Geometric Methods for Sampling, Optimisation, Inference and Adaptive Agents

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Abstract

In this chapter, we identify fundamental geometric structures that underlie the problems of sampling, optimisation, inference and adaptive decision-making. Based on this identification, we derive algorithms that exploit these geometric structures to solve these problems efficiently. We show that a wide range of geometric theories emerge naturally in these fields, ranging from measure-preserving processes, information divergences, Poisson geometry, and geometric integration. Specifically, we explain how (i) leveraging the symplectic geometry of Hamiltonian systems enable us to construct (accelerated) sampling and optimisation methods, (ii) the theory of Hilbertian subspaces and Stein operators provides a general methodology to obtain robust estimators, (iii) preserving the information geometry of decision-making yields adaptive agents that perform active inference. Throughout, we emphasise the rich connections between these fields; e.g., inference draws on sampling and optimisation, and adaptive decision-making assesses decisions by inferring their counterfactual consequences. Our exposition provides a conceptual overview of underlying ideas, rather than a technical discussion, which can be found in the references herein.

Keywords: information geometry; Hamiltonian Monte Carlo; Stein’s method; reproducing kernel; variational inference; accelerated optimisation; dissipative systems; decision theory; active inference.
1 Introduction

Differential geometry plays a fundamental role in applied mathematics, statistics, and computer science, including numerical integration [1–5], optimisation [6–11], sampling [12–16], statistics on spaces with deep learning [17,18], medical imaging and shape methods [19,20], interpolation [21], and the study of random maps [22], to name a few. Of particular relevance to this chapter is information geometry, i.e., the differential geometric treatment of smooth statistical manifolds, whose origin stems from a seminal article by Rao [23] who introduced the Fisher metric tensor on parametrised statistical models, and thus a natural Riemannian geometry that was later observed to correspond to an infinitesimal distance with respect to the Kullback–Leibler (KL) divergence [24]. The geometric study of statistical models has had many successes [25–27], ranging from statistical inference, where it was used to prove the optimality of the maximum likelihood estimator [28], to
the construction of the category of mathematical statistics, generated by Markov morphisms [29,30]. Our goal in this chapter is to discuss the emergence of natural geometries within a few important areas of statistics and applied mathematics, namely optimisation, sampling, inference, and adaptive agents. We provide a conceptual introduction to the underlying ideas rather than a technical discussion, highlighting connections with various fields of mathematics and physics.

The vast majority of statistics and machine learning applications involve solving optimisation problems. Accelerated gradient-based methods [31,32], and several variations thereof, have become workhorses in these fields. Recently, there has been great interest in studying such methods from a continuous-time limiting perspective; see, e.g., [33–40] and references therein. Such methods can be seen as 1st order integrators to a classical Hamiltonian system with dissipation. This raises the question on how to discretise the system such that important properties are preserved, assuming the system has fast convergence to critical points and desirable stability properties. It has been known for a long time that the class of symplectic integrators is the preferred choice for simulating physical systems [1,2,41–48]. These discretisation techniques, designed to preserve the underlying (symplectic) geometry of Hamiltonian systems, also form the basis of Hamiltonian Monte Carlo (HMC) (or hybrid Monte Carlo) methods [13,49]. Originally, such a theory of geometric integration was developed with conservative systems in mind while, in optimisation, the associated system is naturally a dissipative one. Nevertheless, symplectic integrators were exploited in this context [6–8]. More recently, it has been proved that a generalisation of symplectic integrators to dissipative Hamiltonian systems is indeed able to preserve rates of convergence and stability [9], which are the main properties of interest for optimisation. Followup work [10] extended this approach, enabling optimisation on manifolds and problems with constraints. There is also a tight connection between optimisation on the space of measures and sampling which dates back to [50,51]; we will revisit these ideas in relation to dissipative Hamiltonian systems.

Sampling methods are critical to the efficient implementation of many methodologies. Most modern samplers are based on Markov Chain Monte Carlo methods, which include slice samplers [52,53], piecewise-deterministic Markov chains, such as bouncy particle and zig-zag samplers [54–59], Langevin algorithms [60–62], interacting particle systems [63] and the class of HMC methods [12–14,49,64,65]. The original HMC algorithm was introduced in physics to sample distributions on gauge groups for lattice quantum chromodynamics [13]. It combined two approaches that emerged in previous decades, namely the Metropolis-Hastings algorithm and the Hamiltonian formulation of molecular dynamics [66–68]. Modern HMC relies heavily on symplectic integrators to simulate a deterministic dynamic, responsible for generating distant moves between samples and thus reduce their correlation, while at the same time preserving important geometric properties. This deterministic step is then usually combined with a corrective step (originally a Metropolis-Hastings acceptance step) to ensure preservation of the correct target, and with a stochastic process, employed to speed up convergence to the target distribution. We will first focus on the geometry of measure-preserving diffusions, which emerges from ideas formulated by Poincaré and Volterra, and form the building block of many samplers. In particular, we will discuss ways to “accelerate” sampling using irreversibility and hypoellipticity. We will then introduce HMC focusing on its underlying Poisson geometry, the important role played by symmetries, and its connection to geometric integration.

We then discuss the problem of statistical inference, whose practical implementation usually relies upon sampling and optimisation. Given observations from a target distribution, many estimators belong to the family of the so-called $M$ and $Z$ estimators [69], which are obtained by finding the parameters that maximises (or are zeros of) a parametrised set of functions. These include the maximum likelihood and minimum Hyvärinen score matching estimators [70,71], which are also particular instances of the minimum score estimators induced by scoring rules that quantify
the discrepancy between a sample and a distribution [72]. The Monge–Kantorovich transportation problem [73] motivates another important class of estimators, namely the minimum Kantorovich and \( p \)-Wasserstein estimators, whose implementation use the Sinkhorn discrepancy [74–76]. Our discussion of inference builds upon the theory of Hilbertian subspaces and, in particular, reproducing kernels. These inference schemes rely on the continuity of linear functionals, such as probability and Schwartz distributions, over a class of functions to geometrise the analysis of integral probability metrics which measure the worse case integration error. We shall explain how maximum mean, kernelised, and score matching discrepancies arise naturally from topological considerations.

Models of adaptive agents are the basis of algorithmic-decision-making under uncertainty. This is a difficult problem that spans multiple disciplines such as statistical decision theory [77], game theory [78], control theory [79], reinforcement learning [80], and active inference [81]. To illustrate a generic use case for the previous methodologies we consider active inference, a unifying formulation of behaviour—subsuming perception, planning and learning—as a process of inference [81–84]. We describe decision-making under active inference using information geometry, revealing several special cases that are established notions in statistics, cognitive science and engineering. We then show how preserving this information geometry in algorithms enables adaptive algorithmic decision-making, endowing robots and artificial agents with useful capabilities, including robustness, generalisation and context-sensitivity [85,86]. Active inference is an interesting use case because it has yet to be scaled—to tackle high dimensional problems—to the same extent as established approaches, such as reinforcement learning [87]; however, numerical analyses generally show that active inference performs at least as well in simple environments [88–94], and better in environments featuring volatility, ambiguity and context switches [91,92].

2 Accelerated optimisation

We shall be concerned with the problem of optimisation of a function \( V : \mathcal{M} \to \mathbb{R} \), i.e., finding a point that maximises \( V(q) \), or minimises \( -V(q) \), over a smooth manifold \( \mathcal{M} \). We will assume this function is differentiable to construct algorithms that rely on the flows of smooth vector fields guided by the derivatives of \( V(q) \).

Many algorithms in optimisation are given as a sequence of finite differences, represented by iterations of a mapping \( \Psi_{\delta t} : \mathcal{M} \to \mathcal{M} \), where \( \delta t > 0 \) is a step size. The analysis of such finite difference iterations is usually challenging, relying on painstaking algebra to obtain theoretical guarantees; such as convergence to a critical point, stability, and rates of convergence to a critical point. Even when these algorithms are seen as discretisations of a continuum system, whose behaviour is presumably understood, it is well-known that most discretisations break important properties of the system.

2.1 Principle of geometric integration

Fortunately, here comes into play one of the most fundamental ideas of geometric integration: many numerical integrators are very close—exponentially in the step size—to a smooth dynamics generated by a shadow vector field (a perturbation of the original vector field). This allows us to analyse the discrete trajectory implemented by the algorithm using powerful tools from dynamical systems and differential geometry, which are a priori reserved to smooth systems. Crucially, while numerical integrators typically diverge significantly from the dynamics they aim to simulate, geometric integrators respect the main properties of the system. In the context of optimisation this means respecting stability and rates of convergence. This was first demonstrated in [9] and further extended in [10]; our following discussion will be based on these works.
The simplest way to construct numerical methods to simulate the flow of a vector field $X$ arises when it is given by a sum, $X = Y + Z$, and the flows of the individual vector fields $Y$ and $Z$ are—analytically or numerically—tractable. In such a case, we can approximate the exact flow $\Phi_t X = e^{tX}$, for step size $\delta t > 0$, by composing the individual flows $\Phi_{\delta t} Y = e^{\delta tY}$ and $\Phi_{\delta t} Z = e^{\delta tZ}$. The simplest composition is given by $\Psi_{\delta t} X = \Phi_{\delta t}^Y \circ \Phi_{\delta t}^Z$. The Baker–Campbell–Hausdorff (BCH) formula then yields

$$e^{\delta tY} \circ e^{\delta tZ} = e^{\delta tX}, \quad X = (Y + Z) + \frac{1}{2}[Y, Z] \delta t + \frac{1}{12} ([Y, [Y, Z]] - [Z, [Y, Z]]) \delta t^2 + \cdots,$$

where $[Y, Z] = YZ - ZY$ is the commutator between $Y$ and $Z$. Thus, the numerical method itself can be seen as a smooth dynamical system with flow map $\Psi_{\delta t} X = e^{\delta tX}$. The goal of geometric integration is to construct numerical methods for which $X$ shares with $X$ the critical properties of interest; this is usually done by requiring preservation of some geometric structure.

Recall that a numerical map $\Psi_{\delta t} X$ is said to be of order $r \geq 1$ if $|\Psi_{\delta t} X - \Phi_{\delta t}^X| = O(\delta t^{r+1})$; we abuse notation slightly and let $| \cdot |$ denote a well-defined distance over manifolds (see [95] for details).

Thus, the expansion (1) also shows that the error in the approximation is $|\Psi_{\delta t} X - \Phi_{\delta t}^X| = O(\delta t^2)$, i.e., we have an integrator of order $r = 1$. One can also consider more elaborate compositions, such as

$$\Psi_{\delta t} X = \Phi_{\delta t/2}^Y \circ \Phi_{\delta t/2}^Z \circ \Phi_{\delta t/2}^Y,$$

which is more accurate since the first term in (1) cancels out, yielding an integrator of order $r = 2$.\footnote{Higher-order methods are constructed by looking for appropriate compositions that cancel first terms in the BCH formula [43]. However, methods for $r > 2$ tend to be expensive numerically, with not so many benefits (if any) over methods of order $r = 2$.}

### 2.2 Conservative flows and symplectic integrators

As a stepping stone, we first discuss the construction of suitable conservative flows, namely flows along which some function $f : \mathcal{X} \to \mathbb{R}$ is constant, where $\mathcal{X}$ is the phase space manifold of the system, i.e., the space in which the dynamics evolves. Such flows, which are amongst the most well-studied due to their importance in physics, will enable us to obtain our desired “rate-matching” optimisation methods and will also be central in our construction of geometric samplers.

To construct vector fields along the derivative of $f$ we shall need brackets. Geometrically, these are morphisms $\mathcal{X}^* \to \mathcal{X}$, also known as contravariant tensors of rank 2 in physics, where $\mathcal{X}^*$ is the dual space of $\mathcal{X}$. Note that on Riemannian manifolds (e.g., $\mathcal{X} = \mathbb{R}^n$) both spaces are isomorphic. In Euclidean space, $x \in \mathcal{X} = \mathbb{R}^n$, we define such $B$-vector fields in terms of a state-dependent matrix $B = B(x)$ as\footnote{We denote by $x^i$ the $i$th component of $x$ and $\partial_i \equiv \partial / \partial x^i$. We also use Einstein’s summation convention, i.e., repeated upper and lower indices are summed over.}

$$X_f^B(x) \equiv B^i_j(x) \partial_i f(x) \partial_j.$$

Any vector field that depends linearly and locally on $f$ may be written in this manner. Notice that a decomposition $f = \sum_a f_a$ induces a decomposition $X_f^B = \sum_a X_{f_a}^B$ that is amenable to the splitting integrators previously mentioned. Importantly, vector fields that preserve $f$ correspond to bracket vector fields in which $B$ is antisymmetric [96]. Constructing conservative flows is thus straightforward. Unfortunately, it is a rather more challenging task to construct efficient discretisations that retain this property; most well-known procedures, namely discrete-gradient and projection methods, only give rise to integrators that require solving implicit equations at every step, and they may break other important properties of the system.
For a particular class of conservative flows, it is possible to construct splitting integrators that—
extactly—preserve another function \(\tilde{f}\) that remains close to \(f\). Indeed, going back to the BCH formula (1), we see that if we were to approximate a conservative flow of \(X^B_f = X^B_{f_1} + X^B_{f_2}\) by composing the flows of \(X^B_{f_1}\) and \(X^B_{f_2}\), and, crucially, if we had a bracket for which the commutators can be written as

\[
[X^B_{f_1}, X^B_{f_2}] = X^B_{f_3},
\]

for some function \(f_3\), and so on for all commutators in (1), then the right-hand side of the BCH formula would itself be an expansion in terms of a vector field \(X^B_f\) for some shadow function \(\tilde{f} = f + f_3 \delta t + f_4 \delta t^2 + \cdots\). In particular, \(\tilde{f}\) would inherit all the properties of \(f\), i.e., properties common to \(B\)-vector fields. This is precisely the case for Poisson brackets, written \(B \equiv \Pi\), which are antisymmetric brackets for which the Jacobi identity holds:

\[
[X^\Pi_f, X^\Pi_g] = X^\Pi_{\{f,g\}}, \quad \{f, g\} \equiv \partial_i f \Pi^{ij} \partial_j g.
\]

where \(\{f, g\}\) is the Poisson bracket between functions \(f\) and \(g\). The BCH formula then implies

\[
\tilde{f} = (f_1 + f_2) + \frac{1}{2}(f_1, f_2) \delta t + \frac{1}{12} (\{f_1, \{f_1, f_2\}\} + \{f_2, \{f_2, f_1\}\}) \delta t^2 + \cdots.
\]

Such an integrator can thus be seen as a Poisson system itself, generated by the above asymptotic shadow \(\tilde{f}\), which is exactly preserved.

