
Optimal Continuous DR-Submodular Maximization and Applications to Provable Mean Field Inference

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Abstract

Mean field inference in probabilistic models is generally a highly nonconvex problem. Existing optimization methods, e.g., coordinate ascent algorithms, typically only find local optima.

In this work we propose provable mean field methods for probabilistic log-submodular models and its posterior agreement (PA) with strong approximation guarantees. The main algorithmic technique is a new Double Greedy scheme, termed DR-DoubleGreedy, for *continuous* DR-submodular maximization with box-constraints. This one-pass algorithm achieves the *optimal* $1/2$ approximation ratio, which may be of independent interest. We validate the superior performance of our algorithms with baseline results on both synthetic and real-world datasets.

1. Introduction

Consider the following scenario: You want to build a recommender system for n products to sell. Let \mathcal{V} contain all the products. The system is expected to recommend a subset of products $S \subseteq \mathcal{V}$ to the user. This recommendation should reflect relevance and diversity of the user’s choice, such that it will raise the readiness to buy. The two most important components in building such a system are (1) learning a utility function $F(S)$, which measures the utility of any subset of products, and (2) inference, i.e., finding the subset Ω^* with the highest utility given the learnt function $F(S)$. The above task can be achieved using a class of probabilistic graphical models that devise a distribution on all subsets of \mathcal{V} . Such a distribution is known as a point process. Specifically, it defines $p(S) \propto \exp(F(S))$, which renders subsets of products S with high utility to be very likely sug-

gested. In general, inference in point processes is #P-hard. One resorts to approximate inference methods via either variational techniques such as mean field approximations (Wainwright et al., 2008) or sampling.

In this paper we develop mean field methods with provable guarantees. Both of the two components in the recommender system example above can be achieved via provable mean field methods since (i) the latter provide approximate inference given a utility function and, (ii) by using proper differentiation techniques, the iterative process of mean field approximation can be unrolled to serve as a differentiable layer (Zheng et al., 2015), thus enabling the backpropagation of the training error to parameters of $F(S)$. Thereby, learning $F(S)$ in an end-to-end fashion can utilize modern deep learning and stochastic optimization techniques.

The most important property which we require on $F(S)$ is *submodularity*, which naturally models relevance and diversity. Djolonga & Krause (2014) have used submodular functions $F(S)$ to define two classes of point processes: $p(S) \propto \exp(F(S))$ is termed probabilistic log-submodular models, while $p(S) \propto \exp(-F(S))$ is called probabilistic log-supermodular models. They are strict generalizations of classical point processes, such as DPPs (Kulesza et al., 2012). The variational techniques from Djolonga & Krause (2014) and Djolonga et al. (2016) focus on giving tractable upper bounds of the log-partition functions. Our work provides provable *lower* bounds through mean field approximation, which also completes the picture of variational inference for probabilistic submodular models (PSMs).

The most frequently used algorithm for mean field approximation is the CoordinateAscent algorithm¹. It maximizes the ELBO objective in a coordinate-wise manner. CoordinateAscent has been shown to reach stationary points/local optima. However, local optima may be arbitrarily poor, as we demonstrate in §A, and CoordinateAscent can get stuck in these poor local optima without extra techniques, which motivates our pursuit to develop provable methods.

We first investigate the properties of mean field approxi-

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¹It is known under various names in the literature, e.g., iterated conditional modes (ICM), naive mean field algorithm, etc.

mation for probabilistic log-submodular models, and show that it falls into a general class of nonconvex problems, called *continuous DR-submodular maximization with box-constraints*. Continuous submodular optimization is a class of well-behaved nonconvex programs, which has attracted considerable attention recently. Then we propose a new one-epoch algorithm for this general class of nonconvex problem, called DR-DoubleGreedy. It achieves the *optimal* $1/2$ approximation ratio in linear time. Lastly, we extend one-epoch algorithms to multiple epochs, resulting in provable mean field algorithms, termed DG-MeanField.

Typical Application Domains. Recommender systems are just one illustrating example. There are numerous scenarios that can benefit from the mean field method in this work. These settings include, but not limited to, existing applications of submodular models, such as diversity models (Tschitschek et al., 2016; Djolonga et al., 2016), experimental design using approximate submodular objectives (Bian et al., 2017b), variable selection (Krause & Guestrin, 2005), data summarization (Lin & Bilmes, 2011a), dictionary learning (Krause & Cevher, 2010) etc. Another category of applications is conducting model validation using information-theoretic criteria. In order to infer the hyperparameters in the model $F(S)$, practitioners do validation by splitting the training data into multiple folds, and then train models on them. *Posterior-Agreement* (PA, Buhmann (2010); Bian et al. (2016)) provides an information-theoretic criterion for the models trained on these folds, to measure the fitness of one specific hyperparameter configuration. We show in §2.2 that PA can be efficiently approximated by the techniques developed in this work.

Contributions. We contribute in the following respects: i) We propose an *optimal* algorithm for the general problem of continuous DR-submodular maximization with box-constraints, which runs in linear time. ii) Based on the optimal algorithm, we propose provable mean field approaches for probabilistic log-submodular models and its PA. iii) We also present efficient polynomial methods to evaluate the multilinear extensions for a large category of practical objectives, which are used for optimizing the mean field objectives. iv) Extensive experimental evaluations on real-world and synthetic data support our theory.

1.1. Problem Statement and Related Work

Notation. Boldface letters, e.g. \mathbf{x} , represent vectors. Boldface capital letters, e.g. \mathbf{A} , denote matrices. x_i is the i^{th} entry of \mathbf{x} , A_{ij} the $(ij)^{\text{th}}$ entry of \mathbf{A} . We use \mathbf{e}_i to denote the standard i^{th} basis vector. $f(\cdot)$ is used to specify a continuous function, and $F(\cdot)$ to represent a set function. $[n] := \{1, \dots, n\}$. Given two vectors \mathbf{x}, \mathbf{y} , $\mathbf{x} \leq \mathbf{y}$ means $\forall i, x_i \leq y_i$. $\mathbf{x} \vee \mathbf{y}$ and $\mathbf{x} \wedge \mathbf{y}$ is defined as coordinate-wise maximum and coordinate-wise minimum, respectively.

