Driving black-box quantum thermal machines with optimal power/efficiency trade-offs using reinforcement learning

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The optimal control of non-equilibrium open quantum systems is a challenging task but has a key role in improving existing quantum information processing technologies. We introduce a general model-free framework based on Reinforcement Learning to identify out-of-equilibrium thermodynamic cycles that are Pareto optimal trade-offs between power and efficiency for quantum heat engines and refrigerators. The method does not require any knowledge of the quantum thermal machine, nor of the system model, nor of the quantum state. Instead, it only observes the heat fluxes, so it is both applicable to simulations and experimental devices. We test our method identifying Pareto-optimal trade-offs between power and efficiency in two systems: an experimentally realistic refrigerator based on a superconducting qubit, where we identify non-intuitive control sequences that reduce quantum friction and outperform previous cycles proposed in literature; and a heat engine based on a quantum harmonic oscillator, where we find cycles with an elaborate structure that outperform the optimized Otto cycle.

INTRODUCTION

Thermal machines convert between thermal and mechanical energy in a controlled manner. Examples include heat engines such as steam and Otto engines, that extract useful work from a temperature difference, and refrigerators, that extract heat from a cold bath. Quantum thermal machines (QTMs) perform thermodynamic cycles via nanoscale quantum systems. QTMs could find applications in heat management at the nanoscale [1], or for on-chip active cooling [2, 3]. Quantum thermodynamics is a rapidly growing research area that aims at the understanding, design and optimization of QTMs [4]. A fundamental open question is whether quantum effects can boost the performance of QTMs [2, 4, 5]. Conversely, understanding how to optimally control the non-equilibrium dynamics of open quantum systems can improve existing quantum information processing technologies.

Nowadays it is possible to construct quantum devices in platforms such as trapped ions [6, 7], electron spins associated with nitrogen-vacancy centers [8], circuit quantum electrodynamics [9], and quantum dots [10], and to control their state through time-dependent controls, such as electro-magnetic pulses or gate voltages. The heat flow across these systems has been measured [11–14], and recent experimental realizations of QTMs have been reported [15–22].

The two main quantities that describe the performance of a heat engine (refrigerator) are the extracted power (cooling power) and the efficiency (coefficient of performance). Optimizing such quantities is an extremely challenging task: (i) having to operate in finite time, the state can be driven far from equilibrium, where the thermal properties of the system are model-specific; (ii) the optimization is a search over the space of all possible time-dependent controls, which increases exponentially with the number of time points describing the cycle; (iii) there is a trade-off between high power and high efficiency, so that a good balance between the two is sought; (iv) in experimental devices, often subject to undesired effects such as noise and decoherence [23], we could have a limited knowledge of the actual model describing the dynamics of the QTM.

The optimization of QTMs [4, 24] is generally carried out in specific regimes, or assuming a-priori a specific shape of the control-cycle. Within the regimes of either slow driving [25–34] or fast driving, general strategies have been recently derived [35–37]. Outside these regimes, specific cycle structures have been considered [38–43], such as the Otto cycle [44–59]. Shortcuts to adiabaticity [60–68] and variational strategies [69–71] have been employed. The impact of quantum effects on the performance of QTMs is not straightforward. Several studies have found quantum advantages [54, 55, 59, 72–74], while coherence-induced power losses were reported [46, 52, 58, 69, 75, 76].

In general, there is no guarantee that these regimes and cycles are optimal. Recently, Reinforcement-Learning (RL) has been used to find cycles that maximize the power of QTMs without making assumptions on the cycle structure [77], however this approach requires a model of the quantum system, which restricts its practical applicability. This calls for the development of robust and general strategies that overcome all above-mentioned difficulties (i-iv).

We propose a RL-based method with the following properties: (i) it finds cycles yielding near Pareto-optimal trade-offs between power and efficiency, i.e. the family of cycles such that it is not possible to improve either power...
Quantum Thermal Machine

Computer Agent
Hot bath Quantum System
Cold bath

FIG. 1. Schematic representation of a quantum thermal machine controlled by a computer agent. A quantum system (gray circle) can be coupled to a hot (cold) bath at inverse temperatures $\beta_H$ ($\beta_C$), represented by the red (blue) square, enabling a heat flux $J_H(t)$ ($J_C(t)$). The quantum system is controlled by the computer agent through a set of experimental control parameters $\vec{u}(t)$, such as an energy gap or an oscillator frequency, that control the power exchange $P(t)$, and through a discrete control $d(t) = \{\text{Hot, Cold, None}\}$ that determines which bath is coupled to the system. $J_H(t)$ and $J_C(t)$ denote the heat flux flowing out respectively from the hot and cold bath at time $t$.

Our method only relies on the following two assumptions:

(i) the RL agent can measure the heat fluxes $J_C(t)$ and $J_H(t)$ (or their averages over a time period $\Delta t$);

(ii) $J_C(t)$ and $J_H(t)$ are functions of the control history $(\vec{u}(t-T), d(t-T), ..., (\vec{u}(t), d(t)))$, where $T$ is the timescale over which the QTM remembers past controls.

In particular, we do not assume that we have a microscopic model of the inner workings of the quantum system, in contrast to previous work [77]. In that sense, our quantum system is a “black-box”. Any theoretical model or experimental device satisfying these requirements can be optimized by our method. The timescale $T$ is finite because of energy dissipation and naturally emerges by making the minimal assumption that the coupling of the quantum system to the thermal baths drives the system towards a thermal state within some timescale $T$. Such a timescale can be rigorously identified e.g. within the weak system-bath coupling regime, and in the reaction coordinate framework that can describe non-Markovian and strong-coupling effects [101].

The thermal machines we consider are the heat engine and the refrigerator. Up to an internal energy contribution that vanishes after each cycle, the instantaneous power of a heat engine equals the extracted heat:

$$P_{\text{heat}}(t) = J_C(t) + J_H(t),$$

and the cooling power of a refrigerator is:

$$P_{\text{cool}}(t) = J_C(t).$$

The entropy production is given by

$$\Sigma(t) = -\beta_C J_C(t) - \beta_H J_H(t),$$

where we neglect the contribution of the quantum system’s entropy since it vanishes after each cycle.

**Machine Learning Problem**

Our goal is to identify optimal cycles, i.e. periodic functions $\vec{u}(t)$ and $d(t)$ that maximize a trade-off between power and efficiency on the long run. We thus

Setting: Black-box Quantum Thermal Machine

We describe a QTM by a quantum system, acting as a “working medium”, that can exchange heat with a hot (H) or cold (C) thermal bath characterized by inverse temperatures $\beta_H < \beta_C$ (Fig. 1). Our method can be readily generalized to multiple baths, but we focus the description on two baths here.

We can control the evolution of the quantum system and exchange work with it through a set of time-dependent continuous control parameters $\vec{u}(t)$ that enter in the Hamiltonian $H[\vec{u}(t)]$ of the quantum system [100], and through a discrete control $d(t) = \{\text{Hot, Cold, None}\}$ that determines which bath is coupled to the system. $J_H(t)$ and $J_C(t)$ denote the heat flux flowing out respectively from the hot and cold bath at time $t$.

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define the reward function \( r_c(t) \) which measures the power/efficiency trade-off at time \( t \):

\[
r_c(t) = c \frac{P(t)}{P_0} - (1 - c) \frac{\Sigma(t)}{\Sigma_0},
\]

(4)

where \( P(t) \) is the power of a heat engine (Eq. 1) or cooling power of a refrigerator (Eq. 2), and \( P_0, \Sigma_0 \) are reference values to normalize the power and entropy production. \( c \in [0, 1] \) is a weight that determines the trade-off between power and efficiency.

As in Ref. [77], we are interested in cycles that maximize the long-term performance of QTM; we thus maximize the return \( \langle r_c \rangle (t) \), where \( \langle \cdot \rangle(t) \) indicates the exponential moving average of future values:

\[
\langle r_c \rangle (t) = \kappa \int_0^\infty e^{-\kappa \tau} r_c(t + \tau) \, d\tau.
\]

(5)

Here \( \kappa \) is the inverse of the averaging timescale, that will in practice be chosen much longer than the cycle period, such that \( \langle r_c \rangle (t) \) is approximately independent of \( t \).

For \( c = 0 \), we are maximizing the average power \( \langle r_0 \rangle = \langle P \rangle / P_0 \). For \( c = 1 \), we are minimizing the average entropy production \( \langle r_1 \rangle = -\langle \Sigma \rangle / \Sigma_0 \), which corresponds to maximizing the efficiency. For intermediate values of \( c \), the maximization of \( \langle r_c \rangle \) describes possible Pareto-optimal trade-offs between power and efficiency (see “Optimizing the entropy production” in Methods for details).