Poisson brackets and their dynamics are the most important class of conservative dynamical systems, describing many physical systems, including all of fluid and classical mechanics. The two main classes of Poisson brackets are constant antisymmetric matrices on Euclidean space, and symplectic brackets for which \(\Pi^{ij}(x)\) is invertible at every point \(x\). Its inverse is denoted by \(\Omega_{ij} = (\Pi^{-1})_{ij}\), and called a symplectic form. In this case, the function \(f\) is called a Hamiltonian, denoted \(f = H\). The invertibility of the Poisson tensor \(\Pi^{ij}\) implies that such a bracket exists only on even-dimensional spaces. Darboux theorem then ensures the existence of local coordinates \(x \equiv (q^1, \ldots, q^d, p_1, \ldots, p_d)\) in which the symplectic form can be represented as \(\Omega = (\begin{smallmatrix}0 & I \\ -I & 0\end{smallmatrix})\). Dynamically, this corresponds to the fact that these are 2nd order differential equations, requiring not only a position \(q \in \mathcal{M}\) but also a momentum \(p \in T^*_q\mathcal{M}\).\(^3\) Note that if \(H = p_i\) then \(X_H = \partial/\partial q^i\), and conversely if \(H = q^i\) then \(X_H = -\partial/\partial p_i\). Thus, a change in coordinate \(q^i\) is generated by its conjugate momentum \(p_i\), and vice-versa. Thus, the only way to generate dynamics on \(\mathcal{M}\) in this case is by introducing a Hamiltonian depending on both position and momentum. From a numerical viewpoint, the extended phase space introduces extra degrees of freedom that allow us to incorporate “symmetries” in the Hamiltonian, which facilitate integration. Indeed, in practice, the Hamiltonian usually decomposes into a potential energy, associated to position and independent of momentum, and a kinetic energy, associated to momentum and invariant under position changes, both generating tractable flows. Thanks to this decomposition, we are able to construct numerical methods through splitting the vector field. Note also that, for symplectic brackets, the existence of a shadow Hamiltonian can be guaranteed beyond the case of splitting methods, e.g., for variational integrators—which use a discrete version of Hamilton’s principle of least action—and more generally for most symplectic integrators in which the symplectic bracket is preserved up to topological considerations described by the 1st de Rham cohomology of phase space.

\(^3\)More precisely, the dynamics evolve on the cotangent bundle \(X = T^*\mathcal{M}\), with coordinates \(x = (q, p)\); momentum \(p \in T^*_q\mathcal{M}\) and velocity \(v = dq/dt \in T_q\mathcal{M}\) are equivalent on the Riemannian manifolds that are used in practice. \(\mathcal{M}\) is called the configuration manifold with coordinates \(q\).
2.3 Rate-matching integrators for smooth optimisation

Having obtained a vast family of smooth dynamics and integrators that closely preserve $f$, we can now apply these ideas to optimisation. Vector fields for which a Hamiltonian function $f = H$ *dissipates* can be written as a bracket vector field $X_H^B$ for some negative semi-definite matrix $B$ [96]. Let us consider a concrete example in $\mathcal{X} = \mathbb{R}^{2d}$ in the form of a (generalised) conformal Hamiltonian system [8,9,97]. Consider thus the Hamiltonian

$$H(q,p) = \frac{1}{2} p_i g^{ij} p_j + V(q),$$

(6)

where $g_{ij}$ is a constant symmetric positive definite matrix with inverse $g^{ij}$. The associated vector field is $X_B^H = g^{ij} p_j \partial_{q_i} - [\partial_q V + \gamma(t) p_i] \partial_{p_i}$, with $\gamma(t) > 0$ being a “damping coefficient.” This is associated to the negative definite matrix

$$B \equiv \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix} - \gamma(t) \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}.$$  

(7)

The equations of motion are

$$\frac{dq}{dt} = g^{ij} p_j, \quad \frac{dp_i}{dt} = -\frac{\partial V}{\partial q_i} - \gamma(t)p_i,$$

(8)

and obey

$$\frac{dH}{dt} = -\gamma(t) p_i g^{ij} p_j \leq 0,$$

(9)

so the system is *dissipative*. Suppose $V(q)$ has a minimizer $q^* \equiv \arg \min_q V(q)$ in some region of interest and, without loss of generality, has value $V^* \equiv V(q^*) \equiv 0$. Then $H > 0$ and $dH/dt < 0$ outside such a critical point, implying that $H$ is also a (strict) Lyapunov function; the existence of such a Lyapunov function implies that trajectories starting in the neighborhood of $q^*$ will converge to $q^*$. In other words, the above system provably solves the optimisation problem

$$\min_{q \in \mathbb{R}^d} V(q).$$

(10)

Two common choices for the damping are the constant case, $\gamma(t) = \gamma$, and the asymptotic vanishing case, $\gamma(t) = r/t$ for some constant $r \geq 3$ (other choices are also possible). When $V(q)$ is a convex function (resp. strongly convex function with parameter $\mu > 0$) it is possible to show the following convergence rates [37]:

| $V(q(t)) - V^*$         | convex       | $\mu$-strongly convex | damping                  |
|-------------------------|--------------|------------------------|--------------------------|
| $O(t^{-1})$             | $O\left(\exp\left\{-\sqrt{\mu/\lambda_1^2(g)t}\right\}\right)$ | $\gamma(t) = \text{const.}$ |
| $O(\lambda_1^2(g)t^{-2})$ | $O(t^{-2r/3})$ | $\gamma(t) = r/t$    |

(11)

where $\lambda_1(g)$ is the largest eigenvalue of the metric $g$. The *convergence rates* of this system are therefore known under such convexity assumptions. Ideally, we want to design optimisation methods that preserve these rates, i.e., are “rate-matching”, and are also numerically stable. As we will see, such geometric integrators can be constructed by leveraging the shadow Hamiltonian property of
symplectic methods on higher-dimensional conservative Hamiltonian systems [9] (see also [98,99]). This holds not only on $\mathbb{R}^{2d}$ but on general settings, namely on arbitrary smooth manifolds [9,10].

In the conformal Hamiltonian case, the dissipation appears explicitly in the equations of motion. It is however theoretically convenient to consider an equivalent *explicit time-dependent* Hamiltonian formulation. Consider the following coordinate transformation into system (8):

\[ p \mapsto e^{-\eta(t)}p, \quad H(q,p) \mapsto e^{\eta(t)}H(q,e^{-\eta(t)}p), \quad \eta(t) \equiv \int \gamma(t) dt. \] (12)

It is easy to see that (8) is equivalent to standard Hamilton’s equations,

\[ \frac{dq^i}{dt} = \frac{\partial H}{\partial p^i}, \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q^i}, \]

with the explicit time-dependent Hamiltonian

\[ H(t,q,p) = \frac{1}{2} e^{-\eta(t)} p^i g^{ij} p_j + e^{\eta(t)} V(q). \] (13)

The rate of change of $H$ along the flow now satisfies

\[ \frac{dH}{dt} = \frac{\partial H}{\partial t} \neq 0, \] (14)

so the system is *nonconservative*; this equation is equivalent to (9).

Going one step further, let us now promote $t$ to a new coordinate and introduce its (conjugate) momentum $u$. Consider thus the higher-dimensional Hamiltonian

\[ K(t,q,u,p) \equiv \frac{1}{2} e^{-\eta(t)} p^i g^{ij} p_j + e^{\eta(t)} V(q) + u. \] (15)

Note that $t$ and $u$ are two arbitrary canonical coordinates. Denoting the time parameter of this system by $s$, Hamilton’s equations read

\[ \frac{dt}{ds} = 1, \quad \frac{du}{ds} = -\frac{\partial K}{\partial t}, \quad \frac{dq^i}{ds} = e^{-\eta(t)} g^{ij} p_j, \quad \frac{dp_i}{ds} = -e^{\eta(t)} \frac{\partial V}{\partial q^i}. \] (16)

This system is *conservative* since $dK/ds = 0$. Now, if we fix coordinates as

\[ t = s, \quad u(s) = -H(s,q(s),p(s)), \] (17)

the conservative system (16) reduces precisely the original dissipative system (13); the 2nd equation in (16) reproduces (14), and the remaining equations are equivalent to the equations of motion associated to (13), which in turn are equivalent to (8) as previously noted. Formally, what we have done is to embed the original dissipative system with phase space $\mathbb{R}^{2d}$ into a higher-dimensional conservative system with phase space $\mathbb{R}^{2d+2}$. The dissipative dynamics thus lies on a hypersurface of constant energy, $K = 0$, in high dimensions; see [9] for details. The reason for doing this procedure, called *symplectification*, is purely theoretical: since the theory of symplectic integrators only accounts for conservative systems, we can now extend this theory to dissipative settings by applying a symplectic integrator to (13) and then fixing the relevant coordinates (17) in the resulting method. Geometrically, this corresponds to integrating the time flow exactly [9,98]. In [9] such a procedure was defined under the name of *presymplectic integrators*, and these connections hold not only for the specific example above but also for general non-conservative Hamiltonian systems.
We are now ready to explain why this approach is suitable to construct practical optimisation methods. Let $\Psi_{\delta s}: \mathbb{R}^{2d+2} \to \mathbb{R}^{2d+2}$ be a symplectic integrator of order $r \geq 1$ applied to system (15). Denote by $(t_k, q_k, u_k, p_k)$ the numerical state, obtained by $k = 0, 1, \ldots$ iterations of $\Psi_{\delta s}$. Time is simulated over the grid $s_k = (\delta s)k$, with step size $\delta t > 0$. Because a symplectic integrator has a shadow Hamiltonian we have

$$\hat{K}(t_k, q_k, u_k, p_k) = K(t(s_k), q(s_k), u(s_k), p(s_k)) + O(\delta s^r).$$

Enforcing (17), the coordinate $t_k$ becomes simply the time discretization $s_k$, which is exact, and so is $u_k = u(t_k)$ since it is a function of time alone; importantly, $u$ does not couple to any of the other degrees of freedom so it is irrelevant whether we have access to $u(s)$ or not. Replacing (15) into the above equation we conclude:

$$\hat{H}(t_k, q_k, p_k) = H(t_k, q(t_k), p(t_k)) + O(\delta t^r),$$

(18)

where we now denote $t_k = (\delta t)k$, for $k = 0, 1, \ldots$. Hence, the time-dependent Hamiltonian also has a shadow, thanks to the cancellation of the variable $u$. In particular, if we replace the explicit form of the Hamiltonian (13) we obtain\(^4\)

$$V(q_k) - V^* = V(q(t_k)) - V^* + O(e^{-\eta(t_k)}\delta t^r).$$

(19)

Therefore, the known rates (11) for the continuum system are nearly preserved—and so would be any rates of more general time-dependent (dissipative) Hamiltonian systems. Moreover, as a consequence of (18), the original time-independent Hamiltonian (6) of the conformal formulation is also closely preserved, i.e., within the same bounded error in $\delta t$—recall transformation (12). However, this is also a Lyapunov function, hence the numerical method respects the stability properties of the original system as well.\(^5\)

In short, as a consequence of having a shadow Hamiltonian, such geometric integrators are able to reproduce all the relevant properties of the continuum system. These arguments are completely general; namely, they ultimately rely on the BCH formula, the existence of bracket vector fields and the symplectification procedure. Under these basic principles, no discrete-time analyses were necessary to obtain guarantees for the numerical method; which may not be particularly enlightening from a dynamical systems viewpoint and are only applicable on a (painful) case-by-case basis.

Let us now present an explicit algorithm to solve the optimisation problem (10). Consider a generic (conservative) Hamiltonian $H(q, p)$, evolving in time $s$. The well-known leapfrog or Störmer-Verlet method, the most used symplectic integrator in the literature, is based on the composition (2) and reads [2]

\[
\begin{align*}
p_{k+1/2} &= p_k - (\delta s/2)\partial_q H(q_k, p_{k+1/2}), \\
q_{k+1} &= q_k - (\delta s/2) \left[ \partial_p H(q_k, p_{k+1/2}) + \partial_p H(q_{k+1}, p_{k+1/2}) \right], \\
p_{k+1} &= p_{k+1/2} - (\delta s/2)\partial_q H(q_{k+1}, p_{k+1/2}).
\end{align*}
\]

\(^4\)The kinetic part only contributes to the small error since $g$ is positive definite and $|p_k - p(t_k)| = O(\delta t^r)$. There are several technical details we are omitting, such as Lipschitz conditions on the Hamiltonian and on the numerical method, which we refer to [9] for details.

