Hierarchical structure of complex systems

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Dynamical system (X, Φ)

$J \; \ldots \; \mathbb{R} \cap [0, \infty)$ or $\mathbb{Z} \cap [0, \infty)$

$\Phi \colon J \times X \to X$

1. $\Phi(0, x) = x$ for all $x \in X$,
2. $\Phi(t + s, x) = \Phi(t, \Phi(s, x))$ for all $t, s \in J$ and $x \in X$.

Definition

Let (X, Φ) and (Y, Ψ) be two dynamical systems with the same time set J. A map $\Xi \colon X \to Y$ is a *coarse graining* if for all $t \in J$,

$$\begin{array}{ccc} X & \xrightarrow{\Phi_t} & X \\ {\scriptstyle \Xi}\big\downarrow & & \big\downarrow{\scriptstyle \Xi} \\ Y & \xrightarrow{\Psi_t} & Y \end{array}$$

or symbolically $\Xi(\Phi_t(x)) = \Psi_t(\Xi(x))$ for all $t \in J$ and $x \in X$.

Kernel condition

Theorem (Rowe et al [1])

V and W ... open sets in $\mathbb{R}^n$ and $\mathbb{R}^m$
Φ_1 a continuously differentiable function on V
$\Xi\colon V \to W$ a smooth map such that its level sets are connected by smooth paths. Then Ξ is a coarse graining of the system Φ_1 if and only if for all $\boldsymbol{x} \in V$

$$(D\Phi_1)_{\boldsymbol{x}} \cdot T_{\boldsymbol{x}} \subseteq \ker (D\Xi)_{\Phi_1(\boldsymbol{x})}, \tag{1}$$

where $T_{\boldsymbol{x}} \subseteq \ker (D\Xi)_{\boldsymbol{x}}$ is a tangent space at $\boldsymbol{x}$ defined as a linear span of a set of all velocities realised by smooth paths passing through $\boldsymbol{x}$ and attaining values within the same level set of Ξ.

Lattices

Proposition

Linear coarse grainings of a system (Φ_1, X), where X is a subset of a linear space, form a complete modular lattice.
Aggregations also form a complete (but not modular) lattice.

Definition

The following class of maps on Λ_n was introduced by Vose in [2].

Definition

Let $\mathcal{G}$ be a heuristic, a Random Heuristic Search (RHS) with parameter r is a DTMC with state space $\frac{1}{r}X_n^r \subset \Lambda_n$ where X_n^r denotes the set of all possible vectors in $\mathbb{Z}_{\geq 0}^n$ that add up to r (so there are $\binom{n+r-1}{r}$ states). The transition probabilities are given by

$$\mathbb{P}\left[\frac{1}{r}\boldsymbol{v} \to \frac{1}{r}\boldsymbol{w}\right] = \frac{r!}{\boldsymbol{w}!}\left(\mathcal{G}\left(\frac{1}{r}\boldsymbol{v}\right)\right)^{\boldsymbol{w}}.$$

Polynomial model

$$(T(\boldsymbol{p}))_i = \sum_{\boldsymbol{v}:|\boldsymbol{v}|\leq d} \frac{1}{\boldsymbol{v}!}\alpha_{i,\boldsymbol{v}}\boldsymbol{p}^{\boldsymbol{v}},$$

Theorem

Let T be a polynomial map on $\mathbb{R}^n$ as above. An aggregation of variables $\Xi\colon \mathbb{R}^n \to \mathbb{R}^m$ is a valid coarse graining if and only if $\Xi(\boldsymbol{v}) = \Xi(\boldsymbol{w})$ implies $\Xi(\boldsymbol{\alpha}_{\boldsymbol{v}}) = \Xi(\boldsymbol{\alpha}_{\boldsymbol{w}})$ for all $\boldsymbol{v}, \boldsymbol{w} \in \mathbb{Z}^n_{\geq 0}$.

n-type reaction model of degree d

$$T(\boldsymbol{p}) = \sum_{k=0}^{d} \rho_k \left(\sum_{\boldsymbol{v}:|\boldsymbol{v}|=k} \binom{k}{\boldsymbol{v}} \boldsymbol{\tau}_{\boldsymbol{v}} \boldsymbol{p}^{\boldsymbol{v}} \right),$$

Theorem

Let $\mathcal{G}$ be an n-type reaction model of the degree d. A partition $\mathcal{A}$ of the set $\{1, 2, \ldots, n\}$ is a valid aggregation if and only if $\Xi(\boldsymbol{v}) = \Xi(\boldsymbol{w})$ implies $\Xi(\boldsymbol{\tau}_{\boldsymbol{v}}) = \Xi(\boldsymbol{\tau}_{\boldsymbol{w}})$ for all $\boldsymbol{v}, \boldsymbol{w} \in \mathbb{Z}^n_{\geq 0}$ where Ξ is an aggregation associated to partition $\mathcal{A}$.

n-type reaction model of degree d

Observation

A partition $\{C_1, C_2, \ldots, C_m\}$ of a set of particle types will be a valid aggregation if and only if for each $k \in \mathbb{N}$ and each $\boldsymbol{u} \in \mathbb{Z}^m_{\geq 0}, |\boldsymbol{u}| = k$ there exists a well defined probability vector $\tilde{\boldsymbol{\tau}}_{\boldsymbol{u}} \in \mathbb{R}^m$ $(=\Xi(\boldsymbol{\tau}_{\boldsymbol{v}})$, where $\Xi(\boldsymbol{v}) = \boldsymbol{u})$ whose j^{th} entry is probability that in k-degree reaction of $(\boldsymbol{u})_1, (\boldsymbol{u})_2, \ldots, (\boldsymbol{u})_m$ particles of a coarse grained type $C_1, C_2, \ldots, C_m$ respectively (in total k of them) produce a particle of type C_j.

