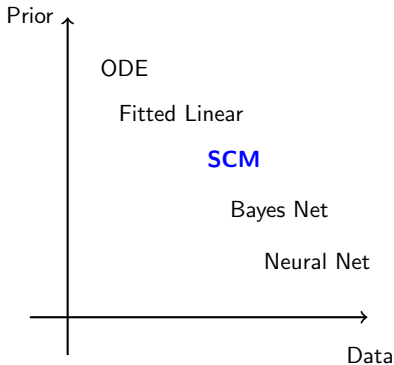
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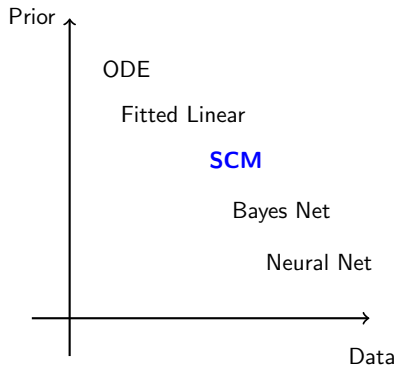
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Structural causal models rely on a strong prior given by *causality* [14, 15].



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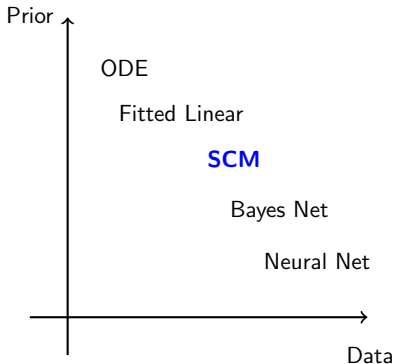
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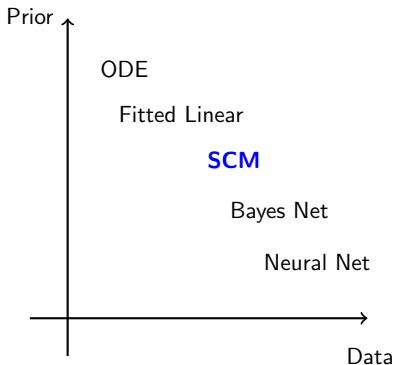
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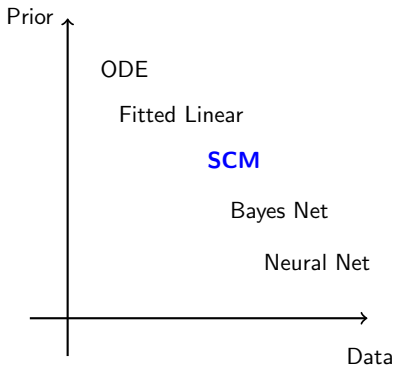
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- It discriminates *correlations* and *causes*.
- It allows for reasoning about *interventions*.
- It allows for reasoning about *counterfactuals*.
- It implies a *causality ladder* of reasoning.

A Motivating Example

SCMs represent **causal systems**.



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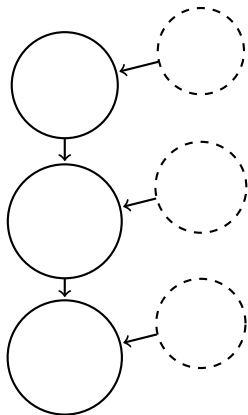
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SCMs integrates a *graphical model* and *probabilities distributions*.

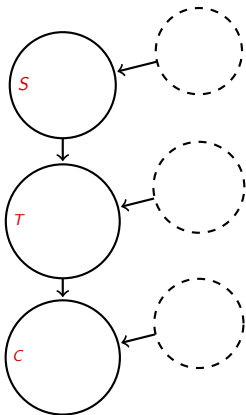
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We express a **SCM** as $\mathcal{M} = \langle \mathcal{X}, \mathcal{U}, \mathcal{F}, \mathcal{P} \rangle$ [14, 15]:



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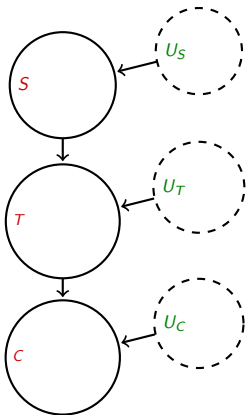
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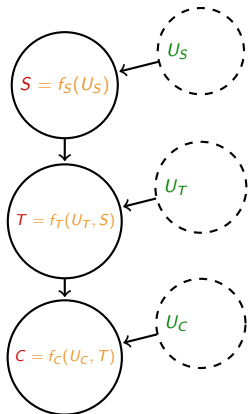
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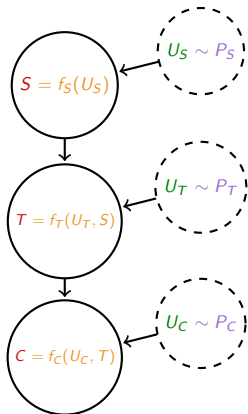
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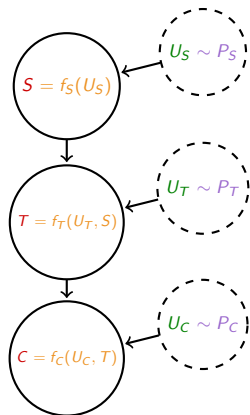
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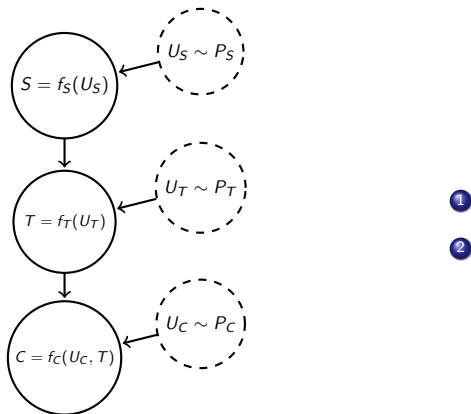


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Every SCM \mathcal{M} implies a (joint) **distribution** $P_{\mathcal{M}}$: $P_{\mathcal{M}}(S, T, C)$

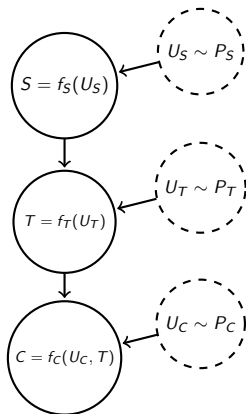
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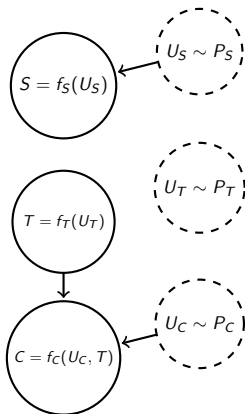
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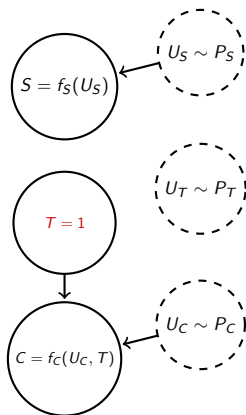


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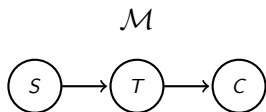
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Structural Causal Models (SCMs) - Distributions

An *intervention* ι defines a new **intervened model** \mathcal{M}_ι with new distributions.

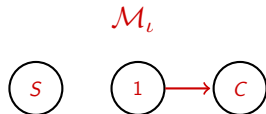
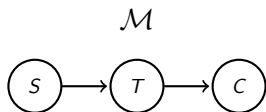
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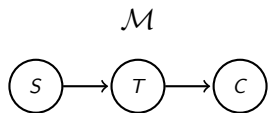
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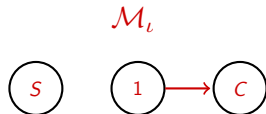


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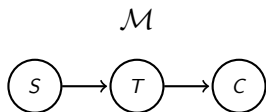


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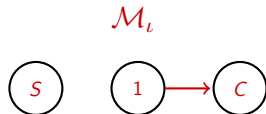


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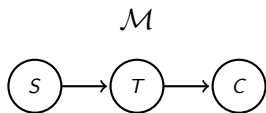
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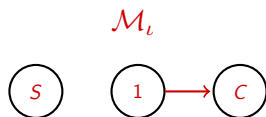
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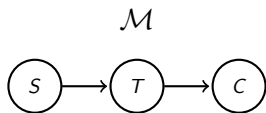
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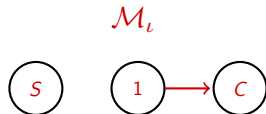
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$P_{\mathcal{M}_\iota}(C|S) = P_{\mathcal{M}}(C|S, do(T = 1))$

2. Causal Abstraction

Levels of Abstraction

Systems may be represented at different **levels of abstraction** (LoA) [7].