\(^5\)Naturally, all these results hold for suitable choices of step size, which can be determined by a linear stability analysis of the particular numerical method under consideration.
According to our prescription, replacing the higher-dimensional Hamiltonian (15), imposing the gauge fixing conditions (17), and recalling that \( u \) cancels out, we obtain the following method.\(^6\)

\[
\begin{align*}
p_{k+1/2} &= p_k - (\delta t/2)e^{\eta(t_k)}\partial_q V(q_k), \\
q_{k+1} &= q_k - (\delta t/2)[e^{-\eta(t_k)} + e^{-\eta(t_{k+1})}]g^{-1}p_{k+1/2}, \\
p_{k+1} &= p_{k+1/2} - (\delta t/2)e^{\eta(t_{k+1})}\partial_q V(q_{k+1}),
\end{align*}
\]

(20)

where we recall that \( \delta t > 0 \) is the step size and \( t_k = (\delta t)k \), for iterations \( k = 0, 1, \ldots \). This method, which is a dissipative generalisation of the leapfrog, was proposed in [9] and has very good performance when solving unconstrained problems (10). In a similar fashion, one can extend any (known) symplectic integrator to a dissipative setting; the above method is just one such example.

2.4 Manifold and constrained optimisation

Following [10], we briefly mention how the previous approach can be extended in great generality, i.e., to an optimisation problem

\[
\min_{q \in \mathcal{M}} V(q),
\]

(21)

where \( \mathcal{M} \) is an arbitrary Riemannian manifold. There are essentially two ways to solve this problem through a (dissipative) Hamiltonian approach. One is to simulate a Hamiltonian dynamics on \( T^*\mathcal{M} \) by incorporating the metric of \( \mathcal{M} \) in the kinetic part of the Hamiltonian. Another is to consider a Hamiltonian dynamics on \( \mathbb{R}^n \) and embed \( \mathcal{M} \) into \( \mathbb{R}^n \) by imposing several constraints,\(^7\)

\[
\psi_a(q) = 0, \quad a = 1, \ldots, m.
\]

(22)

This constrained case turns out to be particularly useful since we typically are unable to compute the geodesic flow on \( \mathcal{M} \), but are able to construct robust constrained sympletic integrators for it.

As an example of the first approach, consider \( \mathcal{M} = \mathcal{G} \) being a Lie group, with Lie algebra \( \mathfrak{g} \) and generators \( \{T_i\} \). The analogous of Hamiltonian (13) is given by \( H = -\frac{1}{4g}e^{-\eta(t)} \text{Tr}(P^2) + e^{\eta(t)}V(Q) \), where \( g > 0 \) is a constant, \( Q \in \mathcal{G} \) and \( P \in \mathfrak{g} \) (they can be seen as matrices). The method (20) can be adapted to this setting, resulting in the following algorithm [10] (recall footnote 6):

\[
\begin{align*}
P_{k+1/2} &= e^{-\Delta \eta_k} \left\{ P_k - (\delta t/2) \text{Tr} \left[ \partial_Q V(Q_k) \cdot Q_k \cdot P_k \right] P_k \right\}, \\
Q_{k+1} &= Q_k \exp \left[ (\delta t/2) \text{cosh}(\Delta \eta_k)g^{-1}P_{k+1/2} \right]; \\
P_{k+1} &= e^{-\Delta \eta_k} P_{k+1/2} - (\delta t/2) \text{Tr} \left[ \partial_Q V(Q_{k+1}) \cdot Q_{k+1} \cdot P_{k+1} \right] P_k,
\end{align*}
\]

(23)

\(^6\) In a practical implementation, it is convenient to make the change of variables \( p_k \mapsto e^{\eta(t_k)}p_k \) into (20); recall the transformations (12). In this case the method reads

\[
\begin{align*}
p_{k+1/2} &= e^{-\Delta \eta_k} \left\{ p_k - (\delta t/2)\partial_q V(q_k) \right\}, \\
q_{k+1} &= q_k - \delta t \text{cosh}(\Delta \eta_k)g^{-1}p_{k+1/2}, \\
p_{k+1} &= e^{-\Delta \eta_k} p_{k+1/2} - (\delta t/2)\partial_q V(q_{k+1}),
\end{align*}
\]

where \( \Delta \eta_k \equiv \eta(t_{k+1/2}) - \eta(t_k) = \int_{t_k}^{t_{k+1/2}} \gamma(t)dt \). Note that only a half-step difference of \( \eta(t) \) appears in these updates. The algorithm is thus written in the same variables as the conformal representation (8). The advantage is that we do not have large or small exponentials, which can be problematic numerically. Furthermore, when solving optimisation problems, it is convenient to set the matrix \( g = (\delta t)I \); this was noted in [8] but can also be understood from the rates (11) since then the step size \( \delta t \) disappears from some of these formulas.

\(^7\) Theoretically, there is no loss of generality since Nash or Whitney embedding theorems tells us that any smooth manifold \( \mathcal{M} \) can be embedded into \( \mathbb{R}^n \) for sufficiently large \( n \).
where \((\partial Q V(Q))_{ij} = \partial V / \partial Q_{ji}\) is a matrix.

As an example of the second approach, one can constrain the integrator on \(\mathbb{R}^n\) to define a symplectic integrator on \(\mathcal{M}\) via the discrete constrained variational approach [5] by introducing Lagrange multipliers, i.e., by considering the Hamiltonian \(H + e^{v(t)} \sum a \lambda^a \psi_a(q)\), where \(H\) is the Hamiltonian (13). In particular, the method (20) can be constrained to yield [10]

\[
\begin{align*}
    p_{k+1/2} &= e^{-\Delta \eta_k} \Lambda(q_k) \left[ p_k - (\delta t/2) \partial_q V(q_k) \right], \\
    \bar{p}_{k+1/2} &= p_{k+1/2} - (\delta t/2) e^{-\Delta \eta_k} [\partial_q \psi(q_k)]^\top \lambda, \\
    q_{k+1} &= q_k - \delta t \cosh(\Delta \eta_k) g^{-1} \bar{p}_{k+1/2}, \\
    0 &= \psi_a(q_{k+1}) \quad (a = 1, \ldots, m), \\
    p_{k+1} &= \Lambda(q_{k+1}) \left[ e^{-\Delta \eta_k} \bar{p}_{k+1/2} - (\delta t/2) \partial_q V(q_{k+1}) \right],
\end{align*}
\]

where we have the projector \(\Lambda(q) \equiv I - R_{q}^{-1}(q) \partial_q \psi(q) g^{-1}\) with \(R_{q}(q) \equiv \partial_q \psi(q) g^{-1} \partial_q \psi(q)^\top\), and \((\partial_q \psi)_{ij} \equiv \partial \psi_i / \partial q_j\) is the Jacobian matrix of the constraints; \(\lambda = (\lambda_1, \ldots, \lambda_m)^\top\) is the vector of Lagrange multipliers and \(\Delta \eta_k \equiv \int_{t_k}^{t_{k+1/2}} \gamma(t) dt\) accounts for the damping. In practice, the Lagrange multipliers are determined by solving the (nonlinear) algebraic equations for the constraints, i.e., the 2nd to 4th updates above are solved simultaneously. The above method consists in a dissipative generalisation of the well-known RATTLE integrator from molecular dynamics [100–103].

It is possible to generalise any other (conservative) symplectic method to this (dissipative) optimisation setting on manifolds. In this general setting, there still exists a shadow Hamiltonian so that convergence rates and stability are closely preserved numerically [10] (similarly to (18) and (19)). In particular, one can also consider different types of kinetic energy, beyond the quadratic case discussed above, which may perform better in specific problems [8]. This approach therefore allows one to adapt existing symplectic integrators to solve optimisation problems on Lie groups and other manifolds commonly appearing in machine learning, such as Stiefel, Grassmanians, or to solve constrained optimisation problems on \(\mathbb{R}^n\).

### 2.5 Gradient flow as a high friction limit

Let us provide some intuition why simulating 2nd order systems is expected to yield faster algorithms. It has been shown that several other accelerated optimisation methods\(^8\) are also discretisations of system (8) [38]. Moreover, in the large friction limit, \(\gamma \to \infty\), this system reduces to the 1st order gradient flow, \(dq/dt = -\partial_q V(q)\) (assuming \(g \propto I\)), which is the continuum limit of standard, i.e., nonaccelerated methods [38]. The same happens in more general settings; when the damping is too strong, the second derivative becomes negligible and the dynamics is approximately 1st order.

As an illustration, consider Figure 1 (left) where a particle immersed in a fluid falls under the influence of a potential force \(-\partial_q V(q)\), that plays the role of “gravity”, and is constrained to move on a surface. In the underdamped case, the particle is under water, which is not so viscous, so it has acceleration and moves fast (even oscillate). In the overdamped case, the particle is in a highly viscous fluid, such as honey, and the drag force \(-\gamma p\) is comparable or stronger to \(-\partial_q V(q)\), thus the particle moves slowly since it cannot accelerate; during the same elapsed time \(\delta t\), an accelerated particle would travel a longer distance. We can indeed verify this behaviour numerically. In Figure 1 (right) we run algorithm (23) in the underdamped and overdamped regimes when solving

---

\(^8\)Besides accelerated gradient based methods, accelerated extensions of important proximal-based methods such as proximal point, proximal-gradient, alternating direction method of multipliers (ADMM), Douglas-Rachford, Tseng splitting, etc., are implicit discretizations of (8); see [38] for details.
Riemannian Gradient Descent
Lie Group (overdamped)
Lie Group (underdamped)

\[ \gamma \to \infty \quad \gamma = O(1) \]

overdamped (honey) 1st order  
underdamped (water) 2nd order

an optimisation problem on the \( n \)-sphere, i.e., on the Lie group \( SO(n) \).\(^9\) We can see that, in the overdamped regime, this method has essentially the same dynamics as the Riemannian gradient descent [104], which is nonaccelerated and corresponds to a 1st order dynamics; all methods use the same step size, only the damping coefficient is changed.

2.6 Optimisation on the space of probability measures

There is a tight connection between sampling and optimisation on the space of probability measures which goes back to [50, 51]. Let \( \mathcal{P}_2(\mathbb{R}^n) \) be the space of probability measures on \( \mathbb{R}^n \) with finite second moments, endowed with a Wasserstein-2 metric \( W_2 \). The gradient flow of a functional \( F[\mu] \) on the space of probability measures is the solution to the partial differential equation

\[ \partial_t \mu(q,t) = -\nabla_{W_2} F[\mu(q,t)], \]

which, under sufficient regularity conditions, is equivalent to [50, 51, 105]

\[ \partial_t \mu = \partial \cdot \left( \mu \frac{\delta F[\mu]}{\delta \mu} \right), \quad (25) \]

where \( \partial \equiv \partial_q \) and \( \partial \cdot \) are the derivative and the divergence operators on \( \mathbb{R}^n \), respectively. The evolution of this system solves the optimisation problem

\[ \rho \equiv \arg \min_{\mu \in \mathcal{P}_2(\mathbb{R}^n)} F[\mu], \quad (26) \]

i.e., \( \mu(q,t) \to \rho(q) \) as \( t \to \infty \) in the sense of distributions. We can consider the analogous situation with a dissipative flow induced by the conformal Hamiltonian tensor (7) on the space of probability measures; we set \( g = I \) and \( \gamma(t) = \gamma = \text{const.} \) for simplicity. Thus, instead of (25), we have a conformal Hamiltonian system in Wasserstein space given by the continuity equation

\[ \partial_t \mu = \partial \cdot \left( \mu B \partial \frac{\delta F[\mu]}{\delta \mu} \right), \quad (27) \]

\(^{9}\)The details are not important here, but this problem minimises the Hamiltonian of a spherical spin glass (see [10] for details). The same behaviour is seen with the constrained method (24) as well.
where now $\partial \equiv (\partial_q, \partial_p)$ and $\mu$ is a measure over $\mathcal{P}_2(\mathbb{R}^d)$. Let $F$ be the free energy defined as

$$ F[\mu] \equiv U[\mu] - \beta^{-1} S[\mu], \quad U[\mu] \equiv \mathbb{E}_\mu[H], \quad S[\mu] \equiv \mathbb{E}_\mu[-\log \mu], $$

(28)

where $U$ is the (internal) energy, $H$ is the Hamiltonian (6), $S$ is the Shannon entropy, and $\beta$ is the inverse temperature. The functional derivative of the free energy equals

$$ \frac{\delta F}{\delta \mu} = H + \beta^{-1} \log \mu = \frac{1}{2} ||p||^2 + V(q) + \beta^{-1} \log \mu. $$

(29)

In particular, the minimiser of $F$ is the stationary density

$$ \rho(q,p) = Z_\beta^{-1} e^{-\beta H(q,p)}, \quad Z_\beta \equiv \mathbb{E}_\mu[e^{-\beta H(q,p)}]. $$

(30)

Note also that the free energy (28) is nothing but the KL divergence (up to a constant which is the partition function):

$$ \text{KL}[\mu | \rho] \equiv \mathbb{E}_\mu[\log(\mu/\rho)] = \beta F[\mu] - \log Z_\beta. $$

Therefore, the evolution of $\mu$ as given by the conformal Hamiltonian system (27) minimises the divergence from the stationary density (30). Replacing (29) into (27) we obtain

$$ \partial_t \mu = -\partial_q \cdot [\mu p] + \partial_p \cdot [\mu \partial_q V(q) + \gamma \mu p] + \gamma \beta^{-1} \partial_p^2 \mu, $$

which is nothing but the Fokker-Planck equation associated to the underdamped Langevin diffusion

$$ dq_t = p_t dt, \quad dp_t = -\partial_q V(q_t) dt - \gamma p_t dt + \sqrt{2\gamma \beta^{-1}} dw_t, $$

(31)

where $w_t$ is a standard Wiener process. Thus, the underdamped Langevin can be seen as performing accelerated optimisation on the space of probability measures. A quantitative study of its speed of convergence is given by the theory of hypocoercivity [106–108].

