# What Energy Functions can be Minimized via Graph Cuts?

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**Abstract**

In the last few years, several new algorithms based on graph cuts have been developed to solve energy minimization problems in computer vision. Each of these techniques constructs a graph such that the minimum cut on the graph also minimizes the energy. Yet because these graph constructions are complex and highly specific to a particular energy function, graph cuts have seen limited application to date. In this paper we characterize the energy functions that can be minimized by graph cuts. Our results are restricted to energy functions with binary variables. However, our work generalizes many previous constructions, and is easily applicable to vision problems that involve large numbers of labels, such as stereo, motion, image restoration and scene reconstruction. We present three main results: a necessary condition for any energy function that can be minimized by graph cuts; a sufficient condition for energy functions that can be written as a sum of functions of up to three variables at a time; and a general-purpose construction to minimize such an energy function. Researchers who are considering the use of graph cuts to optimize a particular energy function can use our results to determine if this is possible, and then follow our construction to create the appropriate graph.

## 1 Introduction and summary of results

Many of the problems that arise in early vision can be naturally expressed in terms of energy minimization. The computational task of minimizing the energy is usually quite difficult, as it generally requires minimizing a non-convex function in a space with thousands of dimensions. If the functions have a restricted form they can be solved efficiently using dynamic programming [2]. However, researchers typically have needed to rely on general purpose optimization techniques such as simulated annealing [3, 10], which is extremely slow in practice.

In the last few years, however, a new approach has been developed based on graph cuts. The basic technique is to construct a specialized graph for the energy function to be minimized, such that the minimum cut on the graph also minimizes the energy (either globally or locally). The minimum cut in turn can be computed very efficiently by max flow algorithms. These methods have been successfully used for a wide variety of vision problems including image restoration [7, 8, 12, 14], stereo and motion [4, 7, 8, 13, 16, 19, 20], voxel occupancy [22], multi-camera scene reconstruction [17] and medical imaging [5, 6, 15]. The output of these algorithms is generally a solution with some interesting theoretical quality guarantee. In some cases [7, 12, 13, 14, 19] it is the global minimum, in other cases a local minimum in a strong sense [8] that is within a known factor of the global minimum. The experimental results produced by these algorithms are also quite good. For example, two recent evaluations of stereo algorithms using real imagery with dense ground truth [21, 23] found that the best overall performance was due to algorithms based on graph cuts.

Minimizing an energy function via graph cuts, however, remains a technically difficult problem. Each paper constructs its own graph specifically for its individual energy function, and in some of these cases (especially [8, 16, 17]) the construction is fairly complex. The goal of this paper is to precisely characterize the class of energy functions that can be minimized via graph cuts, and to give a general-purpose graph construction that minimizes any energy function in this class. Our results play a key role in [17], provide a significant generalization of the energy minimization methods used in [4, 5, 6, 8, 12, 15, 22], and show how to minimize an interesting new class of energy functions.

In this paper we only consider energy functions involving binary-valued variables. At first glance this restriction seems severe, since most work with graph cuts considers energy functions with variables that have many possible values. For example, the algorithms presented in [8] for stereo, motion and image restoration use graph cuts to address the standard pixel labeling problem that arises in early vision. In a pixel labeling problem the variables represent individual pixels, and the possible values for an individual variable represent, e.g., its possible displacements or intensities. However, many of the graph cut methods that handle multiple possible values actually consider a pair of labels at a time. Even though we only address binary-valued variables, our results therefore generalize the algorithms given in [4, 5, 6, 8, 12, 15, 22]. As an example, we will show in section 4.1 how to use our results to solve the pixel-labeling problem, even though the pixels have many possible labels. An additional argument in favor of binary-valued variables is that any cut effectively assigns one of two possible values to each node of the graph. So in a certain sense any energy minimization construction based on graph cuts relies on intermediate binary variables.

