Bargaining with entropy and energy

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Statistical mechanics is based on interplay between energy minimization and entropy maximization. Here we formalize this interplay via axioms of cooperative game theory (Nash bargaining) and apply it out of equilibrium. These axioms capture basic notions related to joint maximization of entropy and minus energy, formally represented by utilities of two different players. We predict thermalization of a non-equilibrium statistical system employing the axiom of affine covariance—related to the freedom of changing initial points and dimensions for entropy and energy—together with the contraction invariance of the entropy-energy diagram. Whenever the initial non-equilibrium state is active, this mechanism allows thermalization to negative temperatures. Demanding a symmetry between players fixes the final state to a specific positive-temperature (equilibrium) state. The approach solves an important open problem in the maximum entropy inference principle, \textit{viz.}, generalizes it to the case when the constraint is not known precisely.

Interplay between entropy and energy is fundamental for equilibrium statistical mechanics \cite{1–5}. The interplay is based on the fact that the equilibrium (positive-temperature) Gibbs distribution can be obtained via maximizing entropy for a fixed energy, or via minimizing energy for a fixed entropy \cite{1–5}. The entropy maximization reflects the tendency of an isolated system towards maximal disorder. The energy minimization relates to finding a more stable (passive) state \cite{4}.

Here we show that the competition between entropy and energy can be formalized via axioms of cooperative game theory (bargaining) \cite{7–9} and applied out of equilibrium. Now entropy $S$ and minus energy $U = -E$ are payoffs of two players that tend to maximize them “simultaneously”; see Table I of \cite{10} for a game theory—statistical physics dictionary. While non-cooperative game theory focuses on rational actions to be chosen given payoffs only, the bargaining provides an axiomatic description of interaction between the players that should reach a compromise \cite{6–8}. Hence bargaining is suitable for formalizing interaction mechanisms to be applied in physics \cite{11}. We apply it when known thermodynamic principles do not suffice for predicting system’s behavior. Given a non-equilibrium initial state with entropy larger than $k_B \ln 2$, and using certain plausible axioms on the relaxation process, we can show that the final state is an equilibrium one, with the sign of temperature depending on the initial state. The final state is fixed to a specific positive-temperature state, if the symmetry between players is assumed. Thus we derive thermalization via game theory. As an application of our results we resolve a major open problem in the maximum entropy inference method \cite{12, 13} generalizing it to those cases, where the constraint is not known precisely.

**Entropy-energy diagram.** We study a classical system with discrete states $i = 1, \ldots, n$ and respective energies $\{\varepsilon_i\}_{i=1}^n$. A statistical (generally non-equilibrium) state of the system is given by probabilities

$$\{p_i \geq 0\}_{i=1}^n, \quad \sum_{i=1}^n p_i = 1. \quad (1)$$

The entropy and minus average energy for such a state are, respectively \cite{1–5}:

$$S[p] = -k_B \sum_{i=1}^n p_i \ln p_i, \quad U[p] = -\sum_{i=1}^n \varepsilon_i p_i, \quad (2)$$

where $k_B$ is Boltzmann’s constant. The Gibbsian equilibrium states are obtained by maximizing $S[p]$ over (1) under a fixed $U = U[p]$ \cite{1–5}:

$$\pi_i = e^{-\beta \varepsilon_i} / Z, \quad Z = \sum_{i=1}^n e^{-\beta \varepsilon_i}, \quad \beta = 1 / (k_B T), \quad (3)$$

![FIG. 1: A typical example of entropy-energy diagram. Entropy is $S$ and the minus energy $U = -E$ for 4-level system with energies: $\varepsilon_1 = 0, \varepsilon_2 = 1, \varepsilon_3 = 2.5, \text{ and } \varepsilon_4 = 3$. Maximal (minimal) entropy curves are denoted by blue (black). All physically acceptable values of entropy and energy are inside of the domain bounded by blue and black curves. States below red dashed lines (both are lower than ln 2) are excluded by Axiom 2. Green dashed line shows $U_{av} = -\frac{1}{4} \sum_{i=1}^4 \varepsilon_i$; it separates $\beta > 0$ from $\beta < 0$; cf. (4). Black point denotes a possible initial state. States inside dashed blue lines hold axiom 4. Magenta lines denote initial states that produce the same final state (9).](image-url)
where the inverse temperature $\beta$ is uniquely determined from $U[p] = U$. The same result—but restricted to the positive-temperature branch $\beta > 0$—is obtained upon maximizing $U[p]$ under fixed $S$ [4, 5]. This is why we frequently employ the minus energy together with entropy: both are maximized in equilibrium.