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Thermodynamics example:

Low-level / Base model:

Microscopic description $\mathbf{x}, \dot{\mathbf{x}}$.

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Macroscopic description P, T, V .

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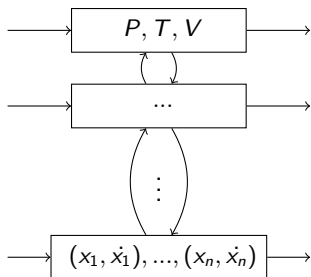
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LoA may be inaccessible, so we may want to *shift* among LoAs.

- 1 We need a *mapping* between LoAs.
- 2 We want the mapping to be *consistent*.

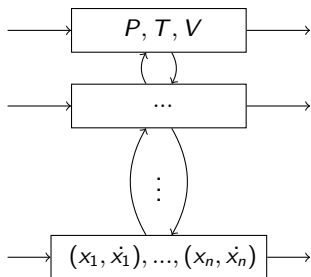
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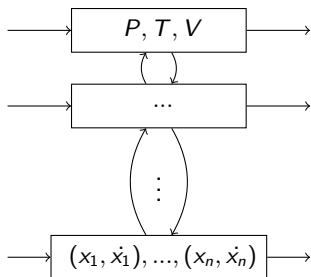
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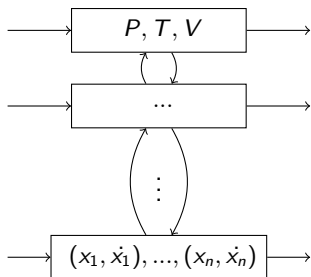
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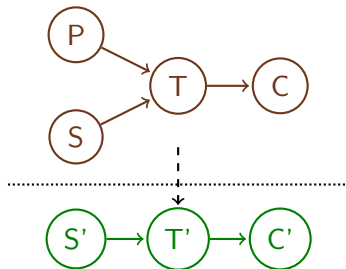
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Lung cancer scenario example:



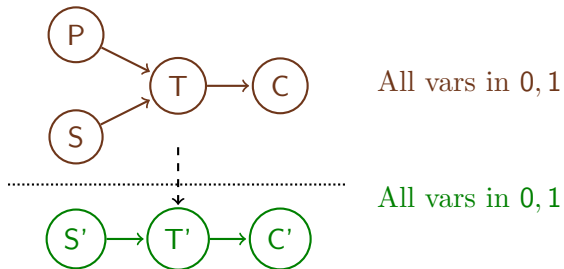
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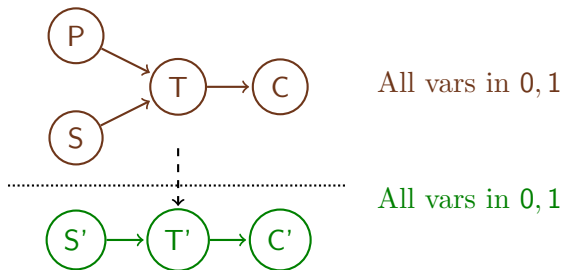
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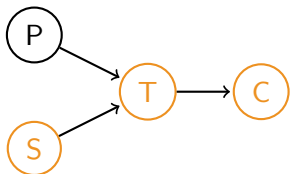
- The *transformation* approach [18, 2]
- The **α -abstraction** approach [17, 16]
- The Φ -*abstraction* approach [12, 13]

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An α -abstraction $\langle R, a, \alpha_i \rangle$ [17, 16] is defined as:

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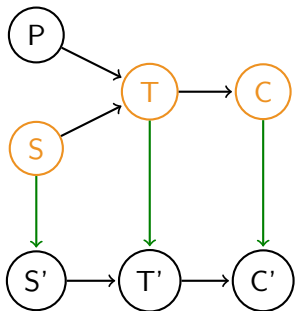


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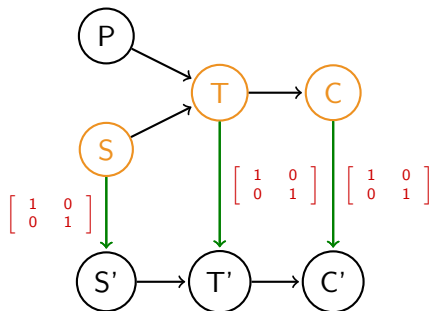
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- α_i : a collection of surjective functions between *outcomes*.