### 1.1 Summary of our results

In this paper we consider two classes of energy functions. Let $\{x_1, \ldots, x_n\}$, $x_i \in \{0, 1\}$ be a set of binary-valued variables. We define the class $\mathcal{F}^2$ to be functions that can be written as a sum of functions of up to 2 variables at a time,

$$E(x_1, \ldots, x_n) = \sum_i E^i(x_i) + \sum_{i<j} E^{i,j}(x_i, x_j). \tag{1}$$

We define the class $\mathcal{F}^3$ to be functions that can be written as a sum of functions of up to 3 variables at a time,

$$E(x_1, \ldots, x_n) = \sum_i E^i(x_i) + \sum_{i<j} E^{i,j}(x_i, x_j) + \sum_{i<j<k} E^{i,j,k}(x_i, x_j, x_k). \tag{2}$$

Obviously, the class $\mathcal{F}^2$ is a strict subset of the class $\mathcal{F}^3$. Note that there is no restriction on the signs of the energy functions or of the individual terms.

The main result in this paper is a precise characterization of the functions in $\mathcal{F}^3$ that can be minimized using graph cuts, together with a graph construction for minimizing such functions. Moreover, we give a necessary condition for all other classes which must be met for a function to be minimized via graph cuts.

Our results also identify an interesting class of class of energy functions that have not yet been minimized using graph cuts. All of the previous work with graph cuts involves a neighborhood system that is defined on pairs of pixels. In the language of Markov Random Fields [10, 18], these methods consider first-order MRF's. The associated energy functions lie in $\mathcal{F}^2$. Our results allow for the minimization of energy functions in the larger class $\mathcal{F}^3$, and thus for neighborhood systems involving triples of pixels.

### 1.2 Organization

The rest of the paper is organized as follows. In section 2 we give an overview of graph cuts. In section 3 we formalize the problem that we want to solve. Section 4 contains our main theorem for the class of functions $\mathcal{F}^2$ and shows how it can be used to solve pixel labeling problems. Section 5 contains our main theorems for other classes. An example of our graph construction is provided in section 6. Proofs of our theorems, together with the details of our graph constructions, are deferred to section 7. A summary of the actual graph constructions is given in the appendix.

## 2 Overview of graph cuts

Suppose $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a directed graph with non-negative edge weights that has two special vertices (terminals), namely the source $s$ and the sink $t$. An $s$-$t$-cut (or just a cut as we will refer to it later) $C = S, T$ is a partition of vertices in $\mathcal{V}$ into two disjoint sets $S$ and $T$, such that $s \in S$ and $t \in T$. The cost of the cut is the sum of costs of all edges that go from $S$ to $T$:

$$c(S,T) = \sum_{u \in S, v \in T, (u,v) \in \mathcal{E}} c(u,v).$$

The minimum $s$-$t$-cut problem is to find a cut $C$ with the smallest cost. Due to the theorem of Ford and Fulkerson [9] this is equivalent to computing the maximum flow from the source to sink. There are many algorithms which solve this problem in polynomial time with small constants [1, 11].

It is convenient to denote a cut $C = S, T$ by a labeling $f$ mapping from the set of the nodes $\mathcal{V} - \{s, t\}$ to $\{0, 1\}$ where $f(v) = 0$ means that $v \in S$, and $f(v) = 1$ means that $v \in T$. We will use this notation later.

## 3 Representing energy functions with graphs

Let us consider a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with terminals $s$ and $t$, thus $\mathcal{V} = \{v_1, \ldots, v_n, s, t\}$. Each cut on $\mathcal{G}$ has some cost; therefore, $\mathcal{G}$ represents the energy function mapping from all cuts on $\mathcal{G}$ to the set of nonnegative real numbers. Any cut can be described by $n$ binary variables $x_1, \ldots, x_n$ corresponding to nodes in $\mathcal{G}$ (excluding the source and the sink): $x_i = 0$ when $v_i \in S$, and $x_i = 1$ when $v_i \in T$. Therefore, the energy $E$ that $\mathcal{G}$ represents can be viewed as a function of $n$ binary variables: $E(x_1, \ldots, x_n)$ is equal to the cost of the cut defined by the configuration $x_1, \ldots, x_n$ ($x_i \in \{0, 1\}$). Note that the configuration that minimizes $E$ will not change if we add a constant to $E$.

