A view of Estimation of Distribution Algorithms through the lens of Expectation-Maximization

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Abstract

We show that under mild conditions, Estimation of Distribution Algorithms (EDAs) can be written as variational Expectation-Maximization (EM) that uses a mixture of weighted particles as the approximate posterior. In the infinite particle limit, EDAs can be viewed as exact EM. Because EM sits on a rigorous statistical foundation and has been thoroughly analyzed, this connection provides a coherent framework with which to reason about EDAs. Importantly, the connection also suggests avenues for possible improvements to EDAs owing to our ability to leverage general statistical tools and generalizations of EM. For example, we make use of results about known EM convergence properties to propose an adaptive, hybrid EDA-gradient descent algorithm; this hybrid demonstrates better performance than either component of the hybrid on several canonical, non-convex test functions. We also demonstrate empirically that although one might hypothesize that reducing the variational gap could prove useful, it actually degrades performance of EDAs. Finally, we show that the connection between EM and EDAs provides us with a new perspective on why EDAs are performing approximate natural gradient descent.

1 Model-based optimization

Many practical problems of interest can be cast as optimizing a function $f : \mathcal{Z} \rightarrow \mathbb{R}$ over a space of discrete or continuous inputs, $\mathcal{Z}$. The solution to this problem is given by $z^* = \arg\max_{z \in \mathcal{Z}} f(z)$. In many settings, such as reinforcement learning [1], protein and molecule design [2], black-box optimization [3], Bayesian optimization [4] and combinatorial optimization [5][6], this optimization problem is transformed into the related problem, $\theta^* = \arg\max_{\theta} \mathbb{E}_{p(z|\theta)}[f(z)]$, where $p(z|\theta)$ is a probability density over $\mathcal{Z}$, parameterized by $\theta \in \mathbb{R}^D$, for $D$ parameters. That is, the search over $\mathcal{Z}$
is replaced by a search over a parameterized family of distributions on $Z$. Herein we refer to this as model-based optimization (MBO). When $p(z|\theta)$ has the capacity to represent a point mass centered on $z^*$, then these two formulations have the same objective values at their respective optima. Reasons for using the MBO formulation include the desire to obtain a set of good candidates rather than a single candidate [2], enabling of rigorous analysis of associated optimization algorithms [5], and the leveraging of probabilistic formulation to incorporate auxiliary information [2].

**Estimation of Distribution Algorithms** A common approach to solving the MBO objective is with a class of iterative algorithms known as Estimation of Distribution Algorithms (EDAs) [3,7], of which the Covariance Matrix Adaptation Evolution Strategy (CMA-ES) [3,9] and Cross Entropy Method (CEM) [10] are perhaps the most well-known. The general template for an EDA is as follows. Beginning with an initial parameter setting, $\theta^{(0)}$, of the “search model”, $p(z|\theta)$, an EDA algorithm generally proceeds in three steps at each iteration $t = 0, 1, 2, ...$:

1. Draw $N$ samples, $\{z_i\}_{i=1}^N$, from $p(z|\theta^{(t)})$.
2. Evaluate $f(z_i)$ for each $z_i$.
3. Find a $\theta^{(t+1)}$ that uses the samples and corresponding function evaluations to move $p(z|\theta)$ towards regions of $Z$ that have large function values.

The final step can be performed in a variety of ways, but is typically done by solving

$$\theta^{(t+1)} = \arg\max_\theta \sum_{i=1}^N f(z_i) \log p(z_i|\theta),$$  \hspace{1cm} (1)

which is simply a weighted maximum likelihood problem with weights, $f(z_i)$.

In some variations of EDAs, $f(z)$ is transformed monotonically through a shaping function [11–13], which alters convergence properties but does not change the optima.

An important aspect of any EDA is the choice of search model. Many EDAs use exponential family models, most commonly the multivariate Gaussian used in CMA-ES. However, Bayesian networks [14], Boltzmann machines [15,16], Markov Random Fields [17], Variational Autoencoder [2], and others [18] have also been used. The choice of search model is driven by prior knowledge and empirics. Variants of some EDAs include re-using samples from previous iterations, and/or smoothing of the parameter estimates across iterations [2,8,19]; however, for clarity of exposition, we do not consider these variations.

**Our contributions** We (i) show that under mild conditions EDAs can be viewed as variational Expectation-Maximization (EM) [20] with an approximate posterior given by a set of weighted particles (i.e., a mixture of delta functions); and, as exact EM in the limit of infinite particles [21], (ii) derive insights from this viewpoint that suggest an improved adaptive hybrid EDA-gradient descent approach, and show that it demonstrates superior performance than either of its component algorithms; we also show empirically that reducing the variational gap is not helpful and likely harmful, and (iii) show that the equivalence between EM and EDAs provides a new perspective on why EDAs can be seen to be performing approximate natural gradient descent.

2 Related Work

The Information Geometry Optimization (IGO) [19] framework encompasses a large class of MBO approaches by discretizing a natural gradient flow. Instantiations of IGO are most readily seen as tantamount to using the “log derivative trick” on the MBO objective, combined with natural gradient, as in Natural Evolution Strategies [11,12]. However, Ollivier et al. use the IGO framework to unify numerous approaches for tackling MBOs, including EDAs such as CEM [10] and CMA-ES [8]. The IGO framework does not make use of EM in achieving its unification, directly or otherwise; therefore, IGO provides a complementary viewpoint to that presented herein.

Staines et al. introduce the notion of variational optimization to tackle MBOs by considering the MBO formulation of the original optimization problem as an upper bound to be minimized; they clearly delineate when the bound can be satiated, sufficient conditions for it to be convex, and for when the derivative of the MBO objective exists [22]. However, they do not connect to the EDA literature.
In the reinforcement learning (RL) community, EM has been used to explain why the Relative Payoff Procedure is guaranteed, in some circumstances, to improve at each iteration [23]. Wierstra et al. directly use EM with heuristic add-ons such as a “forget factor” to optimize an MBO objective with a Gaussian density [24]. The relationship between parameter-based policy search and Expectation-Maximization is also discussed in [25][26]. These papers are focused on problems in RL and do not make connections to the EDA literature.

