

# Dark Control: A Unified Account of Default Mode Function by Control Theory and Reinforcement Learning

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## Abstract

The default mode network (DMN) is believed to subserve the human baseline mental activity. Its highest energy consumption in the brain and its intimate coupling with conscious awareness are both pointing towards an important functional roles. Many research streams support its evolutionarily adaptive role as envisioning mental scenarios to simulate the future.

The present concept paper proposes to explain *how* the DMN may actually implement such continuous assessment and prediction of the environment to guide action choices.

DMN function is recast in mathematical terms of control theory and reinforcement learning based on Markov decision processes. We argue that our formal account of DMN function naturally accommodates as special cases previously proposed cognitive accounts such as *predictive coding*. A process model for the neural implementation of continuous future predictions potentially realized in the DMN could offer insight into the statistical mechanisms underlying human behavior and provide a parsimonious explanation of experimental findings in animals and humans.

**keywords:** systems biology, mind wandering, cognitive science, artificial intelligence, reinforcement learning

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## 1 Introduction

When left unperturbed, the human brain is not at rest. Rather, the brain continues to metabolize large quantities of oxygen and glucose energy to maintain neuronal computation in the absence of behavioral focus (Kenet et al., 2003; Fiser et al., 2004). The baseline energy demand is surprisingly weakly modulated with task demand (Raichle et al., 2001). At the opposite, during sleep, the decoupling of brain structures discarded the idea of the DMN being only a passive network resonance and rather supported its important role in the sustenance of conscious awareness (Horovitz et al., 2009). This dark matter of brain physiology begs the question of underlying biological purpose (Raichle, 2006). What has early been described as the "stream of consciousness" in psychology (James, 1890) found a potential neurobiological manifestation in the so-called "default mode network" (DMN) (Shulman et al., 1997; Raichle et al., 2001). This set of some of the highest regions in the human association cortex (Mesulam, 1998; Margulies et al., 2016) consistently increase in neural activity during unfocused everyday mind wandering (Raichle et al., 2001). The DMN may subserve important functions in higher-order control of human behavior following the notion of "a hierarchy of brain systems

with the DMN at the top and the salience and dorsal attention systems at intermediate levels, above thalamic and unimodal sensory cortex” (Carhart-Harris and Friston, 2010). In the beginning of the 21st century, brain imaging may have been the first technique to allow for the discovery of a unique brain network that subserves baseline mental activities (Raichle et al., 2001; Bzdok and Eickhoff, 2015).

## 1.1 Default mode network: higher-order control of the organism

The human DMN is responsible for a large part of the brain’s baseline activity, which typically decreases during psychological experiments. The standard mode of neural information maintenance and manipulation has been argued to mediate evolutionarily conserved functions (Brown, 1914; Binder et al., 1999; Buzsáki, György, 2006). In line with this, the DMN contains hotspots of highest energy consumption in the entire central nervous system (Raichle et al., 2001), which persists to a substantial degree during sleep and under anesthesia (Buckner et al., 2008). Today, many authors believe that the DMN implements probabilistic estimation of past, hypothetical, and future events (Fox et al., 2005; Hassabis et al., 2007; Schacter et al., 2007; Binder et al., 2009; Buckner et al., 2008). This brain network might have emerged to continuously predict environmental events using mental imagery as an evolutionary advantage. However, information processing in the DMN has also repeatedly been shown to directly impact human behavior. Goal-directed task performance improved with decreased activity in default mode areas (Weissman et al., 2006) and increased DMN activity was linked to more task-independent, yet sometimes useful thoughts (Mason et al., 2007; Seli et al., 2016). Gaining insight into the function of the DMN is particularly challenging because this network appears to simultaneously control perception-action cycles and maintain baseline contemplations across time, space, and content domains.

The present work takes the perspective of a human agent faced with the choice of the next action and being guided by rich reenactment of really-happened, hypothetically conceived, and estimated futures to optimize behavioral performance. A particularly attractive computational framework to describe, quantify, and predict autonomously acting systems like the brain is proposed to be the combination of control theory and reinforcement learning (RL). It is known that, the more the external world is predictable, the more mental activity becomes detached from the actual sensory environment (Antrobus et al., 1966; Pope and Singer, 1978). Conversely, the more the ongoing executed task is unknown and unpracticed, the less stimulus-independent thoughts occur (Filler and Giambra, 1973; Teasdale et al., 1995; Christoff et al., 2016). These “offline” processes may however contribute to optimized control of the organism. **(XXX Guillaume: What about the idea of model free control being also remote of environment? - danilo: hmm, let’s keeping thinking about this)** Informed by outcomes of performed action, the DMN dynamics are constantly adapted in feedback loops shaped by prediction error. A DMN framework incorporating RL can naturally embed human behavior into the tension between exploitative action with immediate gains and exploratory action with longer-term reward outcomes.

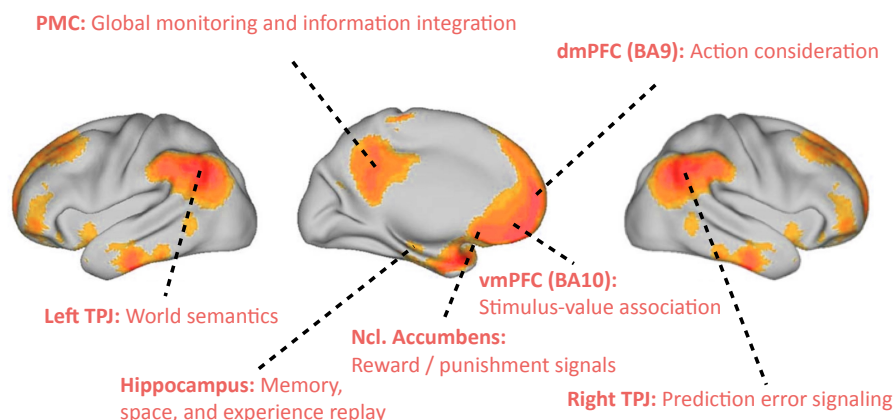
## 1.2 Towards a formal account of DMN function

We argue that DMN implication in a diversity of humans’ most advanced cognitive processes can be parsimoniously recast as prediction error minimization based on pervasive probabilistic simulations, thus maximizing action outcome across multiple time scales. Such a purposeful optimization objective may be solved by a stochastic approximation based on a brain implementation of Markov Chain Monte Carlo (MCMC) sampling (Tenenbaum et al., 2011). In this context, *control* refers to the influence that an agent exerts when interacting with the environment to encourage preferred states. Even (necessarily imperfect) memory recall, random day-time mind-wandering, and dreams during sleep may provide meaningful building blocks to iteratively improve the predictive DMN machinery to optimize the behavior of the organism. It has indeed been proposed earlier that the human brain’s energy budget is largely dedicated to “the development and maintenance of [a] probabilistic model of anticipated events” (Raichle and Gusnard, 2005). This idea has been invigorated by empirical evidence from

neuroscientific experiments (Körding and Wolpert, 2004; Fiser et al., 2004). The present paper proposes a process model that satisfies this contention.

## 2 Known neurobiological properties of the default mode network

We begin by a neurobiological deconstruction of the DMN based on experimental findings in the neuroscience literature. This walkthrough across network nodes will outline the individual functional profiles, paving the way for their functional interpretation within our formal account (next section).



**Fig 1.** Neurobiological overview of the DMN ... Please add a figure caption

### 2.1 The posteromedial cortex: global monitoring and information integration

The midline structures of the DMN, including the posteromedial cortex (PMC) and the medial prefrontal cortex (mPFC), are probably responsible for the highest turn-over of glucose energy consumption (Raichle et al., 2001). These metabolic characteristics go hand-in-hand with functional neuroimaging analyses (Andrews-Hanna et al., 2010) in suggesting that the PMC and mPFC potentially represent the functional backbone of the DMN.

The PMC myelinates relatively late during postnatal development in monkeys (Goldman-Rakic, 1987), which is generally considered to be a sign of evolutionary sophistication (Flechsfig, 1920). Normal and disturbed metabolic fluctuations in the human PMC have been repeatedly related to phenomena of changed conscious awareness (Cavanna and Trimble, 2006). Indeed, the PMC has long been speculated to reflect constant computation of environmental statistics and its internal representation as an inner "mind's eye" (Cavanna and Trimble, 2006; Leech and Sharp, 2014). For instance, Bálint's syndrome is a neurological disorder of conscious awareness that results from damage in the parietal cortex (Bálint et al., 1909). Patients are plagued by an inability to combine various individual features of the visual environment into an integrated whole (i.e., simultanagnosia) as well as an inability to direct action towards currently unattended environmental objects (i.e., optic ataxia). This can be viewed as a high-level impairment in gathering information about alternative objects (i.e., exploration) as well as leveraging these environmental opportunities (i.e., exploitation). Congruently, the human PMC was coupled in two functional connectivity analyses with the amygdala, involved in significance evaluation, and the nucleus accumbens (NAc), involved in reward evaluation. Specifically, among all parts of the PMC, the ventral posterior cingulate cortex was most connected to the laterobasal nuclei group of the amygdala (Bzdok et al., 2015). This amygdalar subregion has been proposed to continuously scan environmental input for biological significance assessment.

