Informative Path Planning for Anomaly Detection in Environment Exploration and Monitoring

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Abstract

An unmanned autonomous vehicle (UAV) is sent on a mission to explore and reconstruct an unknown environment from a series of measurements collected by Bayesian optimization. The success of the mission is judged by the UAV’s ability to faithfully reconstruct any anomalous feature present in the environment (e.g., extreme topographic depressions or abnormal chemical concentrations). We show that the criteria commonly used for determining which locations the UAV should visit are ill-suited for this task. We introduce a number of novel criteria that guide the UAV towards regions of strong anomalies by leveraging previously collected information in a mathematically elegant and computationally tractable manner. We demonstrate superiority of the proposed approach in several applications.

1 Introduction

With the rise of automation and artificial intelligence, a growing number of tasks deemed too tedious or too perilous for humans have been delegated to unmanned autonomous vehicles (UAV). This includes missions related to environment exploration and monitoring in which a UAV is tasked with producing a map for a quantity of interest (e.g., pollutant concentration, terrain elevation, or vegetation growth) by collecting measurements at various locations across a region of interest (e.g., a reservoir, a city, or a crop) [1–5]. The data collected by the UAV can be used to construct a statistical model for the quantity of interest, which in turn can be used for analysis and policy making. Of course, the statistical model is only as good as the measurements made by the UAV. Therefore, the question of data collection (i.e., how, when, and where to make measurements) is of paramount importance, especially from the standpoint of detecting abnormalities in the environment (see Broader Impact).

Path-planning algorithms for environment exploration come in two flavors. Approaches in which the UAV decides on its next move one step at a time are referred to as myopic [6–8]. Myopic algorithms are suitable for most situations but lack a mechanism for anticipation, which may be problematic in cases where path-planning decisions may have negative long-term consequences (e.g., the UAV gets stuck because of maneuverability constraints). On the other hand, non-myopic algorithms operate on sequences of destinations, which allows them to look further into the future [8–11]. The main tool for this is the partially observable Markov decision process, which assigns a reward to each admissible sequence of actions. Non-myopic approaches are computationally complex and incredibly expensive, which is why myopic approaches are often preferred—including in the present work.

The flagship feature of myopic algorithms is that they naturally lend themselves to Bayesian optimization [12, 13], allowing the UAV to a) incorporate prior belief about the environment, and b) decide on its next move by compromising between exploration of the space and exploitation of the available information. At the heart of Bayesian optimization is the acquisition function, which guides the UAV throughout the mission. Many acquisition functions have been proposed for environment exploration [3, 7, 8, 14, 15] but they all have one major flaw, namely, they have no robust mechanism to identify
anomalous environmental features. For example, the approach of Marchant and Ramos [3] requires
the user to specify the values of two ad hoc parameters which must be tuned on a case-by-case basis,
with no foolproof guidelines on how to do so.

The main contribution of this work is the introduction of two novel acquisition functions that are
specifically designed for anomaly detection in environment exploration. The proposed acquisition
functions have the following advantages:

1. They are based on a probabilistic treatment of what constitutes an anomaly, thereby elimi-
nating the need for ad hoc parameters;
2. Their computational complexity is comparable with that of traditional acquisition functions,
making them suitable for online path planning and monitoring; and
3. They provide the UAV’s operator with a mechanism to distill any prior beliefs they may
have about the locations of anomalies while allowing the UAV to refine the operator’s beliefs
“on the fly” as more information is collected.

2 Problem Formulation

2.1 Bayesian Optimization for Environment Exploration

We consider the problem of environment exploration in which a UAV is tasked with reconstructing
the spatial distribution of a quantity of interest \( f : \mathbb{R}^2 \to \mathbb{R} \) over a region of interest \( \mathcal{X} \subset \mathbb{R}^2 \).
(We assume that \( f \) is Lipschitz continuous and \( \mathcal{X} \) is compact.) To reconstruct the map \( f \), the UAV
is allowed to explore the space \( \mathcal{X} \) and collect measurements at locations that it deems informative.
Uncertainty in observations is modeled with additive Gaussian noise, so that each measurement made
by the UAV can be written as

\[
y = f(x) + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2),
\]

where \( x = [x_1, x_2]^T \) is a vector of coordinates identifying the UAV’s position in the Euclidean plane.
The combination of position \( x \) and orientation \( \theta \) (with \( \theta = 0 \) taken to coincide with the \( x_1 \)-axis)
completely determines the pose of the UAV.

To reconstruct the map \( f \), one strategy is for the UAV to visit a large number of precomputed
locations that densely cover the search space. In practice, however, this approach is intractable
because exploration missions are always done on a budget with limited time and resources. A
better strategy is for the UAV to proceed sequentially, deciding on its next destination based on
the information it has collected up to this point. This information can be leveraged to construct a
surrogate model \( \tilde{f} \) for the map \( f \), which the UAV can improve every time a new measurement point
is added. At each iteration the next destination is selected by minimizing an acquisition function
\( a : \mathbb{R}^2 \to \mathbb{R} \) which guides the UAV in its exploration of the space. Once the allocated budget is
exhausted, the mission is terminated and the surrogate model constructed by the UAV can be used in
analyses as a substitute for the unknown map \( f \) (Algorithm 1).

Algorithm 1 Sequential path planning for environment reconstruction.