Finally, parenthetically, EM is used inside of the model fitting part of evolutionary algorithms for binary latent variables in [27], which is conceptually orthogonal to our contributions.

In contrast to these works, we provide an exposition of how a broad class of EDAs can be viewed as EM, from which we derive insights that yield a promising new EDA approach.

3 Connection between EDAs, EM and gradient descent

First we review the Free Energy viewpoint of EM. On that basis, we then describe the connection between EM and EDAs before concluding the section with an exposition of how EM connects to gradient-based optimization.

3.1 Expectation-Maximization (EM)

EM is a method for performing maximum likelihood parameter estimation in latent variable models that exploits the structure of the joint likelihood between latent and observed variables. Intuitively, each E-step imputes the latent variables, and the subsequent M-step then uses these “filled in” data to do standard maximum likelihood, typically in closed form. EM iterates between these E- and M-steps until convergence. We use the Free Energy interpretation of EM and its accompanying generalizations [28] in order to most easily connect EDAs to EM.

Let \( y \) and \( z \) be respectively observed and latent variables. The task of maximum likelihood is to find \( \phi = \arg \max_{\phi} \log L(\phi) \) where \( \log L(\phi) = \log p(y|\phi) = \log \int p(y, z|\phi)dz \), for some model density \( p \) parameterized by \( \phi \). In [28], the authors define a function known as the free energy, given by:

\[
F(q, \phi) = \mathbb{E}_{q(z)}[\log p(y, z|\phi)] + H(q),
\]

where \( q(z) \) is any density over the latent variables and \( H(q) \) is the entropy of \( q \). The free energy lower bounds the log-likelihood, \( \log L(\phi) \geq F(q, \phi) \), and this bound is satisfied only when \( q(z) = p(z|y, \phi) \). If the posterior cannot be obtained exactly (e.g., analytically), one may approximate it to get a variational EM algorithm [20]. The variational posterior can be either a parameterized variational family, \( q(z|\psi) \), or an implicit one based on a set of samples as in Monte Carlo EM [29][30]. The sample-based posterior takes the form, \( q(z) = \frac{1}{N} \sum_i \delta_{z_i}(z) \) with \( z_i \) drawn from \( p(z|y, \phi) \).

In variational EM, typically the bound cannot be satisfied, leading to a variational gap given by \( D_{KL}(q(z)||p(z|y, \phi)) \), where \( D_{KL} \) denotes the KL divergence—equal to zero if and only if \( q \) is equal to the posterior \( p(z|y, \phi^{(t)}) \).

EM and variational EM can both be viewed as alternating coordinate descent on the free energy function. The alternating updates at iteration \( t \) are given by:

- **E-step:** \( q^{(t+1)} = \arg \max_q F(q, \phi^{(t)}) \). It can be shown that this is equivalent to minimizing the variational gap by solving \( q^{(t+1)}(z) = \arg \min_q D_{KL}(q(z)||p(z|y, \phi^{(t)})). \) This is where EM intuitively imputes the “missing” data, \( \{z_i\} \).

- **M-step:** \( \phi^{(t+1)} = \arg \max_{\phi} F(q^{(t+1)}, \phi) = \arg \max_{\phi} \mathbb{E}_{q^{(t+1)}(z)}[\log p(y, z|\phi)] \), which is tantamount to doing weighted maximum likelihood of \( p(y, z|\phi) \) with weights \( q^{(t+1)} \).

When the variational gap can be driven to zero, as in exact EM, this procedure is guaranteed to never decrease the likelihood. Moreover, its convergence properties, to both local and global minima, have been carefully studied (e.g., [21][28][31]). Rigorous generalizations of variational and exact EM to partial E- and M-steps also emerge naturally from this viewpoint [28].
3.2 Estimation of Distribution Algorithms as variational Expectation-Maximization

As described in the introduction, EDAs seek to solve the MBO objective,

\[
\theta^{t+1} = \arg\max_{\theta} \mathbb{E}_{q^{t+1}(z)} \left[ \log p(z | \theta) \right] + \mathbb{E}_{q^{t+1}(z)} \left[ \log f(z) \right]
\]

where \( f(z) \) is the function to be optimized, \( p(z | \theta) \) is what we refer to as the \textit{search model}, parameterized by \( \theta \), and we define \( L_{EDA}(\theta) \equiv \log \mathbb{E}_{q(z)} [f(z)] \)—which can be thought of as an EDA ‘log marginal likelihood’.

Note that it is common in EDAs to monotonically transform \( f(z) \) with a shaping function, \( W(\cdot) \), which may be, for example, a cumulative density function (CDF) \cite{2}, an exponential \cite{1}, or a quantile-based transformation \cite{10,19}. Although this transformation does not change the optima, it may alter the optimization dynamics. Often this shaping function is changed at each iteration in a sample-dependent, adaptive manner (which links these methods to annealed versions of EM and VI \cite{22,33}). In such a setting, the connection that we will show between EDA and EM holds within each full iteration, and the insights derived from this connection have bearing on the entire algorithm. For notational simplicity, we drop the \( W(\cdot) \) and assume that \( f(z) \) has already been transformed.

