

22.09.2025 | Yavar Taheri Yeganeh

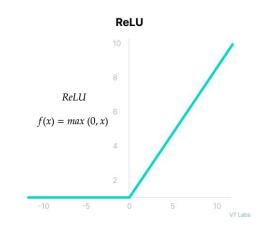
Neuroscience in Machine Learning and Al

Arterial Neural Networks

Modern Machine Learning Universal Function Approximators

Inspired by Biological Neural Networks

ReLU Activation Function



Deep Learning

Inspired by neural firings in the brain "Neurons either fire or do not fire (binary activation)"

Convolutional Neural Networks

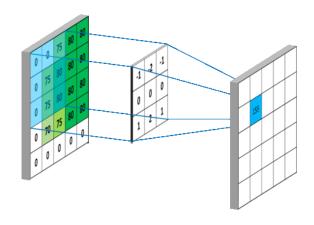
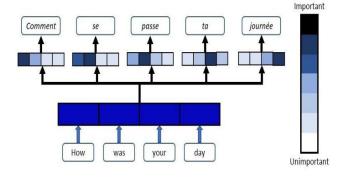


Image Processing Computer Vision

Inspired by the visual processing in the brain (the hierarchical structure of the visual cortex)

Attention Mechanism



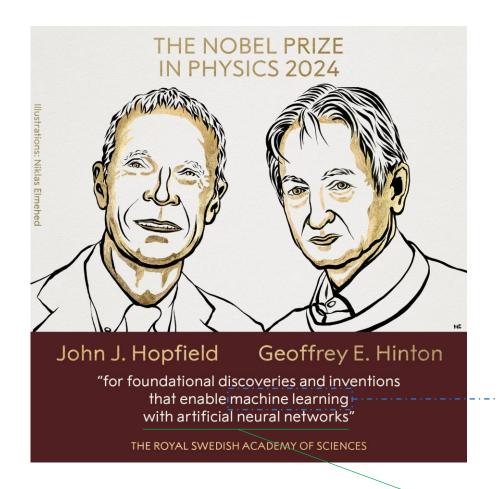
Transformers LLMs (e..g, ChatGPT)

Connections to modulations of neural activities in the brain (selectively focus on specific stimuli)





Neuroscience in Machine Learning and Al



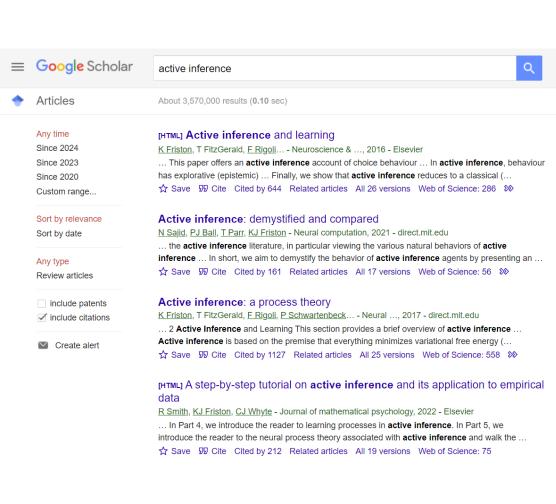


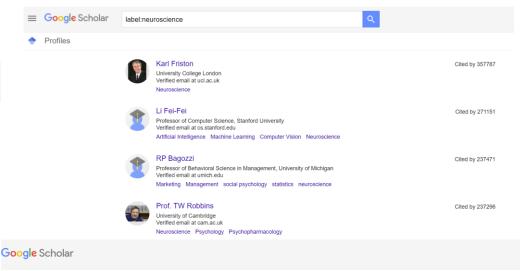
Notably impacted by concepts from Neuroscience (and with Mathematics and Physics)





