Product Distribution Field Theory

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This paper presents a novel way to approximate a distribution governing a system of coupled particles with a product of independent distributions. The approach is an extension of mean field theory that allows the independent distributions to live in a different space from the system, and thereby capture statistical dependencies in that system. It also allows different Hamiltonians for each independent distribution, to facilitate Monte Carlo estimation of those distributions. The approach leads to a novel energy-minimization algorithm in which each coordinate Monte Carlo estimates an associated spectrum, and then independently sets its state by sampling a Boltzmann distribution across that spectrum. It can also be used for high-dimensional numerical integration, (constrained) combinatorial optimization, and adaptive distributed control. This approach also provides a simple, physics-based derivation of the powerful approximate energy-minimization algorithms semi-formally derived in [10,11]. In addition it suggests many improvements to those algorithms, and motivates a new (bounded rationality) game theory equilibrium concept.

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I. INTRODUCTION

Mean Field Approximations (MFA’s) have many applications outside of physics, combinatorial optimization by mean-field annealing being perhaps the most prominent of them [2,3]. One problem with MFA’s is that because they treat all particles as independent, they can be a poor approximation of the desired distribution. Another is that especially in large systems with complex Hamiltonians, they can be expensive to evaluate.

We extend MFA’s by introducing coordinate transformations that allow us to convert a coupled distribution into a decoupled one. This allows us to improve the accuracy of the MFA. It also allows us to employ Monte Carlo mean-field annealing for optimal adaptive control. We also introduce separate Hamiltonians for each particle. This allows us to exploit recent results in collectives theory [4] to speed up MFA evaluations. This extended MFA justifies heuristics recently found to beat simulated annealing in adaptive control problems by orders of magnitude [5,6,7]. It also provides novel ways to do (constrained) combinatorial optimization, a novel (bounded rational) game theory equilibrium concept [8,9], and a way to calculate such equilibria.

II. SELF-CONSISTENT DISTRIBUTIONS

Let ζ be a space with elements z and cardinality |ζ|. A semi-coordinate system of ζ, Ξ, is a space ξ having elements x = (ξ1, . . . , ξM) together with a surjective map from ξ to ζ, written as ξi(z). ξ(z) need not be invertible; the (semi-)coordinates of a point x ∈ ξ may not be unique. No a priori restriction is made on whether ξ and ζ are countable, uncountable, time-extended, etc.

The space of possible probability distributions (or density functions, as the case may be) over ξ is P†.

Any p ∈ P† induces a distribution over ζ, p(z) = ∫ dx p(x)δ(z − ζ(x)). (We implicitly assume integral measures and delta functions that match ξ.) Expressions like “p(ξ) = p′(ξ)”, “p(ξ, i) = p′(ξ, i)”, and “p(ξ, i, j) = p′(ξ, i, j)”, where p, p′ ∈ P†, mean ∀x ∈ ξ, p(x) = p′(x), p(x) = p′(x), and p(x) = p′(x) ∀j ≠ i, respectively. P is the set of all product distributions over ξ, i.e., the submanifold of all p ∈ P† obeying p(ξ) = Πi p(ξi). We will use the obvious parameterization of elements of P as the vectors of their marginal distributions, written q = (q(ξ1, . . . , ξM(ξ))M). Note that changing ζ(ξ) with ξ fixed will change the manifold P in general but won’t affect Q, the space of all q.

We are interested in self-consistent q that obey qi(ξi) = Ai(ξi, q, . . . , qM) ∀i for some functions {Ai}. By Brouwer’s theorem, for any smooth {Ai}, the map q → {Ai(ξi, q, . . . , qM)} (which we call parallel Brouwer updating) has at least one fixed point. Here we consider such Ai that set qi by minimizing a functional of (q1, . . . , qM). As an example, that functional might be the same for all i, for each one measuring the error of (q1, . . . , qM). We write the cross entropy from p to p′ as S(p || p′) ≡ −∫ dx p(x)ln[p′(x)].
private Hamiltonians implicit in \( i \)'s temperatures. The associated fixed points obey

\[
q^\beta_i(\xi_i) = \frac{n_i(\xi_i)}{N_i(h_{i|1},q^\beta)} e^{-[h_{i|1},q^\beta](\xi_i)}
\]

where \( N_i({U}|_{i,p}) \) is the partition function and the bracket notation indicates expectation conditioned on the value of the subscripted coordinate: for any \( U \) and \( p \in \mathcal{P}^i \), \( [U]_{i,p}(\xi_i) \equiv \int dx_i p(x_i | \xi_i) dx_i | \xi_i \).