To link \cite{3} to EM, we introduce a density, \( q(z) \), which allows us to derive a lower bound on \( L_{EDA}(\theta) \) using Jensen’s inequality:

\[
L_{EDA}(\theta) = \log \mathbb{E}_{p(z | \theta)} [f(z)]
\]

\[
= \log \mathbb{E}_{q(z)} \left[ \frac{p(z | \theta) f(z)}{q(z)} \right]
\]

\[
\geq \mathbb{E}_{q(z)} \left[ \log p(z | \theta) f(z) \right] + H(q)
\]

\[
= F(q, \theta),
\]

where \( F \) is the same free energy function appearing in the previous section on EM, except that the complete likelihood is replaced with the term \( f(z)p(z | \theta) \). When \( f(z)p(z | \theta) \) is normalizable, then it can be shown that \( F(q, \theta) - L_{EDA}(\theta) = -D_{KL}(q(z) || \tilde{p}(z | \theta)) \), where we define the ‘tilted density’

\[
\tilde{p}(z | \theta) = \frac{p(z | \theta) f(z)}{\int_Z p(z | \theta) f(z) dz},
\]

which is the EDA counterpart to the exact posterior in EM. We can now construct a coordinate ascent algorithm on the free energy defined in \cite{6} that mirrors the EM algorithm. In particular, this algorithm iterates between E-steps that solve \( q^{t+1}(z) = \arg\min_q D_{KL}(q(z) || \tilde{p}(z | \theta^{t+1})) \), and M-steps that solve \( \theta^{t+1} = \arg\max_{\theta} \mathbb{E}_{q^{t+1}(z)} \left[ \log p(z | \theta) f(z) \right] \). To make the precise connection between practically implemented EDA and EM, we introduce a particular approximate posterior for the E-step that is given by a mixture of weighted particles:

\[
q^{t+1}(z) = \sum_{i=1}^{N} \frac{f(z_i) \delta_{z_i}(z)}{\sum_{i=1}^{N} f(z_i)},
\]

where \( \{z_i\}_{i=1}^{N} \) are samples drawn from \( p(z | \theta^{t+1}) \), as in EDAs. Using this posterior approximation, the M-step amounts to solving the objective:

\[
\theta^{t+1} = \arg\max_{\theta} \mathbb{E}_{q^{t+1}(z)} \left[ \log p(z | \theta) \right] + \mathbb{E}_{q^{t+1}(z)} \left[ \log f(z) \right]
\]

\[
= \arg\max_{\theta} \int_Z q^{t+1}(z) \log p(z | \theta) dz
\]

\[
= \arg\max_{\theta} \frac{1}{\sum_{i=1}^{N} f(z_i)} \sum_{i=1}^{N} \int_Z f(z_i) \delta_{z_i}(z) \log p(z | \theta) dz
\]

\[
= \arg\max_{\theta} \sum_{i=1}^{N} f(z_i) \log p(z_i | \theta),
\]

which is exactly the final step in one iteration of EDA \cite{1}. Therefore, we can view EDA as an EM algorithm that uses the particle-based posterior approximation given by \cite{9}. In the limit of infinite
particles we trivially obtain \( \lim_{N \to \infty} q^{(t+1)}(z) = \tilde{p}(z|\theta^{(t)}) \) by the Law of Large Numbers. In this limit, the approximate posterior exactly matches the tilted distribution—the EDA “exact posterior”—and our algorithm inherits the same guarantee as exact EM, such as guaranteed improvement of the objective function at each iteration, as well as local and global convergence properties [28, 31, 34].

In the finite sample case of EDAs we are not performing exact EM. Instead, we are performing a “weak” form of variational EM—we say weak because typically in a variational setting, one would minimize the KL-divergence between the approximate posterior and the true posterior within the variational class, which is not done in EDAs. A “stronger” variational EDA EM would entail finding the \( N \) weighted particles in the approximate posterior that minimizes the variational gap—a generally intractable problem, but one that we explore in Section 5.

From this exposition it’s also interesting to note that EDA can be seen as performing Importance Sampling [35] with proposal distribution, \( p(z|\theta^{(t)}) \), (sampled in the E-step), and then using importance weights \( p(z|\theta)f(z)/p(z|\theta) = f(z) \) in the posterior-averaged “complete log likelihood”, \( \mathbb{E}_{q^{(t+1)}(z)} [\log(p(z|\theta)f(z))] \), in the M-step, to correct for the fact that these samples were not taken form the exact posterior.

### 3.3 Connection to gradient-based methods

Instead of using EDAs, one could alternatively solve the MBO objective directly with gradient descent (or natural gradient descent) where updates are given by \( \theta^{(t+1)} = \theta^{(t)} + \alpha(\nabla L_{EDA})(\theta^{(t)}) \), and \( \alpha \) is a step size parameter. This is known as REINFORCE [36] in the RL community and is related to IGO-ML [19]. Typically, one cannot compute the gradient term exactly, in which case the “log derivative trick”, \( \nabla_{\theta} \mathbb{E}_{p(z|\theta)}[f(z)] |_{\theta=\theta^{(t)}} = \mathbb{E}_{p(z|\theta^{(t)})}[f(z)\nabla_{\theta} \log p(z|\theta)|_{\theta=\theta^{(t)}}] \) (which, notably, does not require the gradient of \( f(z) \) [37]) is often is often combined with Monte Carlo estimation to arrive at an update:

\[
\theta^{(t+1)} = \theta^{(t)} + \alpha \sum_{i=1}^{N} f(z_i)\nabla_{\theta} \log p(z_i|\theta)|_{\theta=\theta^{(t)}}, \tag{14}
\]

where \( \{ z_i \} \) are samples drawn from \( p(z|\theta^{(t)}) \).

We can connect the gradient based optimization in (14) to the EDA “EM” optimization presented in Section 3.2. In particular, consider the partial M-step version of EM, where instead of fully solving for the new parameter, one instead performs one gradient step [28, 31]—so called “first-order” EM. Instantiating first-order EM into EDA “EM” by partially solving the objective in (13) with a single gradient step (with step size \( \alpha \) ) will result in the same update as (14). In other words, performing “first-order” EM in the EDA context is identical to performing gradient descent on the original MBO objective. In our experiments, we refer to “first-order” EM for EDAs as \( SGD \). It’s interesting to note that as one performs more gradient steps within an M-step, one traces out a continuum of methods between gradient descent on the original objective, and EM.

In the next section we describe how we leverage the viewpoint of EDAs as EM to propose a new algorithm with promising results.