Neuroscience: Active Inference Trend







Karl Friston

Q



Associative Learning and Active Inference

P Anokhin, A Sorokin, M Burtsev, K Friston Neural Computation, 1-34

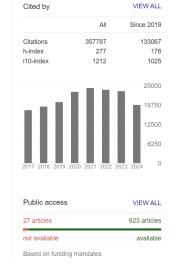
Karl Friston

<u>University College London</u>

Verified email at ucl.ac.uk - <u>Homepage</u>

Neuroscience

TITLE	CITED BY	YEAR
On the Minimal Theory of Consciousness Implicit in Active Inference CJ Whyte, AW Corcoran, J Robinson, R Smith, RJ Moran, T Parr, arXiv preprint arXiv:2410.06633		2024
A cortical field theory–dynamics and symmetries GK Cooray, V Cooray, K Friston Journal of Computational Neuroscience, 1-18		2024
A Mathematical Perspective on Neurophenomenology L Da Costa, L Sandved-Smith, K Friston, MJD Ramstead, AK Seth arXiv preprint arXiv:2409.20318		2024
Possible principles for aligned structure learning agents L Da Costa, T Gavenčiak, D Hyland, M Samiel, C Dragos-Manta, arXiv preprint arXiv:2410.00258		2024
The Inherent Normativity of Concepts WY So, KJ Friston, V Neacsu Minds and Machines 34 (4), 40		2024
A theory of generalised coordinates for stochastic differential equations L Da Costa, N Da Costa, C Heins, J Medrano, GA Pavliotis, T Parr, arXiv preprint arXiv:2409.15532		2024







Active Inference: Concept

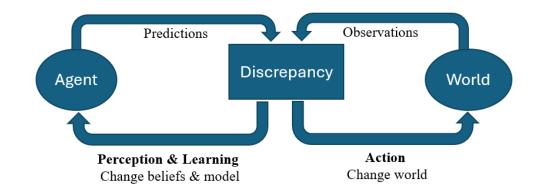
Theory of Biological Brains

Based on Predictive Coding: Both are grounded on Generative Model and Predictions

Perception and Learning are driven by Prediction Errors.

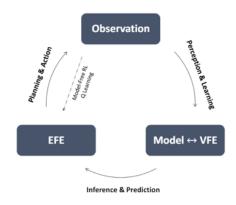
Observations are influenced by actions: **Observation** (action)

Predictive Coding → Active Inference



Free Energy Principle: Minimizing surprise $(-\ln p(observation|model)$ or Free Energy) Active Inference unifies perception, learning, and action:

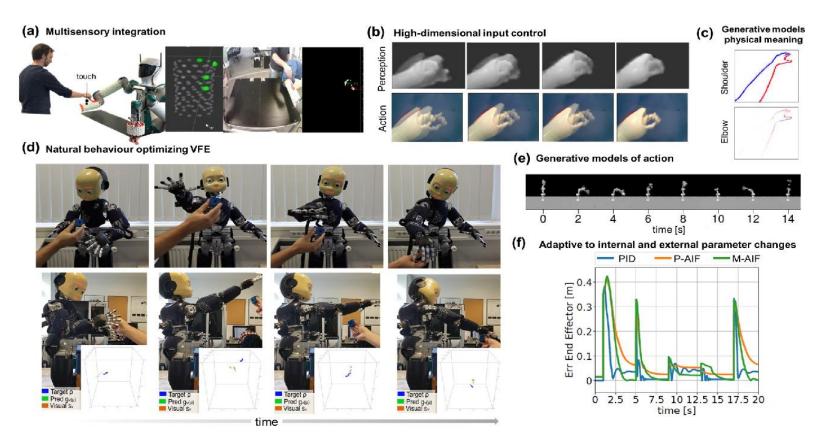
- Variational Free Energy: Perception & Learning Model
- Expected Free Energy: Action







Active Inference: Robotics



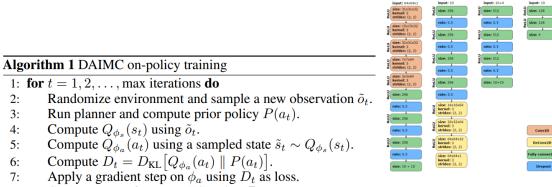
Navigation of Autonomous Vehicles [3]

Robot Control [2]



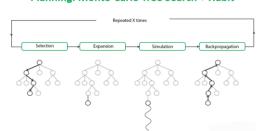


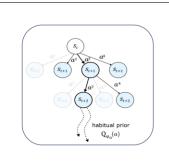
Active Inference: Against Model-Free (DAIMC [4])