We can efficiently minimize $E$ by computing the minimum $s$-$t$-cut on $\mathcal{G}$. This naturally leads to the question: what is the class of energy functions $E$ for which we can construct a graph that represents $E$?

We can also generalize our construction. Above we used each node (except the source and the sink) for encoding one binary variable. Instead we can specify a subset $\mathcal{V}_0 = \{v_1, \ldots, v_k\} \subset \mathcal{V} - \{s, t\}$ and introduce variables only for the nodes in this set. Then there may be several cuts corresponding to a configuration $x_1, \ldots, x_k$. If we define the energy $E(x_1, \ldots, x_k)$ as the minimum among the costs of all such cuts, then the minimum $s$-$t$-cut on $\mathcal{G}$ will again yield the configuration which minimizes $E$.

We will summarize the graph constructions that we allow in the following definition.

**Definition 3.1** *A function $E$ of $n$ binary variables is called* graph-representable *if there exists a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with terminals $s$ and $t$ and a subset of nodes $\mathcal{V}_0 = \{v_1, \ldots, v_n\} \subset \mathcal{V} - \{s, t\}$ such that for any configuration $x_1, \ldots, x_n$ the value of the energy $E(x_1, \ldots, x_n)$ is equal to a constant plus the cost of the minimum $s$-$t$-cut among all cuts $C = S, T$ in which $v_i \in S$, if $x_i = 0$, and $v_i \in T$, if $x_i = 1$ ($1 \leq i \leq n$). We say that $E$ is* exactly represented *by $\mathcal{G}$, $\mathcal{V}_0$ if this constant is zero.*

The following lemma is an obvious consequence of this definition.

**Lemma 3.2** *Suppose the energy function $E$ is graph-representable by a graph $\mathcal{G}$ and a subset $\mathcal{V}_0$. Then it is possible to find the exact minimum of $E$ in polynomial time by computing the minimum $s$-$t$-cut on $\mathcal{G}$.*

In this paper we will give a complete characterization of the classes $\mathcal{F}^2$ and $\mathcal{F}^3$ in terms of graph representability, and show how to construct graphs for minimizing graph-representable energies within these classes. Moreover, we will give a necessary condition for all other classes which must be met for a function to be graph-representable. Obviously, it would be sufficient to consider only the class $\mathcal{F}^3$, since $\mathcal{F}^2 \subset \mathcal{F}^3$. However, the condition for $\mathcal{F}^2$ is simpler so we will consider it separately.

Note that the energy functions we consider can be negative, as can the individual terms in the energy functions. However, the graphs that we construct must have non-negative edge weights. All previous work that used graph cuts for energy minimization dealt with non-negative energy functions and terms; our results have no such restrictions.

# 4 The class $\mathcal{F}^2$

Our main result for the class $\mathcal{F}^2$ is the following theorem.

**Theorem 4.1 ($\mathcal{F}^2$ theorem)** *Let $E$ be a function of $n$ binary variables from the class $\mathcal{F}^2$, i.e.*

$$E(x_1, \dots, x_n) = \sum_i E^i(x_i) + \sum_{i<j} E^{i,j}(x_i, x_j).$$

*Then $E$ is graph-representable if and only if each term $E^{i,j}$ satisfies the inequality*

$$E^{i,j}(0,0) + E^{i,j}(1,1) \leq E^{i,j}(0,1) + E^{i,j}(1,0).$$

## 4.1 Example: pixel-labeling via expansion moves

We now show how to apply this theorem to solve the pixel-labeling problem. In this problem, are given the set of pixels $\mathcal{P}$ and the set of labels $\mathcal{L}$. The goal is to find a labeling $l$ (i.e. a mapping from the set of pixels to the set of labels) which minimizes the energy

$$E(l) = \sum_{p \in \mathcal{P}} D_p(l_p) + \sum_{p,q \in \mathcal{N}} V_{p,q}(l_p, l_q)$$

where $\mathcal{N} \subset \mathcal{P} \times \mathcal{P}$ is a neighborhood system on pixels. Without loss of generality we can assume that $\mathcal{N}$ contains only ordered pairs $p, q$ for which $p < q$ (since we can combine two terms $V_{p,q}$ and $V_{q,p}$ into one term). We will show how our method can be used to derive the expansion move algorithm developed in [8].