### 4 An adaptive, hybrid EDA-gradient algorithm

It is well-known that EM can exhibit super-linear convergence behaviour near a local optimum and in plateau regions, but can exhibit extremely slow convergence rates otherwise—in regions where gradient-based methods can do better [34, 38]. In order to get the best of both worlds Salakhutdinov et al. leverage a precise analysis of EM, including how to diagnose in an on-line, data-driven manner when EM is likely to be in a poor convergence phase. The technically correct diagnostic to achieve this requires difficult computations of the derivatives of the EM “mapping matrix” (the implicit matrix that maps \( \theta^{(t)} \rightarrow \theta^{(t+1)} \)); instead, they propose to use the entropy of the posterior as a proxy to this quantity, using the intuition that both quantities inform on how much “information” EM has about the latent variables at any given point in the algorithm. This intuition follows from a technical condition that holds when, for example, the expected complete log likelihood of the M-step has a single optimum, such as for (mixtures of) Gaussians, (mixtures of) Factor Analysis, HMMs, and probabilistic (mixtures of) Principle Components Analysis [34]. For the gradient-based method, they
Figure 1: One run of each of (a) EDA, (b) SGD, and (c) Hybrid over 5000 iterations, on a two-dimensional Rastrigin function (global minimum at zero). To keep the plots uncluttered, only the first 1000 iterations are shown, which are representative. The summary of results in (d) shows the minimum value achieved by each of SGD and Hybrid over all iterations, with the hybrid showing a clear win. EDA is not shown in this plot because its values are orders of magnitude worse—see panel a)—and would make the differences between SGD and Hybrid difficult to see. Overall, the hybrid approach achieves better optima.

use conjugate gradient descent (CGD) with a line search; they find that the hybrid method never does worse, and often performs better than both standard EM and SGD.

On this basis, we explore an analogous adaptive, hybrid EDA-gradient approach, although we use the SGD updates described in [14] without a line search, instead using AdaGrad [39] to control the learning rate; we do so in the hopes of better understanding the source of differences in performance—differences that do not depend on a line search. Our hybrid, denoted Hybrid, therefore switches between (i) standard EDA [13] which we denote EDA, and (ii) a gradient-based approach [14] which we denote SGD (we augment this by using natural gradients). As in [34], we switch from SGD to EDA when the estimated posterior entropy is above a specified cutoff, $\tau$, and vice versa.

4.1 Experiments

We compared our Hybrid method to the pure EDA and SGD algorithms, in the minimization of 2- and 20- dimensional Rastrigin and Ackley functions—canonical multi-modal, non-convex functions commonly used to benchmark optimization approaches [8].

We used a Gaussian search model with diagonal covariance matrix and $N = 100$ particles at each iteration. Each algorithm had a fixed budget of 50,000 function evaluations (which amounts to a maximum of 5,000 EM iterations). Crucially, as in [12], each algorithms was allowed to randomly restart after convergence until such time as the function budget was used up because this ties in to practical use cases. Convergence was determined to be the point at which $\sqrt{\frac{\operatorname{det}(\Sigma)}{d}} < 0.001$, where $\Sigma$ is the covariance matrix of the search model and $d$ is the dimensionality of the search space. Restarts were randomly initialized with particles drawn from a Gaussian with unit variance and mean randomly positioned on the hypersphere of radius $r$ centered at the global minimum (the origin)—the larger $r$, the further the initialization is from the global optimum. The radius, $r$, was set to 20 and 30 for the Rastrigin and Ackley functions, respectively, to make the optimizations sufficiently difficult.
such that none of the methods tended to reach the global minimum—this, allowed us to better distinguish the relative performance of methods, whose ordering was not sensitive this setting.

As in [8, 10, 12, 19], we used an adaptive shaping function, $W(\cdot)$, to monotonically transform the function values $f(z)$. In particular, we use a sigmoid weighting function given by

$$W_{\theta(t)}(f(z)) = \frac{1}{1 + \exp\left(\frac{f(z) - \mu_t}{\sigma_t^2}\right)} - 1,$$

where $\mu_t = \mathbb{E}_{p(z|\theta(t))}[f(z)]$ and $\sigma_t^2 = \text{Var}_{p(z|\theta(t))}[f(z)]$ were estimated from samples at each iteration. This sigmoid shaping function is much like the CDF used in [2], but is differentiable which was useful for Section 5.

We approximated the entropy of our approximate posterior, a collection of weighted particles, by using the entropy of the search model itself, which can be shown to be

$$H_t = \frac{1}{2} \log(\det(2\pi e \Sigma)).$$

We found that this quantity tends to lie in the range $[-d, d]$ during the course of the optimizations, and therefore chose $\tau = 0$ as the entropy cutoff, $\tau$, for switching in Hybrid. Even in the case where it is not a priori obvious how to set the $\tau$, this hyper-parameter can readily be set for new problems based on empirics from a few sample runs.

As shown in Figures 1 and 2, EDA converges very quickly, but to poor local minima. In constrast, SGD converges very slowly, but to better local minima. Hybrid effectively balances these two extremes by converging to similar local optima as SGD, but much more quickly. This allows Hybrid to more effectively use its iteration budget by restarting more often, and consequently finding lower values of $f(z)$ (Figure 1d, 2). For this reason, on a practical use case with limited budget, one would expect Hybrid on average to obtain better optima then either SGD or EDA.

As an aside, we note that EM implicitly sets its own step-size. However, in [40], using an “overrelaxed bound optimization” technique, an adaptive step size is used instead of the implicit one. The authors demonstrate that this provides faster convergence. We tried using such an approach for EDAs, and indeed, found it converged more quickly, but to worse local optima, and did not pursue this avenue further.

In summary: we leveraged our insights about EDA viewed as EM to propose an adaptive, hybrid EDA-SGD method that demonstrates better performance than either of its component methods on several canonical test functions in both low and high dimensions.

