A BANDIT-LEARNING APPROACH TO MULTIFIDELITY APPROXIMATION*

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Abstract. Multifidelity approximation is an important technique in scientific computation and simulation. In this paper, we introduce a bandit-learning approach for leveraging data of varying fidelities to achieve precise estimates of the parameters of interest. Under a linear model assumption, we formulate a multifidelity approximation as a modified stochastic bandit and analyze the loss for a class of policies that uniformly explore each model before exploiting. Utilizing the estimated conditional mean-squared error, we propose a consistent algorithm, adaptive explore-then-commit (AETC), and establish a corresponding trajectorywise optimality result. These results are then extended to the case of vector-valued responses, where we demonstrate that the algorithm is efficient without the need to worry about estimating high-dimensional parameters. The main advantage of our approach is that we require neither hierarchical model structure nor a priori knowledge of statistical information (e.g., correlations) about or between models. Instead, the AETC algorithm requires only knowledge of which model is a trusted high-fidelity model, along with (relative) computational cost estimates of querying each model. Numerical experiments are provided at the end to support our theoretical findings.

Key words. multifidelity, bandit learning, linear regression, Monte Carlo, consistency

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1. Introduction. Computational models are ubiquitous tools in different aspects of science and engineering, from the discovery of new constitutive laws in physics and mechanics to the design of novel systems such as multifunctional materials. Such models are primarily developed to describe the system of interest accurately such that they can replace time-consuming real-life experiments. In addition to accuracy, an important aspect to consider is the computational cost of model evaluations, which typically increases as the accuracy of the model increases. The trade-off between cost and accuracy constitutes a fundamental challenge in computational science that has been the subject of active research. This challenge has given rise to a widely studied class of methods that involves several computational models with various levels of accuracy and cost. In different contexts and formulations, such methods are called multifidelity, multilevel, multiresolution, etc. The common theme among all these methods is the availability of several models that describe the same system of interest but with varying accuracy and computational cost.

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1.1. Multifidelity models. The notion of fidelity may have different meanings in different problems. A typical scenario corresponds to the level of discretization for solving PDEs, where the finest mesh is referred to as the high-fidelity model and coarser meshes are lower-fidelity models. Other common multifidelity settings include the interpolation and regression models [20, 21], projection-based reduced-order models [50, 46, 29, 9], machine learning models [54, 17, 15], and other reduced-order models [41, 38]. The multifidelity setting considered in this paper is a general abstraction that includes low-fidelity models instantiated as coarse discretizations, via reduced-order models (e.g., reduced-basis methods), or other types of emulators such as Gaussian processes [31, 45].

Combining the low-fidelity models with the high-fidelity model to accelerate computational efficiency is a fruitful idea in engineering science [44]. It can be construed as a model management strategy with three main categories of approaches: (1) adaptation of the low-fidelity model to the high-fidelity model by the use of high-fidelity information; approaches based on model correction fall into this category [19, 1, 2]; (2) fusion of multiple fidelity modes such as control variate approaches [11, 30, 40, 34, 27]; and (3) filtering approaches such as importance sampling where low-fidelity models serve as filters and determine when to use the high-fidelity model [16, 22, 39, 42]. The method developed in this paper belongs to the realm of fusion approaches, where we assume in particular that a subset of low-fidelity models can be combined in a linear way to effectively predict the value of the high-fidelity model.

- 1.2. Bandit learning. The idea of bandit learning first appeared in a study [51] of treatment design problems in clinical trials. It was later developed as a powerful tool to study sequential decision-making problems in an uncertain environment. The primary goal of bandit learning is to find an adaptive strategy that produces close-tooptimal decisions by minimizing the loss or regret. The uncertainty in an environment can be modeled using different mechanisms, such as random feedback [35, 5, 18, 47], adversarial manipulation [7, 6, 13], Markov chains [3, 26, 32], etc., giving rise to a wealth of bandit setups that find use in numerous applications in practice [10, 57]. Regret, which plays a role similar to a loss function in statistical learning, can be chosen in various forms, often depending on the specific application of interest. For example, cumulative loss [5, 7] is widely used as regret to measure the overall performance of a strategy, and a discounted version [26] can be used to account for elapsed time during the strategy. In other situations where only the final decision matters, the loss at a fixed (final) step is adopted [14, 4, 23]. Despite the diversity of choices for regret, the overall goal is quite thematic: find a strategy that performs similarly to an oracle by investing a reasonable amount of computational complexity in a procedure that adaptively learns. The key philosophy behind bandit learning thus lies in efficiently learning a competitive strategy and then utilizing the learned knowledge for future use. A comprehensive treatment of the subject can be found in, for instance, [37, 12].
- 1.3. Related work. Our approach in this article centers around using non-hierarchical linear regression for constructing a multifidelity estimator. The idea of using linear regression for multifidelity approximation is not completely new. For instance, recent work has introduced a general linear regression framework to study telescoping-type estimators in multifidelity inference [48, 49]. This work treats different fidelities as factor models with heterogeneous noise structure. Assuming that the covariance matrix of the noise is known, the authors proposed a reweighted least squares estimator which is shown to be the best linear unbiased estimator for the

quantity of interest (under a fixed allocation choice). This framework offers a uniform perspective on many well-studied multifidelity and multilevel estimators [24, 25, 27, 43] and provides certain limits on their theoretical performance. However, the construction utilizes oracle information about model correlations, which are often not known beforehand and must first be learned from the data, placing practical restrictions on immediate deployment of such procedures. There is limited work on multifidelity methods with nonhierarchical dependence, i.e., methods that do not necessarily assume an ordering of models based on cost/accuracy [28], and algorithms for identifying nonhierarchical relationships are an area of active research.

In [56], the authors proposed to compute a high-fidelity model using a linear combination of low-fidelity surrogates corrected by a deterministic discrepancy function. This approach is easy to implement and allows classical tools to be used in the analysis. Nevertheless, certain drawbacks exist: The assumption on the discrepancy function can be restrictive when noise pollutes data in a random fashion, and realizing the optimal performance of the method requires selecting the "best" surrogate model in practice, which is a nontrivial task when the computational budget is limited.

The work [33] has a similar title to this paper, but the setup and goals considered there are completely different.

1.4. Contributions of this paper. This paper provides techniques to address some of the challenges identified in section 1.3 that limit the applicability of current approaches. Under a type of linear model assumption (that is slightly stronger than what is assumed in [48]), we introduce a bandit-learning approach that, under a budget constraint, facilitates computational learning of the relation between different models before an exploitation choice is committed. Our algorithm seeks to identify the best selection of regressors by investing a portion of the budget in an exploration phase. This selection is then utilized in an exploitation phase to construct a surrogate for the high-fidelity model, which is significantly less expensive but exhibits comparable accuracy.

We make three contributions in this paper:

- We formulate multifidelity approximation as a bandit-learning-type problem under a linear model assumption. In particular, we introduce the uniform exploration policies and define their associated loss (regret). We also derive an asymptotic formula for their loss as the computational budget goes to infinity.
- We propose an adaptive explore-then-commit (AETC) algorithm (Algorithm 5.1) that automatically identifies a trade-off point between exploration and exploitation. We prove that the estimator produced by the algorithm is consistent and asymptotically matches the best regression model with optimal exploration. In particular, this algorithm requires only model cost information and identification of a high-fidelity model. No model correlations or statistics are needed as input.
- We initially consider scalar-valued responses, but subsequently generalize
 to vector-valued high-fidelity models and demonstrate that the algorithm is
 efficient despite some potentially high-dimensional parameter estimation
 procedures.

Our numerical results strongly support our theoretical findings. Our methodology enjoys great generality as it does not require any particular knowledge of the models, i.e., hierarchical structure or correlation statistics. The procedure requires only the identification of a trusted high-fidelity model, the ability to query the models themselves, and a relative cost estimate of each model relative to the high-fidelity model. It is worth mentioning that our approach can be extended to estimate more complicated statistics such as the cumulative distribution functions of quantities of interest [55], but the assumptions there are more subtle and caution must be practiced.

The rest of the paper is organized as follows. In section 2, we introduce the abstract setup of multifidelity approximation with which we will be working in the rest of the paper, followed by a brief review of the key ideas behind stochastic bandits. In section 3, we formulate a multifidelity approximation as a modified bandit-learning problem, and in section 4, we prove consistency of the estimators used during the exploitation phase and derive a nonasymptotic convergence rate. In section 5, we propose an adaptive algorithm, AETC, based on the estimated conditional mean-squared errors from the analysis and establish a trajectorywise optimality result for it. In section 6, we extend our results developed in the previous sections to the case of vector-valued high-fidelity models and justify the efficiency of the estimation procedures where high-dimensional parameters are involved. In section 7, we provide a detailed study of the novel AETC algorithm via numerical experiments that verifies our theoretical statements and demonstrates the utility of the AETC algorithm. In section 8, we conclude by summarizing the main results in the paper.

2. Background.

2.1. Notation. Fix $n \in \mathbb{N}$. We let Y, X_1, \ldots, X_n be random vectors (possibly of different dimensions) representing the high-fidelity model and n surrogate low-fidelity models, respectively. Let c_i $(i \in [n])$ and c_0 be the respective cost of sampling X_i and Y. For example, in parametrized PDEs, X_i is the approximate solution given by the ith solver under random coefficients of a PDE, and Y is the solution given by the most accurate solver, which is assumed to be the ground truth. The cost c_i corresponds to the computational time. We make no assumptions about the accuracy or costs of X_i relative to those of X_{i+1} . In particular, the index i does not represent an ordering based on cost, accuracy, or hierarchy. For X_i $(i \in [n])$ and Y, let f_i and f be output quantity of interest maps that bring X_i and Y, respectively, to $f_i(X_i) \in \mathbb{R}^{k_i}$ and $f(Y) \in \mathbb{R}^{k_0}$, which are the quantities of practical interest. Understanding the mean of f(Y) is crucial for many simulation problems in engineering.