**RESULTS**

Deep reinforcement learning for black-box quantum thermal machines

In RL, a computer agent must learn to master some task by repeated interactions with some environment. Here we develop an RL approach where the agent maximizes the return (5) and the environment is the QTM with its controls (Fig. 2a). To solve the RL problem computationally, we discretize time as \( t_i = i\Delta t \). By time-discretizing the return (5), we obtain a discounted return whose discount factor \( \gamma = \exp(-\kappa \Delta t) \) determines the averaging timescale and expresses how much we are interested in future or immediate rewards (see “Reinforcement Learning Implementation” in Methods for details).

At each time step \( t_i \), the agent employs a policy function \( \pi(a|s) \) to choose an action \( a_i = \{\vec{u}(t_i), d(t_i)\} \) based on the state \( s_i \) of the environment. Here, \( \vec{u}(t) \) are the continuous controls over the quantum system and \( d(t) \in \{\text{Hot}, \text{Cold}, \text{None}\} \) is a discrete control that selects the bath the system is coupled to. All controls are considered to be constant during time step of duration \( \Delta t \). The aim of RL is to learn an optimal policy function \( \pi(a|s) \) that maximizes the return.

In order to represent a black-box quantum system whose inner mechanics are unknown, we define the control history during a time interval of length \( T \) as the observable state:

\[
s_i = (a_{i-N}, a_{i-N+1}, \ldots, a_{i-1}),
\]

(6)

where \( N = T/\Delta t \). Therefore, the state of the quantum system is implicitly defined by the sequence of the agent’s \( N \) recent actions.

To find an optimal policy we employ the soft actor-critic algorithm, that relies on learning also a value function \( Q(s, a) \), generalized to a combination of discrete and continuous actions [78–81]. The policy function \( \pi(a|s) \) plays the role of an “actor” that chooses the actions to perform, while a value function \( Q(s, a) \) plays the role of a “critic” that judges the choices made by the actor, thus providing feedback to improve the actor’s behavior. We further optimize the method for a multi-objective set-
ting by introducing a separate critic for each objective, i.e. one value function for the power, and one for the entropy production. This allows us to vary the weight $c$ during training, thus enhancing convergence (see “Reinforcement Learning Implementation” in Methods for details).

We learn the functions $\pi(a|s)$ and $Q(s, a)$ using a deep NN architecture inspired by WaveNet, an architecture that was developed for processing audio signals [102] (See Figs. 2b-c). We introduce a “convolution block” to efficiently process the time-series of actions defining the state $s_i$. It consists of a 1D convolution with kernel size and stride of 2, such that it halves the length of the input. It is further equipped with a residual connection to improve trainability [103] (see “Reinforcement Learning Implementation” in Methods for details). The policy $\pi(a_i|s_i)$ is described by a NN that takes the state $s_i$ as input, and outputs parameters $\mu$ and $\sigma$ describing the probability distribution from which action $a_i$ is sampled (Fig. 2b). The value function $Q(s_i, a_i)$ is computed by feeding $(s_i, a_i)$ into a NN, and outputting $Q(s_i, a_i)$ (Fig. 2c). Both $\pi(a_i|s_i)$ and $Q(s_i, a_i)$ process the state by feeding it through multiple convolution blocks (upper orange boxes in Figs. 2b and 2c), each one halving the length of the time-series, such that the number of blocks and of parameters in the NN is logarithmic in $N$. Then a series of fully-connected layers produce the final output.

The policy and value functions are determined by minimizing the loss functions in Eqs. (39) and (49) using the ADAM optimization algorithm [104]. The gradient of the loss functions is computed off-policy, over a batch of past experience recorded in a replay buffer, using back-propagation (see “Reinforcement Learning Implementation” in Methods for details).

Pareto-optimal cycles for a superconducting qubit refrigerator

We first consider a refrigerator based on an experimentally realistic system: a superconducting qubit coupled to two resonant circuits that behave as heat baths [52] (Fig. 3a). Such a system was experimentally studied in the steady-state in Ref. [11]. The system Hamiltonian is given by [52, 58, 66]:

$$\hat{H}[u(t)] = -E_0 [\Delta \hat{\sigma}_z + u(t) \hat{\sigma}_x],$$  

(7)

where $E_0$ is a fixed energy scale, $\Delta$ characterizes the minimum gap of the system, and $u(t)$ is our control parameter. In this setup the coupling to the baths, described by the commonly employed Markovian master equation [105–108], is fixed, and cannot be controlled. However, the qubit is resonantly coupled to the baths at different energies. The $u$-dependent coupling strength to the cold (hot) bath is described by the function $\gamma_u^{(C)}$ ($\gamma_u^{(H)}$), respectively (Fig. 3f). As in Ref. [66], the coupling strength is, respectively, maximal at $u = 0$ ($u = 1/2$), with a resonance width determined by the “quality factor” $Q_C$ ($Q_H$) (see “Physical model” in Methods for details). This allows us to choose which bath is coupled to the qubit by tuning $u(t)$.

In Fig. 3 we show an example of our training procedure to optimize the return $\langle r_c \rangle$ at $c = 0.6$ using $N = 128$ steps determining the RL state, and varying $c$ during training from 1 to 0.6 (Fig. 3c). In the early stages of the training,
the return $\langle r_c \rangle$, computed as in Eq. (28) but over past rewards, and the running averages of the cooling power $\langle P_{\text{cool}} \rangle_i$ and of the negative entropy production $-\langle \Sigma \rangle_i$ all start off negative (Fig. 3b), and the corresponding actions are random (left panel of Fig. 3d). Indeed, initially the RL agent has no experience controlling the QTM, so random actions are performed, resulting in heating the cold bath, rather than cooling it, and in a large entropy production. However, with increasing steps, the chosen actions exhibit some structure (Fig. 3d), and the return $\langle r_c \rangle$ increases (Fig. 3b). While both the power and the negative entropy production initially increase together, around step 100k we see that $-\langle \Sigma \rangle$ begins to decrease. This is a manifestation of the fact that power and entropy production cannot be simultaneously optimized. Indeed, the agent learns that in order to further increase the return, it must “sacrifice” some entropy production to produce a positive and larger cooling power. In fact, the only way to achieve positive values of $\langle r_c \rangle_i$ is to have a positive cooling power, which inevitably requires producing entropy. Eventually all quantities in Fig. 3b reach a maximum value, and the corresponding final deterministic cycle (i.e. the cycle generated by policy switching off stochasticity, see “Reinforcement Learning Implementation” in Methods for details) is shown in Fig. 3e as thick black dots.

For the same system, Ref. [66] proposed a smoothed trapezoidal cycle $u(t)$ oscillating between the resonant peaks at $u = 0$ and $u = 1/2$ and optimized the cycle time (Fig. 3c, dashed line). While this choice outperformed a sine and a trapezoidal cycle [52], the cycle found by our RL agent produces a larger return (Fig. 3b). The optimal trapezoidal cycle found for $c = 0.6$ is shown in Fig. 3e as a dashed line (see “Comparing with the trapezoidal and Otto cycle” in Methods for details).

Fig. 4 compares optimal cycles for different trade-offs between cooling power and coefficient of performance $\eta_{\text{cool}}$, the latter defined as the ratio between the average cooling power, and the average input power. This is achieved by repeating the optimization for various values of $c$. To demonstrate the robustness of our method, the optimization of $\langle r_c \rangle$ was repeated 5 times for each choice of $c$ (variability shown with error bars in Fig. 4a, and as separate points in Fig. 4b). The RL method substantially outperforms the trapezoidal cycle by producing larger final values of the return $\langle r_c \rangle$ at all values of $c$ (Fig. 4a), and by producing a better Pareto front (Fig. 4b). The RL cycles simultaneously yield higher power by more than a factor of 10, and a larger $\eta_{\text{cool}}$, for any choice of the power-efficiency trade-off. As expected the period of the RL cycles increases as $c$ decreases and the priority shifts from high power to high $\eta_{\text{cool}}$ (Figs. 4c-f, black dots). However, the period is much shorter than the corresponding optimized trapezoidal cycle (dashed line), and the optimal control sequence is quite unintuitive, even going beyond the resonant point at $u = 1/2$.

As argued in [52, 58, 66], the generation of coherence in the instantaneous eigenbasis of the quantum system, occurring because $[\hat{H}(u_1), \hat{H}(u_2)] \neq 0$ for $u_1 \neq u_2$, causes power losses that increase with the speed of the cycle. We find that we can interpret the power enhancement achieved by our cycle as a mitigation of such detrimental effect: indeed, we find that trapezoidal cycles operated at the same frequency as the RL cycle generate twice as much coherence as the RL cycles (see “Generation of coherence” in Methods for details). In either case, cycles with higher power tend to generate more coherence.

