Joint M-Best-Diverse Labelings as a Parametric Submodular Minimization

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Abstract

We consider the problem of jointly inferring the *M*-best diverse labelings for a binary (high-order) submodular energy of a graphical model. Recently, it was shown that this problem can be solved to a global optimum, for many practically interesting diversity measures. It was noted that the labelings are, so-called, nested. This nestedness property also holds for labelings of a class of parametric submodular minimization problems, where different values of the global parameter γ give rise to different solutions. The popular example of the parametric submodular minimization is the monotonic parametric max-flow problem, which is also widely used for computing multiple labelings. As the main contribution of this work we establish a close relationship between diversity with submodular energies and the parametric submodular minimization. In particular, the joint M-best diverse labelings can be obtained by running a non-parametric submodular minimization (in the special case - max-flow) solver for M different values of γ in parallel, for certain diversity measures. Importantly, the values for γ can be computed in a closed form in advance, prior to any optimization. These theoretical results suggest two simple yet efficient algorithms for the joint M-best diverse problem, which outperform competitors in terms of runtime and quality of results. In particular, as we show in the paper, the new methods compute the exact M-best diverse labelings faster than a popular method of Batra et al., which in some sense only obtains approximate solutions.

1 Introduction

A variety of tasks in machine learning, computer vision and other disciplines can be formulated as energy minimization problems, also known as *Maximum-a-Posteriori* (MAP) or *Maximum Likelihood* (ML) estimation problems in undirected graphical models (Markov or Conditional Random Fields). The importance of this problem is well-recognized, which can be seen by the many specialized benchmarks [36, 21] and computational challenges [10] for its solvers. This motivates the task of finding *the most probable* solution. Recently, a slightly different task has gained popularity, both from a practical and theoretical perspective. The task is not only to find the most probable solution but multiple *diverse* solutions, all with low energy, see e.g., [4, 31, 22, 23]. The task is referred to as the "*M*-best-diverse problem" [4], and it has been used in a variety of scenarios, such as: (a) Expressing uncertainty of the computed solutions [33]; (b) Faster training of model parameters [16]; (c) Ranking of inference results [40]; (d) Empirical risk minimization [32]; (e) Loss-aware optimization [1]; (f) Using diverse proposals in a cascading framework [39, 35].

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In this work we build on the recently proposed formulation of [22] for the M-best-diverse problem. In this formulation all M configurations are inferred *jointly*, contrary to the well-known method [4, 31], where a sequential, greedy procedure is used. Hence, we term it "joint M-best-diverse problem". As shown in [22, 23], the joint approach qualitatively outperforms the sequential approach [4, 31] in a number of applications. This is explained by the fact that the sequential method [4] can be considered as an approximate and greedy optimization technique for solving the joint M-best-diverse problem. While the joint approach is superior with respect to quality of its results, it is inferior to the sequential method [4] with respect to runtime. For the case of binary submodular energies, the approximate solver in [22] and the exact solver in [23] are several times slower than the sequential technique [4] for a normally sized image. Obviously, this is a major limitation when using it in a practical setting. Furthermore, the difference in runtime grows with the number M of configurations.

In this work, we show that in case of binary submodular energies an *exact* solution to the joint M-best-diverse problem can be obtained significantly faster than the approximate one with the sequential method [4]. Moreover, the difference in runtime grows with the number M of configurations.

Related work

The importance of the considered problem can be justified by the fact that a procedure of computing M-best solutions to discrete optimization problems was proposed over 40 years ago, in [28]. Later, more efficient specialized procedures were introduced for MAP-inference on a tree [34], junction-trees [30] and general graphical models [41, 13, 3]. However, such methods are however not suited for the scenario where *diversity* of the solutions is required, since they do not enforce it explicitly.

Structural Determinant Point Processes [27] is a tool for modelling probability distributions of structured models. Unfortunately, an efficient sampling procedure to obtain diverse configurations is feasible only for tree-structured graphical models. The recently proposed algorithm [8] to find *M* best modes of a distribution is also limited to chains and junction chains of bounded width.

Training of M independent graphical models to produce multiple diverse solutions was proposed in [15], and was further explored in [17, 9]. In contrast, we assume a single fixed model where configurations with low energy (hopefully) correspond to the desired output.

The work of [4] defines the M-best-diverse problem, and proposes a solver for it. However, the diversity of the solutions is defined sequentially, with respect to already extracted labelings. In contrast to [4], the work [22] defined the "joint M-best-diverse problem" as an optimization problem of a *single joint energy*. The most related work to ours is [23], where an efficient method for the joint M-best-diverse problem was proposed for submodular energies. The method is based on the fact that for submodular energies and a family of diversity measures (which includes e.g., Hamming distance) the set of M diverse solutions can be totally ordered with respect to the partial labeling order. In the binary labeling case, the M-best-diverse solutions form a nested set. However, although the method [23] is a considerably more efficient way to solve the problem, compared to the general algorithm proposed in [22], it is still considerably slower than the sequential method [4]. Furthermore, the runtime difference grows with the number M of configurations.

Interestingly, the above-mentioned "nestedness property" is also fulfilled by minimizers of a parametric submodular minimization problem [12]. In particular, it holds for the monotonic max-flow method [25], which is also widely used for obtaining diverse labelings in practice [7, 20, 19]. Naturally, we would like to ask questions about the relationship of these two techniques, such as: "Do the joint M-best-diverse configurations form a subset of the configurations returned by a parametric submodular minimization problem?", and conversely "Can the parametric submodular minimization be used to (efficiently) produce the M-best-diverse configurations?" We give positive answers to both these questions.

Contribution

• For binary submodular energies we provide a relationship between the joint M-best-diverse and the parametric submodular minimization problems. In case of "concave node-wise diversity measures" ¹ we give a closed-form formula for the parameters values, which corresponds to the joint M-best-diverse labelings. The values can be computed in advance, prior to any optimization, which allows to obtain each labeling independently.