Computing the expectation of f(Y) may not seem challenging at all: under mild assumptions on the distribution of Y, a Monte Carlo (MC) procedure exploits the law of large numbers using an ensemble of independent samples to accurately estimate the mean of f(Y). However, in practice, obtaining numerous samples of Y can be computationally expensive if c_0 is large. This motivates the idea of estimating $\mathbb{E}[f(Y)]$ using low-fidelity model outputs $f_i(X_i)$, which often contain some information about f(Y) and are cheaper to sample. For instance, when $f_i(X_i)$ and f(Y) are scalars and the correlation between them is high, one can construct an unbiased estimator for $\mathbb{E}[f(Y)]$ by taking a telescoping sum of the low-fidelity models plus a few samples of the ground truth f(Y). Optimizing over the allocation parameters under a minimum variance criterion leads to the multifidelity Monte Carlo (MFMC) estimator. It is shown in [43] that the MFMC method outperforms MC by a substantial margin on several test datasets. However, successful implementation of the method requires both knowledge of statistical information of and between the models, as well as a hierarchical structure, neither of which may be known beforehand. More precisely, in MFMC, a training stage is required to learn correlations between models, and guidance on how to perform this training is heuristic. Our procedure is a principled approach that effects a similar type of training in an automated way and is accompanied by theoretical guarantees. In the rest of this section, we introduce a general framework in terms of learning the high-fidelity model from its surrogates. Our method utilizes ideas from bandit learning and therefore is less reliant on any existing knowledge of the models. We will need a general linear model assumption that has been widely used in statistics. For simplicity, we assume $k_i = 1$ for $i \in [n]$ and denote

$$(2.1) X^{(i)} := f_i(X_i) \in \mathbb{R}.$$

We will first deal with the case where f(Y) is a scalar, i.e., $k_0 = 1$. The result will be generalized to the vector-valued responses in section 6.

2.2. Linear regression. Let $S \subseteq [n]$ be a selection of low-fidelity models with |S| = s > 0. Suppose f(Y) and $\{X^{(i)}\}_{i \in S}$ satisfy the following *linear model assumption*:

$$(2.2) f(Y) = X_S^T \beta_S + \varepsilon_S,$$

where

$$X_S = (1, (X^{(i)})_{i \in S})^T \in \mathbb{R}^{s+1}$$

is the regressor vector, which includes a constant (intercept) term; $\beta_S \in \mathbb{R}^{s+1}$ is the coefficient vector; and $\varepsilon_S \in \mathbb{R}$ is model noise, which we assume is independent of X_S . For convenience, we assume in the following discussion that ε_S is a centered sub-Gaussian random variable with variance σ_S^2 .

Note that even though (2.2) considers only linear interactions with X_S , it is not overly restrictive as it appears. Indeed, a key assumption implied by (2.2) is that the conditional expectation of f(Y) given X_S (i.e., $\mathbb{E}[f(Y)|X_S]$) is a linear function of X_S . By definition, $\mathbb{E}[f(Y)|X_S]$ is a measurable function of X_S , which can be approximated using polynomials of X_S on any compact set under appropriate regularity assumptions. When the linearity assumption is violated, one can add higher-order terms of X_S as new regressors to fit a larger linear model to mitigate the model misspecification effect. This procedure will not incur additional computational cost. Nevertheless, identifying an optimal set of appropriately expressive regressors (features) is a much harder problem that goes beyond the scope of this paper.

Our goal is to seek an efficient estimator for $\mathbb{E}[f(Y)]$, so taking the expectation of (2.2) yields

(2.3)
$$\mathbb{E}[f(Y)] = \mathbb{E}[X_S^T]\beta_S.$$

The term $\mathbb{E}[X_S]$ on the right-hand side of (2.3) can be estimated by averaging the independent joint samples of X_S , which is the same as the MC applied to the conditional expectation $\mathbb{E}[f(Y)|X_S]$.

What is gained from sampling from $f(Y)|X_S$ instead of f(Y)? The two major advantages are as follows:

- The N-sample MC estimator for $\mathbb{E}[f(Y)]$ based on sampling f(Y) has mean-squared error (MSE) $\mathbb{V}[f(Y)]/N$, where $\mathbb{V}[\cdot]$ denotes the variance. The same procedure via sampling $f(Y)|X_S$ has MSE $\mathbb{V}[\mathbb{E}[f(Y)|X_S]]/N$. Since conditioning does not increase variance, the numerator of the latter is bounded by the numerator of the former for any fixed N.
- Given a fixed budget, when $\sum_{i \in S} c_i \ll c_0$, the number of affordable samples for $f(Y)|X_S$ is much larger than f(Y), which can significantly reduce the variance of the estimator.

 $\begin{array}{c} {\rm Table} \ 1 \\ {\it Notation} \ used \ throughout \ this \ article. \end{array}$

$X^{(i)}$	the ith regressor
f(Y)	the response variable (vector)
k_i, k_0	the dimension of $X^{(i)}$ and $f(Y)$
m	the number of samples for exploration
n	the number of regressors
B	total budget
S	the model index set (indices of regressors used in regression)
$(c_i)_{i=0}^n/c_{\text{epr}}/c_{\text{ept}}(S)$	cost parameters/total cost/cost of model S
N_S	the affordable samples in model S
β_S	coefficients (matrix) of model S
$X_{\mathrm{epr},\ell}$	the ℓ th sample in the exploration phase
Z_S	the design matrix in the exploration phase in model S
ε_S/η_S	the noise variable/vector in model S
x_S	the mean of the regressors in model S
Σ_S	the covariance matrix of the regressors in model S
σ_S^2	the variance in model S (single response)
Q	the weight matrix in defining the Q -weighted risk
Γ_S	the covariance matrix of the noise in the case of vector-valued response

Both observations provide some heuristics that (2.3) may give rise to a better estimator for $\mathbb{E}[f(Y)]$ under certain circumstances.

In practice, neither the best model index set S (which is referred to as model S in the rest of the article) nor the corresponding β_S is known. Thus, we cannot avoid expending some resources to estimate β_S for every model $S \subseteq [n]$ before deciding which model can best predict $\mathbb{E}[f(Y)]$. One possible way to achieve this is via bandit learning.

2.3. Stochastic bandits. This section provides a brief overview of the philosophy behind bandit learning, and in particular we focus on stochastic bandits, which is the subfield most relevant to our procedure.

Consider a multiarmed bandit setup: we are faced with k slot machines or arms, where $k \in \mathbb{N}$ is fixed. At each integer time t, a player pulls exactly one arm and this player will receive a reward. Rewards generated from the same arm at different times are assumed to be independent and identically distributed (i.i.d.); rewards generated from different arms are independent and their distributions are stationary in time. Given a fixed (time) horizon N, the goal of stochastic bandit learning is to seek a policy with small "regret." A policy $\pi = (\pi_1, \dots, \pi_N) \in [k]^N$ is a random sequence of choices adapted to the natural filtration generated by the past observations and actions. "Regret" is a special type of loss function that measures the quality of a policy. In the classical setup, the regret of a policy π is defined as

$$(2.4) \qquad R_N(\pi) := N\mu_{\max} - \mathbb{E}\left[\sum_{t \in [N]} z_t(\pi)\right] \\ = \sum_{i \in [k]} T_N(i)\Delta_i, \qquad T_N(i) = \mathbb{E}\left[\#\{t \le N, \pi_t = i\}\right],$$

where $z_t(\pi)$ is the reward received at time t under policy π (i.e., corresponds to reward π_t at time t), μ_i is the expectation of the reward distribution of arm i, $\mu_{\max} := \max_{i \in [k]} \mu_i$, and $\Delta_i := (\mu_{\max} - \mu_i)$ is the *suboptimality* gap of arm i. Intuitively, (2.4) measures the difference between the average total reward under π compared to the best (oracle) mean reward, which is generally not known.

Algorithm 2.1. Explore-then-commit algorithm for stochastic bandits

```
Input: m: the number of explorations on each arm Output: \pi = (\pi_t)_{t \in [N]}

1: if t \leq mk then

2: \pi_t = \lceil t \mod k \rceil

3: else

4: \pi_t = \arg\max_{i \in [k]} \widehat{\mu}_i(mk), where \widehat{\mu}_i(mk) = \frac{1}{m} \sum_{t=m \cdot (i-1)+1}^{m \cdot i} z_t(\pi)

5: end if
```

In practice we assume that the true reward distributions are not available, and so it is necessary to expend effort estimating the expected reward of each arm. A simple idea to estimate these average rewards is to pull each arm a fixed number of times m, and use the gathered data to estimate the mean rewards. Such a process is called an *exploration* stage in bandit learning. Based on the estimated rewards, we can then make a decision about which arm performs the best and repeatedly select it for the remaining time (the *exploitation* phase) until the horizon is reached. A direct combination of the exploration and exploitation gives the explore-then-commit (ETC) algorithm, shown in Algorithm 2.1.

The success of the ETC algorithm closely depends on the input parameter m, which dictates how many times each arm is pulled in the exploration phase, and is therefore indicative of the cost of this phase. A small m may result in poor estimation (and thus poor exploration), and in this case there is a considerable chance that the chosen exploitation strategy will be suboptimal. A large m, on the other hand, leaves little room for exploitation, and regret will then be dominated by the exploration phase. A good choice of m lies in finding the right trade-off point between exploration and exploitation. When k=2 and reward distributions are sub-Gaussian, a near-optimal m can be explicitly computed [37, Chapter 6]. However, such explicit expressions often rely on the knowledge of the suboptimality gaps Δ_i , which are not available in general. More useful algorithms which can be viewed as adaptive generalizations of the ETC include the upper-confidence bound algorithm [5] and the elimination algorithm [8].