Finally, $\mathbf{x}|_i(k)$ is the operation of setting the i^{th} entry of \mathbf{x} to k , while keeping all the others unchanged, i.e., $\mathbf{x}|_i(k) = \mathbf{x} - x_i \mathbf{e}_i + k \mathbf{e}_i$.

All of the mean field approximation problems investigated in this work fall into the following nonconvex maximization problem:

$$\underset{\mathbf{x} \in [\mathbf{a}, \mathbf{b}]}{\text{maximize}} \quad f(\mathbf{x}), \quad (\text{P})$$

where $f : \mathcal{X} \rightarrow \mathbb{R}$ is continuous DR-submodular, $\mathcal{X} = \prod_{i=1}^n \mathcal{X}_i$, each \mathcal{X}_i is an interval (Bach, 2015; Bian et al., 2017c). Continuous DR-submodular functions define a subclass of continuous submodular functions with the additional diminishing returns (DR) property: $\forall \mathbf{a} \leq \mathbf{b} \in \mathcal{X}$, $\forall i \in [n], \forall k \in \mathbb{R}_+$ it holds $f(k\mathbf{e}_i + \mathbf{a}) - f(\mathbf{a}) \geq f(k\mathbf{e}_i + \mathbf{b}) - f(\mathbf{b})$. If f is differentiable, DR-submodularity is equivalent to ∇f being an *antitone* mapping from \mathbb{R}^n to \mathbb{R}^n . If f is twice-differentiable, DR-submodularity is equivalent to all of the entries of $\nabla^2 f(\mathbf{x})$ being non-positive. A function f is DR-supermodular iff $-f$ is DR-submodular.

Background & Related Work. Submodularity is one of the most important properties in combinatorial optimization and has many applications for machine learning, with strong implications for both guaranteed minimization and approximate maximization in polynomial time (Krause & Golovin, 2012). Continuous extensions of submodular set functions play an important role in submodular optimization. Representative instances include the Lovász extension (Lovász, 1983), multilinear extension (Calinescu et al., 2007; Vondrák, 2008; Chekuri et al., 2014; 2015) and the softmax extension for DPPs (Gillenwater et al., 2012). Results on guaranteed optimizations have been extended to continuous domains recently, for both minimization (Bach, 2015; Staib & Jegelka, 2017) and maximization (Bian et al., 2017c;a; Wilder, 2017; Chen et al., 2018; Mokhtari et al., 2018). Specifically, Bach (2015) studies continuous submodular minimization without constraints. He also discusses the possibility of using the technique for mean field inference of probabilistic log-supermodular models. Bian et al. (2017c;a) characterize continuous submodularity using the DR property and propose provable algorithms for maximization.

Most related to this work is the classical problem of unconstrained submodular maximization (USMs), which has been studied in binary (Buchbinder et al., 2012), integer (Soma & Yoshida, 2017) and continuous domains (Bian et al., 2017c). For the general problem (P), at first glance one may consider discretization-based methods: Discretizing the continuous domain and transform (P) to be an integer optimization problem, then solve it using the reduction (Ene & Nguyen, 2016) or the integer Double Greedy algorithm (Soma & Yoshida, 2017). However, discretization-based methods are not appropriate for (P): Firstly, discretization

will inevitably introduce errors for the original continuous problem (P); Secondly, the computational cost is often high². Thus we turn to continuous methods.

The shrunken Frank-Wolfe algorithm (Bian et al., 2017a) provides a $1/e$ approximation guarantee and sublinear rate of convergence for (P), but it is still computationally too expensive: In each iteration it calculates the full gradient, which costs n times as much as computing a partial derivative.

Based on the above analysis, the most promising algorithm to consider would be the Double Greedy algorithm (Bian et al., 2017c), which needs to solve $\mathcal{O}(n)$ 1-D subproblems, and achieves a $1/3$ guarantee for continuous *submodular* maximization. Since it only needs $f(\mathbf{x})$ to be continuous submodular, we call it `Submodular-DoubleGreedy` in the sequel. In this work we propose a new Double Greedy scheme, achieving the optimal $1/2$ approximation ratio (Bian et al., 2017c, Proposition 5) of (P).

Posterior-Agreement (PA) is developed as an information-theoretic criterion for model selection (Gorbach et al., 2017) and algorithmic validation (Gronskiy & Buhmann, 2014; Bian et al., 2016). It originates from the approximation set coding framework of Buhmann (2010). Recently, Buhmann et al. (2018) prove rigorous asymptotics of PA on two typical combinatorial problems: Sparse minimum bisection and Lawler’s quadratic assignment problem. Djolonga & Krause (2014; 2015) study variational inference for PSMs. They propose L-Field to give upper bounds for log-supermodular models through optimizing the subdifferentials.

Contemporary with the development of this work³, Niazadeh et al. (2018) proposed an optimal algorithm for DR-submodular maximization, which is based on a zero-sum game analysis. Their algorithm (Algorithm 4 of Niazadeh et al. (2018), termed BSCB: Binary-Search Continuous Bi-greedy) needs to estimate the partial derivative of the objective, which is not needed in our algorithm. Furthermore, our algorithm is arguably easier to interpret and implement than BSCB. For further comparison of these two algorithms, we provide a simple example in §C. We did extensive experiments (see §5 for details on experimental statistics) to compare them, the results show that both algorithms generate better promising solutions, however, our algorithm produces better solutions than BSCB in most of the experiments.

²e.g., the method from Soma & Yoshida (2017) reaches $\frac{1}{2+\epsilon}$ -approximation in $O(\frac{|V|}{\epsilon}) \log(\frac{\Delta}{\delta}) \log(B)(\theta + \log(B))$ time, B : #grids of discretization, Δ : the maximal positive marginal gain, δ : minimum positive marginal gain. We conducted a study of discretization-based method and defer the results to §G.2

³This work is extended from Bian et al. (2018).