• Our theoretical results suggest a number of efficient algorithms for the joint *M*-best-diverse

¹Precise definition is given in Sections 2 and 3.

problem. We describe and experimentally evaluate the two simplest of them, sequential and parallel. Both are considerably faster than the popular technique [4] and are as easy to implement. We demonstrate the effectiveness of these algorithms on two publicly available datasets.

2 Background and Problem Definition

Energy Minimization Let $2^{\mathcal{A}}$ denote the powerset of a set \mathcal{A} . The pair $\mathcal{G} = (\mathcal{V}, F)$ is called a *hyper-graph* and has \mathcal{V} as a finite set of variable nodes and $F \subseteq 2^{\mathcal{V}}$ as a set of factors. Each variable node $v \in \mathcal{V}$ is associated with a variable y_v taking its values in a finite set of labels L_v . The set $L_{\mathcal{A}} = \prod_{v \in \mathcal{A}} L_v$ denotes the Cartesian product of sets of labels corresponding to a subset $\mathcal{A} \subseteq \mathcal{V}$ of variables. Functions $\theta_f : L_f \to \mathbb{R}$, associated with factors $f \in F$, are called *potentials* and define local costs on values of variables and their combinations. Potentials θ_f with |f| = 1 are called *unary*, with |f| = 2 pairwise and |f| > 2 high-order. Without loss of generality we will assume that there is a unary potential θ_v assigned to each variable $v \in \mathcal{V}$. This implies that $F = \mathcal{V} \cup \mathcal{F}$, where $\mathcal{F} = \{f \in F : |f| \ge 2\}$. For any non-unary factor $f \in \mathcal{F}$ the corresponding set of variables $\{y_v : v \in f\}$ will be denoted by y_f . The energy minimization problem consists in finding a labeling $y^* = (y_v : v \in \mathcal{V}) \in L_{\mathcal{V}}$, which minimizes the total sum of corresponding potentials:

$$\arg\min_{\boldsymbol{y}\in L_{\mathcal{V}}} E(\boldsymbol{y}) = \arg\min_{\boldsymbol{y}\in L} \sum_{v\in\mathcal{V}} \theta_v(y_v) + \sum_{f\in\mathcal{F}} \theta_f(\boldsymbol{y}_f).$$
(1)

Problem (1) is also known as *MAP-inference*. Labeling y^* satisfying (1) will be later called *a solution* of the energy-minimization or MAP-inference problem, shortly MAP-labeling or MAP-solution.

Unless otherwise specified, we will assume that $L_v = \{0, 1\}, v \in \mathcal{V}$, i.e. each variable may take only two values. Such energies will be called *binary*. We also assume that the logical operations \leq and \geq are defined in a natural way on the sets L_v . The case, when the energy E decomposes into unary and pairwise potentials only, we will term as *pairwise case* or *pairwise energy*.

In the following, we use brackets to distinguish between upper index and power, i.e. $(\mathcal{A})^n$ means the *n*-th power of \mathcal{A} , whereas *n* is an upper index in the expression \mathcal{A}^n . We will keep, however, the standard notation \mathbb{R}^n for the *n*-dimensional vector space and skip the brackets if an upper index does not make mathematical sense such as in the expression $\{0, 1\}^{|\mathcal{V}|}$.

Joint-DivMBest Problem Instead of searching for a single labeling with the lowest energy, one might ask for a set of labelings with low energies, yet being significantly different from each other. In [22] it was proposed to infer such M diverse labelings $\{y^1, \ldots, y^M\} \in (L)^M$ jointly by minimizing

$$E^{M}(\{\boldsymbol{y}\}) = \sum_{i=1}^{M} E(\boldsymbol{y}^{i}) - \lambda \Delta^{M}(\{\boldsymbol{y}\})$$
⁽²⁾

w.r.t. $\{\boldsymbol{y}\} := \boldsymbol{y}^1, \ldots, \boldsymbol{y}^M$ for some $\lambda > 0$. Following [22] we use the notation $\{\boldsymbol{y}\}$ and $\{\boldsymbol{y}\}_v$ as shortcuts for $\boldsymbol{y}^1, \ldots, \boldsymbol{y}^M$ and y_v^1, \ldots, y_v^M correspondingly. Function Δ^M defines diversity of arbitrary M labelings, i.e. $\Delta^M(\{\boldsymbol{y}\})$ takes a large value if labelings $\{\boldsymbol{y}\}$ are in a certain sense diverse, and a small value otherwise.

In the following, we will refer to the problem (1) of minimizing the energy E itself as to *the master* problem for (2).

Node-Wise Diversity In what follows we will consider only *node-wise diversity measures*, i.e. those which can be represented in the form

$$\Delta^{M}(\{\boldsymbol{y}\}) = \sum_{v \in \mathcal{V}} \Delta^{M}_{v}(\{\boldsymbol{y}\}_{v})$$
(3)

for some *node diversity measure* $\Delta_v^M \colon \{0,1\}^M \to \mathbb{R}$. Moreover, we will stick to *permutation invariant* diversity measures. In other words, such measures that $\Delta_v^M(\{y\}_v) = \Delta_v^M(\pi(\{y\}_v))$ for any permutation π of variables $\{y\}_v$.

Let the expression $[\![A]\!]$ be equal to 1 if A is true and 0 otherwise. Let also $m_v^0 = \sum_{m=1}^M [\![y_v^m = 0]\!]$ count the number of 0's in $\{y\}_v$. In the binary case $L_v = \{0, 1\}$, any permutation invariant measure can be represented as

$$\Delta_v^M(\{\boldsymbol{y}\}_v) = \bar{\Delta}_v^M(m_v^0).$$
⁽⁴⁾

To keep notation simple, we will use Δ_v^M for both representations: $\Delta_v^M(\{y\}_v)$ and $\bar{\Delta}_v^M(m_v^0)$.