The above results provide a tight connection between sampling and optimisation. Interestingly, by the same argument as used in section 2.5 (see Figure 1), the high friction limit, $\gamma \to \infty$, of the underdamped Langevin diffusion (31) yields the overdamped Langevin diffusion [38,107]

$$ dq_t = -\nabla V(q_t) dt + \sqrt{2\beta^{-1}} dw_t, $$

(32)

which corresponds precisely to the gradient flow (25) on the free energy functional $F[\mu]$ [51,105], where now $\mu = \mu(q,t) \in \mathcal{P}_2(\mathbb{R}^d)$. Thus, in the same manner that a 2nd order damped Hamiltonian system may achieve accelerated optimisation compared to a 1st order gradient flow, the underdamped Langevin diffusion (31) may achieve accelerated sampling compared to the overdamped Langevin diffusion (32). Such an acceleration has indeed been demonstrated [109] in continuous-time and for a particular discretisation.

### 3 Hamiltonian-based accelerated sampling

The purpose of sampling methods is to efficiently draw samples from a given target distribution $\rho$ or, more commonly, to calculate expectations with respect to $\rho$:

$$ \int_X f \, d\rho \approx \frac{1}{n} \sum_{k=0}^{n-1} f(x_k). $$

(33)
However, generating i.i.d. samples \( \{x_k\} \) is usually practically infeasible, even for finite sample spaces, as in high dimensions probability mass tends to concentrate in small regions of the sample space, while regions of high probability mass tend to be separated by large regions of negligible probability. Moreover, \( \rho \) is usually only known up to a normalisation constant [110]. To circumvent this issue, MCMC methods rely on constructing ergodic Markov chains \( \{x_n\}_{n \in \mathbb{N}} \) that preserve the target distribution \( \rho \). If we run the chain long enough \( (n \to \infty) \), Birkhoff’s ergodic theorem guarantees that the estimator on the right-hand side of (33) converges to our target integral on the left-hand side almost surely [111]. An efficient sampling scheme is one that minimises the variance of the MCMC estimator. In other words, fewer samples will be needed to obtain a good estimate. Intuitively, good samplers are Markov chains that converge as fast as possible to the target distribution.

### 3.1 Optimising diffusion processes for sampling

As many MCMC methods are based on discretising continuous-time stochastic processes, the analysis of continuous-time processes is informative of the properties of efficient samplers.

Diffusion processes possess a rich geometric theory, extending that of vector fields, and have been widely studied in the context of sampling. They are Markov processes featuring almost surely continuous sample paths (i.e., no jumps) and correspond to the solutions of stochastic differential equations (SDEs). While a deterministic flow is given by a first order differential operator—namely, a vector field \( X \) as used in §2—diffusions require specifying a set of vector fields \( X, Y_1, \ldots, Y_N \), where \( X \) represents the (deterministic) drift and \( Y_i \) the directions of the (random) Wiener processes \( w_i^t \), and are characterised by a second order differential operator of the form \( \mathcal{L} \equiv X + Y_i \circ Y_i \), known as the generator of the process. Equivalently, diffusions can be written as Stratonovich SDEs:

\[
\text{dx}_t = X(x_t) dt + Y_i(x_t) \circ dw_i^t,
\]

(34)

For a smooth positive target measure \( \rho \), the complete family of \( \rho \)-preserving diffusions is given by (up to a topological obstruction contribution) [112]

\[
dx_t = \text{curl}_\rho(A) dt + \frac{1}{2} \text{div}_\rho(Y_i) Y_i dt + Y_i \circ dw_i^t,
\]

(34)

for a choice of antisymmetric bracket \( A \). Here \( \text{curl}_\rho \) is a differential operator on multi-vector fields, generalising the divergence on vector fields \( \text{div}_\rho \) of \( \rho \), and is induced via an isomorphism \( \rho^\sharp \) defined by \( \rho \) which allows to transfer the calculus of twisted differential forms to a measure-informed calculus on multi-vector fields [112]. The ergodicity of (34) is essentially characterised by Hörmander’s hypoellipticity condition; i.e., whether the Lie algebra of vector fields generated by \( \{Y_i, [X, Y_i]\}_{i=1}^N \) spans the tangent spaces at every point [107,113,114]. On Euclidean space the above complete class of measure preserving diffusions can be given succinctly by Itô SDEs [115]:

\[
dx_t = -(A + S)(x_t) \partial V (x_t) dt + \partial \cdot (A + S)(x_t) dt + \sqrt{2S(x_t)} dw_t,
\]

(35)

where \( S, A \) reduce to symmetric and antisymmetric matrix fields and \( V \) is the negative Lebesgue log-density of \( \rho \).

There are two well-studied criteria describing sampling efficiency in Markov processes: 1) the worst-case asymptotic variance of the MCMC estimator (33) over functions in \( L^2(\rho) \), and 2) the spectral gap. The spectral gap is the lowest non-zero eigenvalue of the (negative) generator \(-\mathcal{L}\) on \( L^2(\rho) \). When it exists, it is an exponential convergence rate of the density of the process to the target density [107,116,117]. Together, these criteria yield confidence intervals on the non-asymptotic variance of the MCMC estimator, which determines sampling performance [118].
A fundamental criterion for efficient sampling is non-reversibility [116, 119, 120]. A process is non-reversible if it is statistically distinguishable from its time-reversal when initialised at the target distribution [107]. Measure-preserving diffusions are non-reversible precisely when $A \neq 0$ [121]. Intuitively, non-reversible processes backtrack less often and thus furnish more diverse samples [122]. Furthermore, non-reversibility leads to mixing, which accelerates convergence to the target measure. It is well known that removing non-reversibility worsens the spectral gap and the asymptotic variance of the MCMC estimator [116, 119, 120]. In diffusions with linear coefficients, one can construct the optimal non-reversible matrix $A$ to optimise the spectral gap [123, 124] or the asymptotic variance [120]. However, there are no generic guidelines on how to optimise non-reversibility in arbitrary diffusions. This suggests a two-step strategy to construct efficient samplers: 1) optimise reversible diffusions, and 2) add a non-reversible perturbation $A \neq 0$ [125].

Diffusions on manifolds are reversible when $A \equiv 0$, and thus have the form $dx_t = \frac{1}{2} \text{div}_\rho(Y_t)Y_t dt + Y_t \circ dw_t$, which on Euclidean space reads

$$dx_t = -S(x_t)\nabla V(x_t)dt + \partial \cdot S(x_t)dt + \sqrt{2S(x_t)}dw_t.$$  (36)

The spectral gap and the asymptotic variance of the MCMC estimator are the same optimality criteria in reversible Markov processes [126]. When $S$ is positive definite everywhere, it defines a Riemannian metric $g$ on the state space. The generator is then the elliptic differential operator

$$\mathcal{L} = \nabla_g + \Delta_g,$$  (37)

where $\nabla_g$ is the Riemannian gradient and $\Delta_g$ is the Laplace-Beltrami operator, i.e., the Riemannian counterpart of the Laplace operator. Thus, reversible (elliptic) diffusions (37) are the natural generalisation of the overdamped Langevin dynamics (32) to Riemannian manifolds [127]. Optimising $S$ to improve sampling amounts to endowing the state space with a suitable Riemannian geometry that exploits the structure of the target density. For example, sampling is improved by directing noise along vector fields that preserve the target density [128]. When the potential $V$ is strongly convex, the optimal Riemannian geometry is given by $g \equiv \partial^2 V$ [129, 130]. Sampling can also be improved in hypoelliptic diffusions with degenerate noise (i.e., when $S$ is not positive definite). Intuitively, the absence of noise in some directions of space leads the process to backtrack less often and thus yield more diverse samples. For instance, in the linear case, the optimal spectral gap is attained for an irreversible diffusion with degenerate noise [131]. However, degenerate diffusions can be very slow to start with, as the absence of noise in some directions of space make it more difficult for the process to explore the state space [131].

Underdamped Langevin dynamics (31) combines all the desirable properties of an efficient sampler: it is irreversible, has degenerate noise, and achieves accelerated convergence to the target density [132]. We can optimise the reversible part of the dynamics (i.e., the friction $\gamma$) to improve the asymptotic variance of the MCMC estimator [133]. Lastly, we can significantly improve underdamped Langevin dynamics by adding additional non-reversible perturbations to the drift [134].

One way to obtain MCMC algorithms is to numerically integrate diffusion processes. As virtually all non-linear diffusion processes cannot be simulated exactly, we ultimately need to study the performance of discrete algorithms instead of their continuous counterparts. Alarmingly, many properties of diffusions can be lost in numerical integration. For example, numerical integration can affect ergodicity [135]. An irreversible diffusion may sample more poorly than its reversible counterpart after integration [136]. This may be because numerical discretisation can introduce, or otherwise change, the amount of non-reversibility [136]. The invariant measure of the diffusion and its numerical integration may differ, a feature known as bias. We may observe very large bias even in the simplest schemes, such as the Euler-Maruyama integration of overdamped Langevin [60].
Luckily, there are schemes whose bias can be controlled by the integration step size \[137\]; yet, this precludes using large step sizes. Alternatively, one can remove bias by supplementing the integration step with a Metropolis-Hastings corrective step; however, this makes the resulting algorithm reversible. In conclusion, designing efficient sampling algorithms with strong theoretical guarantees is a non-trivial problem that needs to be addressed in its own right.

3.2 Hamiltonian Monte Carlo

Constructing measure-preserving processes, in particular diffusions, is relatively straightforward. A much more challenging task consists of constructing efficient sampling algorithms with strong theoretical guarantees. We now discuss an important family of well-studied methods, known as **Hamiltonian Monte Carlo** (HMC), which can be implemented on any manifold, for any smooth fully supported target measure that is known up to a normalising constant. Some of these methods can be seen as an appropriate geometric integration of the underdamped Langevin diffusion, but it is in general simpler to view them as combining a geometrically integrated deterministic dynamics with a simple stochastic process that ensures ergodicity.

The **conservative** Hamiltonian systems previously discussed provide a natural candidate for the deterministic dynamics. Indeed, given a target measure \( \rho \propto e^{-V} \mu_\mathcal{M} \), with \( \mu_\mathcal{M} \) a Riemannian measure (such as the Lebesgue measure \( dq \) on \( \mathcal{M} = \mathbb{R}^d \)), if we interpret the negative log-density \( V(q) \) as a potential energy, i.e., a function depending on *position* \( q \), one can then plug in the potential within Newton’s equation to obtain a deterministic proposal that is well-defined on any manifold, as soon as the acceleration and derivative operators have been replaced by their curved analogues

\[
\begin{align*}
\dot{q} &= -\frac{\partial V(q)}{\partial q}, \\
\dot{v} &= \frac{\partial V(q)}{\partial q}.
\end{align*}
\]

with given initial conditions for the position \( q \) and velocity \( v = dq/dt \). This is a 2nd order system which evolves in the tangent bundle, \((q,v) \in T\mathcal{M})

The resulting flow is conservative since it corresponds to a Hamiltonian system as discussed in section §2.2, with Hamiltonian \( H(q,v) \equiv \frac{1}{2}||v||_q^2 + V(q) \), where \( ||v||_q^2 \) is the Riemannian squared-norm, which is \( v^Tg(q)v \) when \( \mathcal{M} = \mathbb{R}^d \) and \( g(q) \) is the Riemannian metric; this is the manifold version of the Hamiltonian (6). This system preserves the symplectic measure \( \mu_\mathcal{M}(q,v) = det(g(q))dqdv \), and thus also the canonical distribution \( \mu \propto e^{-H(q,v)}\mu_\mathcal{M} \), which is the product of the target distribution over position with the Gaussian measures on velocity (with covariance \( g \)). For instance, on \( \mathcal{M} = \mathbb{R}^d \),

\[
\mu(q,v) \propto \rho(q) \times \mathcal{N}(0,g^{-1}(q))(v) \propto e^{-V(q)} \sqrt{\text{det}g(q)}dq \times \sqrt{\text{det}g(q)}e^{-\frac{1}{2}v^Tg(q)v}dv.
\]