We can choose \( A_i \) based on objective functions other than the free energy; the important thing is to incorporate a concave function like entropy, to avoid the expensive process of checking the borders of \( Q \) for fixed points. For example, all the local minima of \( F_{h_i}(q) \) over \( Q \) are interior to \( Q \). Moreover, for any fixed \( q_{i|1} \) there is only one local minimum over \( Q \).

The following six examples all have uniform \( \mu \). \( \xi = \zeta \) (as in conventional MFA’s) in all but the fifth example:

**Example 1:** Let \( m_i = 1 \) \( \forall i \). Then at \( q^\beta \) each coordinate \( i \) obeys its own canonical ensemble and is independent of the values of the other coordinates. It is coupled to its own heat bath, with its own effective Hamiltonian set by the distributions over the other coordinates, \( [h_{i|1},q^\beta](\xi_i) \).

In contrast, if \( \forall i, m_i = 2 \) and \( h_{i|2} = g(h_{i|1})^2 \), each \( q^\beta_i(\xi_i) \) is a Gaussian over the values \( [h_{i|1},q^\beta](\xi_i) \) rather than a Boltzmann distribution over them. In this case \( \beta_1 \) and \( \beta_2 \) specify the mean and variance of \( h_{i|1} \).

**Example 2:** We have a team game when \( \forall i, i', j, m_i = m_{i'}, h_i = h_{i'} \). In a team game we have a single shared objective function trading off entropy and expected values of the Hamiltonians. For \( m = 1 \) we define the world Hamiltonian \( H \) as the single shared private Hamiltonian. For this the minimizer of the free energy over all \( \mathcal{P}^1 \) is the joint canonical ensemble distribution, \( p^{\beta H} \). In contrast, \( q^{\beta H} \), the minimizer over \( \mathcal{P} \), is an MFA for \( p^{\beta H} \). Since \( \zeta \) is arbitrary, by gradually increasing \( \beta \) one can converge on a \( q \) that is a delta function about the \( z \) that minimizes \( H(z) \). Since \( \zeta \) is arbitrary, this optimization algorithm can be applied for any underlying space one wishes to search. In particular, parallel Brower updating with gradually increasing \( \beta \) is equivalent to mean-field annealing [1].

In general \( q^{\beta H}(\xi_i) \neq p^{\beta H}(\xi_i) \), the marginal of \( p^{\beta H}(\xi) \). However the \( q^{\beta H} \) with the lowest free energy is the \( q \) that best approximates \( p^{\beta H} \), as measured by \( KL(q^{\beta H}, p^{\beta H}) \).

To have the fixed points equal the marginals we must instead have the \( \{ A_j \} \) minimize \( KL(p^{\beta H}, q^{\beta H}) \).

**Example 3:** One way to enforce a constraint \( f(z) = 0 \) is via a generalization of penalty functions. Say we have an \( m = 1 \) team game with world Hamiltonian \( H \). Choose the objective function \( \int dp(x) [\beta H(z(x)) + \beta f(\xi(x))]^2 - S(p) \). Then for \( \beta \rightarrow \infty \) our constraint will be enforced, if possible. Often the solution is on \( Q \)’s border though, which slows the search — finite \( \beta_f \) moves the solution(s) to the interior of \( Q \), by weakening the constraint. Alternatively, choose the objective function \( \int dp(x) [\beta H(x) + \lambda f(\xi(x))]^2 + \gamma \lambda^2 - S(p) \), where \( \gamma \geq 0 \) is a constant. Minimizing over both \( p \in Q \) and \( \lambda \in \mathbb{R} \) forces \( f(z) = 0 \) if \( \gamma = 0 \), while nonzero \( \gamma_i \) weakens the constraint but forces the fixed point \( q(\beta) \) inside \( Q \).