Fig. 1 shows a typical entropy-energy diagram on the $(U, S)$ plane. The maximum entropy curve $S(U)$ holds

$$S(U_{\text{av}}) = \ln n, \quad U_{\text{av}} = -\frac{1}{n} \sum_{k=1}^{n} \epsilon_k.$$  \hfill (4)

For $U > U_{\text{av}}$ ($U < U_{\text{av}}$) $S(U)$ refers to $\beta > 0$ ($\beta < 0$). No probabilistic states are possible below the minimum entropy curve $S_{\text{min}}(U) = \min_{p, U[p]=U} (S[p])$. The maximum entropy curve is smooth and bounds a convex domain due to concavity of $S[p]$ [0 < $\epsilon$ < 1] [4, 5]: $S[p] + (1-\epsilon)q \geq \epsilon S[p] + (1-\epsilon)S[q]$. Now $S_{\text{min}}(U)$ is an irregular curve, because minima of a concave function $S[p]$ are reached for vertices of the allowed probability domain that combines (1) with constraint $U[p] = U$. Hence only two probabilities are non-zero; see §1 of [10] for details. We have [cf. Fig. 1]:

$$S_{\text{min}}(U) \leq k_B \ln 2, \quad S_{\text{min}}(-\epsilon_i) = 0.$$  \hfill (5)

**Statement of the problem.** We emphasize that all above features of the entropy-energy diagram hold for arbitrary large, but finite values of $n$. Let the statistical system be found initially at some point of the entropy-energy diagram. We want to predict the long-time state of this system, knowing that its entropy and minus energy tend not to decrease. An example of this situation is when a thermally isolated statistical system is subject to external fields that extract energy. (Recall that any process is thermally isolated if the environment is included into the system.) Now in two extreme cases thermodynamics can determine the long-time state [1–3]: firstly, if the work-extraction process is very slow, then the entropy is conserved and work-extraction entails decreasing energy. Consequently, through the extraction of as much work as possible, the system will finally reach equilibrium along the constant entropy [1–3]. Secondly, when no work-extraction is present and the system is completely isolated, its entropy will increase till it finally reaches equilibrium along the constant energy path.

Now what if both processes occur simultaneously, i.e. when both entropy and minus energy increase, can one still show that the system will reach a thermal equilibrium? If yes, can one bound its temperature?

The standard thermodynamics cannot answer these two questions due to insufficient information. (E.g. it can predict the final state (3) if we know that the system is attached to a thermal bath at inverse temperature $\beta$; but we do not make such an assumption.) The questions can be answered within more detailed, non-equilibrium statistical mechanical theories [4, 5]. But such theories make a number of dynamical assumptions, e.g. they assume that internal constituents of the system move according to quantum Hamiltonian dynamics during the whole system’s evolution [4, 5]. Or they assume that the systems is of hydrodynamic type with smooth density, velocity and pressure fields [1]. The direct validity of such assumptions is difficult to address, hence a specific axiomatic approach is required [23].

Here we address the above question via axioms of bargaining games [6–8]; see Table I of [10] for a detailed comparison between bargaining theory and statistical physics. Given the initial state $(U_i, S_i)$, we look for the final state $(U_f, S_f) = (U[p_f], S[p_f])$. Axioms below will determine this final state on the entropy-energy diagram.

**Axiom 1:** Once both $S$ and $U$ tend to increase, then at least one of them should increase to some extent:

$$U_i \leq U_f, \quad S_i \leq S_f,$$  \hfill (6)

where at least one inequality is strict. In game theory (6) relates to individual rationality of players [8, 9].

**Axiom 2:** The choice of initial conditions. We shall assume a non-equilibrium initial (probabilistic) state, with entropy $S_i > k_B \ln 2$. This is a class of sufficiently macroscopic states for our purposes. In concrete cases this condition can be made weaker; e.g. for the case of Fig. 1 we can allow all initial states above dotted red lines. Now Axioms 1 and 2 ensure that the domain of allowed final states on the entropy-energy diagram is a convex set.

**Axiom 3:** Affine-covariance. If the entropy-energy diagram $(U, S)$ (including $(U_i, S_i)$) is transformed as

$$(U, S) \rightarrow (a^{-1}U + d, b^{-1}S + c), \quad a > 0, b > 0,$$  \hfill (7)

where $c$ and $d$ are arbitrary, then the final state is transformed via the same rule (7) [7]. The freedom to translate energy and entropy by an arbitrary amount is well-known in physics; hence the factors $c$ and $d$ in (7). In (7), $a$ and $b$ account for the fact of different dimensions for $S[p]$ and $U[p]$ [cf. (2)], and the possibility of changing those dimensions without changing physics. We shall apply (7) also for dimensionless $a$ and $b$.

**Axiom 4:** Contraction invariance (Independence of irrelevant alternatives) [7]. Let $D'$ be a subset of the original entropy-energy phase-diagram $D$, and $D'$ contains both $(S_i, U_i)$ and $(S_f, U_f)$. If $D$ now the set of allowed final states is restricted (contracted) from $D$ to $D'$, then it still holds that $(U_i, S_i) \rightarrow (U_f, S_f)$.

Axiom 4 tells about any subset $D'$, but below we shall need it only for full-measure, well-behaved subsets that are similar to $D$. The restriction to those subsets can be realized via suitable external fields.

Contraction invariance plays an important role in decision theory [6–8]. The intuition behind this axiom is physical: it assumes that the actual evolution $(U_i, S_i) \rightarrow (U_f, S_f)$ amounts to selecting the “best” state via binary comparisons of diagram points. Hence restricting the set
of alternatives—provided that the “best” states are still allowed—cannot change the “best”.