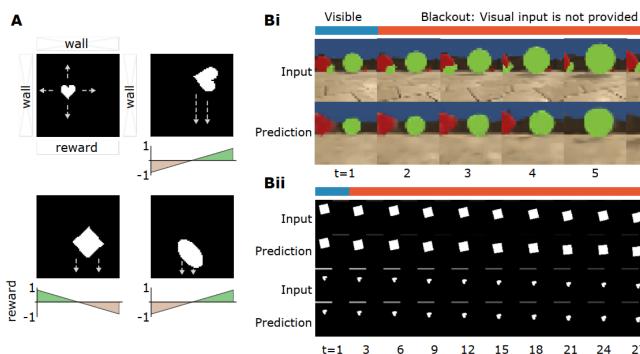


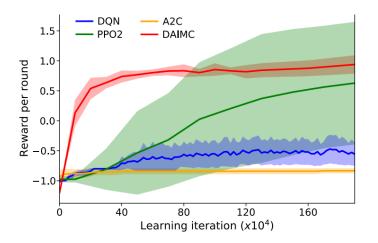
- Compute ω_{t+1} from Eq. (10) using D_t .
- Apply action $\tilde{a}_t \sim P(a_t)$ to the environment and sample a new observation \tilde{o}_{t+1} .
- Compute μ, σ from $P_{\theta_s}(s_{t+1}|\tilde{s_t}, \tilde{a_t})$.
- Compute $Q_{\phi_s}(s_{t+1})$ using \tilde{o}_{t+1} . 11:
- Apply a gradient step on θ_s using $D_{\text{KL}}[Q_{\phi_s}(s_{t+1}) \parallel \mathcal{N}(\mu, \sigma^2/\omega_t)]$.
- Apply a gradient step on ϕ_s , θ_o using $-\mathbb{E}_{Q(s_{t+1})}\left[\log P_{\theta_o}(o_{t+1}|s_{t+1})\right]$ + $D_{\mathrm{KL}}[Q_{\phi_s}(s_{t+1}) \parallel \mathcal{N}(\tilde{\mu}, \tilde{\sigma}^2/\omega_t)].$ 14: **end for**

Planning: Monte-Carlo Tree Search + Habit









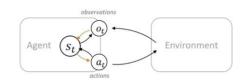


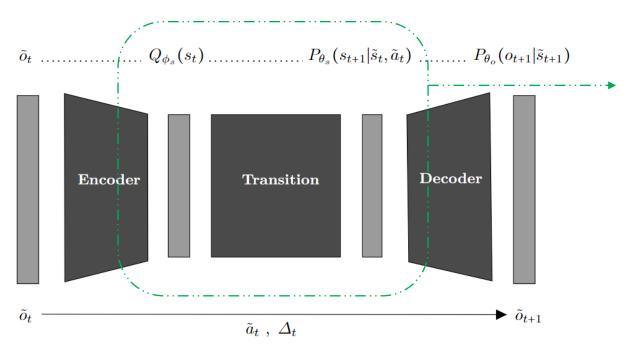


Active Inference: Core

The core of the formalism is the Generative Model.

Realization of this formalism is through Deep Learning: Generative Modeling and Inferences





space of the model

State (i.e., representation)

Variational Auto Encoder





06/10/2025

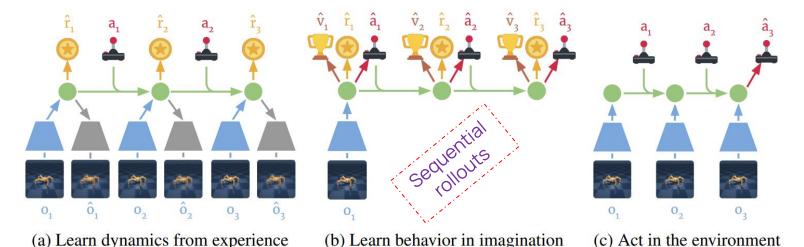
World-Modelling and Model-Based RL

Model-Based RL

- Use a model for making decisions
- Engaging methods for policy improvement and planning

World Models

- Build an internal predictive/generative model of the world (often task agnostic)
- Focuses on modelling and representations, either latent or ambient
- Learning policy (or planning) in model imaginations (roll outs)



General agents contain world models

Jonathan Richens 1 David Abel 1 Alexis Bellot 1 Tom Everitt 1

Abstract

Are world models a necessary ingredient for flexible, goal-directed behaviour, or is model-free learning sufficient? We provide a formal answer to this question, showing that any agent capable of generalizing to multi-step goal-directed tasks must have learned a predictive model of its environment. We show that this model can be extracted from the agent's policy, and that increasing the agents performance or the complexity of the goals it can achieve requires learning increasingly accurate world models. This has a number of consequences: from developing safe and general agents, to bounding agent capabilities in complex environments, and providing new algorithms for learning an agent's world model.