Given the stochastic nature of RL, we also compared the cycles obtained across the 5 independent training runs, finding that cycles are typically quite robust, displaying only minor changes (see Fig. 8 of Methods for four cycles found in independent training runs corresponding to Figs. 4c-f).
Pareto-optimal cycles for a quantum harmonic oscillator engine

We now consider a heat engine based on a collection of non-interacting particles confined in a harmonic potential [46] (Fig. 5a). The Hamiltonian is given by

\[ \hat{H}[u(t)] = \frac{1}{2m} \hat{p}^2 + \frac{1}{2} m(u(t)w_0)^2 \hat{q}^2, \]  

(8)

where \( m \) is the mass of the system, \( w_0 \) is a reference frequency and \( \hat{p} \) and \( \hat{q} \) are the momentum and position operators. The control parameter \( u(t) \) allows us to change the frequency of the oscillator. Here, at every time step we let the agent choose which bath (if any) to couple to the oscillator. The coupling to the baths, characterized by the thermalization rates \( \Gamma_\alpha \), is modeled using the Lindblad master equation as in Ref. [46] (see “Physical model” in Methods for details). In contrast to the superconducting qubit case, \( c \) is held constant during training.

Fig. 5 reports the results on the optimal trade-offs between extracted power and efficiency \( \eta_{\text{heat}} \), the latter defined as the ratio between the extracted power and the input heat, in the same style of Fig. 4. In this setup, we compare our RL-based results to the well-known Otto cycle. The authors of Ref. [46] study this system by optimizing the switching times of an Otto cycle, i.e. the duration of each of the 4 segments, shown as a dashed lines in Figs. 5d-e, composing the cycle (see “Comparing with the trapezoidal and Otto cycle” in Methods for details).

The RL method produces cycles with a larger return and with a better power-efficiency Pareto-front with respect to the Otto cycle (Fig. 5b,c). The cycle power found by the RL method significantly outperforms the Otto engine. For \( c = 1 \), a high-power cycle is found (Fig. 5d and corresponding blue dots in Figs. 5b-c) but at the cost of a lower efficiency than the Otto cycles. However, at \( c = 0.5 \), the RL method finds a cycle that matches the maximum efficiency of the Otto cycles, while delivering a \( \sim 30\% \) higher power (Fig. 5e and corresponding blue dots in Figs. 5b-c).

Remarkably, our black-box RL method finds a cycle with roughly the same maximum power as in a previous RL method [77] that relies on observing the internal quantum state of the system (compare Fig. 5d, with Fig. 5c of Ref. [77]).

Interestingly, as shown in Figs. 5d-e, the cycles found by the RL agent share many similarities with the Otto cycle: both alternate between the hot and cold bath (orange and blue portions) with a similar period. However, there are some differences: at \( c = 1 \), the RL cycle ramps the value of \( u \) while in contact with the bath, eliminating the unitary stroke (Fig. 5d). Instead, at \( c = 0.5 \), the RL agent employs a unitary stroke that is quite different respect to a linear ramping of \( u \) (Fig. 5e, green dots). As in the superconducting qubit case, the enhanced performance of the RL cycle may be interpreted as a mitigation of quantum friction [46, 76].

Also in this setup, we verified that the discovered cycles are quite robust across the 5 independent training runs, displaying only minor changes (see Fig. 9 of Methods for two cycles found in independent training runs).
corresponding to Figs. 5d-e).

**DISCUSSION**

We introduced a model-free framework, based on Reinforcement Learning, to discover Pareto-optimal thermodynamic cycles that describe the best possible trade-off between power and efficiency of out-of-equilibrium quantum thermal machines (heat engines and refrigerators). The only inputs our algorithm requires are the heat fluxes of the QTM. It can therefore be used both for the theoretical optimization of known systems, and potentially of experimental devices for which no model is known, and in the absence of any measurement performed on the quantum system. Using state-of-the-art machine learning techniques, we demonstrate the validity of our method applying it to two different prototypical setups. Our black-box method discovered new uninitiative and elaborate cycles that outperform previously proposed cycles and are on par with a previous RL method performed on the quantum system. Using state-of-the-art quantum thermal machines (heat engines and refrigerators). The only inputs our algorithm requires are the heat fluxes of the QTM. It can therefore be used both across independent training runs.

Our method paves the way for a systematic use of RL in the field of quantum thermodynamics. Future directions include investing larger systems to uncover the impact of quantum many-body effects on the performance of QTM, optimizing systems in the presence of noise, and optimizing trade-offs that include power fluctuations [109–112].

**METHODS**

**Optimizing the entropy production**

Here we discuss the relation between optimizing the power and the entropy production, or the power and the efficiency. We start by noticing that we can express the efficiency of a heat engine $\eta_{\text{heat}}$ and the coefficient of performance of a refrigerator $\eta_{\text{cool}}$ in terms of the averaged power and entropy production, i.e.

$$
\eta_{\nu} = \eta_{\nu}^{(c)} [1 + \langle \Sigma \rangle / (\beta_{\nu} \langle P_{\nu} \rangle)]^{-1},
$$

where $\nu = \text{heat, cool}$, $\eta_{\text{heat}}^{(c)} \equiv 1 - \beta_{\text{H}} / \beta_{\text{C}}$ is the Carnot efficiency, $\eta_{\text{cool}}^{(c)} \equiv \beta_{\text{H}} / (\beta_{\text{C}} - \beta_{\text{H}})$ is the Carnot coefficient of performance, and where we defined $\beta_{\text{heat}} \equiv \beta_{\text{C}}$ and $\beta_{\text{cool}} \equiv \beta_{\text{C}} - \beta_{\text{H}}$. We now observe that, thanks to this dependence of $\eta_{\nu}$ on $\langle P_{\nu} \rangle$ and $\langle \Sigma \rangle$, optimizing a trade-off between high power and high efficiency yields all the Pareto optimal trade-offs between high power and low entropy-production up to a change of $c$.

Mathematically, we want to prove that the cycles that maximize

$$
\langle G_{\nu}(c) \rangle = c \langle P_{\nu} \rangle + (1 - c) \eta_{\nu}
$$

for some value of $c \in [0, 1]$, also maximize the return in Eq. (5) for some (possibly different) value of $c \in [0, 1]$. To simplify the proof and the notation, we consider the following two functions

$$
F(a, b, \theta) = aP(\theta) - b\Sigma(P(\theta), \eta(\theta)),
$$

$$
G(a, b, \theta) = aP(\theta) + b\eta(\theta),
$$

where $P(\theta)$ and $\eta(\theta)$ represent the power and efficiency of a cycle parameterized by a set of parameters $\theta$, $a > 0$ and $b > 0$ are two scalar quantities, and

$$
\Sigma(P, \eta) = \frac{\eta^{(c)}(c) - \eta}{\eta} \beta_\nu P
$$

is obtained by inverting Eq. (9).

We wish to prove the following. Given some weights $a_1 > 0$ and $b_1 > 0$, let $\theta_1$ be the value of $\theta$ that locally maximizes $G(a_1, b_1, \theta)$. Then, it is always possible to identify positive weights $a_2 > 0$, $b_2 > 0$ such that the same parameters $\theta_1$ (i.e. the same cycle) is a local maximum for $F(a_2, b_2, \theta)$. In the following, we will use that

$$
\partial P \Sigma \geq 0 \quad \partial P \Sigma < 0,
$$

and that the Hessian $H^{(\Sigma)}$ of $\Sigma(P, \eta)$ is given by

$$
H^{(\Sigma)} = \begin{pmatrix}
0 & -\beta_\nu \eta^{(c)} \\
-\beta_\nu \eta^{(c)} & 2\beta_\nu P \eta^{(c)}
\end{pmatrix}.
$$

**Proof:** by assumption, $\theta_1$ is a local maximum for $G(a_1, b_1, \theta)$. Denoting with $\partial_i$ the partial derivative in $(\theta)_i$, we thus have

$$
0 = \partial_i G(a_1, b_1, \theta_1) = a_1 \partial_i P(\theta_1) + b_1 \partial_i \eta(\theta_1).
$$

Now, let us compute the derivative in $\theta$ of $F(a_2, b_2, \theta)$, where $a_2 > 0$ and $b_2 > 0$ are two arbitrary positive coefficients. We have

$$
\partial_i F(a_2, b_2, \theta_1) = (a_2 - b_2 \partial P \Sigma) \partial_i P(\theta_1) - (b_2 \partial P \Sigma) \partial_i \eta(\theta_1).
$$

Therefore, if we choose $a_2$ and $b_2$ such that

$$
\begin{pmatrix}
a_1 \\
b_1
\end{pmatrix} = \begin{pmatrix}
1 - \partial P \Sigma \\
\partial P \Sigma
\end{pmatrix} \begin{pmatrix}
a_2 \\
b_2
\end{pmatrix},
$$

thanks to Eq. (15) we have that

$$
0 = \partial_i F(a_2, b_2, \theta_1),
$$

meaning that the same parameters $\theta_1$ that nullifies the gradient of $G$, nullifies also the gradient of $F$ at a different choice of the weights, given by Eq. (17). The invertibility of Eq. (17) (i.e. a non-null determinant of the matrix) is guaranteed by Eq. (13). We also have to make sure that if $a_1 > 0$ and $b_1 > 0$, then also $a_2 > 0$ and $b_2 > 0$. To do this, we invert Eq. (17), finding

$$
\begin{pmatrix}
a_2 \\
b_2
\end{pmatrix} = \begin{pmatrix}
1 - \partial P \Sigma / (\partial \eta \Sigma) \\
0 - 1 / (\partial \eta \Sigma)
\end{pmatrix} \begin{pmatrix}
a_1 \\
b_1
\end{pmatrix}.
$$
It is now easy to see that also the weights $a_2$ and $b_2$ are positive using Eq. (13).