Moreover, the pushforward under the projection \( \text{Proj} : (q,v) \mapsto q \) is precisely the target measure: \( \text{Proj}_*\mu = \rho \). Concretely, the samples generated by moving according to Newton’s law, after ignoring their velocity component, have \( \rho \) as their law. The main critical features and advantages in using Hamiltonian systems arises from their numerical implementation. Indeed, the flow of (38) is only tractable for the simplest target measures, namely those possessing a high degree of symmetry. In order to proceed, we must devise suitable numerical approximations which, unfortunately, not only break such symmetries but may lose key properties of the dynamics such as stationarity (typically not retained by discretisations). However, as we saw in section §2.2, most symplectic integrators have a **shadow Hamiltonian** and thus generate discrete trajectories that are close to the associated bona fide (shadow) Hamiltonian dynamics, that in particular preserve the shadow canonical distribution.
Most integrators used in sampling, such as the leapfrog, are geodesic integrators. These are splitting methods (see section §2.1) obtained by splitting the Hamiltonian \( H(q,v) = H_1(q,v) + H_2(q) \), where \( H_1(q,v) = \frac{1}{2}||v||^2_q \) and \( H_2(q) = V(q) \) are to be treated as independent Hamiltonians in their own right. Both of these Hamiltonians generate dynamics that might be tractable: the Riemannian component \( H_1 \), associated to the Riemannian reference measure, induces the geodesic flow, while the target density component \( H_2 \) gives rise to a vertical gradient flow, wherein the velocity is shifted by the direction of maximal density change, i.e., \((q,v) \mapsto (q,v - \delta t \nabla_q V(q))\). The Jacobi identity and the BCH formula imply these integrators do possess a shadow Hamiltonian \( \tilde{H} \), and reproduce its dynamics. Such a shadow can in fact be explicitly obtained from (5) by computing iterated Poisson brackets; e.g., on \( M = \mathbb{R}^d \) and for \( \tilde{H}(q,v) = (1/2)v^Tg + V(q) \), the three-stage geodesic integrator

\[
\tilde{H}(q,v) = H(q,v) + \delta t^2 \left[ c_1 \partial V(q)^T g^{-1} \partial V(q) + c_2 v^T \partial^2 V(q)v \right] + O(\delta t^4),
\]

for some constants \( c_1 \) and \( c_2 \). As an immediate consequence, these symplectic integrators preserve the reference symplectic measure \( \mu_0 \) and can be used as a (deterministic) Markov proposal, which when combined with the Metropolis-Hastings acceptance step that depends only on the target density, gives rise to a measure-preserving process. Moreover, the existence of the shadow Hamiltonian ensures that the acceptance rate will remain high for distant proposals, allowing small correlations. However, since Hamiltonian flows are conservative, they remain stuck within energy level sets, which prevents ergodicity. It is thus necessary to introduce another measure-preserving process, known as the heat bath or thermostat, that explores different energy levels; the simplest such process corresponds to sampling a velocity from a Gaussian distribution. Bringing these ingredients together, we thus have the following HMC algorithm: given \( z^n = (q,v) \), compute \( z^{n+1} \) according to

1. **Heat bath:** sample a velocity according to a Gaussian, \( v^\dagger \sim \mathcal{N}(0,g^{-1}(q)) \).

2. **Shadow Hamiltonian dynamics:** move along the Hamiltonian flow generated by the geodesic integrator, \( z^* = \Psi_{\delta t}(z^\dagger) \), where \( z^\dagger = (q,v^\dagger) \).

3. **Metropolis correction:** accept \( z^* \) with probability \( \min \{1,e^{-\Delta H}\} \), where \( \Delta H = H(z^*) - H(z^\dagger) \).

If accepted then set \( z^{n+1} = z^* \), otherwise set \( z^{n+1} = (q_i,-v_i) \).

The above rudimentary HMC method (originally known as Hybrid Monte Carlo) was proposed for simulations in lattice quantum chromodynamics with \( M \) being the special unitary group, \( SU(n) \), and used a Hamiltonian dynamics ingeniously constructed from the Maurer-Cartan frame to compute the partition function of discretised gauge theories [13]. This method has later been applied in molecular dynamics and statistics [12,49,64,139,140].

While the above discussion provides a justification for the use of Hamiltonian mechanics, a more constructive argument from first principles can also be given. From the family of measure-preserving dynamics, which as we have seen can be written as \( \text{curl}_\mu(A) \) (recall (34)), we want to identify those suited to practical implementations (here \( \mu \) could be any distribution on some space \( F \) having the target \( \rho \) has a marginal). Only for the simplest distributions \( \mu \) we can hope to find brackets \( A \) for which the flow of \( \text{curl}_\mu(A) \) is tractable. Instead, the standard approach to geometrically integrate this flow relies as before on splitting methods, which effectively decompose \( \mu \propto e^{-\sum H_t} \mu_F \) into simpler components by decomposing the reference measure from the density and taking advantage of any product structure of the density, so that \( \text{curl}_\mu(A) = \text{curl}_{\mu_F}(A) + \sum X^A_{H_t} \).

There are three critical properties underpinning the success of HMC in practice. The first two are the preservation of the reference measure and the existence of a conserved shadow Hamiltonian
for the numerical method. These imply that we remain close to preserving \( \mu \) along the flow, and in particular leads to Jacobian-free Metropolis corrections with good acceptance rates for distant proposals (see [141] for examples of schemes with Jacobian corrections). Achieving these properties yield strong constraints on the choice of \( A \) [142]; the shadow property is essentially exclusive to Poisson systems, for which the conservation of a common reference measure is equivalent to the triviality of the modular class in the first Poisson cohomology group [143]. In particular, Poisson brackets that admit such an invariant measure have been carefully analysed and are known as unimodular; the only unimodular Poisson bracket that can be constructed on general manifolds seems to be precisely the symplectic one.

The third critical property is the existence of splittings methods for which all the composing flows are either tractable or have adequate approximations, namely the geodesic integrators. Indeed, as we have seen, the flow \( \Phi^{H2} \)—induced by the potential \( H_2(q) = V(q) \)—is always tractable, independently of the complexity of the target density; this is possible mainly due to the extra “symmetries” resulting from implementing the flow on a higher-dimensional space \( TM \) rather than \( M \). On the other hand, one key consideration for the tractability of the the geodesic flow \( \Phi^{H1} \)—induced by the kinetic energy \( H_1(q,v) \)—is the choice of Riemannian metric; for most cases, it is numerically hard to implement \( \Phi^{H1} \) since several implicit equations need to be solved. In general, it is desirable to use a Riemannian metric that reflects the intrinsic symmetries of the sample space, mathematically described by a Lie group action. Indeed, by using an invariant Riemannian metric, one greatly simplifies the equations of motion of the geodesic flow, reducing the usual 2nd order Euler-Lagrange equations to the 1st order Euler-Arnold equations [144–146], with tractable solutions in many cases of interest, e.g., for naturally reductive homogeneous spaces; including \( \mathbb{R}^d \), the space of positive definite matrices, Stiefel manifolds, Grassmannian manifolds, and many Lie groups. In such cases, it is possible to find a Riemannian metric whose geodesic flow is known and given by the Lie group exponential [16, 147, 148]. For the other main class of spaces, namely those given by constraints, if one chooses the restriction of the Euclidean metric, then the RATTLE scheme discussed in optimisation (see section §2.4) is a suitable symplectic integrator [103, 149–152] (perhaps up to a reversibility check). Occasionally, it may be suitable to use a Riemannian metric associated to the target distribution rather than the sample space; e.g., when it belongs to a statistical manifold. In that case, any choice of (information) divergence gives rise to an information tensor that may be used in the HMC algorithm. Notably, this is the case in Bayesian statistics, wherein attempting to find a Riemannian metric that locally matches the Hessian of the posterior motivates the use of the Fisher information tensor summed with the Hessian of the prior, giving rise to the Riemannian HMC [127, 153]. When a Riemannian metric whose geodesic flow is unknown is chosen, one can use the trick of increasing the dimension of the phase space to add symmetries to derive explicit symplectic integrators [154, 155].

Once we have an integrator for the geodesic flow, another important consideration is the construction and tuning of the overall integrator, i.e., the specific composition of \( \Phi^{H_1}_{\delta t} \) and \( \Phi^{H_2}_{\delta t} \). Traditional numerical integrators are tuned to provide highly accurate approximations for the trajectories in the limit \( \delta t \to 0 \); for instance, a forth order Runge-Kutta method. However, samplers aim to have the largest possible step size \( \delta t \) in order to reduce correlations. One approach consists in tuning the integrator to obtain good density preservation in the Gaussian case. Another approach consists in tuning the integrator to ensure the shadow Hamiltonian \( \tilde{H} \) agrees with \( H \) up to the desired order; see [156–161]. We note that when the target density contains two components, one computationally expensive and the other computationally cheap, it may be desirable to further split the potential \( H_2(q) = V(q) \) to obtain higher acceptance rates [162–164]. In order to achieve ergodicity in HMC methods, it is usually sufficient to randomise the trajectory length of the integrator [165–167]. However, deriving guarantees on the rate of convergence of HMC is difficult, though recent work have
established sufficient conditions for geometric ergodicity [15, 168].

Let us also briefly mention some useful upgrades that have been proposed in recent years. First, whenever the Metropolis step rejects the proposed sample, the (expensive) computation of the numerical trajectory is wasted, and several modifications have been proposed to address this issue, for example by granting the method extra integration steps when the proposal is rejected [169, 170], or using a dynamic integration with a termination criterion that aims to ensure the motion is long enough to avoid random walks, but short enough that we do not waste computational effort, such as the No-U-Turn sampler [171].

Second, the Metropolis algorithm gives rise to a reversible method which, as discussed above, usually has slower convergence properties. Modern HMC methods bypass this issue by replacing the heat bath by an Ornstein-Uhlenbeck process, which ensures the overall algorithm is irreversible. In this case, the overall HMC method can be viewed as a geometric integration of the underdamped Langevin diffusion [106, 172, 173]. The connection between HMC and Langevin diffusion originates from the desire to replace the Gaussian heat bath with a partial momentum refreshment, yielding a more accurate simulation of dynamical properties and higher acceptance rates [174].

Third, many modifications of the rudimentary HMC algorithm only provide improvements when the acceptance rate is sufficiently high. A third class of upgrades improves the acceptance rate by using the fact that the shadow Hamiltonian is exactly preserved by the integrator. These shadow HMC methods sample from a biased target distribution, defined by the (truncated) shadow Hamiltonian, and correct the bias in the samples via an importance sampler [138, 175, 176].

Finally, the Metropolis step can be replaced with a multinomial correction that uses the entire numerical trajectory, accepting a given point along it according to the degree by which it distorts the target measure [64]. Some methods entirely skip the accept/reject step, in particular those relying on approximate gradients and surrogates [177, 178], such as the stochastic HMC methods; such methods approximate the potential $V(q)$ and its derivative when they are given by a sum over data points, $V(q) = \sum_i V_i(q)$, by a cheaper sum over a uniformly sampled minibatches [179] (these are commonly called stochastic gradients in machine learning). However, this may break the shadow property and reduce the scalable and robust properties of HMC methods [180].

4 Statistical inference with kernel-based discrepancies

The problem of parameter inference consists of estimating an element $\theta^* \in \Theta$ using a sequence of random functions (or estimators) $\hat{\theta}_n : \Omega \to \Theta$, with $\hat{\theta}_n$ determined by a set of measurements $\{q_1, \ldots, q_n\}$ representing the available experimental data. In the statistical context, we search for the optimal approximation $\mu_{\theta^*}$ of the target measure $\rho$ within a statistical model $\{\mu_\theta : \theta \in \Theta\}$, with respect to a discrepancy $D : P \times P \to [0, \infty]$ over the set of probability measures $P$. A common choice of discrepancy is the KL-divergence, and the resulting inference problem can be implemented via the asymptotically optimal maximum likelihood estimators [69]. As in many applications we are interested in computing expectations, a particularly suitable notion of discrepancies are the integral probability pseudometrics (IPM) [181], which quantify the worse-case integration error with respect to a family of functions $\mathcal{F}$

$$d_\mathcal{F}(\rho, \mu) \equiv \sup_{f \in \mathcal{F}} \left| \int f d\rho - \int f d\mu \right|.$$

An apparent difficulty arises with IPMs in that we need to compute a supremum, which will be intractable for most choices of $\mathcal{F}$. Observe, however, that if $\mathcal{F}$ were the unit ball of a normed vector space $\mathcal{H}$, and integration with respect to $\rho$ and $\mu$ was a continuous linear functional on $\mathcal{H}$, then $d_\mathcal{F}(\rho, \mu)$ would correspond to the distance between $\rho$ and $\mu$ in the dual norm over the dual $\mathcal{H}^*$,
\[ d_F(\rho, \mu) = \|\rho - \mu\|_\ast. \]

Conveniently, reproducing kernel Hilbert spaces (RKHS) are precisely Hilbert spaces over which the Dirac distributions \( \delta_x : f \mapsto f(x) \) act continuously [182–184], and, more generally, the probability distributions that act continuously by integration on a RKHS are exactly those for which all elements of \( \mathcal{H} \) are integrable [185]. Denoting by \( \mathcal{P}_H \) the set of such probability distributions, so that by definition \( \delta_x \in \mathcal{P}_H \), we can define the Maximum Mean Discrepancy (MMD) as

\[ \text{MMD} : \mathcal{P}_H \times \mathcal{P}_H \rightarrow [0, \infty), \quad \text{MMD}[\rho | \mu] = \|\rho - \mu\|, \]

where we further used the Riesz representation isomorphism to view \( \rho, \mu \in \mathcal{P}_H \subset \mathcal{H}^\ast \approx \mathcal{H} \) as elements of \( \mathcal{H} \). The map \( \mathcal{P}_H \rightarrow \mathcal{H} \) is usually referred to as the mean embedding [186,187].