2. Applications to Mean Field Approximation

2.1. Classical Mean Field Inference

Mean field inference aims to approximate the intractable distribution $p(S) \propto \exp(F(S))$ by a fully factorized surrogate distribution $q(S|\mathbf{x}) := \prod_{i \in S} x_i \prod_{j \notin S} (1 - x_j)$, $\mathbf{x} \in [0, 1]^n$. This can be achieved by maximizing the (ELBO) objective, which provides a lower bound for the log-partition function, $(\text{ELBO}) \leq \log Z = \log \sum_{S \subseteq V} \exp(F(S))$. Specifically, the optimization problem is,

$$\begin{aligned} \max_{\mathbf{x} \in [0, 1]} f(\mathbf{x}) &:= \overbrace{\mathbb{E}_{q(S|\mathbf{x})}[F(S)]}^{\text{multilinear extension of } F(S): f_{\text{mt}}(\mathbf{x})} \\ &= \sum_{i=1}^n [x_i \log x_i + (1 - x_i) \log(1 - x_i)] \\ &= f_{\text{mt}}(\mathbf{x}) + \sum_{i \in V} H(x_i), \quad (\text{ELBO}) \quad (1) \end{aligned}$$

where $H(x_i) := -[x_i \log x_i + (1 - x_i) \log(1 - x_i)]$ is the binary entropy function and by default $0 \log 0 = 0$. $f_{\text{mt}}(\mathbf{x}) := \mathbb{E}_{q(S|\mathbf{x})}[F(S)]$ is the multilinear extension of $F(S)$. The above (ELBO) is continuous DR-submodular w.r.t. \mathbf{x} , thus falling into the general problem class (P). At first glance, $f_{\text{mt}}(\mathbf{x})$ seems to require an exponential number of operations for evaluation; we show in §4 that $f_{\text{mt}}(\mathbf{x})$ and its gradients can be computed precisely in polynomial time for many classes of practical objectives, such as facility location, FLID (Tschitschek et al., 2016), set cover (Lin & Bilmes, 2011b) and graph cuts. Maximizing (ELBO) to optimality provides the tightest lower bound of $\log Z$ in terms of the KL divergence $\mathbb{KL}(q||p)$. We put details in §D.

2.2. Mean Field Inference of Posterior-Agreement (PA)

In addition to the traditional mean field objective (ELBO) in (1), here we further formulate a second class of mean field objectives. They come from Posterior-Agreement (PA) for probabilistic log-submodular models, which is an information-theoretic criterion to conduct model and algorithmic validation (Buhmann, 2010; Buhmann et al., 2018; Bian et al., 2016).

Let us again consider the recommender system example: usually there are some hyperparameters in the model/utility function $F(S)$ that require adaptation to the input data. One natural way to do so is through model validation: Split the training data into multiple folds, train a model on each fold D and infer a “noisy” posterior distribution $p(S|D)$. PA measures the agreement between these “noisy” posterior distributions.

Assume w.l.o.g. that there are two folds of data D', D'' in the sequel. In the PA framework, we have two consecutive targets: 1) Direct inference based on the two posterior distributions $p(S|D')$ and $p(S|D'')$. This task amounts to find the MAP solution of the PA distribution (which is discussed

in the next paragraph), it can be approximated by standard mean field inference. 2) Use the PA objective (3) as a criterion for model validation/selection. Since in general the PA objective (3) is intractable, we will still use mean field lower bounds and some upper bounds of Djolonga & Krause (2014) to obtain estimates for it.

Mean Field Approximation of the Posterior-Agreement Distribution. A probabilistic log-submodular model is a special case of a Gibbs random field with unit temperature and $-F(S)$ as the energy function. In PA framework, we explicitly keep β as the inverse temperature, $p_\beta(S|D) := \frac{\exp(\beta F(S|D))}{\sum_{\tilde{S} \subseteq V} \exp(\beta F(\tilde{S}|D))}$, $\forall S \subseteq V$, where D is the dataset used to train the model $F(S|D)$. The PA distribution is defined as,

$$p^\text{PA}(S) \propto p_\beta(S|D') p_\beta(S|D'') \propto \exp[\beta(F(S|D') + F(S|D''))].$$

Note that its log partition function is still intractable. In order to approximate $p^\text{PA}(S)$, we use mean field approximation with a surrogate distribution $q(S|\mathbf{x}) := \prod_{i \in S} x_i \prod_{j \notin S} (1 - x_j)$,

$$\begin{aligned} \log Z^\text{PA} &= \log \sum_{S \subseteq V} \exp[\beta(F(S|D') + F(S|D''))] \\ &\geq \beta \mathbb{E}_{q(S|\mathbf{x})}[F(S|D')] + \beta \mathbb{E}_{q(S|\mathbf{x})}[F(S|D'')] \quad (2) \\ &\quad + \sum_{i \in V} H(x_i). \quad (\text{PA-ELBO}) \end{aligned}$$

Maximizing (PA-ELBO) in (2) still falls into the general problem class (P) (see § D for details). Maximizing (PA-ELBO) also serves as a building block for the second target below.

Lower Bounds for the Posterior-Agreement Objective. The PA objective is used to measure the agreement between two posterior distributions motivated by an information-theoretic analogy (Buhmann et al., 2018; Bian et al., 2016). By introducing the same surrogate distribution $q(S|\mathbf{x})$, one can easily derive that,

$$\begin{aligned} \log \sum_{S \subseteq V} p_\beta(S|D') p_\beta(S|D'') \quad (\text{PA objective}) \quad (3) \\ \geq \underbrace{\mathbb{H}(q) + \beta \mathbb{E}_q F(S|D') + \beta \mathbb{E}_q F(S|D'')}_{(\text{PA-ELBO}) \text{ in (2)}} \\ - \log Z(\beta; D') - \log Z(\beta; D'') \end{aligned}$$

where $\mathbb{H}(q)$ is the entropy of q , $Z(\beta; D')$ and $Z(\beta; D'')$ are the partition functions of the two noisy distributions, respectively. In order to find the best lower bound for PA objective, one need to maximize w.r.t. $q(S|\mathbf{x})$ the (PA-ELBO) objective, at the same time, find the upper bounds for $\log Z(\beta; D') + \log Z(\beta; D'')$. The latter can be achieved using techniques from Djolonga & Krause (2014). We summarize the details in § E to make it self-contained.