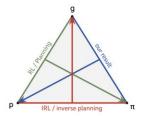


Figure 1: Our result complements previous insights from planning and inverse RL. While planning uses a world model and a goal to determine a policy, and IRL and inverse planning use an agent's policy and a world model to identify its goal, our result uses an agent's policy and its goal to identify a world model

RSSM Sequence model: $h_t = f_{\phi}(h_{t-1}, z_{t-1}, a_{t-1})$ $z_t \sim q_{\phi}(z_t \mid h_t, x_t)$

Dynamics predictor: $\hat{z}_t \sim p_{\phi}(\hat{z}_t \mid h_t)$

Reward predictor: $\hat{r}_t \sim p_\phi(\hat{r}_t \mid h_t, z_t)$

Continue predictor: $\hat{c}_t \sim p_{\phi}(\hat{c}_t \mid h_t, z_t)$ Decoder: $\hat{x}_t \sim p_{\phi}(\hat{x}_t \mid h_t, z_t)$

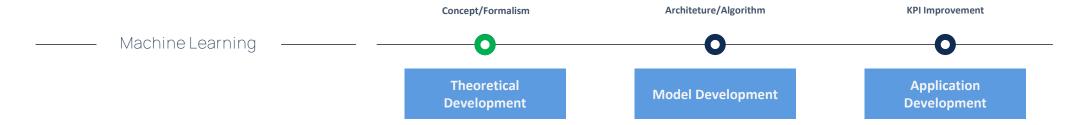
Dreamer learns policy with Actor-Critic

in model imaginations [5]





Motivation



Promises of Deep Learning: Generative Models:

- Bayesian and Probabilistic
- Representation Learning for both latent and ambient spaces
- Utilizes the observatory (cheap and raw) data

Promises of Active Inference (AIF):

- Bayesian Framework: Integrates perception, learning, and action
- Model-Driven
- Adaptability
- Intrinsic Objectives: Exploration to resolve uncertainty
- End-to-End Action: Doesn't require high-quality reward signals

Promises of Word-Model RL Agents:

- Planning via imagination
- Generalization & Sample-efficient
- Reduced reliance on rewards

Problem:

AlF agents struggle in delayed and long-horizon environments due to reliance on:

- Immediate predictions.
- Exhaustive planning.

Train a Policy within the Generative World-Model via Active Inference Conencting: DL, AIF, RL





Overshooting Trick: Integrating Policy

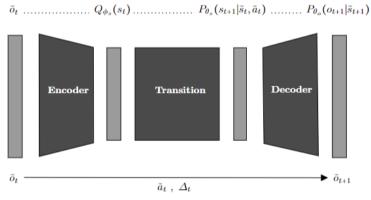


Figure 3: The agent's architecture and generative framework resemble that of a VAE. The line on top represents the agent simulating the future and making a prediction, while on the bottom, the agent receives a new observation after Δ_t of taking an action, \tilde{a}_t .

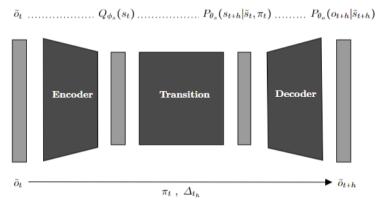
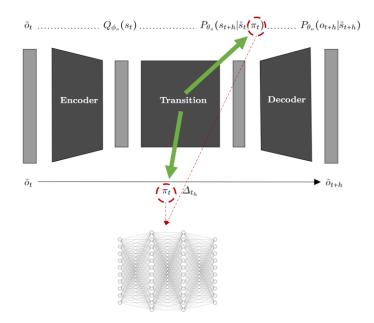


Figure 4: The agent's architecture and generative framework with an an impact/update/planning horizon, h (e.g., 100).



Selecting an impact/update/planning horizon: h (e.g., 300)





Formalism: Deep Active Inference (DAIF)

Model Learning (Calibration): Variational Free Energy

$$\theta^* = \arg\min_{\theta} \left(\mathbb{E}_{Q_{\phi}(s_t, a_t)} \left[\log Q_{\phi}(s_t, a_t) - \log P_{\theta}(o_t, s_t, a_t) \right] \right)$$