### 5 Decreasing the EDA variational gap is not helpful

As shown in Section 3.2, EDA is doing a “weak” form of variational EM—“weak” in the sense that it is not actually optimizing the variational family. This suggests a possible improvement to EDA where the $N$ weighted particles used in the approximate posterior (9) are adjusted to reduce the variational gap. We explored this possibility by using Stein Variational Gradient Descent (SVGD) [41] to iteratively propagate particles such that collectively they better approximate the specified target distribution—in this case, the EDA “exact posterior” (8). Although rigorously derived, intuitively, SVGD pushes the $i^{th}$ particle in the direction of the gradient of $\log \tilde{p}(z_i|\theta)$ with respect to $z_i$, while maintaining a repulsive force between the particles to ensure diversity. SVGD depends on the choice of a kernel, for which we used a Radial Basis Function (RBF) kernel with length-scale parameter chosen as suggested in [41]. Additionally, to keep the method black-box, we used a finite difference
Figure 3: EDA with SVGD updates to minimize the Rastrigin function (a) in two dimensions, and (b) in 20 dimensions. Bars represent the value of $f(z)$ at convergence, averaged over 100 optimizations, with error bars representing the corresponding standard deviation. Note that the function value at the global minimum is zero. As more and more SVGD updates are performed at each E-step (horizontal axis), the variational gap is reduced; however, the value of the objective function we are minimizing gets correspondingly worse. Degraded performance owing to SVGD is worse in higher dimensions.

for the gradient of $\log f(z_i)$ (required for (8)) after verifying that it recapitulated the analytical gradient, although there are entirely gradient-free SVGD approaches emerging [42].

In order to test the potential utility of reducing the variational gap in EDA, we used an increasing number of SVGD updates in the E-step of EDA during minimizations of the Rastrigin function. We use the same experimental setup described in the previous section but without a function evaluation budget, such that for each setting, $M$, of the number of SVGD updates, we ran exactly 100 optimizations to convergence. Removing the evaluation budget allows us to clearly determine if decreasing the variational gap is helpful—if it is, then one should compare it to other approaches with a function budget experimental set-up. Here we used $r = 10$ to best expose differences between the varying number of SVGD updates, but our conclusions are not sensitive to this setting. As shown in Figure 3, as we decrease the variational gap by using an increasing number of SVGD updates, performance tends to degrade.

Although it has conventionally been deemed beneficial to reduce the variational gap—indeed, this is precisely what is done in variational inference—results are emerging that suggest it is not always advantageous to do so. For example, in [43], reducing the variational gap in VAEs is shown to be potentially harmful. Similarly, our results show that using SVGD in the E-step of EDAs yields worse performance. However, we speculate that the reason for this may be quite different than in [43]. We speculate that SVGD within EDA may degrade performance because it more quickly converges to ‘closest’ local optimum, rather than more thoroughly exploring the landscape. In other words, in MBO, the existence of a variational gap may induce better exploration, similarly to how stochasticity in SGD may be doing so, although this latter point itself remains in debate [44].

In summary: We showed that decreasing the EDA ‘variational gap’, by way of Stein Variational gradient descent, in the EDA ‘E-step’, tends to degrade the performance of EDAs.

6 Relationship of EDAs to natural gradient descent by way of EM

Akimoto et al. showed that CMA-ES, a particular EDA, can be viewed as approximate natural gradient descent (NGD) [45]. This result also emerges from the IGO framework of Ollivier et al. [19] who additionally show that CEM and several other EDAs can be viewed as NGD. Malago et al. show how EDAs using MRF for the search model can be interpreted as performing NGD [46].

One might wonder whether using the relationship between EDA and EM might provide a different perspective on these connections. Indeed, it turns out that Chrétien and Hero showed that EM can be formulated as an optimization method known as the proximal point method (PPM)—in particular they showed that EM is using the PPM with the reverse KL divergence to maximize the log-likelihood.
We have shown an explicit connection between Estimation of Distribution Algorithms and Expectation-Maximization. From this mapping we leveraged insights that yielded a promising new approach, a hybrid EDA-gradient method, which may have implications in numerous fields, such as RL, where one or the other approach are used, but to the best of our knowledge, never both. For example, REINFORCE type algorithms are gradient-based \cite{36}, while Reward Reweighted Regression type algorithms are EDA-based \cite{1}. Furthermore, we anticipate that the connection between EDAs and EM may spur further improvements.

In light of EDAs as EM, one can ask whether this viewpoint sheds any light on the choice of EDA search models. Suppose for a moment that rather than a sample-based approximate posterior, one instead used a parametric posterior, as in standard VI. In such a case, when the search model were in

\textbf{7 Discussion}

We have shown an explicit connection between Estimation of Distribution Algorithms and Expectation-Maximization. From this mapping we leveraged insights that yielded a promising new approach, a hybrid EDA-gradient method, which may have implications in numerous fields, such as RL, where one or the other approach are used, but to the best of our knowledge, never both. For example, REINFORCE type algorithms are gradient-based \cite{36}, while Reward Reweighted Regression type algorithms are EDA-based \cite{1}. Furthermore, we anticipate that the connection between EDAs and EM may spur further improvements.

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\textbf{In summary:} EM is a PPM with KL divergence; linearization of the EM PPM is mirror descent; a second order approximation of the KL divergence in mirror descent yields NGD. Thus in the infinite sample limit of EDAs, they can be seen as approximate NGD.

A result related to that of EM performing approximate NGD has previously been shown. Specifically, Sato, and later others, showed that for exponential family models with hidden variables and a conjugate prior (to the joint observed and hidden model), that classical (non-amortized) mean-field variational inference is performing NGD \cite{51}–\cite{53}. In contrast, the result we describe is for any exact EM, and is only approximate NGD.

On a separate note, Salimbeni \textit{et al}. demonstrate empirically that the best step size in NGD (according to a Brent line search to find the best step size at each iteration) increases over iterations to 1.0, for Gaussian approximations to several models \cite{54}. This result nicely aligns with the fact shown herein that that EM implicitly sets its own step size, and that EM, viewed as approximate NGD, has a step size of precisely 1.0.

\textbf{In summary:} EM is a PPM with KL divergence; linearization of the EM PPM is mirror descent; a second order approximation of the KL divergence in mirror descent yields NGD. Thus in the infinite sample limit of EDAs, they can be seen as approximate NGD.

