

Formal verification of complex systems: model-based and data-driven methods

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Automated formal verification: successes and frontiers

automated, sound, formal

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- automated, sound, formal
- industrial impact in verification of

protocols, hardware circuits, and software

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- industrial impact in verification of

protocols, hardware circuits, and software

- asserts properties over given model of a system
- scalable and useful on "unsophisticated" models

Automated formal verification: pushing the envelope

• verification of physical systems (cyber-physical systems)

- dynamical models with uncertainty, noise (for CPS)
- bridging the gap between data and models
- principled integration of learning and verification

Building automation systems: an exemplar of CPS

- cyber-physical systems: integration of physical/analogue with cyber/digital
- building automation systems as a CPS exemplar

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• smart energy initiatives at Oxford CS

Building automation systems - a CPS exemplar

Building automation system setup in rooms 478/9 at Oxford CS

- advanced modelling for smart buildings
- application: certifiable energy management
	- \bullet control of temperature, humidity, $CO₂$
	- ² model-based predictive maintenance of devices
	- **3** fault-tolerant control
	- ⁴ demand-response over smart grids

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- model $CO₂$ dynamics, under the effect of
	- \bullet occupants: room full $(F)/$ empty (E)
	- 2 window: open (O)/closed (C)
	- **3** air circulation: ON/OFF

$$
x_{k+1} = x_k + \frac{\Delta}{V} \left(-\mathbb{1}_{ON} m x_k + \mu_{\{O,C\}} (C_{out} - x_k) \right) + \mathbb{1}_F C_{occ}
$$

- $x z$ one $CO₂$ level
- \bullet Δ sampling time
- *V* zone volume
- *m* air inflow (when ON)
- **●** μ [○] air exchange with outside (when O)
- \bullet μ_C air leakage with outside (when C)
- \bullet C_{out} outside $CO₂$ level
- \bullet C_{occ} CO₂ by occupants (when F)

- model $CO₂$ dynamics, under the effect of
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$$
x_{k+1} = x_k + \frac{\Delta}{V} \left(-1_{ON} m x_k + \mu_{\{O,C\}} (C_{out} - x_k) \right) + 1_F C_{occ}
$$

þ

• model $CO₂$ dynamics, under the effect of

- occupants: room empty E
- 2 window: closed C
- air circulation: ON

- **Q** occupants: room full F
- 2 window: closed C
- **3** air circulation: ON

• model $CO₂$ dynamics, under the effect of

- **Q** occupants: room full F
- ² window: open O
- ³ air circulation: ON

$$
x_{k+1} = x_k + \frac{\Delta}{V} (-mx_k + \mu_O(C_{out} - x_k)) + C_{occ}
$$

0 12 0 12 0 12 0 12 0

• model $CO₂$ dynamics, under the effect of

- occupants: room empty E
- 2 window: closed C
- air circulation: ON

 (F,C) $(0,0)$

 (E,C) (E,Q)

 \bullet model CO₂ dynamics, under the effect of

 \bullet occupants: room full $(F)/$ empty (E)

- 2 window: open (O)/closed (C)
- air circulation: ON

model with *hybrid* dynamics

- model $CO₂$ dynamics, under the effect of
	- \bullet occupants: room full $(F)/$ empty (E)
	- 2 window: open (O)/closed (C)
	- ³ air circulation: OFF

model with *hybrid* dynamics

data-driven analysis

data-driven analysis model learning (with data), and model-based verification

disconnect between data-driven learning and model-based verification

disconnect between data-driven learning and model-based verification

principled integration of learning and verification

Overview of method

Parametric Markov chains

Parametric Markov chains

$$
\mathcal{G} = (\Theta, S, \mathbb{T}_{\theta}, \rightarrow, \mathbf{AP}, L)
$$

S – set of states **T**_θ – mapping $S \times S \rightarrow [0, 1]$ expressed in terms of $\theta \in \Theta$ Θ – set of all possible valuations of *θ*, vector of parameters \rightarrow – starting states

Parametric Markov chains

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\mathcal{G} = (\Theta, S, \mathbb{T}_{\theta}, \rightarrow, \mathsf{AP}, L)
$$

S – set of states

- **T**_{*θ*} mapping $S \times S \rightarrow [0, 1]$ expressed in terms of $\theta \in \Theta$
- Θ set of all possible valuations of *θ*, vector of parameters
- \rightarrow starting states
- L labelling function, mapping states into $2^{\rm AP}$, ${\rm AP}$ alphabet

• denote by $M(\theta) \in \mathcal{G}$ a model parameterised by $\theta \in \Theta$

• property *φ* specified in PCTL, e.g.