Decision (Planning & Action): Expected Free Energy

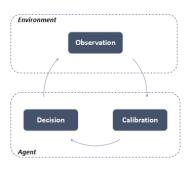
$$G(\pi,\tau) = \underbrace{-\mathbb{E}_{Q(\theta|\pi)Q(s_{\tau}|\theta,\pi)Q(o_{\tau}|s_{\tau},\theta,\pi)} \left[\log P(o_{\tau}|\pi)\right]}_{+\mathbb{E}_{Q(\theta|\pi)} \left[\mathbb{E}_{Q(o_{\tau}|\theta,\pi)} H(s_{\tau}|o_{\tau},\pi) - H(s_{\tau}|\pi)\right]} \underbrace{1}_{+\mathbb{E}_{Q(\theta|\pi)Q(s_{\tau}|\theta,\pi)} H(o_{\tau}|s_{\tau},\theta,\pi) - \mathbb{E}_{Q(s_{\tau}|\pi)} H(o_{\tau}|s_{\tau},\pi)\right]}_{+\mathbb{E}_{Q(\theta|\pi)Q(s_{\tau}|\theta,\pi)} H(o_{\tau}|s_{\tau},\theta,\pi) - \mathbb{E}_{Q(s_{\tau}|\pi)} H(o_{\tau}|s_{\tau},\pi)\right]} \underbrace{3}$$

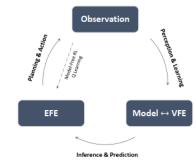
1) Extrinsic Value 2) State Epistemic Uncertainty 3) Parameter Epistemic Uncertainty

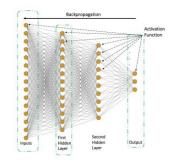
Policy Optimization via Gradients

- 1. Integrate the encoded policy parameters $\hat{\pi}(\phi_a)$ in the model and EFE: $G_{ heta}(ilde{o},\phi_a)$
- 2. Take the gradient of EFE w.r.t parameters: $\phi_a \leftarrow \phi_a \alpha \nabla_{\phi_a} \mathbb{E} [G(\phi_a)]$







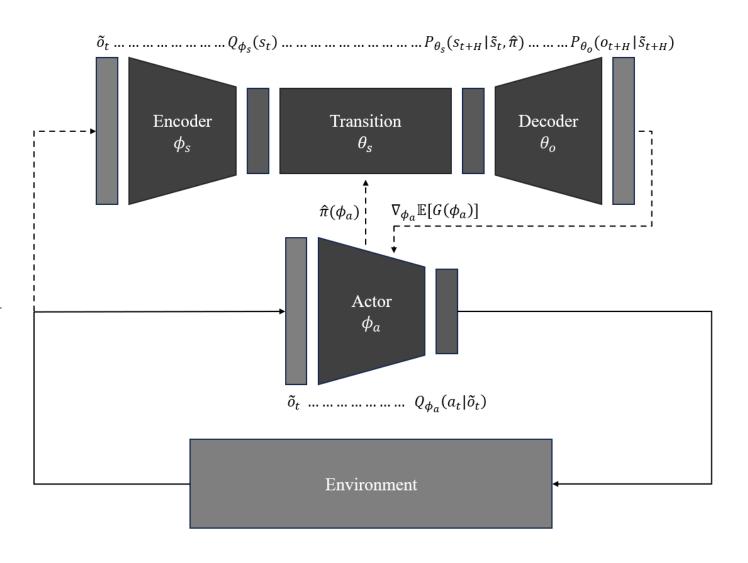






DAIF: Architecture

- Actor directly interact with the environment.
- Actor parameters are encoded and integrated into transition.
- Model predicts H steps into future in a single rollout.
- Gradient of policy parameters are taken via EFE of the prediction of the H steps into future.