1: Input: Number of iterations \( n_{\text{iter}} \)
2: Initialize: Surrogate model \( \tilde{f} \) on initial dataset of input–output pairs \( D_0 = \{x_i, y_i\}_{i=1}^{n_{\text{init}}} \)
3: for \( n = 0 \) to \( n_{\text{iter}} \) do
4: Select next destination as \( x_{n+1} = \arg\min_{x\in\mathcal{X}} a(x; \tilde{f}, D_n) \)
5: Collect measurement \( y_{n+1} \) at location \( x_{n+1} \)
6: Augment dataset: \( D_{n+1} = D_n \cup \{x_{n+1}, y_{n+1}\} \)
7: Update surrogate model
8: return Final surrogate model

Algorithm 1 is at the foundation of Bayesian optimization [13] and Bayesian experimental design
[16]. Its success is conditioned on two key components: a) the surrogate model \( \tilde{f} \), which encapsulates
the UAV’s belief about what the environment looks like given the data it has collected; and b) the
acquisition function \( a \), upon which the UAV relies to plan its next move.
2.2 Model Selection

For the surrogate model $\bar{f}$, we use a Bayesian approach based on Gaussian process (GP) regression [17]. This choice is appropriate because Gaussian processes a) are agnostic to the inner workings of the unknown map $f$, b) provide a way to quantify uncertainty associated with noisy observations, and c) are robust, versatile, easy to implement, and relatively inexpensive to train. For a dataset $D = \{X, y\}$ of input–output pairs and a zero-mean GP with covariance function $k(x, x')$, the random process $\bar{f}(x)$ conditioned on $D$ follows a normal distribution with posterior mean and variance

$$
\mu(x) = k(x, X)K^{-1}y,
$$

$$
\sigma^2(x) = k(x, x) - k(x, X)K^{-1}k(X, x),
$$

respectively, where $K = k(X, X) + \sigma^2 I$. The posterior mean can be used to predict the value of the model at any point $x$, and the posterior variance to quantify uncertainty in prediction at that point.

In GP regression, the choice of covariance function is crucial as it is the main building block for practitioners to encode structure (e.g., symmetry or invariance) in the model. In this work we use the radial-basis-function (RBF) kernel with automatic relevance determination,

$$
k(x, x') = \sigma_f^2 \exp\left(-\frac{(x - x')^T\Theta^{-1}(x - x')}{2}\right),
$$

where $\Theta$ is a diagonal matrix containing the lengthscales for each dimension. Other choices are possible (e.g., Matérn kernel [7]), but the properties of the RBF kernel will come in handy later. For a given dataset, the hyper-parameters appearing in (3) are trained by maximum likelihood estimation.

2.3 Acquisition Functions for Environment Exploration

In environment exploration, the role of the acquisition function is to favor exploration of regions where uncertainty is high. We briefly review two common approaches to achieving this.

**Uncertainty sampling (US):** The most intuitive approach is for the UAV to go where the predictive variance of the GP model is the largest [18], that is,

$$
a_{US}(x) = \sigma^2(x).
$$

This approach is tantamount to minimizing the mean squared error between $\bar{f}$ and $f$ [19, 20], and therefore ensures that model uncertainty is distributed somewhat evenly over the search space.

**Integrated variance reduction (IVR):** Another approach is to consider the effect of observing a hypothetical “ghost” point $x$ on the overall model variance [21]. This effect is measured by

$$
a_{IVR}(x) = \int [\sigma^2(x') - \sigma^2(x'; x)] \, dx' = \frac{1}{\sigma^2(x)} \int \text{cov}^2(x, x') \, dx',
$$

where $\sigma^2(x'; x)$ is the predictive variance at $x'$ had $x$ been observed, and $\text{cov}^2(x, x')$ is the posterior covariance between $x$ and $x'$ [22]. Therefore, maximizing IVR has the effect of maximally reducing the overall model variance.

If the UAV operator wants to focus exploration on certain regions of the search space, or if they have prior beliefs about where relevant environmental features might be located, then it is possible to bias exploration by incorporating a prior $p_x(x)$ over the input space in US and IVR. (Formally, $p_x$ is a density with respect to the Lebesgue measure.) The prior acts as a sampling weight, leading to

$$
a_{US-IW}(x) = \sigma^2(x)p_x(x),$$

$$
a_{IVR-IW}(x) = \frac{1}{\sigma^2(x)} \int \text{cov}^2(x, x')p_x(x') \, dx',
$$

where the suffix “IW” stands for “input-weighted”. We note that if no prior knowledge is available, then $p_x$ can be chosen uniform, in which case US-IW and IVR-IW reduce to US and IVR, respectively.

The idea of using a prior $p_x$ as a sampling weight was first suggested by Sacks et al. [23] in the context of sequential design of computer experiments. To the best of our knowledge, it has never been applied to problems related to environment exploration as a way of emphasizing certain regions...
of the input space. The closest instance of which we are aware is the work of Oliveira et al. [24, 25] in which a prior is placed on the input space in order to account for localization noise, i.e., the error in estimating the UAV’s position resulting from imperfections in the UAV’s sensors, actuators, and motion controllers. This is quite different from the proposed approach in which the UAV’s position is assumed to be known with exactitude and the input prior is used as a mechanism to highlight certain regions of the search space before the mission starts.