**Example 4:** Consider a team game with \( m = m' \) and \( h_j(x) = h_j(x_j) \in \mathbb{N}^+ \forall j \leq m' \). Here \( p^\theta \) is an MFA for the grand canonical ensemble of a system with \( m' \) particle types and Hamiltonian \( h_{m'|1} \): \( z_i \) encodes the states of all type \( i \) particles, and \( h_i \) counts their number [4].

**Example 5:** Say \( \zeta(\cdot) \) is bijective but \( \xi \neq \zeta \). Then \( \zeta(\cdot) \) is akin to a rotation, in that each \( \xi_i \) couples multiple components of \( \zeta \). More generally, \( |\xi| \neq |\zeta| \) means \( \zeta \) is an \( M \)-dimensional representation of an \( M' < M \)-dimensional system. This allows arbitrary distributions over \( \xi \) to be expressed as a product distribution.

As an illustration, say \( \zeta \) is two-dimensional with elements \((z_1, z_2)\). Take \( \zeta_1 = \zeta_1 \) and have an additional \( \xi \) coordinate for each separate value of \( z_1 \), which we write as \( \zeta_{z_1} \). So there are \( 1 + |\zeta_1| \) coordinates altogether. Have each \( \xi_i \) contain \(|\zeta_2|\) elements, i.e., \(|\zeta_2| \) separate subsets of \( \zeta \) and label those subsets by the values \( z_2 \in \zeta_2 \).

Example 6:** Formally, when \( \xi = \zeta \), and \( H(\xi) \) the objective function one wants to minimize. The goal in optimal control is to find argmin\( H(\xi) \) \( \xi \). Have the \( q_{i \geq 2} \) fixed to \( p(\xi_{z_1} \mid \xi_1) \), the distribution relating the plant variable and the control variables. Take \( m_1 = 1, h_{11}(\xi) = H(\xi_1) \), and redefine \( F_{h_1} \) to involve the entropy of just \( \xi_1 \) rather than all of \( \xi \). Annal \( \beta \rightarrow \infty \), so that \( q_1(\xi_1) \) becomes a single delta function.

Write the resultant \( p^{\beta H} \) as \( \xi_1 \prod_{i \geq 2} q_i(\xi_i) \). This distribution minimizes \( \sum_{x_1} h_{11}(\xi_1) q_{1|x_1} \prod_{i \geq 2} q_i(x_i) = \sum_{x_1} h_{11}(\xi_1) q_{1|x_1} p(\xi_{z_1} \mid x_1) = \sum_{x_1} \mathcal{H}(\xi) p(\xi_{z_1} \mid x_1) = \sum_{x_1} \mathcal{H}(\xi_{z_1}) p(\xi_{z_1} \mid x_1) = \mathcal{H}(\xi_{z_1}) \) for fixed \( x_1 \).

So \( z_1 = x_1 \) solves our optimal control problem.

As an alternative interpretation of \( q^\beta \), say we have a rationality functional \( R(U, q_i) \) that measures how peaked any \( q_i \) is about argmax\( x_i U(x_i) \) for any \( U : \xi \rightarrow \mathbb{R} \). We require that \( R(U, q_i) = \beta \) if \( q_i(\xi_i) \propto \mu(\xi_i) e^{-\beta U(\xi_i)} \), and that the \( q_i \) satisfying \( R(U, q_i) = \beta \) that has maximal entropy is \( \mu(\xi_i) e^{-\beta U(\xi_i)} N_i(U) \). Now say we are told the \( \{ \beta_i^* \} \), the rationalities of the \( M \) players for their associated effective Hamiltonians \( \{ [h_{i|1},q_i] \} \). Then the information-theoretic optimal estimate for the associated
q is the minimizer over q and the {λi} of the free energy
\[ H_q = H - \sum \lambda_i f_i(R(h_{i1}, q_i)) - f_i(\beta^*) - \sum \beta^*_i \] for any monotonically increasing functions \{f_i\}. At any local minimum of this free energy \( q = q^g \) with \( \beta^* = \beta^*_i \forall i \).