Causal Abstractions (CAs) - Consistency

We want an abstraction to guarantee *interventional consistency*.

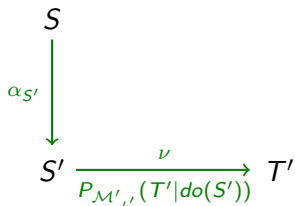
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$$S' \xrightarrow[\mathcal{P}_{\mathcal{M}'_\nu, (T'|do(S'))}]{\nu} T'$$

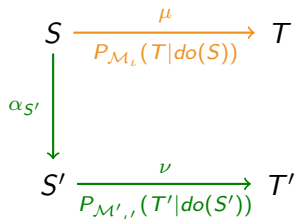
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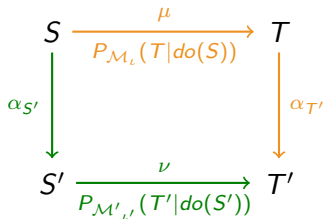
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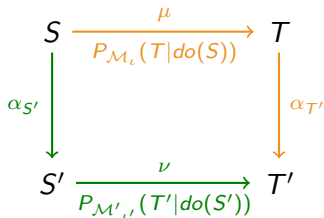
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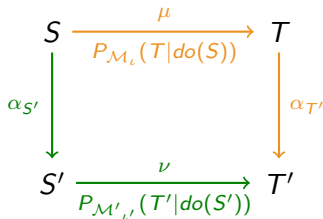
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- Ideally, mechanisms and abstractions *commute*.

Causal Abstractions (CAs) - Consistency

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- Ideally, mechanisms and abstractions *commute*.
- Otherwise, we compute an abstraction error as the *worst-case discrepancy* over all possible interventions:

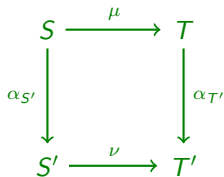
$$E_{\alpha}(S', T') = \max_l D(\alpha_{T'} \cdot \mu, \nu \cdot \alpha_{S'})$$

Causal Abstractions (CAs) - Abstraction Error

An abstraction implies multiple *causal mechanism diagrams*:

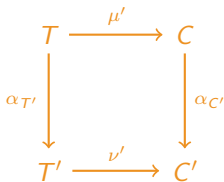
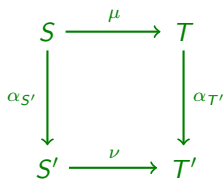
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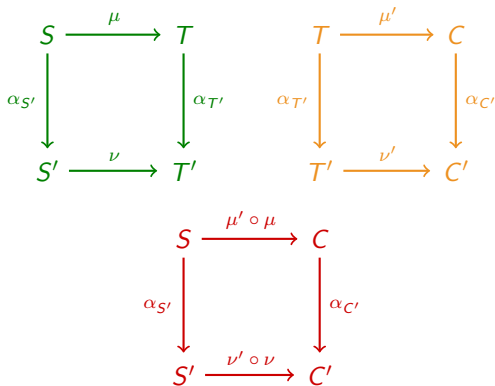
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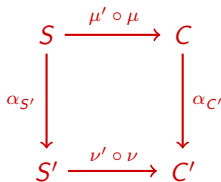
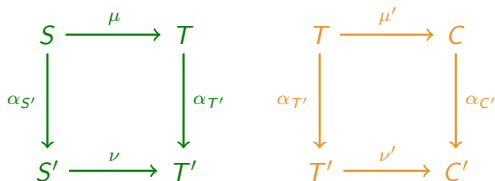
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A **(global) abstraction error**
[17] $e(\alpha)$ is the maximum
abstraction error over all
diagrams.

$$e(\alpha) = \sup_{\mathbf{X}', \mathbf{Y}' \subseteq \mathcal{X}'} E_{\alpha}(\mathbf{X}', \mathbf{Y}')$$

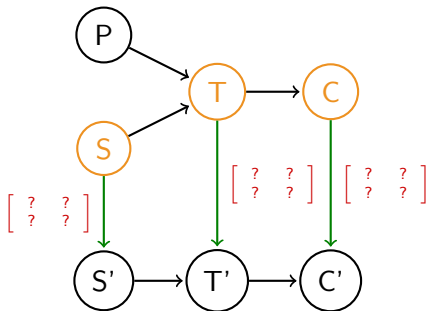
3. Abstraction Learning

Joint work of FMZ, M. Drávucz, G. Apachitei, W.D. Widanage and T. Damoulas

Problem statement [22]

