Free Energy and Active Inference in Biological Systems
M23SC3.101 ITB- Technical Report

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Abstract

A consistent and sufficiently general definition of life that explains the vast variety of observed processes is an important question for biologists. This technical paper explores the Free Energy Principle, developed through large contributions by Karl Friston which is an important step in answering this question. It represents a powerful generalization of definitions for what are considered 'biological' systems using the methods of Statistical Mechanics and Bayesian Inference. Active Inference is a process that is considered central to what we term as 'biological systems' in this framework. By integrating the specific process theories of the respective fields there are attempts to model fields as diverse as neuronal dynamics, population ecology, and intracellular kinetics using the FEP[1].

1 Introduction and Motivation

> *"How can the events in space and time which take place within the spatial boundary of a living organism be accounted for by physics and chemistry?"*
> Erwin Schrodinger, "What is Life"[2](1944)

Schrodinger's perspective about life acting as a localized negative entropy extractor was revolutionary in many respects and led to many developments in Biology.

Building upon work motivated by Schrodinger, the Free Energy Principle is an important step in answering the question of Life and Biological self-organization.

Here we reverse the question [3] and ask, given a definition of a "system" that appears to be "living", what sort of dynamics, internally and in its interactions with the environment, to show the behavior it does.

The definitions of "system" and "living" crucially underpin most of the mathematical formalism that is derived in the FEP. It may be shown that given that we choose these definitions, biological self-organization is an inevitable and emergent property of the systems under consideration.

2 Defining Systems: Markov Blankets

The FEP defines a system as a subset of the partition of some abstract state space. Borrowing ideas from Bayesian networks [4], Systems are characterized not only by internal and external states but also by a boundary between them which marks that the subsets on either side of it are causally independent. This is justified by the assumption that if the coupling of systems is based explicitly on short-range forces, then distant states must necessarily be uncoupled.[5]

This leads to the notion of a **Markov Blanket**; The structure of the boundary states i.e. Markov blanket in a Bayesian network is necessarily isomorphic to three kinds of structures[4]:

1. Children of a set (the set of states that are influenced)
2. Parents of a set (the set of states that influence it)
3. The parents of its children

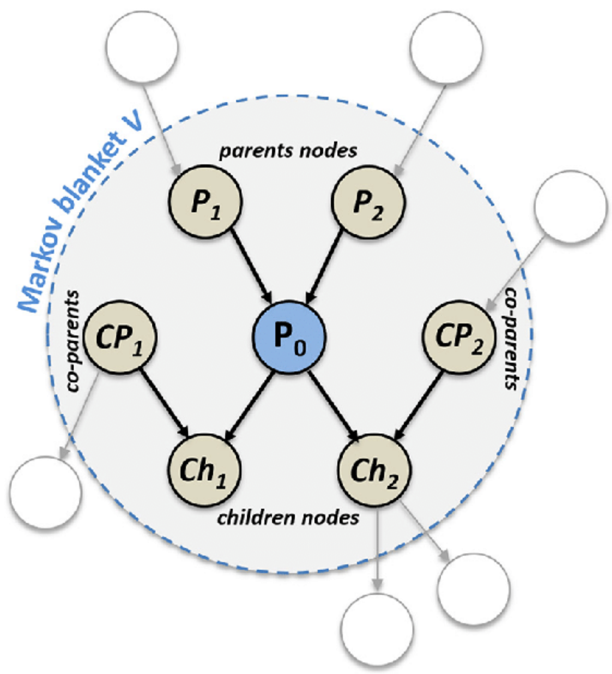

Figure 1: The Three Types of Node Substructures that may be seen in Markov Blankets

This definition of 'thingness' in terms of causal independence and Markov Blankets may be considered an axiom for this theory.
There is another way to arrive at this formulation of Internal, External, and Blanket states.