While other acquisition functions exist, either they are computationally more complex or they have narrower applicability than those previously discussed. For example, the mutual information in general cannot be written in closed form and thus loses out to US, the latter being a good approximation for the former [16, 18]. Likewise, the upper confidence bound (UCB), the expected improvement (EI), and the probability of improvement (PI) are not appropriate for environment reconstruction because they are designed for optimization, not exploration [26, 27]. And while UCB, EI and PI each contain an ad hoc parameter that controls the trade-off between exploration and exploitation, setting the value of that parameter to a large number in order to favor exploration is moot because in that limit UCB, EI and PI are equivalent to US (see Section S1). Variants of these criteria [3, 8, 28, 29] suffer from the same shortcomings.

3 Methods

In this section, we introduce two novel acquisition functions for reconstruction of anomalous environment. Both share three critical features: a) they leverage information collected previously by the UAV and assign more weight to regions of the search space where the map $f$ is thought to exhibit strong anomalies; b) they allow incorporation of a prior $p_\mu(x)$ over the search space, with expectations about potential benefits being similar to those discussed earlier for US-IW and IVR-IW; and c) their computational complexity is comparable to that of traditional acquisition functions.

3.1 Output-Informed Acquisition Functions for Anomalous Environment

We begin with a definition of what constitutes an anomalous environment. A map $f : \mathcal{X} \to \mathbb{R}$ is anomalous if the conditional probability density function (pdf) of the output $p_f(x)$ is heavy-tailed. (A pdf is heavy-tailed when at least one of its tails is not exponentially bounded.) Heavy tails are the manifestation of high-impact events occurring with low probability, and are therefore appropriate to characterize anomalies in output values. Heavy-tailed distributions commonly arise in the study of risk [30] and extreme events [31] but as far as we know they have not been considered in the context of environment exploration. In what follows, we drop the conditional notation for clarity.

The proposed definition suggests a strategy for the UAV to decide on its next destination. At each iteration, the UAV can use the pdf of the GP mean $p_\mu$ as a proxy for $p_f$ and select the next destination so that uncertainty in $p_\mu$ is most reduced. The latter can be quantified by

$$a_L(x) = \int \left| \log p_{\mu_+}(y) - \log p_{\mu_-}(y) \right| \, dy,$$

where $\mu_+ (x'; x)$ denotes the upper and lower confidence bounds at $x'$ had the data point $\{x, \mu(x)\}$ been collected, that is, $\mu_+ (x'; x) = \mu(x') \pm \sigma^2(x'; x)$. The use of logarithms in (8) places extra emphasis on the pdf tails in which critical information about abnormal features is encapsulated.

The above metric enjoys attractive convergence properties [32] but is cumbersome to compute (let alone minimize) and therefore unsuitable for online path planning. To combat this, we show that $a_L(x)$ is bounded above (up to a multiplicative constant) by

$$a_B(x) = \int \sigma^2(x'; x) \frac{p_x(x')}{p_\mu(\mu(x'))} \, dx'$$

Equation (9) is a massive improvement over (8) from the standpoint of reducing complexity. More importantly, it reveals an unexpected connection between the metric $a_L$ (whose primary focus is the reduction of uncertainty in pdf tails) and the IVR-type acquisition functions of Section 2.3. Indeed, it only takes a few lines to show that $a_B(x)$ is strictly equivalent to

$$a_{IVR-LW}(x) = \frac{1}{\sigma^2(x)} \int \text{cov}^2(x, x') \frac{p_x(x')}{p_\mu(\mu(x'))} \, dx',$$
which is clearly a cousin of (5) and (7), with the ratio \( p_x(x)/p_{\mu}(\mu(x)) \) playing the role of a sampling weight. By the same logic, we introduce

\[
a_{US-LW}(x) = \sigma^2(x) \frac{p_x(x)}{p_{\mu}(\mu(x))}
\]

(11)
as the “likelihood-weighted” (LW) counterpart of US and US-IW. For details about the derivation, we refer the reader to Section S2.

3.2 The Likelihood Ratio and its Benefits

In the importance-sampling literature, the ratio

\[
w(x) = \frac{p_x(x)}{p_{\mu}(\mu(x))}
\]

is referred to as the likelihood ratio [33]. The likelihood ratio is important in cases where some points are more important than others in determining the value of the output. When used in an acquisition function, it acts as a sampling weight, assigning to each point \( x \in \mathcal{X} \) a measure of relevance defined in probabilistic terms. For points with equal probability of being observed “in the wild” (i.e., same \( p_x \)), the likelihood ratio assigns more weight to those that have a large impact on the magnitude of output (i.e., small \( p_{\mu} \)). For points with equal impact on the output (i.e., same \( p_{\mu} \)), it promotes those with higher probability of occurrence (i.e., large \( p_x \)). In other words, the likelihood ratio favors points associated with abnormal output values over points associated with frequent, average output values.

In environment exploration, the likelihood ratio can be beneficial in two ways. First, it incorporates field information through the GP mean \( \mu(x) \) in such a way that a) no additional ad hoc parameter is introduced; b) anomalous regions are naturally accentuated due to the probabilistic dependence on the density \( p_{\mu} \); and c) it does not discriminate between abnormally small and abnormally small output values, which is a tremendous advantage over approaches based on PI, EI or UCB. Second, the likelihood ratio preserves the possibility for the operator to distill prior belief through the density \( p_x \). But the fact that the input prior is weighted by the output density \( p_{\mu} \) enables the UAV to correct and refine the operator’s beliefs on the fly as more information is collected. Thus, the likelihood ratio provides a mechanism for the UAV to strike an informed balance between its own representation of the environment and the operator’s guidelines. We will see that this feature significantly improves performance in situations where the operator’s beliefs are imprecise or erroneous.