Example 1 (Hamming distance diversity). *Consider the common node diversity measure, the sum of Hamming distances between each pair of labels:*

$$\Delta_{v}^{M}(\{\boldsymbol{y}\}_{v}) = \sum_{i=1}^{M} \sum_{j=i+1}^{M} [\![\boldsymbol{y}_{v}^{i} \neq \boldsymbol{y}_{v}^{j}]\!].$$
(5)

This measure is permutation invariant. Therefore, it can be written as a function of the number m_0^n .

$$\Delta_v^M(m_v^0) = m_v^0 \cdot (M - m_v^0).$$
(6)

Minimization Techniques for Joint-DivMBest Problem Direct minimization of (2) has so far been considered as a difficult problem even when the master problem (1) is easy to solve. We refer to [22] for a detailed investigation of using general MAP-inference solvers for (2). In this paragraph we briefly summarize existing *efficient* minimization approaches for (2).

As shown in [22] the sequential method DivMBest [4] can be seen as a greedy algorithm for approximate minimization of (2), by finding one solution after another. The sequential method [4] is used for diversity measures that can be represented by sum of diversity measures between each pair of solutions, i.e. $\Delta^M(\{y\}) = \sum_{m_1=1}^{M} \sum_{m_2=m_1+1}^{M} \Delta^2(y^{m_1}, y^{m_2})$. For each $m = 1, \ldots, M$ the method sequentially computes

$$\boldsymbol{y}^{m} = \operatorname*{arg\,min}_{\boldsymbol{y} \in L_{\mathcal{V}}} \left[E(\boldsymbol{y}) - \lambda \sum_{i=1}^{m-1} \Delta^{2}(\boldsymbol{y}, \boldsymbol{y}^{i}) \right] .$$
(7)

In case of a node diversity measure (3), this algorithm requires sequentially solving M energy minimization problems (1), with only modified unary potentials comparing to the master problem (1). It typically implies that an efficient solver for the master problem can also be used to obtain its diverse solutions.

In [23] an efficient approach for (2) was proposed for submodular energies E. An energy E(y) is called submodular if for any two labelings $y, y' \in L_{\mathcal{V}}$ it holds

$$E(\boldsymbol{y} \vee \boldsymbol{y}') + E(\boldsymbol{y} \wedge \boldsymbol{y}') \le E(\boldsymbol{y}) + E(\boldsymbol{y}'), \qquad (8)$$

where $y \lor y'$ and $y \land y'$ denote correspondingly the node-wise maximum and minimum with respect to the natural order on the label set L_v .

In the following, we will use the term *the higher labeling*. The labeling y is *higher* than the labeling y' if $y_v \ge y'_v$ for all $v \in \mathcal{V}$. So, the labeling $y \lor y'$ is higher than y and y'. Since the set of all labelings is a lattice w.r.t. the operation \ge , we will speak also about *the highest labeling*.

It was shown in [23] that for submodular energies, under certain technical conditions on the diversity measure Δ_v^M (see Lemma 2 in [23]), the problem (2) can be reformulated as a submodular energy minimization and, therefore, can be solved either exactly or approximately by efficient optimization techniques (e.g., by reduction to the min-cut/max-flow in the pairwise case). However, the size of the reformulated problem grows at least linearly with M (quadratically in the case of the Hamming distance diversity (5)) and therefore even approximate algorithms require longer time than the DivMBest (7) method. Moreover, this difference in runtime grows with M.

The mentioned transformation of (2) into a submodular energy minimization problem is based on the theorem below, which plays a crucial role in obtaining the main results of this work. We first give a definition of the "nestedness property", which is also important for the rest of the paper.

Definition 1. An *M*-tuple $(\boldsymbol{y}^1, \ldots, \boldsymbol{y}^M) \in (L_{\mathcal{V}})^M$ is called nested if for each $v \in \mathcal{V}$ the inequality $y_v^i \leq y_v^j$ holds for $1 \leq i \leq j \leq M$, i.e. for $L_{\mathcal{V}} = \{0, 1\}$, $y_v^i = 1$ implies $y_v^j = 1$ for j > i.

Theorem 1. [Special case of Thm. 1 of [23]] For a binary submodular energy and a node-wise permutation invariant diversity, there exists a nested minimizer to the Joint-DivMBest objective (2).

Parametric submodular minimization Let $\gamma \in \mathbb{R}^{|\mathcal{V}|}$, $i = \{1, ..., k\}$ be a vector of parameters with the coordinates indexed by the node index $v \in \mathcal{V}$. We define the parametric energy minimization as the problem of evaluating the function

$$\min_{\boldsymbol{y}\in L_{\mathcal{V}}} E^{\boldsymbol{\gamma}}(\boldsymbol{y}) := \min_{\boldsymbol{y}\in L} \left[E(\boldsymbol{y}) + \sum_{v\in\mathcal{V}} \gamma_v y_v \right]$$
(9)

for all values of the parameter $\gamma \in \Gamma \subseteq \mathbb{R}^{|\mathcal{V}|}$. The most important cases of the parametric energy minimization are



Figure 1: Hamming distance (left) and linear (right) diversity measures for M = 5. Value m is defined as $\sum_{m=1}^{M} [\![y_v^m = 0]\!]$. Both diversity measures are concave.

• the monotonic parametric max-flow problem [14, 18], which corresponds to the case when E is a binary submodular pairwise energy and $\Gamma = \{\nu \in \mathbb{R}^{|\mathcal{V}|} : \nu_v = \gamma_v(\lambda)\}$ and functions $\gamma_v \colon \Lambda \to \mathbb{R}$ are non-increasing for $\Lambda \subseteq \mathbb{R}$.

• a subclass of the parametric submodular minimization [12, 2], where E is submodular and $\Gamma = \{\gamma^1, \gamma^2, \dots, \gamma^k \in \mathbb{R}^{|\mathcal{V}|} : \gamma^1 \ge \gamma^2 \ge \dots \ge \gamma^k\}$, where operation \ge is applied coordinate-wise.