The putative role of the PMC in continuous integration of relevant environmental information and ensuing top-level control of action on the environment is supported by a number of neuroscience experiments. Electrophysiological recordings in animals implicated the PMC in strategic decision making (Pearson et al., 2009), risk assessment (McCoy and Platt, 2005), outcome-contingent behavioral modulation (Hayden et al., 2009), as well as approach-avoidance behavior (Vann et al., 2009). Neuron spiking activity in the PMC allowed distinguishing whether a monkey would pursue an exploratory or exploitative behavioral strategy during food foraging (Pearson et al., 2009). Further, single-cell recordings in the monkey PMC demonstrated this brain region's sensitivity to subjective target utility (McCoy and Platt, 2005) and integration across individual decision-making instances (Pearson et al., 2009). This DMN node encoded the preference of or aversion to options with uncertain reward outcomes and its spiking activity was more associated with subjectively perceived relevance of a chosen object than by its factual value, based on an internal currency of value (McCoy and Platt, 2005). In fact, direct stimulation of PMC neurons promoted exploratory actions, which would otherwise be shunned (Hayden et al., 2008). Graded changes in firing rates of PMC neurons indicated changing choices in upcoming trials and their neural patterns were distinct from spike firings that indicated choosing either option. Similarly in humans, the DMN has been shown to gather and integrate information over different parts of auditory narratives in an fMRI study (Simony et al., 2016).

The retrosplenial portion of the PMC can subserve representation of action possibilities and evaluation of reward contingencies by integration with information from memory and different perspective frames. Regarding memory recall, retrosplenial lesions have been consistently associated with anterograde and retrograde memory impairments of various kinds of sensory information in rabbits and humans (Vann et al., 2009). Regarding perspective frames, the retrosplenial subregion of the PMC has been proposed to mediate between the organism's egocentric (i.e., focused on sensory input) and allocentric (i.e., focused on world knowledge) viewpoints in animals and humans (Epstein, 2008; Burgess, 2008; Valiquette and McNamara, 2007).

Consequently, the PMC may contribute to overall DMN function by monitoring the subjective outcomes of possible decisions and integrating that information with memory, perspective frames, and reward outcomes into higher-level strategies. Perceived value, that differs across individuals, may update statistical assessment of the environment to predict delayed reward opportunities in the future. In doing so, the PMC may continuously adapt to changes in both the external environment and its internal representation to enable strategic behavior in volatile environments.

## 2.2 The prefrontal cortex: stimulus-value association and action consideration

Analogous to the PMC, the dorsomedial PFC (dmPFC) of the DMN is believed to subserve supra-sensory processes across time, space, and content domains to exert top-down control. In comparison to the PMC, however, dmPFC function may be closer to a "mental sketchpad" (Goldman-Rakic et al., 1996), as it potentially subserves the de-novo generation and manipulation of meaning representations instructed by stored semantics and memories.

Generally, patients with neurological lesions in the prefrontal cortex are known to struggle with adaption to novel situations and stimuli (Stuss and Benson, 1986). The dmPFC may subserve inference, representation, and assessment of one's own and other individuals' action considerations. Specifically, neural activity in the human dmPFC reflected expectations about other peoples' actions and errors in these predictions. Neural activity in the dmPFC indeed explained the proficiency decline of inferring other peoples' thoughts in aging humans (Moran et al., 2012). Some dmPFC neurons in macaque monkeys exhibited a preference for processing others', rather than own, behavior with fine-grained adjustment of contextual circumstances (Yoshida et al., 2010). In fact, the topographically neighboring dorsal anterior cingulate cortex has also been linked to computing values and efforts of persisting a behavioral plan versus switching the environmental context in several lesion studies (Kolling et al., 2016). Such highly abstract neural computations necessarily rely on the generation of probabilistic internal information drawing from episodic memory recall, generative construction processes, and

explicit knowledge of the external world. In a computational neuroimaging experiment, dorsomedial PFC activity preferentially modeled the consequences of action choices that were not actually executed, whereas ventromedial PFC (vmPFC) activity modeled especially value outcomes of performed actions in the environment (Nicolle et al., 2012).

Comparing to the dmPFC, the vmPFC probably subserves subjective value evaluation and risk estimation of relevant environmental stimuli. This DMN node is more closely associated with orchestrating adaptive behavior by bottom-up-driven processing of what matters now, probably drawing on sophisticated value representations (O'Doherty et al., 2015). Quantitative lesion findings across 344 human individuals confirmed a substantial impairment in value-based decision making (Gläscher et al., 2012). Indeed, the vmPFC is preferentially connected with reward-related and limbic areas. The vmPFC is well known to have monosynaptical connections with the NAc in axonal tracing studies in monkeys (Haber et al., 1995). Congruently, the gray-matter volume of the vmPFC and NAc correlated with indices of value-guided behavior and reward attitudes in humans (Lebreton et al., 2009). NAc activity is thought to reflect reward prediction signals from dopaminergic pathways (Schultz, 1998) that not only channel action towards basic survival needs but also subserve RL in humans more broadly (O'Doherty et al., 2015). This is consistent with diffusion MRI tractography in humans and monkeys (Croxson et al., 2005) that quantified the NAc to be more connected to the vmPFC than dmPFC in both species. Two functional connectivity analyses in humans strongly connected the vmPFC with the NAc, hippocampus (HC), and PMC. In line with these connectivity findings in animals and humans, the vmPFC is often proposed to be involved in (external) emotional reactions and own (visceral) arousal (Damasio et al., 1996). Real or imagined bodily states could be mapped in the vmPFC as a bioregulatory disposition governing cognition and decision making. In neuroeconomic studies of human decision making, the vmPFC consistently reflects an individuals subjective valuation (Behrens et al., 2008). This may be why performance within and across participants was related to state encoding in the vmPFC. Such a “cognitive map” of the action space was argued to encode the current task state even when states are unobservable from sensory input, which was shown to be critical for behavior (Schuck et al., 2016).

## 2.3 The hippocampus: memory, space, and experience replay

The DMN midline is probably closely linked with the HC in the medial temporal lobe (Vincent et al., 2006) – a region long known to be involved in memory operations and spatial navigation in animals and humans.

While the HC is traditionally believed to allow remembering the past, there is now increasing evidence for a role in constructing mental models in general (Zeidman and Maguire, 2016; Schacter et al., 2007; Gelbard-Sagiv et al., 2008; Javadi et al., 2017). Its recursive anatomical architecture may be specifically designed to allow reconstructing entire episodes of experience from memory fragments. Indeed, hippocampal damage is not only associated with an impairment in reexperiencing the past (i.e., amnesia), but also imagining one's own future and fictitious experiences more broadly (Hassabis et al., 2007). Mental scenes created by HC-lesioned patients exposed a lack of spatial integrity, richness in detail, and overall coherence. Single-cell recordings in the animal HC revealed some constantly active neuronal ensembles whose firing coincided with specific locations in space during environmental navigation. London taxi drivers, individuals with high performance in spatial navigation, were shown to exhibit increased gray-matter volume in the HC (Maguire et al., 2000). Indeed, when an animal is choosing between alternative paths, the corresponding neuronal populations in the HC spike one after another (Johnson and Redish, 2007). These neuronal patterns appear to also indicate upcoming behavior (Pfeiffer and Foster, 2013).

HC function probably extend beyond simple forms of encoding and reconstruction of memory and spatial information. Based on large-scale recordings of hippocampal neuronal populations, complex spiking patterns can be followed across extended periods including their modification of input-free self-generated patterns after environmental events (Buzsáki, 2004). Specific spiking sequences, which were elicited in experimental task conditions, have been shown to be reenacted spontaneously during quiet wakefulness and sleep (Hartley et al., 2014; O'Neill et al., 2010). Moreover, spike sequences measured in hippocampal place cells of rats



featured re-occurrence directly after experimental trials as well as directly before upcoming experimental trials (Diba and Buzsáki, 2007). Such hippocampal ensembles burst during rest and sleep have been proposed to be critical in communicating local information to the neocortex for long-term storage, potentially also in the nodes of the DMN. These HC-subervised mechanisms probably contribute to advanced cognitive processes that require recollecting autobiographical memory episodes, as well as reexperiencing or newly generating mental scenarios (Hassabis et al., 2007).

The HC thus orchestrates experience of environmental aspects for consolidations based on reenactment and for integration into rich mental scene construction (Deuker et al., 2016; Bird et al., 2010). In this way, the HC may contribute to improving ongoing perception of and action on the environment (Zeidman and Maguire, 2016).

## 2.4 The right and left TPJ: prediction error signaling and world semantics

The DMN emerges with its midline structures early in human development (Doria et al., 2010). However, the right and left TPJ may become fully integrated into this canonical network only after birth. The TPJs are known to exhibit hemispheric differences based on cytoarchitectonic borders and gyrification pattern (Seghier, 2013). Neuroscientific investigations on hemispheric functional specialization have highlighted the right versus left cerebral hemisphere as dominant for attention versus language functions.