Hence Axioms 1—4 imply thermalization: the final state is on the maximum entropy curve. Negative-temperature states are allowed by this derivation for $U_i < U_{av}$. Such initial states are active, i.e. $(p_i - p_j)(\varepsilon_i - \varepsilon_j) > 0$ at least for one pair $(i, j)$.

More information on the final state is contained in

Axion 5: Symmetry. We made $U$ and $S$ dimensionless via (7). If the domain of allowed final states (6) is symmetric—i.e. it contains a point $(U, S)$ if and only if it contains $(S, U)$—and so is the initial state $(U_i = S_i)$, then the final state is also symmetric $(S_F, S_i)$, provided that there are no reasons to regard the players asymmetrically.

Nash [6] and his followers [8] argued that the only final state satisfying axioms 1—5 is

$$\left(U_N, S_N\right) = \arg\max_{\left(U, S\right)} \left[\left(U - U_i\right)(S - S_i)\right],$$

where the maximum is reached on the maximum entropy curve restricted by (6). Since this curve is concave, the argmax in (9) is unique; see §2.1 of [10]. Eq. (9) shows that $(U_N, S_N)$ refer to a $\beta_N > 0$; cf. (3).

However, Refs. [6, 8] derive (9) by making an additional assumption, viz. the domain restricted by (6) can enlarged into a larger domain; see §2.2 of [10] for details. We cannot employ this assumption, since it is completely unphysical. We shall derive (9) using axioms 1—5, but without the assumption. Fig. 3 shows a typical example of the maximal entropy curve $s(u)$—denoted by $\mathcal{B}$ in Fig. 3—in coordinates (8) with $U = \mathcal{O} \equiv (0, 0)$. The domain of states $\mathcal{B}A\mathcal{O}$ allowed by Axiom 1 is not symmetric in the sense of Axiom 5. But it has the largest symmetric subset $\mathcal{B}O\mathcal{K}\mathcal{C} \subset \mathcal{B}A\mathcal{O}$, where $K$ is the solution of $s(\hat{u}) = \hat{u}$, and $\mathcal{K}$ is the inverse function $s^{-1}(u)$ of $s(u)$; see Fig. 3. For $\mathcal{B}O\mathcal{K}\mathcal{C}$ Axiom 5 + thermalization lead to $\mathcal{K}$ as the final state. Hence for the original domain $\mathcal{B}A\mathcal{O}$ the final state is located on the line $\mathcal{K}\mathcal{A}$ (possibly including $\mathcal{K}$); see Axiom 4 and the result that the final state is located on $\mathcal{B}A\mathcal{O}$. In coordinates (8) the state (9) is given as $(u_N, s(u_N))$ with $u_N = \arg\max_u \left[u s(u)\right]$. This is the point $\mathcal{N}$ on Fig. 3. Now $\mathcal{N} \in \mathcal{K}\mathcal{A}$, as seen from working out concave function $s(u)$ for $u \simeq \hat{u}:

$$us(u) - us(\hat{u}) = \hat{u}(u - \hat{u})\left[1 + s'(\hat{u})\right],$$

$$s(u) - s^{-1}(u) = \left[s'(\hat{u})^2 - 1\right] \left[u - \hat{u}\right] / s'(\hat{u}),$$

where $s'(u) = ds/du$ and factors $\mathcal{O}[(u - \hat{u})^2]$ were neglected. Now for $-1 < s'(u) < 0$ we have the situation shown on Fig. 3, where $u_N > \hat{u}$ and $s(u) > s^{-1}(u)$ for $u > \hat{u}$. For $-1 > s'(u)$ we have the analogue of Fig. 3, where $u_N < \hat{u}$, and the solution is located on $\mathcal{B}\mathcal{K}$. For $1 > s'(\hat{u}) > 0$, we always get $u_N > \hat{u}$.

The same restricting of the final state will be done after transformation (7) with $b = 1$ and $c = d = 0$, where $s(u) \rightarrow s(au)$. We choose $a = a_0$ such that

$$\arg\max_u \left[u s(a_0 u)\right] = \hat{u}_0, \quad \hat{u}_0 = s(a_0 \hat{u}_0),$$

where

\begin{fig2}

\textbf{FIG. 2.} The set of states in coordinates (8) for $U_i > U_{av}$ (black and green curves) and $U_i < U_{av}$ (dotted and dashed blue curves). In both cases the initial state is shifted to $(0, 0)$ via (7). $\mathcal{F}$ and $\mathcal{G}$ are tentative final states for (resp.) first and second scenario.

\textbf{Thermalization.} We have two possibilities for the initial state $(U_i, S_i)$ [see (4) and Fig. 2, 1]: $U_i \geq U_{av}$ or $U_i < U_{av}$. Both scenarios are studied in coordinates

$$u = U - U_i, \quad s = S - S_i,$$

which is done by (7) with $a = b = 1$; see Fig. 2.

