




pymdp: A Python library for active inference in discrete state spaces

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Statement of Need

Active inference is an account of cognition and behavior in complex systems which brings together action, perception, and learning under the theoretical mantle of Bayesian inference (Friston et al., 2009, 2012, 2015, 2017). Active inference has seen growing applications in academic research, especially in fields that seek to model human or animal behavior (Adams et al., 2021; Holmes et al., 2021; Parr et al., 2020). The majority of applications have focused on cognitive neuroscience, with a particular focus on modelling decision-making under uncertainty (Schwartenbeck et al., 2015; Smith et al., 2020; Smith, Kirlic, et al., 2021). Nonetheless, the framework has broad applicability and has recently been applied to diverse disciplines, ranging from computational models of psychopathology (Montague et al., 2012; Smith, Kirlic, et al., 2021), control theory (Baoumy et al., 2021; Baltieri & Buckley, 2019; Millidge et al., 2020) and reinforcement learning (Fountas et al., 2020; Millidge, 2020; Sajid et al., 2021; Tschantz, Baltieri, et al., 2020; Tschantz, Millidge, et al., 2020), through to social cognition (Adams et al., 2021; Tison & Poirier, 2021; Wirkuttis & Tani, 2021) and even real-world engineering problems (Fox, 2021; Martínez et al., 2021; Moreno, 2021). While in recent years, some of the code arising from the active inference literature has been written in open source languages like Python and Julia (Çatal et al., 2020; T. W. van de Laar & Vries, 2019; Millidge, 2020; Tschantz, Seth, et al., 2020; Ueltzhöffer, 2018), to-date, the most popular software for simulating active inference agents is the DEM toolbox of SPM (Friston et al., 2008; Smith, Friston, et al., 2021), a MATLAB library originally developed for the statistical analysis and modelling of neuroimaging data (Penny et al., 2007). DEM contains a reliable, reproducible set of functions for studying active inference, but the use of the toolbox can be restrictive for researchers in settings where purchasing a MATLAB license is financially costly. And although active inference researchers have relied heavily on DEM for simulating and fitting models of behavior, most of its functionality is restricted to single MATLAB scripts or functions, particularly one called `spm_MDP_VB_X.m`, that lack modularity and often must be customized for applications on a domain-specific basis. Increasing interest in active inference, manifested both in terms of sheer number of cited research papers as well as diversifying applications across disciplines, has thus created a need for generic, widely-available, and user-friendly code for simulating active inference in open-source scientific computing languages like Python. The software we present here, `pymdp`, represents a significant step in this direction: namely, we provide the first open-source package for simulating active inference with discrete state-space generative

models. The name pymdp derives from the fact that the package is written in the **Python** programming language and concerns discrete, Markovian generative models of decision-making, which take the form of Markov Decision Processes or **MDPs**.

pymdp is a Python package that is directly inspired by the active inference routines contained in DEM. However, pymdp has a modular, flexible structure that allows researchers to build and simulate active inference agents quickly and with a high degree of customization. We developed pymdp in the hopes that it will increase the accessibility and exposure of the active inference framework to researchers, engineers, and developers with diverse disciplinary backgrounds. In the spirit of open-source software, we also hope that it spurs new innovation, development, and collaboration in the growing active inference and wider Bayesian modelling communities.

Summary

pymdp offers a suite of robust, tested, and modular routines for simulating active inference agents equipped with *partially-observable Markov Decision Process* (POMDP) generative models. Mathematically, a POMDP comprises a joint distribution over observations o , hidden states s , control states u and hyperparameters ϕ : $P(o, s, u, \phi)$. This joint distribution further factorizes into a set of categorical and Dirichlet distributions: the likelihoods and priors of the generative model. With pymdp, one can build a generative model using a set of prior and likelihood distributions, initialize an agent, and then link it to an external environment to run active inference processes – all in a few lines of code. The Agent and Env (environment) APIs of pymdp are built according to the standardized framework of OpenAIGym commonly used in reinforcement learning, where an agent and environment object recursively exchange observations and actions over time (Brockman et al., 2016).