One generalization of stochastic bandits pertaining to the multifidelity approximation problem of our interest is budget-limited bandits [52], where each arm has a cost for pulling, and the number of pulls is constrained by a total budget instead of the time horizon. Similar algorithms as well as the regret analysis in the stochastic bandits can be carried out in the budget-limited setup [52, 53].

- 3. A bandit-learning perspective of the multifidelity problem. In this section, we demonstrate that multifidelity approximation fits into a modified framework of bandit learning, which we exploit to develop an algorithm. Since our multifidelity goal is different from that in classical stochastic bandits, both the action set and the loss function (regret) must be tailored. We begin with the former.
- **3.1.** Action sets and uniform exploration policies. Our goal is to construct a regression-based MC estimator for $\mathbb{E}[f(Y)]$ using the best regression model. However, the relationship between f(Y) and X_S is unknown, requiring us to first estimate the coefficient vector β_S in (2.3) for each S and then decide which model is optimal. As a consequence, the action set contains both the exploration and exploitation options for each $S \subseteq [n]$. Denote by \mathcal{A} the set of actions. Then, we can write \mathcal{A} as

(3.1)
$$\mathcal{A} = \{a_{\text{epr}}(S), a_{\text{ept}}(S)\}_{S \subset [n]},$$

where

 $a_{\mathrm{epr}}(S)$: collect a sample of $(X_S, f(Y))$,

 $a_{\mathrm{ent}}(S)$: use the remaining budget to sample X_S .

As opposed to stochastic bandits, actions here are highly correlated. For example, exploration will not be allowed whenever an exploitation action is triggered (which exhausts the budget), separating exploration and exploitation into two distinct phases. In addition, action $a_{\rm epr}(S)$ yields data for every S' satisfying $S' \subset S$. For simplicity, we specialize our action set to consider only uniform exploration policies, i.e., each exploration yields a sample of all regressors, incurring the cost

(3.2)
$$c_{\text{epr}} := \sum_{i=0}^{n} c_i.$$

This procedure is similar to the ETC algorithm (Algorithm 2.1) where arms are explored to the same degree during exploration.

Let B>0 be a given, fixed total budget, and let m>n+1 be the number of exploration actions. (We will specify how m is chosen later.) The budget $B_{\rm epr}$ spent on exploration under a uniform exploration policy π and the budget $B_{\rm ept}$ remaining for exploitation are given by

$$B_{\text{epr}} = c_{\text{epr}} m,$$
 $B_{\text{ept}} = B - B_{\text{epr}}.$

During exploration, each action yields a sample of the form

$$X_{ ext{epr},\ell} = \left(1, X_\ell^{(1)}, \dots, X_\ell^{(n)}, f(Y_\ell)\right)^T, \qquad \qquad \ell \in [m],$$

where the subscript ℓ is a sampling index. For $S \subseteq [n]$, let $X_{\text{epr},\ell}|_S \in \mathbb{R}^{s+1}$ (including the intercept term) and $X_{\text{epr},\ell}|_Y \in \mathbb{R}$ be the restriction of $X_{\text{epr},\ell}$ to model S and f(Y), respectively. The coefficient vector β_S in (2.2) can be estimated by a standard least squares procedure:

$$\widehat{\beta}_S = Z_S^{\dagger} X_{\text{epr}}|_Y,$$

where

$$Z_S = \left(X_{\mathrm{epr},1}|_S, \dots, X_{\mathrm{epr},m}|_S\right)^T, \qquad X_{\mathrm{epr}}|_Y = \left(X_{\mathrm{epr},1}|_Y, \dots X_{\mathrm{epr},m}|_Y\right)^T$$

are the design matrix and data vector, respectively, and Z_S^{\dagger} is the Moore Penrose pseudoinverse of Z_S . For simplicity, we will assume that the design matrix has full rank in the following discussion, so that $Z_S^{\dagger} := (Z_S^T Z_S)^{-1} Z_S^T$. In exploitation, one selects an action $a_{\rm ept}(S)$ for some $S \subseteq [n]$ and uses (2.3) to build an MC estimator for $\mathbb{E}[f(Y)]$. The true coefficient vector β_S is unknown but can be replaced by the estimate $\widehat{\beta}_S$, yielding the linear regression Monte Carlo (LRMC) estimator associated with model S,

(3.4)
$$\mathsf{LRMC}_S = \frac{1}{N_S} \sum_{\ell \in [N_S]} X_{S,\ell}^T \widehat{\beta}_S,$$

where N_S is the number of affordable samples to exploit model S,

$$N_S = \left\lfloor rac{B_{ ext{ept}}}{c_{ ext{ept}}(S)}
ight
floor = \left\lfloor rac{B - c_{ ext{exp}} m}{c_{ ext{ept}}(S)}
ight
floor, \qquad \qquad c_{ ext{ept}}(S) := \sum_{i \in S} c_i,$$

and $X_{S,\ell}$ are i.i.d. samples of X_S which are independent of the samples in the exploration stage. Here we choose not to reuse samples from the exploration phase during the exploitation process for convenience of analysis.

Remark 3.1. A similar analysis of the LRMC estimator that reuses or recycles the exploration data can be carried out but with more complicated notation. For most applications that we consider, where $m/N_S \ll 1$ (since the high-fidelity model is often substantially more expensive than the low-fidelity emulators), reuse has little impact on the estimator in general. Regardless of analysis, one can always recycle exploration samples in a practical setting; our numerical results show that recycling exploration samples has negligible impact on the performance of our procedure for the examples we have tested. See Appendix SM1 for a theoretical justification and Figure 2 in section 7 for numerical evidence.

We will show in section 4 that for fixed $S \subseteq [n]$, LRMC_S defined in (3.4) is, almost surely, a consistent estimator for $\mathbb{E}[f(Y)]$, and we will provide a convergence rate.

3.2. Loss function. The loss function used in bandit learning is called regret, which is often defined by the reward difference between a policy and an oracle. In our case, it is more convenient to define loss as a quantity that we wish to minimize. Note that the output of a uniform exploration policy π is an LRMC estimator (3.4), where the selected model S satisfies $\pi_{m+1} = a_{\text{ept}}(S)$. One way to measure the immediate quality of (3.4) is through the following conditional MSE on $\widehat{\beta}_S$:

$$\left. \mathsf{MSE}_{S} \right|_{\widehat{\beta}_{S}} = \mathbb{E} \left[\left(\mathsf{LRMC}_{S} - \mathbb{E}[f(Y)] \right)^{2} \left| \widehat{\beta}_{S} \right| \right].$$

The LRMC_S alone, despite being an unbiased estimator (which is easily verified using independence), is not a sum of i.i.d. random variables unless conditioned on $\widehat{\beta}_S$. Once conditioned, LRMC_S becomes a sum of i.i.d. random variables that is a biased estimator for $\mathbb{E}[f(Y)]$. Define the following statistics of X_S :

$$x_S = \mathbb{E}[X_S],$$
 $\Sigma_S = \text{Cov}[X_S].$

By writing $\mathsf{MSE}_S|_{\widehat{\beta}_S}$ using the bias-variance decomposition, we obtain

$$\begin{aligned} \mathsf{MSE}_{S}|_{\widehat{\beta}_{S}} &= \left(x_{S}^{T}(\widehat{\beta}_{S} - \beta_{S})\right)^{2} + \mathbb{V}\left[\mathsf{LRMC}_{S}\big|\widehat{\beta}_{S}\right] \\ &= (\widehat{\beta}_{S} - \beta_{S})^{T}x_{S}x_{S}^{T}(\widehat{\beta}_{S} - \beta_{S}) + \frac{1}{N_{S}}\widehat{\beta}_{S}^{T}\Sigma_{S}\widehat{\beta}_{S}, \end{aligned}$$

$$(3.6)$$

where $\mathbb{V}[\cdot|\widehat{\beta}_S]$ is the $\widehat{\beta}_S$ -conditional variance operator. Note that (3.6) decomposes the loss incurred in the exploration and exploitation phases by the bias term and the variance term, respectively. The average conditional MSE of the LRMC is defined as (3.6) averaged over the randomness of the model noise ε_S in exploration:

$$\overline{\mathsf{MSE}}_{S}|_{\widehat{\beta}_{S}} := \mathbb{E}_{\varepsilon_{S}} \left[\mathsf{MSE}_{S}|_{\widehat{\beta}_{S}} \right]
= \frac{1}{N_{S}} \left[\beta_{S}^{T} \Sigma_{S} \beta_{S} + \sigma_{S}^{2} \operatorname{tr} \left(\Sigma_{S} (Z_{S}^{T} Z_{S})^{-1} \right) \right] + \sigma_{S}^{2} \operatorname{tr} \left(x_{S} x_{S}^{T} (Z_{S}^{T} Z_{S})^{-1} \right).$$

Note that $\overline{\mathsf{MSE}}_S|_{\widehat{\beta}_S}$ defined in (3.7) is random, and one could alternatively define it by averaging all the randomness (both ε_S and Z_S). However, this approach is more difficult to analyze due to the term $\mathbb{E}[(Z_S^T Z_S)^{-1}]$. In the following discussion, we will use (3.7) as the *loss function* associated with the uniform exploration policy π to examine its average quality in terms of estimating $\mathbb{E}[f(Y)]$.

4. Consistency of the LRMC estimator. In this section, we will show that the LRMC estimators constructed in the previous section are consistent estimators for $\mathbb{E}[f(Y)]$. The result can be derived as a corollary of a nonasymptotic estimate of the convergence rate of the $\hat{\beta}_S$ -conditional MSE. The following definition will be used in the subsequent analysis.