This problem is shown in [8] to be NP-hard if $|\mathcal{L}| > 2$. [8] gives an approximation algorithm for minimizing this energy. A single step of this algorithm is an operation called an $\alpha$-expansion. Suppose that we have some current configuration $l^0$, and we are considering a label $\alpha \in \mathcal{L}$. During the $\alpha$-expansion operation a pixel $p$ is allowed either to keep its old label $l_p^0$ or to switch to a new label $\alpha$: $l_p = l_p^0$ or $l_p = \alpha$. The key step in the approximation algorithm presented in [8] is to find the optimal expansion operation, i.e. the one that leads to the largest reduction in the energy $E$. This step is repeated until there is no choice of $\alpha$ where the optimal expansion operation reduces the energy.

[8] constructs a graph which contains nodes corresponding to pixels in $\mathcal{P}$. The following encoding is used: if $f(p) = 0$ (i.e., the node $p$ is in the source set) then $l_p = l_p^0$; if $f(p) = 1$ (i.e., the node $p$ is in the sink set) then $l_p = \alpha$.

Note that the key technical step in this algorithm can be naturally expressed as minimizing an energy function involving binary variables. The binary variables correspond to pixels, and the energy we wish to minimize can be written formally as

$$E(x_{p_1}, \ldots, x_{p_n}) = \sum_{p \in \mathcal{P}} D_p(l_p(x_p)) + \sum_{p,q \in \mathcal{N}} V_{p,q}(l_p(x_p), l_q(x_q)), \qquad (3)$$

where

$$\forall p \in \mathcal{P} \qquad l_p(x_p) = \begin{cases} l_p^0, & x_p = 0 \\ \alpha, & x_p = 1. \end{cases}$$

We can demonstrate the power of our results by deriving an important restriction on this algorithm. In order for the graph cut construction of [8] to work, the function $V_{p,q}$ is required to be a metric. In their paper, it is not clear whether this is an accidental property of the construction (i.e., they leave open the possibility that a more clever graph cut construction may overcome this restriction).

Using our results, we can easily show this is not the case. Specifically, by the $\mathcal{F}^2$ theorem (theorem 4.1), the energy function given in equation 3 is graph-representable if and only if each term $V_{p,q}$ satisfies the inequality

$$V_{p,q}(l_p(0), l_q(0)) + V_{p,q}(l_p(1), l_q(1)) \leq V_{p,q}(l_p(0), l_q(1)) + V_{p,q}(l_p(1), l_q(0))$$

or

$$V_{p,q}(\beta, \gamma) + V_{p,q}(\alpha, \alpha) \leq V_{p,q}(\beta, \alpha) + V_{p,q}(\alpha, \gamma)$$

where $\beta = l_p^0$, $\gamma = l_q^0$. If $V_{p,q}(\alpha, \alpha) = 0$, then this is the triangle inequality:

$$V_{p,q}(\beta, \gamma) \leq V_{p,q}(\beta, \alpha) + V_{p,q}(\alpha, \gamma)$$

This is exactly the constraint on $V_{p,q}$ that was given in [8].

## 5 More general classes of energy functions

We begin with several definitions. Suppose we have a function $E$ of $n$ binary variables. If we fix $m$ of these variables then we get a new function $E'$ of $n-m$ binary variables; we will call this function a *projection* of $E$. The notation for projections is as follows.