It is known [38] that in these two cases, (i) the highest minimizers $y^1, \ldots, y^k \in L_{\mathcal{V}}$ of E^{γ^i} , $i = \{1, \ldots, k\}$ are nested and (ii) the parametric problem (9) is solvable efficiently by respective algorithms [14, 18, 12]. In the following, we will show that for a submodular energy E the Joint-DivMBest problem (2) reduces to the parametric submodular minimization with the values $\gamma^1 \ge \gamma^2 \ge \ldots \ge \gamma^M \in \mathbb{R}^{|\mathcal{V}|}$ given in closed form.

3 Joint *M*-Best-Diverse Problem as a Parametric Submodular Minimization

Our results hold for the following subclass of the permutation invariant node-wise diversity measures: **Definition 2.** A node-wise diversity measure $\Delta_v^M(m)$ is called concave if for any $1 \le i \le j \le M$ it holds

$$\Delta_v^M(i) - \Delta_v^M(i-1) \ge \Delta_v^M(j) - \Delta_v^M(j-1).$$
⁽¹⁰⁾

There are a number of practically relevant concave diversity measures:

Example 2. Hamming distance diversity (6) is concave, see Fig. 1 for illustration.

Example 3. *Diversity measures of the form*

$$\Delta_v^M(m_v^0) = -\left(\left|m_v^0 - (M - m_v^0)\right|\right)^p = -\left(\left|2m_v^0 - M\right|\right)^p \tag{11}$$

are concave for any $p \ge 1$. Here $M - m_v^0$ is the number of variables labeled as 1. Hence, $|m_v^0 - (M - m_v^0)|$ is an absolute value of the difference between the numbers of variables labeled as 0 and 1. It expresses the natural fact that a distribution of 0's and 1's is more diverse, when their amounts are similar.

For p = 1 we call the measure (11) *linear*; for p = 2 the measure (11) coincides with the Hamming distance diversity (6). An illustration of these two cases is given in Fig. 1.

Our main theoretical result is given by the following theorem:

Theorem 2. Let *E* be binary submodular and Δ^M be a node-wise diversity measure with each component Δ_v^M , $v \in V$, being permutation invariant and concave. Then a nested *M*-tuple $(\mathbf{y}^m)_{m=1}^M$ minimizing the Joint-DivMBest objective (2) can be found as the solutions of the following *M* problems:

$$\boldsymbol{y}^{m} = \operatorname*{arg\,min}_{\boldsymbol{y}_{\mathcal{V}}} \left[E(\boldsymbol{y}) + \sum_{v \in \mathcal{V}} \gamma_{v}^{m} y_{v} \right] , \qquad (12)$$

where $\gamma_v^m = \lambda \left(\Delta_v^M(m) - \Delta_v^M(m-1) \right)$. In the case of multiple solutions in (12) the highest minimizer must be selected.

We refer to the supplement for the proof of Theorem 2 and discuss its practical consequences below. First note that the sequence $(\gamma^m)_{m=1}^M$ is monotone due to concavity of Δ_v^M . Each of the M optimization problems (12) has the same size as the master problem (1) and differs from it by unary potentials only. Theorem 2 implies that γ^m in (12) satisfy the monotonicity condition: $\gamma^1 \ge \gamma^2 \ge \ldots \ge \gamma^M$. Therefore, equations (12) constitute the parametric submodular minimization problem as defined above, which reduces to the monotonic parametric max-flow problem for pairwise E. Let $|\cdot|$ denote the largest integer not exceeding an argument of the operation.

Corollary 1. Let Δ_v^M in Theorem 2 be the Hamming distance diversity (6). Then it holds: 1. $\gamma_v^m = \lambda(M - 2m + 1)$.

2. The values γ_v^m , m = 1, ..., M are symmetrically distributed around 0: $-\gamma_v^m = \gamma_v^{M+1-m} \ge 0$, for $m \le \lfloor (M+1)/2 \rfloor$ and $\gamma_v^m = 0$, if m = (M+1)/2.

3. Moreover, this distribution is uniform, that is $\gamma_v^{m+1} - \gamma_v^m = 2\lambda$, $m = 1, \dots, M$.

4. When M is odd, the MAP-solution (corresponding to $\gamma^{(M+1)/2} = 0$) is always among the M-best-diverse labelings minimizing (2).

Corollary 2. Implications 2 and 4 of Corollary 1 hold for any symmetrical concave Δ_v^M , i.e., those where $\Delta_v^M(m) = \Delta_v^M(M + 1 - m)$ for $m \leq \lfloor (M + 1)/2 \rfloor$.

Corollary 3. For linear diversity measure the value γ_v^m in (12) is equal to $\lambda \cdot sgn\left(\frac{M}{2} - m\right)$, where sgn(x) is a sign function, i.e., sgn(x) = [x > 0] - [x < 0]. Since all γ_v^m for $m < \frac{M}{2}$ are the same, this diversity measure can give only up to 3 different diverse labelings. Therefore, this diversity measure is not useful for M > 3, and can be seen as a limit of useful concave diversity measures.

4 Efficient Algorithmic Solutions

Theorem 2 suggests several new computational methods for minimizing the Joint-DivMBest objective (2). All of them are more efficient than those proposed in [23]. Indeed, as we show experimentally in Section 5, they outperform even the sequential DivMBest method (7).

The simplest algorithm applies a MAP-inference solver to each of the M problems (12) sequentially and independently. This algorithm has the same computational cost as DivMBest (7) since it also sequentially solves M problems of the same size. However, already its slightly improved version, described below, performs faster than DivMBest (7).

Sequential Algorithm Theorem 2 states that solutions of (12) are nested. Therefore, from $y_v^{m-1} = 1$ it follows that $y_v^m = 1$ for labelings y^{m-1} and y^m obtained according to (12). This allows to reduce the size and computing time for each subsequent problem in the sequence.² Reusing the flow from the previous step gives an additional speedup. In fact, when applying a push relabel or pseudoflow algorithm in this fashion the total work complexity is asymptotically the same as of a single minimum cut [14, 18] of the master problem. In practice, this strategy is efficient with other min-cut solvers (without theoretical guarantees) as well. In our experiments we evaluated it with the dynamic augmenting path method [6, 24].