Definition 4.1 (a-Orlicz norm). The a-Orlicz (a \geq 1) norm of a random variable W is defined as

$$||W||_{\psi_{\alpha}} := \inf\{C > 0 : \mathbb{E}[\exp(|W|^{\alpha}/C^{\alpha})] \le 2\}.$$

Theorem 4.2. Fix $S \subseteq [n]$. Suppose X_S satisfies

$$(4.1) \qquad \max \left\{ \sup_{\|\theta\|_2 = 1} \mathbb{E}[\langle X_S, \theta \rangle^4]^{1/4}, \|\|X_S\|_2\|_{\psi_1} \right\} \leq K < \infty, \qquad K \geq 1$$

where $\|\cdot\|_{\psi_1}$ is the 1-Orlicz norm, and $\Lambda_S := \mathbb{E}[X_S X_S^T] = x_S x_S^T + \Sigma_S$ is invertible. Then, for large m, with probability at least $1 - m^{-2}$,

$$(4.2) \hspace{1cm} \textit{MSE}_S|_{\widehat{\beta}_S} \lesssim \frac{\beta_S^T \Sigma_S \beta_S}{N_S} + (s+1) \sigma_S^2 \frac{\log m}{m},$$

where the implicit constant in \lesssim is independent of m.

Theorem 4.2 implies the following consistency result of the LRMC estimator, which follows immediately from (4.2) and an application of the Borel-Cantelli lemma.

COROLLARY 4.3 (consistency of the LRMC). Let $\{B_k\}_{k=1}^{\infty}$ satisfy $\lim_{k \uparrow \infty} B_k = \infty$, and let m_k, N_k be the respective exploration round and exploitation samples satisfying $\min(m_k, N_k) \to \infty$. For fixed $S \subseteq [n]$, denote $\mathsf{LRMC}_{S,k}$ the LRMC estimator under budget B_k , and $\widehat{\beta}_{S,k}$ the corresponding estimator for β_S . Then, for almost every sequence $\{\widehat{\beta}_{S,k}\}_{k=1}^{\infty}$, $\mathsf{LRMC}_{S,k} \stackrel{\mathbb{P}}{\to} \mathbb{E}[f(Y)]$ as $k \to \infty$.

Without a nonasymptotic convergence rate, a strong consistency result for the LRMC estimator can be established using existing results in [36, Theorem 1]. In fact, a sufficient condition for the estimator $\hat{\beta}_S$ (hence $\hat{\sigma}_S^2$) to be strongly consistent is that the largest and smallest eigenvalues of $(Z_S^T Z_S)^{-1}$, λ_{\max} and λ_{\min} , satisfy $\lambda_{\min} \to \infty$ and $\log \lambda_{\max}/\lambda_{\min} \to 0$ as $m \to \infty$ a.s., which is verifiable under the condition (4.1).

5. Algorithms. In this section, we first analyze the asymptotic loss associated with uniform exploration policies. Then, we propose an AETC algorithm based on the estimated average MSEs, which selects the optimal exploration round and the best model to commit for large budget almost surely. For convenience, we will ignore all integer rounding effects in the rest of the discussion.

5.1. Oracle loss of uniform exploration policies. A uniform exploration policy spends the first m rounds on exploration and then chooses a fixed model S among the subsets of [n] for exploitation. Fixing B and for each S, the optimal exploration $m_S(B)$ balances the terms in expression (3.7). The best uniform exploration policy is the one that stops exploring at time $m_S(B)$ and then picks model S for exploitation, where model S has the smallest average conditional MSE computed at the optimal exploration round $m_S(B)$. In order to develop computable expressions, we will be mainly concerned with the case when B tends to infinity.

To find the optimal m for fixed S, note that for sufficiently large m, the law of large numbers tells us that almost surely from (3.7),

$$\overline{\mathsf{MSE}}_{S}|_{\widehat{\beta}_{S}} = \frac{1}{N_{S}} \left(\beta_{S}^{T} \Sigma_{S} \beta_{S} + \sigma_{S}^{2} \operatorname{tr} \left(\Sigma_{S} (Z_{S}^{T} Z_{S})^{-1} \right) \right) + \sigma_{S}^{2} \operatorname{tr} \left(x_{S} x_{S}^{T} (Z_{S}^{T} Z_{S})^{-1} \right)
\simeq \frac{c_{\operatorname{ept}}(S)}{B - c_{\operatorname{epr}} m} \left(\beta_{S}^{T} \Sigma_{S} \beta_{S} + \frac{1}{m} \sigma_{S}^{2} \operatorname{tr} \left(\Sigma_{S} \Lambda_{S}^{-1} \right) \right) + \frac{1}{m} \sigma_{S}^{2} \operatorname{tr} \left(x_{S} x_{S}^{T} \Lambda_{S}^{-1} \right)
\simeq \frac{1}{B - c_{\operatorname{epr}} m} c_{\operatorname{ept}}(S) \beta_{S}^{T} \Sigma_{S} \beta_{S} + \frac{1}{m} \sigma_{S}^{2} \operatorname{tr} \left(x_{S} x_{S}^{T} \Lambda_{S}^{-1} \right),$$
(5.1)

where $A_1(m) \simeq A_2(m)$ means that $A_1(m)/A_2(m) \to 1$ as $m \to \infty$ with probability 1. Denoting

$$(5.2) k_1(S) = c_{\text{ept}}(S)\beta_S^T \Sigma_S \beta_S, k_2(S) = \sigma_S^2 \operatorname{tr}(x_S x_S^T \Lambda_S^{-1}) \le (s+1)\sigma_S^2,$$

the asymptotically best m for exploiting model S can be found by minimizing (5.1):

(5.3)
$$m_S = \operatorname*{arg\,min}_{1 < m < B/c_{\rm epr}} \frac{k_1(S)}{B - c_{\rm epr}m} + \frac{k_2(S)}{m} = \frac{B}{c_{\rm epr} + \sqrt{\frac{c_{\rm epr}k_1(S)}{k_2(S)}}},$$

where the latter equality can be computed explicitly since (5.1) is a strictly convex function of m in its domain. The $\overline{\mathsf{MSE}}_S|_{\widehat{\mathcal{G}}_S}$ corresponding to $m=m_S$ is

$$(5.4) \qquad \overline{\mathsf{MSE}}_S^*|_{\widehat{\beta}_S} = \frac{\left(\sqrt{k_1(S)} + \sqrt{c_{\mathrm{epr}}k_2(S)}\right)^2}{B} \propto \left(\sqrt{k_1(S)} + \sqrt{c_{\mathrm{epr}}k_2(S)}\right)^2.$$

The best model is the one that has the smallest $\overline{\mathsf{MSE}}_S^*|_{\widehat{\beta}_S}$ under the optimal exploration round:

$$(5.5) \hspace{1cm} S^* = \mathop{\arg\min}_{S \subseteq [n]} \overline{\mathsf{MSE}}_S^*|_{\widehat{\beta}_S} = \mathop{\arg\min}_{S \subseteq [n]} \left(\sqrt{k_1(S)} + \sqrt{c_{\mathrm{epr}} k_2(S)} \right)^2,$$

where the right-hand side is assumed to have a unique minimizer. The uniform exploration policy π^* with exploration round count $m = m_{S^*}$ (more precisely ($\lfloor m_{S^*} \rfloor$)) and exploitation action $a_{\text{ept}}(S^*)$ achieves the smallest asymptotic loss among all uniform exploration policies; such a policy is referred to as a perfect uniform exploration policy. Note that determination of this optimal policy requires oracle information and thus cannot be directly applied in practice. We will provide a solution for this in the next section.

Remark 5.1. For every $S \subseteq [n]$, one can verify that the numerator in (5.4) is bounded by $2(k_1(S) + c_{\text{epr}}k_2(S))$. On the other hand, the MC estimator using the

high-fidelity samples alone has MSE of a similar form with numerator $c_0\mathbb{V}[f(Y)]$ (section 2.2). Taking the quotient of the two quantities yields

$$\begin{split} \frac{2(k_1(S) + c_{\mathrm{epr}}k_2(S))}{c_0 \mathbb{V}[f(Y)]} &\overset{(5.2)}{\leq} \frac{2[c_{\mathrm{ept}}(S)\beta_S^T \Sigma_S \beta_S + c_{\mathrm{epr}}(s+1)\sigma_S^2]}{c_0 \mathbb{V}[f(Y)]} \\ &\overset{(2.2)}{\leq} 2\left[\frac{c_{\mathrm{ept}}(S)}{c_0} + \frac{c_{\mathrm{epr}}(s+1)}{c_0} \frac{\sigma_S^2}{\mathbb{V}[f(Y)]}\right]. \end{split}$$

This can be unconditionally bounded by 2(n+1)(n+2) for all $S \subseteq [n]$ and can be significantly smaller than 1 if both

$$\frac{c_{\rm ept}(S)}{c_{\rm epr}} \ll 1, \qquad \frac{\sigma_S^2}{\mathbb{V}[f(Y)]} \ll 1.$$

This implies that the best uniform exploration policies are at most a constant (which only depends on n) worse than the classical MC and can be significantly better if (5.6) is satisfied for at least one S (which is often the case in practice).