Corollaries

Corollary

Let M be a transition matrix of a Markov chain over a set of states $\Omega = \{1, 2, \ldots, n\}$. A partition of Ω is a valid coarse graining if and only if there is a well defined transition probability from any state in the piece C of the partition to the piece D.

Corollaries

Definition

The equivalence relation on a search space is *contiguous* if for all $i, j, k \in \Omega$ we have

$$i \equiv k \text{ and } i \to j \to k \implies i \equiv j \equiv k. \quad (2)$$

Corollary

Let the heuristic $\mathcal{G}$ be as above. The equivalence relation on Ω is compatible (i.e. gives coarse graining) with $\mathcal{G}$ if and only if it is contiguous.

Corollaries

Definition

The equivalence relation $\equiv$ on a search space is *contiguous* with respect to selection map P if for all $i, j, k \in \Omega$ we have

$$i \equiv k \text{ and } P(i,j) \neq P(k,j) \implies i \equiv j \equiv k. \tag{3}$$

Corollary

Let P be a selection map on Ω. Let the heuristic $\mathcal{G}$ defined by

$$(\mathcal{G}(p_1, \ldots, p_n))_i = 2p_i \sum_{k \in \Omega} P(i,k) p_k. \tag{4}$$

The equivalence relation on Ω is compatible (i.e. gives coarse graining) with $\mathcal{G}$ if and only if it is contiguous with respect to P.

Subset sum problem (SSP)

We can reduce any 'Subset sum problem' (SSP) to the problem of finding (at least one of the) finest aggregations that is coarser than the initial one. Namely, let $S = \{a_1, a_2, \ldots, a_n\}$ be a set for which we want to solve the SSP. Let s denote the sum of the elements in S. Let $v = (a_1, a_2, \ldots, a_n, -s)$ and let v^+, v^- be the positive and the negative parts of v respectively so that $v = v^+ - v^-$. Normalise v^+ and v^- to be probability distributions (note that the scaling factor will be the same) and scale v accordingly keeping the same notation. Finally set M to be $n+1 \times n+1$ transition matrix having first row v^+ and all the other rows v^-. It should be clear now that the question 'Does the Markov chain given with M have a non-trivial aggregation that glues states 1 and 2 together?' is equivalent to the question 'Does the set S have a non-empty subset whose sum is zero?'.

SSP to CG

Example

Let $S_1 = \{1, 2, -3, 4\}$ and $S_2 = \{2, -3, 5, -6\}$.

$$v_1 = (1/7, 2/7, -3/7, 4/7, -4/7), v_1^+ = (1/7, 2/7, 0, 4/7, 0),$$
$$v_1^- = (0, 0, 3/7, 0, 4/7), v_2 = (2/9, -3/9, 5/9, -6/9, 2/9),$$
$$v_2^+ = (2/9, 0, 5/9, 0, 2/9), v_2^- = (0, 3/9, 0, 6/9, 0),$$

$$M_1 = \begin{bmatrix} 1/7 & 2/7 & 0 & 4/7 & 0 \\ 0 & 0 & 3/7 & 0 & 4/7 \\ 0 & 0 & 3/7 & 0 & 4/7 \\ 0 & 0 & 3/7 & 0 & 4/7 \\ 0 & 0 & 3/7 & 0 & 4/7 \end{bmatrix}, M_2 = \begin{bmatrix} 2/9 & 0 & 5/9 & 0 & 2/9 \\ 0 & 3/9 & 0 & 6/9 & 0 \\ 0 & 3/9 & 0 & 6/9 & 0 \\ 0 & 3/9 & 0 & 6/9 & 0 \\ 0 & 3/9 & 0 & 6/9 & 0 \end{bmatrix}.$$

The first system has a valid aggregation $\{\{1, 2, 3\}, \{4, 5\}\}$ or equivalently a space spanned with the set $\{(1, -1, 0, 0, 0), (0, 1, -1, 0, 0), (0, 0, 0, 1, -1)\}$ is left invariant for M_1 and $1, 2, -3$ is a zero sum subset of S_1.
On the other hand, set S_2 does not have a non-empty, zero summing subset and in the first step of the proposed algorithm we get the 'merger' vector $v_2 = (1, -1, 0, 0, 0) \cdot M_2$ which means 'lump everything together'.

Previous reasoning can be extended to show that existence of any non trivial aggregation of Markov chain is a NP-complete problem. Namely, let S be the set for which we want to solve the SSP. Let v^+ and v^- be defined as before. Choose $n+1$ different numbers in the interval $(1/2, 1]$ and denote them with $\lambda_1, \dots \lambda_{n+1}$. Let M be a $n+1 \times n+1$ transition matrix having for the i^{th} row vector $\lambda_i v^+ + (1-\lambda_i)v^-$. It is now easy to see that any non trivial aggregation would give zero summing subset of S and conversely any such subset would imply that the partition $\{\hat{S}, \hat{S}^c\}$, where we denoted set of indices representing elements of zero summing subset S with $\hat{S}$, is a valid aggregation of the Markov chain given by M.

Theorem

The existence of a non-trivial aggregation coarse graining for a Markov chain is an NP-complete problem.

Unanswered questions

- Is there an universal separable compact space which coarse grains to any dynamical system?
- ...

The End!

Thank you!

References

[1] Jonathan E. Rowe, Michael D. Vose, and Alden H. Wright, *Differentiable coarse graining*, Theoret. Comput. Sci. **361** (2006), no. 1, 111–129. MR2254227 (2007h:68171)

[2] Michael D. Vose, *The simple genetic algorithm*, Complex Adaptive Systems, MIT Press, Cambridge, MA, 1999. Foundations and theory, A Bradford Book. MR1713436 (2000h:65024)