The system of interest is defined on some state space $X \in R^d$ and is immersed in the environment. The system evolves in time with a deterministic law and the environment adds a random noise to its evolution. Hence, its dynamics may be modeled by a set of stochastic differential equations of the form:

$$\dot{x}(\tau) = f(x) + \omega(\tau) \tag{1}$$

Now, the systems of interest for us are systems whose probability is characterized by tending to certain states over long periods. If being a 'thing' separate from others were not defined in such a way, the deterministic evolution of the probability distribution by the Fokker-Planck equation would make the property of 'thingness' would itself be meaningless in this framework.
These states are called **pullback attractors** in terms of Dynamical Systems theory, which is a set of states that our system tends to orbit with time, regardless of our initial conditions. Stochastic differential equations are solved through two mathematical formulations, usually:

1. The Fokker Planck Equation, which gives deterministic evolution in the probability densities

$$\dot{p}(x, \tau) = \nabla \cdot (\Gamma \nabla - f(x)) p(x, \tau) \tag{2}$$

2. Path Integral Formulation, that gives the probability of a path given its action.

$$A(x[\tau]) = -\ln p(x[\tau] \mid x_0) = \frac{\tau}{2} \ln\left(|(4\pi)^n \Gamma|\right) + \int_0^\tau dt\, L(x, \dot{x}), \tag{3}$$

Here, the Lagrangian is given by:

$$L(x, \dot{x}) = \frac{1}{2} (\dot{x} - f) \cdot \frac{1}{2\Gamma} (\dot{x} - f) + \nabla \cdot f.$$

Pullback attractors imply Non-equilibrium Steady State Solutions to the Fokker-Planck Equation, which simply means that the system may have stable and deterministic probability distributions away from equilibrium.

Using this and manipulating the Hessian and Jacobian of the Probability Distributions we may come to the same partitioning of the states, Under the assumptions of **Sparse Coupling** [3]. This is intuitive, because if we assume that the interactions in the system are short-range, then we will naturally derive Causal Independence of distant states.

3 Perception-Action Coupling

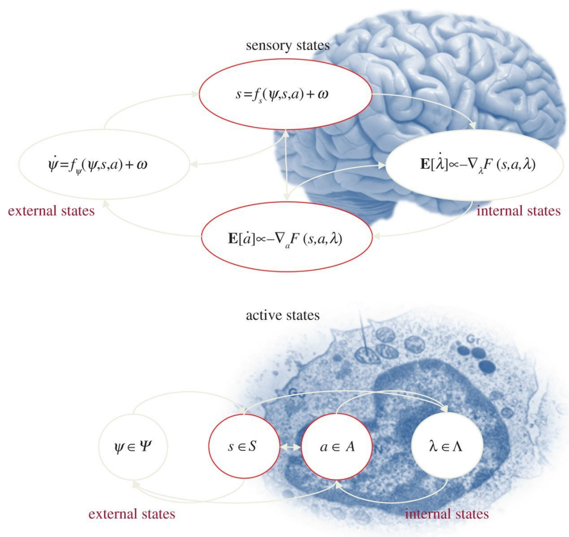

Figure 2: Circular Causality in Perception-Action[4]

By separating the states that are directly affected by external states and those that are not, we further divide the whole state space. The state space is partitioned into 4 subsets as follows:

a sample space Ω or non-empty set from which random fluctuations or outcomes $\omega \in \Omega$ are drawn

external states $\Psi : \Psi \times A \times \Omega \to \mathbb{R}$ states of the world that cause sensory states and depend on action

sensory states $S : \Psi \times A \times \Omega \to \mathbb{R}$ the agent's sensations that constitute a probabilistic mapping from action and external states

action states $A : S \times \Lambda \times \Omega \to \mathbb{R}$ an agent's action that depends on its sensory and internal states

internal states $\Lambda : \Lambda \times S \times \Omega \to \mathbb{R}$ the states of the agent that cause action and depend on sensory states

Figure 3: Mathematical Model for the Partitioning of the State Space in terms of Random Dynamical Systems[4]

4 Free Energy Principle

4.1 G-density and R-density

There are two types of probability density functions important in the Free Energy Principle. Let v here stand for environmental variables, and let ϕ denote the sensory inputs respectively. There is a one to many mapping between environmental variables and the corresponding sensory states.