5.2. An adaptive ETC algorithm. Finding a uniform exploration policy is impossible without oracle access to β_S , Σ_S , x_S , σ_S^2 , and Λ_S^{-1} . These quantities, despite being unknown, can be estimated at any particular time t in exploration (t > s + 1):

(5.7)

$$\widehat{eta}_S(t) = Z_S^\dagger X_{ ext{epr}}|_Y ext{ (using the first t samples)}, \qquad \qquad \widehat{x}_S(t) = rac{1}{t} \sum_{\ell \in [t]} X_{ ext{epr},\ell}|_S,$$

$$\widehat{\Sigma}_S(t) = \frac{1}{t-1} \sum_{\ell \in [t]} (X_{\mathrm{epr},\ell}|_S - \widehat{x}_S(t)) (X_{\mathrm{epr},\ell}|_S - \widehat{x}_S(t))^T,$$

$$\widehat{\sigma}_S^2(t) = \frac{1}{t-s-1} \sum_{\ell \in [t]} \left(X_{\mathrm{epr},\ell}|_Y - X_{\mathrm{epr},\ell}|_S \widehat{\beta}_S \right)^2, \qquad \qquad \widehat{\Lambda}_S^{-1}(t) = \left(\frac{1}{t} Z_S^T Z_S \right)^{-1}.$$

Note that $\widehat{\sigma}_S^2(t)$ is an unbiased estimator for σ_S^2 when the noise is Gaussian. Plugging (5.7) into (3.7) and ignoring the higher-order term $\sigma_S^2 \operatorname{tr} \left(\Sigma_S(Z_S^T Z_S)^{-1} \right)$ yields the sample estimator for $\overline{\mathsf{MSE}}_{S}|_{\widehat{\beta}_S}$ at time t:

$$(5.8) \qquad \widehat{\overline{\mathsf{MSE}}}_S|_{\widehat{\beta}_S}(t) = \frac{1}{B - c_{\mathtt{enr}} t} \widehat{\beta}_S^T(t) \widehat{\Sigma}_S(t) \widehat{\beta}_S(t) + \frac{1}{t} \widehat{\sigma}_S^2(t) \operatorname{tr} \Big(\widehat{x}_S(t) \widehat{x}_S^T(t) \widehat{\Lambda}_S^{-1}(t) \Big).$$

We call (5.8) the *empirical average conditional MSE* of model S at time t, which we subsequently call the empirical MSE. Correspondingly, we define more empirical estimates of quantities that were previously defined in terms of oracle information:

(5.9)

$$\begin{split} k_{1,t}(S) &= c_{\text{ept}}(S) \widehat{\beta}_S^T(t) \widehat{\Sigma}_S(t) \widehat{\beta}_S(t), \qquad k_{2,t}(S) = \widehat{\sigma}_S^2(t) \operatorname{tr} \Big(\widehat{x}_S(t) \widehat{x}_S^T(t) \widehat{\Lambda}_S^{-1}(t) \Big), \\ m_S(t) &= \frac{B}{c_{\text{epr}} + \sqrt{\frac{c_{\text{epr}} k_{1,t}(S)}{k_{2,t}(S)}}}, \qquad \overline{\mathsf{MSE}}_S^*|_{\widehat{\beta}_S}(t) = \frac{\Big(\sqrt{k_{1,t}(S)} + \sqrt{c_{\text{epr}} k_{2,t}(S)}\Big)^2}{B}. \end{split}$$

To mimic the idea of a perfect uniform exploration policy, we start by collecting the smallest necessary number of exploration samples to make the above estimation possible, which requires |S|+2 exploration rounds. For $t\geq |S|+2$, we use the collected exploration data to compute (5.7), (5.8), (5.9), from which we can estimate the best empirical MSE for each model S. At this point, if $m_S(t)>t$, then more exploration is needed for model S, and the optimal empirical MSE is approximately $\overline{\text{MSE}}_S^*|_{\widehat{\beta}_S}(t) = \widehat{\overline{\text{MSE}}}_S|_{\widehat{\beta}_S}(m_S(t))$. Otherwise, the best trade-off point has passed and stopping immediately yields the minimal empirical MSE, which equals $\widehat{\overline{\text{MSE}}}_S|_{\widehat{\beta}_S}(t)$. An algorithm could use the estimated optimal expected MSEs to determine which model is currently most favorable for exploitation. But another exploration round should transpire if $m_S(t)$ for this favorable model is larger than the current step t.

During implementation, we use the above procedure once t exceeds a relatively small number, i.e., the maximum number of regressors plus one. The estimation error of the second term in (5.8) is of constant order and cannot be ignored at the beginning. If it becomes pathologically close to zero during the initial stages of the algorithm, exploration may terminate after only a few rounds. To combat this deficiency, we employ a common regularization in bandit learning: For every S, we additively augment $k_{2,t}(S)$ with a small regularization parameter α_t , which decays to 0 as $t \to \infty$. For large B, adding α_t encourages the algorithm to explore at the beginning, but the encouragement becomes negligible as $\alpha_t \to 0$. Putting the ideas together yields Algorithm 5.1, the AETC algorithm for multifidelity approximation.

Remark 5.2. Algorithm 5.1 is an adaptive version of the ETC algorithm (Algorithm 2.1). To better comprehend Algorithm 5.1, note that the first "for" loop (steps 2–3) involves collecting a minimum number of samples to make the parameters that will be used estimable. The "while" loop (steps 5 17) determines the exploration

Algorithm 5.1. AETC algorithm for multifidelity approximation (single-valued case)

```
Input: B: total budget, c_i: cost parameters, \alpha_t \downarrow 0: regularization parameters
   Output: (\pi_t)_t
 1: compute the maximum exploration round M = \lfloor B/c_{\rm epr} \rfloor
 2: for t \in [n+2] do
       \pi_t = a_{\mathrm{epr}}([n])
 4: end for
    while n+2 \le t \le M do
 5:
        for S \subseteq [n] do
 6:
          compute k_{1,t}(S), k_{2,t}(S) using (5.7), (5.9), and set k_{2,t}(S) \leftarrow k_{2,t}(S) + \alpha_t
 7:
          compute m_S(t) using (5.9)
 8:
          compute the optimal expected MSE using (5.8): h_S(t) = \widehat{\overline{\mathsf{MSE}}}_{S}|_{\widehat{\beta}_S}(m_S(t) \vee t)
 9:
10:
        find the optimal model S^*(t) = \arg \min_{S \subseteq [n]} h_S(t)
11:
        if m_{S^*(t)}(t) > t then
12:
          \pi_{t+1} = a_{\text{epr}}([n]) \text{ and } t \leftarrow t+1
13:
14:
           \pi_t = a_{\text{ept}}(S^*(t)) and t \leftarrow M + 1
15:
16:
        end if
17: end while
```

rate adaptively based on the estimated optimal MSE. In particular, the inner "for" loop (steps 6–10) computes for each $S \subseteq [n]$ the expected optimal mean-squared error under the current budget, and step 11 selects the best model based on the estimated values. The "if-else" procedure (steps 12 15) then decides if more exploration is needed based on the information of the selected best model.

5.3. AETC consistency and optimality. Algorithm 5.1 ensures that both exploration and exploitation go to infinity as $B \to \infty$. (See Appendix SM3.) As a consequence, almost surely, the model chosen by Algorithm 5.1 for exploitation converges to S^* and the corresponding exploration is asymptotically optimal.

THEOREM 5.3. Let m(B) be the exploration round chosen by Algorithm 5.1 under budget B, and let S(B) be the model for exploitation, i.e., $S(B) = S^*(m(B))$. Suppose (4.1) holds uniformly for all $S \subseteq [n]$, and $\lim_{t\to\infty} \alpha_t = 0$. Then, with probability 1,

$$\lim_{B\to\infty}\frac{m(B)}{m_{S^*}}=1,$$

$$\lim_{B \to \infty} S(B) = S^*,$$

where S^* and m_{S^*} are the model choice and exploration round count given oracle information defined in (5.5) and (5.3), respectively.

Proof. See Appendix SM3.
$$\Box$$

Theorem 5.3 concludes that as the budget goes to infinity, both the exploration round count and the chosen exploitation model will converge to the optimal ones given by the perfect uniform exploration policies for almost every realization. However, this does not imply that the loss of the corresponding policy π asymptotically matches the loss of the perfect uniform exploration policy. Indeed, the formula defining the loss in (3.7) assumes m is deterministic and cannot be applied when m=m(B) is chosen in an adaptive (and random) manner.

Selecting α_t is often considered an art in bandit learning and for us is mostly used for theoretical analysis. In practice, we observe that it is sufficient to choose α_t as a sequence with exponential decay in t.

Remark 5.4. Let N(B) denote the number of affordable samples for exploiting under budget B. (5.10a) implies that both m(B) and N(B) diverge as B goes to infinity. In addition, one can see from the proof that $S^*(t) = S^*$ for sufficiently large t almost surely. These combined with Theorem 4.2 imply that the estimators produced by Algorithm 5.1 are almost surely consistent.

6. Vector-valued responses and efficient estimation.

6.1. Vector-valued high-fidelity models. We now generalize the results in the previous section to the case of vector-valued responses, i.e., $k_0 > 1$. Let

$$f(Y) = (f^{(1)}(Y), \dots, f^{(k_0)}(Y))^T \in \mathbb{R}^{k_0}$$

denote the response vector. The linear model assumption in (2.2) is modified as follows:

$$(6.1) f(Y) = \beta_S X_S + \varepsilon_S,$$

where $\varepsilon_S = (\varepsilon_S^{(1)}, \dots, \varepsilon_S^{(k_0)})^T \sim \mathcal{N}(0, \Gamma_S)$ is a centered multivariate normal distribution with covariance matrix Γ_S , and $\beta_S = (\beta_S^{(1)}, \dots, \beta_S^{(k_0)})^T \in \mathbb{R}^{k_0 \times (s+1)}$ is the

coefficient matrix for model S. For fixed S, one may use (3.3) to estimate the coefficients $\beta_S^{(j)}$ by $\widehat{\beta}_S^{(j)}$ for $j \in [k_0]$, and the corresponding LRMC estimators can be built similarly as in (3.4). To generalize the MSE, we consider a common class of quadratic risk functionals to measure the quality of the LRMC estimators. Let $Q \in \mathbb{R}^{q \times l}$, and let $\widehat{\theta}$ be an estimator for $\theta \in \mathbb{R}^l$ where q is arbitrary. The Q-risk of $\widehat{\theta}$ is defined as

$$(6.2) \qquad \qquad \mathrm{Risk}(\widehat{\theta}) = \mathbb{E}\left[\left\| Q(\widehat{\theta} - \theta) \right\|_2^2 \right] = \mathbb{E}\left[(\widehat{\theta} - \theta)^T Q^T Q(\widehat{\theta} - \theta) \right],$$

where we suppress the notational dependence of Risk on Q. We use the following conditional Q-risk on the estimated coefficient matrix $\widehat{\beta}_S$ in place of (3.5):

$$(6.3) \qquad \mathsf{Risk}_S|_{\widehat{\beta}_S} := \mathsf{Risk}(\mathsf{LRMC}_S)|_{\widehat{\beta}_S} = \mathbb{E}\left[\|Q(\mathsf{LRMC}_S - \mathbb{E}[f(Y)])\|_2^2\,|\widehat{\beta}_S|\right],$$

where above $Q \in \mathbb{R}^{q \times k_0}$ for arbitrary q. A result similar to Theorem 4.2 can be obtained for the LRMC estimator under (6.3).