To conclude the proof, we show that $\theta_1$ is a local maximum for $F(a_2, b_2, \theta)$ by showing that its Hessian is negative semi-definite. Since, by hypothesis, $\theta_1$ is a local maximum for $G(a_1, b_1, \theta)$, we have that the Hessian matrix

$$H^{(G)}_{ij} = \partial_{ij} G(a_1, b_1, \theta_1) = a_i \partial_{ij} P + b_i \partial_{ij} \eta \quad \text{(20)}$$

is negative semi-definite. We now compute the Hessian $H^{(F)}$ of $F(a_2, b_2, \theta)$ in $\theta = \theta_1$:

$$H^{(F)}_{ij} = a_2 \partial_{ij} P - b_2 [\partial_P \Sigma \partial_{ij} P + \partial_\eta \Sigma \partial_{ij} \eta + Q_{ij}], \quad \text{(21)}$$

where

$$Q_{ij} = \left( \partial_P \Sigma \partial_{ij} \right) H^{(\Sigma)} \left( \partial_P \Sigma \partial_{ij} \right), \quad \text{(22)}$$

and $H^{(\Sigma)}$ is the Hessian of $\Sigma(P, \eta)$ computed in $P(\theta_1)$ and $\eta(\theta_1)$. Since we are interested in studying the Hessian of $F(a_2, b_2, \theta_1)$ in the special point $(a_2, b_2)$ previously identified, we substitute Eq. (19) into Eq. (21), yielding

$$H^{(F)}_{ij} = H^{(G)}_{ij} + \frac{b_1}{\partial_\eta \Sigma} Q_{ij}, \quad \text{(23)}$$

We now prove that $H^{(F)}_{ij}$ is negative semi-definite since it is the sum of negative semi-definite matrices. By hypothesis $H^{(G)}_{ij}$ is negative semi-definite. Recalling Eq. (13) and that $b_1 > 0$, we now need to show that $Q_{ij}$ is positive semi-definite. Plugging Eq. (14) into Eq. (22) yields

$$Q_{ij} = \beta_{[\nu]} \eta^{(c)}_{[\nu]} \partial_\eta \partial_{ij} \eta R_{ij}, \quad \text{(24)}$$

where

$$R_{ij} = 2 P + S_{ij} + S_{ij}^T, \quad S_{ij} = - \frac{\partial_P}{\partial_\eta} \Sigma, \quad \text{(25)}$$

We now show that if $R_{ij}$ is positive semi-definite, then also $Q_{ij}$ is positive semi-definite. By definition, $Q_{ij}$ is positive semidefinite if, for any set of coefficient $a_i$, we have that $\sum_{ij} a_i Q_{ij} a_j \geq 0$. Assuming $R_{ij}$ to be positive semi-definite, and using that $\beta_{[\nu]} \eta^{(c)}_{[\nu]} \eta > 0$, we have

$$\sum_{ij} a_i Q_{ij} a_j = \beta_{[\nu]} \eta^{(c)}_{[\nu]} \sum_{ij} x_i R_{ij} x_j \geq 0, \quad \text{(26)}$$

where we define $x_i \equiv \partial_i \eta a_i$. We thus have to prove the positivity of $R_{ij}$. We prove this showing that it is the sum of 3 positive semi-definite matrices. Indeed, the first term in Eq. (25), $2 P$, is proportional to a matrix with 1 in all entries. Trivially, this matrix has 1 positive eigenvalue, and all other ones are null, so it is positive semi-definite. At last, $S_{ij}$ and its transpose have the same positivity, so we focus only on $S_{ij}$. $S_{ij}$ is a matrix with all equal columns. This means that it has all null eigenvalues, except for a single one that we denote with $\lambda$. Since the trace of a matrix is equal to the sum of the eigenvalues, we have $\lambda = \text{Tr}[S] = \sum_{ii} S_{ii}$. Using the optimality condition in Eq. (15), we see that each entry of $S$ is positive, i.e. $S_{ij} > 0$. Therefore $\lambda > 0$, thus $S$ is positive semi-definite, concluding the proof that $H^{(F)}_{ij}$ is negative semi-definite.

To conclude, we notice that we can always renormalize $a_2$ and $b_2$, preserving the same exact optimization problem. This way, a value of $c \in [0, 1]$ can be identified.

Reinforcement Learning Implementation

As discussed in the main text, our goal is to maximize the return $\langle r_c \rangle (t)$ defined in Eq. (5). To solve the problem within the RL framework, we discretize time as $t_i = i \Delta t$. At every time-step $t_i$, the aim of the agent is to learn an optimal policy that maximizes, in expectation, the time-discretized return $\langle r_c \rangle_i$. The time-discrete reward and return functions are given by:

$$r_{i+1} = \Delta t^{-1} \int_{t_i}^{t_{i+1}} r_c(t) dt, \quad \text{(27)}$$

$$\langle r_c \rangle_i = (1 - \gamma) \sum_{j=0}^{\infty} \gamma^j r_{i+j}. \quad \text{(28)}$$

Eq. (28) is the time-discrete version of Eq. (5), where the discount factor $\gamma = \exp(-\kappa \Delta t)$ determines the averaging timescale and expresses how much we are interested in future or immediate rewards.

To be precise, plugging Eq. (27) into Eq. (28) gives $\langle r_c \rangle(t)$ (up to an irrelevant constant prefactor) only in the limit of $\Delta t \to 0$. However, also for finite $\Delta t$, both quantities are time-averages of the reward, so they are equally valid definitions to describe a long-term trade-off maximization.

As in Ref. [77], we use a generalization of the soft-actor critic (SAC) method, first developed for continuous actions [78, 79], to handle a combination of discrete and continuous actions [80, 81]. We further tune the method to stabilize the convergence in a multi-objective scenario. We here present an overview of our implementation of SAC putting special emphasis on the differences with respect to the standard implementation. However, we refer to [78–81] for additional details. Our method, implemented with PyTorch, is based on modifications and generalizations of the SAC implementation provided by Spinning Up from OpenAI [113]. All code and data to reproduce the experiments is available online (see Data Availability and Code Availability sections).

The SAC algorithm is based on policy iteration, i.e. it consists of iterating multiple times over two steps: a policy evaluation step, and a policy improvement step. In the policy evaluation step, the value function of the current policy is (partially) learned, whereas in the policy improvement step a better policy is learned by making
use of the value function. We now describe these steps more in detail.

In typical RL problems, the optimal policy \( \pi^*(s|a) \) is defined as the policy that maximizes the expected return defined in Eq. (28), i.e.:

\[
\pi^* = \arg \max_{\pi} \mathbb{E}_\pi \left[ \sum_{k=0}^{\infty} \gamma^k r_{k+1} \middle| s_0 = s \right],
\]  

(29)

where \( \mathbb{E}_\pi \) denotes the expectation value choosing actions according to the policy \( \pi \). The initial state \( s_0 = s \) is sampled from \( \mu_\pi \), i.e. the steady-state distribution of states that are visited by \( \pi \). In the SAC method, balance between exploration and exploitation \cite{114} is achieved by introducing an Entropy-Regularized maximization objective. In this setting, the optimal policy \( \pi^* \) is given by

\[
\pi^* = \arg \max_{\pi} \mathbb{E}_\pi \left[ \sum_{k=0}^{\infty} \gamma^k \left( r_{k+1} + \alpha H[\pi(\cdot|s_k)] \right) \middle| s_0 = s \right],
\]  

(30)

where \( \alpha \geq 0 \) is known as the “temperature” parameter that balances the trade-off between exploration and exploitation, and

\[
H[P] = \mathbb{E}_{x \sim P}[-\log P(x)]
\]  

(31)

is the entropy of the probability distribution \( P \). Notice that we replaced the unknown state distribution \( \mu_\pi \) with \( B \), which is a replay buffer populated during training by storing the observed one-step transitions \((s_k, a_k, r_{k+1}, s_{k+1})\).