Parallel Algorithm The M problems (12) are completely independent, and their highest minimizers recover the optimal M-tuple $(\mathbf{y^m})_{\mathbf{m}}$ according to Theorem 2. They can be solved fully in parallel or, using p < M processors, in parallel groups of M/p problems per processor, incrementally within each group. The overhead is only in copying data costs and sharing the memory bandwidth.

Alternative approaches One may suggest that for large M it would be more efficient to solve the full parametric maxflow problem [18, 14] and then "read out" solutions corresponding to the desired values γ^m . However, the known algorithms [18, 14] would perform exactly the incremental computation described in the sequential approach above plus an extra work of identifying all breakpoints. This is only sensible when M is larger than the number of breakpoints or the diversity measure is not known in advance (e.g., is itself parametric). Similarly, parametric submodular function minimization can be solved in the same worst case complexity [12] as non-parametric, but the algorithm is again incremental and would just perform less work when the parameters of interest are known in advance.

5 Experimental Evaluation

We base our experiments on two datasets: (i) The interactive foreground/background image segmentation dataset utilized in several papers [4, 31, 22, 23] for comparing diversity techniques; (ii) A new

²By applying "symmetric reasoning" for the label 0, further speed-ups can be achieved. However, we stick to the first variant in our experiments.

Table 1: Interactive segmentation. The quality measure is a per-pixel accuracy of the best segmentation, out of M, averaged over all test images. The runtime is in milliseconds (ms). The quality for M = 1 is 91.57. Parametric-parallel is the fastest method followed by Parametric-sequential. Both achieve higher quality than DivMBest, and return the same solution as loint-DivMBest.

uon as joint-Dividest.	M=2		M=6		M=10	
	quality	time (ms)	quality	time (ms)	quality	time (ms)
DivMBest [4]	93.16	2.6	95.02	11.6	95.16	15.4
Joint-DivMBest [23]	95.13	5.5	96.01	17.2	96.19	80.3
Parametric-sequential (1 core)	95.13	2.2	96.01	5.5	96.19	8.4
Parametric-parallel (6 cores)	95.13	1.9	96.01	4.3	96.19	6.2

dataset for foreground/background image segmentation with binary pairwise energies derived from the well-known PASCAL VOC 2012 dataset [11]. Energies of the master problem (1) in both cases are binary and pairwise, therefore we use their reduction [26] to the min-cut/max-flow problem to obtain solutions efficiently.

Baselines Our main competitor is the fastest known approach for inferring M diverse solutions, the DivMBest method [4]. We made its efficient re-implementation using dynamic graph-cut [24]. We also compare our method with Joint-DivMBest [23], which provides an exact minimum of (2) as our method does.

Diversity Measure In all of our experiments we use the Hamming distance diversity measure (5). Note that in [31] more sophisticated diversity measures were used e.g., the *Hamming Ball*. However, the DivMBest method (7) with this measure requires to run a very time-consuming *HOP-MAP* [37] inference technique. Moreover, the experimental evaluation in [23] suggests that the exact minimum of (2) with Hamming distance diversity (5) outperforms DivMBest with a *Hamming Ball* distance diversity.

Our Method We evaluate both algorithms described in Section 4, i.e., sequential and parallel. We refer to them as Parametric-sequential and Parametric-parallel respectively. We utilize the dynamic graph-cut [24] technique for Parametric-sequential, which makes it comparable to our implementation of DivMBest. The max-flow solver of [6] is used for Parametric-parallel together with *OpenMP* directives. For the experiments we use a computer with 6 physical cores (12 virtual cores), and run Parametric-parallel with M threads.

Parameters λ (from (7) and (2)) were tuned via cross-validation for each algorithm and each experiment separately.

5.1 Interactive Segmentation

The basic idea is that after a user interaction, the system provides the user with M diverse segmentations, instead of a single one. The user can then manually select the best one and add more user scribbles, if necessary. Following [4] we consider only the first iteration of such an interactive procedure, i.e., we consider user scribbles to be given and compare the sets of segmentations returned by the system.

The authors of [4] kindly provided us their 50 super-pixel graphical model instances. They are based on a subset of the PASCAL VOC 2010 [11] segmentation challenge with manually added scribbles. An instance has on average 3000 nodes. Pairwise potentials are given by contrast-sensitive Potts terms [5], which are submodular in the binary case. This implies that Theorem 2 is applicable.

Quantitative comparison and runtime of the different algorithms are presented in Table 1. As in [4], our quality measure is a per-pixel accuracy of the best solution for each test image, averaged over all test images. As expected, Joint-DivMBest and Parametric-* return the same, exact solution of (2). The measured runtime is also averaged over all test images. Parametric-parallel is the fastest method followed by Parametric-sequential. Note that on a computer with fewer cores, Parametric-sequential may even outperform Parametric-parallel because of the parallelization overheads.

5.2 Foreground/Background Segmentation

The Pascal VOC 2012 [11] segmentation dataset has 21 labels. We selected all those 451 images from the validation set for which the ground truth labeling has only two labels (background and one



Figure 2: Foreground/background segmentation. (a) Intersection-over-union (IoU) score for the best segmentation, out of M. Parametric represents a curve, which is the same for Parametric-sequential, Parametric-parallel and Joint-DivMBest, since they exactly solve the same Joint-DivMBest problem. (b) DivMBest uses dynamic graph-cut [24]. Parametric-sequential uses dynamic graph-cut and a reduced size graph for each consecutive labeling problem. Parametric-parallel solves M problems in parallel using OpenMP.

of the 20 object classes) and which were *not* used for training. As unary potentials we use the output probabilities of the publicly available fully convolutional neural network FCN-8s [29], which is trained for the Pascal VOC 2012 challenge. This CNN gives unary terms for all 21 classes. For each image we pick only two classes: the background and the class-label that is presented in the ground truth. As pairwise potentials we use the contrastive-sensitive Potts terms [5] with a 4-connected grid structure.