The TPJ in the right hemisphere (RTPJ) has been shown to be intimately related to supra-modal prediction and error signaling. It is probably central for action initiation during externally structured tasks and sensorimotor control by integrating supra-modal stimulus-guided attention (Corbetta and Shulman, 2002). Involvement of this DMN node was repeatedly reported in multi-step action execution (Hartmann et al., 2005), visuo-proprioceptive conflict (Balslev et al., 2005), and multi-modal detection of sensory changes across visual, auditory, or tactile stimulation in a multi-modal fMRI study (Downar et al., 2000). In humans, direct electrical stimulation of the RTPJ during neurosurgery was associated with altered perception and stimulus awareness (Blanke et al., 2002). It was argued that the RTPJ encodes actions and ensuing outcomes without necessarily relating those to outcome value (Liljeholm et al., 2013; Hamilton and Grafton, 2008; Jakobs et al., 2009). Neural activity in the RTPJ has been argued to be responsible for stimulus-driven attentional reallocation to salient and surprising sources of information as a circuit breaker that recalibrates control and maintenance systems (Bzdok et al., 2013; Corbetta et al., 2008). Indeed, patients with RTPJ damage have particular difficulties with multistep actions (Hartmann et al., 2005). In the face of large discrepancies between actual and previously predicted environmental events the RTPJ acts as a potential switch between externally-oriented mind sets focussed on the sensory world and internally-oriented mind sets focussed on self-relevant mental scene construction. Transient RTPJ lesion in humans for instance diminished the impact of predicted intentions of other individuals (Young et al., 2010), a capacity believed to be enabled by the DMN. The RTPJ might hence be an important relay that shifts away from the internally directed baseline processes to, instead, deal with (unexpected) environmental objects and events.

The TPJ in the left hemisphere (LTPJ), in turn, exhibits a close topographical relationship to Wernicke's area involved in understanding spoken and written language. Neurological patients with damage caused to Wernicke's area have a major impairment of language comprehension when listening to others or reading a book. Their speech preserves natural rhythm and about normal syntax, yet the voiced sentences are devoid of meaning (i.e., aphasia). Abstracting from the typical semantic interpretations in linguistics and neuropsychology, the LTPJ probably mediates access to and integration of world knowledge, such as required during action considerations (Binder and Desai, 2011; Seghier, 2013). For instance, LTPJ lesions also entail problems in recognizing others' pantomimed action towards objects without obvious relation to processing explicit language content (Varney and Damasio, 1987). Inner speech also hinges on knowledge recall about the physical and inter-personal world. Indeed, the internal production of verbalized thought ("language of the mind") was closely related to the LTPJ in a multivariate analysis of brain volume (Geva et al., 2011). Further, episodic memory recall and

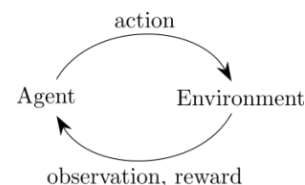
imagination strongly draw on reassembling world knowledge. Isolated building blocks of world statistics probably get reassembled in internally generated visual scenarios that navigate present action, weigh hypothetical possibilities, and forecast the future. The LTPJ may hence facilitate the automated prediction of events by incorporating experience-derived representations of the world into ongoing action, planning, and problem solving.

### 3 Reinforcement learning: a process model for DMN function

We now argue the outlined neurobiological properties and potential functions of the DMN nodes to be sufficient for implementing all components of a full-fledged RL algorithm. Recalling past experience, considering candidate actions, random sampling of possible scenarios, as well as evaluating instantaneous, delayed, and expected reward outcomes are key components of intelligent RL agents that are plausible to intersect in the DMN.

RL is a problem-solving technique in which, through interactions with an environment, an agent learns to reach goals, optimize reward signals, and minimize costs in an iterative trial-by-error fashion. At a given moment, each taken *action*  $a$  triggers an *partially observed* change in the *state* of the environment  $s \rightarrow s'$ , accompanied by environmental feedback signals as *reward*  $r = r(s, a)$  (or *punishment*, since it can be negative) collected by the agent. This is illustrated in Fig. 2. In this view, the environment is partially controlled by the action of the agent and the reward can be thought of as satisfaction – or punishment – accompanying the execution of an action.

Action may be delayed to achieve substantial increases in expected reward that can grow with time. The environment is generally taken as stochastic, that is, changing in random ways. In addition, the environment is only *partially observed* in the sense that only part of the current state is observed by the agent (Starkweather et al., 2017). The volatility of the environment is realistic in a computational model which sets out to explain DMN function. We argue that a functional account of the DMN based on RL can naturally embed human behavior in the tension between exploitative action with immediate gains and explorative action with longer-term reward outcomes (Dayan and Daw, 2008). DMN implication in a diversity of particularly advanced cognitive processes can be parsimoniously explained as probabilistic mental scene simulations coupled with prediction error minimization to calibrate action trajectories and maximize reward outcomes at different time scales. Such a purposeful optimization objective may be solved by a stochastic approximation based on a brain implementation of MCMC sampling (Tenenbaum et al., 2011).



**Fig 2.** RL in a nutshell

#### 3.1 Partially Observable Markov Decision Processes

We argue that the brain in general and the DMN in particular are a physical system governed by the laws of physics and can be locally described by Markov processes at a sufficiently coarse scale. Indeed, as noted in Tegmark (2016), any system obeying the laws of classical physics can be accurately modeled as a Markov process as long as the time step is sufficiently short. The process has *memory* if the next state depends not only on the current state but also on some finite number of past states. Rational probabilistic planning can be reformulated as a standard memoryless Markov process by simply expanding the definition of the state  $s$  to include elements of the past.

In artificial intelligence and machine learning, a popular computational model for multi-step decision processes in such an environment are *Partially Observable Markov Decision Processes (POMDPs)*. A POMDP formalizes a sequential decision process in which it is assumed that environment dynamics are determined by a Markov process, but the agent cannot directly observe the underlying state. Instead, the agent tries to optimize a *subjective* reward signal (i.e., is likely to be different for another agent in the same state). This is performed alongside



each transition in the environments state space, and maintains a probability distribution over the set of possible states, based on a set of observations and observation probabilities. This is a minimal amount of assumptions that can be made about an environment, and is characteristic of so-called *model-free RL*, which we propose as a useful formal framework for DMN function.

Model-free RL is plausible to be realizable in the human brain. Indeed, it has long been proposed (Dayan and Daw, 2008) that there is a rather direct mapping of model-free RL learning algorithms onto aspects of the brain. The neurotransmitter dopamine could serve as a “teaching signal” to better estimate value associations and action policies by controlling synaptic plasticity at targets such as the ventral and dorsolateral striatum. In contrast, *model-based RL* would start off with some mechanistic assumptions about the dynamics of the world. These can be assumptions about the physical laws governing the agent’s world or constraints on the state space and transitions between states. For instance, if a rat in a maze knows that standing still will produce no change in the environment, and in particular will not eventually lead to finding the food. In our present model-free RL framework, a rat might represent such knowledge about the world as follows:

- $r(s, \text{“stand still”}) = 0$  if  $s$  does not correspond to a cell / chamber containing food.
- $p(s'|s, \text{“stand still”}) = 1$  if  $s' = s$  and 0 otherwise.
- etc.

**Definition.** Mathematically, a POMDP is simply a quintuplet  $(\mathcal{S}, \mathcal{A}, r, p, \mu)$  where

- $\mathcal{S}$  is the set of states, such as  $\mathcal{S} = \{\text{happy, sad}\}$ .
- $p : \mathcal{S} \times \mathcal{A} \times \mathcal{S} \rightarrow [0, 1]$ ,  $(s, a, s') \mapsto p(s'|s, a)$ , the probability of moving to state  $s'$  if action  $a$  is taken from state  $s$ . In addition, one requires that such transitions be Markovian. Consequently, the future states are independent of past states and only depend on the present.
- $\mathcal{A}$  is the set of actions, such as  $\mathcal{A} = \{\text{read, run, laugh, sympathize, empathize}\}$ .
- $r : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$  is the reward function, so that  $r(s, a)$  is the instant reward for taking action  $a$  in state  $s$ .
- $\mu : \mathcal{S} \rightarrow [0, 1]$  is the prior probability on the states so that  $\mu(s)$  is the probability that the environment starts off in state  $s$ .

### 3.2 Long-term rewards and action policies

The behavior of the agent is governed by some kind of *policy*. It maps states of the world to a set of candidate actions to perform given this state. Starting a time  $t = 0$ , a policy  $\pi$  generates a trajectory of action cascades / trajectories as follows

**observe transition:**  $s_1 \sim p(s|s_0, a_0)$  **and collect reward**  $R_0 = r(s_0, a_0)$   
**choose action:**  $a_1 \sim \pi(a|s_1)$   
**observe transition:**  $s_2 \sim p(s|s_1, a_1)$ , **and collect reward**  $R_1 = r(s_1, a_1)$   
 ...  
**choose action:**  $a_t \sim \pi(a|s_t)$   
**observe transition:**  $s_{t+1} \sim p(s|s_t, a_t)$ , **and collect reward**  $R_t = r(s_t, a_t)$   
 ...

**Time-invariance assumption:** It is assumed that the underlying MDP is stationary – i.e., has reached steady-state conditions – so that the dynamics of the process are equivalent over sufficiently long time windows of equal length.

Since an action taken in the present moment  $t$  might have repercussions in the far future, it turns out that the quantity to optimize is not the instantaneous rewards  $r(s, a)$ , but a

cumulative reward estimate which takes into account expected reward in the future. A common approach to modeling this accumulation is the time-discounted *cumulative reward*

$$G^\pi = \sum_{t=0}^{\infty} \gamma^t R_t = R_0 + \gamma R_1 + \gamma^2 R_2 + \dots + \gamma^t R_t + \dots \quad (1)$$

This random variable<sup>1</sup> measures the cumulative reward of following a policy  $\pi$ .