Definition 1 (R-density)**.** *Representational density is an internal model of the organism. It is a probability distribution over all possible sensory states. We denote it as* $q(v)$

Definition 2. *Generative Density is a system's model of the causes of the sensory input in terms of the environmental variables. It is hence a joint probability distribution between the environmental variables and sensory input* $p(v, \phi)$

In the proofs that follow all the probability densities are normalized, unless otherwise stated.

Because of how the Markov boundary of an organism is defined, it may not directly perceive information about the environment (external states). It needs to perform a process of Bayesian Inference, using the sensory input data to infer information about the environment.

The G-density may be factorized into an organisms prior belief about the world, and the likelihood of that belief being true.

$$p(v, \varphi) = p(\varphi)|v * p(v)$$

So, using these quantities, and a stimulus from the environment $\varphi = \phi$ we may calculate the posterior using Bayes theorem:

$$p(\phi|v) = \frac{p(\phi|v)p(v)}{\int p(\phi|v)p(v)dv} \tag{4}$$

The integral at the bottom is often intractable due to an exponential number of states to account for. So, we use a method known as Variational Bayes to solve this problem.

4.2 Variational Bayes

This is a method that helps us to approximately solve the integral in the denominator of (3). We introduce an auxillary probability density, which in our case would be the previously defined R-density. This is the organism's current "best guess" at the generative density. We model the difference between the organisms present best guess and the generative density using some information theoretical metric. In most cases, we use the Kullback Leibler Divergence between these two distributions, given by:

$$D_{KL}(q(v)||p(v|\varphi)) = \int \frac{\ln q(v)}{p(v|\varphi} q(v)dv = F + \ln p(\varphi) \tag{5}$$

Where

$$F = \int dvq(v) \frac{\ln q(v)}{p(\varphi, v)}$$

has been defined as the **Variational Free Energy**.

Minimizing this Free Energy has two benefits:

Table 1. Mathematical objects relating to the VFA.

Symbol	Name	Description
ϑ	**Environmental variables**	**These refer to all states outside of the brain and include both environmental and bodily variables.**
φ	Sensory data	Signals caused by the environment (or body).
$q(\vartheta)$	R-density	Organism's (implicit) probabilistic representation of environmental states which cause sensory data.
$p(\varphi, \vartheta)$	G-density	Joint probability distribution relating environmental states and sensory data. This is necessary to specify the Laplace-encoded energy and is usually specified in terms of a likelihood and prior
$p(\vartheta)$	Prior density	Organism's prior beliefs, encoded in the brain's state, about environmental states.
$p(\varphi\|\vartheta)$	Likelihood density	Organism's implicit beliefs about how environmental states map to sensory data.
$p(\vartheta\|\varphi)$	Posterior density	The inference that a perfectly rational agent (with incomplete knowledge) would make about the environment's state upon observing new sensory information, given the organism's prior assumptions.
$p(\varphi)$	Sensory density	Probability density of the sensory input, encoded in the brain's state, which cannot be directly quantified given sensory data alone.
$-\ln p(\varphi)$	Surprisal	*Surprise* or *self-information* in information-theory terminology, which is equal to the negative of *log model evidence* in Bayesian statistics.
$F(\vartheta, \varphi)$	Variational free energy (VFE)	The quantity minimised under the FEP which forms an upper bound on surprisal allows the approximation of the posterior density.

Figure 4: Table representing relevant quantities in Variational Bayes taken from [6]

1. It is a good approximation to the Bayesian Posterior, which is not intractable. In particular, we see that the numerator depends only on R-density which we are free to specify, and the G-density the organism already has. The second term, which represents the surprisal (in information-theoretic terms) of sensory input, is independent of the R-density.