Quantitative Comparison and Runtime As quality measure we use the standard Pascal VOC measure for semantic segmentation – average intersection-over-union (IoU) [11]. The unary potentials alone, i.e., output of FCN-8s, give 82.12 IoU. The single best labeling, returned by the MAP-inference problem, improves it to 83.23 IoU.

The comparisons with respect to runtime and accuracy of results are presented in Fig. 2a and 2b respectively. The increase in runtime with respect to M for Parametric-parallel is due to parallelization overhead costs, which grow with M. Parametric-parallel is a clear winner in this experiment, both in terms of quality and runtime. Parametric-sequential is slower than Parametric-parallel but faster than DivMBest. The difference in runtime between these three algorithms grows with M.

6 Conclusion and Outlook

We have shown that the M labelings, which constitute a solution to the Joint-DivMBest problem with binary submodular energies, and concave node-wise permutation invariant diversity measures can be computed in parallel, independently from each other, as solutions of the master energy minimization problem with modified unary costs. This allows to build solvers which run even faster than the approximate method of Batra et al. [4]. Furthermore, we have shown that such Joint-DivMBest problems reduce to the parametric submodular minimization. This shows a clear connection of these two practical approaches to obtaining diverse solutions to the energy minimization problem.

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Supplementary Materials: Joint M-Best-Diverse Labelings as a Parametric Submodular Minimization

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Below we provide two proofs of Theorem 2. The first one is restricted to pairwise energies. It is based on representing the submodular Joint-DivMBest problem (2) in the form of minimizing a convex multilabel energy. This problem is known as Convex MRF or as total variation (TV) regularized optimization with convex data terms. Thresholding theorems [8, 6, 5, 3, 9] then allow to break the problem into independent minimization and connect it to parametric mincut. This approach reveals an important link between our problem and the mentioned methods. It is also the shorter one. However, it is limited by the existing thresholding theorems and does not fully cover e.g., the higher order case (as discussed below).

The second proof is both more general (applies to arbitrary submodular energies) and simpler than the respective proves of the related results. It is self contained and uses only basic concepts of submodular function minimization, revealing the true simplicity of central fact that allows the problem to decouple.

7 Pairwise Case

For pairwise energies it holds $f = \{u, v\}, u, v \in \mathcal{V}$. Therefore, we will denote θ_f as $\theta_{u,v}$. The energy of the master problem (1) then reads

$$E(y) = \sum_{v \in \mathcal{V}} \theta_v(y_v) + \sum_{uv \in \mathcal{F}} \theta_{u,v}(y_u, y_v).$$
(13)

It is known [2] and straightforward to check that in the binary case it holds

$$E(y) = \text{const} + \sum_{v \in \mathcal{V}} a_v y_v + \sum_{uv \in \mathcal{F}} \Theta_{u,v} |y_u - y_v|, \qquad (14)$$

where $a_v = \theta_v(1) - \theta(0)$ and $\Theta_{u,v} = \theta_{u,v}(0,1) + \theta_{u,v}(1,0) - \theta_{u,v}(0,0) - \theta_{u,v}(1,1)$. For submodular E, the values $\Theta_{u,v}$ are non-negative. In what follows, we will use the representation (14) and omit the constant in it, since it does not influence any further considerations.

A nested *M*-tuple $\{\boldsymbol{y}\} := (\boldsymbol{y}^1, \dots, \boldsymbol{y}^M)$ is unambiguously specified by $|\mathcal{V}|$ numbers $m_v^0 \in \{0, \dots, M\}, v \in \mathcal{V}$, where m_v^0 defines a number of labelings, which are assigned the label 0 in the node v. The link between the two representations is given by

$$m_v^0 = \sum_m [\![y_v^m = 0]\!], \tag{15}$$

$$y_v^m = m \le m_v^0. \tag{16}$$

In other words, labelings y^m are superlevel sets of $m^0: \mathcal{V} \to \{0, \dots, M\}$.

Let us write the Joint-DivMBest objective (2) as a function of m^0 . The label $m \in \{0, ..., M\}$ denotes that exactly m out of M labelings in $\{y\}$ are assigned the label 0 in the node v. The unary cost assigned to a label m in the node v is equal to $a_v(M-m)$, since exactly (M-m) labelings out of M are assigned the label 1 in the node v. The pairwise cost for a pair of labels $\{m, n\}$ in the

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neighboring nodes $\{u, v\} \in \mathcal{F}$ is equal to $\Theta_{u,v}|m-n|$, since exactly |m-n| labelings switch their label 0 to the label 1 between nodes u and v. Therefore

$$\sum_{i=1}^{M} E(\boldsymbol{y}^{i}) = \sum_{v \in \mathcal{V}} a_{v}(M - m_{v}^{0}) + \sum_{uv \in \mathcal{F}} \Theta_{u,v} |m_{u}^{0} - m_{v}^{0}|, \qquad (17)$$

where m_v^0 is defined as in (15).

Adding a node-wise diversity measure $\sum_{v \in \mathcal{V}} \lambda \Delta_v^M(\{y\}_v) = \sum_{v \in \mathcal{V}} \lambda \Delta_v^M(m_v^0)$ and regrouping terms, one obtains that the Joint-DivMBest objective (2) is equivalent to

$$\sum_{v \in \mathcal{V}} \left(a_v (M - m_v^0) - \lambda \Delta_v^M(m_v^0) \right) + \sum_{uv \in \mathcal{F}} \Theta_{u,v} |m_u^0 - m_v^0|$$
(18)

and must be minimized with respect to the labeling $m^0 \in \{0, \dots, M\}^{\mathcal{V}}$.

Since the diversity measure $\lambda \Delta_v^M(m_v^0)$ is concave w.r.t. m_v^0 , the unary factors $a_v(M - m_v^0) - \lambda \Delta_v^M(m_v^0)$ are convex. The pairwise factors $\Theta_{u,v}|m_u^0 - m_v^0|$ are also convex w.r.t. $m_u^0 - m_v^0$ due to non-negativity of $\Theta_{u,v}$.