**Where is “value” buffered in the DMN ?** The amygdala is known to be involved in evaluation of biological significance, whereas the NAc is involved in reward evaluation. Both are known to be connected to the vmPFC of the DMN.

The goal of the RL agent is then to adapt this policy so as to maximize  $G^\pi$ . In the definition of cumulative reward  $G^\pi$  above, the constant  $\gamma$  ( $0 \leq \gamma < 1$ ) is the reward *discount factor*. Setting  $\gamma = 0$  corresponds to a perfectly shortsighted agent who is solely concerned about its immediate rewards. Such an agent would have no horizon for the future, which is not compatible with long-term goal planning as potentially implemented in the DMN. To allow a learning process to arise, it is necessary that  $0 < \gamma < 1$ .  $\gamma$  can be seen as calibrating risk-seeking valency of the intelligent agent, that is, the decision related to reward-delay trade-off schedules. Such an agent puts relatively more emphasis on rewards expected in a short future and pays less attention to rewards expected at a later time, precisely rewards more than  $1/(1 - \gamma)$  time steps into the future are disregarded. This reduces the variance of expected rewards accumulated across action cascades by limiting the length of this cascades.

### 3.3 The Q-values, state-values, and the advantage function

We can now formulate the purpose of the DMN as finding a policy  $\pi$  for the human agent that maximizes the expected cumulative value of an state-action pair  $(a, s)$ , also known as the *Q-value*, namely

$$Q^\pi(s, a) = \mathbb{E}[G^\pi | s_0 = s, a_0 = a]. \quad (2)$$

In other words, the Q-value  $Q^\pi(s, a)$  corresponds to the expected reward over all possible action trajectories, in which the agent sets out in the environment in state  $s$ , chooses action  $a$ , and then follows the policy  $\pi$  to select future actions. For the brain,  $Q^\pi(s, a)$  defined in (2) provides the subjective utility of executing a specific action; it answers the question “What is the expected utility of taking action  $a$  in this situation?”.  $Q^\pi(s, a)$  offers a formalization of optimal behavior that may well reflect processing aspects of the DMN in human agents.

One can also define the state-value function

$$V^\pi(s) := \mathbb{E}_{a \sim \pi} Q^\pi(s, a) = \mathbb{E}[G^\pi | s_0 = s], \quad (3)$$

which measures the value of each state  $s \in \mathcal{S}$  under the policy  $\pi$ . This serves as a baseline value for any action. Finally, the advantage function is defined by

$$A^\pi(s, a) := Q^\pi(s, a) - V^\pi(s). \quad (4)$$

### 3.4 Efficient computation of optimal behavior

By construction, maximizing the expectation in (2) is computationally intractable in general. This is due to the enormous number of possible action trajectories that the agent often needs to consider simultaneously. One popular solution is called Q-learning. It remedies the issue by only considering the sub-family of *deterministic policies*, which map each state to the single best action to take at the current state. Such policies define deterministic functions from states to actions.

<sup>1</sup>Random as it depends both on the environment’s dynamic and the policy  $\pi$  being played (which can be stochastic).

### 3.4.1 Q-learning

Q-learning (Watkins & Dayan, 1992) generates a *greedy policy* **XXX please add 1-2 sentences why this is interesting in the current context. This statement appears a little alone as it stands.**

$$\pi^*(s) = \operatorname{argmax}_{a \in \mathcal{A}} Q^*(s, a), \quad (5)$$

which maps each state  $s$  to the optimal action which should be taken at that state. Here  $Q^*(s, a) := \max_{\pi} Q^{\pi}(s, a)$ , the optimal Q-value over all policies. The *Bellman equation* (Sutton and Barto, 1998) then takes the simple form

$$\begin{aligned} Q^*(s_0, a_0) &= \mathbb{E}_{s_1 \sim p(s_1 | s_0, a_0)} [r(s, a) + \gamma \max_{a_1 \in \mathcal{A}} Q^*(s_1, a_1)] \\ &= \mathbb{E}_{s_1 \sim p(s_1 | s_0, a_0)} [r(s_0, a_0) + \gamma Q^*(s_1, \pi(s_1))]. \end{aligned} \quad (6)$$

This consistency equation for the optimal (i.e., over all policies) Q-value function provides a recursive decomposition of optimal behavior by dividing the Q-value function into the immediate reward and the discounted rewards of the upcoming states. The optimal Q-value operator  $Q^*$  is a fixed point for this equation. A complicated dynamic programming optimization can be broken into simpler sub-problems at different time points. Exploitation of hierarchical structure in actions considerations has previously been closely related to the medial prefrontal part of the DMN (Koechlin et al., 1999; Braver and Bongiolatti, 2002). Using the Bellman equation, each state can be associated with a certain value to guide action towards a better state, thus improving on the agent's current policy. Note that in (6) the sampling is done only over things which depend on the environment, and so can be learned off-policy by observing state transitions triggered by another behavioral policy, which can be stochastic.

### 3.4.2 Efficient learning via value approximation and experience replay

A practically successful RL approach needs ways to efficiently approximate the state-action value function to allow for scaling to large state and action spaces. In a state  $s \in \mathcal{S}$ , the agent takes an action  $a \in \mathcal{A}$  by sampling from its current policy, and collects a reward  $r$ , after which the environment transitions to a new state  $s' \in \mathcal{S}$ . At the end of this cycle, a new *experience*  $e = (s, a, r, s')$  is produced, which represents an exemplar behavior of the agent and is recorded in replay memory buffer (possibly discarding the oldest entries to make space):

$\mathcal{D} \leftarrow \text{append}(\mathcal{D}, e)$ . At iteration  $k + 1$ , replay then consists in sampling (uniform or importance-weighted <sup>2</sup> ?) mini-batches of experiences  $(s, a, r, s') \sim \mathcal{D}$  from the replay memory  $\mathcal{D}$ . The agent then tries to approximate the would-be Q-value for the state-action pair  $(s, a)$  as predicted by the Bellman equation (6), namely

$$y_k := y_k(s, a, s') = r + \gamma \max_{a'} \tilde{Q}(s', a' | \theta_{k-1}), \quad (7)$$

with the prediction of a parametrized regression model  $(s, a) \mapsto \tilde{Q}(s, a | \theta_{k-1})$ . Here the function  $(s, a) \mapsto \tilde{Q}(s, a | \theta_{k-1})$  is an approximator for the Q-value operator, parameterized by weights  $\theta_k$  (synaptic strengths, etc.).

From a neurobiological perspective, experience replay would be manifested as the re-occurrence of a neuron spiking sequence that also occurs during specific actions. In the human brain, the hippocampus is likely to contribute to such a mechanism, as neuroscience experiments on various animals have repeatedly indicated in rats, mice, cats, rabbits, songbirds, and monkeys Buhry et al. (2011); Nokia et al. (2010); Dave and Margoliash (2000); Skaggs et al. (2007).

Computing an optimal policy then corresponds to finding the parameters  $\theta_k$  which minimize the following mean-squared loss function

$$\mathcal{L}(\theta_k^Q) = \mathbb{E}_{(s, a, r, s') \sim \mathcal{D}} \left[ \frac{1}{2} (\tilde{Q}(s, a | \theta_k) - y_k)^2 \right], \quad (8)$$

<sup>2</sup>e.g weighted by TD error of the state transition  $s \xrightarrow{a} s'$ .

where  $y_k$  is defined in (6). For instance, a general linear model with a kernel  $\phi$  would be of the form

$$\tilde{Q}(s, a|\theta) = \phi(s, a)^T \theta.$$

$\phi(s, a)$  would represent a high-level hand-crafted representation of the state-action pairs  $(s, a)$ , as proposed by (Song et al., 2016) for example. A recently proposed, practically successful alternative approach (Mnih et al., 2015; Silver et al., 2016) is to learn this representation using a deep neural network, leading to the so-called *Deep Q-learning* family of methods which likely are state-of-the-art in RL. The set of  $\theta$  parameters that instantiate the nonlinear interactions between layers of the artificial neural network may find a neurobiological correspondence in the adaptive strengths of axonal connections between neurons from the different levels of the neural processing hierarchy (Mesulam, 1998; Taylor et al., 2015).

Learning of the entire model parameters can effectively be achieved via *backpropagation*, where reward prediction errors (RPEs) – also known as *regret* – percolate from lower to higher processing layers to modulate the choice of future actions

$$\delta\theta_k \propto -\nabla_{\theta_k} \mathcal{L}(\theta_k) = -\mathbb{E}_{(s,a,r,s') \sim \mathcal{D}} \left[ \underbrace{(\tilde{Q}(s, a|\theta_k) - y_k)}_{\text{prediction error}} \underbrace{\nabla_{\theta_k} \tilde{Q}(s, a|\theta_k)}_{\text{averseness}} \right]. \quad (9)$$

### 3.4.3 Link to classical reinforcement learning algorithms

One should note that most classical RL algorithms, including *Temporal Difference (TD)* learning (Sutton and Barto, 1998), REINFORCE (Williams, 1992), and SARSA can be cast in this **please unpack the "this" here** general variational framework. For instance, TD corresponds to the above framework using a linear value approximator with feature encoding  $\phi(s, a) = \delta_{(s,a)}$  = point mass at  $(s, a)$  on the grid  $\mathcal{S} \times \mathcal{A}$ , and so

$$\nabla_{\theta} \tilde{Q}(s, a|\theta) = \phi(s, a) = \delta_{(s,a)}.$$

Whence, the gradient update due to the sample  $(s, a, r, s') \in \mathcal{D}$  is

$$\theta(s, a) \leftarrow \theta(s, a) + \alpha(\tilde{Q}(s, a|\theta) - y),$$

the well-known TD update rule (Sutton and Barto, 1998).