This use of rationality functionals expresses the bounded-rationality assumption that one can get estimates of the effective Hamiltonian by sampling the associated Monte Carlo samples. So we have a minimizer of a single objective functional whose local minima are all interior to \( Q \). As an illustration, choose \( f_i(\beta) \) to be the ideal expected Hamiltonian \( \Delta \ln(N_i(\beta(h_{i1}, q_i))) \), and \( R(U, q_i) = \text{argmin}_\beta KL(q_i || e^{-\beta U} N_i(\beta(h_{i1}, q_i))) \). For such a choice \( f_i(R(h_{i1}, q_i)) \) is the actual expected Hamiltonian, \( \int dx, q_i(x_i)[h_{i1}, q_i](x_i) \).

III. FINDING FIXED POINTS

When we have an \( m = 1 \) team game we can use variants of gradient descent to find minima of the (single) free energy. Another approach for such scenarios is parallel Brouwer updating. More generally, define the free energy gap at \( q \) for coordinate \( i \) as
\[ \ln[N_i(h_{i1}, q_i)] + \int dx, q_i(x_i)[h_{i1}, q_i](x_i) + \int dx, q_i(x_i)\ln\frac{\ln\frac{q_i(x_i)}{h_{i1}(x_i)}}{P(x_i)} \]
This is how much \( F_{hi} \) is reduced if only \( q_i \) undergoes the Brouwer update. Define serial Brouwer updating as only updating one \( q_i \) at a time. In an \( m = 1 \) team game, any such update must reduce \( F_{hi}(p) \), in contrast to the case with parallel Brouwer updating. In greedy serial Brouwer updating, instead of cycling through all \( i \), at each iteration we update only the coordinate with the largest gap; this maximizes the free energy drop in that update.

A practical difficulty with these schemes for finding fixed points is that evaluating \( h_{i1}(q) \) can be very difficult in large systems. An alternative is to use Monte Carlo simple sampling to get estimates of the effective Hamiltonians, and use those to update \( p \). In this scheme, given a \( q \) at iteration \( t \), each \( x_i \) is separately set by randomly sampling \( q_i(t) \), thereby generating \( x(t) \). Next the pair \( (x(t), h_{i1}(x(t))) \) is combined with previous pairs and the update rule to set \( q_i(t+1) \), and then the process repeats.

To simplify the analysis, consider simple gradient descent of the free energy for the \( m = 1 \) team game. Have \( p \) be constant through each successive block of \( \tau \) timesteps, updating only when we go from some block \( m \) to block \( m+1 \), with the update based on observations during block \( m \). Say we have a team game and are at a block-transition, \( t = rm+1 \), and let \( n_i(t) \in n_i(t) \) be all information the algorithm controlling \( q_i \) has at that time, including the associated Monte Carlo samples. So we have a posterior conditional distribution of possible gradient descent directions \( P(\tilde{F}_H(q(t)) | n_i(t)) \), where \( F_{H}(q(t)) \) is the components involving coordinate \( i \) of the projection onto \( P \) of the free energy gradient \( \nabla F_{H,i}(q(t)) \).

In gradient descent updating, that distribution should set the vector to add to \( q_i(t) \) to get \( q_i(t+1) \). More precisely, since agent \( i \) knows \( q_i(t) \), presuming quadratic loss reflects quality of the update, the Bayes-optimal estimate of the gradient is the posterior expected gradient, \[ \int dq_i(t) P(q_i(t) | n_i(t)) \times \tilde{F}_H(q(t)) \]. Expanding, the \( x_i \) component of \( \tilde{F}_H(q) \) is \( u_i(x_i) - \sum u_i(x_i)/|\xi_i| \), where \( u_i(x_i) \equiv \beta[H_{i,q_i}(x_i) + \ln(q(x_i))] \). Rather than evaluate the integral of \( |H_{i,q_i}(\xi_i)| \), we can use a maximum likelihood estimator, i.e., replace that integral with \( (H)_{i,n_i}(\xi_i) \), the average of the observed \( H \) values over the \( \tau_{\xi_i} \) instances (of the just-completed block) when \( \xi_i = x_i \).