Given a partially define
abstraction α in terms of $\langle R, a \rangle$
 can I learn α_i as:

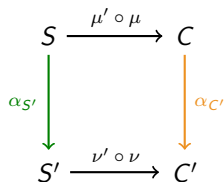
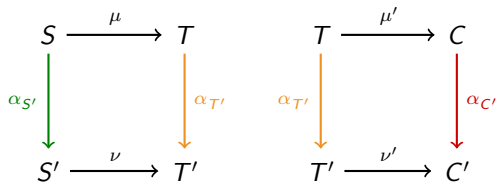
$$\min_{\alpha} e(\alpha)$$



Challenges [22]

(i) *Multiple related problems*

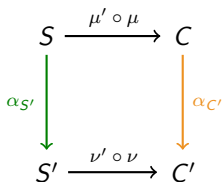
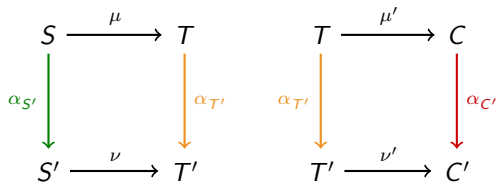
$$\alpha_{S'} = \begin{bmatrix} ? & ? \\ ? & ? \end{bmatrix}, \alpha_{T'} = \begin{bmatrix} ? & ? \\ ? & ? \end{bmatrix}, \alpha_{C'} = \begin{bmatrix} ? & ? \\ ? & ? \end{bmatrix}$$



Challenges [22]

- (i) *Multiple related problems*
- (ii) *Combinatorial optimization*

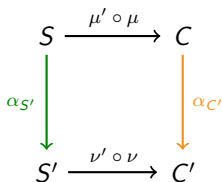
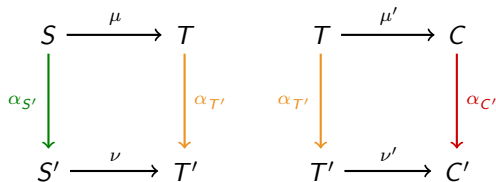
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Challenges [22]

- (i) *Multiple related problems*
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- (iii) *Surjectivity constraints*

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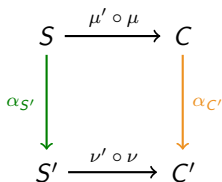
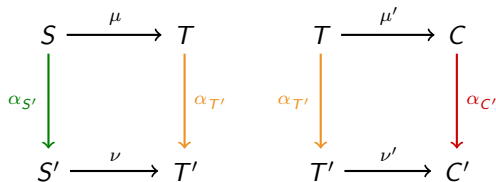
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(i) *Multiple related problems*

(ii) *Combinatorial optimization*

(iii) *Surjectivity constraints*



Baselines: parallel or sequential approaches.

Relaxation and parametrization [22]

We address (ii) *combinatorial optimization* by *relaxing* and *parametrizing* all α_j .

$$\min_{\alpha(\mathbf{W})} e(\alpha(\mathbf{W}))$$

$$\alpha_{S'}, \alpha_{T'}, \alpha_{C'} \in \mathbb{R}^{2 \times 2}$$

$$\begin{bmatrix} 0.7 & 1.2 \\ -0.2 & 3.3 \end{bmatrix}$$

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We add *tempering* $t(W) = \frac{e^{\frac{w_{ij}}{T}}}{\sum_i e^{\frac{w_{ij}}{T}}}$ along the matrix columns to binarize them.

$$\alpha_{S'}, \alpha_{T'}, \alpha_{C'} \in [0, 1]^{2 \times 2}$$

$$\mathcal{L}_1 : \min_{\alpha(\mathbf{W})} e(\alpha(t(\mathbf{W})))$$

$$t \left(\begin{bmatrix} 0.7 & 1.2 \\ -0.2 & 3.3 \end{bmatrix} \right) = \begin{bmatrix} 0.99 & 0.02 \\ 0.01 & 0.98 \end{bmatrix}$$

Enforcing surjectivity [22]

We address (iii) *surjective constraints* through a *penalty function*:

$$\mathcal{L}_2 : \min_{\mathbf{W}} \sum_{\mathbf{W}} \sum_i \left(1 - \max_j t(\mathbf{W})_{ij} \right)$$