3. An Optimal Algorithm for Continuous DR-Submodular Maximization

Unfortunately, problem (P) is generally hard: The 1/2 hardness result (Bian et al., 2017c, Proposition 5) can be easily translated to (P) with details deferred to § B.1. The following question arises naturally: Is it possible to achieve the optimal 1/2 approximation ratio (unless $\text{RP}=\text{NP}$) by properly utilizing the extra DR property in (P)? To affirmatively answer this question, we propose a new Double Greedy algorithm for continuous DR-submodular maximization called DR-DoubleGreedy and prove a 1/2 approximation ratio.

3.1. A Deterministic 1/2-Approximation for Continuous DR-Submodular Maximization

Algorithm 1: DR-DoubleGreedy($f, \mathbf{a}, \mathbf{b}$)

Input: $\max_{\mathbf{x} \in [\mathbf{a}, \mathbf{b}]} f(\mathbf{x})$, $f(\mathbf{x})$ is DR-submodular,
 $[\mathbf{a}, \mathbf{b}] \subseteq \mathcal{X}$; # coordinates n ; additive error level
 $\delta \geq 0$.

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1  $\mathbf{x}^0 \leftarrow \mathbf{a}, \mathbf{y}^0 \leftarrow \mathbf{b}$ ;
2 for  $k = 1 \rightarrow n$  do
3   let  $v_k$  be the coordinate being operated;
4   find  $u_a$  such that
       $f(\mathbf{x}^{k-1}|_{v_k}(u_a)) \geq \max_{u'} f(\mathbf{x}^{k-1}|_{v_k}(u')) - \frac{\delta}{n}$ ,
5    $\delta_a \leftarrow f(\mathbf{x}^{k-1}|_{v_k}(u_a)) - f(\mathbf{x}^{k-1})$ ;
6   find  $u_b$  such that
       $f(\mathbf{y}^{k-1}|_{v_k}(u_b)) \geq \max_{u'} f(\mathbf{y}^{k-1}|_{v_k}(u')) - \frac{\delta}{n}$ ,
7    $\delta_b \leftarrow f(\mathbf{y}^{k-1}|_{v_k}(u_b)) - f(\mathbf{y}^{k-1})$ ;
8    $\mathbf{x}^k \leftarrow \mathbf{x}^{k-1}|_{v_k}(\frac{\delta_a}{\delta_a + \delta_b} u_a + \frac{\delta_b}{\delta_a + \delta_b} u_b)$ ; //update  $\mathbf{x}_k^{\text{th}}$ 
      coordinate to be a convex combination of  $u_a$  &  $u_b$ 
9    $\mathbf{y}^k \leftarrow \mathbf{y}^{k-1}|_{v_k}(\frac{\delta_a}{\delta_a + \delta_b} u_a + \frac{\delta_b}{\delta_a + \delta_b} u_b)$ ;

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Output: \mathbf{x}^n or \mathbf{y}^n ($\mathbf{x}^n = \mathbf{y}^n$)

The pseudocode of DR-DoubleGreedy as summarized in Alg. 1 describes a one-epoch algorithm, sweeping over the n coordinates in one pass. Like the previous Double Greedy algorithms, the procedure maintains two solutions \mathbf{x}, \mathbf{y} , that are initialized as the lower bound \mathbf{a} and the upper bound \mathbf{b} , respectively. In iteration k , it operates on coordinate v_k , and solves the two 1-D subproblems $\max_{u'} f(\mathbf{x}^{k-1}|_{v_k}(u'))$ and $\max_{u'} f(\mathbf{y}^{k-1}|_{v_k}(u'))$, based on \mathbf{x}^{k-1} and \mathbf{y}^{k-1} , respectively. It also allows solving 1-D subproblems approximately with additive error $\delta \geq 0$ ($\delta = 0$ recovers the error-free case). Let u_a and u_b be the solutions of these 1-D subproblems.

Unlike previous Double Greedy algorithms, we change coordinate v_k of \mathbf{x}^{k-1} and \mathbf{y}^{k-1} to be a *convex* combination of u_a and u_b , weighted by respective gains δ_a, δ_b . This convex combination is the key step that utilizes the DR property of f , and it also plays a crucial role in the proof.

Note that the 1-D subproblem has a closed-form solu-

tion for ELBO (1) (and similarly for PA-ELBO (2)). For coordinate i , the partial derivative of the multilinear extension is $\nabla_i f_{\text{mt}}(\mathbf{x})$, and for the entropy term, it is $\nabla H(x_i) = \log \frac{1-x_i}{x_i}$. Then x_i should be updated as $x_i \leftarrow \sigma(\nabla_i f_{\text{mt}}(\mathbf{x})) = (1 + \exp(-\nabla_i f_{\text{mt}}(\mathbf{x})))^{-1}$, where σ is the logistic sigmoid function.

Theorem 1. *Assume the optimal solution of $\max_{\mathbf{x} \in [\mathbf{a}, \mathbf{b}]} f(\mathbf{x})$ is \mathbf{x}^* , then for Alg. 1 it holds,*

$$f(\mathbf{x}^n) \geq \frac{1}{2}f(\mathbf{x}^*) + \frac{1}{4}[f(\mathbf{a}) + f(\mathbf{b})] - \frac{5\delta}{4}. \quad (4)$$

Proof Sketch. The high level proof strategy is to bound the change of an intermediate variable $\mathbf{o}^k := (\mathbf{x}^* \vee \mathbf{x}^k) \wedge \mathbf{y}^k$ through the course of Alg. 1, which is the common framework in the analysis of existing Double Greedy variants (Buchbinder et al., 2012; Gottschalk & Peis, 2015; Bian et al., 2017c; Soma & Yoshida, 2017). The novelty of our method results from the update of \mathbf{x} , \mathbf{y} , which plays a key role in achieving the optimal 1/2 approximation ratio. Furthermore, in the analysis we find a way to utilize the DR property directly, resulting in a succinct proof. We document the details in §B.2, and summarize a sketch here. Firstly, using DR-submodularity, we prove that in each iteration, if we were to flip the 1-D subproblem solutions of \mathbf{x} and \mathbf{y} , it still does not decrease the function value (in the error-free case $\delta = 0$).