Unfortunately, often in very large systems the convergence of \( \langle H \rangle_{i,n_i}(\xi_i) \) is very slow, since the distribution sampled by the Monte Carlo to produce \( n_i \) is very broad. To address this, posit that the differences \( \langle H \rangle_{i,q_i}(x_i) - \langle H \rangle_{i,n_i}(x_i') \) are unchanged when \( x_i, x_i' \in \xi_i \) are when one replaces \( H \) with some \( h_i \). This means that \( q_i(t) \) is unchanged by that replacement. The set of all \( h_i \) guaranteed to have this character, regardless of the form of \( q(x_i, \xi_i) \), is the set of all difference Hamiltonians, \( h_i(\xi) = H(\xi) - D_i(\xi) \) for some function \( D_i \). Now across block \( m \) we are sampling \( P(h_i(\xi)) \) to generate \( n_i \), and then evaluating \( (h_i)_{i,n_i}(x_i) \). The associated variances of values (for each of the \( x_i \)), \( \text{Var}((h_i)_{i,n_i}(x_i)) \), govern the accuracy of the estimate of the free energy gradient. For well-chosen \( D_i \), these variances may be far smaller than when \( h_i = H \). In particular, if the number of coordinates coupled to \( \xi_i \) through \( H \) does not grow as the system does, often such difference Hamiltonian variances will not grow much with system size, whereas the variances \( \text{Var}(H_{i,n_i}(x_i)) \) will grow greatly. Furthermore, very often such a difference Hamiltonian is far easier to evaluate than is \( H \), due to cancellation in subtracting \( D_i \).

More precisely, for practical reasons we want \( i \)'s update algorithm to be robust against misperception of \( q_i \). So for quadratic loss, assuming no \( \tau_{\xi_i} = 0 \), consider the \( h_i \) minimizing \[ \int dq_i P(q_i) [\text{Var}(n_i^a, q_i, h_i) \times (\tilde{F}_H(q(x_i)) - \tilde{F}_n(q_i))^2] \], where \( P(q_i) \) reflects any prior information we might have concerning \( q_i \) (e.g., that it is likely that the associated \( \tilde{F}_H(q) \) is close to that estimated for the previous block of \( \tau \) steps). Here \( \tilde{F}_n(q_i) \) is our estimator for \( \tilde{F}_{H,n}(q) \), and \( n_i^a \) is the Hamiltonian values contained in \( n_i \), the associated \( \xi_i \) values, \( n_i^\xi_i \), being independent of \( h_i \) and \( q_i \), and therefore fixed.

The inner integral is a sum, of the (square of the) bias \( \tilde{F}^i(q_i) - \tilde{F}^i(H(q)) \) with the variance, \( \int d\bar{n}_i^a P(n_i^a | n_i^\xi_i, q_i, h_i) \times (\tilde{F}_H(q) - \tilde{F}_n(q_i))^2 \), where \( \tilde{F}_H(q) \equiv \int d\bar{n}_i^a P(n_i^a | n_i^\xi_i, q_i, h_i) \tilde{F}_H(q_i) \). By only considering difference utilities we guarantee that the bias equals 0. Now expand our variance of vectors as a sum of variances of scalars, one for each \( x_i \). Since \( n_i \) is IID generated that sum is \[ \frac{1}{\tau_{\xi_i}} \sum x_i \text{Var}((h_i)_{i,n_i}(x_i))/\tau_{x_i} \]
The difference Hamiltonian minimizing this is \( H(s) - \sum \frac{\tau_{x_i}}{\tau_{\xi_i}} H(x_i', x_i) \).
replacing the $\tau_{x_{1}}$ with $g(x_{1})\tau_{x_{1}}$. Being independent of $q_{i_{1}}$, this Hamiltonian minimizes our $q_{i_{1}}$ integral, regardless of $P(q_{i_{1}})$. For the same reason it is optimal if the integral is replaced by a worst-case bound over $q_{i_{1}}$.

An extensive series of experiments have been conducted with this optimal Hamiltonian under the approximation of uniform $q(x_{1})$, and under the approximation that $\tau_{x_{1}} = 0$ for one and only one $x_{1}$ value. These experiments compared this Hamiltonian with the team game, for many different $H$, under a variant of the parallel Brouwer update rule $\xi$ [8, 11] that crudely corrected the updating, even when that updating is done correctly. Despite these shortcomings, in the experiments in [8, 11] the result in more accurate updating with parallel Brouwer updating, since we want to raise $\beta$ to below that pre-switch value. An upper bound on the how large that drop in $F_{\xi}$ needs to be is $\max_{x_{1}} \ln(\sum_{x_{2}} \delta_{\xi_{1}}(x_{2}, x_{1}))$.