 $\phi = \mathbb{P}_{\geq 0.99}(\square^{\leq 20}$ safe), $\qquad \phi = \mathbb{P}_{>0.5}(\textsf{safe} \,\, \mathsf{U} \,\, \textsf{reach}), \qquad \textsf{safe}, \textsf{reach} \in \mathrm{AP}$

• probabilistic model checking PCTL properties over Markov chains

- input: Markov chain (*S*, **T**), PCTL formula *φ*
- \bullet output: $\mathsf{Sat}(\phi) = \{z \in S : z \models \phi\}$
- tools: PRISM, STORM, . . .

Parameter synthesis

property *φ* specified in PCTL, e.g.

$$
\phi = \mathbb{P}_{\geq 0.99}(\square^{\leq 20} \; \textsf{safe}), \qquad \phi = \mathbb{P}_{>0.5}(\textsf{safe } \textsf{U} \;\textsf{reach}), \qquad \textsf{safe}, \textsf{reach} \in \textsf{AP}
$$

- classify models in Θ according to property of interest ϕ , that is
- \bullet synthesise parameters *θ* ∈ Θ s.t. *M*(*θ*) satisfies *φ*:

Bayesian inference

$$
p(\theta_j | D) = \frac{\mathbb{P}(D | \theta_j) p(\theta_j)}{\mathbb{P}(D)}
$$

$$
= \frac{\prod_{s' \in S} \mathbb{T}_{\theta}(s_j, s')^{D_{s'_j}^{s'}} p(\theta_j)}{\mathbb{P}(D_{s_j})}
$$

- \bullet *D* overall data gathered (traces) D_{s_j} – traces crossing state s_j , where $\theta_j = \theta_{s_j}$
- $p(\theta_i)$ prior distribution
- $\prod_{s' \in S} \mathbb{T}_{\theta}(s_j, s')^{D_{s_j}^{s'}}$ likelihood, multinomial distribution at state s_j

Bayesian inference

$$
p(\theta_j | D) = \frac{\mathbb{P}(D | \theta_j) p(\theta_j)}{\mathbb{P}(D)}
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$$
= \frac{\prod_{s' \in S} \mathbb{T}_{\theta}(s_j, s')^{D_{s'_j}^{s'}} p(\theta_j)}{\mathbb{P}(D_{s_j})}
$$

- \bullet *D* overall data gathered (traces) D_{s_j} – traces crossing state s_j , where $\theta_j = \theta_{s_j}$
- select as conjugate prior the Dirichlet distribution

$$
p(\theta_j) = \text{Dir}(\theta_j \mid \alpha) \propto \theta_j^{\alpha_1 - 1} (1 - \theta_j)^{\alpha_2 - 1}
$$

for pair $(\theta_j, 1 - \theta_j)$, with $\alpha = (\alpha_1, \alpha_2)$ hyperparameters

Bayesian inference

$$
p(\theta_j \mid D) = \frac{\mathbb{P}(D \mid \theta_j) p(\theta_j)}{\mathbb{P}(D)}
$$

$$
= \frac{\prod_{s' \in S} \mathbb{T}_{\theta}(s_j, s')^{D_{s'_j}^{s'}} p(\theta_j)}{\mathbb{P}(D_{s_j})}
$$

\n- $$
D
$$
 – overall data gathered (traces)
\n- D_{s_j} – traces crossing state s_j , where $\theta_j = \theta_{s_j}$
\n

• under Dirichlet prior, posterior update is analytic

$$
p(\theta_j \mid D) \propto \theta_j^{D_{s_j}^{s_1'}} (1-\theta_j)^{D_{s_j}^{s_2'}} \theta_j^{\alpha_1-1} (1-\theta_j)^{\alpha_2-1}
$$

and obtained updating hyperparameters of Dirichlet distribution, as

$$
p(\theta_j|D) = \text{Dir}(\theta_j \mid D_{s_j} + \alpha)
$$

Confidence computation

Confidence computation

Confidence computation

compute confidence C on whether system S satisfies property *φ* as

$$
C = \mathbb{P}(S \models \phi \mid D) = \int_{\Theta_{\phi}} p(\theta \mid D) d\theta
$$

Case study: setup

pMC model:

• specification:
$$
\phi = \mathbb{P}_{>0.3}(\square^{\leq 20} \neg(E, O))
$$

Case study: setup

- goal: benchmark against statistical model checking (SMC)
- pMC model:

- specification: $\phi = \mathbb{P}_{>0.3}(\square^{\leq 20} \neg(E, O))$
- **•** for selected pMC and property, synthesis yields Θ_{ϕ} (yellow set)

Case study: experiments

data: state trajectories of different length

- attains confidence closer to "true" value than SMC
- extracts information from data more efficiently
- is more robust with limited data

Parametric Markov decision processes

$$
\mathcal{G} = (\Theta, S, A, \mathbb{T}_{\theta}, \rightarrow, \mathsf{AP}, L)
$$

 Θ , S , \rightarrow , L – as before *A* – set of actions **T**_{*θ*} – mapping $S \times A \times S \rightarrow [0, 1]$ expressed in terms of $\theta \in \Theta$

Dual role of actions in pMDP

actions can be employed to shape set Θ*^φ*

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Dual role of actions in pMDP actions can be employed to shape set Θ*^φ* 0 1 1 shape set Θ*^φ* • actions can be chosen to affect confidence level C 0 1

 $integral \rightarrow confidence$ level

reminiscent of exploration/exploitation tradeoff in RL

Overview of method

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Strategy synthesis for experiment design

design experiments to affect confidence calculation

 $\max \{ \mathbb{P}(S \models \phi \mid D), \mathbb{P}(S \not\models \phi \mid D) \}$

Strategy synthesis for experiment design

design experiments to affect confidence calculation

$$
\max\left\{\mathbb{P}(\mathsf{S}\models\phi\,|\,D),\mathbb{P}(\mathsf{S}\not\models\phi\,|\,D)\right\}
$$

expected confidence gain at state-action (*s*, *α*) (and corresp. parameter)

$$
e_{s,\alpha} = \int_{\Theta_{\phi}} \prod_{\theta_i \in \theta} p(\theta_i \mid \mathbb{E}_{s,\alpha}(D_i)) d\theta
$$

Strategy synthesis for experiment design

design experiments to affect confidence calculation

$$
\max\left\{\mathbb{P}(\mathsf{S}\models\phi\,|\,D),\mathbb{P}(\mathsf{S}\not\models\phi\,|\,D)\right\}
$$

e expected confidence gain at state-action (s, α) (and corresp. parameter)

$$
\mathcal{C}_{s,\alpha} = \int_{\Theta_{\phi}} \prod_{\theta_i \in \theta} p(\theta_i \mid \mathbb{E}_{s,\alpha}(D_i)) d\theta
$$

use C*s*,*^α* as a reward for (*s*, *α*)

• synthesise optimal strategy π for experiment design

Case study: setup

- goal: compare optimally synthesised policies vs. random/deterministic ones
- pMDP model:

• specification: $\phi = \mathbb{P}_{>0.3}(\square^{\leq 20} \neg(E, O))$

Case study: setup

- **e** goal: compare optimally synthesised policies vs. random/deterministic ones
- pMDP model:

- specification: $\phi = \mathbb{P}_{>0.3}(\square^{\leq 20} \neg(E, O))$
- **•** for selected pMDP and given ϕ , Θ_{ϕ} is shown in yellow

Case study: experiments

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Extensions to other model classes

- model $CO₂$ dynamics, under the effect of
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- \bullet C_{occ} $CO₂$ by occupants (when F)

Extensions to other model classes

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parametrised LTI model

 $u(t)$ – input

$$
y(t)
$$
 - system output

$$
\tilde{y}(t)
$$
 – measured output

e(*t*) − measurement noise, $e(t) \sim \mathcal{N}(0, \sigma_e^2)$

• model set $\mathcal{G} = \{M(\theta) \mid \theta \in \Theta\}$, where

$$
M(\theta): \begin{cases} x(t+1) = Ax(t) + Bu(t) \\ y(t) = \theta^T x(t) \end{cases}
$$

Applications of method

models for chemical reaction networks , with known stoichiometry, but with uncertain rates, expressed as pMDP

- CRN can be excited by external input, pCT-MDP
- ² limited data access (only to some states) to analyse known property
- **3** quantify confidence
- ⁴ synthesise optimal experiments
- **5** study actions tradeoff
- **•** if stoichiometry is not perfectly known, do network synthesis?

[red text: new theory needed]

- integration of learning and verification
- verification and policy synthesis for Cyber-Physical Systems (CPS)
- application in Building Automation Systems (BAS)

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Thank you for your attention

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