We should not lose sight of the fact that these benefits may be neutralized if the likelihood ratio is not tractable computationally. Fortunately, that is not the case. To see this, we note that to evaluate \( w(x) \), we must estimate the pdf of the posterior mean \( p_{\mu} \), typically at each iteration. This can be done by computing \( \mu(x) \) for a large number of input points and applying kernel density estimation (KDE) to the resulting samples. Fortunately, KDE is to be performed in the (one-dimensional) output space, allowing use of fast FFT-based algorithms which scale linearly with the number of samples [34].

To evaluate (10) without resorting to Monte Carlo integration, we approximate the likelihood ratio with a Gaussian mixture model (GMM):

\[
w(x) \approx \sum_{i=1}^{n_{GM}} \alpha_i \mathcal{N}(x; \omega_i, \Sigma_i).
\]

(13)

When combined with the RBF kernel, the GMM approximation renders the integral in (10) analytic (see Section S3). The number of Gaussian mixtures in (13) can be kept constant throughout the mission or modified in real time, either according to a predefined schedule or by minimizing the Akaike information criterion (AIC) or the Bayesian information criterion (BIC) at each iteration.

For a visually compelling illustration of the benefits provided by the likelihood ratio, we consider the Michalewicz function (S33) with the input space \([0, \pi]^2\) rescaled to the unit square and a Gaussian prior \( p_x(x) = \mathcal{N}(0 + 1/2, 0.011) \). The Michalewicz function is characterized by large regions of “flatland” interrupted by steep valleys and ridges, with its deepest portion accounting for a tiny fraction of the search space. For this function, Figure 1 makes it visually clear that the likelihood ratio gives more emphasis to the area where the quantity of interest \( f(x) \) assumes abnormally small values, taking precedence over the operator’s belief that the UAV should focus solely on the center region. Figure 1 also shows that \( w(x) \) can be approximated satisfactorily with a small number of Gaussian mixtures, a key prerequisite for algorithm efficiency.
4 Results

4.1 Experimental Protocol

To solidify the utility of the likelihood ratio in environment exploration, we perform a series of numerical experiments as per the following protocol. For each example considered, the search space is rescaled to the unit square \([0, 1]^2\) and the UAV’s initial pose is specified as \(x_0 = 0\) and \(\theta_0 = \pi/4\). At each iteration, the UAV’s admissible destinations are constrained to lie on a circular arc with radius \(L\) centered at \(x\) and subtending an angle \(2\alpha\) which bisects \(\theta\). The parameters \(L\) and \(\alpha\) characterize the lookahead distance and field of view of the UAV, respectively. Consecutive destinations are connected by a Dubins path with turning radius \(R\) along which the UAV travels at constant speed \([35]\). This parametrization ensures that the UAV’s path is \(C^1\)-continuous. To avoid situations in which the UAV might venture outside of the search space, we discard from the set of admissible destinations those lying a distance \(2R\) or less from the boundaries of the unit square (Figure 2).

In Algorithm 1, measurements are only collected at destination, and consequently no use is made of the fact that in practice the sampling frequency of the UAV’s sensors is much higher than the frequency of the decision making. This is problematic because it renders the sampling approach in Algorithm 1 suboptimal \([8]\). Therefore, to replicate the conditions of an actual field experiment, we allow the UAV to collect \(M\) measurements during the trip from \(x_n\) to \(x_{n+1}\). To make the most of this additional data, we modify the path-planning policy in Line 4 to

\[
x_{n+1} = \arg \min_{x \in A_n} \int_{S(x_n, x)} a(x'; f, D_n) \, dx',
\]

where \(A_n\) denotes the set of admissible destinations for position \(x_n\), and \(S(x_n, x)\) is the Dubins path from \(x_n\) to candidate destination \(x\). (This approach is known as informative path planning \([8]\).) In general, the integral in (14) is not analytic; in this work, we evaluate it using the trapezoidal rule.

To assess performance of the algorithm, we compute the root mean square error \(\text{rmse}\), log-pdf error \(\text{pdfe}\), distance to minimizer \(\ell\), and simple regret \(r\). (Expressions are given in Section S4.) The root mean square error measures the overall goodness of the GP model with no consideration for anomalies of any kind. In contrast, the log-pdf error judges the model by its ability to reconstruct the tails of the output pdf, which is where abnormal features “live”. The metrics \(\ell\) and \(r\) quantify the model’s ability to predict the locations and output value, respectively, of the map’s global minimizers. These two metrics are appropriate because in the examples considered the global minimizers are associated with abnormally small output values.

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Figure 1: From left to right: Contour plots of the map \(f(x)\), the input pdf \(p_x(x)\), the likelihood ratio \(w(x)\), and the GMM approximation of the likelihood ratio \(w_{GMM}(x)\) with two Gaussian mixtures.