For concave diversity the problem can be solved efficiently in time $O(T(n, m) + n \log M)$ [8], where $n = |\mathcal{V}|, m = |\mathcal{E}|$ and T(n, m) is the complexity of a minimum *s*-*t* cut procedure that can be implemented efficiently as parametric. Even for m^0 ranging in the continuous domain the complexity of the method [8] is polynomial, essentially matching the complexity of a single mincut. In particular, [8, Theorem 3.1] shows that a solution of such convex multilabel energy minimization problem decouples into M problems of the form (12). Our Theorem 2 then follows.

7.1 Related Results and Limitations

For a general (not necessarily concave) permutation invariant nodewise diversity, the problem (17) can be still solved efficiently in time $O(nm \log \frac{n^2}{m}M^2 \log M)$ by either [10] or [1, 9]. On the other hand, the reformulation (14) expressing the regularizer as the function $|m_u^0 - m_v^0|$ holds for the pairwise case only. The results of Hochbaum [8] are as well limited to the pairwise case and involve min-cut / max-flow arguments.

Other related results are as follows. Chan and Esedoglu [5] give a thresholding theorem (related to Theorem 2) for the Rudin-Osher-Fatemi denoising model [11], Darbon and Sigelle [6] for TV-regularized L_1 and L_2 data fidelity problems, Chambolle [3] proposes further generalization towards thresholding of TV-like regularized convex problems in a finite dimensional space. The thresholding theorem of Chambolle [3] is applicable to higher order models, however the conditions on the regularizer are stricter than in Theorem 2: only a certain convex subclass of submodular functions qualifies.

8 General Case

In the following, we identify a simple and general thresholding theorem, applicable to arbitrary submodular (not only pairwise) functions. This constitutes a basis for a general proof of Theorem 2.

8.1 Nestedness

The set of labeling $L_{\mathcal{V}}$ together with the coordinate-wise maximum and minimum operations \lor , \land forms a distributive lattice. The respective partial order $\mathbf{x} \leq \mathbf{y}$ is the coordinate-wise order $(\forall v \in \mathcal{V}) x_v \leq y_v$.

Definition 3. Function $F: L_{\mathcal{V}} \to \mathbb{R}$ is monotone (resp. antitone) if for all $x \leq y$ there holds $F(x) \leq F(y)$ (resp. $F(x) \geq F(y)$).

For example, a linear function $2^{\mathcal{V}} \to \mathbb{R}$: $\mathbf{y} \mapsto \sum_{v=1}^{\mathcal{V}} a_v y_v$ is monotone for $a_v \ge 0$; a multilabel modular function $\sum_{v=1}^{\mathcal{V}} \theta_v(y_v)$ is monotone if $\theta_v(y'_v) \ge \theta_v(y_v)$ for all $y'_v \ge y_v$ and all $v \in \mathcal{V}$. The sum, minimum and maximum of monotone (resp. antitone) functions is monotone (resp. antitone). Note that, e.g., minimum of modular functions is in general not modular.

The following lemma provides sufficient conditions under which the parametric min-cut and the parametric submodular function minimization are monotone. It is essential for the subsequent derivation that we formulate it in a constructive form, i.e., not only existence of nested minimizers is shown but also the way to restore nestedness.

Lemma 1 (See [12] Theorem 6.1). Let $E: L_{\mathcal{V}} \to \mathbb{R}$ be submodular and $F: L_{\mathcal{V}} \to \mathbb{R}$ be antitone. Then for any minimizer x of E and any minimizer y of E + F, the solution $y' = y \lor x$ is a minimizer of E + F and $x \le y'$.

Proof. Since x is a minimizer of E, $E(x) \leq E(y \wedge x)$. Adding this inequality to the submodularity inequality,

$$E(\boldsymbol{x} \vee \boldsymbol{y}) + E(\boldsymbol{x} \wedge \boldsymbol{y}) \le E(\boldsymbol{x}) + E(\boldsymbol{y}), \tag{19}$$

we obtain

$$E(\boldsymbol{x} \vee \boldsymbol{y}) \le E(\boldsymbol{y}). \tag{20}$$

For antitone F and $x \lor y \ge y$ we have $F(x \lor y) \le F(y)$. Adding to (20), we get

$$(E+F)(\boldsymbol{x} \vee \boldsymbol{y}) \le (E+F)(\boldsymbol{y}).$$
(21)

Since y was a minimizer of E + F, it follows that $x \vee y$ is a minimizer of E + F as well.

It follows that the minimal minimizer of E is nested (contained in the case of set functions) in the minimal minimizer of E + F. Symmetrically, if E is submodular and F is monotone, then $x \land y \leq y$ is a minimizer of E + F. Similar results appear in [8], [4, Lemma 3.4] in a somewhat less general form. Fleischer and Iwata [7, Lemma 3.1] proves nestedness under a related condition called a *strong map*. It can be easily shown that for submodular E + F the map $E \rightarrow E + F$ is a strong map iff F is antitone.

8.2 Thresholding Theorem

Let a function $\mathcal{E}: (L_{\mathcal{V}})^M \to \mathbb{R}$ of a tuple $\{y\}$ has the expression

$$\mathcal{E}(\{\boldsymbol{y}\}) = \sum_{m=1}^{M} E_m(\boldsymbol{y}^m), \qquad (22)$$

for some functions $E_m: L_{\mathcal{V}} \to \mathbb{R}$. We will show that such a decomposition holds for the Joint-DivMBest objective E^M (2) under conditions of Theorem 2 (cf. coarea formula in [3]). Consider minimizing the function \mathcal{E} over *nested* tuples $\{y\}$.