THEOREM 6.1. Under the same conditions as in Theorem 4.2 and the joint normality assumption (6.1), the following result holds: For large m, with probability at least $1 - m^{-2}$,

$$(6.4) \qquad \textit{Risk}_S|_{\widehat{\beta}_S} \lesssim \frac{1}{N_S} \operatorname{tr} \left(\Sigma_S \beta_S^T Q^T Q \beta_S \right) + (s+1) \operatorname{tr} \left(Q \Gamma_S Q^T \right) \frac{\log m}{m},$$

where the implicit constant in \leq is independent of m.

Other results in the previous section (including Algorithm 5.1 and Theorem 5.3) can also be generalized to the vector-valued case; since the ideas are similar, we do not restate them here. An extended discussion of the results and the proof of Theorem 6.1 can be found in Appendix SM4. The corresponding algorithm is Algorithm SM4.1.

- **6.2. Efficient estimation.** Estimation for vector-valued responses is more challenging due to the presence of high-dimensional parameters. Nevertheless, we are only interested in some functionals of the high-dimensional parameters, i.e., $\operatorname{tr}(Q\Gamma_SQ^T)$, for instance, instead of Γ_S itself. For these functionals, the plug-in estimators are relatively accurate for $t \gtrsim s+1$. See Appendix SM4 for a discussion that theoretically establishes this point.
- 7. Numerical simulations. In this section we demonstrate performance of the AETC algorithms (Algorithms 5.1 and SM4.1). The regularization parameters α_t are set as $\alpha_t = 4^{-t}$ in all simulations, except in one case (Figure 5) where we investigate how the accuracy of AETC depends on α_t . We will utilize four methods to solve multifidelity problems:
 - (MC) Classical Monte Carlo, where the entire budget is expended over the high-fidelity model.
 - (MFMC) The multifidelity Monte Carlo procedure from [43], which is provided with oracle correlation information in Table 2.
 - (AETC) Algorithm 5.1 (for scalar responses) or SM4.1 (for vector responses).
- (AETC-re) Algorithm 5.1 or SM4.1, but we recycle samples from exploration when computing exploitation estimates. See Remark 3.1.

To evaluate results, we compute and report an empirical MSE over 500 samples. Since both AETC and AETC-re produce random estimators due to the exploration step, the experiment (including both exploration and exploitation) is repeated 200 times with the 0.05-0.50-0.95-quantiles recorded.

Table 2 Oracle information of f(Y) and $X^{(i)}$ (approximated with three digits) in the case of the square domain (top) and the L-shape domain (bottom).

Model	f(Y)	$X^{(1)}$	$X^{(2)}$	$X^{(3)}$	$X^{(4)}$	$X^{(5)}$	$X^{(6)}$
$Corr(\cdot, f(Y))$	1	0.998	0.992	0.976	0.940	0.841	-0.146
Mean	9.641	9.197	8.749	8.287	7.782	7.141	6.160
Standard deviation	0.127	0.113	0.099	0.086	0.072	0.052	0.027
Cost	4096	1024	256	64	16	4	1

Model	f(Y)	$X^{(1)}$	$X^{(2)}$	$X^{(3)}$	$X^{(4)}$	$X^{(5)}$	$X^{(6)}$
$Corr(\cdot, f(Y))$	1	0.999	0.995	0.980	0.932	0.733	-0.344
Mean	25.940	24.256	22.902	21.180	19.054	16.072	12.275
Standard deviation	0.290	0.242	0.195	0.149	0.104	0.061	0.070
Cost	4096	1024	256	64	16	4	1

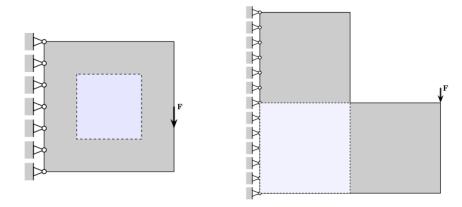


Fig. 1. Geometry, boundary conditions, and loading for two linear elastic structures, the square and the L-shape. The regions in which the vector-valued quantities are investigated are highlighted in light blue.

7.1. Multifidelity finite element approximation for parametric PDEs.

In the first example, we investigate the performance of our approach on a multifidelity parametric solution of linear elastic structures. We consider two scenarios associated with different geometries of the domain, namely square and L-shape structures. The geometry, boundary conditions, and loading in these structures are shown in Figure 1.

The model is an elliptic PDE that governs motion in linear elasticity. In a parametric setting, we introduce the parametric/stochastic version of this governing equation. In a bounded spatial domain D with boundary ∂D , the parametric elliptic PDE is

(7.1)
$$\begin{cases} \nabla \cdot (E(\boldsymbol{p}, \boldsymbol{x}) \nabla u(\boldsymbol{p}, \boldsymbol{x})) = f(\boldsymbol{x}) & \forall (\boldsymbol{p}, \boldsymbol{x}) \in \mathcal{P} \times D, \\ u(\boldsymbol{p}, \boldsymbol{x}) = 0 & \forall (\boldsymbol{p}, \boldsymbol{x}) \in \mathcal{P} \times \partial D, \end{cases}$$

where E, the elasticity matrix dependent on state variables \boldsymbol{x} , is parameterized with the random variables \boldsymbol{p} , and f is the forcing function. We assume that $\boldsymbol{p} \in \mathcal{P}$ is a d-dimensional random variable with independent components $\{p_i\}_{i=1}^d$. The solution of

this parametric PDE is the displacement $u \equiv u(\mathbf{p}, \mathbf{x}) : \mathcal{P} \times D \to \mathbb{R}$. The displacement is used to compute the scalar quantity of interest, the *compliance*, which is the measure of elastic energy absorbed in the structure as a result of loading,

(7.2)
$$\operatorname{cpl} := \int_{D} \nabla u(\boldsymbol{p}, \boldsymbol{x})^{T} E(\boldsymbol{p}, \boldsymbol{x}) \nabla u(\boldsymbol{p}, \boldsymbol{x}) d\boldsymbol{x}.$$

The linear elastic structure is subjected to plane stress conditions and the uncertainty is considered in the material properties, namely the elastic modulus, which manifests in the model through the random parameters p. To model the uncertainty, we consider a random field for the elastic modulus via a Karhunen Loéve (KL) expansion,

(7.3)
$$E(\boldsymbol{p}, \boldsymbol{x}) = E_0(\boldsymbol{x}) + \delta \left[\sum_{i=1}^d \sqrt{\lambda_i} E_i(\boldsymbol{x}) p_i \right],$$

where $\delta = 0.5$, $E_0(\boldsymbol{x}) = 1$ are constants, and the random variables p_i are uniformly distributed on [-1,1] and the eigenvalues λ_i and basis functions E_i are taken from the analytical expressions for the eigenpairs of an exponential kernel on $D = [0,1]^2$. The Poisson's ratio is $\nu = 0.3$, and we use d = 4 parameters. We solve the partial differential equation (7.1) for each fixed \boldsymbol{p} via the finite element method with standard bilinear square isotropic finite elements on a rectangular mesh.

In this example, we form a multifidelity hierarchy through mesh coarsening: Consider n=7 mesh resolutions with mesh sizes $h=\{1/(2^{8-L})\}_{L=1}^7$, where L denotes the level. The mesh associated with L=1 yields the most accurate model (highest fidelity), which is taken as the high-fidelity model in our experiments. To utilize the notation presented earlier in this article, our potential low-fidelity regressors are formed from the compliance computed from various discretizations,

$$X^{(i)} = \operatorname{cpl}^{(i)} \in \mathbb{R}, \qquad i \in [6],$$

where $\mathsf{cpl}^{(i)}$ is the compliance of the solution computed using a solver with mesh size $h = 2^{i-7}$. We provide more details about the discretization and the uncertainty model of this section in Appendix SM5.

The cost for each model is the computation time, which we take to be inversely proportional to the mesh size squared, i.e., h^2 . (This corresponds to employing a linear solver of optimal linear complexity.) We normalize cost so that the model with the lowest fidelity has unit cost. The total budget B ranges from 10^5 to 4×10^5 , and our simulations increment the budget over this range by 0.5×10^5 units. A larger budget simulation can be done but requires more time to generate sufficient high-fidelity data, thus it is not implemented here. We refer to [55] for a further study of the square domain when the budget ranges from 10^5 to 10^7 .

7.1.1. Scalar high-fidelity output. In the first experiment, the response variable is chosen as the compliance of the high-fidelity model, i.e.,

$$f(Y) = \operatorname{cpl}^{(0)} \in \mathbb{R}.$$

Therefore, for AETC we use Algorithm 5.1. The oracle statistics of f(Y) and $X^{(i)}$ are computed over 50000 independent samples and shown in Table 2.

In both cases, the expensive models are more correlated with the high-fidelity model than the cheaper ones. Such hierarchical structure is often a necessary assumption for the implementation of multifidelity methods, the MFMC, for instance.