### 3.4.4 Excursion: the role of the hippocampus

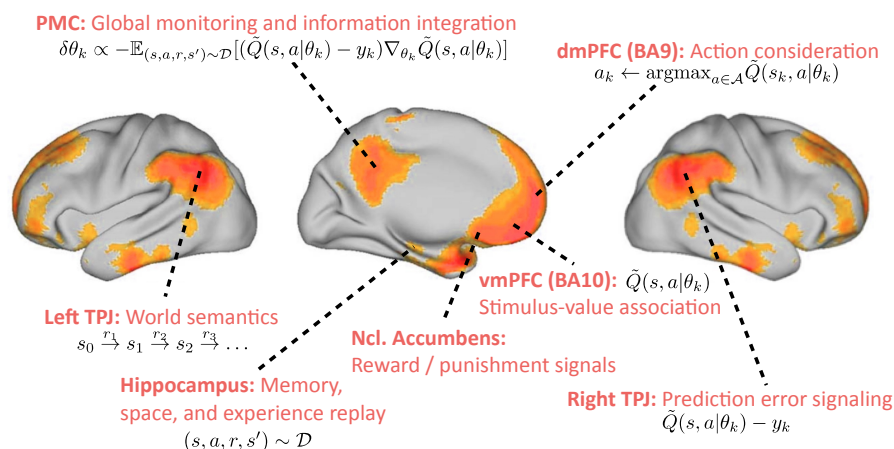
**Does the hippocampus subserve Monte-Carlo sampling?** In RL, Monte-Carlo simulation can be used to update the agent's belief state (Silver and Veness, 2010). Such methods have a sample complexity that is determined only by the underlying difficulty of the POMDP, rather than the size of the state space or observation space, which can be prohibitively large. Monte-Carlo simulation provides a simple method for evaluating the value / fitness of a state. They provide an effective mechanism both for tree search and for belief state updates, breaking the curse of dimensionality and allowing much greater scalability than a RL agent without stochastic resampling procedures.

In the human brain, the HC could contribute to synthesizing imagined sequences of world states, observations and rewards (Aronov et al., 2017; Chao et al., 2017). These simulations would be used to update the value function, without ever looking inside the black box describing the model's dynamics. This would be a simple control algorithm by evaluating all legal actions and selecting the action with highest expected cumulative rewards. In POMDPs, Monte-Carlo simulation provides an effective mechanism both for tree search and for belief-based state updates, breaking the curse of dimensionality and allowing much greater scalability than has previously been possible. **XXX Elvis: refs needed..** Much recent work points to Monte Carlo or stochastic sampling-based approximations as a unifying framework for understanding how Bayesian inference may work practically across all these levels, in minds, brains, and machines. **XXX Elvis: refs needed in last sentence. Plus, should be really bring up Bayesian?** For sampling-based methods it is still almost non-existent beyond the description of receptive fields. **XXX Elvis: rephrase last sentence**

**Does hippocampal replay equal inverse reinforcement-learning?** Given the trace  $s_0, a_0, s_1, \dots$ , of an optimal agent's strategy  $\pi^*$  in a POMDP (called a *teacher's demonstration*), can we figure out what is the (instantaneous) reward function  $r : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$  that the agent is optimizing over a prescribed class of reward functions (e.g., linear rewards  $r(s, a) \equiv \theta^T \phi(s, a)$ )? For instance, given traces of motor actions from an adult to grab a cup on a table, can an observing child figure out what “lagrangian” functional is being minimized by the former? How? Can they reproduce this optimal behavior? Such questions are of course pertinent to our decision-making theory for the DMN. In the general artificial case, the problem has been extensively studied and partially solved by Abbeel and Ng (2004). They are also been rigorously studied in general optimal control literature under the name “inverse optimal control”, but in model-based certain (where the physical dynamics are known, etc.)... IRL is suited for problems in which it's hard to define what the reward function could be (e.g., car-driving, drone maneuvering, etc.) ...

### 3.5 Putting everything together

The DMN is today known to consistently increase in neural activity when humans engage in goal-directed behavior that are detached from current sensory environment (Kenet et al., 2003; Fiser et al., 2004) and it was proposed to be situated at the top of the functional network hierarchies (Carhart-Harris and Friston, 2010; Margulies et al., 2016). Its putative involvement in thinking about the past, the future, and hypothetical possibilities appears to tie in with the implicit computation of action and state cascades as a function of what happened in the past. A policy represents the repertoire of possible actions on the world given a current state. It encodes the probabilities of choosing actions to be executed in a certain situation. The DMN may subserve constant exploration of possible future actions and their cumulative reward outcomes. Implicit computation of future choices provides an explanation for the evolutionary emergence and practical usefulness of mind-wandering in humans.



future scenarios and action outcomes. Our account of DMN function thus acknowledges the unavoidable stochasticity of computation in neuronal processes (Faisal et al., 2008).

From the perspective of our model-free RL agent, *inference* in the human brain reduces to generalization of policy and value adaptations from sampled experiences to successful action choices and reward predictions in future states. As such, plasticity in the DMN arises naturally: If an agent behaving optimally in a given environment moves to novel, yet unexperienced environments, reward prediction errors will massively increase **Please check/simplify sentence**. This will lead to adaptation of the policy until the system converges to a new steady-state of optimal action decisions in volatile environments.

## 4 Relation to other models decision-making and optimal control for the brain

### 4.1 Predictive coding hypothesis

Predictive coding mechanisms (Clark, 2013; Friston, 2008) are a frequently evoked idea in the context of default mode function (Bar et al., 2007). Cortical responses are explained as emerging from continuous functional interaction between higher and lower levels of the neural processing hierarchy. Feed-forward sensory processing is constantly calibrated by top-down modulation from more multi-modal and associative brain regions further away from primary sensory cortical regions. The dynamic interplay between cortical processing levels may enable inferences about the world by reconciling gaps between fresh sensory input and expectations computed from stored prior information. At each stage of neural processing, an internally generated prediction of aspects of sensory sensation is directly compared against the actual environmental input. A prediction error at one of the processing levels incurs plasticity changes of neuronal back projections (i.e., adapting model parameters) to allow for gradually improved future prediction of the environment. In this way, the predictive coding hypothesis offers explanations for the constructive, generative nature of sensory perception (Friston, 2010) and the intimate relation of motor action to sensory expectations (Wolpert et al., 1995; K rding and Wolpert, 2004). Contextual sensorimotor integration of perception-action cycles may be maintained by top-down modulation by a-priori information about the environment.

Predictive coding processes permit updates of the internal representation of the environment to best accommodate and prepare the organism for the constant influx of sensory examples and for reacting to the environment. There are hence a number of common properties between the predictive coding account and the proposed formal account. Importantly, a generative model of how perceived sensory cues arise in the world would be incorporated into the current neuronal wiring. Further, both frameworks are plausibilized by neuroscientific evidence that suggest the human brain to be a “statistical organ” with the biological purpose to generalize from the past to new experiences. Neuroanatomically, axonal back projections indeed outnumber by far the axonal input projections existing in the primate brain (Salin and Bullier, 1995). Moreover, both accounts provide a parsimonious explanation why the human brain decreases processing load devoted to incoming information when the environment is predictable because the internal generative model only requires updating following discrepancies between environmental reality and its internal reinstantiation. Increased computation resources are however allocated when novel stimuli or unexpected events are encountered by the organism. The predictive coding and formal account naturally evoke a mechanism of brain plasticity in that neuronal wiring gets increasingly adapted when faced by unprecedented environmental challenges.

While sensory experience is a generative process from both views, the predictive coding account frames sensory perception of the external world as a generative experience due to the modulatory top-down influence at various stages of sensory input processing. In our RL view, instead, the Markov property of our sequential decision making framework entails the environmental model to be **effectively expressed in the current state of the human agent XXX guys, please double-check**. Further, the hierarchical processing aspect from predictive coding is re-expressed in our account in form of nested prediction of probable upcoming actions, states, and rewards. Both frameworks model the consequences of action. The predictive coding framework is typically explained without explicit parameterization of the



agent's horizon and has a tendency to be presented as emphasizing prediction about the immediate future. In the present account, the horizon of that look into the future is explicitly expressed in the  $\gamma$  parameter of the Bellman equation. Finally, the process of adapting the neuronal connections for improved top-down modulation takes the concrete form of gradient computation and back-propagation in our RL implementation. It is however important to note that the neurobiological plausibility of the back-propagation procedure is controversial (Goodfellow et al., 2016). In sum, the present formal account may serve as a concrete implementation of the long-standing predictive coding account from cognitive neuroscience. MPDs have the advantage of exposing an explicit mechanism for the horizon of future considerations or how the internal model of the world gets updated, and more explicitly reconciles sensory input processing and action consideration. Recasting DMN function in terms of MDPs therefore naturally incorporates a majority of aspects of the prediction coding hypothesis.