For $U_i \geq U_{av}$, all points on and below the maximum entropy curve $\mathcal{B}A$ [apart of $(0, 0)$] are allowed as possible final states; see (6) and Fig. 2. Assume that the final state $\mathcal{F} \equiv (\hat{u}, \hat{s}) \not\in \mathcal{B}A$; cf. Fig. 2. Then there is a point $\mathcal{F}_1 = (a_1 \hat{u}, b_1 \hat{s})$, with $a_1 \geq 1$ and $b_1 \geq 1$ (at least one of these inequalities is strict). We now apply (7) with $a = a_1$, $b = b_1$, and $c = d = 0$ to all point of the diagram. This transforms $\mathcal{F}_1 \rightarrow \mathcal{F}$, and changes the original domain $D = \mathcal{B}O\mathcal{A} \equiv [(0, 0) = \mathcal{O}]$ to smaller domain $D' \subset D$; see Fig. 2, where $D'$ is below the green line. Now $\mathcal{F} \in D'$, due to $\mathcal{F}_1 \rightarrow \mathcal{F}$. But we can regard $D'$ as just a subset of $D$ and apply to it Axiom 4. We now have 2 contradicting facts: following Axiom 4, $\mathcal{F}$ should not change when going to a subset. But it should change, $\mathcal{F} \rightarrow \mathcal{F}_2$ according to (7), i.e. Axiom 3. The contradiction is avoided only if $\mathcal{F}$ is located on the maximum entropy curve $\mathcal{B}A$ [9].

For $U_i < U_{av}$, we can apply (7) only with $a = 1$ and $b > 1$ ($c = d = 0$). Otherwise, $D' \not\subset D$—see Fig. 2 for an example—and then Axiom 4 does not apply. Hence given a tentative final state $\mathcal{G} = (\hat{u}, \hat{s})$ we can reach the above contradiction only if there is a point $\mathcal{G}_1 = (\hat{u}, b \hat{s})$; see Fig. 2. I.e. the set of possible final states coincides with curve $\mathcal{B}\mathcal{C}$ in Fig. 2. Note that for this conclusion we should slightly modify Axiom 1: $U_i > U_i$; cf. (6).

\end{fig2}
i.e. the transformed Nash solution (9) equals \( \hat{u}_0 \). Consider (7) under two other values of \( a: a_2 > a_0 > a_1 \); see Fig. 3. When applying (7) with \( a = a_2 \), the transformed Nash solution lies on BK_2. On that curve, the final state lies between \( K_1 \) and \( K_2 \). Going back to the original curve \( K_A \), we restrict the final state to lay between \( K \) and \( n_2 \) on \( K_A \). Applying (7) with \( a = a_1 \), we further restrict the final state to lay between \( n_1 \) and \( n_2 \); see Fig. 3. For \( a_1 \to a_0 \leftrightarrow a_2 \) we get \( n_1 \to N \leftrightarrow n_2 \), i.e. the final state coincides with (9).

![Entropy-energy diagram in coordinates (8): \( s(u) \) (black), \( s(a_0u) \) (green), \( s(a_1u) \) (magenta) and \( s(a_2u) \) (brown).](image)

**Retrospecting from an equilibrium state (without conservation laws).** Given an equilibrium state \((U(\beta), S(\beta))\) with \( \beta > 0 \) we can identify it with the final state (9), and ask which initial states give rise to it. Such a question is possible to ask within standard thermodynamics only if the conservation law of entropy or energy is there. Note that \((U_N, S_N)\) in (9) is determined from \( \frac{d}{d\beta} [\Delta U(\beta)] = 0 \). This leads to a line \( S - S(\beta) = \beta(U - U(\beta)) \) on the entropy-energy diagram; see magenta lines on Fig. 1. They start from \((U(\beta), S(\beta))\) and end either at a boundary of the diagram, or at a point, where the convexity of the domain is lost.

The maximum entropy method grew out of statistical physics and is widely used in probabilistic inference [12–14]. To recall it: probabilities (1) are not known, but the average value \( U = U[p] = -\sum_{k=1}^n p_k \varepsilon_k \) of a random quantity \( \{-\varepsilon_k\}_{k=1}^n \) is known. Then the most unbiased (least informative) probabilities that correspond to this prior information are derived by maximizing the entropy \( S[p] \) under \( U = U[p] \): \( \max_p S[p] = S(U) \) [13–15]. Applications of the method meet the following problem: if \( \{p_k\}_{k=1}^n \) are not known, and \( U \) is learned from experiments, then it cannot be known precisely [14, 15]; see §3 of [10] for a review of the method and the open problem. Thus we ask how is the method applied if there is weaker prior information, i.e. the average \( U \) is not known precisely, but we only know that it belongs to the interval \( U \in [U_1, U_2] \)? For technical clarity we add another constraint [see (4) and §3.4 of [10] for extensions]:

\[
U \in [U_1, U_2], \quad U_{av} < U_1 < U_2. \tag{13}
\]