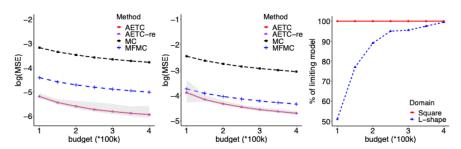


Fig. 2. Comparison of the (\log_{10}) MSE of the LRMC estimator given by the AETC algorithm, the AETC algorithm reusing the exploration samples (AETC-re), the MC estimator, and the MFMC estimator as the total budget increases from 10^5 to 4×10^5 in the case of the square domain (left) and the L-shape domain (middle). The 0.05-0.50-0.95-quantiles are plotted for the LRMC estimator to measure its uncertainty. We also compute the probability (plotted as a percentage) that the AETC algorithm selects the limiting model given by (5.5) (right).

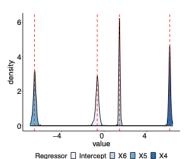
Accuracy results for various multifidelity procedures are shown in the first two plots in Figure 2. As the budget goes to infinity, the model selected by AETC converges to the minimizer given by (5.5), which can be explicitly computed using oracle information. Particularly, solutions to (5.5) in the case of the square domain and the L-shape domain are respectively as follows:

- square domain: $f(Y) \sim X^{(4)} + X^{(5)} + X^{(6)} + \text{intercept};$
- L-shape domain: $f(Y) \sim X^{(3)} + X^{(4)} + X^{(5)} + X^{(6)} + \text{intercept.}$

The regression coefficients for the square domain and L-shape domain are 6.151 $(X^{(4)})$, $-6.509 (X^{(5)})$, $1.444 (X^{(6)})$, -0.640 (intercept), and $5.537 (X^{(3)})$, $-6.606 (X^{(4)})$, $2.559 (X^{(5)})$, $-0.437 (X^{(6)})$, and -1.210 (intercept), respectively. Note that there is a canceling effect for the more expensive regressors due to high correlations. Neither limiting model above will be used by the MFMC estimator as the relationship between cost and correlation does not satisfy the assumption [43, condition (20)]. For every budget level B under our test, we compute the empirical probability (as a percentage) that the limiting model is selected by AETC and plot this in rightmost panel in Figure 2.

Figure 2 shows that for both domain geometries, the AETC algorithm outperforms both MC and MFMC by a notable margin, even though the latter has access to oracle correlation statistics that are not provided to AETC. Little difference between AETC and AETC-re is visible, which is not surprising since the number of the exploitation samples is much larger than the number of exploration rounds. The MSE of AETC is smaller in the case of the square domain than in the L-shape domain under the same budget, for which a possible explanation is that the variance of the surrogate models in the former is smaller than in the latter (Table 2), making the exploration procedure more efficient in the square domain case. Finally, note that as the budget goes to infinity, the MSE of the AETC algorithm decays to zero, and the frequency of AETC exploiting the limiting model given by (5.5) converges to 1, verifying the asymptotic results in Theorem 5.3. The densities of the learned regression coefficients of the limiting model in both cases when $B=4\times 10^5$ are provided in Figure 3.

In this example, despite a deterministic nonlinear relationship between f(Y) and $X^{(i)}$, the conditional expectation $\mathbb{E}[f(X)|X_S]$ does seem to admit a reasonable approximation using an appropriately constructed linear combinations of the low-fidelity model outputs in the selected subsets by AETC. In particular, it can be seen from



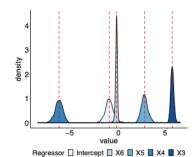


Fig. 3. Densities of the estimated coefficients of the limiting model learned by AETC under budget $B=4\times 10^5$ in 200 experiments in the case of the square domain (left) and the L-shape domain (middle). Red dashed lines correspond to the true values of the coefficients estimated using the whole dataset.

Table 3 Oracle information of f(Y) and $X^{(i)}$ (approximated with three digits) in the case of the square domain with randomness dimension d=20.

Models	f(Y)	$X^{(1)}$	$X^{(2)}$	$X^{(3)}$	$X^{(4)}$	$X^{(5)}$	$X^{(6)}$
$Corr(\cdot, f(Y))$	1	0.998	0.989	0.966	0.914	0.789	-0.135
Mean	9.645	9.200	8.752	8.290	7.784	7.142	6.160
Standard deviation	0.137	0.120	0.104	0.089	0.073	0.052	0.027
Cost	4096	1024	256	64	16	4	1

Figure 3 that the regression coefficients learned by AETC on the limiting model, which are estimated based on less than 25 random exploration samples in both cases, are close to their true values computed using the oracle dataset (50000 independent samples).

In the rest of this section, we focus on the square domain case to further test the performance of AETC. We will take a much larger KL truncation dimension d=20 to inject more randomness into the models. To better demonstrate the behavior of the algorithms in the asymptotic regime, we use a greater budget range than in the previous simulation, i.e., the total budget B ranges from 2×10^5 to 12×10^5 , with budget increment 2×10^5 units. The oracle statistics of f(Y) and $X^{(i)}$ are computed over 50000 independent samples and shown in Table 3.

We first conduct a standard analysis for AETC, including an average MSE comparison with the other two methods and the convergence to the limiting model. As before, we use oracle statistics to compute the limiting model via (5.5), which in this case is given by $f(Y) \sim X^{(4)} + X^{(5)} + X^{(6)} + \text{intercept.}$ Note that this model is different from the one in the previous example where d=4. A plausible explanation, as can be seen from Tables 2 and 3, is that the low-fidelity models are less correlated with the high-fidelity model when d is large, thus AETC leans toward utilizing more low-fidelity models to achieve equally accurate predictions. Moreover, we include two additional plots to summarize the statistics (median) of the exploration/exploitation rate in AETC as opposed to the optimal rates (5.4) computed using the oracle statistics, as well as a plot of the estimation given by AETC along 100 trajectories at different budget. The results are reported in Figure 4.

Figure 4 shows a consistent outperformance of AETC algorithm over the other two methods as in Figure 2 and the expected model convergence. Both the exploration and exploitation rates in AETC asymptotically match the optimal rates computed using

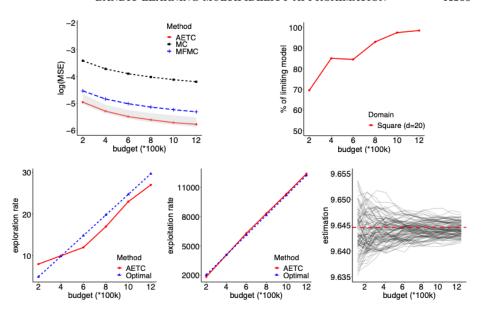


Fig. 4. Comparison of the (\log_{10}) MSE of the LRMC estimator given by the AETC algorithm, the MC estimator, and the MFMC estimator as the total budget increases from 2×10^5 to 12×10^5 in the case of the square domain with KL truncation parameter d=20 (top left). The 0.05-0.50-0.95-quantiles are plotted for the LRMC estimator to measure its uncertainty. We also compute the probability (plotted as a percentage) that the AETC algorithm selects the limiting model given by (5.5) (top right), and the median of the exploration (bottom left) and exploitation (bottom middle) rate in AETC at a different budget. Finally, we provide the estimated values for $\mathbb{E}[f(Y)]$ of the LRMC estimation in AETC at a different budget along 100 random trajectories, with the red dashed line referring to the true value of $\mathbb{E}[f(Y)]$ (bottom right).

the oracle statistics, verifying the statement (5.10a) in Theorem 5.3. Moreover, by plotting the AETC estimation along 100 random trajectories (with multiple evaluation at a different budget), we notice that the LRMC estimator in the AETC algorithm converges to $\mathbb{E}[f(Y)]$ as the budget goes to infinity. This observation is consistent with Remark 5.4.

We next investigate how the performance of AETC depends on the regularization parameters α_t . Besides the default setup $\alpha_t = 4^{-t}$, we consider two alternative choices $\alpha_t = 2^{-t}$ and $\alpha_t = 8^{-t}$, respectively corresponding to a more and a less active exploration strategy in the early stage of learning. We apply AETC with different regularization parameters to the same training dataset under a different total budget, and record the corresponding average MSEs. The simulation results are reported in Figure 5.

It can be seen from Figure 5 that for a large budget, the three exponential-decaying choices for α_t yield similar accuracy results. For a small budget, however, the larger α_t is slightly more accurate, thanks to a more active early-stage exploration enforced by the regularization.

7.1.2. Vector-valued high-fidelity output. The same experiment is repeated when f(Y) is taken as a vector-valued response, and hence we utilize Algorithm SM4.1. We take f(Y) to be defined by nine randomly selected components of the magnitude of the discrete solution (displacement) given by the high-fidelity model within a region

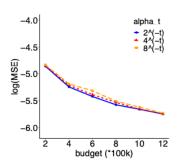


Fig. 5. Comparison of the average (log₁₀) MSE of the AETC algorithm at three different regularization parameters ($\alpha_t = 2^{-t}, 4^{-t}, 8^{-t}$) as the total budget increases from 2×10^5 to 12×10^5 in the case of the square domain with KL truncation d=20.

highlighted in blue in Figure 1, i.e.,

$$f(Y) := \bar{\boldsymbol{u}}^{(0)}|_{T}, \qquad \qquad \bar{\boldsymbol{u}}^{(0)} = \sqrt{\left(\boldsymbol{u}_{x}^{(0)}\right)^{2} + \left(\boldsymbol{u}_{y}^{(0)}\right)^{2}} \in \mathbb{R}_{+}^{2601},$$

where T is a subset of coordinates in the highlighted region in Figure 1 with |T|=9, and the arithmetic operations above are taken componentwise. The full spatial domain of the structures depicted in Figure 1 is in $[0,1]^2$, and the highlighted regions are squares with the size 0.5×0.5 in the center and lower left corner of the square and L-shape structures, respectively. In order to compute the vector-valued quantity at the same points across all resolutions, we evaluate \bar{u} on a fixed 51×51 mesh across different resolutions, where the evaluations are accomplished by using the continuous solution from the finite element approximation.