## 4.2 Semantic hypothesis

Another frequently proposed cognitive account of DMN function revolves around forming logical associations and analogies between the current experience and the conceptual knowledge derived from past experiences (Bar, 2007; Binder et al., 1999). Analogies might naturally tie incoming novel sensory stimuli to explicit world knowledge (i.e., semantics) extracted from the environment (Bar, 2009). The encoding of complex environments could thus be facilitated by association to similar states. Going beyond human language itself, semantic building blocks may provide the basis for mentally envisioning non-existent scenarios that would optimize behavior in the environment by constantly simulating possible future events. Such cognitive processes can afford the internal generation of necessary information that is not presented in the surrounding environment by recombining building blocks of concept knowledge and episodic memories (Hassabis and Maguire, 2009). Indeed, in aging humans, remembering the past and imaging the future equally decreased in the level of detail and were associated with concurrent deficits in forming and integrating relationships between items (Addis et al., 2008; Spreng and Levine, 2006). Further, a constructive account can explain the reciprocal relationship between an egocentric first person perspective and an allocentric birds eye perspective immersed in self-reflection, semantic associations, and autobiographical memories. Cognitive aspects of egocentric-allocentric switching are also closely related to episodic memory, language, problem solving, planning, estimating other people's thoughts, and spatial navigation. These neural processes are likely to build on abstract world knowledge and logical associations for integrating the constituent elements in mental scene construction (Schacter et al., 2007). Such scene generation processes could contribute to interpreting the present and foretelling the future. Mental scene construction has been proposed to imply a distinction between engagement in the sensory environment and internally generated mind-wandering (Buckner and Carroll, 2007). These authors stated that "A computational model [...] will probably require a form of regulation by which perception of the current world is suppressed while simulation of possible alternatives are constructed, followed by a return to perception of the present.". The semantic hypothesis is for instance supported by evidence in animals that could learn a *cognitive map of the environment*, even without reward incentives, and exploit it later for other means (Tolman, 1948).

In comparison, both the semantic hypothesis and MDPs expose mechanisms of how action considerations could be mentally explored. In both accounts, there is also no evidence to indicate that predictions of various levels of complexity, abstraction, timescale and purpose use mechanisms that are qualitatively different. This concurs with DMN activity increases across time, space, and content domains demonstrated in many neuroimaging studies (Spreng et al., 2009). The semantic hypothesis and MDP account provide explanations why hippocampus lesion does not only impair recalling memories, but also hypothetical and future thinking (Hassabis et al., 2007). While both semantic hypothesis and our formal account propose memory-based internally generated information for probabilistic mental models of action outcomes, MDPs render explicit the grounds on which the final action is eventually chosen, namely, the estimated cumulative reward. **The notion of semantic knowledge associations is incorporated into the MDP as the Markov property, that is, the**

**current state directly results from the agent's history of states and actions. The learned estimations of value and action transitions drive stimulus processing and action choice in the present.** The MDPs naturally integrate the former egocentric (more related to current action, state and reward) and the later allocentric (more related to past and future actions, states, and rewards) angles on the world in a same optimization problem. Further, the semantic account of DMN function does not offer a mechanistic explanation how explicit world knowledge and semantic analogies thereof lead to prediction of future actions and states. The semantic hypothesis does not explain why memory recall for scene construction in humans is typically fragmentary and noisy instead of accurate and reliable. In contrast to existing accounts on semantics and mental scene construction, the random and creative aspects of DMN function are explained in MDPs by the advantages of stochastic optimization. Yet, the MDP framework provides an algorithmic explanation in that stochasticity of the parameter space explored by the Monte Carlo solvers achieves better fine-tuning of the action policies and estimation of expected reward outcomes. That is, the purposeful stochasticity of policy and value estimation in MDPs provides a candidate explanation for why humans have evolved imperfect noisy memories as the more advantageous adaptation. In sum, episodic scene construction according to the semantic account is lacking an explicit time and incentive model.

### 4.3 Sentinel hypothesis

Processing self-relevant information was perhaps the first cognitive account that was proposed for the DMN (Gusnard et al., 2001). Since then, many investigators have speculated that neural activity in the DMN may reflect the brain's continuous tracking of relevance in the environment as an advantageous evolutionary adaptation (Buckner et al., 2008; Hahn et al., 2007). According to this cognitive account, the human brain's baseline realizes a "radar" function to detect subjectively salient cues and unexpected events in the environment. Propositions of such a sentinel function have however seldom detailed the mechanisms of how attention and memory resources are exactly reallocated when encountering a salient environmental stimulus. In the present formal account, promising action trajectories are recursively explored by human agents. Conversely, certain branches of candidate action trajectories are detected to be less worthy to become mentally explored. This mechanism, expressed by the Bellman equation, directly implies stratified allocation of attention and working memory load over relevant cues and events in the environment. Further, our account provides a parsimonious explanation for the increasingly recognized observation of the DMN implication in certain goal-directed experimental tasks and in task-unconstrained mind-wandering (Smith et al., 2009; Bzdok et al., 2016). Both cognitive sets may entail DMN recruitment if environmental relevance is processed, manipulated, and used for predicting the future. During tasks, the policy and value estimates may be updated to optimize especially short-term action. At rest, these parameter updates may improve especially mid- and long-term action. The horizon is expressed in the  $\gamma$  parameter in the formal account. We thus provide answers for the unsettled question why the involvement of the same neurobiological brain circuit (i.e., DMN) has been documented for baseline house-keeping functions and specific task performances.

More specifically, environmental stimuli especially important for humans are frequently of social nature. This is probably unsurprising given that the complexity of the social systems is a likely human-defining property (Tomasello, 2009). According to the "social brain hypothesis", the human brain has especially been shaped for forming and maintaining increasingly complex social systems, which allows solving ecological problems by social relationships (Whiten and Byrne, 1988). Indeed, social topics amount to roughly two thirds of human everyday communication (Dunbar et al., 1997), while mind-wandering at daytime and dreams during sleep are rich in stories about people and the complex relationships between them. In line with this, the DMN has been proposed to reflect continuous processing of social information as a physiological baseline of human brain function (Schilbach et al., 2008). This view was later challenged by observing analogues of the DMN in monkeys (Mantini et al., 2011) and rats (Lu et al., 2012), both species with supposedly less advanced social-cognitive capacities. Rather than functional specificity for processing social information, the present formal account can parsimoniously incorporate the dominance of social content in human mental activity as high

value function estimates for information about humans (Baker et al., 2009; Kampe et al., 2001; Krienen et al., 2010). The DMN may thus exert control on the human agent in a way that prioritizes appraisal of and action towards social contexts, without entirely neglecting environmental cues of the physical world. In sum, our account on the DMN directly implies its previously proposed “sentinel” function of monitoring the environment for salient information in general and inherently incorporates the importance of social environmental cues as an important special case.

#### 4.4 The free-energy principle and active inference XXX move to Appendix

In Friston’s free-energy principle (FEP) (Friston, 2010; Friston et al., 2009), the brain is portrayed as biomechanical inference engine which must minimize the long-term average of surprise. Precursors of this theory can be traced back to (Dayan et al., 1995) in which they introduced the so-called *Helmholtz machine*, a hierarchical factorial *directional deep belief-net* (DBN). According to FEP’s account, the goal of the brain is then to optimize over the generative model  $G$ : to iteratively modify its internal representation  $p_G(\mathbf{z}|\mathbf{x})$  about objects in the world, their interactions and dynamics, etc., so as to minimize surprise when these representations are confronted with sensory input  $\mathbf{x}$  during perception cycles. This is called the *generative* model. FEP also postulates a dual model called the *recognition* model, which works in tandem with the generative model  $p_R(\mathbf{z}|\mathbf{x})$ , to accomplish approximate inference. The recognition model dreams / fantasizes imaginary worlds  $\mathbf{z}$  whilst the latter tries to generate sensations  $\mathbf{x}$  which match these dreams!

Because surprisal is intractably difficult to optimize (since we would need to sum over all hidden causes of the sensations), FEP sets out to instead minimize an upper-bound thereupon, namely the free-energy  $F_G^R(\mathbf{x})$  given by

$$\begin{aligned} \text{generative surprise} &:= -\log(p_G(\mathbf{x})) = F_G(\mathbf{x}) \\ &= \underbrace{F_G^R(\mathbf{x})}_{\text{accuracy}} - \underbrace{D_{KL}(P_R(\cdot|\mathbf{x})||P_G(\cdot|\mathbf{x}))}_{\text{complexity}} \\ &\leq F_G^R(\mathbf{x}), \text{ with equality if } p_R(\mathbf{z}|\mathbf{x}) = p_G(\mathbf{z}|\mathbf{x}) \text{ for all } \mathbf{z} \end{aligned} \quad (10)$$

The main algorithm for minimizing free-energy  $F_G^R(\mathbf{x})$  is the *wake-sleep algorithm*. (Dayan et al., 1995). As noted already in (Dayan et al., 1995), a crucial drawback of the wake-sleep algorithm is that it postulates a pair forward (generation) and backward (recognition) models, which together do not correspond to optimization of (a bound of) the marginal likelihood, because of the incorrect KL used therein, etc. Thus the brain could not possibly be running such an algorithm, not even in principle! To the rescue, we note that the recent theory of *variational auto-encoders* (VAEs) (Kingma and Welling, 2013) might provide an efficient alternative to the wake-sleep algorithm, as it overcomes the technical limits of the former, by using a reparametrization trick. For instance, unlike the wake-sleep algorithm for minimizing free-energy, VAEs can be efficiently trained via back-propagation of learning errors.