Figure 2: Schematic of the experimental set-up for environment exploration (not to scale).
On the first iteration, every admissible destination is as good as any other from the UAV’s standpoint because there is only one measurement available (collected at $x_0$). To disambiguate this situation, the first destination $x_1$ is drawn uniformly from the set of admissible destinations $A_0$. This introduces an element of randomness in the problem, which is averaged out by repeating the mission many times, each time with a different choice of $x_1$. For each example considered, we repeat the mission 50 times, and report the median for the four metrics introduced above. (The error bands indicate a quarter of the median absolute deviation.) Experiments were performed on a computer cluster equipped with 40 Intel Xeon E5-2630v4 processors clocking at 2.2 GHz. Our code is available on GitHub.$^1$

### 4.2 Benchmark Results

We evaluate the performance of the proposed criteria on five test functions commonly used in optimization and uncertainty quantification: Ackley, Bird, Bukin06, Michalewicz, and Modified Rosenbrock. (Analytical expressions are given in Section S5.) These functions were chosen because they are representative of what an anomalous environment may look like in real life. For example, the steep ridge of the Bukin06 function is reminiscent of an unusually deep oceanic trench; and the Ackley function is evocative of a substance diffusing away from an abnormally potent source (Figure S1). In each case, the noise variance is specified as $\sigma^2 = 10^{-3}$ and appropriately rescaled to account for the variance of the map $f$. We do not set the parameter $\sigma^2$ beforehand; instead, we let the UAV learn it from data. We use $L = 0.2$, $\alpha = 3\pi/4$, $R = 0.02$ and $M = 3$ for the path-planning algorithm, and $n_{GMM} = 2$ for the GMM approximation of $w(x)$. (We have verified that the results are robust with respect to these parameters.) In the interest of space, results for the Bird, Bukin06 and Modified Rosenbrock functions have been relegated to the Supplementary Material.

![Graphs of benchmark results](image)

(a) Ackley

(b) Michalewicz

Figure 3: For uniform $p_x$, performance of US; US-LW; IVR; IVR-LW.

We first consider the situation in which the UAV’s operator has no prior beliefs about the locations of abnormalities in the search space, and thus a uniform prior is used for $p_x$. For the Ackley and Michalewicz functions, Figure 3 shows that the proposed LW criteria substantially outperform their unweighted counterparts in the three critical metrics $\text{pdfe}$, $\ell$ and $r$, often by more than one full order of magnitude. This is clear evidence that a UAV guided by US-LW or IVR-LW is able to identify environment anomalies more quickly and more efficiently than otherwise (Movies 1 and 2). When

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$^1$Link will be inserted here.
performance is measured in terms of the rmse, US-LW and IVR-LW are on par with US and IVR. This is not surprising since US and IVR are specifically designed for rmse minimization, while US-LW and IVR-LW are not. This is inconsequential from the standpoint of anomaly detection since the rmse only accounts for second-order moments and therefore is not a good indicator of abnormalities, unlike pdfe, ℓ and r. Similar trends are seen for the other test functions (Figure S2 and Movies 3–5).

We next consider the situation in which the UAV’s operator has some prior beliefs about where anomalies may be located and therefore decides to specify the Gaussian prior used in Figure 1 to focus exploration in the central part of the domain. For the Ackley function, this is a good guess, and as a result US-IW, US-LW, IVR-IW, and IVR-LW deliver similar performance, as shown in Figure 4(a) and Movie 6. For this function, the likelihood ratio is not particularly helpful. For the other test functions, however, the operator’s guess is quite poor, which leads to vastly different outcomes. Figures 4(b) and S3 as well as Movies 7–10 are a testament to the likelihood ratio’s ability to correct the operator’s beliefs and refine the UAV’s decision making in a way that makes anomaly detection more efficient. Absent the likelihood ratio, the UAV does not have the ability to depart from the operator’s guidelines, missing out on the critical anomalous features that lie beyond its ascribed area.

![Graphs](a) Ackley

![Graphs](b) Michalewicz

Figure 4: For Gaussian \( p_x \), performance of --- US-IW; --- US-LW; --- IVR-IW; --- IVR-LW.

Finally, we have investigated how computation of the likelihood ratio affects the efficiency of the path-planning algorithm. Table S1 shows that the runtimes for the LW criteria are comparable to those of the other criteria. For the LW criteria, we found that the penalty incurred for computing the likelihood ratio can be largely mitigated if sampling of the posterior mean \( \mu(x) \) is done frugally (i.e., using no more than \( 10^6 \) samples), as was done to generate the results in this section.

5 Conclusion

We have introduced two novel acquisitions functions for informative path planning that are specifically designed for identification of abnormalities in exploration missions. Having ramifications running deep within the field of rare-event quantification, the proposed criteria exploit the unique properties of the likelihood ratio to guide the UAV towards regions of the space in which the quantity of interest is thought to exhibit strong anomalies. Our approach deliver better performance (i.e., faster identification of anomalies) in a number of applications, paving the way for use in more sophisticated path-planning algorithms and more complex environments.
**Broader Impact**

Our method is quite general and therefore has positive implications for a range of commercial, scientific, and military applications in which anomaly detection is critical. For aerial UAVs, our work can be used to detect abnormal concentrations of chemicals, pollutants, or radioactive material in a region of interest; to reconstruct terrain with unknown topography in order to plan large-scale architecture; and to monitor abnormal crop growth in order to optimize agriculture operations. In the military, our algorithm can facilitate the clearing of minefields, having the ability to quickly identify signs of explosive chemicals leaking from landmines and causing abnormalities in the surrounding vegetation [36]. For underwater UAVs, our approach can be used to make detailed maps of the seafloor, of which less is known than of the topography of Mars. Bathymetric anomalies are important for the telecommunications industry and the oil and gas industry to be able to build subsea infrastructure, and also for navigation and coastal management as well as tsunami forecasting [37]. Our method can also improve detection of wreackages of missing crafts as well as other artifacts found in underwater archeological sites, which may be viewed as abnormal features lying on the ocean floor. Potential ethical issues include those related to security vulnerabilities (e.g., in-flight hijacking) as well as disruption of the wildlife in natural environments.