**Definition 5.1** *Let $E(x_1, \ldots, x_n)$ be a function of $n$ binary variables, and let $I$, $J$ be a disjoint partition of the set of indices $\{1, \ldots, n\}$: $I = \{i(1), \ldots, i(m)\}$, $J = \{j(1), \ldots, j(n-m)\}$. Let $\alpha_{i(1)}, \ldots, \alpha_{i(m)}$ be binary constants. A* projection *$E' = E[x_{i(1)} = \alpha_{i(1)}, \ldots, x_{i(m)} = \alpha_{i(m)}]$ is a function of $n-m$ variables defined by*

$$E'(x_{j(1)}, \ldots, x_{j(n-m)}) = E(x_1, \ldots, x_n),$$

*where $x_i = \alpha_i$ for $i \in I$. We say that we* fix *the variables $x_{i(1)}$, ..., $x_{i(m)}$.*

Now we introduce our definition of *regular* functions.

**Definition 5.2**

- *All functions of one variable are regular.*
- *A function $E$ of two variables is called regular if $E(0,0) + E(1,1) \leq E(0,1) + E(1,0)$.*
- *A function $E$ of more than two variables is called regular if all projections of $E$ of two variables are regular.*

Now we are ready to formulate our main theorem for $\mathcal{F}^3$.

**Theorem 5.3 ($\mathcal{F}^3$ theorem)** *Let $E$ be a function of $n$ binary variables from $\mathcal{F}^3$, i.e.*

$$E(x_1, \ldots, x_n) = \sum_i E^i(x_i) + \sum_{i<j} E^{i,j}(x_i, x_j) + \sum_{i<j<k} E^{i,j,k}(x_i, x_j, x_k).$$

*Then $E$ is graph-representable if and only if $E$ is regular.*

We also give a necessary condition for all other classes.

**Theorem 5.4 (regularity)** *Let $E$ be a function of binary variables. If $E$ is not regular then $E$ is not graph-representable.*

Regularity is thus an extremely important property, as it allows energy functions to be minimized using graph cuts. Our last theorem shows that minimizing an arbitrary non-regular function is NP-hard, even if we restrict our attention to $\mathcal{F}^2$.

**Theorem 5.5 (NP-hardness)** *Let $E^2$ be a non-regular function of two variables. Then minimizing functions of the form*

$$E(x_1, \dots, x_n) = \sum_i E^i(x_i) + \sum_{(i,j) \in \mathcal{N}} E^2(x_i, x_j)$$

*where $E^i$ are arbitrary functions of one variable and $\mathcal{N} \subset \{(i,j) | 1 \leq i < j \leq n\}$, is NP-hard.*

## 6 Example constructions

The graph constructions we provide will be based on the following two theorems, which are proved in section 7.

**Theorem 6.1 (additivity)** *The sum of two graph-representable functions is graph-representable.*

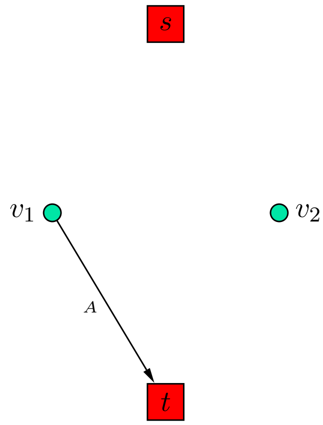
**Theorem 6.2 (regrouping)** *Any regular function from the class $\mathcal{F}^3$ can be rewritten as a sum of terms such that each term is regular and depends on at most three variables.*

It is important to note that the proofs of these theorems are constructive. The additivity theorem's construction has a particularly simple form if the graphs representing the two functions are defined on the same set of vertices (i.e., they differ only in their edge weights). In this case, by simply adding the edge weights together, we obtain a graph that represents the sum of the two functions. If one of the graphs has no edge between two vertices, we can add an edge with weight 0.

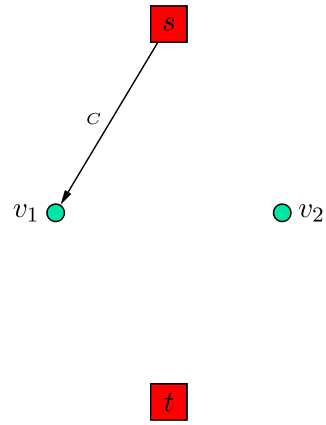
As a result, to complete the constructive part for the $\mathcal{F}^2$ theorem and the $\mathcal{F}^3$ theorem (theorems 4.1 and 5.3), we only need to show how to construct graphs for simple regular functions depending on at most three variables. We can then add the graphs together in the way described in the proof of the additivity theorem.