2. By Jensen's Inequality, the KL Divergence is always non-negative [7]. So, VFE also provides an upper bound on the surprisal of the sensory inputs received by the organism. Minimizing the VFE makes these upper bounds tighter.

$$F \geq -\ln p(\varphi)$$

   If we take expectation on both sides in the above equation, and interpret it from the path integral formulation, we see that the action appears to minimize the entropy. This ties in nicely with the observation that self organizing biological systems seem to locally defy the second law of thermodynamics.

$$\mathbb{E}[F] = \mathbb{E}[-\ln p(\varphi)] = H(\varphi) \tag{6}$$

   This is equivalent to the good regulator theorem in biological self-organization which states that every good regulator is a model of its environment[8].

5 Example working of FEP: Toy Brain

5.1 R-Density encoding: The Laplace Approximation

To actually implement the method described above, the system we have mentioned must have the R-density encoded in a way that it can select a certain distribution to start from.
Considering a concrete example of a brain, it has been suggested that neuronal activities encode sufficient statistics about a family of probability distributions. These are parametrized by some variable μ picked out by the instantaneous state of the brain which encodes the beliefs about the environment at that point in time. Finding the optimal density $q(v;\mu)$ is still an intractable problem, so we make the following further assumptions to obtain a closed form solutions while still maintaining a large level of generality for systems of interest.

1. We assume that the R-density is factorizable into independent sub-densities
2. We assume that the R-density is Gaussian. This is called the **Laplace Approximation**. The sufficient statistics now become parameters (i.e. the Mean and the Variance of the assumed R-density) for the optimization of the VFE. Under these assumptions, minimizing the VFE leads to the following expression:

$$F = \mathbb{E}(\mu, \varphi) - \ln\{2\zeta^*\} \tag{7}$$

Here, ζ^* is a constant variance term that may be removed by considering a fully multivariate Gaussian Distribution that corresponds to the weaker assumption that environment states are only weakly correlated. We get a form similar to (6).

$$\mathbb{E}[\{\mu_\alpha, \varphi_{\alpha\}})] = -\ln p(\{\mu_\alpha, \varphi_\alpha\}) \tag{8}$$

Here $\{\mu_\alpha\}, \{\varphi_\alpha\}$ are vectors representing brain states and sensory states respectively corresponding to environment variables. This equation shows that the brain represents only the most likely environmental causes of sensory data and not the details of their distribution. However, the brain also encodes uncertainties through G-density.

5.2 G-Density: How beliefs about the environment are generated

The approximation for the VFE works by considering an approximate G-density. Here, we specify how these G-densities might be generated from the environment in two models, the static model and the dynamic model which follows the form of the equation (1).

5.2.1 The Static Case

Instead of an $\dot{x}$ term on the LHS, for the static case, we only have the sensory input on the LHS. Consider a model where the organism has only one brain state and only one environmental variable μ. The organism believes that its sensory data is generated from the environment data along with some noise function. It believes that the environmental data itself is modelled as a noisy variation about some mean. These are modelled as follows:

$$\varphi = g(\mu; \theta) + z\bar{\mu} = \mu + w$$

Here, $\bar{\mu}$ is not the mean of the R-density, rather it is the expectation of the prior. In particular, R-density or recognition density, is derived after the system interacts with the environment whereas these are beliefs already encoded in the organism.

Assuming both our noises to be Gaussian, we get the following:

$$p(\phi|\mu) = \frac{1}{\sqrt{2\pi\sigma_z}} \exp\left\{-\frac{(\phi - g(\mu;\theta))^2}{2\sigma_z^2}\right\} .p(\mu) = \frac{1}{\sqrt{2\pi\sigma_w}} \exp\left\{-\frac{(\mu - \bar{\mu})^2}{2\sigma_w^2}\right\}.$$

Substituting the likelihood and the prior densities obtained here into equation(8), we finally get:

$$E(\mu, \phi) = -\ln p(\phi|\mu) - \ln p(\mu) \tag{9}$$

which can be further expanded as:

$$E(\mu, \phi) = \frac{1}{2\sigma_z^2}\varepsilon_z^2 + \frac{1}{2\sigma_w^2}\varepsilon_w^2 + \frac{1}{2}\ln(\sigma_z\sigma_w). \tag{10}$$

Here $\varepsilon_z \equiv \phi - g(\mu;\theta)$,
and $\varepsilon_w \equiv \mu - \bar{\mu}$ are respectively called **Residual Error** and **Prediction Error** respectively. The residual error quantifies how much our expectation deviates from the actual value and the Prediction error is how much the states actually vary about pre-specified $\bar{\mu}$.