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S1 Equivalence Between UCB, PI, and EI in the Limit of Pure Exploration

S1.1 Preliminaries

We begin with a few definitions. To avoid any ambiguity, we follow the convention that the acquisition functions are to be maximized (i.e., UCB, PI and EI are looking to maximize the function $f$).

Uncertainty sampling (US):

$$a_{US}(x) = \sigma^2(x) \quad (S1)$$

Upper confidence bound (UCB):

$$a_{UCB}(x) = \mu(x) + \kappa \sigma(x) \quad (S2)$$

Probability of improvement (PI):

$$a_{PI}(x) = \Phi(\lambda(x)) \quad (S3)$$

Expected improvement (EI):

$$a_{EI}(x) = \sigma(x) \left[ \lambda(x) \Phi(\lambda(x)) + \phi(\lambda(x)) \right] \quad (S4)$$

In the above, \( \Phi \) and \( \phi \) are the cumulative and probability density functions of the standard normal distribution, respectively, and \( \kappa \) is a positive parameter that controls the trade-off between exploration (large \( \kappa \)) and exploitation (small \( \kappa \)). We have also introduced the quantity

$$\lambda(x) = \frac{\mu(x) - y^* - \kappa}{\sigma(x)}, \quad (S5)$$

where \( y^* \) denotes the current best observation.

We first note that the locations and ordering of a function’s extrema are preserved under strictly increasing continuous transformations. Therefore, to prove that UCB, PI and EI are equivalent to US in the limit of pure exploration (i.e., large \( \kappa \)), we only need to show that in that limit, UCB, PI and EI can be expressed as strictly increasing continuous functions of US. We will use the fact that the composition of two strictly increasing functions is also a strictly increasing function.

S1.2 Equivalence Between UCB and US in the Limit of Pure Exploration

It is straightforward to see that for large \( \kappa \),

$$a_{UCB}(x) \sim \kappa \sigma(x). \quad (S6)$$

The function $x \mapsto x^2$ is strictly increasing on $[0, +\infty]$, which completes the proof.
S1.3 Equivalence between PI and US in the Limit of Pure Exploration

For large $\kappa$, we note that

$$a_{PI}(x) \sim \frac{1}{2} \left\{ 1 - \text{erf} \left( \frac{\kappa}{\sqrt{2}\sigma(x)} \right) \right\},$$  \hspace{1cm} (S7)

where we have used the fact that $\Phi(-x) = (1/2)[1 - \text{erf}(x/\sqrt{2})]$ for any $x$. For any $a > 0$, the function $x \mapsto 1 - \text{erf}(a/\sqrt{x})$ is strictly increasing on $[0, +\infty]$, which completes the proof.

S1.4 Equivalence between EI and US in the Limit of Pure Exploration

For large $\kappa$, we have

$$a_{EI}(x) \sim \frac{\sigma(x)}{\sqrt{2\pi}} \exp \left[ -\frac{\kappa^2}{2\sigma^2(x)} \right] - \frac{\kappa^2}{2} \left\{ 1 - \text{erf} \left( \frac{\kappa}{\sqrt{2}\sigma(x)} \right) \right\},$$  \hspace{1cm} (S8)

But for $x \gg 1$, we know that

$$\text{erf}(x) \sim 1 - \frac{\exp(-x^2)}{x \sqrt{\pi}} \left[ 1 - \frac{1}{2x^2} \right].$$ \hspace{1cm} (S9)

It follows that

$$a_{EI}(x) \sim \frac{\sigma(x)}{\sqrt{2\pi}} \exp \left[ -\frac{\kappa^2}{2\sigma^2(x)} \right] - \frac{\kappa^2}{2\sigma^2(x)} \exp \left[ -\frac{\kappa^2}{2\sigma^2(x)} \right] \left[ 1 - \frac{\sigma^2(x)}{\kappa^2} \right],$$  \hspace{1cm} (S10)

and therefore

$$a_{EI}(x) \sim \frac{\sigma^3(x)}{\kappa^2 \sqrt{2\pi}} \exp \left[ -\frac{\kappa^2}{2\sigma^2(x)} \right].$$ \hspace{1cm} (S11)

For any $a > 0$, the function $x \mapsto x^{3/2} \exp(-a/x)$ is strictly increasing on $[0, +\infty]$, which completes the proof.

