Exploration in Online Advertising Systems with Deep Uncertainty-Aware Learning

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ABSTRACT

Modern online advertising systems inevitably rely on personalization methods, such as click-through rate (CTR) prediction. Recent progress in CTR prediction enjoys the rich representation capabilities of deep learning and achieves great success in large-scale industrial applications. However, these methods can suffer from lack of exploration. Another line of prior work addresses the exploration-exploitation trade-off problem with contextual bandit methods, which are recently less studied in the industry due to the difficulty in extending their flexibility with deep models. In this paper, we propose a novel Deep Uncertainty-Aware Learning (DUAL) method to learn CTR models based on Gaussian processes, which can provide predictive uncertainty estimations while maintaining the flexibility of deep neural networks. DUAL can be easily implemented on existing models and deployed in real-time systems with minimal extra computational overhead. By linking the predictive uncertainty estimation ability of DUAL to well-known bandit algorithms, we further present DUAL-based Ad-ranking strategies to boost up long-term utilities such as the social welfare in advertising systems. Experimental results on several public datasets demonstrates the effectiveness of our methods. Remarkably, an online A/B test deployed in the Alibaba display advertising platform shows an 8.2% social welfare improvement and an 8.0% revenue lift.

CCS CONCEPTS

• Information systems → Personalization; Online advertising;
• Computing methodologies → Gaussian processes.

KEYWORDS

click-through rate (CTR), exploration-exploitation trade-off, advertising system, Gaussian process

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1 INTRODUCTION

Online advertising [5] has become one of the most important business in today’s e-commerce platforms, social networks, and news/movie content providers, where billions of Internet users can be reached every day. In current online advertising markets, cost-per-click (CPC) campaigns are widely preferred, where advertisers pay for each click on their advertisements (Ads). The effectiveness of advertising systems therefore largely depends on personalization techniques, such as click-through rate (CTR) prediction, which captures user interests and helps distribute online traffic efficiently, and potentially reduces unpleasant user experiences.

Recently, deep learning-based CTR prediction methods have achieved great success [9, 18, 33, 50, 51] due to their ability to learn rich representations of user behaviors and Ad characteristics. Such models are usually trained in a purely supervised learning manner, where the training data (i.e., Ad impressions and user feedback) are sequentially obtained from online serving. Based on the CTR predictions, a common Ad-ranking strategy derived from the widely used generalized second-price auction [12] is to display Ads according to the ranking of predicted eCPMs (effective cost per mille), which in turn produces the data for further updates of the CTR model (as illustrated in Fig. 1). However, due to lack of exploration [7] (as detailed in Sec. 2), these models can gradually focus on a small subset of Ad candidates and miss out on opportunities to find the unknown better ones, potentially leading to suboptimal predictive performance and unsatisfying social welfare [12].

Exploring in advertising systems can be very expensive. In contrast to supervised learning, another line of prior work in recommendation systems (which is closely related to advertising systems) is formulated as a contextual bandit problem [25, 39], in which the system sequentially displays items to the users based on contextual information of the user and items, and updates its...
We review the importance of CTR prediction in advertising systems and identify their good practices which can be adapted to contextual bandit methods while maintaining the powerful representation capabilities of deep neural networks. The core idea is to learn deep CTR models that can provide uncertainty estimations of the predictions, which is the key to navigating the exploration in contextual bandit problems. In DUAL, possessing a Bayesian perspective of CTR modeling, we impose a Gaussian process (GP) prior distribution to the unknown true function and obtain the predictions as well as the uncertainty estimations from the posterior given the observed data. We present practical learning and inference algorithms for DUAL and an efficient implementation so that it can be easily deployed in real-time systems with minimal extra computational overhead. By combining the uncertainty estimations from DUAL with widely-known bandit algorithms such as UCB [1] and Thompson Sampling [8], we obtain new DUAL-based Ad-ranking strategies, which manage to balance the exploration-exploitation trade-off and improve long-term utilities. Finally, we demonstrate the effectiveness of our proposed methods in terms of predictive performance and long-term social welfare on several public datasets, and identify their good practices in the Alibaba display advertising platform.

To sum up, our main contributions are as follows:

- We present a novel approach to learning deep CTR prediction models, named Deep Uncertainty-Aware Learning (DUAL), which can provide efficient uncertainty estimations along with the predictions and is compatible with existing deep CTR models favored in large-scale industrial applications.
- We propose new DUAL-based Ad-ranking strategies by combining CTR models learned by DUAL with bandit algorithms, to efficiently balance the exploration-exploitation trade-off and optimize long-term utilities in advertising systems.
- We conduct extensive experiments on several public datasets. Results demonstrate the effectiveness of the proposed DUAL approach for learning deep CTR models and DUAL-based strategies for long-term social welfare optimization.
- Remarkably, a two-week online A/B test deployed in the Alibaba display advertising platform shows an 8.2% social welfare improvement and an 8.0% revenue lift.

2 BACKGROUND AND MOTIVATION

We review the importance of CTR prediction in advertising systems and the common manner for learning CTR models. Then we discuss the assumptions and drawbacks behind, which motivate us to move towards a contextual bandit formulation of online advertising.