Lemma 1. *For all $k = 1, \dots, n$, it holds that,*

$$\begin{aligned} f(\mathbf{x}^{k-1}|_{v_k(u_b)}) - f(\mathbf{x}^{k-1}) &\geq -\delta/n, \\ f(\mathbf{y}^{k-1}|_{v_k(u_a)}) - f(\mathbf{y}^{k-1}) &\geq -\delta/n. \end{aligned} \quad (5)$$

Then using the new update rule and the DR property, we show that the loss on intermediate variables $f(\mathbf{o}^{k-1}) - f(\mathbf{o}^k)$ can be upper bounded by the increase of the objective value in \mathbf{x} and \mathbf{y} times 1/2.

Lemma 2. *For all $k = 1, \dots, n$, it holds that,*

$$\begin{aligned} f(\mathbf{o}^{k-1}) - f(\mathbf{o}^k) \\ \leq \frac{1}{2} [f(\mathbf{x}^k) - f(\mathbf{x}^{k-1}) + f(\mathbf{y}^k) - f(\mathbf{y}^{k-1})] + \frac{2.5\delta}{n}. \end{aligned} \quad (6)$$

Given Lemma 2, let us sum for $k = 1, \dots, n$. After rearrangement we reach the final conclusion.

3.2. Multi-epoch Extensions

Though DR-DoubleGreedy reaches the optimal 1/2 guarantee with one epoch, in practice it usually helps to use its output as an initializer, and continue coordinate-wise optimization for additional epochs. Since each step of coordinate update will never decrease the function value, the approximation guarantees will hold. We call this class of algorithms DoubleGreedy-MeanField, abbreviated as

DG-MeanField, and summarize the pseudocode in Alg. 2.

Algorithm 2: DG-MeanField-1/2 & DG-MeanField-1/3

Input: $\max_{\mathbf{x} \in [\mathbf{a}, \mathbf{b}]} f(\mathbf{x})$, e.g., from the ELBO (1) or PA-ELBO (2) objective

- 1 Option I: DG-MeanField-1/3: run Submodular-DoubleGreedy (Bian et al., 2017c) to get a 1/3 initializer $\hat{\mathbf{x}}$;
 - 2 Option II: DG-MeanField-1/2: run DR-DoubleGreedy to get a 1/2 initializer $\hat{\mathbf{x}}$;
 - 3 beginning with $\hat{\mathbf{x}}$, optimize $f(\mathbf{x})$ coordinate by coordinate for T epochs;
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4. Efficient Methods for Calculating Multilinear Extension & its Gradients

In this section we present guaranteed methods to efficiently calculate the multilinear extension $f_{\text{mt}}(\mathbf{x})$ and its gradients in polynomial time⁴. Remember that the multilinear extension is the expected value of $F(S)$ under the surrogate distribution: $f_{\text{mt}}(\mathbf{x}) := \mathbb{E}_{q(S|\mathbf{x})}[F(S)] = \sum_{S \subseteq \mathcal{V}} F(S) \prod_{i \in S} x_i \prod_{j \notin S} (1 - x_j)$. One can verify that the partial derivative of $f_{\text{mt}}(\mathbf{x})$ is,

$$\begin{aligned} \nabla_i f_{\text{mt}}(\mathbf{x}) &= \mathbb{E}_{q(S|\mathbf{x}, x_i=1)}[F(S)] - \mathbb{E}_{q(S|\mathbf{x}, x_i=0)}[F(S)] \\ &= f_{\text{mt}}(\mathbf{x}|_i(1)) - f_{\text{mt}}(\mathbf{x}|_i(0)) \\ &= \sum_{S \subseteq \mathcal{V}, S \ni i} F(S) \prod_{j \in S \setminus \{i\}} x_j \prod_{j' \notin S} (1 - x_{j'}) \\ &\quad - \sum_{S \subseteq \mathcal{V} \setminus \{i\}} F(S) \prod_{j \in S} x_j \prod_{j' \notin S, j' \neq i} (1 - x_{j'}). \end{aligned}$$

4.1. Gibbs Random Fields with Finite Order of Interactions

Let us use $\mathbf{v} \in \{0, 1\}^{\mathcal{V}}$ to equivalently denote the n binary random variables. $F(\mathbf{v})$ corresponds to the negative energy function in Gibbs random fields. If the energy function is parameterized with a finite order of interactions, i.e., $F(\mathbf{v}) = \sum_{s \in \mathcal{V}} \theta_s v_s + \sum_{(s,t) \in \mathcal{V} \times \mathcal{V}} \theta_{s,t} v_s v_t + \dots + \sum_{(s_1, s_2, \dots, s_d)} \theta_{s_1, s_2, \dots, s_d} v_{s_1} \dots v_{s_d}$, $d < \infty$, then one can verify that its multilinear extension has the following closed form,

$$\begin{aligned} f_{\text{mt}}(\mathbf{x}) &= \sum_{s \in \mathcal{V}} \theta_s x_s + \sum_{(s,t) \in \mathcal{V} \times \mathcal{V}} \theta_{s,t} x_s x_t + \dots \\ &\quad + \sum_{(s_1, s_2, \dots, s_d)} \theta_{s_1, s_2, \dots, s_d} x_{s_1} \dots x_{s_d}. \end{aligned} \quad (7)$$

⁴Iyer & Bilmes (2015) give closed-form expressions for the partition functions of submodular point processes for several classes of objectives, which can be treated as the multilinear extensions evaluated at $0.5 * \mathbf{1}$ with proper scaling.

The gradient of this expression can also be easily derived. Given this observation, one can quickly derive the multilinear extensions of a large category of energy functions of Gibbs random fields, e.g., graph cut, hypergraph cut, Ising models, etc. Details are in §F.

4.2. Facility Location & FLID (Facility Location Diversity)

FLID is a diversity model (Tschitschek et al., 2016) that has been designed as a computationally efficient alternative to DPPs. It is in a more general form than facility location. Let $\mathbf{W} \in \mathbb{R}_+^{|\mathcal{V}| \times D}$ be the weights, each row corresponds to the latent representation of an item, with D as the dimensionality. Then

$$\begin{aligned} F(S) &:= \sum_{i \in S} u_i + \sum_{d=1}^D (\max_{i \in S} W_{i,d} - \sum_{i \in S} W_{i,d}) \\ &= \sum_{i \in S} u'_i + \sum_{d=1}^D \max_{i \in S} W_{i,d}, \end{aligned} \quad (8)$$

which models both coverage and diversity, and $u'_i = u_i - \sum_{d=1}^D W_{i,d}$. If $u'_i = 0$, one recovers the facility location objective. The computational complexity of evaluating its partition function is $\mathcal{O}(|\mathcal{V}|^{D+1})$ (Tschitschek et al., 2016), which is exponential in terms of D .