S2 Mathematical Derivation of IVR-LW

We begin with Theorem 1 of Mohamad and Sapsis [1] which states that for small enough $\sigma(x)$,

$$a_L(x) \approx \int_{\mathcal{Y}} \frac{1}{p_\mu(y)} \left| \frac{d}{dy} \mathbb{E}[\sigma^2(x';x) \cdot 1_{\mu(x')=y}] \right| dy,$$  \hspace{1cm} (S12)

where $\mathbb{E}$ is the expectation with respect to $p_\mu$, and $\mathcal{Y}$ is the domain over which the pdf $p_\mu$ is defined. Standard inequalities [2] allow us to bound the above as follows:

$$\int_{\mathcal{Y}} \frac{1}{p_\mu(y)} \frac{d}{dy} \mathbb{E}[\sigma^2(x';x) \cdot 1_{\mu(x')=y}] dy \leq K \int_{\mathcal{Y}} \frac{1}{p_\mu(y)} \mathbb{E}[\sigma^2(x';x) \cdot 1_{\mu(x')=y}] dy,$$ \hspace{1cm} (S13)

where $K$ is a positive constant. But we note that

$$\mathbb{E}[\sigma^2(x';x) \cdot 1_{\mu(x')=y}] = \int_{\mu(x')=y} \sigma^2(x';x) p_\mu(x') dx' \hspace{1cm} (S14a)$$

$$= \int_{\mu(x')=y} \sigma^2(x';x) p_\mu(x') \cdot 1_{\mu(x')=y} dx'. \hspace{1cm} (S14b)$$

Therefore,

$$\int_{\mathcal{Y}} \frac{1}{p_\mu(y)} \mathbb{E}[\sigma^2(x';x) \cdot 1_{\mu(x')=y}] dy = \int_{\mu(x') \in \mathcal{Y}} \frac{\sigma^2(x';x) p_\mu(x')}{p_\mu(\mu(x'))} dx'. \hspace{1cm} (S15)$$

In practice, the domain of integration in (S15) is replaced with the support of the input pdf $p_x$:

$$a_B(x) = \int \sigma^2(x';x) \frac{p_x(x')}{p_\mu(\mu(x'))} dx'.$$ \hspace{1cm} (S16)
Finally, it should be clear that the optimization problem
\[\min_{x \in X} \int \sigma^2(x'; x) \frac{p_x(x')}{p_\mu(\mu(x'))} \, dx'\] (S17)
is strictly equivalent to
\[\max_{x \in X} \int [\sigma^2(x') - \sigma^2(x; x)] \frac{p_x(x')}{p_\mu(\mu(x'))} \, dx',\] (S18)
since the term involving \(\sigma^2(x')\) in (S18) does not depend on the optimization variable \(x\). We can then rewrite the difference of variances using the trick of Gramacy and Lee [3]. We thus obtain
\[\max_{x \in X} \frac{1}{\sigma^2(x)} \int \text{cov}^2(x, x') \frac{p_x(x')}{p_\mu(\mu(x'))} \, dx',\] (S19)
which concludes the derivation of IVR-LW.

S3 Analytical Expressions for IVR-LW with RBF Kernel

With the likelihood ratio being approximated with a GMM, the IVR-LW acquisition function becomes
\[a_{\text{IVR-LW}}(x) = \frac{1}{\sigma^2(x)} \sum_{i=1}^{n_{\text{GMM}}} \beta_i a_i(x),\] (S20)
where each \(a_i\) is given by
\[a_i(x) = \int \text{cov}^2(x, x') \mathcal{N}(x'; \omega_i, \Sigma_i) \, dx'.\] (S21)

Using the formula for the posterior covariance, we get
\[a_i(x) = \int [k(x, x') - k(x, X)K^{-1}k(X, x')]^2 \mathcal{N}(x'; \omega_i, \Sigma_i) \, dx'\] (S22a)
\[= \int k(x, x')k(x', x)\mathcal{N}(x'; \omega_i, \Sigma_i) \, dx'
+ k(x, X)K^{-1} \left[ \int k(X, x')k(x', X)\mathcal{N}(x'; \omega_i, \Sigma_i) \, dx' \right] K^{-1}k(X, x)
- 2k(x, X)K^{-1} \int k(X, x')k(x', x)\mathcal{N}(x'; \omega_i, \Sigma_i) \, dx',\] (S22b)
\[= \hat{k}_i(x, x) + k(x, X)K^{-1} \left[ \hat{k}_i(X, X)K^{-1}k(X, x) - 2\hat{k}_i(x, x) \right],\] (S22c)
where we have defined
\[\hat{k}_i(x_1, x_2) = \int k(x_1, x')k(x', x_2)\mathcal{N}(x'; \omega_i, \Sigma_i) \, dx'.\] (S23)

Therefore, to evaluate \(a_i\) and its gradients, we only need a mechanism to compute \(\hat{k}_i\) and its gradients. For the RBF kernel
\[k(x, x'; \Theta) = \sigma^2 \exp[-(x - x')^T \Theta^{-1} (x - x')/2],\] (S24)
it is straightforward to show that
\[\hat{k}_i(x_1, x_2) = |2\Sigma_i\Theta^{-1} + I|^{-1/2}k(x_1, x_2; 2\Theta)k(x_1 + x_2, \omega_i; \Theta + 2\Sigma_i)\] (S25a)
and
\[\frac{d\hat{k}_i}{dx_1} = \hat{k}_i(x_1, x_2) \left\{ -x_1^T \Theta^{-1} + \frac{1}{2} [\omega_1^T + (x_1 + x_2)^T \Theta^{-1} \Sigma_i] (\Sigma_i + \Theta/2)^{-1} \right\}.\] (S25b)
S4 Analytical Expressions for Error Metrics

Analytical expressions for the error metrics used in Section 4.2 are given below. The index $n$ indicates the current iteration.