2.1 Online Advertising Systems

Currently, most cost-per-click (CPC) advertising platforms sell advertising spaces through online auctions, such as the generalized second-price (GSP) auction [12]. Under GSP auctions, Ads are displayed according to the ranking of their expected values of impression, each of which is referred to as the eCPM and defined as the product of the advertiser’s bid price and the CTR. Such a mechanism is shown to have an equilibrium maximizing the social welfare [12], i.e., the total value obtained by all advertisers, and thus promotes a long-term win-win situation for advertisers and platforms. However, since the true CTRs are inaccessible, the eCPMs are usually estimated with predicted CTRs. Therefore, CTR prediction models play an important role in today’s real-world advertising systems.

2.2 CTR Prediction

CTR prediction models are usually learned from data collected during online serving. The contextual information of each Ad impression and the user feedback are recorded as a data sample. Specifically, this information includes User Info, which contains the user’s profile and historical behaviors; Ad Info, which characterizes the content of the Ad; and Env Info, which records the environmental information such as the scene and the timestamp of the impression.

For algorithmic modeling, the contextual information of each data sample is usually represented as a feature vector. To facilitate subsequent analysis, we introduce user feature denoted by \(X_u\), which is the vectorized representation of the User Info, and let \(X_s\) denote the space of user features, i.e., \(X_u \in X_s\). The Ad feature \(x_a\), Env feature \(x_e\), and their corresponding feature spaces \(X_a\) and \(X_e\) are defined by analogy. We denote the feature vector of the data sample by the concatenation \(x = [x_u^T, x_a^T, x_e^T]^T\). We assume the joint feature space \(X = X_u \times X_a \times X_e\) has a dimension of \(d\), i.e., \(X \subset \mathbb{R}^d\). The feedback is regarded as the binary label \(y \in \{0, 1\}\), whose value takes 1 for positive feedback (i.e., click) and 0 otherwise. Finally, the dataset \(D = \{(x_i, y_i)\}_{i=1}^N\) for training CTR models is composed of all the observed data samples.

Most existing works [9, 51] tackle the CTR prediction task in a purely supervised learning manner, i.e., learning a function \(h\) mapping from \(X\) to the CTR space \([0, 1]\) (or the logit space \(\mathbb{R}\)) by minimizing the empirical risk. Formally, let \(\mathcal{H} \subset \mathbb{R}^N\) be the hypothesis space and \(\ell : (X \times \mathbb{R}) \times \mathcal{H} \rightarrow \mathbb{R}\) be the loss function. Given the training data \(D\), the learning problem is to find an empirical risk minimizer (ERM) \(\hat{h} \in \mathcal{H}\) that minimizes the empirical risk \(\hat{L}(h)\):

\[
\hat{L}(h) = \frac{1}{N} \sum_{i=1}^N \ell(f((x_i, y_i), h)), \quad \hat{h} = \arg\min_{h \in \mathcal{H}} \hat{L}(h).
\]

For CTR prediction, the loss function is usually defined as the negative log-likelihood of the sample \((x, y)\) induced by the model \(h\), i.e.,

\[
\ell((x, y), h) = -\log p(y|x; h)\]

and

\[
p(y|x; h) = y \cdot \sigma(h(x)) + (1 - y) \cdot (1 - \sigma(h(x))),
\]

where we have assumed without loss of generality that the model \(h : X \rightarrow \mathbb{R}\) outputs a logit value and the predicted CTR can be obtained by applying the sigmoid transformation \(\sigma(\cdot) = \frac{1}{1 + e^{-\cdot}}\) to the logit. Finally, practitioners adopt large-scale optimization techniques.
We discuss several assumptions in advertising systems built upon which means the learned model feedback) are listed in each time step. The blue and green dotted lines show the predicted and true CTRs, respectively. Without exploration, the system could consistently display the middle Ad due to its highest CTR prediction. The underestimation of the other two Ads has little chance to be corrected, thus leading to suboptimality. Best viewed in color.

Algorithmic approaches, such as stochastic gradient descent (SGD) [4], to obtain an (approximate) ERM \( \hat{h} \) and make further use, e.g., online serving.

### 2.3 Motivation

We discuss several assumptions in advertising systems built upon CTR prediction models. First, the Ad-ranking strategy derived from the GSP auction assumes perfect eCPM estimations. In other words, the system implements GSP auctions only when the CTR prediction model \( \hat{h} \) during online serving (which can be viewed as the test phase) relies on a key assumption behind supervised learning: the training and test samples are drawn i.i.d. from some fixed underlying data-generating distribution \( p \). Under such an assumption, the best possible model we can aspire to is the expected risk minimizer \( h^* \), which minimizes the expected risk \( L(h) \):

\[
L(h) \equiv \mathbb{E}_{(x,y) \sim p_{X \times Y}} [ℓ((x,y), h)], \quad h^* \in \arg\min_{h \in \mathcal{H}} L(h),
\]

and the uniform convergence bounds [42] guarantee that the performance gap \( L(\hat{h}) - L(h^*) \) will not be too large with high probability, which means the learned model \( h \) is reliable.