As noted in \cite{49}, mirror descent is a linearization of the PPM. In the case of relevance here—a PPM with a KL-divergence—the mirror descent update is

\[ \phi^{(t+1)} = \text{argmax}_\phi \log L(\phi) - D_{KL}(p(z|y, \phi^{(t)})||p(z|y, \phi)) \]

If one uses a second-order Taylor series approximation to the KL divergence, then the resulting approximate mirror descent update is precisely NGD. In particular, the second order approximation is given by

\[ D_{KL}(p(z|y, \phi^{(t)})||p(z|y, \phi)) = \frac{1}{2} (\phi - \phi^{(t)})^\top I(\phi^{(t)}) (\phi - \phi^{(t)}) + O((\phi - \phi^{(t)})^3), \]

where \( I \) is the Fisher information metric \cite{50}. When the KL divergence in mirror descent is replaced with its approximation, we obtain

\[ \phi^{(t+1)} = \text{argmax}_\phi \log L(\phi^{(t)}) + \langle \nabla_\phi \log L(\phi) \rangle_{\phi=\phi^{(t)}} + (\phi - \phi^{(t)})^\top I(\phi^{(t)}) (\phi - \phi^{(t)}), \]

which can be shown to be equivalent to (see Supplementary Information) the standard NGD update rule

\[ \phi^{(t+1)} = \phi^{(t)} + I(\phi^{(t)})^{-1} \nabla_\phi \log L(\phi) \mid_{\phi=\phi^{(t)}}. \]
some sense “conjugate” to \( f(z) \), then the posterior could take on an analytical form. When might such an approach make sense? Suppose one were using EDAs to perform protein design \([2]\), and that \( f(z) \) represented protein stability, and that it could be approximated by using an exponential model of linear additive marginal and pairwise terms. Then if one used a Potts model \([55]\) as the search model, the exact posterior could also be written in this form, and a “parametric” EDA could be pursued.

EDAs are often improved by smoothing, such as exponentially decaying averaging of previous updates, or model-specific schemes such as in CMA-ES \([8]\). We did not employ such smoothing here, but expect that doing so would not alter the message of our paper.

Given the tight connection between EDAs with adaptive shape functions, and annealed versions of EM and VI \([32,33]\), we believe that these latter approaches could benefit from the simple and robust implicit annealing schemes found in the EDA literature, which arise not from an annealing schedule, but from simple quantile transformations and the like.

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References

[1] Jan Peters and Stefan Schaal. Reinforcement learning by reward-weighted regression for operational space control. In Proceedings of the 24th International Conference on Machine Learning, ICML ’07, pages 745–750, New York, NY, USA, 2007. ACM.

[2] David Brookes, Hahnbeom Park, and Jennifer Listgarten. Conditioning by adaptive sampling for robust design. In Proceedings, Intl. Conf. on Machine Learning (ICML), 2019.

[3] Endika Bengoetxea, Pedro Larrañaga, Isabelle Bloch, and Aymeric Perchant. Estimation of distribution algorithms: A new evolutionary computation approach for graph matching problems. In Mário Figueiredo, Josiane Zerubia, and Anil K. Jain, editors, Energy Minimization Methods in Computer Vision and Pattern Recognition, pages 454–469, Berlin, Heidelberg, 2001. Springer Berlin Heidelberg.

[4] James T. Wilson, Frank Hutter, and Marc Peter Deisenroth. Maximizing acquisition functions for Bayesian optimization. Technical report, 2018.

[5] Mark Zlochin, Mauro Birattari, Nicolas Meuleau, and Marco Dorigo. Model-based search for combinatorial optimization: A critical survey. Annals of Operations Research, 131(1-4):373–395, 2004.

[6] Horia Mania, Aurelia Guy, and Benjamin Recht. Simple random search provides a competitive approach to reinforcement learning. arXiv preprint arXiv:1803.07055, 2018.

[7] Shumeet Baluja and Rich Caruana. Removing the genetics from the standard genetic algorithm. In Armand Prieditis and Stuart Russell, editors, Machine Learning Proceedings 1995, pages 38–46. Morgan Kaufmann, San Francisco (CA), 1995.

[8] Nikolaus Hansen and Andreas Ostermeier. Completely derandomized self-adaptation in evolution strategies. Evol. Comput., 9(2):159–195, June 2001.

[9] Freek Stulp and Olivier Sigaud. Path integral policy improvement with covariance matrix adaptation. In Proceedings of the 29th International Conference on International Conference on Machine Learning, ICML’12, pages 1547–1554, USA, 2012. Omnipress.

[10] Reuven Rubinstein and William Davidson. The Cross-Entropy Method for Combinatorial and Continuous Optimization. Methodol. Comput. Appl. Probab., 1:127–190, 1999.

[11] D. Wierstra, T. Schaul, J. Peters, and J. Schmidhuber. Natural evolution strategies. In 2008 IEEE Congress on Evolutionary Computation (IEEE World Congress on Computational Intelligence), pages 3381–3387, June 2008.

[12] Daan Wierstra, Tom Schaul, Tobias Glasmachers, Yi Sun, Jan Peters, and Jürgen Schmidhuber. Natural evolution strategies. Journal of Machine Learning Research, 15:949–980, 2014.

[13] Sun Yi, Daan Wierstra, Tom Schaul, and Jürgen Schmidhuber. Stochastic search using the natural gradient. In Proceedings of the 26th Annual International Conference on Machine Learning, ICML ’09, pages 1161–1168, New York, NY, USA, 2009. ACM.
[14] J. Ocenasek and J. Schwarz. Estimation of distribution algorithm for mixed continuous-discrete optimization problems. In Proceedings of the 29th International Conference on International Conference on Machine Learning, Slovakia, 2012. IOS Press.

[15] Jiaqiao Hu and Ping Hu. Annealing adaptive search, cross-entropy, and stochastic approximation in global optimization. Naval Research Logistics (NRL), 58(5):457–477, aug 2011.