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DAIF: Algorithm

- Actor directly interact with the environment.
- Actor parameters are encoded and integrated into transition.
- Model predicts H steps into future in a single rollout.
- Gradient of policy parameters are taken via EFE of the prediction of the H steps into future.

```
Algorithm 1 Deep AIF Agent Training (per epoch)
 1: Initialize \theta = \{\theta_s, \theta_o\}, \ \phi = \{\phi_s, \phi_a\}, \ \mathcal{M}
                                                                                                                Agent components:
                                                                                                                    Model:
  2: Randomly initialize E
  3: for n = 1, 2, ..., N do
                                                                                                                        Encoder Q_{\phi_a}.
                                                                                                                        Transition P_{\theta_n}.

    ▷ Environment Interaction

             \hat{\pi}_t \leftarrow \Pi(\mathcal{Q}_{\phi_a})
  4:
                                                                                                                         Decoder P_{\theta_-}.
  5:
             for \tau = t + 1, t + 2, ..., t + H do
                                                                                                                    Actor Q_{\phi_a}.
  6:
                     Sample a new observation \tilde{o}_{\tau} from E
                                                                                                                     Actor mapping \Pi.
                     Apply \tilde{a}_{\tau} \sim Q_{\phi_{\alpha}}(a_{\tau}|\tilde{o}_{\tau}) to E
                                                                                                                    Preference mapping \Psi.
  7:
                     Sample a new observation \tilde{o}_{\tau+1} from E
  8:
                                                                                                                Other components:
             \mathcal{M} \leftarrow \mathcal{M} \cup \{(\tilde{o}_t, \hat{\pi}_t, \tilde{o}_{t+H})\}
                                                                                                                     Environment E.
              ▶ MODEL LEARNING
                                                                                                                    Experience Memory \mathcal{M}.
              \{(\tilde{o}_{t'}, \hat{\pi}_{t'}, \tilde{o}_{t'+H})\}^{B_1} \sim \mathcal{M}
10:
             for t' = 1, 2, ..., B_1 do
11:
                                                                                                                Hyperparameters:
                    run Model(\tilde{o}_{t'}, \hat{\pi}_{t'}, \tilde{o}_{t'+H})
12:
                                                                                                                    Iterations N.
                     \mathcal{L}_s \leftarrow \mathcal{L}_s + D_{\text{KL}} \left[ Q_{\phi_s}(s_{t'+H}) || \mathcal{N}(\mu, \sigma^2) \right]
13:
                                                                                                                     Beta \beta.
                    \mathcal{L}_o \leftarrow \mathcal{L}_o - \mathbb{E}_{Q(s_{t'\perp H})} \left[ \log P_{\theta_o}(o_{t'+H} | \tilde{s}_{t'+H}) \right]
14:
                                                                                                                     Horizon H.
                    \mathcal{L}_o \leftarrow \mathcal{L}_o + \beta * D_{KL} \left[ Q_{\phi_s}(s_{t'+H}) || \mathcal{N}(\tilde{\mu}, \tilde{\sigma}^2) \right]
                                                                                                                     Batch size B_1, B_2.
15:
                                                                                                                    Sample size S_1, S_2.
             \theta_s \leftarrow \theta_s - \xi \nabla_{\theta_s} \mathbb{E} [\mathcal{L}_s(\theta_s)]
16:
                                                                                                                    Learning rate \xi, \gamma, \eta, \alpha.
             \phi_s \leftarrow \phi_s - \gamma \nabla_{\phi_s} \mathbb{E} \left[ \mathcal{L}_s(\phi_o) \right]
17:
             \theta_o \leftarrow \theta_o - \eta \nabla_{\theta_o} \mathbb{E} [\mathcal{L}_o(\theta_o)]
                                                                                                                Run Model (\tilde{o}_i, \hat{\pi}, \tilde{o}_{i+H}):
18:
                                                                                                                    Compute Q_{\phi_z}(s_i) using \tilde{o}_i
             ▶ POLICY OPTIMIZATION
              \{\tilde{o}_{\tau}\}^{B_2} \sim \mathcal{M}
                                                                                                                    Sample \tilde{s}_i \sim Q_{\phi_s}(s_i)
19:
                                                                                                                    Compute \mu, \sigma \leftarrow P_{\theta_s}(s_{i+H}|\tilde{s}_i, \hat{\pi})
             for \tau = 1, 2, ..., B_2 do
20:
                                                                                                                    Compute Q_{\phi_s}(\tilde{s}_{i+H}) using \tilde{o}_{i+H}
                     Compute Q_{\phi_s}(s_{\tau}) using \tilde{o}_{\tau}
21:
                                                                                                                    Compute \mu', \sigma' \leftarrow Q_{\phi_s}(\tilde{s}_{i+H})
                     Sample \tilde{s}_{\tau} \sim Q_{\phi_s}(s_{\tau})
22:
                     for s = 1, 2, ..., S_1 do
                                                                                                                    Sample \tilde{s}_{i+H} \sim \mathcal{N}(\mu, \sigma^2)
23:
                           Compute \mu, \sigma \leftarrow P_{\theta_s}(s_{\tau+H}|\tilde{s}_{\tau}, \hat{\pi}_t)
                                                                                                                    Compute P_{\theta_0}(o_{i+H}|\tilde{s}_{i+H})
24:
                           Sample \tilde{s}_{\tau+H} \sim \mathcal{N}(\mu, \sigma^2)
25:
                           Compute P_{\theta_0}(o_{\tau+H}|\tilde{s}_{\tau+H})
26:
                           Compute Q_{\phi_s}(\tilde{s}_{\tau+H}) using \tilde{o}_{\tau+H}
27:
                           Compute \mu', \sigma' \leftarrow Q_{\phi_s}(\tilde{s}_{\tau+H})
28:
                           G \leftarrow G - \log \Psi \left[ P_{\theta_{\alpha}}(o_{\tau+H} | \tilde{s}_{\tau+H}) \right]
29:
                           G \leftarrow G + [H(\mu', \sigma') - H(\mu, \sigma)]
30:
                           for s = 1, 2, ..., S_2 do
31:
                                  Sample \tilde{s}_{\tau+H} \sim P_{\theta_{\tau}}(s_{\tau+H}|\tilde{s}_{\tau}, \hat{\pi}_{\tau}) \triangleright Re
32:
                                 computed with dropout.
                                 Compute \mu'', \sigma'' \leftarrow P_{\theta_2}(o_{\tau+H}|\tilde{s}_{\tau+H})
33:
                                 Sample \tilde{s}_{\tau+H} \sim \mathcal{N}(\mu, \sigma^2)
34:
                                 Compute \mu''', \sigma''' \leftarrow P_{\theta_o}(o_{\tau+H}|\tilde{s}_{\tau+H})
35:
                                 G \leftarrow G + [H(\mu'', \sigma'') - H(\mu''', \sigma''')]
36:
              \phi_a \leftarrow \phi_a - \alpha \nabla_{\phi_a} \mathbb{E}[G(\phi_a)]
37:
```