However, we point out an inherent inconsistency that the distribution of training samples for the CTR model are in fact largely influenced by the ranking of predicted eCPMs, which are in turn interfered by the CTR model itself. This contradicts the assumption behind supervised learning that the data are i.i.d. from a fixed data-generating distribution \( p_{X \times Y} \) and can further lead to lack of exploration: only those Ads that the models believe to have high eCPMs are prone to be displayed and then collected into future data. This is likely to result in inaccurate predictions for those Ads that have rarely or never been displayed, which further violates the assumption of perfect eCPM estimations behind the Ad-ranking strategy. Moreover, since the CTR models are usually regularly retrained to incorporate the latest data, it potentially forms a pernicious feedback loop [7] (see Fig. 1 and a concrete example in Fig. 2), which can gradually lead to consistent inaccuracy in predictive performance, suboptimal auction mechanisms, and even unintended social and economic consequences [6] such as price discrimination [32]. Such self-interference of CTR models motivate us to move towards a contextual bandit formulation of advertising.

### 3 A CONTEXTUAL BANDIT FORMULATION

We now present a joint formulation of the CTR prediction and the Ad-ranking strategy from a contextual bandit [25] perspective, which explicitly takes the sequential nature into consideration to overcome the issue of lack of exploration discussed in Sec. 2.3.

Let \( \mathcal{A} \) be the set of available Ads. Formally, we consider advertising as a decision problem that takes a user feature and an Env feature \((x_u, x_e) \in X_u \times X_e \) as input and outputs an ordering of \( \mathcal{A} \), which describes the Ad-ranking process before an impression. The inputs \((x_u, x_e)\) here are assumed to be drawn i.i.d. from a fixed distribution \( p_{X_u \times X_e} \), which can be viewed as the statistical description of online traffic. We define scoring functions \( s : \mathcal{A} \times X_u \times X_e \rightarrow \mathbb{R} \) that score each Ad \( a \in \mathcal{A} \) given \((x_u, x_e)\). Clearly, any scoring function defines an ordering of \( \mathcal{A} \), and thus corresponds to an Ad-ranking strategy. For example, the strategy that ranks Ads by predicted eCPMs can be represented by the following scoring function:

\[
s_{\text{eCPM}}(a; x_u, x_e) \overset{\text{def}}{=} \sigma(\hat{h}(x_u, x_e, a)) \cdot \text{Bid}(a), \tag{4}
\]

where \( x_e(a) \) and \( \text{Bid}(a) \) are the Ad feature and the bid price of the Ad \( a \), respectively. In the rest of this section, we assume only one Ad is displayed each time, for simplicity. In this case, the winner Ad \( a \) is the top ranking one, i.e., \( a = \arg\max_{a' \in \mathcal{A}} s(a'; x_u, x_e) \).

We further define stochastic Ad-ranking strategies, which hold a distribution \( p(s) \) over scoring functions and output orderings of \( \mathcal{A} \) with randomly sampled scoring functions from \( p(s) \). Note that the deterministic Ad-ranking strategies such as Eq. (4) also fall into this formulation, where all the probability mass of \( p(s) \) is assigned to one single scoring function. We therefore consider stochastic Ad-ranking strategies in the following, without loss of generality. With a slight abuse of notation, we also denote a stochastic strategy by \( s \) and the winner Ad by \( a = s(\mathcal{A}|x_u, x_e) \), where \( s(\mathcal{A}|x_u, x_e) \) is the distribution of winner Ads induced by \( s \).

In advertising systems, we can only observe a stochastic feedback \( y \) for the displayed Ad \( a = s(\mathcal{A}|x_u, x_e) \). Specifically, positive feedback \( y = 1 \) and negative feedback \( y = 0 \) are assumed to be drawn from an unknown conditional distribution \( p_{Y|X} \), i.e., \( y \sim p_{Y|X}(y|x_u, x_e(a), x_e) \). Since the feedback \( y \) only takes values of 1 and 0 in our formulation, the CTR is just the expectation \( \mathbb{E}_{p_{Y|X}}(y|x_u, x_e(a), x_e) \) which we denote by \( \mathbb{E}[y|x] \) for simplicity.

We then define the expected utility of a stochastic strategy \( s \) as:

\[
R(s) = \mathbb{E}_{(x_u,x_e)} - p_{X_u \times X_e} \mathbb{E}_{a \sim s(\mathcal{A}|x_u, x_e)} (\mathbb{E}[y|x] \cdot \text{Bid}(a)), \tag{5}
\]

which can be understood as the “social welfare per impression” provided that all advertisers bid truthfully. The problem of advertising is then transformed to maximizing the expected utility \( R(s) \) w.r.t. the stochastic strategy \( s \). A clear bound on \( R(s) \) is as follows:

\[
R(s) \leq \mathbb{E}_{(x_u,x_e)} - p_{X_u \times X_e} \max_{a \in \mathcal{A}} (\mathbb{E}[y|x] \cdot \text{Bid}(a)) \overset{\text{def}}{=} R(s^*), \tag{6}
\]

where \( s^* \) is the optimal Ad-ranking strategy:

\[
s^*(a; x_u, x_e) \overset{\text{def}}{=} \mathbb{E}[y|x] \cdot \text{Bid}(a). \tag{7}
\]

The interpretation of Eq. (6 & 7) is very intuitive: The utility (social welfare) is maximized when the strategy is able to identify...
and display the Ads with highest true eCPM given the user and environment, which exactly implements the GSP auctions. However, since the true CTRs/eCPMs are unknown, optimizing the strategy $s$ is essentially equivalent to maximizing the black-box eCPM function $E[y(x, a)]$ for the Ad $a$ w.r.t. a $a \in A$, which can be very difficult. To make matters worse, it is even unreliable to get an approximate solution based on historical data, since the optimal Ads may have never been displayed.