The calculation can be extended to the multivariable case easily. The original encoded beliefs are replaced by a vector encoding beliefs about multiple variables. The noise sources are also now represented by a vector. They may be correlated in general [9], but assuming independence simplifies the calculations as the priors and likelihoods may now be expressed as products.

$$p(\{\mu_\alpha\}) = \prod_{\alpha=1}^{N} p(\mu_\alpha), p(\{\mu_\alpha\}) = \prod_{\alpha=1}^{N} \frac{1}{\sqrt{2\pi\sigma_\alpha^2}} \exp\left\{-\frac{(\mu_\alpha - \bar{\mu}_\alpha)^2}{2\sigma_\alpha^2}\right\}$$

$$p(\{\phi_\alpha\}|\{\mu_\alpha\}) = \prod_{\alpha=1}^{N} p(\phi_\alpha|\{\mu_\alpha\}).$$

where α represents an index over all brain states. Solving this under these assumptions, we finally get the following result:

$$E_{static}(\{\phi_\alpha\}, \{\mu_\alpha\}) = \sum_{\alpha=1}^{N}\left[\frac{(\varepsilon_{\alpha w})^2}{2\sigma_{\alpha w}^2} + \frac{1}{2}\ln\sigma_{\alpha w}\right] + \sum_{\alpha=1}^{N}\left[\frac{(\varepsilon_{\alpha z})^2}{2\sigma_{\alpha z}^2} + \frac{1}{2}\ln\sigma_{\alpha z}\right], \tag{11}$$

Intuitively, this result says that the VFE is a quadratic sum of the errors, weighted for precision and another logarithm term. This lends nicely to conceptualizing it as a Loss/Error function which we will do in VFE Minimization.

5.2.2 The Dynamic Case

Here we handle the stochastic differential equation that arises from our modelling of the environment in its full generality.

For the dynamic case where we have equations of the form of (1), we need to utilise **Generalized Coordinates**. At any point in the state space, instead of just taking the state variables into account, we also take the recursively higher order time derivatives of the state vector into account as a part of our vector. So our state vector becomes an infinite dimensional vector that encodes all the information about the instantaneous velocity of the point. The derivative of such a vector μ is defined as:

We make a local linearity assumption, i.e. each dynamical order of each state variable has an independent noise source. This cancels all the cross terms. Additionally let $g_{[n]}$ denote a term in the n^th dynamical order. Our set of equations now becomes:

$$\phi_{\alpha[n]} = g_{\alpha[n]} + z_{\alpha[n]} \tag{12}$$

$$D\mu_{\alpha[n]} = f_{\alpha[n]} + w_{\alpha[n]} \tag{13}$$

With similar calculations and assumptions as in the case of the static case we end up with the following:

$$E_{dynamic}(\{\tilde{\mu}_\alpha\}, \{\tilde{\phi}_\alpha\}) = \sum_{\alpha=1}^{N}\sum_{n=0}^{\infty}\left\{\frac{1}{2\sigma_\alpha^{z[n]}}\left[\varepsilon_\alpha^{z[n]}\right]^2 + \frac{1}{2}\ln\sigma_\alpha^{z[n]}\right\} + \sum_{\alpha=1}^{N}\sum_{n=0}^{\infty}\left\{\frac{1}{2\sigma_\alpha^{w[n]}}\left[\varepsilon_\alpha^{w[n]}\right]^2 + \frac{1}{2}\ln\sigma_\alpha^{w[n]}\right\}, \tag{14}$$

where we have used the auxiliary variables:

$$\varepsilon_\alpha^{z[n]} \equiv \phi_\alpha[n] - g_\alpha[n], \varepsilon_\alpha^{w[n]} \equiv \mu_\alpha[n+1] - f_\alpha[n].$$

We neglect terms of higher dynamical order by setting them equal to the noise at that order. This reflects the fact that the order below is unconstrained and they are free to change to best reflect the sensory data.