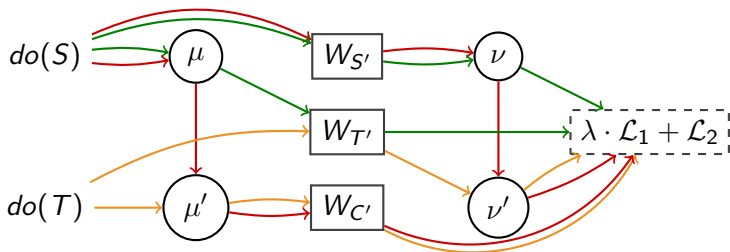
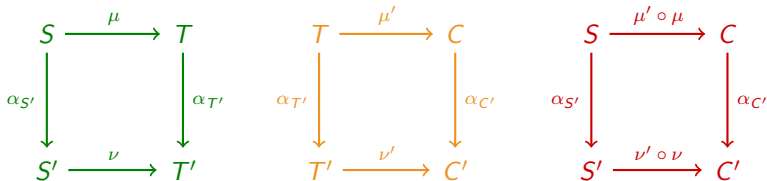
$$\alpha_{S'}, \alpha_{T'}, \alpha_{C'} \in [0, 1]^{2 \times 2}$$

$$\begin{bmatrix} 0.99 & 0.02 \\ 0.01 & 0.98 \end{bmatrix} \overset{\mathcal{L}_2}{\rightsquigarrow}$$

$$(1-0.99)+(1-0.98)$$

Solution by gradient descent [22]

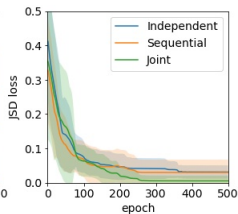
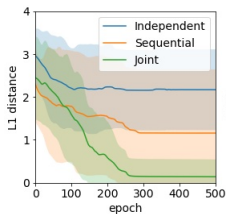
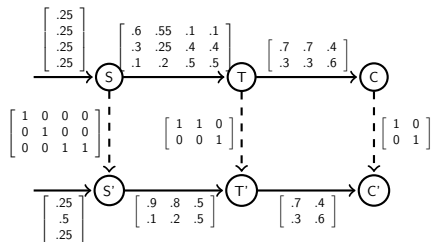
We address (i) multiple related problems by *jointly* solving all the problems via *gradient descent*:



Synthetic Experiments [22]

We evaluated our learning method:

- On multiple synthetic models;
- Against *independent* and *sequential* approach;
- Monitoring *loss functions*, *L1-dist from ground truth*, *wall-clock time*.



Real-World Experiments [22]

We want to model the stage of **coating** in lithium-ion battery manufacturing:

$$\text{Mass Loading} = f(\text{input})$$

Experiments are costly, so we want to integrate data¹ collected by two groups running similar (but not identical) experiments:

LRCS (France)

Collection of few statistics in each a few stages of battery manufacturing [?].

WMG (UK)

Collection of detailed space- and time-dependent measurements during coating.

¹<https://chemistry-europe.onlinelibrary.wiley.com/doi/full/10.1002/batt.201900135>

<https://github.com/mattdravucz/jointly-learning-causal-abstraction/>

Real-World Experiments [22]

We evaluated our learning method:

- Performing abstraction of data from base to abstracted (WMG \rightarrow LRCS);
- Evaluating change in performance using aggregated data when predicting *out-of-sample* (k).

	Training set	Test Set	MSE
(a)	LRCS[$CG \neq k$]	LRCS[$CG = k$]	1.86 ± 1.75
(b)	LRCS[$CG \neq k$] + WMG	LRCS[$CG = k$]	0.22 ± 0.26
(c)	LRCS[$CG \neq k$] + WMG[$CG \neq k$]	LRCS[$CG = k$] + WMG[$CG = k$]	1.22 ± 0.95

4. Current Developments

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- 1 *Foundations* of the frameworks
 - Category theory [13]
 - Measure theory [3]
 - Review [20]
- 2 *Characterization* of these frameworks
 - Measures of abstraction [23]
 - Abstraction with soft interventions [10]
 - Cluster DAGs and do-calculus [1]
 - Causal bandits and abstraction [21]

Current Developments

- ③ *Algorithmic and empirical* development
 - Learning with optimal transport [6]
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And connections to *causal representation learning, reinforcement learning...*

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And connections to *causal representation learning, reinforcement learning...*

More about causal abstraction:

<https://github.com/FMZennaro/CausalAbstraction/>

Thanks!

Thank you for listening!

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