Fortunately, we can make trials (i.e., to display the Ads and get user feedback) to learn more information about the true CTRs and improve the strategy. Specifically, given the user feature and Env feature $(x^t, x^t_e)$ at time $t$, the system is able to determine and display the winner Ad $a^t \sim s(t) (A|x^t, x^t_e)$ according to the strategy $s(t)$, then receives feedback $y^t \sim p(y|x^t, a^t, x^t_e)$, and finally updates the strategy to $s^{t+1}$ based on the observed data $D_t \equiv \{(s^t, y^t)\}_{t=1}^T$. After $T$ rounds, the total utility is $\sum_{t=1}^T (y^t \cdot \text{Bid}(a^t))$, which is the objective we aim to maximize through the sequential decision-making process.

Intuitively, the strategy should favor the Ads with high eCPM predictions as well as the Ads that reveal more information about the CTR function. This is known as the exploration-exploitation trade-off and has been well discussed in previous studies of contextual bandit problems [8, 25, 30]. However, in the advertising/recommendation community, most existing methods impose strong assumptions on the unknown CTR functions, limiting their flexibility. Noticing that the key is to establish the confidence bounds or uncertainty estimations for the unknown functions, we propose a novel method for learning deep CTR models that enables uncertainty estimations, and show how it can be combined with bandit algorithms to obtain new practical Ad-ranking strategies in Sec. 4.

### 4 DEEP UNCERTAINTY-AWARE LEARNING

In this section, we present a novel Deep Uncertainty-Aware Learning (DUAL) method for CTR prediction which enables uncertainty estimations and propose DUAL-based Ad-ranking strategies for the contextual bandit problems of advertising described in Sec. 3.

#### 4.1 DUAL for CTR Prediction

Training CTR prediction models is essentially learning the unknown CTR function $E[y|x]$ w.r.t. the feature vectors $x \in X$ from the observed data $D_t$. Here we equivalently focus on the logit function, defined as $f(x) \equiv \mathbb{E}[y|x]$, which has a range of $\mathbb{R}$ and is thus convenient for analysis. Most existing deep learning-based CTR models approximate $f$ with a parameterized neural network $h$ (as described in Sec. 2.2), which gives point predictions of CTR with no measure of uncertainty. Instead, under a Bayesian perspective of function learning, we impose a prior distribution $p(f)$ to the logit function $f$ and (approximately) infer the posterior distribution $p(f|D_t)$ over functions as the learned model, which gives distributional CTR predictions and thus can provide uncertainty estimations along with the predictions.

The prior distribution expresses our prior belief about the logit function $f$. A common choice of prior distributions over functions is the Gaussian process (GP) [35], which is favored due to its high flexibility for function learning. Below, we describe how we obtain CTR predictions and uncertainties with GPs.

**Gaussian Processes for CTR Prediction.** We assume a GP prior distribution over $f$, i.e., $f \sim GP(m(x), k(x, x'))$, where $m(x) = \mathbb{E}[f(x)]$ is the mean function and $k(x, x') = \text{Cov}[f(x), f(x')]$ is the covariance kernel function. For a thorough introduction of GPs, we refer to Rasmussen and Williams [35].

We aim to estimate the logit $f^* = f(x^*)$ as well as its uncertainty at any feature point $x^* \in X$, given the observed data samples $D_t = \{(s^i, y^i(t))\}_{t=1}^T$ at time $t$. Let $x_t = [x^t(1), \ldots, x^t(l)]^T \in \mathbb{R}^{l \times d}$ be the matrix of the observed feature vectors, $f_t = f(x_t) \in \mathbb{R}^l$ be the vector of the corresponding function values, and $y_t = [y^t(1), \ldots, y^t(l)]^T \in \{0, 1\}^l$ be the vector of user feedback. Each feedback $y$ is viewed as a noisy measurement of the logit $f(x)$, generated from a Bernoulli likelihood model $p(y|f(x)) = \text{Bern}(y; \sigma(f(x)))$. Then the joint likelihood of $y_t, f_t$ and the logit value $f^*$ is:

$$p(y_t, f_t, f^*) = p(y_t, f_t') p(f_t', f^*) = p(f_t', f^*) \prod_{i=1}^l p(y^i_t | f^i(t)).$$

Then the posterior distribution of $f^*$ given $D_t$ can be evaluated as:

$$p(f^*|y_t) = \frac{\int p(y_t, f_t, f^*) \, df_t}{p(y_t)} = \frac{1}{p(y_t)} \int p(y_t, f_t) \, df_t,$$

which is the distributional prediction we desire. However, the posterior is generally intractable since the Bernoulli likelihood is not conjugate to the GP prior. Moreover, since the feature vectors are usually extremely sparse and high-dimensional in advertising systems, it is also challenging to design a proper kernel function that exploits the structural information of the feature space $X$. Inspired by Wilson et al. [45, 46], we propose to address these challenges by 1) incorporating the deep structures into base kernel functions and 2) adopting sparse variational approximate inference for GPs [40], so that we can benefit from both the expressive power of deep models and the ability of GPs to estimate uncertainties.