Introduction

Simulations of active inference are commonly performed in discrete time and space (Da Costa et al., 2020; Friston et al., 2015). This is partially motivated by the mathematical tractability of performing inference with discrete probability distributions, but also by the intuition of modelling choice behavior as a sequence of discrete, mutually-exclusive choices, in e.g. psychophysics or decision-making experiments. The most popular generative models – used to realize active inference in this context – are partially-observable Markov Decision Processes or *POMDPs* (Kaelbling et al., 1998). POMDPs are state-space models that model the environment in terms of hidden states that stochastically change over time, as a function of both the current state of the environment as well as the behavioral output of an agent (control states or actions). Crucially, the environment is *partially-observable*, i.e. the hidden states are not directly observed by the agent, but can only be inferred through observations that relate to hidden states in a probabilistic manner, such that observations are modelled as being generated stochastically from the current hidden state. This necessitates both “perceptual” inference of hidden states as well as control.

As such, in most POMDP problems, an agent is tasked with inferring the hidden state of its environment and then choosing a sequence of control states or actions to change hidden states in a way that leads to desired outcomes (maximizing reward, or occupancy within some preferred set of states).

Usage

In order to enhance the user-friendliness of pymdp without sacrificing flexibility, we have built the library to be highly modular and customizable, such that agents in pymdp can be specified at a variety of levels of abstraction with desired parameterisations. The methods of the Agent class can thus be called in any particular order, depending on the application, and furthermore

92 they can be specified with various keyword arguments that entail choices of implementation
93 details at lower levels.

94 By retaining a modular structure throughout the package's dependency hierarchy, pymdp
95 also affords the ability to flexibly compose different low level functions. This allows users to
96 customize and integrate their active inference loops with desired inference algorithms and policy
97 selection routines. For instance, one could sub-class the Agent class and write a customized
98 `step()` function, that combines whichever components of active inference one is interested in.

99 Related software packages

100 The DEM toolbox within SPM in MATLAB is the current gold-standard in active inference
101 modelling. In particular, simulating an active inference process in DEM consists of defining
102 the generative model in terms of a fixed set of matrices and vectors, and then calling the
103 `spm_MDP_VB_X.m` function to simulate a sequence of trials. pymdp, by contrast, provides a
104 user-friendly and modular development experience, with core functionality split up into different
105 libraries that separately perform the computations of active inference in a standalone fashion.
106 Moreover, pymdp provides the user the ability to write an active inference process at different
107 levels of abstraction depending on the user's level of expertise or skill with the package –
108 ranging from the high level Agent functionality, which allows the user to define and simulate
109 an active inference agent in just a few lines of code, all the way to specifying a particular
110 variational inference algorithm (e.g. marginal-message passing (Parr et al., 2019)) for the
111 agent to use during state estimation. In the DEM toolbox of SPM, this would require setting
112 undocumented flags or else manually editing the routines in `spm_MDP_VB_X.m` to enable or
113 disable bespoke functionality. There has been one recent attempt at creating a comprehensive
114 user-guide for building active inference agents in DEM (Smith, Friston, et al., 2021), though to
115 our knowledge there has not been a package devoted to the open source development of these
116 powerful software tools.

117 A recent related, but largely non-overlapping project is ForneyLab, which provides a set of Julia
118 libraries for performing approximate Bayesian inference via message passing on Forney Factor
119 Graphs (T. van de Laar et al., 2018). Notably, this package has also seen several applications
120 in simulating active inference processes, using ForneyLab as the backend for the inference
121 algorithms employed by an active inference agent (Ergul et al., 2020; T. van de Laar et al.,
122 2021; T. W. van de Laar & Vries, 2019; Vanderbroeck et al., 2019). While ForneyLab focuses
123 on including a rigorous set of message passing routines that can be used to simulate active
124 inference agents, pymdp is specifically designed to help users quickly build agents (regardless of
125 their underlying inference routines) and plug them into arbitrary environments to run active
126 inference in a few easy steps.