Benchmark: AIF vs Realistic Industrial Environment

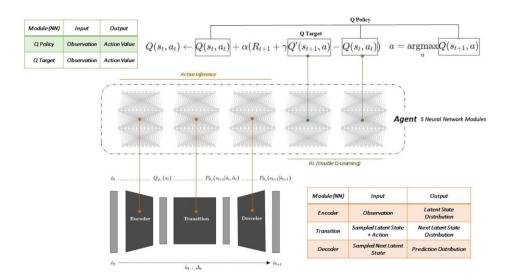
Application

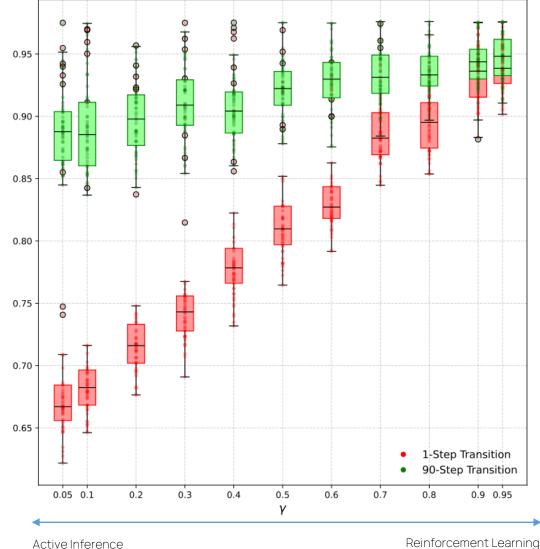
Energy-Efficient Control of simulated workstations within automotive manufacturing system composed of parallel, identical machines.

Challenges

Stochastic - Delayed - Long-horizon - Multi-Modal Observation

Requires extensive planning with horizon of one-shift (~ 3000 actions).









Results: DAIF vs Realistic Industrial Environment

Application

Energy-Efficient Control of simulated workstations within automotive manufacturing system composed of parallel, identical machines.

Challenges

Stochastic - Delayed - Long-horizon - Multi-Modal Observation

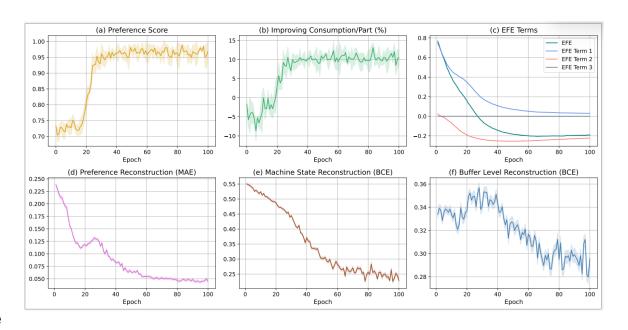
Requires extensive planning with horizon of one-shift (~ 3000 actions).

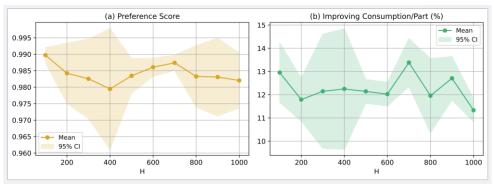
Improving Energy-Efficiency:

Controlling the number of active machines to minimize idle time with negligible production loss.