The angles between the mean embedding of Dirac distributions play a central role in the study of RKHS, and indeed characterise them. They define the reproducing kernel \( k : \mathcal{M} \times \mathcal{M} \rightarrow \mathbb{R} \), \( k(x, y) \equiv \langle \delta_x, \delta_y \rangle \), with \( \langle \cdot, \cdot \rangle \) denoting the inner product on \( \mathcal{H} \), from which we can obtain a practical expression for the squared MMD:

\[ \text{MMD}^2[\rho | \mu] = \int \int k(x, y)(\rho - \mu)(dy)(\rho - \mu)(dx). \]

### 4.1 Topological methods for MMDs

A key feature of RKHS, as identified by Laurent Schwartz, is the fact they are Hilbertian subspaces, i.e., Hilbert spaces continuously embedded within a topological vector space \( \mathcal{T} \), denoted \( \mathcal{H} \hookrightarrow \mathcal{T} \) [188]. In this context, by composing the transpose of the inclusion \( \mathcal{H} \hookrightarrow \mathcal{T} \) with the Riesz isomorphism, we can define a (generalised) mean embedding as the weakly-continuous positive map

\[ \phi : \mathcal{T}^\ast \hookrightarrow \mathcal{H}^\ast \hookrightarrow \mathcal{H}. \]

This mapping allows us to transfer structures between \( \mathcal{H} \) and \( \mathcal{T}^\ast \), an example of which is the MMD, which is nothing else than the pullback of the Hilbert space metric from \( \mathcal{H} \) to \( \mathcal{T}^\ast \). Some important examples of \( \mathcal{T} \) are \( C_0, C_\infty^c \) and \( \mathbb{R}^\mathcal{M} \) (with their canonical topologies), whose duals are the spaces of finite Radon measures, Schwartz distributions, and measures with finite support, respectively [189]. In particular a RKHS, as defined above, is any Hilbert space satisfying \( \mathcal{H} \hookrightarrow \mathbb{R}^\mathcal{M} \). More generally, when \( \mathcal{T} \) is continuously embedded in the space of \( \mathbb{R}^n \)-valued functions on \( \mathcal{M} \)—as in the examples above, which have \( n = 1 \)—then \( \mathcal{H} \) inherits (and can be characterised in terms of) a reproducing kernel \( K : \mathcal{M} \times \mathcal{M} \rightarrow \mathbb{R}^{n \times n} \), defined \( \forall \nu, u \in \mathbb{R}^n \) by

\[ v^\top K(x, y)u = \delta_x^\nu \left[ \phi(\delta_y^u) \right], \]

where \( \delta_x^u : h \mapsto u \cdot h(x) \); but this need not be the case in general, and we will employ Hilbertian subspaces with no reproducing kernel to construct the score-matching discrepancy.

This geometric description of RKHS and MMD allows us to swiftly apply topological methods in their analysis. For example, in order for \( \text{MMD}^2 \) to be a valid notion of statistical divergence, it should accurately discriminate distinct distributions, in the sense that \( \text{MMD}[\rho | \mu] = 0 \) iff \( \rho = \mu \). By construction, MMD will be characteristic to a subset of \( \mathcal{T}^\ast \), that is be able to distinguish its elements, iff \( \phi \) is injective. The Hahn–Banach theorem further shows that this is equivalent to the denseness of \( \mathcal{H} \) in \( \mathcal{T} \), reducing the matter to a topological question [186,189,190]. In many applications, we typically would like \( \mathcal{T}^\ast \) to be the set of probability measures, but the latter is not even a vector space. Instead, just as is commonly done to define (statistical) manifolds, it is
desirable to embed \( \mathcal{P} \) within a more structured space, such as the space of finite Radon measures \( C_0^* \). Characteristicness to \( C_0^* \) is also known as universality in learning theory, since such RKHS are dense in \( L^2(\mu) \) for any \( \mu \in \mathcal{P} \), which enables the method to learn the target function independently of the data-generating distribution [191]. However, in many important cases, we are interested in analysing the denseness of \( \mathcal{H} \) in a space other than \( C_0 \). For instance, in the case of unbounded reproducing kernels, we cannot aim to separate all finite distributions, since the RKHS will contain unbounded functions and the MMD will only be defined on a subset of \( \mathcal{P} \). In the particular case of the KSDs discussed below, which are given by transforming a base RKHS into a Stein RKHS via a differential operator, the characteristicness of the Stein RKHS to a set of probability measures is equivalent to the characteristicness of the base RKHS to more general spaces \( T^* \) of Schwartz distributions [185].

Moreover, the ability of MMD to discriminate distributions is also useful to ensure it further metrises, or at least controls, weak convergence, and thus provide a suitable quantification of the discrepancy between unequal distributions. Indeed, on non-compact locally compact Hausdorff spaces such as \( \mathbb{R}^d \), when \( \mathcal{H} \hookrightarrow C_0 \), then MMD will metrise weak convergence (of probability measures) iff the kernel \( k \) is continuous and \( \mathcal{H} \) is characteristic to the space of finite Radon measures [192]. The fact that the RKHS must separate all finite measures in order to metrise weak convergence results from the fact that otherwise MMD cannot in general prevent positive measures from degenerating into the null measure on non-compact spaces, beyond the family of translation-invariant kernels, for which characteristicness to the sets of probability measures or that of finite measures are in fact equivalent [189]. It is also possible to prevent probability mass from escaping to infinity—when the topology of the sequence of distributions is relatively compact with respect to the weak topology on the space of distributions—since, in that case, standard topological arguments relate MMD and weak convergence via characteristicness to \( \mathcal{P} \) [193]. For example, by Prokhorov’s theorem we may use the tightness of a sequence of distributions to ensure characteristic MMDs detect any loss of mass, and thus control weak convergence [194].

### 4.2 Smooth measures and KSDs

MMD have a computationally tractable expression whenever \( \rho, \mu \) are discrete measures, or at least tractable \( U \)-statistics when their samples are readily available. Many applications involve distributions that are smooth and fully supported, but hard to sample from. Recalling the definition of \( d\mathcal{F}(\rho, \mu) \), it would be useful to construct a MMD for which the set \( \mathcal{F} \) consists of functions whose integral under \( \mu \) is tractable, for example equal to zero; the MMD would then reduce to a double integration with respect to \( \rho \). To achieve this, we will leverage ideas from Stein’s method [195,196], and apply Stein operators to a given RKHS so as to construct a Stein RKHS whose elements have vanishing expectation under a distribution of interest.

#### 4.2.1 The canonical Stein operator and Poincaré duality

To gain intuition on Stein operators, we begin by considering the integral with respect to \( \mu \) as a linear operator on test functions, \( \mu : C_c^\infty(\mathcal{M}) \rightarrow \mathbb{R} \), with \( \mu f \equiv \int f \, d\mu \), and we are interested in generating test functions in the kernel of this operator (i.e., with vanishing expectations). There are two fundamental theorems that help us understand the integral-differential geometry of the manifold: de Rham’s theorem and Poincaré duality. The former relates the topology of the manifold to information on the solutions of differential equations defined over the manifold [197]. The latter (which contains the fundamental theorem of calculus) describes the properties of the integral pairing \( (\alpha, \beta) \mapsto \int \alpha \wedge \beta \) of differential forms, which include the pairing of test functions with smooth
measures \((f, \mu) \mapsto \int f d\mu\). While these results are canonical statements about the manifold, we can turn them into measure-theoretic statements by means of the isomorphism \(\mu^\sharp\). In particular, when \(\mathcal{M}\) is connected, there is an isomorphism between the top compactly supported twisted de Rham cohomology group \(H_p^\mathbb{R}(\mathcal{M})\) (which depends on the topology of \(\mathcal{M}\)) and \(\mathbb{R}\) given by integration, \(\omega \mapsto \int_{\mathcal{M}} \omega\). Applying the transformation \(\mu^\sharp\) to this isomorphism yields the isomorphism of vector spaces

\[
\mu : C^\infty_c(\mathcal{M})/\text{Im(}\text{div}(\cdot)\text{)} \to \mathbb{R},
\]

where \(\text{div}_{\mu|_c} : \mathfrak{x}_c(\mathcal{M}) \to C^\infty_c(\mathcal{M})\) is the divergence operator restricted to the set of compactly supported vector fields \(\mathfrak{x}_c(\mathcal{M})\). Hence, if \(h, f \in C^\infty_c(\mathcal{M})\), then

\[
\int f d\mu = \int h d\mu \iff f = h + \text{div}_{\mu}(X) \quad \text{for some } X \in \mathfrak{x}_c(\mathcal{M}).
\]

Consequently,

\[
\mu^{-1}(\{0\}) = \{\text{div}_{\mu}(X) : X \in \mathfrak{x}_c(\mathcal{M})\}.
\]

Thus, the test functions that integrate to zero are precisely those that can be written as the divergence of compactly supported vector fields. In particular, on compact manifolds, there is a canonical Stein operator, \(\text{div}_\mu\), which turns vector fields into functions with vanishing expectations. For other types of manifolds, one can obtain similar dualities by using other classes of differential forms, such as the square-integrable ones, or by allowing boundaries. For our purposes, the above is sufficient to motivate calling

\[
S_\mu \equiv \text{div}_{\mu|_c} : \mathfrak{x}_\mu \to C^\infty(\mathcal{M})
\]

the canonical Stein operator, whose domain \(\mathfrak{x}_\mu\), called the Stein class, is any set of vector fields satisfying the desired property that \(E_\mu[S_\mu(X)] \equiv \int S_\mu(X)d\mu = 0\), for all \(X \in \mathfrak{x}_\mu\).

If we have a bracket \(B\) on \(\mathcal{M}\), we can turn the canonical Stein operator on vector fields into a 2nd order differential operator acting on functions, the \(B\)-Stein operator on the Stein class

\[
C^\infty_\mu \equiv \{f \in C^\infty(\mathcal{M}) : X_f^B \in \mathfrak{x}_\mu\},
\]

by

\[
S^B_\mu : C^\infty_\mu \to C^\infty(\mathcal{M}), \quad S^B_\mu f \equiv \text{div}_\mu(X_f^B).
\]

If \(\mu = e^{-H}\mu_\mathcal{M}\) then we have the following useful decomposition:

\[
\text{div}_{e^{-H}\mu_\mathcal{M}}(X_f^B) = \text{div}_{\mu_\mathcal{M}}(X_f^B) - X_f^B(H).
\]

Let us give some important examples of bracket Stein operators. When \(B \equiv A\) is antisymmetric, the \(A\)-Stein operator is simply a 1st order differential operator, namely the \(\mu\)-preserving curl vector field \(S_\mu^A = \text{curl}_{\mu}(A)\). When \(B\) is Riemannian, and \(\mu_\mathcal{M}\) is the Riemannian measure, then

\[
S^B_\mu(f) = \nabla \cdot X_f^g - \langle \nabla f, \nabla H \rangle = \Delta f - \langle \nabla f, \nabla H \rangle = \Delta f + \langle \nabla f, \nabla \log d\mu/d\mu_\mathcal{M} \rangle,
\]

where \(\nabla, \Delta, \nabla \cdot, \langle \cdot, \cdot \rangle\) are the Riemannian gradient, Laplacian, divergence, and metric, respectively; the \(g^{-1}\)-Stein operator becomes the Riemannian Stein operator \([21,198,199]\). Hence, the Riemannian Stein operator is the restriction of the canonical Stein operator to gradient vector fields. In general, decomposing the bracket into its symmetric and antisymmetric parts, \(B \equiv S + A\), we obtain the following useful decomposition of the \(B\)-Stein operator:

\[
S^{S+A}_\mu(f) = \text{div}_\mu(X_f^S) + \text{curl}_\mu(A)(f).
\]
In particular, if we restrict ourselves to a symmetric positive semi-definite $B$, associated to a set of vector fields $\{Y_i\}$, $X^B_f \equiv Y_i(f)Y_i$ for any function $f$, then (39) corresponds to the generator of a $\mu$-preserving diffusion. A suitable Stein class is then the domain of the generator, since for any function in that domain $\mathbb{E}_\mu [S^A_\mu f]$ vanishes by the Fokker-Planck equation. The construction of Stein operators via measure-preserving diffusions is known as the Barbour approach \[200\]. In fact, the brackets allow us to define a more general notion of Stein operator acting on 1-forms of Stein operators via measure-preserving diffusions is known as the Barbour approach \[200\]. In particular, if we restrict ourselves to a symmetric positive semi-definite $B$, associated to a set of vector fields (or more general tensor fields) whose image $\mathcal{F}$ under the operator has mean zero under $\mu$. The resulting IPM is then known as a Stein Discrepancy:

$$ds_{\mu}(\mathcal{F})(\mu, \rho) = \sup_{X \in \mathcal{F}} \left| \int S_\mu(X)d\rho \right|.$$ 

The expression $\int S_\mu(X)d\rho$ is precisely the rate of change of the KL divergence along measures satisfying the continuity equation; an observation that leads to Stein variational gradient descent (SVGD) methods to approximate distributions \[198,202\]. Specifically, in SVGD the target measure is approximated using a finite distribution $\sum_i\delta_{x_i}$, where the location of the particles $\{x_i\}$ is updated by moving along the direction that maximises the rate of change of KL within a space of vector fields isomorphic to a RKHS (e.g., the space of gradients of functions in a RKHS).