Recall that upon (13) the same result is obtained by maximizing \( S[p] \) for \( U = U[p] \), or by maximizing \( U[p] \) for \( S = S[p] \). Note that the uncertainty (13) translates into the uncertainty \( S \in [S_1, S_2] \) \((S_1 \equiv S(U_1), S_2 \equiv S(U_2))\) for the maximum entropy. For applying the bargaining axioms—where \( U[p] \) and \( S[p] \) are two utilities that tend to maximize simultaneously—we should define the domain of allowed states \( \Omega \) on the \((U, S)\)-diagram. Now \( \Omega \) is defined by joining two uncertainty intervals:

\[
\Omega = \{(U, S) \mid U \in [U_1, U_2], \ S \in [S_1, S_2] \}. \tag{14}
\]

\( \Omega \) has the form required by Axiom 1 with the initial point \((U_0, S_0) = (U_1, S_2)\); cf. (6). Now Axioms 1–5 apply; see §3.3 of [10] for details. Thus we deduce the bargaining solution for the uncertainty given by (13) [cf. (9)]:

\[
\arg\max_{(U, S)} [U(U_1)(S(S_2))]. \tag{15}
\]

In particular, Axiom 5 is natural here due to the duality between maximizing \( U[p] \) and \( S[p] \). Extensions of (15) to other [than (13)] uncertainty intervals \([U_1, U_2]\) are worked in §3.4 of [10]. Elsewhere we shall explore applications of this generalized maximum-entropy method.

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\[\text{(10) Supplementary material.}\]

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SUPPLEMENTARY MATERIAL

1. Calculation of the minimum entropy for a fixed average energy

Here we show how to minimize entropy

\[ S_{\text{min}}(E) = \min_p S[p], \quad S[p] = -k_B \sum_{i=1}^{n} p_i \ln p_i, \]  

over probabilities \( \{p_i \geq 0\}_{i=1}^{n}, \quad \sum_{i=1}^{n} p_i = 1, \)  

for a fixed average energy \( E = \sum_{i=1}^{n} \varepsilon_i p_i. \)

Energy levels \( \{\varepsilon_i \geq 0\}_{i=1}^{n} \) are given.

Since \( S[p] \) is concave, its minimum is reached for vertices of the allowed probability domain. This domain is defined by the intersection of (17) with probabilities that support constraint (18). Put differently, as many probabilities nullify for the minimum of \( S[p] \), as allowed by (18). Hence at best only two probabilities are non-zero.

We now order different energies as

\[ \varepsilon_1 < \varepsilon_2 < \varepsilon_3 \ldots \]  

and define entropies \( s_{ij}(E) \), where only states \( i \) and \( j \) with \( i < j \) have non-zero probabilities:

\[ s_{ij}(E) = \frac{E - \varepsilon_i}{\varepsilon_j - \varepsilon_i} \ln \frac{\varepsilon_j - E}{\varepsilon_j - \varepsilon_i} - \frac{\varepsilon_j - E}{\varepsilon_j - \varepsilon_i} \ln \varepsilon_j - \varepsilon_i \varepsilon_i \leq E \leq \varepsilon_j. \]  

The minimum entropy \( S_{\text{min}}(E) \) under (18) is found by looking—for a fixed \( E \)—at the minimum over all \( s_{ij}(E) \) whose argument supports that value of \( E \). E.g. \( S_{\text{min}}(E) \) reads from (20) for \( n = 3 \) (3 different energies):

\[ S_{\text{min}}(E) = \min[s_{13}(E), \theta(\varepsilon_2 - E)s_{12}(E) + \theta(E - \varepsilon_2)s_{23}(E)], \]  

where \( \theta(x) \) is the step-function \( (\theta(x > 0) = 1 \) and \( \theta(x < 0) = 0 ) \), and where we assume \( \varepsilon_1 \leq E \leq \varepsilon_3 \). Likewise, for \( n = 4 \):

\[ S_{\text{min}}(E) = \min[s_{14}(E), \theta(\varepsilon_2 - E)s_{12}(E) + \theta(E - \varepsilon_2)s_{23}(E) + \theta(E - \varepsilon_3)s_{34}(E), \theta(\varepsilon_2 - E)s_{12}(E) + \theta(E - \varepsilon_2)s_{24}(E), \theta(\varepsilon_3 - E)s_{13}(E) + \theta(E - \varepsilon_3)s_{34}(E) \]  

where \( \varepsilon_1 \leq E \leq \varepsilon_4 \). Generalizations to \( n > 4 \) are guessed from (22, 23).

2. Features of the Nash solution (9)

2.1 Concavity

Let us write (9) in coordinates (8):

\[ u_N = \arg \max_u \left[ u_0(s(u)) \right], \]  

where (for obvious reasons) the maximization was already restricted to the maximum entropy curve \( s(u) \). Now recall that \( s(u) \) is a concave function. Local maxima of \( u_0(s(u)) \) are found from \( \frac{\partial}{\partial u} s' = s'' \):

\[ [u_0(s)]''|_{u=u_N} = u_N s''(u_N) + s(u_N) = 0. \]  

Calculating

\[ [u_0(s)]'''|_{u=u_N} = -\frac{2s(u_N)}{u_N} + us''(u_N) < 0 \]  

TABLE I: Bargaining theory – statistical mechanics dictionary.