**Deep Kernels.** Existing deep CTR models tackle the sparsity and high-dimensionality with embeddings and learn high-level abstractions of input vectors with neural networks [18, 51]. These models can be summarized as first extracting a compact feature representation $\phi(x; \theta) \in \mathbb{R}^d$ from the input vector $x \in X \subset \mathbb{R}^d$ with a nonlinear mapping $\phi(\cdot; \theta)$ parameterized by $\theta$, and then applying a simple logistic regression to the compact feature $\phi(x; \theta)$. We propose to build up deep kernels by combining base kernels with deep nonlinear mappings. Specifically, given a deep nonlinear mapping $\phi(\cdot; \theta)$ and a base kernel $k_0(x, x')$, such as the RBF kernel $k_0(x, x') = a^2 \cdot \exp(-\|x-x'|^2/2\lambda)$, the composed kernel is defined as:

$$k(x, x') = k_0(\phi(x; \theta), \phi(x'; \theta)).$$

It is clear that this combination is compatible with any structures of deep CTR models and any valid base kernel functions.

**Sparse Variational Approximation of GP Inference.** Inference from Eq. (10) is generally very hard due to the non-conjugacy and the scalability limitation in GPs. Sparse variational GP (SVGP) methods [20, 21, 40] have shown promise in addressing these difficulties.
We present two Ad-ranking strategies based on DUAL, in which
\[ q(\mu, \Sigma)(\phi) = \frac{1}{\sqrt{2\pi}} \exp \left( -\frac{1}{2} (\phi - \mu)^T \Sigma^{-1} (\phi - \mu) \right), \]
where \( \mu \) and \( \Sigma \) are the mean and covariance of the posterior distribution of \( f \) given by the GP.

A common choice of the variational distribution is
\[ q(\mu, \Sigma)(\phi) = \frac{1}{\sqrt{2\pi}} \exp \left( -\frac{1}{2} (\phi - \mu)^T \Sigma^{-1} (\phi - \mu) \right), \]
where \( \mu \) and \( \Sigma \) are the mean and covariance of the posterior distribution of \( f \) given by the GP.

The core idea of SVGP methods is to approximate the posterior with a bunch of learned inducing points that best summarize the observed data. We propose to adopt SVGP methods for efficient and scalable approximate inference of the CTR as well as its uncertainty.

Specifically, let \( Z = [z_1, \ldots, z_M]^T \in \mathbb{R}^{M \times d} \) be a set of \( M \) parameterized vectors in \( X \), called the inducing points, and let \( u = f(Z) \).

Then the joint distribution of \( u, f^*, y^* \) given by the GP is:
\[
p(y^*, f^*, u) = \mathcal{N}(f(Z), k(Z, Z)) \mathcal{N}(\mu, \Sigma) \]  

where \( \mathcal{N}(\mu, \Sigma) \) is the Gaussian distribution.

Thompson Sampling (TS) [8], which are widely studied for decades.

The core idea of SVGP methods is to approximate the posterior distribution of \( f \) with a distribution of \( q(\mu, \Sigma)(\phi) \) that minimizes the KL divergence:
\[
\mathrm{KL}(q(\mu, \Sigma)(\phi) \parallel \mathcal{N}(\hat{f}(Z), \Sigma_f)), \]
where \( \hat{f}(Z) \) is the mean of the posterior distribution of \( f \) given by the GP.

DUAL-TS is a stochastic strategy that scores Ads following the posterior eCPM distribution:
\[
s_{\text{TS}}(a; x_U, x_E) \equiv \sigma(\hat{f}) \cdot \text{Bid}(a), \]
where \( \hat{f} \) is randomly sampled from the posterior in Eq. (13).

Intuitively, both DUAL-UCB and DUAL-TS can balance exploration against exploitation, since both encourage the system to explore new Ads or Ads with few data samples, which are expected to have high posterior uncertainties in their eCPM estimates.

Meanwhile, we also describe a greedy strategy:

**DUAL-Greedy:** DUAL-Greedy scores the Ads with predicted eCPMs while ignoring the uncertainty:
\[
s_{\text{Greedy}}(a; x_U, x_E) \equiv \sigma(\mu(a)) \cdot \text{Bid}(a). \]

Note that it is greedy w.r.t. the maximum a posteriori (MAP) estimates \( \mu(a) \), in which the prior still plays an important role (See Eq. (14)). If we choose a GP prior with a constant mean function \( m(x) = C \) and set a higher constant \( C \), the predictions to new Ads or Ads with few samples will also be higher. Under such circumstances, DUAL-Greedy will be inclined to display these Ads even if it ignores uncertainty. This suggests that with a properly specified prior, DUAL-Greedy also has the potential to conduct exploration.

It is also worth noting that the common paradigm of advertising, i.e., training a deep CTR model in the purely supervised learning manner (as described in Sec. 2.2) and ranking Ads by predicted eCPMs (as in Eq. (4)), can be viewed as a special case of the greedy strategy, to which we refer as the DNN-Greedy strategy. This can be argued by comparing Eq. (4) with Eq. (18) and the fact that \( \hat{h} \) corresponds to a MAP estimate of the logit function \( f \) in the non-parametric sense if we choose an uninformative prior [31] over \( f \). Therefore, we conjecture that DUAL-Greedy can also improve over DNN-Greedy as we can choose a more appropriate and informative prior, which is empirically verified in Sec. 6.2.

### 4.3 Practical Techniques for DUAL

We describe several practical techniques for applying DUAL in real-world CTR prediction tasks.