For the square domain, T is taken as a randomly selected 3×3 block of pixels from the 51×51 solution vector corresponding to the highlighted region in Figure 1. For the L-shape domain, T is taken as nine randomly sampled components from the 51×51 -dimensional solution vector corresponding to the highlighted region in Figure 1. For both cases, Q is the identity matrix I_9 , so the Q-risk defined in (6.3) is simply the sum of the MSE of each response. We show oracle information of the correlations between $X^{(i)}$ and $f^{(j)}(Y)$, $i \in [6]$, $j \in [9]$ in Figure 6.

For both domain structures, cheaper models have some strong correlations with the high-fidelity model, implying that the cost-correlation hierarchical structure (an assumption for MFMC) is violated. We thus compare only the MC estimator with AETC (for vector-valued high-fidelity output). The oracle limiting models to which AETC will converge are

- square domain: $f(Y) \sim X^{(4)} + X^{(5)} + X^{(6)} + \text{intercept};$
- L-shape domain: $f(Y) \sim X^{(3)} + X^{(4)} + X^{(5)} + X^{(6)} + \text{intercept.}$

The details of the results are given in Figure 7, which are consistent with the conclusion drawn from Figure 2.

7.2. Mixture of reduced-order models. In this example, we consider a multifidelity problem using the same model as in the previous section on the square domain, but we generate different types of reduced-order models (or surrogate models) which approximate the compliance of the solution to (7.1). We will use the compliance computed via the finite element method on a $2^6 \times 2^6$ mesh as the ground truth, i.e., the surrogate model $X^{(1)}$ in the first table in Table 2 is treated as the high-fidelity model



	×	2	2	*	X	9	- 1
Y1	0.551	0.568	0.583	0.564	0.272	-0.726	0.8
Y2					0.567	0.899	0.6
Y3	-0.331	-0.276			0.321	0.666	0.4
Y4	0.544	0.562	0.581	0.568	0.283	-0.736	-0.2
Y5	-0.492	-0.48	-0.453	-0.367		0.958	0
Y6	-0.543	-0.529	-0.499	-0.407		0.954	-0.2
Y7	0.794	0.803	0.807	0.772	0.47	-0.709	-0.4
Y8	-0.518	-0.51	-0.488	-0.41		0.94	-0.6
Y9	0.668	0.679	0.687	0.659	0.351	-0.796	-0.8

Fig. 6. Correlations between $X^{(i)}$ and $f^{(j)}(Y)$, $i \in [6]$, $j \in [9]$ in the case of the square domain (top) and the L-shape domain (bottom). The entry associated to indices (Xi, Yj) is the value of $Corr(X^{(i)}, f^{(j)}(Y))$.

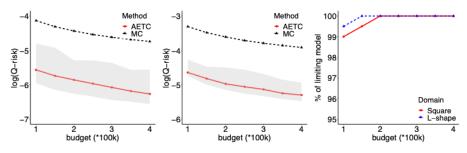


Fig. 7. Comparison of the (\log_{10}) Q-risk of the LRMC estimator given by the AETC algorithm and the MC estimator as the total budget increases from 10^5 to 4×10^5 in the case of the square domain (left) and the L-shape domain (middle). The 0.05-0.50-0.95-quantiles are plotted for the LRMC estimator to measure its uncertainty. We also compute the probability (plotted as a percentage) that the AETC algorithm selects the limiting model given by (SM4.11) (right).

Y. We explore two classes of choices for reduced-order models:

- Gaussian process (GP) emulators. Low-fidelity regressors $X^{(i)}$ for $i \in [6]$ are generated as the mean of GP emulators built on compliance data from Y. We use an exponential covariance kernel and optimize hyperparameters by maximizing the log-likelihood. For $n_T = 10,100,1000$ training points in parameter space, this defines models $X^{(1)}$, $X^{(3)}$, $X^{(5)}$, respectively. We then select nonoptimal hyperparameters with the same training data $n_T = 10,100,1000$, which defines models $X^{(2)}$, $X^{(4)}$, $X^{(6)}$, respectively. The cost of these models is given by the cost of training, optimization, and evaluation of the GP averaged over 2×10^4 different values of p. We perform each experiment five times and report the average time (cost) for each model in Table 4.
- Projection-based model reduction with proper orthogonal decomposition (POD). We generate k POD basis functions from high-fidelity displacement data, we use this to form a rank-k Galerkin projection of the finite element

Table 4

Oracle information of f(Y) and $X^{(i)}$. The numerator of the asymptotic average conditional MSE estimate (5.4) is also shown.

Model	f(Y)	$X^{(1)}$	$X^{(2)}$	$X^{(3)}$	$X^{(4)}$	$X^{(5)}$
$Corr(\cdot, f(Y))$	1	0.993	0.414	1-2e-05	0.401	1-1e-06
Mean	9.197	9.195	9.147	9.197	9.045	9.197
Standard deviation	0.113	0.122	0.556	0.113	0.335	0.113
Cost	9233.69	0.31	0.31	2.31	2.33	30.79
(5.4) with $S = \{i\}$	-	4.202	203.025	0.358	214.676	3.574

Model	$X^{(6)}$	$X^{(7)}$	$X^{(8)}$	$X^{(9)}$	$X^{(10)}$	$X^{(11)}$	$X^{(12)}$
$Corr(\cdot, f(Y))$	1-2e-04	0.999	1-2e-04	1-5e-05	1-8e-06	≈ 1	≈ 1
Mean	9.196	9.189	9.194	9.195	9.197	9.197	9.197
Standard deviation	0.114	0.113	0.113	0.113	0.113	0.113	0.113
Cost	31.29	0.18	0.45	0.68	0.85	1.03	2.02
(5.4) with $S = \{i\}$	6.226	0.732	0.243	0.180	0.137	0.119	0.230

formulation, and models $X^{(i)}$ for $i=(7,\ldots,12)$ are the compliances computed from the projected systems of rank k=(1,2,3,4,5,10), respectively. The cost of this procedure is taken as *only* the cost of solving the rank-k projected system and does *not* include the time required to collect POD training data or the time required to compute the POD modes.

More details about the experimental setup above are given in Appendix SM6. The oracle statistics and costs for the GP and POD low-fidelity models are shown in Table 4. Note that here we have not normalized the cost relative to the low-fidelity model.

We now apply the (scalar response) AETC algorithm to this multifidelity setup, with the total budget ranging from 10^5 to 2×10^5 , incremented by 0.2×10^5 in our experiments. We have 12 low-fidelity models in total, and exhausting all of them for selection would require complexity on the order of $2^{12}-1$. Since the AETC algorithm generally produces an efficient combination of relatively cheap regressors, we set the maximal number of regressors in the model to be five to accelerate computation, i.e., we explore only for $s=|S|\leq 5$. (We could have used the full model, which would not incur too much an increase in computation time but would require taking more exploration samples to start with, which is a waste of resources.)

The performance of AETC is compared to the direct MC estimator applied to f(Y), and the results are reported in the first plot in Figure 8. The figure shows that AETC is more efficient than the MC estimator by a substantial margin in terms of the MSE. To better see how this is reflected in practice, we fix the budget to be $B=10^5$, run 200 experiments of both AETC and MC, and compute the difference between the estimated values of $\mathbb{E}[f(Y)]$ and the ground truth. This is illustrated in the second plot in Figure 8. Since this multifidelity setup contains surrogates obtained from different types of methods, we investigate which are chosen by AETC for exploitation. This information is given in the last plot in Figure 8. The most frequent models chosen by the AETC are between models $X^{(10)}$ and $X^{(11)}$, both of which have near-perfect correlation with f(Y) with only a moderate cost. In fact, $X^{(11)}$ is also the oracle limiting model given by (5.5), although the convergence is rather slow due to the competitor $X^{(10)}$, which has an extremely high correlation but a slightly cheaper cost. The other models which have been selected by the AETC are the other POD models as well as their combinations with models $X^{(1)}$ and $X^{(2)}$. These models correspond to the lowest-fidelity models in each method of approximation and are often cheap to sample from with reasonably high correlation.

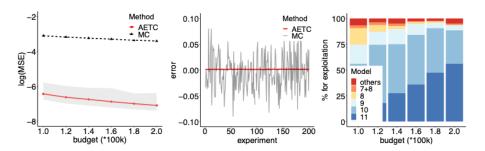


Fig. 8. The left plot is the (\log_{10}) MSE of the estimators as the budget increases, with the 0.05-0.5-0.95-quantiles plotted for the AETC algorithm to measure the uncertainty in the exploration. The middle plot compares the estimation error of the AETC algorithm by plotting instances of the error over each of 200 experiments for a fixed total budget $B=10^5$. The right plot shows the empirical probability (plotted as a percentage) of certain models being selected by AETC for exploitation.

8. Conclusions. We have proposed a novel algorithm for the multifidelity problem based on concepts from bandit learning. Our proposed AETC procedures, Algorithms 5.1 and SM4.1, operate under the assumption of a linear relationship between low-fidelity features and a high-fidelity output. Their exploration phase expends resources to learn about model relationships in order to discover an effective linear relationship. The exploitation phase leverages the cost savings by regressing on low-fidelity features to produce an LRMC estimate of the high-fidelity output. Under the linear model assumption, we show the consistency of the LRMC, whose MSE can be partitioned into a component stemming from exploration, and another from exploitation. This partition allows us to construct the AETC algorithm, which is an adaptive procedure operating under a specified budget that decides how much effort to expend in exploration versus exploitation and also identifies an effective linear regression low-fidelity model. We show that, for a large budget, our AETC algorithms explore and exploit optimally.

The main advantage of our approach is that no a priori statistical information or hierarchical structure about models is required, and very little knowledge about model relationships is needed: AETC needs only an identification of which model is the trusted high-fidelity one, along with a specification of the cost of sampling each model. The algorithm proceeds from this information alone, which is a distinguishing feature of our approach compared to alternative multifidelity and multilevel methods, and can be used to tackle situations when a natural cost versus accuracy hierarchy is difficult to identify, and when relationships between models are not known.

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