Utilities of players | Entropy and minus energy
---|---
Joint actions of players | Probabilities of states for the physical system
Feasible set of utility values | Entropy-energy diagram
Defection point | Initial state
Pareto set | Maximum entropy curve for positive inverse temperatures \( \beta > 0 \)

we see that solutions \( u_N \) of (25) are indeed local maxima due to \( s''(u) < 0 \) (concavity) and \( u \geq 0, s(u) \geq 0 \), as seen from (8).

We shall now show that this local maximum is unique and hence coincides with the global maximum. For any concave function \( s(u) \) we have for \( u_1 \neq u_2 \):

\[
s(u_1) - s(u_2) < s'(u_2)(u_1 - u_2),
\]

which produces after re-working and using (25) for \( u \neq u_N \):

\[
us(u) - u_N s(u_N) < s'(u_N)(u - u_N)^2 = -\frac{s(u_N)}{u_N} (u - u_N)^2 < 0.
\]

Hence \( u_N \) is the unique global maximum of \( us(u) \).

2.2 Comments on the textbook derivation of (9).

In the main text we emphasized that the derivation of the solution (9) for the axiomatic bargaining problem that was proposed by Nash [1] and is reproduced in textbooks [2-4] has a serious deficiency. Namely, (9) is derived under an additional assumption, viz. that one can enlarge the domain of allowed state on which the solution is searched for. This is a drawback already in the game-theoretic set-up, because it means that the payoffs of the original game are (arbitrarily) modified. In contrast, restricting the domain of available states can be motivated by forbidding certain probabilistic states (i.e. joint actions of the original game), which can and should be viewed as a possible part of negotiations into which the players engage. For physical applications this assumption is especially unwarranted, since it means that the original (physical) entropy-energy phase diagram is arbitrarily modified.
FIG. 4: Entropy-energy diagram in coordinates (8). Blue curve: $s(u)$. The affine freedom is chosen such that the Nash solution (9) coincides with the point (1, 1). The original domain of allowed states is filled in yellow. This domain is not symmetric with respect to $s = u$. The domain below $AA_1$ is symmetric with respect to $s = u$.

We now demonstrate on the example of Fig. 4 how specifically this assumption is implemented. Fig. 4 shows an entropy-energy diagram in relative coordinates (8) with $s(u)$ being the maximum entropy curve. The affine transformation were chosen such that the Nash solution (9) coincides with the point (1, 1). Now recall (25). Once $s(u_N) = u_N = 1$, then $\frac{ds(u_N)}{du} = -1$, and since $s(u)$ is a concave function, then all allowed states lay below the line $2 - u$; see Fig. 4. If now one considers a domain of all states ($u \geq 0, s \geq 0$) (excluding the initial point (0, 0)) lying below the line $2 - u$ (this is the problematic move!), then (1, 1) is the unique solution in that larger domain. Moving back to the original domain and applying the contraction invariance axiom, we get that (1, 1) is the solution of the original problem.

3. Maximum entropy method and its open problem

3.1 Maximum entropy method: a reminder

The method originated in the cross-link between information theory and statistical mechanics [6]. It applies well to quasi-equilibrium statistical mechanics [7, 8], and developed to become an inference method (for recovering unknown probabilities) with a wide range of applications; see e.g. [7–10].

As a brief reminder: let we do not know probabilities (17), but we happen to known that they hold a constraint:

$$U = U[p] \equiv \sum_{k=1}^{n} u_k p_k,$$

with $\{u_k\}_{k=1}^{n}$ being realizations of some random variable $U$. We refrain from calling $U$ energy (or minus energy), since applications of the method are general.

Now if we know precisely the average $U$ in (29), then unknown probabilities (17) can be recovered from maximizing the entropy (16) under constraint (29). In a well-defined sense this amounts to minimizing the number of assumption to be made additionally for recovering probabilities [9]. The outcome of the maximization is well-known and was already given by us in the main text:

$$\pi_i = e^{-\beta u_i}/Z, \quad Z = \sum_{i=1}^{n} e^{-\beta u_i},$$

where the Lagrange multiplier $\beta$ is determined from (29).

The method has a number of desirable features [9]. It also has several derivations reviewed in [7–9]. Importantly, the method is independent from other inference practices, though it does have relations with Bayesian statistics [12–14] and causal decision making [12].