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IV. AVOIDING LOCAL MINIMA

Say we have an $m = 1$ team game, are ultimately interested in annealing $\beta$, and are currently at a local minimum $q^{H} \in \mathcal{Q}$ of the shared free energy. Then to break out of that minimum we can simply raise $\beta$ and restart the updating, since we want to raise $\beta$ anyway, and in general doing so will change the $F_{H}$ so that the Lagrange gaps become nonzero.

A way to break free without changing the free energies is to switch to a coordinate system $\xi$ for $\xi$, and thereby change $\mathcal{P}$. As an example, $\xi = \xi_{1} \xi_{2}$ can join two components of $\xi$ into an aggregate coordinate. Since we can now have statistical dependencies between those two components, the $\xi^{2}$ space product distributions map to a superset of $\mathcal{P}$. In general the local minima of that superset do not coincide with local minima of $\mathcal{P}$.

Less trivially, say $\xi^{2} = \xi$, and $\xi(\cdot)$ is the identity map for all but a few components, indicated as indices $1 \rightarrow n$. Have $\xi(\cdot)$ be a bijection, so that for any fixed $x_{n+1}^{2} = x_{n+1}^{2} - M$, the effect of the coordinate transformation is merely to “shuffle” the associated mapping taking coordinates $1 \rightarrow n$ to $\xi$. Say we have a $m = 1$ team game, and set $q_{n+1}^{\xi_{1}} = q_{n+1}^{\xi_{1}}$. This means we can estimate the expectations of $\beta H$ conditioned on possible $x_{1}^{1}$, from the Monte Carlo samples conditioned on $\xi(x_{1}^{1} \rightarrow 0)$. So for any $\xi(\cdot)$ we can estimate $E(H)$ as $\int dx_{1}^{1} \rho_{\xi_{1}}^{2}(x_{1}^{1} \rightarrow 0) E(H | \xi(x_{1}^{1} \rightarrow 0))$. Now entropy is the sum of the entropy of coordinates $n + 1 \rightarrow M$ plus that of coordinates $1 \rightarrow n$. Accordingly, for any choice of $\xi(\cdot)$ and $q_{1}^{\xi_{1} \rightarrow n}$, we can approximate $L_{\xi}^{H}$ as (our associated estimate of) $E(H)$ minus the entropy of $p_{1}^{\xi_{1} \rightarrow n}$, minus a constant unaffected by choice of $\xi(\cdot)$.

So for finite and small enough $|\xi_{1} \rightarrow n|$, we can use our estimates $E(H | \xi(x_{1}^{1} \rightarrow 0))$ to search for the “shuffling” $\xi(\cdot)$ and distribution $q_{1}^{\xi_{1} \rightarrow n}$ that minimizes $L_{\xi}^{H}$ (penalizing by the bias plus variance expression if we intend to do more Monte Carlo). The search can involve a series of free energy descents over $\xi_{1}^{\xi_{1} \rightarrow n}$ for each possible $\xi(\cdot)$, or use cruder heuristics, like having $q_{1}^{\xi_{1} \rightarrow n} = \delta_{\xi_{1} \rightarrow n}$, and only varying $\xi(\cdot)$. Not only should this coordinate transformation lower the free energy, it should also result in a new surface through $\mathcal{P}^{1}$ that is no longer at a local minimum. More generally, for arbitrary $\xi^{2}$ we can bound $F_{\xi}^{2} \geq F_{\xi_{1}}^{2} \geq F_{\xi_{1}}^{2} - \max_{x_{1}} [\ln(\sum_{x_{2}} \delta_{\xi_{1}}(x_{2}, x_{1}))]$ (and similarly for uncountable $\xi^{2}$). So if after switching to $\xi^{2}$ we can then reduce $F_{\xi_{1}}^{2}$ to less than the value $F_{\xi_{1}}^{2}$ had when we made the switch, then we know we have also reduced $F_{\xi_{1}}^{2}$ to below that pre-switch value. An upper bound on the how large that drop in $F_{\xi_{1}}^{2}$ needs to be is $\max_{x_{1}} [\ln(\sum_{x_{2}} \delta_{\xi_{1}}(x_{2}, x_{1}))]$.

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