We now show the technique such that $f_{\text{mt}}(\mathbf{x})$ and $\nabla_i f_{\text{mt}}(\mathbf{x})$ can be evaluated in $\mathcal{O}(Dn^2)$ time. Firstly, for one $d \in [D]$, let us sort $W_{i,d}$ such that $W_{i_d(1),d} \leq W_{i_d(2),d} \leq \dots \leq W_{i_d(n),d}$. After this sorting, there are D permutations to record: $i_d(l), l = 1, \dots, n, \forall d \in [D]$. Now, one can verify that,

$$\begin{aligned} f_{\text{mt}}(\mathbf{x}) &= \sum_{i \in [n]} u'_i x_i + \sum_d \sum_{S \subseteq \mathcal{V}} \max_{i \in S} W_{i,d} \prod_{m \in S} x_m \prod_{m' \notin S} (1 - x_{m'}) \\ &= \sum_{i \in [n]} u'_i x_i + \sum_d \sum_{l=1}^n W_{i_d(l),d} x_{i_d(l)} \prod_{m=l+1}^n [1 - x_{i_d(m)}]. \end{aligned}$$

Sorting costs $\mathcal{O}(Dn \log n)$, and from the above expression, one can see that the cost of evaluating $f_{\text{mt}}(\mathbf{x})$ is $\mathcal{O}(Dn^2)$. By the relation that $\nabla_i f_{\text{mt}}(\mathbf{x}) = f_{\text{mt}}(\mathbf{x}|_i(1)) - f_{\text{mt}}(\mathbf{x}|_i(0))$, the cost is also $\mathcal{O}(Dn^2)$. For $\nabla_i f_{\text{mt}}(\mathbf{x})$, there exists a refined way to calculate this derivative, which we explain in §F.

4.3. Set Cover Functions

Suppose there are $|C| = \{c_1, \dots, c_{|C|}\}$ concepts, and n items in \mathcal{V} . Give a set $S \subseteq \mathcal{V}$, $\Gamma(S)$ denotes the set of concepts covered by S . Given a modular function $\mathbf{m} : 2^C \mapsto \mathbb{R}_+$, the set cover function is defined as $F(S) = \mathbf{m}(\Gamma(S))$. This function models coverage in maximization, and also the notion of complexity in minimization problems

(Lin & Bilmes, 2011b). Let us define an inverse map Γ^{-1} , such that for each concept c , $\Gamma^{-1}(c)$ denotes the set of items v such that $\Gamma^{-1}(c) \ni v$. So the multilinear extension is,

$$\begin{aligned} f_{\text{mt}}(\mathbf{x}) &= \sum_{i \in \mathcal{V}} \mathbf{m}(\Gamma(S)) \prod_{m \in S} x_m \prod_{m' \notin S} (1 - x_{m'}) \\ &= \sum_{c \in C} m_c \left[1 - \prod_{i \in \Gamma^{-1}(c)} (1 - x_i) \right]. \end{aligned} \quad (9)$$

The last equality is achieved by considering the situations where a concept c is covered. One can observe that both $f_{\text{mt}}(\mathbf{x})$ and $\nabla_i f_{\text{mt}}(\mathbf{x})$ can be evaluated in $\mathcal{O}(n|C|)$ time.

4.4. General Case: Approximation by Sampling

In the most general case, one may only have access to the function values of $F(S)$. In this scenario, one can use a polynomial number of sample steps to estimate $f_{\text{mt}}(\mathbf{x})$ and its gradients. Specifically: 1) Sample k times $S \sim q(S|\mathbf{x})$ and evaluate function values for them, resulting in $F(S_1), \dots, F(S_k)$. 2) Return the average $\frac{1}{k} \sum_{i=1}^k F(S_i)$. According to the Hoeffding bound (Hoeffding, 1963), one can easily derive that $\frac{1}{k} \sum_{i=1}^k F(S_i)$ is arbitrarily close to $f_{\text{mt}}(\mathbf{x})$ with increasingly more samples: With probability at least $1 - \exp(-k\epsilon^2/2)$, it holds that $|\frac{1}{k} \sum_{i=1}^k F(S_i) - f_{\text{mt}}(\mathbf{x})| \leq \epsilon \max_S |F(S)|$, for all $\epsilon > 0$.

5. Experiments

The objectives under investigation are ELBO (1) and PA-ELBO (2). We set $\beta = 1$ in PA-ELBO. We tested on the representative FLID model the following algorithms and baselines: The first category is one-epoch algorithms, including ① Submodular-DoubleGreedy (Bian et al., 2017c) with 1/3 approximation guarantee, ② BSCB (Alg. 4 of Niazadeh et al. (2018), where we chose $\epsilon = 10^{-3}$) with 1/2 guarantee and ③ DR-DoubleGreedy (Alg. 1) with 1/2 guarantee.

The second category contain multiple-epoch algorithms: ④ CoordinateAscent-0: initialized as $\mathbf{0}$ and coordinate-wisely improving the solution; CoordinateAscent-1: initialized as $\mathbf{1}$; CoordinateAscent-Random: initialized as a uniform vector $U(\mathbf{0}, \mathbf{1})$. ⑤ DG-MeanField-1/3. ⑥ DG-MeanField-1/2 from Alg. 2. ⑦ BSCB-Multiepoche, which is the multi-epoch extension of BSCB: After the first epoch, it continues to improve the solution coordinate-wisely.