Theorem 3 (Thresholding). Let $E_m : L_{\mathcal{V}} \to \mathbb{R}$ be submodular for each m and $(E_m - E_{m-1})$ be antitone for each m > 1. Then the joint problem,

$$\min_{\{\boldsymbol{y}\}} \sum_{m=1}^{M} E_m(\boldsymbol{y}^m) \quad s.t. \; \{\boldsymbol{y}\} \text{ is nested},$$
(23)

decouples into independent problems

$$\sum_{m} \min_{\boldsymbol{y} \in L_{\mathcal{V}}} E_m(\boldsymbol{y}). \tag{24}$$

Where "decouples" means that the optimal values of both problems are equal and there is a simple mapping between their optimal solutions.

Proof. We will prove the theorem by constructing, out of independent minimizers \hat{y}^m , m = 1, ..., M, a nested tuple of independent minimizers $\{\bar{y}\}$.

Assume that $\hat{y}^k \not\geq \hat{y}^m$ for k > m. The function E_k can be expressed as

$$E_k = E_m + F, (25)$$

where $F = \sum_{l=m+1}^{k} (E_l - E_{l-1})$ is antitone (by conditions of the theorem). We have: \hat{y}^m minimizes E_m , \hat{y}^k minimizes E_k . By the nestedness Lemma 1, it must be that $\hat{y}^k \vee \hat{y}^m$ also minimizes E_k . Moreover, $\hat{y}^k \vee \hat{y}^m \ge \hat{y}^m$.

By going in m in order from 1 to M and replacing \hat{y}^{m+1} with $\hat{y}^{m+1} \vee \hat{y}^m$ we obtain a tuple which is nested and each modifications has preserved optimality to (24). Let $\{\bar{y}\}$ be the resulting nested tuple. It is feasible to the joint problem (23) and optimal to decoupled problem (24). Since also (23) is lower bounded by (24), the tuple $\{\bar{y}\}$ is optimal to (23).

Corollary 4. Let elements of the tuple $\{\hat{y}\}$ be defined as the highest minimizers of E_m :

$$\hat{\boldsymbol{y}}^m = \bigvee \underset{\boldsymbol{y} \in L_{\mathcal{V}}}{\operatorname{arg\,min}} E_m(\boldsymbol{y}) \,. \tag{26}$$

Then under conditions of Theorem 3 the tuple $\{\hat{y}\}$ is nested and optimal to (23).

Proof. The highest minimizer in (26), i.e., the maximum of the set of optimal solutions exists since the set of minimizers to a submodular function on a lattice is a lattice itself [12]. Since for each k > m, (i) the replacement $\hat{y}^k \lor \hat{y}^m$ is a minimizer of $E_k(y)$ (with the same substantiation as in the proof of Theorem 3) and (ii) \hat{y}^k is the highest minimizer of E_k , it therefore holds $\hat{y}^k \lor \hat{y}^m \le \hat{y}^k$. This is however the case only when $\hat{y}^k \ge \hat{y}^m$.

8.3 Application to Submodular Joint-DivMBest Problem

Let $L_{\mathcal{V}} = \{0, 1\}^{\mathcal{V}}$ and the master energy E be submodular. Then the Joint-DivMBest problem according to Theorem 1 has the form

$$\min_{\{\boldsymbol{y}\}} \sum_{m=1}^{M} E(\boldsymbol{y}^m) - \Delta^M(\{\boldsymbol{y}\}) \text{ s.t. } \{\boldsymbol{y}\} \text{ is nested.}$$
(27)

In order to apply Theorem 3, we need to express the objective of this problem in the form (23). Since the master energy $E(\boldsymbol{y}^m)$ is the same for all m, clearly $E - E \equiv 0$ is an antitone function of \boldsymbol{y} . It remains to express $\Delta^M(\{\boldsymbol{y}\})$ in the form (23). Recall that any permutation invariant diversity measure $\Delta_v^M(\{\boldsymbol{y}_v\})$ expresses as a function $g_v(x)$, where $x = \sum_{m=1}^M [\![\boldsymbol{y}_v^m = 0]\!]$. Any function $g_v: \{0, \ldots M\} \to \mathbb{R}$ can be expressed as a prefix (cumulative) sum:

$$g_v(x) = g_v(0) + \sum_{m=1}^M \gamma_v^m [\![m \le x]\!] = g_v(0) + \sum_{m \le x} \gamma_v^m,$$
(28)

where $\gamma_v^m = g_v(m) - g_v(m-1)$ for $m \in \{1, ..., M\}$.

For concave diveristy measures, the discrete derivatives γ_v^m of g_v are monotone non-increasing in m. For a nested tuple $\{y\}$ we have $y_v^m = [\![m \le x]\!]$, and it holds

$$\Delta^{M}(\{\boldsymbol{y}\}) = \sum_{v \in \mathcal{V}} g_{v}(0) + \sum_{m=1}^{M} F_{m}(\boldsymbol{y}^{m})$$
(29)

for $F_m(\boldsymbol{y}^m) = \sum_{v \in \mathcal{V}} \gamma_v^m y_v^m$.

Since the constant term $\sum_{v \in \mathcal{V}} g_v(0)$ can be ignored we proved that $\Delta^M(\{y\})$ decomposes as (22). It remains to show that $-(F_m(y) - F_{m-1}(y))$ is antitone to fulfill conditions of Theorem 3 w.r.t. $-\Delta^M(\{y\})$.

Indeed, the difference $F_m(\mathbf{y}) - F_{m-1}(\mathbf{y})$ expresses as $\sum_{v \in \mathcal{V}} a_v y_v$ with $a_v = \gamma_v^m - \gamma_v^{m-1}$. Since γ_v^m is non-decreasing w.r.t. m, it holds $a_v \ge 0$ and $F_m - F_{m-1}$ is monotone. It implies $-(F_m - F_{m-1})$ is antitone.

As a result, the Joint-DivMBest problem (27) has the expression satisfying conditions of Theorem 3. Thus Theorem 2 holds. $\hfill \Box$

The study of the question which multilabel diversity measures have expression as a sum with monotone differences is left for the future work.

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