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References

- Adams, R. A., Vincent, P., Benrimoh, D., Friston, K. J., & Parr, T. (2021). Everything is connected: Inference and attractors in delusions. *Schizophrenia Research*.
- Baoumy, M., Pezzato, C., Corbato, C. H., Hawes, N., & Ferrari, R. (2021). Towards stochastic fault-tolerant control using precision learning and active inference. *arXiv*. <https://arxiv.org/abs/2109.05870>
- Baltieri, M., & Buckley, C. L. (2019). PID control as a process of active inference with linear generative models. *Entropy*, 21(3), 257. <https://doi.org/10.3390/e21030257>
- Brockman, G., Cheung, V., Pettersson, L., Schneider, J., Schulman, J., Tang, J., & Zaremba, W. (2016). OpenAI gym. *arXiv*. <https://arxiv.org/abs/1606.01540>
- Çatal, O., Verbelen, T., Nauta, J., De Boom, C., & Dhoedt, B. (2020). Learning perception and planning with deep active inference. *IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, 3952–3956. <https://doi.org/10.1109/ICASSP40776.2020.9054364>
- Da Costa, L., Parr, T., Sajid, N., Veselic, S., Neacsu, V., & Friston, K. J. (2020). Active inference on discrete state-spaces: A synthesis. *Journal of Mathematical Psychology*, 99, 102447. <https://doi.org/10.1016/j.jmp.2020.102447>
- Ergul, B., Laar, T. van de, Koudahl, M., Roa-Villescas, M., & Vries, B. de. (2020). Learning where to park. *International Workshop on Active Inference*, 125–132.
- Fountas, Z., Sajid, N., Mediano, P. A. M., & Friston, K. J. (2020). Deep active inference agents using monte-carlo methods. *Advances in Neural Information Processing Systems*. <https://proceedings.neurips.cc/paper/2020/hash/865dfbde8a344b44095495f3591f7407-Abstract.html>
- Fox, S. (2021). Active inference: Applicability to different types of social organization explained through reference to industrial engineering and quality management. *Entropy*, 23(2), 198. <https://doi.org/10.3390/e23020198>
- Friston, K. J., Daunizeau, J., & Kiebel, S. J. (2009). Reinforcement learning or active inference? *PLoS ONE*, 4(7), e6421. <https://doi.org/10.1371/journal.pone.0006421>
- Friston, K. J., FitzGerald, T., Rigoli, F., Schwartenbeck, P., & Pezzulo, G. (2017). Active inference: A process theory. *Neural Computation*, 29(1), 1–49. https://doi.org/10.1162/NECO_a_00912
- Friston, K. J., Rigoli, F., Ognibene, D., Mathys, C., Fitzgerald, T., & Pezzulo, G. (2015). Active inference and epistemic value. *Cognitive Neuroscience*, 6(4), 187–214. <https://doi.org/10.1080/17588928.2015.1020053>
- Friston, K. J., Samothrakis, S., & Montague, R. (2012). Active inference and agency: Optimal control without cost functions. *Biological Cybernetics*, 106(8–9), 523–541. <https://doi.org/10.1007/s00422-012-0512-8>