Developing on Ref. \cite{77}, we generalize such approach to a combination of discrete and continuous actions in the following way. Let us write an arbitrary action \( a \) as \( a = (u, d) \), where \( u \) is the continuous action and \( d \) is the discrete action (for simplicity, we describe the case of a single continuous action, though the generalization to multiple variables is straightforward). From now on, all functions of \( a \) are also to be considered as functions of \( u, d \). We decompose the joint probability distribution of the policy as

\[
\pi(u, d|s) = \pi_D(d|s) \cdot \pi_C(u|d, s),
\]  

(32)

where \( \pi_D(d|s) \) is the marginal probability of taking discrete action \( d \), and \( \pi_C(u|d, s) \) is the conditional probability density of choosing action \( u \), given action \( d \) (D stands for “discrete”, and C for “continuous”). Notice that this decomposition is an exact identity, thus allowing us to describe correlations between the discrete and the continuous action. With this decomposition, we can write the entropy of a policy as

\[
H[\pi(\cdot|s)] = H_D^\pi(s) + H_C^\pi(s),
\]  

(33)

where

\[
H_D^\pi(s) = H[\pi_D(\cdot|s)], \quad H_C^\pi(s) = \sum_d \pi_D(d|s) H[\pi_C(\cdot|d, s)],
\]  

(34)

correspond respectively to the entropy contribution of the discrete (D) and continuous (C) part. These two entropies take on values in different ranges: while the entropy of a discrete distribution with \(|D| \) discrete actions is non-negative and upper bounded by \( \log(|D|) \), the (differential) entropy of a continuous distribution can take on any value, including negative values (especially for peaked distributions). Therefore, we introduce a separate temperature for the discrete and continuous contributions replacing the definition of the optimal policy in Eq. (30) with

\[
\pi^* = \arg \max_{\pi} \mathbb{E}_\pi \left[ \sum_{k=0}^{\infty} \gamma^k \left( r_{k+1} + \alpha_D H_D^\pi(s_k) + \alpha_C H_C^\pi(s_k) \right) \middle| s_0 = s \right],
\]  

(35)

where \( \alpha_C \geq 0 \) and \( \alpha_D \geq 0 \) are two distinct “temperature” parameters. This is one of the differences with respect to Refs. \cite{77–79}. Equation (35) defines our optimization objective. Accordingly, we define the value function \( Q^\pi(s, a) \) of a given policy \( \pi \) as

\[
Q^\pi(s, a) = \mathbb{E}_\pi \left[ r_1 + \sum_{k=1}^{\infty} \gamma^k \left( r_{k+1} + \alpha_D H_D^\pi(s_k) + \alpha_C H_C^\pi(s_k) \right) \middle| s_0 = s, a_0 = a \right].
\]  

(36)

Its recursive Bellman equation therefore reads

\[
Q^\pi(s, a) = \mathbb{E}_{\xi \sim \mathcal{N}(0, 1)} \left[ r_1 + \gamma \left( Q^\pi(s_1, a_1) + \alpha_D H_D^\pi(s_1) + \alpha_C H_C^\pi(s_1) \right) \middle| s_0 = s, a_0 = a \right].
\]  

(37)

As in Ref. \cite{78, 79}, we parameterize \( \pi_C(u|d, s) \) as a squashed Gaussian policy, i.e. as the distribution of the variable

\[
\tilde{u}(\xi|d, s) = u_a + \frac{u_b - u_a}{2} \left[ 1 + \tanh(\mu(d, s) + \sigma(d, s) \cdot \xi) \right],
\]  

\( \xi \sim \mathcal{N}(0, 1) \),

(38)

where \( \mu(d, s) \) and \( \sigma(d, s) \) represent respectively the mean and standard deviation of the Gaussian distribution, \( \mathcal{N}(0, 1) \) is the normal distribution with zero mean and unit variance, and where we assume that \( U = [u_a, u_b] \). This is the so-called reparameterization trick.

We now describe the policy evaluation step. In the SAC algorithm, we learn two value functions \( Q_{\phi_i}(s, a) \) described by the learnable parameters \( \phi_i \) for \( i = 1, 2 \). \( Q_{\phi_i}(s, a) \) is a function approximator, e.g. a neural network. Since \( Q_{\phi_i}(s, a) \) should satisfy the Bellman Eq. (37), we define the loss function for \( Q_{\phi_i}(s, a) \) as the mean square difference between the left and right hand side of Eq. (37), i.e.

\[
L_Q(\phi_i) = \mathbb{E}_{(s, a, r, s') \sim B} \left[ (Q_{\phi_i}(s, a) - y(r, s'))^2 \right],
\]  

(39)
where

\[ y(r, s') = r + \gamma \mathop{\mathbb{E}}_{a' \sim \pi(\cdot|s')} \left[ \min_{j=1,2} Q_{\phi_{\text{ targ},j}}(s', a') + \alpha_D H_D(s') + \alpha_C H_C(s') \right]. \tag{40} \]

Notice that in Eq. (40) we replaced \( Q^{\pi} \) with \( \min_{j=1,2} Q_{\phi_{\text{ targ},j}} \), where \( \phi_{\text{ targ},j} \), for \( j = 1, 2 \), are target parameters which are not updated when minimizing the loss function; instead, they are held fixed during backpropagation, and then they are updated according to Polyak averaging, i.e.

\[ \phi_{\text{ targ},i} \leftarrow \rho_{\text{ polyak}} \phi_{\text{ targ},i} + (1 - \rho_{\text{ polyak}}) \phi_i, \tag{41} \]

where \( \rho_{\text{ polyak}} \) is a hyperparameter. This change was shown to improve learning [78, 79]. In order to evaluate the expectation value in Eq. (40), we use the decomposition in Eq. (32) to write

\[ \mathop{\mathbb{E}}_{a' \sim \pi(\cdot|s')} \left[ \right] = \sum_{d'} \pi_D(d'|s') \mathop{\mathbb{E}}_{u' \sim \pi_C(\cdot|d', s')} \left[ \right], \tag{42} \]

where we denote \( a' = (u', d') \). Plugging Eq. (42) into Eq. (40) and writing the entropies explicitly as expectation values yields

\[ y(r, s') = r + \gamma \sum_{d'} \pi_D(d'|s') \left( \mathop{\mathbb{E}}_{u' \sim \pi_C(\cdot|d', s')} \left[ \min_{j=1,2} Q_{\phi_{\text{ targ},j}}(s', d', u') - \alpha_C \log \pi_C(u'|d', s') \right] - \alpha_D \log \pi_D(d'|s') \right). \tag{43} \]

We then replace the expectation value over \( u' \) in Eq. (43) with a single sampling \( u' \sim \pi_C(\cdot|d', s') \) (therefore one sampling for each discrete action) performed using Eq. (38). This corresponds to performing a full average over the discrete action, and a single sampling of the continuous action.

We now turn to the policy improvement step. Since we introduced two separate temperatures, we cannot use the loss function introduced in Refs. [78, 79]. Therefore, we proceed in two steps. Let us define the following function

\[ Z_\pi(s) = - \mathop{\mathbb{E}}_{a \sim \pi(\cdot|s)} \left[ Q^{\pi_{\text{old}}}(s, a) - \alpha_D H_D^\pi(s) - \alpha_C H_C^\pi(s) \right], \tag{44} \]

where \( Q^{\pi_{\text{old}}}(s, a) \) is the value function of some given “old policy” \( \pi_{\text{old}} \), and \( \pi \) is an arbitrary policy. First, we prove that if a policy \( \pi_{\text{new}} \) satisfies

\[ Z_{\pi_{\text{new}}}(s) \leq Z_{\pi_{\text{old}}}(s) \tag{45} \]

for all values of \( s \), then \( \pi_{\text{new}} \) is a better policy than \( \pi_{\text{old}} \) as defined in Eq. (35). Next, we will use this property to define a loss function that implements the policy improvement step. Equation (45) implies that

\[ \mathop{\mathbb{E}}_{a \sim \pi_{\text{old}}(\cdot|s)} \left[ Q^{\pi_{\text{old}}}(s, a) - \alpha_D H_D^\pi(s) - \alpha_C H_C^\pi(s) \right] \leq \mathop{\mathbb{E}}_{a \sim \pi_{\text{new}}(\cdot|s)} \left[ Q^{\pi_{\text{old}}}(s, a) - \alpha_D H_D^\pi(s) - \alpha_C H_C^\pi(s) \right]. \tag{46} \]