For example, consider an arbitrary regular function in $\mathcal{F}^2$,

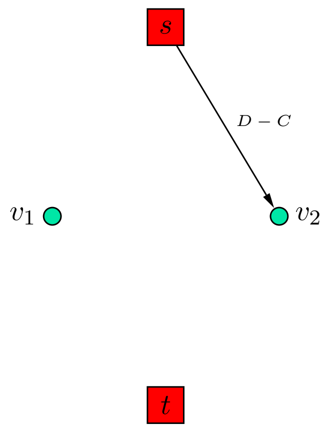
$$E(x_1, \dots, x_n) = \sum_i E^i(x_i) + \sum_{i<j} E^{i,j}(x_i, x_j).$$



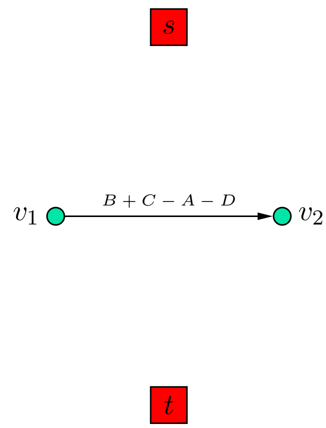

(a) Graph for $\begin{array}{|c|c|}\hline A & A \\ \hline 0 & 0 \\ \hline\end{array}$ (case 1)



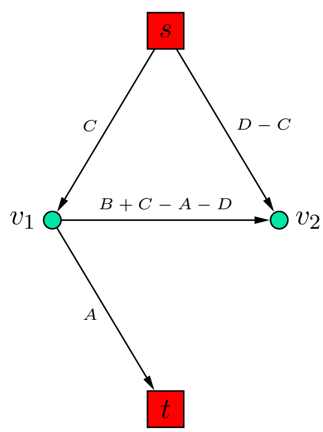

(b) Graph for $\begin{array}{|c|c|}\hline 0 & 0 \\ \hline C & C \\ \hline\end{array}$ (case 1)



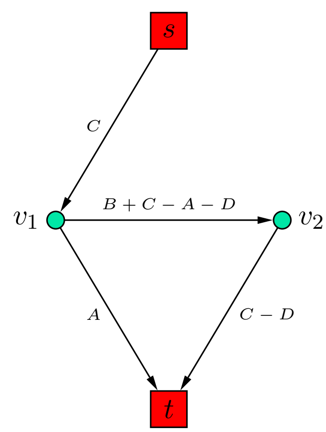

(c) Graph for $\begin{array}{|c|c|}\hline 0 & D-C \\ \hline 0 & D-C \\ \hline\end{array}$ (case 1)




(d) Graph for $\begin{array}{|c|c|}\hline 0 & B+C-A-D \\ \hline 0 & 0 \\ \hline\end{array}$ (case 1)




(e) Graph for $\begin{array}{|c|c|}\hline A & B \\ \hline C & D \\ \hline\end{array}$ (case 1)




(f) Graph for $\begin{array}{|c|c|}\hline A & B \\ \hline C & D \\ \hline\end{array} + \begin{array}{|c|c|}\hline C-D & C-D \\ \hline C-D & C-D \\ \hline\end{array}$ (case 2)

Figure 1: Graph construction for various cases (see text for details)

We can write $E^{i,j}$ as a table

$$\begin{array}{|c|c|}\hline E^{i,j}(0,0) & E^{i,j}(0,1) \\ \hline E^{i,j}(1,0) & E^{i,j}(1,1) \\ \hline \end{array} = \begin{array}{|c|c|}\hline A & B \\ \hline C & D \\ \hline \end{array}$$

We know that $E$ is graph-representable just in case $A + D \leq B + C$, so all we must do is construct the appropriate graph for an arbitrary $E^{i,j}$ that obeys this inequality.