##### 4.4.1 Comparison to our proposed theory

On the surface, a common point between the FEP and our proposed RL-based framework is placing the minimization of a surprise signal at the core of brain function. Indeed in RL, surprise minimization is subsumed by accurate prediction of rewarding outcomes in the future. A “free-energy” agent is barely a biomechanical machine which has the tendency to resist undesired / harmful phase-transitions. (Friston, 2010; Friston et al., 2009; Ortega and Braun, 2013). Such a theory cannot by itself, explain the emergence of strategic behavior inherent in humans (e.g., cite dark-room experiment).

**XXX: add tons of more examples and connections XXX: integrate aspects from section “The MARKOV DECISION PROBLEM” in Dayan and Daw XXX: integrate aspects from WakeNsleep by Hinton XXX: integrate aspects from**

Friston2014(Dropbox) on active inference XXX: integrate aspects from Sutton/Barto book chapter

## 5 Conclusion

What brain function could be important enough for the existence and survival of the human species to warrant constant, high energy costs? MDPs provide an attractive process model how the human association cortex might implement supra-modal representation and control of the environment to optimize the organism's fate. This idealized process model explains a number of previous experimental observations in the DMN by a simple but non-trivial mechanism. From the computational view of a Markovian sequential decision process, behavior unfolds by integrating happened past events and possible future events to guide action choice in the present context. This functional account is more compatible with the DMN's poorly understood involvement across autobiographical memory recall, problem solving, abstract reasoning based on internally generated scenes, social cognition, as well as delay discounting and self-related prospection. MDPs provide a mathematical formalism how optimal substructure in the environment can be recursively exploited when confronted with complicated decisions. Improvement of the internal world model by injecting stochasticity in the recall of past actions and outcomes may explain why very accurate memories have been disfavored in human evolution and why human creativity might be adaptive. In principle, neuroscientific experiments can be designed that operationalize the set of action, value, and state variables that determine the behavior of intelligent RL systems. The proposed machine-learning perspective on DMN biology is hence not only practically computable but also yields falsifiable neuroscientific hypotheses. At the least, we propose an alternative vocabulary to describe and interpret experimental findings in neuroscience studies on the DMN. Ultimately, the DMN can be viewed as a functional integrator from the relatively recent events to anticipated upcoming events in order to constantly improve action in our dynamic world.

## Acknowledgment

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## A Free-energy principles!

The so-called free-energy principle in its present form (including notions like “generative density”, “recognition density”, etc.) can be traced back to works of Dayan & Hinton (Dayan et al., 1995) in which they introduced the so-called *Helmholtz machine*, a hierarchical factorial directional deep belief-net (DBN). In this subsection, we will develop from first-principles, the bare-bones minimalistic ideas needed to build a free-energy principle for general decision-making. This ideas were first developed by Hinton et al. in the early 90s in building their Helmholtz machine. Theories like Friston’s free-energy principle and active-inference will then emerge as particular instances of this general framework, with particular design choices. For instance, the Friston theory axiomatizes that the brain uses a (problematic, as it implicitly assumes that posterior of each hidden unit is factorial) wake-sleep algorithm to train the underlying Helmholtz machine, etc.



## A.1 Helmholtz free-energy and the generative model

| symbol                | description   |
|-----------------------|---|
| $\langle X \rangle_p$ | Expectation (a.k.a average, a.k.a mean value) of the random quantity $X$ w.r.t to the probability density $p$ , formally defined by $\langle E \rangle_p := \sum_z p(z)X(z)$ .    |
| $\mathcal{H}(p)$      | Information-theoretic entropy of a probability density $p$ , formally defined by $\mathcal{H}(p) := -\sum_z p(z) \log(p(z))$ , with the usual convention $0 \log(0) := 0$ .       |
| $D_{KL}(q  p)$        | The Kullback-Leibler divergence between the probability densities $q$ and $p$ respectively, formally defined by $D_{KL}(q  p) := \sum_z q(z) \log(q(z)/p(z))$ .                   |
| $\mathbf{x}$          | Observations. In Friston's free-energy principle this has a decomposition in to two terms: the brain's internal state $b$ and sensory inputs $s$ , i.e $\mathbf{x} = (s, b)$ .    |
| $\mathbf{z}$          | Hidden variables. This should be understood as the unobservable states of the external environment (to which the brain is trying to adapt by learning).                           |
| $p_G(. \mathbf{x})$   | Generative density for ...  |
| $p_R(. \mathbf{x})$   | Recognition density for ... Does some kind of predictive coding (?).  |
| $F_G(\mathbf{x})$     | Helmholtz free-energy for a model $p_G$ of generating the observation $\mathbf{x}$ . This measures the surprise incurred upon observing $\mathbf{x}$ generated by the model $G$ . |
| $F_G^R(\mathbf{x})$   | Variational Helmholtz free-energy from model $G$ to $R$ . Note that $F_G^G = F_G$ .   |

**Table 1.** Table of notations.

Our starting point will be to build an approximation  $p_G$  for the true density  $p$  of the observations, so that this approximate density corresponds to the partition function of thermodynamic system. So,

$$\begin{aligned}
 \text{generative surprise} &= -\log(p_G(\mathbf{x})) = -\log(p_G(\mathbf{x})) \times 1 = -\log(p_G(\mathbf{x})) \sum_{\mathbf{z}} p_G(\mathbf{z}|\mathbf{x}) \\
 &= -\sum_{\mathbf{z}} p_G(\mathbf{z}, \mathbf{x}) \log(p_G(\mathbf{x})) = -\sum_{\mathbf{z}} p_G(\mathbf{z}|\mathbf{x}) \log(p_G(\mathbf{z}, \mathbf{x})/p_G(\mathbf{z}|\mathbf{x})) \\
 &= \sum_{\mathbf{z}} p_G(\mathbf{z}|\mathbf{x}) \log(p_G(\mathbf{z}|\mathbf{x})) - \sum_{\mathbf{z}} p_G(\mathbf{z}|\mathbf{x}) \log(p_G(\mathbf{z}, \mathbf{x})) \\
 &= -\langle \log(p_G(., \mathbf{x})) \rangle_{p_G(.|\mathbf{x})} - \mathcal{H}(p_G(.|\mathbf{x})) \\
 &= \langle E_G(., \mathbf{x}) \rangle_{p_G(.|\mathbf{x})} - \mathcal{H}(p_G(.|\mathbf{x}))
 \end{aligned} \tag{11}$$

where  $E_G(\mathbf{z}, \mathbf{x})$  is the energy at *macrostate*  $\mathbf{z}$  of a fictive thermodynamic system defined by setting

$$E_G(\mathbf{z}, \mathbf{x}) := -\log(p_G(\mathbf{z}, \mathbf{x})), \tag{12}$$

The last quantity in (11) is nothing but *Helmholtz free-energy* (at unit temperature!), defined formally by

$$F_G(\mathbf{x}) := \langle E_G(., \mathbf{x}) \rangle_{p_G(.|\mathbf{x})} - \mathcal{H}(p_G(.|\mathbf{x})). \tag{13}$$

Thus,

**Fact A.1.** *Generative surprise and generative Helmholtz free-energy are different views on exactly the same object.*

The goal of the brain is then to optimize over the generative model  $G$ : to iteratively or analytically modify the generative density  $p_G(.|\mathbf{x})$ , so as to minimize surprise. It turns out that a direct attempt to attack this optimization problem by gradient descent on the free-energy  $F_G(\mathbf{x})$  is futile: the parameter update steps are not “very clean”, and require rather

cumbersome and heavy computations. A workaround is then to introduce a second density  $p_R(\cdot|\mathbf{x})$  called a *recognition* density to work in tandem with the generative density  $p_G(\cdot|\mathbf{x})$ , as a trick for doing approximate inference. The former dreams / fantacizes whilst the latter tries to generate sensations which match these dreams! This primal-dual idea, first proposed in Hinton et al. 1995, is at the heart of the general free-energy principle that we will introduce shortly.

## A.2 Variational Helmholtz free-energy and the bottom-up recognition sub-model

In this subsection, we will present an insightful upper bound for the generative surprise (i.e. generate Helmholtz free-energy), called the *variational* (Helmholtz) free-energy. As an avant-gout of what is to come shortly, let's just note that the well-known *free-energy principle* is simply a workaround whereby the minimization surprise (intractable) is replaced with the minimization a carefully chosen upper bound thereof.