**Inducing Points & Regularization in Hidden Space.** Noticing that the inducing points \( Z \) always appear in the deep kernel, i.e., \( k(Z, Z) = k_h(\phi(Z), \phi(Z)) \), we directly parameterize \( Z^* \equiv \phi(Z, \theta) \in \mathbb{R}^{M \times d} \) in the hidden space instead of \( Z \in \mathbb{R}^{M \times d} \) in the input space, which extremely reduces the number of parameters to learn.

However, this raises a new issue of training when using kernels like RBF as the base kernel. Specifically, with a randomly initialized \( \theta \) and \( Z^* \), it is very likely to happen that \( \phi(\cdot; \theta) \) maps input data \( x_U \) to somewhere far from \( Z^* \) in the hidden space, which can cause gradient saturation and failure in learning. Inspired by prior work [21] that initializes the inducing points using K-means clustering, we propose to regularize the inducing points \( Z^* \) and the mapping parameters \( \theta \) with a clustering loss \( \mathcal{R}(D_\theta) \):
\[
\mathcal{R}(D_\theta) = \frac{1}{t} \sum_{i=1}^{t} \left\| \mathcal{Z}(x_y; \theta) - z_i^* \right\|^2, \]
where \( c_i = \arg \min_{m \in [M]} \| z_m^* - \phi(x_i; \theta) \| \) is the index of nearest inducing point of \( \phi(x_i; \theta) \). This regularization encourages the inducing points to track the data in the hidden space while the mapping \( \theta \) is deforming during training.

**Temperature Control.** We incorporate a temperature \( \tau \) to control the strength of the prior, which is a common practice in Bayesian
inference [44]. Specifically, we modified the ELBO in Eq. (15) to:
\[
\mathcal{L}_r(D_t) = \frac{1}{l} \sum_{i=1}^{l} \mathbb{E}_{q(f^{(i)} \mid u, S)} [\log p(y^{(i)} \mid f^{(i)})] - \tau \cdot \text{KL}[q(u) \parallel p(u)].
\]  

Then, the final loss function for practical training of DUAL is:
\[
O(\theta, Z', \nu, S; r, \lambda) = -\mathcal{L}_r(D_t) + \lambda \cdot \mathcal{R}(D_t),
\]
where both \( \tau \) and \( \lambda \) are tunable hyperparameters.

### 4.4 Computational and Memory Complexity

In addition to the deep mapping parameters \( \theta \), DUAL introduces variational parameters \( Z' \in \mathbb{R}^{M \times d'} \), \( \nu \in \mathbb{R}^{M} \) and \( S \in \mathbb{R}^{M \times M} \). The extra memory complexity is therefore \( O(Md' + M^2) \). Note that one can use structured covariance approximations such as a diagonal covariance \( S = \text{diag}(s_1, \ldots, s_M) \) to further reduce the parameters.

The terms of \( \alpha_1 \triangleq K_{uu}^{-1}(\nu - m(Z)) \) and \( \alpha_2 \triangleq K_{uu}^{-1}(K_{uu} - S) K_{uu}^{-1} \) in Eq. (14) are independent with \( x \) and thus can be precomputed before performing inference. During online inference, after computing the deep nonlinear mapping \( \phi(x'; \theta) \), we need to 1) calculate \( \beta \triangleq k(x', Z) = k_0(\phi(x'; \theta), Z') \), which costs \( O(Md') \) time; and 2) calculate \( \beta_0 \) and \( \beta \alpha_1 \) and \( \beta \alpha_2 \beta' \), which costs \( O(M^2) \) time. Therefore, the extra computational complexity of obtaining the predictive mean and variance is also \( O(Md' + M^2) \), which is almost equivalent to the complexity of an additional \( M \)-dimensional layer in deep networks for a moderate \( M \). We also empirically observe that it cause minimal additional computational overhead in large deep CTR models.

## 5 RELATED WORK

### CTR Prediction

CTR prediction has proven to be an important personalization technique in modern recommendation/advertising systems. Recently, deep learning approaches have been introduced in CTR prediction methods with great success [9, 13, 18, 19, 50, 51], due to their rich representation ability. Cheng et al. [9] combine wide linear models and deep neural networks to enjoy both memorization and generalization abilities. Zhou et al. [50] introduce recurrent units to model the evolving processes in user interests. These works mainly focus on designing better model structures and learning more effective representations of user interests. We instead propose a learning approach without specifying a concrete deep structure. Our work can be viewed as a complementary approach to these existing deep CTR prediction methods, in that it enables uncertainty estimation for arbitrary deep CTR model structures.

### Exploration-Exploitation Trade-off

The issue of exploration-exploitation trade-off in recommendation/advertising systems has been discussed for decades [2, 25, 30, 41]. Early approaches [34, 39] adopt context-free models, e.g., multi-armed bandit (MAB), in which no information is shared among users or items. To address this challenge, recent research commonly considers the contextual bandit setting [14, 23, 25], where users/items are related through features. Li et al. [25] propose LinUCB, which assumes a linear dependence between the feedback and the features. Later, the dependence assumption is extended to logistic [8, 11] and generalized linear [14, 27]. Although these methods greatly reduce the problem complexity, their assumptions are too strict and the flexibility is limited. Vanchinathan et al. [41] propose to manage the exploration-exploitation trade-off in list recommendation problem based on Gaussian process bandits [23, 38], which is close to our idea. However, our method is compatible with deep CTR models and thus can handle high-dimensional sparse data through embedding techniques, which is not available in all above-mentioned methods.