One subtlety is that $A, B, C, D$ can be positive or negative, while the weights on the graphs edges must be non-negative. As a result, there are several different cases depending on the signs of various quantities.

For example, suppose $A > 0, C > 0, D - C > 0$; we will call this "case 1". Then we can re-write the table as

$$\begin{array}{|c|c|}\hline A & B \\ \hline C & D \\ \hline \end{array} = \begin{array}{|c|c|}\hline A & A \\ \hline 0 & 0 \\ \hline \end{array} + \begin{array}{|c|c|}\hline 0 & 0 \\ \hline C & C \\ \hline \end{array} + \begin{array}{|c|c|}\hline 0 & D-C \\ \hline 0 & D-C \\ \hline \end{array} + \begin{array}{|c|c|}\hline 0 & B+C-A-D \\ \hline 0 & 0 \\ \hline \end{array}$$

The quantities in the first 3 tables are non-negative by assumption, and the last is non-negative by regularity. The graphs for each of these tables are shown in figure 1(a)–(d), and the combined graph is shown in figure 1(e).

It is easy to verify that each graph provides the stated penalty; for example, the graph shown in figure 1(a) provides a penalty of $A$ just in case $x_1 = 0$, which is true just in case the edge from the source $s$ to vertex $v_1$ is not cut. If this edge is not cut, then the edge from $v_1$ to the sink $t$ is cut, and the penalty of $A$ is imposed. The argument for the next 2 tables is very similar. The graph shown in figure 1(d) provides a penalty just in case both the edge from $s$ to $v_1$ and the edge from $v_2$ to $t$ are not cut, i.e. when $x_1 = 0$ and $x_2 = 1$.

The combined graph shown in figure 1(e) is just the sum of all the edges. Note that there is no edge from $v_2$ to $t$, which implies that $x_2 = 0$ when we compute the minimum cut. This in fact follows in case 1: regularity implies $B - A \geq D - C$, and in case 1 $D - C > 0$ so we have $B > A$, which together with $D > C$ implies that the minimum is reached with $x_2 = 0$. However, this is only the case for this particular term, and for the energy function as a whole the graphs corresponding to many edges will in general be added together.

The combined graph for a different case, called "case 2", is shown in figure 1(f). In this case we assume $A > 0, C > 0, C - D > 0$. Here we first add the constant $C - D$ to the table and then construct the graph that minimizes it. We have

$$\begin{array}{|c|c|}\hline A & B \\ \hline C & D \\ \hline\end{array} + \begin{array}{|c|c|}\hline C-D & C-D \\ \hline C-D & C-D \\ \hline\end{array} = \begin{array}{|c|c|}\hline A & A \\ \hline 0 & 0 \\ \hline\end{array} + \begin{array}{|c|c|}\hline 0 & 0 \\ \hline C & C \\ \hline\end{array} + \begin{array}{|c|c|}\hline C-D & 0 \\ \hline C-D & 0 \\ \hline\end{array} + \begin{array}{|c|c|}\hline 0 & B+C-A-D \\ \hline 0 & 0 \\ \hline\end{array}$$

Each table on the right hand side corresponds to an obvious edge in the graph shown in figure 1(f).

# 7 Proofs

The proofs in this section are organized as follows. Section 7.1 gives a constructive proof of the additivity theorem (theorem 6.1). Section 7.2 proves some basic lemmas. Sections 7.3 and 7.4 construct graphs for regular functions of two and three variables, respectively. (These constructions are summarized in the appendix). Section 7.5 gives a constuctive proof of the regrouping theorem (theorem 6.2). In section 7.6 we prove the regularity theorem (theorem 5.4), which gives a necessary condition for graph representability, as well as the corresponding directions for the $\mathcal{F}^2$ and $\mathcal{F}^3$ theorems. Finally, in section 7.7 we prove the NP-hardness theorem (theorem 5.5) which shows the intractability of energy minimization in the absence of regularity.