- 181 Friston, K. J., Trujillo-Barreto, N., & Daunizeau, J. (2008). DEM: A variational treatment of
182 dynamic systems. *NeuroImage*, 41(3), 849–885. [https://doi.org/10.1016/j.neuroimage.](https://doi.org/10.1016/j.neuroimage.2008.02.054)
183 [2008.02.054](https://doi.org/10.1016/j.neuroimage.2008.02.054)
- 184 Holmes, E., Parr, T., Griffiths, T. D., & Friston, K. J. (2021). Active inference, selective
185 attention, and the cocktail party problem. *Neuroscience & Biobehavioral Reviews*, 131,
186 1288–1304.
- 187 Kaelbling, L. P., Littman, M. L., & Cassandra, A. R. (1998). Planning and acting in
188 partially observable stochastic domains. *Artificial Intelligence*, 101(1-2), 99–134. [https://doi.org/10.1016/S0004-3702\(98\)00023-X](https://doi.org/10.1016/S0004-3702(98)00023-X)
189 [https://doi.org/10.1016/S0004-3702\(98\)00023-X](https://doi.org/10.1016/S0004-3702(98)00023-X)
- 190 Laar, T. van de, Cox, M., Senoz, I., Bocharov, I., & Vries, B. de. (2018). ForneyLab: A toolbox
191 for biologically plausible free energy minimization in dynamic neural models. *Conference*
192 *on Complex Systems*. [https://biaslab.github.io/pdf/forneylab/van_de_laar_forneylab_](https://biaslab.github.io/pdf/forneylab/van_de_laar_forneylab_biologically_plausible_free_energy_minimization.pdf)
193 [biologically_plausible_free_energy_minimization.pdf](https://biaslab.github.io/pdf/forneylab/van_de_laar_forneylab_biologically_plausible_free_energy_minimization.pdf)
- 194 Laar, T. van de, Senoz, I., Özçelikkale, A., & Wymeersch, H. (2021). Chance-constrained
195 active inference. *arXiv Preprint arXiv:2102.08792*.
- 196 Laar, T. W. van de, & Vries, B. de. (2019). Simulating active inference processes by message
197 passing. *Frontiers in Robotics and AI*, 6, 20. <https://doi.org/10.3389/frobt.2019.00020>
- 198 Martínez, E. C., Kim, J. W., Barz, T., & Bournazou, M. N. C. (2021). Probabilistic modeling
199 for optimization of bioreactors using reinforcement learning with active inference. *Computer*
200 *Aided Chemical Engineering*, 50, 419–424. [https://doi.org/10.1016/B978-0-323-88506-5.](https://doi.org/10.1016/B978-0-323-88506-5.50066-8)
201 [50066-8](https://doi.org/10.1016/B978-0-323-88506-5.50066-8)
- 202 Millidge, B. (2020). Deep active inference as variational policy gradients. *Journal of Mathe-*
203 *matical Psychology*, 96, 102348. <https://doi.org/10.1016/j.jmp.2020.102348>
- 204 Millidge, B., Tschantz, A., Seth, A. K., & Buckley, C. L. (2020). On the relationship between
205 active inference and control as inference. *International Workshop on Active Inference*, 3–11.
206 https://doi.org/10.1007/978-3-030-64919-7_1
- 207 Montague, P. R., Dolan, R. J., Friston, K. J., & Dayan, P. (2012). Computational psychiatry.
208 *Trends in Cognitive Sciences*, 16(1), 72–80. <https://doi.org/10.1016/j.tics.2011.11.018>
- 209 Moreno, A. R. (2021). *PID control as a process of active inference applied to a refrigera-*
210 *tion system*. [https://projekter.aau.dk/projekter/files/415131289/1034_PID_Control_as_](https://projekter.aau.dk/projekter/files/415131289/1034_PID_Control_as_Active_Inference.pdf)
211 [Active_Inference.pdf](https://projekter.aau.dk/projekter/files/415131289/1034_PID_Control_as_Active_Inference.pdf)
- 212 Parr, T., Markovic, D., Kiebel, S. J., & Friston, K. J. (2019). Neuronal message passing
213 using mean-field, bethe, and marginal approximations. *Scientific Reports*, 9(1), 1–18.
214 <https://doi.org/10.1038/s41598-018-38246-3>
- 215 Parr, T., Rikhye, R. V., Halassa, M. M., & Friston, K. J. (2020). Prefrontal computation as
216 active inference. *Cerebral Cortex*, 30(2), 682–695.
- 217 Penny, W. D., Friston, K. J., Ashburner, J. T., Kiebel, S. J., & Nichols, T. E. (2007). *Statistical*
218 *parametric mapping: The analysis of functional brain images*. [https://doi.org/10.1016/](https://doi.org/10.1016/B978-0-12-372560-8.X5000-1)
219 [B978-0-12-372560-8.X5000-1](https://doi.org/10.1016/B978-0-12-372560-8.X5000-1)
- 220 Sajid, N., Ball, P. J., Parr, T., & Friston, K. J. (2021). Active inference: Demystified and
221 compared. *Neural Computation*, 33(3), 674–712. https://doi.org/10.1162/neco_a_01357
- 222 Schwartenbeck, P., FitzGerald, T., Mathys, C., Dolan, R., & Friston, K. J. (2015). The
223 dopaminergic midbrain encodes the expected certainty about desired outcomes. *Cerebral*
224 *Cortex*, 25(10), 3434–3445. <https://doi.org/10.1093/cercor/bhu159>
- 225 Smith, R., Friston, K. J., & Whyte, C. (2021). A step-by-step tutorial on active inference and
226 its application to empirical data. *PsyArXiv*. <https://doi.org/10.31234/osf.io/b4jmf>