**Root mean square error:**

$$\text{rmse}(n) = \min_{k \in [0, n]} \sqrt{\frac{1}{N} \sum_{i=1}^{N} (f(x_i) - \mu_k(x_i))^2},$$  
(S26)

where $\{x_i\}_{i=1}^{N}$ is a set of $10^5$ samples uniformly distributed over the input space, and $\mu_k$ denotes the posterior mean of the GP model at iteration $k$.

**Log-pdf error:**

$$\text{pdfe}(n) = \min_{k \in [0, n]} \int |\log p_f(y) - \log p_{\mu_k}(y)| \, dy,$$  
(S27)

where the densities are estimated using $10^5$ samples uniformly distributed over the input space.

**Distance to minimizer:**

$$\ell(n) = \min_{k \in [0, n]} \|x^* - x^*_k\|^2,$$  
(S28)

where $x^*$ and $x^*_k$ are the minimizers for the true map $f$ and the GP mean $\mu_k$, respectively.

**Simple regret:**

$$r(n) = \min_{k \in [0, n]} f(x^*_k) - f(x^*)$$  
(S29)

S5 Analytical Expressions for Benchmark Test Functions

Analytical expressions for the synthetic test functions considered in Section 4.2 are given below. Contour plots are shown in Figure S1. Further details can be found in Jamil and Yang [5].

**Ackley function:**

$$f(x) = -a \exp \left[ -b \sqrt{x_1^2 + x_2^2} / 2 \right] - \exp \left[ (\cos cx_1 + \cos cx_2) / 2 \right] + a + \exp(1),$$  
(S30)

where $a = 20$, $b = 0.2$, and $c = 2\pi$.

**Bird function:**

$$f(x) = \sin(x_1) \exp[(1 - \cos x_2)^2] + \cos(x_2) \exp[(1 - \sin x_1)^2] + (x_1 - x_2)^2$$  
(S31)

**Bukin function:**

$$f(x) = 100\sqrt{|x_2 - 0.01x_1^2| + 0.01|x_1 + 10|}$$  
(S32)

**Michalewicz:**

$$f(x) = -\sin(x_1) \sin^{2m}(x_1^2 / \pi) - \sin(x_2) \sin^{2m}(2x_2^2 / \pi),$$  
(S33)

where $m$ controls the steepness of the valleys and ridges. In this work we use $m = 10$.

**Modified Rosenbrock:**

$$f(x) = 74 + 100(x_2 - x_1^2)^2 + (1 - x_1)^2 - 400 \exp[-10(x_1 + 1)^2 - 10(x_2 + 1)^2]$$  
(S34)
Figure S1: Contour plots of the test functions considered in Section 4.2.
Figure S2: For uniform $p_x$, performance of US; US-LW; IVR; IVR-LW.
Figure S3: For Gaussian $p_x$, performance of US-IW; US-LW; IVR-IW; IVR-LW.
Table S1: Average time per iteration (in seconds) for the missions completed in Section 4.2.

|                  | US  | US-IW | US-LW | IVR  | IVR-IW | IVR-LW |
|------------------|-----|-------|-------|------|--------|--------|
| Ackley           | 0.90| 1.05  | 1.20  | 0.96 | 1.56   | 1.65   |
| Bird             | 1.07| 1.13  | 1.26  | 1.11 | 1.58   | 1.67   |
| Bukin06          | 0.92| 0.95  | 1.19  | 0.99 | 1.41   | 1.62   |
| Michalewicz      | 1.10| 1.17  | 1.40  | 1.17 | 1.64   | 1.84   |
| Modified Rosenbrock | 1.10| 1.19  | 1.32  | 1.16 | 1.65   | 1.59   |
**Movie captions**

**Movie 1:** Comparison of IVR (pink) and IVR-LW (dark green) for the Ackley function with uniform $p_x$ and the parameters given in Section 4.1.

**Movie 2:** Comparison of IVR (pink) and IVR-LW (dark green) for the Michalewicz function with uniform $p_x$ and the parameters given in Section 4.1.

**Movie 3:** Comparison of IVR (pink) and IVR-LW (dark green) for the Bird function with uniform $p_x$ and the parameters given in Section 4.1.

**Movie 4:** Comparison of IVR (pink) and IVR-LW (dark green) for the Bukin06 function with uniform $p_x$ and the parameters given in Section 4.1.

**Movie 5:** Comparison of IVR (pink) and IVR-LW (dark green) for the Modified Rosenbrock function with uniform $p_x$ and the parameters given in Section 4.1.

**Movie 6:** Comparison of IVR-IW (pink) and IVR-LW (dark green) for the Ackley function with Gaussian $p_x$ and the parameters given in Section 4.1.

**Movie 7:** Comparison of IVR-IW (pink) and IVR-LW (dark green) for the Michalewicz function with Gaussian $p_x$ and the parameters given in Section 4.1.

**Movie 8:** Comparison of IVR-IW (pink) and IVR-LW (dark green) for the Bird function with Gaussian $p_x$ and the parameters given in Section 4.1.

**Movie 9:** Comparison of IVR-IW (pink) and IVR-LW (dark green) for the Bukin06 function with Gaussian $p_x$ and the parameters given in Section 4.1.

**Movie 10:** Comparison of IVR-IW (pink) and IVR-LW (dark green) for the Modified Rosenbrock function with Gaussian $p_x$ and the parameters given in Section 4.1.

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