$\mathbf{Agent}(\phi)$	Production Loss [%]	EN Saving [%]
DQN (0.93)	4.82 ± 0.34	10.87 ± 0.76
DQN (0.94)	3.34 ± 0.23	9.92 ± 0.69
DAIF	2.59 ± 0.16	12.49 ± 0.04
DQN (0.95)	1.27 ± 0.05	7.00 ± 0.07
DQN (0.96)	1.27 ± 0.09	7.62 ± 0.12
DQN (0.97)	1.20 ± 0.05	7.72 ± 0.10
DQN (0.98)	0.54 ± 0.04	2.72 ± 0.19
DQN (0.99)	0.40 ± 0.03	2.46 ± 0.01

Production loss versus energy-saving (EN) across reward parameters ϕ of DQN agents (best model-free RL) against the DAIF agent .





Performance of the agents versus overshooting horizon H.





DAIF: Promises

Derived from a Bayesian-grounded framework (heuristic-free)

Natively scalable to both discrete and continuous action spaces

A unified explore-exploit gradient

Effective encoding of long-horizon dynamics

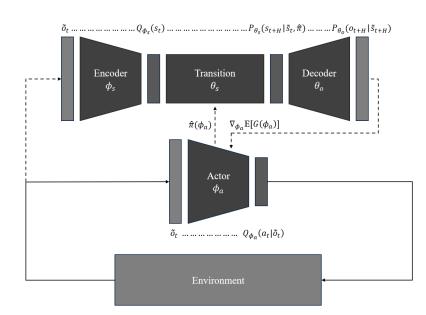
Capturing distinct forms of epistemic uncertainty, providing an intrinsic drive for model refinement

Reliance on observations (cheap, raw data), instead of often expensive, engineered reward signals

A degree of interpretability

Inherent adaptability in non-stationary settings via AIF

Minimal computational cost during both inference (model-free) and planning (EFE calculated in a single H-step forward pass)







DAIF: Potential

Scope: Data-Driven Decision Making or Optimization:

Sequential decision making under uncertainty (POMDP)

- Control / Planning / Search
- Reasoning / Inference / Search
- Generation / Synthesis

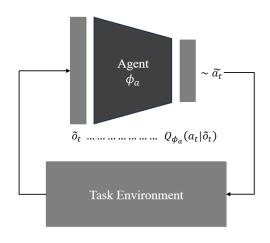
Domains:

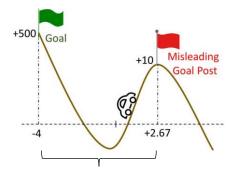
- Robotics
- Production Control
- Healthcare
- Drug Discovery / Protein Design
- •

Settings:

Delayed and Long-Horizon Environments

- Stochastic & Partial Observability
- Delayed/Sparse/Expensive Reward (i.e., Scarce high-quality data)
- Long Horizon





Two sparse rewards [1]







Future Work

DAIF is a concept: Generative world model with multi-step latent transitions + differentiable policy; backpropagates EFE through long horizons without tree search; scales to all spaces while keeping the explore-exploit balance.

Next steps

Generative Model (DL): Try diffusion/flow-matching world models instead of VAE.

Sample efficiency (DL): Still needs experience collection every H steps; aim to reduce data needs.

Sequence aggregation: Replace slow recurrent unrolling with set-based pooling of H embeddings (with simple positional encodings) or operator-learning for resolution-invariant aggregation.

Optimization (RL): Explore actor-critic training and add regularization to stabilize/variance-reduce EFE gradients.

EFE Methods (AIF): Improving distinct term estimations (e.g., sampling).

Adaptation (AIF): Focus on rapid learning in non-stationary environments.

Expanding Experimental: In addition to more domains, looking a range of settings.

Reasoning Model: Exploring potential for reasoning tasks.

Big picture: Bridges generative world-modelling with active inference and RL—compact, end-to-end probabilistic agents





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References

Yeganeh, Yavar Taheri, Mohsen Jafari, and Andrea Matta. "Deep Active Inference Agents for Delayed and Long-Horizon Environments." *arXiv preprint arXiv:2505.19867* (2025).





- [1] Chakraborty, Souradip, et al. "Dealing with sparse rewards in continuous control robotics via heavy-tailed policies." arXiv preprint arXiv:2206.05652 (2022).
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