### Uncertainty Modeling in Deep Structures

Recently, there has been growing research interest in quantifying predictive uncertainty in deep neural networks [3, 15, 17, 24], which can be viewed as alternative ways to estimate uncertainties in deep CTR models. Most of the existing work resorts to Bayesian neural networks (BNN), where a prior distribution is imposed on the parameters of the neural network. The predictive uncertainty is then induced from the posterior distribution over parameters given the training data, which is obtained by variational inference [3, 16] or MCMC [15, 43] methods. Another line of research focuses on ensemble learning [24], such as bagging [31], where multiple networks are trained to produce uncertainty estimates. However, most BNNs and ensemble methods cost significantly more inference time or storage, which is too expensive to practice in large-scale industrial applications. On the contrary, our method only needs \( O(Md' + M^2) \) additional computational and memory cost. Wilson et al. [45, 46] share a similar idea of combining GPs with deep kernels. However, our work differs in two respects. First, we parameterize the inducing points in the compact hidden space instead of the input space (which could be high-dimensional and sparse), thus greatly saving the number of parameters. Second, their learning process includes two pre-training stages and a joint fine-tuning stage, which is difficult to handle in industrial practice. We instead achieve end-to-end training with a clustering regularization.

## 6 EXPERIMENTS

We present experimental results of the proposed method on several public datasets to demonstrate its effectiveness. We first examine the predictive performance of DUAL when it is combined with several state-of-the-art deep CTR models. Then, we verify the efficacy of the proposed DUAL-based strategies in long-term social welfare maximization. Finally, we share the results and techniques of a two-week online A/B test in the Alibaba display advertising platform.

Throughout the experiments, we use RBF base kernels in DUAL, i.e., \( k_0(x, x') = a^2 \cdot \exp(-\frac{\|x - x'\|^2}{2a^2}) \). We adopt Adam [22] to optimize all model parameters. Hyperparameters and detailed experimental settings will be specified later for each task. Code is available at https://github.com/duchao0726/DUAL.

### 6.1 CTR Prediction

DUAL can be treated as a complementary component to deep CTR models which enables uncertainty estimation, as described in Sec. 4.1. One common concern would be: does DUAL improve or hurt the predictive performance of the origin CTR models? To answer this question, we combine several state-of-the-art deep CTR models with DUAL and compare them with the original models.

We conduct the evaluation on two subsets of Amazon dataset [29]: Books and Electronics. The data are preprocessed in the same way as in Zhou et al. [50]. After preprocessing, Books consists of 1, 086, 120 training samples and 121, 216 test samples. Electronics consists of 346, 110 training samples and 38, 696 test samples.

The comparison is performed on five popular deep CTR models, including DNN [51], Wide&Deep [9], PNN [33], DIN [51], and DIEN [50]. The network structures and the embedding layers of the
We report the average and standard deviation of test AUC estimates with DUAL consistently producing better or comparable results. We provide a sensitivity analysis of hyperparameters.

The regularization coefficient is chosen from \( \lambda \) variational distribution, i.e., \( \mathcal{S} \). We use diagonal covariances for the variational distribution, i.e., \( S = \text{diag}(s_1, \ldots, s_M) \). This results in an \( O(M) \) (4M in our case) variational parameters, which is negligible compared to the number of weights in the deep neural networks and embedding layers. The number of inducing points \( M \) is set to 200. We choose \( m(x) = 0 \) for the mean function of the GP prior. The regularization coefficient is chosen from \( \lambda = \{0.01, 0.1, 1.0\} \) and the temperature \( \tau \) is set inversely proportional to the size of each dataset. For the RBF base kernel, we choose the amplitude \( a \in \{0.1, 0.3\} \) and the lengthscale \( l \in \{1.5, 3.0\} \) manually. We also provide a sensitivity analysis of hyperparameters.

Table 1 and Table 2 show the comparison of the predictive results. We report the average and standard deviation of test AUC estimates of 32 repeated runs for each result. For DUAL we use the predictive mean as the prediction. We observe that learning these models with DUAL consistently produces better or comparable results. We also test the vanilla models with larger MLPs (200-90-2 FC layers) which incorporate more parameters than DUAL and observe no improvement compared to the original ones. This suggests that the improvements obtained from DUAL are not simply due to the slightly more parameters. Fig. 4 shows the histograms of CTR predictions on test data from the vanilla DNN and the DNN learned with DUAL. We observe that DUAL makes much less overconfident predictions, which is as expected since the predictive mean of DUAL averages all possibilities. (Recall the example in Fig. 2. When only one negative sample is observed, the prediction of an ideal ERM is 0%, whereas DUAL will produce a positive predictive mean.) It suggests that DUAL can be more robust to overfitting, benefiting from its Bayesian formalism and awareness of uncertainty.