We now use this inequality to show that \( \pi_{\text{new}} \) is a better policy. Starting from the Bellmann equation (37) for \( Q^{\pi_{\text{old}}} \), we have

\[ Q^{\pi_{\text{old}}}(s, a) = \mathop{\mathbb{E}}_{a' \sim \pi_{\text{old}}(\cdot|s)} \left[ r_1 + \gamma \left( Q^{\pi_{\text{old}}}(s_1, a_1) + \alpha_D H_D^{\pi_{\text{old}}}(s_1) + \alpha_C H_C^{\pi_{\text{old}}}(s_1) \right) \right]_{s_0 = s, a_0 = a} \leq \mathop{\mathbb{E}}_{a' \sim \pi_{\text{new}}(\cdot|s)} \left[ r_1 + \gamma \left( Q^{\pi_{\text{old}}}(s_1, a_1) + \alpha_D H_D^{\pi_{\text{new}}}(s_1) + \alpha_C H_C^{\pi_{\text{new}}}(s_1) \right) \right]_{s_0 = s, a_0 = a} = \mathop{\mathbb{E}}_{a' \sim \pi_{\text{new}}(\cdot|s)} \left[ r_1 + \gamma \left( \alpha_D H_D^{\pi_{\text{new}}}(s_1) + \alpha_C H_C^{\pi_{\text{new}}}(s_1) \right) \right]_{s_0 = s, a_0 = a} + \gamma \mathop{\mathbb{E}}_{a' \sim \pi_{\text{new}}(\cdot|s)} \left[ Q^{\pi_{\text{old}}}(s_1, a_1) \right]_{s_0 = s, a_0 = a} \leq \cdots \leq Q^{\pi_{\text{new}}}(s, a). \tag{47} \]

Using a strategy similar to that described in Refs. [78, 114], in Eq. (47) we make a repeated use of inequality (46) and of the Bellmann equation for \( Q^{\pi_{\text{new}}}(s, a) \) to prove that the value function of \( \pi_{\text{new}} \) is better or equal to the value function of \( \pi_{\text{old}} \).

Let \( \pi_\theta(a|s) \) be a parameterization of the policy function that depends on a set of learnable parameters \( \theta \). We define the following loss function

\[ L_\pi(\theta) = \mathop{\mathbb{E}}_{a \sim \pi(\cdot|s)} \left[ -Q^{\pi_{\text{old}}}(s, a) - \alpha_D H_D^{\pi_{\text{old}}}(s) - \alpha_C H_C^{\pi_{\text{old}}}(s) \right]. \tag{48} \]

Thanks to Eqs. (44) and (45), this choice guarantees us to
find a better policy by minimizing $L_\pi(\theta)$ with respect to $\theta$. In order to evaluate the expectation value in Eq. (48), as before we implicitly average over the discrete action and perform a single sample of the continuous action, and we replace $Q^{\text{old}}$ with $\min_j Q_{\phi_j}$. Recalling the parameterization in Eq. (38), this yields

$$L_\pi(\theta) = \mathbb{E}_{s \sim B} \left[ \sum_d \pi_{D,\theta}(d|s) \left( \alphaD \log \pi_{D,\theta}(d|s) + \alphaC \log \pi_{C,\theta}(\hat{u}_\theta(\xi|d,s)|d,s) - \min_j Q_{\phi_j}(s, \hat{u}_\theta(\xi|d,s), d) \right) \right],$$

$$\xi \sim \mathcal{N}(0,1).$$

(49)

We have defined and shown how to evaluate the loss functions $L_Q(\phi)$ and $L_\pi(\theta)$ that allow us to determine the value function and the policy [see Eqs. (39), (43) and (49)]. Now, we discuss how to automatically tune the temperature hyperparameters $\alphaD$ and $\alphaC$. Ref. [79] shows that constraining the average entropy of the policy to a certain value leads to the same exact SAC algorithm with the addition of an update rule to determine the temperatures. Let $\bar{H}_D$ and $\bar{H}_C$ be respectively the fixed average values of the entropy of the discrete and continuous part of the policy. We can then determine the corresponding temperatures $\alphaD$ and $\alphaC$ minimizing the following two loss functions

$$L_D(\alphaD) = \alphaD \mathbb{E}_{s \sim B} \left[ H_D^\alpha(s) - \bar{H}_D \right],$$

$$L_C(\alphaC) = \alphaC \mathbb{E}_{s \sim B} \left[ H_C^\alpha(s) - \bar{H}_C \right].$$

(50)

As usual, we evaluate the entropies by explicitly taking the average over the discrete actions, and taking a single sample of the continuous action. To be more specific, we evaluate $L_D$ by computing

$$L_D(\alphaD) = \alphaD \mathbb{E}_{s \sim B} \left[ - \sum_d \pi_D(d|s) \log \pi_D(d|s) - \bar{H}_D \right],$$

and $L_C$ by computing

$$L_C(\alphaC) = \alphaC \mathbb{E}_{s \sim B} \left[ - \sum_d \pi_D(d|s) \mathbb{E}_{u \sim \pi_C(\cdot|d,s)} \left[ \log \pi_C(u|d,s) \right] - \bar{H}_C \right]$$

(52)

and replacing the expectation value over $u$ with a single sample.

To summarize, the SAC algorithm consists of repeating over and over a policy evaluation step, a policy improvement step, and a step where the temperatures are updated. The policy evaluation step consists of a single optimization step to minimize the loss functions $L_Q(\phi_i)$ (for $i = 1, 2$), given in Eq. (39), where $y(r, s)$ is computed using Eq. (43). The policy improvement step consists of a single optimization step to minimize the loss function $L_\pi(\theta)$ given in Eq. (49). The temperatures are then updated performing a single optimization step to minimize $L_D(\alphaD)$ and $L_C(\alphaC)$ given respectively in Eqs. (51) and (52). In all loss functions, the expectation value over the states is approximated with a batch of experience sampled randomly from the replay buffer $B$.

We now detail how we parameterize $\pi(a|s)$ and $Q(s, a)$. The idea is to develop an efficient way to process the state that can potentially be a long time-series of actions. To this aim, we introduce a “convolution block” as a building element for our NN architecture. The convolution block, detailed in Fig. 6, takes an input of size $(C_{\text{in}}, L_{\text{in}})$, where $C_{\text{in}}$ is the number of channels and $L_{\text{in}}$ is the length of the time-series, and produces an output of size $(C_{\text{out}}, L_{\text{out}})$. In this image $L_{\text{in}} = 4$. The output is produced by stacking a 1D convolution of kernel size and stride of 2, and a non-linearity (left branch). A residual connection (right branch), consisting only of linear operations, is added to improve trainability.

Using the decomposition in Eq. (32) and the parameterization in Eq. (38), the quantities that need to be parameterized are the discrete probabilities $\pi_D(d|s)$, the averages $\mu(d, s)$ and the variances $\sigma(d, s)$, for $d = 1, \ldots, |D|$, $|D| = 3$ being the number of discrete actions. The architecture of the neural network that we use for the policy function is shown in Fig. 7a. The state, composed of the time-series $s_\iota = (a_{\iota-1}, \ldots, a_{\iota-1})$ which has shape $(C_{\text{in}}, L_{\text{in}} = N)$, is fed through a series of 1D convolutional blocks, which produce an output of length $(C_{\text{out}}, L = 1)$. The number of input channels $C_{\text{in}}$ is determined by stacking the components of $\bar{u}$ (which, for simplicity, is a single real number $u$ in this appendix) and by using a one-hot encoding of the discrete actions. We then feed this output, together with the last action which has a privileged position, to a series of fully connected NNs with ReLU activations. Finally, a linear network outputs $W(d|s), \mu(d, s)$ and $\log(\sigma(d, s))$, for all $d = 1, \ldots, |D|$. The probabilities $\pi_D(d|s)$ are then produced applying the
We introduce two separate value functions, one for each objective (P for the power, and Σ for the entropy production).

\begin{align}
Q^P(s,a) &= E_\pi \left[ r_1^{(P)} + \sum_{k=1}^{\infty} \gamma^k (r_{k+1}^{(P)} + \alpha_D H_D^P(s_k)) | s_0 = s, a_0 = a \right], \\
Q^\Sigma(s,a) &= E_\pi \left[ r_1^{(\Sigma)} + \sum_{k=1}^{\infty} \gamma^k (r_{k+1}^{(\Sigma)} + \alpha_D H_D^\Sigma(s_k)) | s_0 = s, a_0 = a \right],
\end{align}

(53)

where

\begin{align}
r_{i+1}^{(P)} &= \frac{1}{\Delta t} \int_{t_i}^{t_i+\Delta t} P(\tau) d\tau, \\
r_{i+1}^{(\Sigma)} &= \frac{1}{\Delta t} \int_{t_i}^{t_i+\Delta t} \Sigma(\tau) d\tau,
\end{align}

(54)

represent respectively the normalized average power and average entropy production during each time-step. Since the value functions in Eq. (53) are identical to Eq. (36) up to a change of the reward, they separately satisfy the same Bellmann equation as in Eq. (37), with \( r_1 \) replaced respectively with \( r_1^{(P)} \) and \( r_1^{(\Sigma)} \). Therefore, we learn each value functions minimizing the same loss function \( L_Q \) given in Eq. (39), with \( r_1 \) replaced with \( r_1^{(P)} \) or \( r_1^{(\Sigma)} \). Both value functions are parameterized using the same architecture, but separate and independent parameters. We now turn to the determination of the policy. Comparing the definition of \( r_1 \) given in the main text with Eq. (54), we see that \( r_{i+1} = a_{i+1}^{(P)} - (1-c)r_{i+1}^{(\Sigma)} \). Using this property, and comparing Eq. (36) with Eq. (53), we see that

\begin{align}
Q^\pi(s,a) &= cQ^P\pi(s,a) - (1-c)Q^\Sigma(s,a).
\end{align}

(55)

Therefore, we learn the policy minimizing the same loss function as in Eq. (49), using Eq. (55) to compute the value function. To summarize, this method allows us to vary \( c \) dynamically during training. This requires learning two value functions, one for each objective, and storing in the replay buffer the two separate rewards \( r_1^{(P)} \) and \( r_1^{(\Sigma)} \).