For all algorithms, we use the same random order to process the coordinates within each epoch. We are trying to understand: 1) In terms of DR-submodular maximization, how good are the solutions returned by one-epoch algorithms? 2) For multi-epoch algorithms, how good are the realized lower bounds? For small scale problems we can calculate the true log-partitions exhaustively, which serves as a

Table 1: Summary of results on ELBO objective (1) and PA-ELBO objective (2). Sub-DG stands for Submodular-DoubleGreedy, DR-DG stands for DR-DoubleGreedy. Boldface numbers indicate the best mean of function values returned. For ELBO, the mean and standard deviation were calculated for 10 FLID models trained on 10 folds of the data. For PA-ELBO, the mean and standard deviation were calculated for models trained over 45 pairs of folds. More details are in the experimental section.

Category	D	ELBO objective (1)			PA-ELBO objective (2)		
		Sub-DG	BSCB	DR-DG	Sub-DG	BSCB	DR-DG
furniture $n=32$	2	2.078 \pm 0.091	2.771 \pm 0.123	3.035 \pm 0.059	0.918 \pm 0.768	2.287 \pm 0.399	2.402 \pm 0.159
	3	1.835 \pm 0.156	2.842 \pm 0.128	3.026 \pm 0.099	1.296 \pm 1.176	2.536 \pm 0.439	2.693 \pm 0.181
	10	1.375 \pm 0.194	2.951 \pm 0.161	2.917 \pm 0.103	1.504 \pm 1.110	2.764 \pm 0.405	2.882 \pm 0.248
carseats $n=34$	2	2.089 \pm 0.166	2.863 \pm 0.090	3.045 \pm 0.069	1.218 \pm 1.189	2.106 \pm 0.308	2.383 \pm 0.173
	3	1.890 \pm 0.146	3.003 \pm 0.110	3.138 \pm 0.082	1.598 \pm 1.422	2.413 \pm 0.397	2.718 \pm 0.194
	10	1.390 \pm 0.232	3.100 \pm 0.140	3.003 \pm 0.157	1.975 \pm 1.587	2.670 \pm 0.332	2.957 \pm 0.244
safety $n=36$	2	1.934 \pm 0.402	2.727 \pm 0.212	2.896 \pm 0.098	1.263 \pm 1.187	2.088 \pm 0.290	2.335 \pm 0.121
	3	1.867 \pm 0.453	2.830 \pm 0.191	2.970 \pm 0.110	1.477 \pm 1.150	2.359 \pm 0.354	2.636 \pm 0.158
	10	1.546 \pm 0.606	2.916 \pm 0.191	2.920 \pm 0.149	1.716 \pm 1.209	2.507 \pm 0.287	2.723 \pm 0.138
strollers $n=40$	2	2.042 \pm 0.181	2.829 \pm 0.144	2.928 \pm 0.060	0.587 \pm 0.673	1.883 \pm 0.238	2.171 \pm 0.171
	3	1.814 \pm 0.264	2.958 \pm 0.146	2.978 \pm 0.077	0.837 \pm 0.835	2.119 \pm 0.243	2.496 \pm 0.165
	10	1.328 \pm 0.544	3.065 \pm 0.162	2.910 \pm 0.140	1.225 \pm 1.023	2.412 \pm 0.230	2.706 \pm 0.252
media $n=58$	2	3.221 \pm 0.066	3.309 \pm 0.055	3.493 \pm 0.051	0.372 \pm 0.286	1.477 \pm 0.128	1.336 \pm 0.101
	3	3.276 \pm 0.082	3.492 \pm 0.083	3.712 \pm 0.079	0.418 \pm 0.366	1.736 \pm 0.177	1.762 \pm 0.095
	10	2.840 \pm 0.183	3.894 \pm 0.122	3.924 \pm 0.114	0.653 \pm 0.727	2.309 \pm 0.244	2.524 \pm 0.130
health $n=62$	2	3.197 \pm 0.067	3.174 \pm 0.074	3.516 \pm 0.043	0.528 \pm 0.264	1.679 \pm 0.112	1.654 \pm 0.066
	3	3.231 \pm 0.055	3.306 \pm 0.108	3.707 \pm 0.064	0.621 \pm 0.405	1.918 \pm 0.144	2.023 \pm 0.085
	10	2.633 \pm 0.115	3.508 \pm 0.120	3.675 \pm 0.110	0.808 \pm 0.755	2.256 \pm 0.175	2.384 \pm 0.110
toys $n=62$	2	3.543 \pm 0.047	3.454 \pm 0.091	3.856 \pm 0.044	0.491 \pm 0.138	1.789 \pm 0.187	1.735 \pm 0.058
	3	3.362 \pm 0.055	3.412 \pm 0.070	3.736 \pm 0.051	0.456 \pm 0.149	1.794 \pm 0.197	1.763 \pm 0.065
	10	3.037 \pm 0.138	3.706 \pm 0.108	3.859 \pm 0.119	0.547 \pm 0.301	2.218 \pm 0.269	2.287 \pm 0.105
diaper $n=100$	2	3.500 \pm 0.058	3.517 \pm 0.058	3.636 \pm 0.043	0.295 \pm 0.158	1.119 \pm 0.063	0.665 \pm 0.116
	3	3.739 \pm 0.080	3.753 \pm 0.065	3.974 \pm 0.065	0.337 \pm 0.240	1.429 \pm 0.111	1.141 \pm 0.120
	10	3.423 \pm 0.110	4.150 \pm 0.120	4.203 \pm 0.086	0.386 \pm 0.504	1.969 \pm 0.201	2.009 \pm 0.199
feeding $n=100$	2	3.942 \pm 0.041	3.808 \pm 0.024	3.970 \pm 0.036	0.393 \pm 0.034	0.894 \pm 0.022	0.501 \pm 0.029
	3	4.333 \pm 0.031	4.095 \pm 0.032	4.390 \pm 0.031	0.503 \pm 0.072	1.232 \pm 0.041	0.893 \pm 0.046
	10	4.611 \pm 0.053	4.553 \pm 0.079	4.860 \pm 0.056	0.608 \pm 0.239	1.808 \pm 0.087	1.820 \pm 0.078
gear $n=100$	2	3.311 \pm 0.046	3.150 \pm 0.037	3.430 \pm 0.040	0.232 \pm 0.068	1.019 \pm 0.048	0.590 \pm 0.043
	3	3.538 \pm 0.048	3.347 \pm 0.045	3.721 \pm 0.050	0.303 \pm 0.132	1.257 \pm 0.085	1.020 \pm 0.064
	10	3.065 \pm 0.083	3.550 \pm 0.050	3.670 \pm 0.067	0.312 \pm 0.232	1.566 \pm 0.130	1.514 \pm 0.072
bedding $n=100$	2	3.406 \pm 0.080	3.374 \pm 0.088	3.620 \pm 0.062	0.525 \pm 0.121	1.932 \pm 0.194	2.001 \pm 0.080
	3	3.648 \pm 0.106	3.564 \pm 0.083	3.876 \pm 0.081	2.499 \pm 0.972	2.250 \pm 0.269	2.624 \pm 0.066
	10	3.355 \pm 0.161	3.799 \pm 0.144	3.912 \pm 0.082	3.919 \pm 0.045	2.578 \pm 0.358	3.157 \pm 0.091
apparel $n=100$	2	3.560 \pm 0.094	3.527 \pm 0.046	3.784 \pm 0.059	0.332 \pm 0.519	1.557 \pm 0.140	1.492 \pm 0.189
	3	3.878 \pm 0.092	3.755 \pm 0.062	4.140 \pm 0.063	0.445 \pm 0.675	1.922 \pm 0.235	2.231 \pm 0.202
	10	3.751 \pm 0.087	4.084 \pm 0.075	4.425 \pm 0.066	0.505 \pm 1.005	2.368 \pm 0.333	2.953 \pm 0.238
bath $n=100$	2	2.957 \pm 0.087	3.024 \pm 0.032	3.198 \pm 0.056	0.266 \pm 0.306	1.091 \pm 0.071	0.827 \pm 0.184
	3	3.062 \pm 0.085	3.195 \pm 0.058	3.448 \pm 0.058	0.347 \pm 0.436	1.358 \pm 0.117	1.307 \pm 0.177
	10	2.497 \pm 0.135	3.426 \pm 0.076	3.438 \pm 0.089	0.502 \pm 0.644	1.715 \pm 0.163	1.777 \pm 0.214