Sensitivity Analysis. We now investigate the influence of several hyperparameters on DUAL. Here we consider the experiments of learning the DNN models with DUAL on the Book dataset. Fig. 3 shows the results produced with different hyperparameters. First, we observe that the performance increases as the regularization coefficient \( \lambda \) increases from 0 to \( 10^{-3} \), which verifies the effectiveness of the proposed regularization technique for DUAL. For the temperature \( \tau \), we find that using the reciprocal of the number of data points produces good results. We observe that using more inducing points can improve the predictive performance. However, we do not observe significant improvement with \( M \) larger than 200. Finally, we find that the RBF base kernel has a considerable influence on the results. We thus manually choose the lengthscale \( l \) and the amplitude \( a \) of the RBF base kernel for each experiment.

6.2 Long-Term Social Welfare Maximization

We evaluate DUAL-based Ad-ranking strategies on the Yahoo! R6B dataset [48], which contains around 28 million lines of log data collected from the Today Module on Yahoo!’s frontpage within 15 days of October 2011. Each line consists of the following information:

- a 136-dimensional multi-hot user feature;
- a candidate set of available news articles and the ID of the one displayed, which was randomly drawn from the candidate set;
- a binary label indicating whether the user clicked the article.

The dataset contains 652 different articles and the average size of the candidate sets is 38. The random recommendations in the data collection process make the dataset perfectly unbiased, which allows us to evaluate the strategies with offline replay [26]. We treat each news article as an Ad and assume that their bid prices are all
equal to 1 for simplicity. In this case, the social welfare (SW) is just the number of total clicks. We compare the following strategies:

- **DUAL-TS**, **DUAL-UCB**, and **DUAL-Greedy** as described in Sec. 4.2. For **DNN-Greedy** we choose $\kappa = 1$ by manual search.
- **DUAL-TS** and **DUAL-UCB**. The predictions from a random picked model and the mean/variance of the predictions of all models are used in the TS and UCB strategies, respectively.

- **BNN-TS** and **BNN-UCB**. We learn a Bayesian deep CTR model using dropout approximation [15], where dropout is performed in both training and inference time. The predictive distribution is approximated with multiplicative stochastic forward passes. The samples and the estimated mean/variance are then used in the TS and UCB strategies, respectively.
- **Ensemble-TS** and **Ensemble-UCB**. We train an ensemble of 5 deep CTR models with bagging [31]. The predictions from a random picked model and the mean/variance of the predictions of all models are used in the TS and UCB strategies, respectively.
- **Random** selection of Ads. This acts as a trivial baseline.

For all deep structures, the same embedding technique is adopted to deal with the sparse inputs. In specific, we use a 6-dimensional embedding layer and sum pooling to convert the multi-hot user features to dense vectors and another 6-dimensional embedding layer to encode the Ad IDs, resulting in 12-dimensional compact embedding representations. For DUAL-based strategies, we use MLPs with 16-2 FC layers after the embedding layers in the deep kernels and $M = 8$ inducing points. For all other methods, the deep CTR models are built with larger MLPs with 16-8-2 FC layers after the embedding layers, for fair comparison.

For each strategy, we use the first 80,000 log entries as the initial data to pre-train its CTR model(s). After initialization, the remaining log entries are replayed to evaluate the strategies, according to the unbiased offline evaluation method proposed by Li et al. [26]. Specifically, each strategy is asked to re-rank the candidate set in each log entry and to determine the winner Ad again. If the winner Ad happens to be the one recorded as displayed in the log entry, the strategy will collect the corresponding Ad ID, the user feature, and the label as a new data sample, otherwise skip the log entry. To simulate the daily/hourly updates of CTR models in real-world systems, we update the strategies every 80,000 log entries, resulting around 2,200 data samples collected between each update and 337 total updates during each replay. We choose the best hyperparameters for each strategy by manual search.

Fig. 5a & 5b show the final cumulative SW and the daily CTRs obtained by each strategy. Results are averaged over 32 repeated runs for each experiment. First, we notice that DUAL-Greedy achieves better results than DNN-Greedy, which verifies our conjecture in Sec. 4.2. Then, we observe that DUAL-TS offers consistent performance improvements over greedy and $\epsilon$-greedy approaches, which suggests that the uncertainties provided by DUAL can help to balance the exploration-exploitation efficiently. Specifically, DUAL-TS improves DNN-Greedy by 30.7% and improves DNN-$\epsilon$-Greedy by 10.0%, benefiting from exploration.

Moreover, we find that DUAL-TS achieves better performance compared to other TS/UCB strategies that use BNN or ensemble to estimate uncertainty. As pointed out in Sec. 5, BNN and ensemble methods consume much more resources and are therefore impractical for large-scale real-world systems, whereas DUAL does not incur additional computational and memory burden. Fig. 5c shows the computational and memory costs of different strategies. Notably, DUAL-TS yields a similar final cumulative SW result as Ensemble-TS with only 20% computational and memory overhead.

We also observe that DUAL-TS significantly outperforms DUAL-UCB. Our conjecture is that the deterministic nature of DUAL-UCB might lead to “greedy exploration” that over explores a deterministic subset of Ads between successive updates, inhibiting the efficiency.

6.3 Online A/B Testing

We have deployed our method in the Alibaba display advertising platform and conducted an online A/B test for two weeks in October 2020. Comparing with the previous state-of-the-art method used online, DUAL-TS increased the cumulative revenue by 8.0% and the social welfare by 8.2%, during the A/B test. To our best knowledge, this is the first large-scale industrial display advertising system that benefits from exploration-exploitation trade-off using uncertainty estimation in deep CTR models, without increasing computational overhead. Remarkably, it had served the main traffic (over tens of
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