At last, when we refer to “final deterministic cycle”, we are sampling from the policy function “switching off the stochasticity”, i.e. choosing continuous actions \( a \) setting \( \xi = 0 \) in Eq. (38), and choosing deterministically the discrete action with the highest probability.

**Physical model**

As discussed in the main text, we describe the dynamics of the two analyzed QTMs employing the Lindblad master equation that can be derived also for non-adiabatic drivings [108], in the weak system-bath coupling regime performing the usual Born-Markov and secular approximation [105–107] and neglecting the Lamb-shift contribution. This approach describes the time-evolution of the reduced density matrix of the quantum
system, $\hat{\rho}(t)$, under the assumption of weak system-bath interaction. Setting $\hbar = 1$, the master equation reads
\[
\frac{\partial}{\partial t} \hat{\rho}(t) = -i \left[ \hat{H}[\tilde{u}(t)], \hat{\rho}(t) \right] + \sum_{\alpha} D_{\tilde{u}(t),d(t)}^{(\alpha)}[\hat{\rho}(t)], \tag{56}
\]
where $\hat{H}[\tilde{u}(t)]$ is the Hamiltonian of the quantum system that depends explicitly on time via the control parameters $\tilde{u}(t)$, $[\cdot, \cdot]$ denotes the commutator, and $D_{\tilde{u}(t),d(t)}^{(\alpha)}$, known as the dissipator, describes the effect of the coupling between the quantum system and bath $\alpha = H, C$. Without loss of generality, the dissipator protocols, we are not impacted by possible inaccuracies of the master equation subject to fast parameter driving [115], provided that $\Delta t$ is not smaller than the bath timescale. Without loss of generality, the dissipators can be expressed as [106, 107]
\[
P_{\tilde{u}(t),d(t)}^{(\alpha)} = \lambda_{\alpha}[d(t)] \sum_{k} \gamma_{k,\tilde{u}(t)}^{(\alpha)} \left( \hat{A}_{k,\tilde{u}(t)}^{(\alpha)} \hat{\rho} \hat{A}_{k,\tilde{u}(t)}^{(\alpha)*} \right) - \frac{1}{2} \hat{\gamma}_{k,\tilde{u}(t)}^{(\alpha)} \hat{\rho} \hat{\gamma}_{k,\tilde{u}(t)}^{(\alpha)*} - \frac{1}{2} \hat{\gamma}_{k,\tilde{u}(t)}^{(\alpha)*} \hat{\rho} \hat{\gamma}_{k,\tilde{u}(t)}^{(\alpha)} \hat{\rho}, \tag{57}
\]
where $\lambda_{\alpha}[d(t)] \in \{0, 1\}$ are functions that determine which bath is coupled to the quantum system, $\hat{A}_{k,\tilde{u}(t)}^{(\alpha)}$ are the Lindblad operators, and $\gamma_{k,\tilde{u}(t)}^{(\alpha)}$ are the corresponding rates. In particular, $\lambda_{H}(\text{Hot}) = 1$, $\lambda_{C}(\text{Cold}) = 0$, while $\lambda_{H}(\text{Cold}) = 0$, $\lambda_{C}(\text{Cold}) = 1$, and $\lambda_{H}(\text{None}) = \lambda_{C}(\text{None}) = 0$. Notice that both the Lindblad operators and the rates can depend on time through the value of the control $\tilde{u}(t)$. Their explicit form depends on the details of the system, i.e. on the Hamiltonian describing the dynamics of the overall system including the bath and the system-bath interaction. Below, we provide the explicit form of $\hat{A}_{k,\tilde{u}(t)}^{(\alpha)}$ and $\gamma_{k,\tilde{u}(t)}^{(\alpha)}$ used to model the two setups considered in this manuscript. We adopt the standard approach to compute the instantaneous power and heat currents [24]
\[
P(t) \equiv -\text{Tr} \left[ \hat{\rho}(t) \frac{\partial}{\partial t} \hat{H}[\tilde{u}(t)] \right],
\]
\[
J_{\alpha}(t) \equiv \text{Tr} \left[ \hat{H}[\tilde{u}(t)] D_{\tilde{u}(t),d(t)}^{(\alpha)} \right], \tag{58}
\]
that guarantees the validity of the first law of thermodynamics $\partial U(t)/\partial t = -P(t) + \sum_{\alpha} J_{\alpha}(t)$, the internal energy being defined as $U = \text{Tr}[\hat{\rho}(t)\hat{H}[\tilde{u}(t)]]$.

In the superconducting qubit refrigerators, we employ the model first put forward in Ref. [52], and further studied in Refs. [58, 66]. In particular, we consider the following Lindblad operators and corresponding rates (identifying $k = \pm$):
\[
\hat{A}_{\alpha,\pm}(t) = -i |e_u(t)\rangle \langle g_u(t)|, \quad \hat{A}_{\alpha,-}(t) = +i |g_u(t)\rangle \langle e_u(t)|, \tag{59}
\]
where $|g_u(t)\rangle$ and $|e_u(t)\rangle$ are, respectively, the instantaneous ground state and excited state of Eq. (7). The corresponding rates are given by $\gamma_{\alpha,\pm}(t) = S_\alpha[\Delta \epsilon_u(t)]$, where $\Delta \epsilon_u(t)$ is the instantaneous energy gap of the system, and
\[
S_\alpha(\Delta \epsilon) = \frac{g_\alpha}{2} \frac{1}{1 + Q_\alpha^2 (\Delta \epsilon/\omega_\alpha - \omega_\alpha/\Delta \epsilon)^2} e^{\gamma_{\alpha}(\Delta \epsilon)} - 1 \tag{60}
\]
is the noise power spectrum of bath $\alpha$. Here $\omega_\alpha, Q_\alpha$ and $g_\alpha$ are the base resonance frequency, quality factor and coupling strength of the resonant circuit acting as bath $\alpha = H, C$ (see Refs. [52, 66] for details). As in Ref. [66], we choose $\omega_C = 2E_0 \Delta$ and $\omega_H = 2E_0 \sqrt{\Delta^2 + 1/4}$, such that the C (H) bath is in resonance with the qubit when $u = 0$ ($u = 1/2$). The width of the resonance is governed by $Q_\alpha$. The total coupling strength to bath $\alpha$, plotted in Fig. 3f, is quantified by
\[
\gamma_u(t) \equiv \gamma_{\alpha,\text{+}}(t) + \gamma_{\alpha,\text{-}}(t). \tag{61}
\]
In the quantum harmonic oscillator based heat engine, following Ref. [46], we describe the coupling to the baths through the Lindblad operators $\hat{A}_{\alpha,\text{+}}(t) = \hat{a}_{\alpha,\text{+}}(t)$, $\hat{A}_{\alpha,\text{-}}(t) = \hat{a}_{\alpha,\text{-}}(t)$ and corresponding rates $\gamma_{\alpha,\text{+}}(t) = \Gamma_\alpha n(\beta_{\alpha} u(t) \omega_0)$ and $\gamma_{\alpha,\text{-}}(t) = \Gamma_\alpha [1 + n(\beta_{\alpha} u(t) \omega_0)]$, where we identify $k = \pm$, $\hat{a}_{\alpha,\text{+}}(t) = (1/\sqrt{2}) \sqrt{\omega C} \hat{q} + i/\sqrt{\omega C} \hat{p}$ and $\hat{a}_{\alpha,\text{-}}^\dagger(\alpha, t)$ are respectively the (control dependent) lowering and raising operators, $\Gamma_\alpha$ is a constant rate setting the thermalization timescale of the system coupled to bath $\alpha$, and $n(x) = [\exp(x) - 1]^{-1}$ is the Bose-Einstein distribution.