When $S_\mu$ is the canonical Stein operator, there is a canonical Stein class, provided by Stokes’ theorem, which essentially only depends on the manifold: for a connected manifold $\mathcal{M}$, viewing integration as an operator on smooth $\mu$-integrable functions, then $\int f d\mu = 0 \iff \int d\alpha = 0$, where $f = \text{div}_\mu(\mu^\ast(\alpha))$. Unfortunately, Stokes’ theorem usually does not provide a practical description of the differential forms that satisfy $\int d\alpha = 0$, aside from the compactly supported case. There are, however, several choices of Stein class constructed from Hilbertian subspaces that lead to computationally tractable Stein discrepancies. One route consists in constructing a RKHS of mean-zero functions as the image of another RKHS under a Stein operator. In this case, we can use $S_\mu$ to map a given RKHS of $\mathbb{R}^d$-valued functions $\mathcal{H}$, with (matrix-valued) reproducing kernel $K$, into a Stein RKHS of $\mathbb{R}$-valued functions $S_\mu(\mathcal{H})$ associated to a Stein reproducing kernel $k_\mu$, given by (here $q$ is the Lebesgue density of $\mu$)

$$k_\mu(x, y) = \frac{1}{q(x)q(y)} \partial_y \cdot \partial_x \cdot (q(x)K(x, y)q(y)).$$

The resulting Stein discrepancy can be thought of as an MMD that depends only on $\rho$ and is known as kernel Stein discrepancy \[203\]:

$$\text{KSD}[\rho]^2 \equiv \text{MMD}[\rho \mid \mu]^2 = \iint \frac{1}{q(x)q(y)} \partial_y \cdot \partial_x \cdot (q(x)K(x, y)q(y)) d\rho(y)d\rho(x).$$

Another class of discrepancies relies on a choice of bracket $B$ together with a corollary from Stokes’ theorem: $\int S_\mu^B(\alpha)d\rho = \int \alpha(X^B_{H^K})d\rho$, where $e^{-H}$ and $e^{-K}$ are the densities of $\rho$ and $\mu$ with respect to a common smooth measure (below the Riemannian one), while $B^*$ is the dual bracket (the transpose of $B$). We can thus re-write the Stein discrepancy as

$$\sup_{\alpha \in \mathcal{A}} \left| \int \alpha(X^B_{H^K})d\rho \right| \quad (40)$$
over some family of 1-forms $\mathcal{A}$. As we did previously, we can “remove” the supremum by re-writing the above as a supremum over some unit ball of a continuous linear functional. This can be achieved once we have a Riemannian metric $\langle \cdot, \cdot \rangle$, which induces a natural inner product that is central to the theory of Harmonic forms, namely $\langle \alpha, \beta \rangle_{\mu} \equiv \int \langle \alpha, \beta \rangle d\mu$. In particular, taking as $\mathcal{A}$ the smooth compactly supported 1-forms in the unit ball of $L^2(T^*\mathcal{M}, \mu)$—the Hilbert space of square $\mu$-integrable 1-forms—the Stein discrepancy recovers a generalisation of the score matching [71]:

$$SM_B[\rho \mid \mu] = \int \|X_{H-K}^*\|^2 d\rho = \mathbb{E}_{\rho} \left[ \|X_{H-K}^*\|^2 \right].$$

(41)

It is worth noting that, while $L^2(T^*\mathcal{M}, \mu)$ is not a RKHS, and does not have a reproducing kernel, it remains a Hilbertian subspace of the space of de Rham currents. When $B$ is Riemannian we recover the Riemannian score matching [21]

$$SM_G[\rho \mid \mu] = \int \|\nabla H - \nabla K\|^2 d\rho,$$

while in Euclidean space (41) yields the diffusion score matching [204].

4.3 Information geometry of MMDs and natural gradient descent

MMDs and Stein discrepancies have proved to be important tools in a wide range of contexts, from hypothesis testing and training generative neural networks to measuring sample quality [128, 205–209]. In the context of statistical inference, once we have chosen a suitable discrepancy, $D$, and a statistical model, $\{\mu_\theta\}$, our aim is to find the best approximation of the target distribution within the model; this corresponds to solving the optimisation problem $\theta^* \in \arg \min_{\theta \in \Theta} D[\rho \mid \mu_\theta]$. As mentioned previously, computing the value of the discrepancy $D[\rho \mid \mu_\theta]$ is computationally challenging. Fortunately, we can often obtain robust Stein discrepancy estimators for smooth statistical models, whose distributions have a smooth positive Lebesgue density, as well as MMD estimators for generative model that are easy to sample from but have intractable model densities.

In either case, once we have an estimator $\hat{D}_m$ based on $m$ samples from the target, we must solve the approximate optimisation problem $\theta^*_m \in \arg \min_{\theta \in \Theta} \hat{D}_m[\rho \mid \mu_\theta]$. When the function $\hat{D}_m[\rho \mid \mu_\theta]$ is smooth, this may be done via the accelerated Hamiltonian-based optimisation methods previously discussed (section §2). If $D$ is a divergence function, one can also usually improve the speed of convergence by following the **natural gradient descent**, associated with the information Riemannian metric $g_\theta$ induced by $D$ [210–213]. In practice, this leads to implementing the update

$$\hat{\theta}_{t+1} = \hat{\theta}_t - \gamma_t \hat{\theta}^{-1}_t \partial_{\theta_t} \hat{D}_m[\rho \mid \mu_\theta],$$

where $\{\gamma_t\}$ is an appropriate sequence of step sizes, and $\hat{\theta}^{-1}_t$ is the inverse of a regularised estimate of the information tensor [214]. Finally, note that there is a deep connection between divergences and the geometric mechanics discussed in sampling and optimisation, as any divergence may be interpreted as a **discrete Lagrangian**, and hence generates a symplectic structure and integrator [215].

4.3.1 Minimum Stein discrepancy estimators

When the model $\{\mu_\theta\}$ consists of smooth measures with positive densities $\{q_\theta\}$, and we have access to samples $\{x_\ell\}$ from the target, the Stein discrepancies offer a flexible family of inference methods. For SM we can use the estimator

$$\hat{SM}_m[\rho \mid \mu_\theta] = \frac{1}{m} \sum_{\ell=1}^m \left( \|B^T \partial_x \log q_\theta\|_2^2 + 2\partial_x \cdot (BB^T \partial_x \log q_\theta) \right)(x_\ell)$$

(41)
combined with the following expression for the information tensor:

$$(g_{\theta})_{ij} = \int B^T \partial_x \partial_{\theta_i} \log q_{\theta} \cdot B^T \partial_x \partial_{\theta_j} \log q_{\theta} \, d\mu_{\theta}.$$ 

For KSD it is convenient to choose a family of matrix kernels $K_{\theta}(x, y) = B_{\theta}(x)k(x, y)B_{\theta}(y)^T$, for some scalar kernel $k$, and parameter-dependent matrix function $B_{\theta}$. Denoting the associated Stein reproducing kernel by $k_{\mu_{\theta}, \theta}$, we have the unbiased estimator

$$K_{\text{KSD}} m[\rho] = \frac{1}{m(m-1)} \sum_{i \neq j} k_{\mu_{\theta}, \theta}(x_i, x_j),$$

and information tensor

$$(g_{\theta})_{ij} = \iint (\partial_x \partial_{\theta_i}) B_{\theta}(x)k(x, y)B^T_{\theta}(y)\partial_x \partial_{\theta_j} \log q_{\theta} d\mu_{\theta}(x) d\mu_{\theta}(y).$$

The parameters $B$ and $k$, and the choice of statistical model, can often be adjusted to achieve characteristiness, consistency, bias-robustness, and obtain central limit theorems; see [204] for details, and for numerical experiments showing an acceleration induced by the information Riemannian metric.

4.3.2 Likelihood-free inference with generative models

For many applications of interests, the densities of the model, $\{\mu_{\theta}\}$, cannot be evaluated or differentiated. We thus need density-free inference methods. This is the case, for instance, in the context of generative models wherein $\mu_{\theta}$ is the pushforward of a distribution $\mu$, from which we can sample efficiently, with respect to a generator function $T_{\theta}$. Then, the minimum Stein discrepancy estimators based on KSD and SM, or other discrepancies that rely on the scores, are intractable. The MMDs are suited to this case since they depend on the target and model only through integration, which can be straightforwardly estimated using the samples. The associated information tensor is

$$(g_{\theta})_{ij} = \iint (\partial_x \partial_{\theta_i}) B_{\theta}(x)k(x, y)B^T_{\theta}(y)\partial_x \partial_{\theta_j} \log q_{\theta} \, d\mu_{\theta}(x) \, d\mu_{\theta}(y).$$

Under appropriate choices of kernels and models one can derive theoretical guarantees, such as concentration/generalisation bounds, consistency, asymptotic normality, and robustness; see, e.g., [209,216,217]. Moreover, many approaches to kernel selection in a wide range of contexts have been studied, which include the median heuristic or maximising the power of hypothesis tests, and in practice mixtures of Gaussian kernels are often employed [209,216,218–221].

5 Adaptive agents through active inference

The previous sections have established some of the mathematical fundamentals of optimisation, sampling and inference. In this final section, we close with a generic use case called active inference. Active inference is a general framework for describing and designing adaptive agents that unifies many aspects of behaviour—including perception, planning and learning—as processes of inference. Active inference emerged in the late 2000s as a unifying theory of human brain function [82–84,222], and has since been applied to simulate a wide range of behaviours in neuroscience [81,223], machine learning [88,94,224], and robotics [85,86]. In what follows, we derive the objective functional
overarching decision-making in active inference and describe its information geometric structure, revealing several special cases that are established notions in statistics, cognitive science and engineering. Finally, we exploit this geometric structure in a generic framework for designing adaptive agents.

5.1 Modelling adaptive decision-making

5.1.1 Behaviour, agents and environments

We define behaviour as the interaction between an agent and its environment. Together the agent and its environment form a system that evolves over time according to a stochastic process \( x \). This definition entails a notion of time \( T \), which may be discrete or continuous, and a state space \( X \), which should be a measure space (e.g., discrete space, manifold, etc.). A stochastic process \( x \) is a time-indexed collection of random variables \( x_t \) on the state space. More concisely, it is a random variable over trajectories on the state space \( T \to X \):

\[
x : \Omega \to (T \to X), \omega \mapsto x(\omega) \iff x_t : \Omega \to X, \omega \mapsto x(\omega)(t) \quad \forall t \in T.
\]

We denote by \( P \) the probability density of \( x \) on the space of paths \( T \to X \) with respect to a pre-specified base measure.

Typically, systems comprising an agent and its environment have three sets of states: external states are unknown to the agent and constitute the environment; the observable states are those agent’s states that the agent sees but cannot directly control; finally, the autonomous states are those agent’s states that the agent sees and can directly control. This produces a partition of the state space \( X \) into states external to the agent \( S \) and states belonging to the agent \( \Pi \), which themselves comprise observable \( O \) and autonomous states \( A \). As a consequence, the system \( x \) can be decomposed into external \( s \), observable \( o \), and autonomous \( a \) processes:

\[
X \equiv S \times \Pi \equiv S \times O \times A \implies x \equiv (s, \pi) \equiv (s, o, a),
\]

here written as random interacting trajectories on their respective spaces (see Figure 2 for an illustration).

5.1.2 Decision-making in precise agents

The description of behaviour adopted so far could, in principle, describe particles interacting with a heat bath [107] as well as humans interacting with their environment (see Figure 2). We would like a description that accounts for purposeful behaviour [81,225–229]. So what distinguishes people from small particles? An obvious distinction is that human behaviour is subject to classical as opposed to statistical mechanics. In other words, people are precise agents, with conservative dynamics.

**Definition 5.1** (Precise agent). An agent is precise when it evolves deterministically in a (possibly) stochastic environment, i.e., when \( P(\pi \mid s) \) is a Dirac measure for any \( s \). For example,

\[
ds_t = f(s_t, \pi_t)dt + dw_t, \quad d\pi_t = g(s_t, \pi_t)dt.
\]

At any moment in time \( t \), the agent has access, at most, to its past trajectory \( \pi_{\leq t} \), and has agency over its future autonomous trajectory \( a_{>t} \). We define a decision to be a choice of autonomous trajectory in the future given available knowledge \( a_{>t} \mid \pi_{\leq t} \). We interpret \( P(s, o \mid \pi_{\leq t}) \) as expressing the agent’s preferences over external and observable trajectories given available data, and \( P(s, o \mid a_{>t}, \pi_{\leq t}) \) as expressing the agent’s predictions over external and observable paths given
Figure 2: Partitions and agents. This figure illustrates a human (agent $\pi$) interacting with its environment (external process $s$), and the resulting partition into external $s$, observable $o$, and autonomous $a$ processes. The external states are the environment, which the agent does not have direct access to, but which is sampled through the observable states. These could include states of the sensory epithelia (e.g., eyes and skin). The autonomous states constitute the muscles and nervous system that factor available information into decisions. In the example of human behaviour, the environment causes observations (i.e., sensations), which informs a nervous and muscular response, which in turn influences the environment. In general, autonomous responses may be informed by all past agent states $\pi \leq t = (o \leq t, a \leq t)$ (the information available to the agent at time $t$), which means that the systems we are describing are typically non-Markovian.