Invoking (12) and applying Bayes rule, we get the Gibbs distribution

$$p_G(\mathbf{z}|\mathbf{x}) = \frac{p_G(\mathbf{z}|\mathbf{x})}{p_G(\mathbf{x})} = \frac{\exp(-E_G(\mathbf{z}, \mathbf{x}))}{Z_G(\mathbf{x})} = \frac{\exp(-E_G(\mathbf{z}, \mathbf{x}))}{Z_G(\mathbf{x})}, \quad (14)$$

where  $Z_G(\mathbf{x}) := \log(p_G(\mathbf{x})) = \sum_{\mathbf{z}'} \exp(-E_G(\mathbf{z}', \mathbf{x}))$ , the normalizing *partition function* for the model 12. Whence, for any macrostate  $\mathbf{z}$ , we have  $p_G(\mathbf{x}) = Z_G(\mathbf{x}) = \exp(-E_G(\mathbf{z}, \mathbf{x}))/p_G(\mathbf{z}|\mathbf{x})$ , and so it holds that

$$F_G(\mathbf{x}) \stackrel{(11)}{=} -\log(p_G(\mathbf{x})) = -\log(Z_G(\mathbf{x})) = E_G(\mathbf{z}, \mathbf{x}) + \log(p_G(\mathbf{z}|\mathbf{x})). \quad (15)$$

Now, in the above equation, the LHS only depends on the generative model  $G$  and the data point  $\mathbf{x}$ : it doesn't depend on the hidden variable  $\mathbf{z}$ , etc. So, taking expectations w.r.t an arbitrary density<sup>3</sup>  $p_R(\cdot|\mathbf{x})$  yields

$$\begin{aligned} F_G(\mathbf{x}) &= -\log(Z_G(\mathbf{x})) = \langle E_G(\cdot, \mathbf{x}) \rangle_{P_R(\cdot|\mathbf{x})} + \sum_{\mathbf{z}} p_R(\mathbf{z}|\mathbf{x}) \log(p_G(\mathbf{z}|\mathbf{x})) \\ &= \langle E_G(\cdot, \mathbf{x}) \rangle_{P_R(\cdot|\mathbf{x})} - \mathcal{H}(p_R(\cdot|\mathbf{x})) - \sum_{\mathbf{z}} p_R(\mathbf{z}|\mathbf{x}) \log(p_R(\mathbf{z}|\mathbf{x})/p_G(\mathbf{z}|\mathbf{x})) \\ &= F_G^R(\mathbf{x}) - D_{KL}(P_R(\cdot|\mathbf{x})||P_G(\cdot|\mathbf{x})), \end{aligned} \quad (16)$$

where  $F_G^R(\mathbf{x})$  is the *variational* Helmholtz free-energy from  $R$  to  $G$  defined by

$$F_G^R(\mathbf{x}) := \langle E_G(\cdot, \mathbf{x}) \rangle_{P_R(\cdot|\mathbf{x})} - \mathcal{H}(p_R(\cdot|\mathbf{x})) \quad (17)$$

and  $D_{KL}(P_R(\cdot|\mathbf{x})||P_G(\cdot|\mathbf{x}))$  is the Kullback-Leibler divergence between the  $p_R(\cdot|\mathbf{x})$  and the generative density  $p_G(\cdot|\mathbf{x})$ . Note that  $F_G^G = F_G$ .

## A.3 A general free-energy principle

We can resume the situation as follows<sup>4</sup>:

$$\begin{aligned} \text{generative surprise} &:= -\log(p_G(\mathbf{x})) = F_G(\mathbf{x}) \\ &= \underbrace{F_G^R(\mathbf{x})}_{\text{accuracy}} - \underbrace{D_{KL}(P_R(\cdot|\mathbf{x})||P_G(\cdot|\mathbf{x}))}_{\text{complexity}} \\ &\leq F_G^R(\mathbf{x}), \text{ with equality if } p_R(\mathbf{z}|\mathbf{x}) = p_G(\mathbf{z}|\mathbf{x}) \text{ for all } \mathbf{z} \end{aligned} \quad (18)$$

<sup>3</sup>conditioning in  $P_R(\cdot|\mathbf{x})$  is because this density is selected from a world in which the sensory inputs and internal brain state vector  $\mathbf{x}$  is assumed already observed.

<sup>4</sup>Where we have used the fact that KL divergence is always nonnegative.

## A.4 Helmholtz machines and the wake-sleep algorithm

**Assumption:** In both generative and recognition components of the network, there is conditional independence of neurons in the same layer, given the data (i.e input from lower more primitive layers). Precisely

$$p_G(\mathbf{z}^{(l)}|\mathbf{x}) = \prod_{k=1}^{h_l} p_G(\mathbf{z}_k^{(l)}|\mathbf{x}), \quad p_R(\mathbf{z}^{(l)}|\mathbf{x}) = \prod_{k=1}^{h_l} p_R(\mathbf{z}_k^{(l)}|\mathbf{x})$$

## A.5 Friston’s active-inference and agency

This is nothing but an application of the Dayan’s wake-sleep algorithm for training a Helmholtz machine model of the brain...

The following critics can be made:

- As noted by Dayan et al. (*Variants of Helmholtz machines*), the inter-neuronal intra-layer independence assumption which is at the center of the HM becomes severely problematic as it is agnostic to the known organization of cortical layers...
- A drawback of the wake-sleep algorithm is that it requires a concurrent models (generative and recognition), which together do not correspond to optimization of (a bound of) the marginal likelihood (because of the incorrect KL used therein, etc.).
- Also, note that the wake-sleep algorithm doesn’t do backprop! This is due to technical difficulty in getting derivatives of loss function w.r.t recognition weights  $\mathbf{W}^R$ ).
- This difficulty was removed in the 2010s by (Kingma and Welling, 2013), and other groups, via a “reparametrization trick”.

## A.6 Minimizing free-energy via backprop: variational auto-encoders

Here, we present a way to alleviate some conceptual and computational issues with the free-energy framework presented thus far, by using the recent *variational auto-encoder* (VAE) theory (Kingma and Welling, 2013). Define the data-dependent auxiliary random function

$$f_{G,R}(\cdot, \mathbf{x}) : \mathbf{z} \mapsto \log(p_G(\mathbf{z}, \mathbf{x})) - \log(p_R(\mathbf{z}|\mathbf{x})). \quad (19)$$

Then we can rewrite the variational free-energy as

$$\begin{aligned} F_G^R(\mathbf{x}) &:= \langle E_G(\cdot, \mathbf{x}) \rangle_{p_R(\cdot|\mathbf{x})} - \mathcal{H}(p_R(\cdot|\mathbf{x})) = \langle E_G(\cdot, \mathbf{x}) + \log(p_R(\cdot|\mathbf{x})) \rangle_{p_R(\cdot|\mathbf{x})} \\ &= \langle -\log(p_G(\cdot, \mathbf{x})) + \log(p_R(\cdot|\mathbf{x})) \rangle_{p_R(\cdot|\mathbf{x})} \\ &= -\langle f_{G,R} \rangle_{p_R(\cdot|\mathbf{x})} \approx -\frac{1}{M} \sum_{m=1}^M f_{G,R}(\mathbf{z}^{(m)}), \text{ with } \mathbf{z}^{(1)}, \dots, \mathbf{z}^{(M)} \sim p_R(\cdot|\mathbf{x}), \text{ and } M \rightarrow \infty. \end{aligned}$$

**Problem:** How do we sample from the recognition density  $p_R(\cdot|\mathbf{x})$  in such a way that the sampling process is differentiable w.r.t the weights of the recognition network  $\mathbf{W}^R$  ?

**Solution: the reparametrization trick.**

- Choose  $\epsilon \sim p_{\text{noise}}$  (noise distribution, independent of  $\mathbf{W}^R$ )
- Set  $\mathbf{z} = g(\mathbf{W}^R, \mathbf{x}, \epsilon)$ , where  $g$  is an appropriate class  $\mathcal{C}^1$  function
  - results in a sample  $\mathbf{z} \sim p_R(\cdot|\mathbf{x})$ , from the correct posterior

The mapping  $g$  should be taught of as a “blurring” function which produces noisy versions  $\mathbf{z}$ , called *sensations*, of the true world state  $\mathbf{x}$ . The result is a scheme for training DBNs via good-old backprop! Refer to Fig. vae.pdf. Some examples of the reparametrization trick for a number of choices of the posterior distribution are given in Tab. 2.

| Posterior   | $p_R(. \mathbf{x})$             | noise                               | $g(\mathbf{W}^R, \mathbf{x}, \epsilon)$ | Also   |
|-------------|---------------------------------|-------------------------------------|---|--|
| Normal      | $\mathcal{N}(\mu, \sigma)$      | $\epsilon \sim \mathcal{N}(0, 1)$   | $\mu + \sigma \odot \epsilon$           | Location-scale family: Laplace, Elliptical, Students t, Logistic, Uniform, Triangular, ...           |
| Exponential | $\exp(\lambda)$                 | $\epsilon \sim \mathcal{U}([0, 1])$ | $-\log(1 - \epsilon)/\lambda$           | Invertible CDF: Cauchy, Logistic, Rayleigh, Pareta, Weibull, Reciprocal, Gompert, Gumbel, Erlan, ... |
| Other       | $\log \mathcal{N}(\mu, \sigma)$ | $\epsilon \sim \mathcal{N}(0, 1)$   | $\exp(\mu + \sigma \odot \epsilon)$     | Gamma, Dirichlet, Beta, Chi-squared, F, ...  |

**Table 2.** Reparametrization trick (Kingma and Welling, 2013) for a variety of models.

## A.7 GANs and other likelihood-free methods

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