Training details

We now provide additional practical details and the hyper parameters used to produce the results of this manuscript.

In order to enforce sufficient exploration in the early stage of training, we do the following. As in Ref. [113], for a fixed number of initial steps, we choose random actions sampling them uniformly withing their range. Furthermore, for another fixed number of initial steps, we do not update the parameters to allow the replay buffer to have enough transitions. $B$ is a first-in-first-out buffer, of fixed dimension, from which batches of transitions $(s_k, a_k, r_{k+1}, s_{k+1}, a_{k+1})$ are randomly sampled to update the NN parameters. After this initial phase, we repeat a policy evaluation, a policy improvement step and a temperature update step $n_{\text{updates}}$ times every $n_{\text{updates}}$ steps. This way, the overall number of updates coincides with the number of actions performed on the QTM. The optimization steps for the value function and the policy are performed using the ADAM optimizer with the standard hyper parameters used to produce the results of this manuscript.

After the first phase of training, we perform another policy evaluation step (i.e., a policy improvement step), followed by a new policy evaluation step and a temperature update step $n_{\text{updates}}$ times every $n_{\text{updates}}$ steps. This way, the overall number of updates coincides with the number of actions performed on the QTM. The optimization steps for the value function and the policy are performed using the ADAM optimizer with the standard hyper parameters used to produce the results of this manuscript.
particular, we vary them exponentially during each step according to
\[ H_a(n_{\text{steps}}) = H_{a,\text{end}} + (H_{a,\text{start}} - H_{a,\text{end}}) \exp\left(-n_{\text{steps}}/H_{a,\text{decay}}\right), \tag{62} \]

where \( a = C, D \), \( n_{\text{steps}} \) is the current step number, and \( H_{a,\text{start}}, H_{a,\text{end}} \) and \( H_{a,\text{decay}} \) are hyperparameters. In the superconducting qubit refrigerator case, we schedule the parameter \( c \) according to a Fermi distribution, i.e.
\[ c(n_{\text{step}}) = c_{\text{end}} + (c_{\text{start}} - c_{\text{end}}) \left[ 1 + \exp \left( \frac{n_{\text{step}} - c_{\text{mean}}}{c_{\text{decay}}} \right) \right]^{-1}. \tag{63} \]

In the harmonic oscillator engine case, to improve stability while training for lower values of \( c \), we do not vary \( c \) during training, as we do in the superconducting qubit refrigerator case. Instead, we discourage the agent from never utilizing one of the two thermal baths by adding a negative reward if, withing the last \( N = 128 \) actions describing the state, less than 25 describe a coupling to either bath. In particular, if the number of actions \( N_\alpha \) where \( d = \alpha \), with \( \alpha = \text{Hot}, \text{Cold} \) is less than 25 in the state time-series, we sum to the reward the following penalty
\[ r_{\text{penalty}} = -1.4 \frac{25 - N_\alpha}{25}. \tag{64} \]

This penalty has no impact on the final cycles where \( N_\alpha \) is much larger than 25.

All hyperparameters used to produce the results of the superconducting qubit refrigerator and of the harmonic oscillator heat engine are provided respectively in Tables I and II, where \( c \) refers to the weight at which we are optimizing the return.

**Convergence of the RL approach**

The training process presents some degree of stochasticity, such as the initial random steps, the stochastic sampling of actions from the policy function, and the random sampling of a batch of experience from the replay buffer to compute an approximate gradient of the loss functions. We thus need to evaluate the reliability of our approach.

As shown in the main text, specifically in Figs. 4 and 5, we ran the full optimization 5 times. Out of 65 trainings in the superconducting qubit refrigerator case, only 4 failed, and out of the 55 in the harmonic oscillator engine, only 2 failed, where by failed we mean that the final return was negative. In such cases, we ran the training an additional time.

Figs. 4a and 5b display an error bar corresponding to the standard deviation, at each value of \( c \), computed over the 5 repetitions. Instead, in Figs. 4b and 5c we display one black dot for each individual training. As we can see, the overall performance is quite stable and reliable.

At last, we discuss the variability of the discovered cycles. The cycles shown in Figs. 4c-f and 5d-e were chosen by selecting the largest return among the 5 repetitions. In Figs. 8 and 9 we display cycles discovered in the last of the 5 repetition, i.e. chosen without any post-selection. They correspond to the same setups and parameters displayed in Figs. 4c-f and 5d-e. As we can see, 5 out of the 6 displayed cycles are very similar to the ones displayed in Figs. 4c-f and 5d-e, with a very slight variability. The only exception is Fig. 8b, where the cycle has a visibly shorter period and amplitude than the one shown in Fig. 4d. Despite this visible difference in the cycle shape, the return of the cycle shown in Fig. 8b is 0.382 compared to 0.385 of the cycle shown in Fig. 4b.
We therefore conclude that, up to minor changes, the cycles are generally quite stable across multiple trainings.

**Comparing with the trapezoidal and Otto cycle**

In Figs. 4 and 5 we compare the performance of our method respectively against optimized trapezoidal cycles and optimized Otto cycles. We now detail how we perform such comparison.

In the refrigerator based on a superconducting qubit, we consider the trapezoidal cycle proposed in Ref. [52, 66], i.e. we fix

$$u(t) = \frac{1}{4} \left(1 + \frac{\tanh(a \cos \Omega t)}{\tanh(a)}\right)$$  \hspace{0.5cm} (65)

with $a = 2$, and we optimize $\langle r_e \rangle$ with respect to frequency $\Omega$. In the heat engine case based on a quantum harmonic oscillator, we fix an Otto cycle as described in Ref. [46], i.e. a trapezoidal cycle consisting of the 4 strokes shown in Figs. 5d-e as a dashed line, and we optimize over the duration of each of the 4 strokes. In particular, we first performed a grid search in the space of these four durations for $c = 1$. After identifying the largest power, we ran the Newton algorithm to further maximize the return. We then ran the Newton algorithm for all other values of $c$.

**Generation of coherence**

In order to quantify the coherence generated in the instantaneous eigenbasis of the Hamiltonian in the refrigerator based on a superconducting qubit, we evaluated the time average of relative entropy of coherence [116], defined as

$$C(\dot{\rho}(t)) = S(\hat{\rho}_{\text{diag}}(t)) - S(\hat{\rho}(t)),$$  \hspace{0.5cm} (66)

where $S(\hat{\rho}) = -\text{Tr}[\hat{\rho} \ln \hat{\rho}]$ is the Von Neumann entropy, and

$$\hat{\rho}_{\text{diag}}(t) = \langle g_{u(t)}|\hat{\rho}(t)|g_{u(t)}\rangle \cdot |g_{u(t)}\rangle \langle g_{u(t)}| + \langle e_{u(t)}|\hat{\rho}(t)|e_{u(t)}\rangle \cdot |e_{u(t)}\rangle \langle e_{u(t)}|$$  \hspace{0.5cm} (67)

is the density matrix, in the instantaneous eigenbasis $|g_{u(t)}\rangle$ and $|e_{u(t)}\rangle$, with the off-diagonal terms canceled out.

We compute the time-average of the relative entropy of coherence generated by the final deterministic cycle found by the RL agent, and compare it to the coherence generated by a trapezoidal cycle operated at the same speed, i.e. with the same period. As we can see in Table III, the trapezoidal cycles generate twice as much coherence as the RL cycles shown in Figs. 4c-f, i.e. corresponding to $c = 1, 0.8, 0.6, 0.4$.

| $c$  | RL    | Trapez. |
|------|-------|---------|
| 1    | 0.068 | 0.13    |
| 0.8  | 0.050 | 0.12    |
| 0.6  | 0.054 | 0.092   |
| 0.4  | 0.035 | 0.090   |

**TABLE III.** Coherence generated by the final deterministic cycles identified by the RL method (RL column) and generated by a trapezoidal cycle operated at the same speed (Trapez. column) at the values of $c$ shown in the first column. These values correspond to the cycles shown in Figs. 4c-f.

**DATA AVAILABILITY**

All raw data was generated with the accompanying code and is available in Figshare (https://doi.org/10.6084/m9.figshare.19180907).

**CODE AVAILABILITY**

The code used to generate all results is available on GitHub (https://github.com/PaoloAE/paper_rl_blackbox_thermal_machines).
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COMPETING INTERESTS

The authors declare no competing interests. P.A.E. and F.N. are authors of a patent application containing aspects of this work (Application to the European Patent Office, file number: 21 191 966.7).

AUTHOR CONTRIBUTIONS

P.A.E. and F.N. designed the research and method. P.A.E. wrote the computer code and carried out the numerical calculations. P.A.E. and F.N. analysed the data and wrote the manuscript.
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