3.2 The open problem

But from where could we know $U$ in (29) precisely? This can happen in those (relatively rare) cases when our knowledge is based on some symmetry or a law of nature. Otherwise, we have to know $U$ from a finite number of experiments or—which within subjective probability and management science [11]—from an expert opinion. The former method will never provide us with a precise value of $U$, simply because the number of experiments is finite. Opinions coming from experts do naturally have certain uncertainty, or there can be at least two slightly different expert opinions that are relevant for the decision maker. Thus in all those cases we can stick to a weaker form of prior information, viz. that $U$ is known to belong to a certain interval

$$U \in [U_1, U_2], \quad U_1 < U_2.$$

This problem was recognized by the founder of the method [15], who did not offer any specific solution for it. Further studies attempted to solve the problem in several different ways:

- Following Ref. [16], which studies the entropy maximization under more general type of constraints (not just a fixed average), one can first fix $U$ by (29), calculate the maximum entropy $S(U)$, and then maximize $S(U)$ over $U \in [U_1, U_2]$, which will mean maximizing entropy (16) under constraint (31). This produces:

$$\max_{p, U \in [U_1, U_2]} S[p] = S(U_1) \quad \text{for} \quad U_1 \geq U_{av}$$

$$= S(U_2) \quad \text{for} \quad U_2 \leq U_{av}$$

$$= \ln n \quad \text{for} \quad U_1 < U_{av} < U_2.$$
Such a solution is not acceptable; e.g. in the regime (32) it does not change when increasing \( U_2 \). I.e. the solution does not feel the actual range of uncertainty implied in (31).

- What is wrong with the simplest possibility that will state \( S(\frac{U_1+U_2}{2}) \)—i.e. the maximum entropy at the center of the interval—as the solution to the problem? Taking the arithmetic average of the interval independently from the underlying problem seems arbitrary.

Another issue is that each value of \( U \) from the interval \([U_1, U_2]\) is mapped to the (maximum) entropy value making up an interval of entropy values. For \( U_1 \geq U_{av} \) this interval is \([S_2, S_1]\), where \( S_1 = S(U_1) \) and \( S_2 = S(U_2) \). Denoting by \( U(S) \) the inverse function of \( U \), we can take \( U(\frac{S_1+S_2}{2}) \) instead of \( S(\frac{U_1+U_2}{2}) \).

- Ref. [17] assumes that (though the precise value of the average is not known) we have a probability density \( \rho(U) \) for \( U \). Following obvious rules, the knowledge of \( \rho(U) \) translates into the joint density \( \rho(\tau_1, ..., \tau_n) \) for maximum-entropy probabilities (30). While this is technically well-defined, it is not completely clear what is the meaning of probability density \( \rho(U) \) over the average. One possibility is that the random variable \( U \) is sampled independently \( M \) times (\( M \) is necessarily finite), and the probability density of the empiric mean

\[
\frac{1}{M} \sum_{\alpha=1}^{M} u_{[\alpha]}, \tag{36}
\]

is identified with \( \rho(U) \). This possibility is however problematic, since it directly relates probability of the empiric mean with the probability of the average. E.g. if we shall sample independently \( M \) times from (30), then the average of the empiric mean equals \( \int dUU\rho(U) \), but the empiric mean itself is not distributed via \( \rho(U) \).

- Given (30), one can regard \( \beta \) as an unknown parameter, and then apply standard statistical methods for estimating it [18]. Thus within this solution the maximum entropy method is not generalized: its standard outcome serves as the initial point for applying standard tools of statistics. This is against the spirit of the maximum entropy method that is meant to be an independent inference principle [15].

- Yet another route for solving the problem was discussed in Ref. [15]. (We mention this possibility, also because it came out as the first reaction when discussing the above open problem with practitioners of the maximum entropy method [19].) It amounts to the situation, where in addition to the empiric mean (36) one also fixes the second empiric moment \( \frac{1}{M} \sum_{\alpha=1}^{M} u_{[\alpha]}^2 \) as the second constraint in maximizing (16). It is hoped that since identifying the sample mean (36) with the average \( U \) is not sufficiently precise for a finite \( M \), then fixing the second moment will account for this lack of precision. This suggestion was not worked out in detail, but it is clear that it cannot be relevant to the question we are interested in. Indeed, its implementation will amount to fixing two different constraints, i.e. in addition to knowing precisely the average \( U \) in (29), it will also fix the second moment \( U' = \sum_{k=1}^{n} u_k^2 p_k \) thereby assuming more information than the precise knowledge of \( U \) entails.

3.3 Solving the problem via bargaining

Main premises of this solution is that we should simultaneously account for both the uncertainty in \( U \) and in \( S \), and that we should account for the duality of optimization, i.e. that the maximum entropy result can be also obtained via the optimization of \( U[p] \) under a fixed \( S = S[p] \).

Let us first of all add an additional restriction in (31):

\[
U \in [U_1, U_2], \quad U_{av} = \frac{1}{n} \sum_{k=1}^{n} u_k < U_1 < U_2, \tag{37}
\]

\[
S(U) = \max_{p, U = U[p]} S[p]. \tag{38}
\]
The case $U_{\text{av}} > U_2$ is treated similarly to (37) with obvious generalizations explained below. The general case (31) is more difficult and will be addressed at the end of the next chapter.

We now know that the maximum entropy solution (30) can be recovered also by maximizing $U$ over $\{p_1\}_{i=1}^n$ for a fixed entropy. Note that the uncertainty (37) translates into an uncertainty

$$S \in [S_2, S_1], \quad S_1 = S(U_1), \quad S_2 = S(U_2), \quad (39)$$

in the maximum entropy. We now take the joint uncertainty domain $\Omega$ in the maximum entropy. We now take the joint uncertainty point (40) does already connect with the maximum entropy (37). On the other hand, is obtained by the inverse function $U(S) = \max_{p, S = S(p)} U(p)$ of $S(U)$.