- 227 Smith, R., Kirlic, N., Stewart, J. L., Touthang, J., Kuplicki, R., Khalsa, S. S., Feinstein,
228 J., Paulus, M. P., & Aupperle, R. L. (2021). Greater decision uncertainty characterizes
229 a transdiagnostic patient sample during approach-avoidance conflict: A computational
230 modelling approach. *Journal of Psychiatry & Neuroscience*, 46(1), E74. [https://doi.org/](https://doi.org/10.1503/jpn.200032)
231 [10.1503/jpn.200032](https://doi.org/10.1503/jpn.200032)
- 232 Smith, R., Schwartenbeck, P., Stewart, J. L., Kuplicki, R., Ekhtiari, H., Paulus, M. P., &
233 Tulsa 1000 Investigators. (2020). Imprecise action selection in substance use disorder:
234 Evidence for active learning impairments when solving the explore-exploit dilemma. *Drug*
235 *and Alcohol Dependence*, 215, 108208. <https://doi.org/10.1016/j.drugalcdep.2020.108208>
- 236 Tison, R., & Poirier, P. (2021). Communication as socially extended active inference: An
237 ecological approach to communicative behavior. *Ecological Psychology*, 33, 197–235.
238 <https://doi.org/10.1080/10407413.2021.1965480>
- 239 Tschantz, A., Baltieri, M., Seth, A. K., & Buckley, C. L. (2020). Scaling active inference.
240 *2020 International Joint Conference on Neural Networks (IJCNN)*, 1–8. [https://doi.org/](https://doi.org/10.1109/IJCNN48605.2020.9207382)
241 [10.1109/IJCNN48605.2020.9207382](https://doi.org/10.1109/IJCNN48605.2020.9207382)
- 242 Tschantz, A., Millidge, B., Seth, A. K., & Buckley, C. L. (2020). Reinforcement learning through
243 active inference. *Bridging AI and Cognitive Science at the International Conference on*
244 *Learning Representations*. https://baicsworkshop.github.io/pdf/BAICS_37.pdf
- 245 Tschantz, A., Seth, A. K., & Buckley, C. L. (2020). Learning action-oriented models through
246 active inference. *PLoS Computational Biology*, 16(4), e1007805. [https://doi.org/10.1371/](https://doi.org/10.1371/journal.pcbi.1007805)
247 [journal.pcbi.1007805](https://doi.org/10.1371/journal.pcbi.1007805)
- 248 Ueltzhöffer, K. (2018). Deep active inference. *Biological Cybernetics*, 112(6), 547–573.
249 <https://doi.org/10.1007/s00422-018-0785-7>
- 250 Vanderbroeck, M., Baioumy, M., Lans, D. van der, Rooij, R. de, & Werf, T. van der. (2019).
251 Active inference for robot control: A factor graph approach. *Student Undergraduate*
252 *Research E-Journal*!, 5, 1–5.
- 253 Wirkuttis, N., & Tani, J. (2021). Leading or following? Dyadic robot imitative interaction using
254 the active inference framework. *IEEE Robotics and Automation Letters*, 6(3), 6024–6031.
255 <https://doi.org/10.1109/LRA.2021.3090015>