[16] V. A. Shim, K. C. Tan, J. Y. Chia, and A. Al Mamun. Multi-objective optimization with estimation of distribution algorithm in a noisy environment. Evolutionary Computation, 21(1):149–177, March 2013.

[17] Siddhartha Shakya and John McCall. Optimization by estimation of distribution with deum framework based on markov random fields. International Journal of Automation and Computing, 4(3):262–272, Jul 2007.

[18] Stefan Kern, Sybille D. Müller, Nikolaus Hansen, Dirk Büche, Jiri Ocenasek, and Petros Koumoutsakos. Learning probability distributions in continuous evolutionary algorithms – a comparative review. Natural Computing, 3(1):77–112, Mar 2004.

[19] Yann Ollivier, Ludovic Arnold, Anne Auger, and Nikolaus Hansen. Information-Geometric Optimization Algorithms: A Unifying Picture via Invariance Principles. Technical report, 2017.

[20] Matthew J Beal. Variational Algorithms for Approximate Bayesian Inference. PhD thesis, 1998.

[21] A. P. Dempster, N. M. Laird, and D. B. Rubin. Maximum likelihood from incomplete data via the em algorithm. Journal of the Royal Statistical Society, Series B, 39(1):1–38, 1977.

[22] J Staines and D Barber. Optimization by variational bounding. In European Symposium on ANNs, 2013.

[23] Peter Dayan and Geoffrey E. Hinton. Using expectation-maximization for reinforcement learning. Neural Comput., 9(2):271–278, February 1997.

[24] D. Wierstra, T. Schaul, J. Peters, and J. Schmidhuber. Fitness expectation maximization. In PPSN 2008, pages 337–346, Berlin, Germany, September 2008. Max-Planck-Gesellschaft, Springer.

[25] Thomas Furmston, Guy Lever, and David Barber. Approximate newton methods for policy search in markov decision processes. Journal of Machine Learning Research, 17:227:1–227:51, 2016.

[26] Jens Kober and Jan R. Peters. Policy search for motor primitives in robotics. In D. Koller, D. Schuurmans, Y. Bengio, and L. Bottou, editors, Advances in Neural Information Processing Systems 21, pages 849–856. Curran Associates, Inc., 2009.

[27] Enrico Guiraud, Jakob Drefs, and Jörg Lücke. Evolutionary expectation maximization. In Proc. Genet. Evol. Comput. Conf. - GECCO ’18, pages 442–449, New York, New York, USA, 2018. ACM Press.

[28] Radford M. Neal and Geoffrey E. Hinton. A View of the EM Algorithm that Justifies Incremental, Sparse, and other Variants. pages 355–368, 2012.

[29] Brian S Caffo, Wolfgang Jank, and Galin L. Jones. Ascent-based monte carlo expectation-maximization. Journal of the Royal Statistical Society. Series B: Statistical Methodology, 67(2):235–251, 2005.

[30] Gersende Fort and Eric Moulines. Convergence of the monte carlo expectation maximization for curved exponential families. Ann. Statist., 31(4):1220–1259, 08 2003.

[31] Sivaraman Balakrishnan, Martin J. Wainwright, and Bin Yu. Statistical guarantees for the em algorithm: From population to sample-based analysis. Ann. Statist., 45(1):77–120, 02 2017.

[32] Thomas Hofmann. Unsupervised learning by probabilistic latent semantic analysis. Machine Learning, 42(1):177–196, Jan 2001.

[33] Stephan Mandt, James McInerney, Farhan Abrol, Rajesh Ranganath, and David M. Blei. Variational tempering. In AISTATS, volume 51, pages 704–712. JMLR.org, 2016.

[34] Ruslan Salakhutdinov, Sam Roweis, and Zoubin Ghahramani. Optimization with EM and Expectation-Conjugate-Gradient. In Proceedings, Intl. Conf. on Machine Learning (ICML), pages 672–679, 2003.
[35] David J. C. MacKay. Information theory, inference, and learning algorithms. Cambridge University Press, 2003.

[36] Ronald J. Williams. Simple statistical gradient-following algorithms for connectionist reinforcement learning. Mach. Learn., 8(3-4):229–256, May 1992.

[37] Benjamin Recht. A tour of reinforcement learning: The view from continuous control. arXiv, abs/1806.09460, 2018.

[38] Lei Xu and Michael I. Jordan. On convergence properties of the EM algorithm for Gaussian mixtures. Neural Comput., 8(1):129–151, January 1996.

[39] John Duchi, Elad Hazan, and Yoram Singer. Adaptive subgradient methods for online learning and stochastic optimization. J. Mach. Learn. Res., 12:2121–2157, July 2011.

[40] Ruslan Salakhutdinov and Sam Roweis. Adaptive overrelaxed bound optimization methods. In Proceedings of the International Conference on Machine Learning, volume 20, pages 664–671, 2003.

[41] Qiang Liu and Dilin Wang. Stein variational gradient descent: A general purpose bayesian inference algorithm. In Neural Information Processing Systems, pages 2370–2378, 2016.

[42] Jun Han and Qiang Liu. Stein variational gradient descent without gradient. In Jennifer Dy and Andreas Krause, editors, Proceedings of the 35th International Conference on Machine Learning, volume 80, pages 1900–1908, 2018.

[43] Tom Rainforth, Adam R. Kosiorek, Tuan Anh Le, Chris J. Maddison, Maximilian Igl, Frank Wood, and Yee Whye Teh. Tighter variational bounds are not necessarily better. In Proceedings of the 35th International Conference on Machine Learning, ICML 2018, Stockholm, Sweden, July 10-15, 2018, pages 4274–4282, 2018.

[44] Arvind Neelakantan, Luke Vilnis, Quoc V. Le, Ilya Sutskever, Lukasz Kaiser, Karol Kurach, and James Martens. Adding gradient noise improves learning for very deep networks. CoRR, abs/1511.06807, 2015.