natural upper bound of ELBO. All algorithms are implemented in Python3, and source code will be public on the author’s homepage.

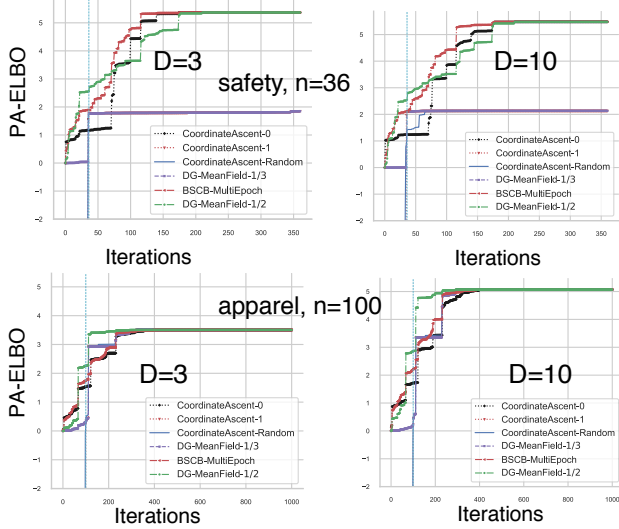


Figure 1: PA-ELBO on Amazon data. The figures trace trajectories of multi-epoch algorithms. Cyan vertical line shows the one-epoch point.

Real-world Dataset. We tested the mean field methods on the trained FLID models from Tschitschek et al. (2016) on Amazon Baby Registries dataset. After preprocessing, this dataset has 13 categories, e.g., “feeding” & “furniture”. One category contains a certain number of registries over the ground set of this category, e.g., “strollers” has 5,175 registries with $n = 40$. One can refer to Table 1 for specific dimensionalities on each of the category⁵. For each category, three classes of models were trained, with latent dimensions $D = 2, 3, 10$, respectively, on 10 folds of the data.

5.1. Results on One-epoch Algorithms

Table 1 summarizes the outputs of one-epoch algorithms for both ELBO and PA-ELBO objectives. For each category, the results of FLID models with three dimensionalities ($D = 2, 3, 10$) are reported.

ELBO Objective. The results are summarized in columns 3 to 5 in Table 1. The mean and standard deviation are calculated for 10 FLID models trained on 10 folds of the data. One can observe that both DR-DoubleGreedy and BSCB improve over the baseline Submodular-DoubleGreedy, which has only a $1/3$ approximation guarantee. Furthermore, DR-DoubleGreedy generates better solutions than

BSCB for almost all of the cases, though they have the same approximation guarantees.

PA-ELBO objective. The results are summarized in columns 6 to 8 in Table 1. For each category, out of the 10 folds of data, we have $\binom{10}{2} = 45$ pairs of folds. For each pair of folds, one PA-ELBO objective is defined. The mean and standard deviation are computed for these 45 pairs for each category and each latent dimensionality D . One can still observe that DR-DoubleGreedy and BSCB significantly improve over Submodular-DoubleGreedy. Moreover, DR-DoubleGreedy usually produces better solutions than BSCB.

5.2. Results on Multi-epoch Algorithms

PA-ELBO Objective. Figure 1 shows representative results on PA-ELBO objectives. One can see that after one epoch, DG-MeanField-1/2 usually returns the best solution. However, CoordinateAscent is quite sensitive to initializations. After sufficiently many iterations, most multi-epoch algorithms converge to similar function values. This is consistent with the intuition since after one epoch, all algorithms are using the same strategy: conducting coordinate-wise maximization. However, for CoordinateAscent with unlucky initializations, e.g., for category “safety” (row 1), it may get stuck in poor local optima.

More Experiments. Due to space limit, the results on ELBO objectives along with the true log-partition values are put into §G.1, the experimental study of the discretization-based algorithm (Soma & Yoshida, 2017) are put in to §G.2, and synthetic results are deferred to §G.4.

6. Conclusions

Probabilistic structured models play an important role in machine learning today, especially models with submodular costs. We have proposed a novel Double Greedy scheme with optimal $1/2$ approximation ratio for the general problem of box-constrained continuous DR-submodular maximization. Based on the optimal scheme, we present provable mean field algorithms for probabilistic log-submodular models and their posterior agreement score.

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⁵More details on this dataset can be found in Gillenwater et al. (2014).

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