6 VFE Minimization: Recognition Dynamics and Active Inference

We have already demonstrated how minimizing the VFE corresponds to minimizing KL divergence between the G-Density and the R-Density. We have also shown how the R-density and G-density may be approximated and generated from an organisms model about the environment respectively.

Continuing with the running example of brain states, if we outline a method for the minimization that we have explained, it is the beginning of a biological **Process Theory**.

In the FEP it is suggested that neuronal states change so as to implement a gradient descent on the VFE. This is called Recognition Dynamics.

$$\mu^{\alpha}_{t+1} = \mu^{\alpha}_{t} - \kappa\mu^{\wedge}_{\alpha} \cdot \nabla\mu_{\alpha} E(\{\mu_{\alpha}\}, \{\phi_{\alpha}\}) \tag{15}$$

In the continuous limit, this becomes a differential equation of the form:

$$\dot{\mu}_{\alpha} = -\kappa\mu^{\wedge}_{\alpha} \cdot \nabla\mu_{\alpha} E(\{\mu_{\alpha}\}, \{\phi_{\alpha}\}) \tag{16}$$

As in any gradient descent, the objective function settles to its minima. In this case, our objective function is the Laplace Approximation of the Free Energy, so we settle to a minimum of free energy which is what we wanted.

The problem with including higher order dynamical terms is that they introduce coupling between the Differential equations. We can however account for this by noting that the motion of a point in generalized coordinates is different from the encoding of the trajectory that the brain will encode. This leads to a general version of the VFE minimization as:

This gives us a model for the updating of the neuronal states in the brain.

$$\mu^{\alpha}_{t+1}[n] - \mu^{\alpha}_{t}[n] = -\kappa\mu^{\wedge}_{\alpha}[n] \cdot \nabla\mu^{\sim}_{\alpha} E(\{\mu^{\sim}_{\alpha}\}, \{\phi^{\sim}_{\alpha}\}) \tag{17}$$

6.1 Active Inference

The systems active states are not directly involved in the Free Energy Term. However, by changing the sensory variables in a way that the G-density conforms more closely to the R-density, action (which may be modeled as any kind of response to stimulus etc.) can contribute to minimizing the Free Energy.

The crucial claim in this context is that the brain has an **inverse model**. This inverse model represents how the sensory inputs change with action. It has been well argued that this exists[11][12], and hence we may write using the Laplace encoded energy change for action:

$$\frac{dE(\mu, \phi)}{da} \equiv \frac{d\phi}{da}\frac{\partial E(\mu, \phi)}{\partial \phi}. \tag{18}$$

So, we write the same gradient descent formula we wrote for recognition dynamics, but now in terms of action.

$$\dot{a} = -\kappa_a \frac{d\phi}{da}\frac{dE(\mu, \phi)}{d\phi}, \tag{19}$$

This may then be written for generalized coordinates as:

$$\dot{a} = -\kappa_a \sum_{\alpha} \frac{d\phi^{\sim}_{\alpha}}{da} \cdot \nabla\phi^{\sim}_{\alpha} E(\{\mu^{\sim}_{\alpha}\}, \{\phi^{\sim}_{\alpha}\}). \tag{20}$$

This is an agent based model for action. [3] may be consulted for an in depth calculation and simulation of our model for an agent.

7 Further Directions for Research

1. The FEP is an evolving framework and recent formulations that focus more on the Langevin Dynamics and Random Dynamical Systems formulation and solving the stochastic differential equations governing the dynamics of the system through the Fokker Planck Equation or a Path Integral Formulation [3]. Learning about the specifics of the mathematical formalism more rigorously may be enriching to the understanding of the FEP.

2. The free energy has already been used to model neuronal dynamics and mathematical psychology. The application of specific process theories is an open question that continues to be researched. There are already attempts to use it to model Intracellular kinetics, and population ecology etc. and there are a vast number of fields that it may be used to model owing to the generality of the principle.

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