[45] Youhei Akimoto, Yuichi Nagata, Isao Ono, and Shigenobu Kobayashi. Bidirectional relation between cma evolution strategies and natural evolution strategies. In Robert Schaefer, Carlos Cotta, Joanna Kołodziej, and Günter Rudolph, editors, Parallel Problem Solving from Nature, PPSN XI, pages 154–163, Berlin, Heidelberg, 2010. Springer Berlin Heidelberg.

[46] L. Malagò, M. Matteucci, and G. Pistone. Natural gradient, fitness modelling and model selection: A unifying perspective. In IEEE Congress on Evolutionary Computation, pages 486–493, June 2013.

[47] Stephane Chrétien and Alfred O Hero III. Acceleration of the em algorithm via proximal point iterations. In Proceedings of the IEEE International Symposium on Information Theory (ISIT), 1998.

[48] Stéphane Chrétien and Alfred O. III Hero. Kullback proximal algorithms for maximum-likelihood estimation. IEEE transactions on information theory, 46(5):1800–1810, 2000.

[49] Amir Beck and Marc Teboulle. Mirror descent and nonlinear projected subgradient methods for convex optimization. Operations Research Letters, 31(3):167–175, 2003.

[50] James Martens. New insights and perspectives on the natural gradient method. arXiv preprint arXiv:1412.1193, 2014.

[51] Masa-Aki Sato. Online model selection based on the variational bayes. Neural Comput., 13(7):1649–1681, July 2001.

[52] James Hensman, Magnus Rattray, and Neil D. Lawrence. Fast variational inference in the conjugate exponential family. In Peter L. Bartlett, Fernando C. N. Pereira, Christopher J. C. Burges, Léon Bottou, and Kilian Q. Weinberger, editors, Advances in Neural Information Processing Systems, volume 25, Cambridge, MA, 00 2012.

[53] Matthew D. Hoffman, David M. Blei, Chong Wang, and John Paisley. Stochastic variational inference. J. Mach. Learn. Res., 14(1):1303–1347, May 2013.

[54] Hugh Salimbeni, Stefanos Eleftheriadis, and James Hensman. Natural gradients in practice: Non-conjugate variational inference in gaussian process models. In Uncertainty In Artificial Intelligence, 03 2018.
[55] Debora S. Marks, Lucy J. Colwell, Robert Sheridan, Thomas A. Hopf, Andrea Pagnani, Riccardo Zecchina, and Chris Sander. Protein 3d structure computed from evolutionary sequence variation. *PLOS One*, 6(12):1–20, 12 2011.
Supplementary Information: A view of Estimation of Distribution Algorithms through the lens of Expectation-Maximization

S1 Additional hybrid EDA-gradient experiments

![Figure S1: Trajectory plots in the style of Fig. 1a for the remaining tested functions. In particular, they represent one run each of (left) EDA (regular EDA), (center) SGD (single gradient step partial M-step), and (right) Hybrid (switching between EDA and SGD), over 5000 iterations (only first 1000 iterations shown), on (a-c) a twenty-dimensional Rastrigin function, (d-f) two-dimensional Ackley function, and (g-i) twenty-dimensional Ackley function, using the same experimental set-up as the results in Figure 1. Global minima of all functions are zero.](image)

S2 Equivalence between Expectation-Maximization and the proximal point method

In Section 6, we discuss the equivalence between EM and using the proximal point method (PPM) with reverse KL divergence to maximize the log-likelihood function. Here, we provide the
derivation of this equivalence, beginning with a formulation of the PPM:

\[
\phi^{(t+1)} = \arg\max_{\phi} \log \mathcal{L}(\phi) - D_{KL}(p(z|y, \phi^{(t)})||p(z|y, \phi))
\]

\[
= \arg\max_{\phi} \log p(y|\phi) - \int p(z|y, \phi^{(t)}) \log \frac{p(z|y, \phi^{(t)})}{p(z|y, \phi)} \, dz
\]

\[
= \arg\max_{\phi} \log p(y|\phi) + \int p(z|y, \phi^{(t)}) \log p(z|y, \phi) \, dz
\]

\[
= \arg\max_{\phi} \int p(z|y, \phi^{(t)}) \log p(y|\phi) + \log p(z|y, \phi) \, dz
\]

\[
= \arg\max_{\phi} \int p(z|y, \phi^{(t)}) \log p(y, z|\phi) \, dz.
\]

Note that the last line is precisely the update rule for EM.

**S3 Details of natural gradient descent**

Recall from Section 6 that replacing the log-likelihood with its linearization and the KL-divergence with its second-order Taylor series approximation in the PPM formulation of EM yields the update

\[
\phi^{(t+1)} = \arg\max_{\phi} \log \mathcal{L}(\phi^{(t)}) + \langle \nabla_{\phi} \log \mathcal{L}(\phi) \rangle_{\phi=\phi^{(t)}} - \frac{1}{2} (\phi - \phi^{(t)})^\top I(\phi^{(t)})(\phi - \phi^{(t)}).
\]

One can further derive a closed-form update by taking the derivative of the \(\arg\max\) argument on the right-hand side, setting it equal to zero as per first-order optimality conditions, and solving:

\[
\nabla_{\phi} \left( \log \mathcal{L}(\phi^{(t)}) + \langle \nabla_{\phi} \log \mathcal{L}(\phi) \rangle_{\phi=\phi^{(t)}} - \frac{1}{2} (\phi - \phi^{(t)})^\top I(\phi^{(t)})(\phi - \phi^{(t)}) \right)_{\phi=\phi^{(t+1)}} = 0
\]

\[
\Rightarrow \nabla_{\phi} \log \mathcal{L}(\phi)_{\phi=\phi^{(t)}} - I(\phi^{(t)})(\phi^{(t+1)} - \phi^{(t)}) = 0
\]

\[
\Rightarrow \phi^{(t+1)} = \phi^{(t)} + I(\phi^{(t)})^{-1} \nabla_{\phi} \log \mathcal{L}(\phi)_{\phi=\phi^{(t)}}.
\]

This establishes the equivalence between the standard natural gradient descent update rule and the mirror descent update derived using the PPM formulation of EM as a starting point.