A decision. Crucially, decision-making in (precise) agents is a functional of the agent’s predictions and preferences\(^{10}\)

\[
- \log P(a_{>t} \mid \pi_{\leq t}) = \mathbb{E}_{P(s,o \mid a_{>t}, \pi_{\leq t})}[- \log P(a_{>t} \mid \pi_{\leq t})] = \mathbb{E}[\log P(s,o \mid a_{>t}, \pi_{\leq t}) - \log P(s, o, a_{>t} \mid \pi_{\leq t})] \\
= \mathbb{E}[\log P(s \mid a_{>t}, \pi_{\leq t}) - \log P(s, o \mid \pi_{\leq t}) + \log P(o \mid s, a_{>t}, \pi_{\leq t}) - \log P(a_{>t} \mid s, o, \pi_{\leq t})] \\
= 0
\]

\[
\Rightarrow - \log P(a_{>t} \mid \pi_{\leq t}) = \mathbb{E}_{P(s,o \mid a_{>t}, \pi_{\leq t})}[\log P(s \mid a_{>t}, \pi_{\leq t}) - \log P(s, o \mid \pi_{\leq t})].
\]  

(EFE)

This functional is known as an expected free energy (EFE) \cite{81,84,231} because it resembles the expectation of the free energy functional (a.k.a. evidence lower bound \cite{232}) used in approximate Bayesian inference \cite{84,226}. We define active inference as Hamilton’s principle of least action on expected free energy\(^{11}\) that expresses the most likely decision $a_{>t}$, where

\[
a_{>t} \equiv \arg \min_{a_{>t}} - \log P(a_{>t} \mid \pi_{\leq t}).
\]  

(AIF)

5.1.3 The information geometry of decision-making

Interestingly, active inference (AIF) looks like it describes agents that engage in purposeful behaviour. Indeed, we can rearrange the expected free energy (EFE) in several ways, each of which reveals a fundamental trade-off that underwrites decision-making. This allows us to relate active inference to information theoretic formulations of decision-making that predominate in statistics.

\(^{10}\)Under the precise agent assumption (Definition 5.1) it is straightforward to show that $\mathbb{E}_{P(s,o \mid a_{>t}, \pi_{\leq t})}[\log P(o \mid s, a_{>t}, \pi_{\leq t}) - \log P(a_{>t} \mid s, o, \pi_{\leq t})] = 0$ when the path space $\mathcal{T} \rightarrow \mathcal{X}$ is countable \cite{230}. Presumably, this equality can be extended to more general path spaces by a limiting argument.

\(^{11}\)As a negative log density over paths, the expected free energy is an action in the physical sense of the word.
Figure 3: Decision-making under active inference. This figure illustrates various imperatives that underwrite decision-making under active inference in terms of several constructs that predominate in statistics, cognitive science and engineering. These formulations are disclosed when one removes certain sources of uncertainty. For example, if we remove ambiguity, decision-making minimises risk, which corresponds to aligning predictions with preferences about the external course of events. This aligns with prospect theory of human choice behaviour in economics [233] and underwrites modern approaches to control as inference [234–236], variously known as Kalman duality [237,238], KL control [239] and maximum entropy reinforcement learning [240]. If we further remove preferences, decision-making maximises the entropy of external trajectories. This maximum entropy principle [241,242] allows one to least commit to a pre-specified external trajectory and therefore keep options open. If we reintroduce ambiguity, but ignore preferences, decision-making maximises intrinsic value or expected information gain [243]. This underwrites Bayesian experimental design [244] and active learning in statistics [245], intrinsic motivation and artificial curiosity in machine learning and robotics [246–250]. This is mathematically equivalent to optimising expected Bayesian surprise and mutual information, which underwrites visual search [251,252] and the organisation of our visual apparatus [253–255]. Lastly, if we remove intrinsic value, we are left with maximising extrinsic value or expected utility. This underwrites expected utility theory [78], game theory, optimal control [256,257] and reinforcement learning [80]. Bayesian formulations of maximising expected utility under uncertainty are also known as Bayesian decision theory [77]. To ease notation, we omitted to condition every distribution in the figure by $\pi \leq t$.
that enable to recognise the external course of events. This leads to a type of observational bias commonly known as the streetlight effect [258]: when a person loses their keys at night, they initially search for them under the streetlight because the resulting observations (“I see my keys under the streetlight” or “I do not see my keys under the streetlight”) accurately disambiguate external states of affairs.

Similarly, decision-making maximises extrinsic and intrinsic value [259]:

\[
-\log P(a_{>t} \mid \pi \leq t) = \mathbb{E}_{P(o_{a_{>t}, \pi \leq t})} \left[ \text{KL} \left[ P(s \mid o, a_{>t}, \pi \leq t) \mid P(s \mid o, \pi \leq t) \right] \right] \\
- \mathbb{E}_{P(o_{a_{>t}, \pi \leq t})} \left[ \log P(o \mid \pi \leq t) \right] - \mathbb{E}_{P(o_{a_{>t}, \pi \leq t})} \left[ \text{KL} \left[ P(s \mid o, a_{>t}, \pi \leq t) \mid P(s \mid a_{>t}, \pi \leq t) \right] \right].
\]

Extrinsic value refers to the (log) likelihood of observations under the model of preferences. This corresponds to an expected utility or expected reward in behavioural economics, control theory and reinforcement learning [78, 80]. In short, maximising extrinsic value leads to sampling observations that are likely under the model of preferences. Intrinsic value refers to the amount of information gained about external courses of events. This measures the expected degree of belief updating about external trajectories under a decision, with versus without future observations. Making decisions to maximise information gain leads to a goal-directed form of exploration [231], driven to answer “What would happen if I did that?” [247]. Interestingly, this decision-making procedure underwrites Bayesian experimental design in statistics [244], which describes optimal experiments as those that maximise expected information gain. In summary, decision-making weighs the imperatives of maximising utility and information gain, which suggests a principled solution to the exploration-exploitation dilemma [260].

5.2 Realising adaptive agents

We now show how active inference affords a generic recipe to generate adaptive agents.

5.2.1 The basic active inference algorithm

Active inference specifies an agent by a prediction model \( P(s, o \mid a) \), expressing the distribution of external and observable paths given autonomous paths, and a preference model \( P(s, o) \), expressing the preferred external and observable trajectories. To aid intuition, we will refer to autonomous states as actions. At any time \( t \), the agent knows past observations and actions \( \pi \leq t = (o_{\leq t}, a_{\leq t}) \), and must make a decision \( a_{>t} \). In discrete time, active inference proceeds by assessing the expected free energy of each possible decision and then executing the best one:

1. Preferential inference: infer preferences about external and observable trajectories, i.e.,

   \[
   \text{Approximate } P(s, o \mid \pi \leq t) \text{ by } Q(s, o). \quad (43)
   \]

2. For each possible sequence of future actions \( a_{>t} \):

   (a) Perceptual inference: infer external and observable paths under the action sequence, i.e.,

   \[
   \text{Approximate } P(s, o \mid a_{>t}, \pi \leq t) \text{ by } Q(s, o \mid a_{>t}). \quad (44)
   \]
(b) Planning as inference: assess the action sequence by evaluating its expected free energy (EFE), i.e.,
\[ -\log Q(a_{>t}) \equiv \mathbb{E}_{Q(s,o\mid a_{>t})} \left[ \log Q(s \mid a_{>t}) - \log Q(s,o) \right]. \]  

3. Decision-making: execute the most likely decision \( a_{t+1} \) according to
\[ a_{t+1} = \arg \max Q(a_{t+1}), \quad Q(a_{t+1}) = \sum_{a_{>t}} Q(a_{t+1} \mid a_{>t}) Q(a_{>t}). \]  

5.2.2 Sequential decision-making under uncertainty

A common model of sequential decision-making under uncertainty is a partially observable Markov decision process (POMDP). A POMDP is a discrete time model of how actions influence external and observable states. In a POMDP, 1) each external state depends only on the current action and previous external state \( P(s_t \mid s_{t-1}, a_t) \), and 2) each observation depends only on the current external state \( P(o_t \mid s_t) \). One can additionally specify 3) a distribution of preferences over external trajectories \( P(s) \). Together, 1) & 2) forms the agent’s (POMDP) prediction model, and 2) & 3) forms the agent’s (hidden Markov) preference model, which defines an active inference agent. A simple simulation of active inference on a POMDP is provided in Figure 4; implementation details on generic POMDPs are available in [81,91,261,262]. For more complex simulations of sequential decision-making (e.g., involving hierarchical POMDPs), please see [88,91,223,224,263–265].

5.2.3 World model learning as inference

Due to a lack of domain knowledge, it may be challenging to specify an agent’s prediction and preference model. For example, how do external states map to observations? Should external states be represented in a discrete or continuous state space?

In active inference, generative models are learned by inferring their parameters [81,91,268] and structure [81,263,269–271]. Suppose there is an unknown parameter (or structure variable) \( m \) in the prediction model, the preference model or both. By definition, each alternative parameterisation \( m \) entails different predictions \( P(o,s \mid a,m) \) and preferences \( P(o,s \mid m) \). Since unknowns are simply external states, we treat the parameter as an additional external state. We equip the space of parameters with a prior distribution \( P(m) \), and define the agent with an augmented prediction (resp. preference) model that combines the different alternatives \( P(o,s,m \mid a) \equiv P(o,s \mid a,m)P(m) \) (resp. \( P(a,s,m) \equiv P(a,s \mid m)P(m) \)). The parameter can then be inferred along with other external states during preferential (43) or perceptual (44) inference [81,91,268]. Better yet, having specified priors over parameters that are independent of actions, we can infer them separately, for example, after fixed-length sequences of decisions to reduce computational cost [81,268].

All this says that a prior \( P(m) \) and some data \( \pi_{<t} \) leads to approximate posterior beliefs \( Q(m) \approx P(m \mid \pi_{<t}) \) about model parameters. But what are the right priors? One way to answer this question lies in optimising a free energy functional \( F \) (a.k.a. an evidence lower bound [232]):

\[
F \equiv \mathbb{E}_{Q(m)} \left[ -\log P(m, \pi_{<t}) \right] - S \left[ Q(m) \right] = \text{KL} \left[ Q(m) \mid P(m) \right] - \mathbb{E}_{Q(m)} \left[ \log P(\pi_{<t} \mid m) \right].
\]

Choosing priors that minimise free energy leads to parsimonious models that explain the data at hand [272]. This follows since maximising accuracy increases the likelihood of the data under
Figure 4: Sequential decision-making in a T-Maze environment. Left: The agent’s prediction model is a partially observed Markov decision process (see text) represented here as a Bayesian network [266]. The colour scheme illustrates the problem at $t = 2$: the agent must make a decision (in red) based on previous actions and observations (in grey), which are informative about external states and future observations (in white). Right: $s_t$: The T-Maze has four possible spatial locations: middle, top-left, top-right, bottom. One of the top locations contains a reward (in red), while the other contains a punishment (in black). The reward’s location determines the context. The bottom arm contains a cue whose colour (blue or green) discloses the context. Together, location and context determine the external state. $a_t$: The agent observes its spatial location. In addition, when it is at the top of the Maze, it observes the reward or the punishment; when it is at the bottom, it observes the colour of the cue. $P(s_t)$: The agent prefers being at the reward’s location ($- \log P(s_t) = +3$) and avoid the punishment’s location ($- \log P(s_t) = -3$). All other states have a neutral preference ($- \log P(s_t) = 0$). $o_0$: The agent is in the middle of the Maze and is unaware of the context. $a_1$: Visiting the bottom or top arms have a lower ambiguity than staying, as they yield observations that disclose the context. However, staying or visiting the bottom arm are safer options, as visiting a top arm risks receiving the punishment. By acting to minimise both risk and ambiguity (42) the agent goes to the bottom. $o_1$: The agent observes the colour of the cue and hence determines the context. $a_2$: All actions have equal ambiguity as the context is known. Collecting the reward has a lower risk than staying or visiting the middle, which themselves have a lower risk than collecting the punishment. Thus, the agent visits the arm with the reward. See [267] for more details.
5.2.4 Scaling active inference

We conclude by identifying promising scaling methods for active inference that enable computationally tractable implementations in a variety of applications.

Planning for all possible courses of action is computationally expensive as the number of action sequences is exponential in the length of the sequence. One way to finesse this is by planning only for intelligently chosen subsets of action sequences, using sampling algorithms such as Monte-Carlo tree search [87, 224, 274–276]. Monte-Carlo sampling can be also be used to finesse the expectations inherent in assessing action sequences (45) [224]. A complementary approach is to assess actions, instead of action sequences, by conditioning future actions to be optimal in the sense that they minimise the expected free energy [228, 277]. This idea leads to a backward form of planning, where the agent plans for the best action at the last time-step, followed by the best action at the penultimate time-step, and so on, until the present. Crucially, it leads to smarter agents [228, 277] whose computational complexity scales linearly (as opposed to exponentially) in the length of action sequences [278].

Scalable inference methods [279] can be used to make active inference more efficient [280]. For example, we can train neural networks to predict the various posterior distributions, including the posterior over actions [88, 224, 281]. While training, the output of the neural network can be used as an initial conditions for variational inference [282], resulting in accurate inferences whose computational cost decrease as the network learns. Additionally, optimising free energy reduces to efficient message passing schemes, when one imposes certain simplifying restrictions to the family of candidate distributions [283–287].

A much cheaper implementation of active inference exists for continuous states evolving in continuous time. The method frames perception and decision-making as variational inference, by simulating a gradient flow on free energy in an extended state space [82, 226]. Furthermore, it can be combined with discrete active inference to operate efficiently in generative models combining discrete and continuous states [288]. As an example, high-dimensional observations in the continuous domain (e.g., speech) processed through continuous active inference are converted into discrete, abstract representations (e.g., semantics) [281]. Based on these representations, the agent makes high-level, categorical decisions (e.g., “I want to move over there”), which contextualise low-level, continuous actions (e.g., the continuous motion of a limb towards the goal location) [289].

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