Axiom 5 will go as stated in the main text and demands symmetry between maximizing $S$ and maximizing $U$. Altogether, Axioms 1', 2, 3', 4 and 5 suffice for deriving

$$\arg\max_{(U, S)} [(U - U_1)(S - S_2)], \quad (43)$$

as the solution of the problem with uncertainty interval (37).

3.4 Generalizing the solution to other types of uncertainty intervals

Uncertainty intervals that instead of (37) hold

$$U \in [U_1, U_2], \quad U_1 < U_2 < U_{\text{av}}, \quad (44)$$

are straightforward to deal with. Now relevant points on the maximum entropy curve can be reached by entropy maximization for a fixed $U = U[p]$, or minimizing $U[p]$ for a fixed entropy $S = S[p]$. Hence the initial point and Axiom 1' now read [cf. (40, 41)]:

$$\arg\max_{(U, S)} [(U - U_1)(S - S_2)]. \quad (43)$$

Instead of (43), the solution under (44, 45) will read:

$$\arg\max_{(U, S)} [(U_2 - U)(S - S_1)]. \quad (47)$$

Let us now take the case, where $[U_1, U_2]$ holds neither (37), nor (44), i.e. it holds:

$$U \in [U_1, U_2], \quad U_1 < U_2 < u_{\text{av}}. \quad (48)$$

Note that the discussion after (9) of the main text assumed only affine transformations of $U$ only, but we could consider affine transformations of $S$ only with the same success; see Fig. 3. Note as well that instead of affine transformation (42) we can apply $U \to a^{-1}U + d$ [i.e. we can reformulate axiom (42)], if the initial state (40) is parametrized as $(U_1, S_1) = (U_1, S_2) = (U_1, S_2)$ at the inverse function $U(S) = \max_{p, S = S(p)} U(p)$ of $S(U)$.

We define $\Omega$ as above by joining together uncertainties of $U$ and $S$, i.e. by including all points $(U, S)$, where $U \in [U_1, U_2]$ [see (48)], but where $S \in \min\{S_1, S_2\}$, $\ln n$. The latter interval, due to (48), is where the maximum entropy values are contained. It is clear that generically $\Omega$ has a structure of a right “triangle” formed by by two legs and a convex curve instead of the hypotenuse. Depending on whether $S_2 < S_1$ or $S_1 < S_2$, we apply to $\Omega$ either (40) with Axiom 1' (41), or (45) with Axiom 1'' (46). Axioms 2, 3', 4, 5 apply without changes. Hence

---

1 The reason of this restriction is that for being able to deduce thermalization using only the restricted affine-covariance (42), we anyhow need to require the strict inequality $U_1 < U_1$; cf. the discussion after (8).

2 We emphasize that for the present problem—where we have an uncertainty interval $[U_1, U_2]$ for $U$—the inapplicability of the affine transformation $U \to a^{-1}U + d$ is expected for at least two reasons. Firstly, the uncertainty interval $[U_1, U_2]$ does generally change under this transformation, which indicates on altogether a different problem. Secondly, the very definition of the initial point (40) does already connect with the maximum entropy curve; hence we do not expect the full freedom with respect to affine transformations to retain.
the initial point and solution reads, respectively in two regimes:

\[ S_2 = S(U_2 > 0) = S(U_1 < 0). \] (53)

Indeed, now interpolating from \( S_2 < S_1 \) will lead to (50), which is different as compared with interpolating (52) from \( S_1 < S_2 \). Thus we state that under (53) the prior information (48) does not suffice for drawing a unique conclusion with the bargaining method.

Fig. 5 illustrates all the above solution on an entropy-energy diagram. Two examples of the set \( \Omega \) are shown by blue, green (dashed) and red (dashed) lines. Brown dashed lines show an example of \((U_1, U_2) (U_1 < U_2)\), where the domain of states allowed according to Axiom 1 is not convex: it will cross the minimum entropy curve \( S_{\min}(U) \) denoted by black lines on Fig. 5. Hence such values of \((U_1, U_2)\) are not allowed. Fig. 5 shows two examples of allowed intervals \((U_1, U_2)\): \((U_1, U_2) = (-8.35, -3.375)\) and \((U_1, U_2) = (-3.375, -0.425)\). The corresponding values of \( S_1 = S(U_1) \) and \( S_2 = S(U_2) \) are \((\ln 2, \ln 4)\) and \((\ln 4, \ln 2)\). Blue arrows join the initial states with corresponding Nash solutions (43, 47).

It is seen that for \((U_1, U_2) = (-8.35, -0.425)\), where \( S_1 = S_2 = \ln 2 \), there are two Nash solutions denoted by dashed magenta arrows on Fig. 5. For this case (53) the existing prior information does not allow to single out a unique solution.

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