## 7.1 Constructive proof of the additivity theorem

Proof: Let us assume for simplicity of notation that $E'$ and $E''$ are functions of all $n$ variables: $E' = E'(x_1, \ldots, x_n)$, $E'' = E''(x_1, \ldots, x_n)$. By the definition of graph representability, there exist constants $K'$, $K''$, graphs $\mathcal{G}' = (\mathcal{V}', \mathcal{E}')$, $\mathcal{G}'' = (\mathcal{V}'', \mathcal{E}'')$ and the set $\mathcal{V}_0 = \{v_1, \ldots, v_n\}$, $\mathcal{V}_0 \subset \mathcal{V}' - \{s, t\}$, $\mathcal{V}_0 \subset \mathcal{V}'' - \{s, t\}$ such that $E' + K'$ is exactly represented by $\mathcal{G}'$, $\mathcal{V}_0$ and $E'' + K''$ is exactly represented by $\mathcal{G}''$, $\mathcal{V}_0$. We can assume that the only common nodes of $\mathcal{G}'$ and $\mathcal{G}''$ are $\mathcal{V}_0 \cup \{s, t\}$. Let us construct the graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ as the combined graph of $\mathcal{G}'$ and $\mathcal{G}''$: $\mathcal{V} = \mathcal{V}' \cup \mathcal{V}''$, $\mathcal{E} = \mathcal{E}' \cup \mathcal{E}''$.

Let $\tilde{E}$ be the function that $\mathcal{G}$, $\mathcal{V}_0$ exactly represents. Let us prove that $\tilde{E} \equiv E + (K' + K'')$ (and, therefore, $E$ is graph-representable).

Consider a configuration $x_1, \ldots, x_n$. Let $C' = S', T'$ be the cut on $\mathcal{G}'$ with the smallest cost among all cuts for which $v_i \in S'$ if $x_i = 0$, and $v_i \in T'$ if $x_i = 1$ $(1 \leq i \leq n)$. According to the definition of graph representability,

$$E'(x_1, \ldots, x_n) + K' = \sum_{u \in S', v \in T', (u,v) \in \mathcal{E}'} c(u, v)$$

Let $C'' = S'', T''$ be the cut on $\mathcal{G}''$ with the smallest cost among all cuts for which $v_i \in S''$ if $x_i = 0$, and $v_i \in T''$ if $x_i = 1$ $(1 \le i \le n)$. Similarly,

$$E''(x_1, \ldots, x_n) + K'' = \sum_{u \in S'', v \in T'', (u,v) \in \mathcal{E}''} c(u,v)$$

Let $S = S' \cup S''$, $T = T' \cup T''$. It is easy to check that $C = S, T$ is a cut on $\mathcal{G}$. Thus,

$$\tilde{E}(x_1, \ldots, x_n) \le \sum_{u \in S, v \in T, (u,v) \in \mathcal{E}} c(u,v)$$

$$= \sum_{u \in S', v \in T', (u,v) \in \mathcal{E}'} c(u,v) + \sum_{u \in S'', v \in T'', (u,v) \in \mathcal{E}''} c(u,v)$$

$$= (E'(x_1, \ldots, x_n) + K') + (E''(x_1, \ldots, x_n) + K'') = E(x_1, \ldots, x_n) + (K' + K'').$$

Now let $C = S, T$ be the cut on $\mathcal{G}$ with the smallest cost among all cuts for which $v_i \in S$ if $x_i = 0$, and $v_i \in T$ if $x_i = 1$ $(1 \le i \le n)$, and let $S' = S \cap \mathcal{V}'$, $T' = T \cap \mathcal{V}'$, $S'' = S \cap \mathcal{V}''$, $T'' = T \cap \mathcal{V}'$. It is easy to see that $C' = S', T'$ and $C'' = S'', T''$ are cuts on $\mathcal{G}'$ and $\mathcal{G}''$, respectively. According to the definition of graph representability,

$$E(x_1, \ldots, x_n) + (K' + K'') = (E'(x_1, \ldots, x_n) + K') + (E''(x_1, \ldots, x_n) + K'')$$

$$\le \sum_{u \in S', v \in T', (u,v) \in \mathcal{E}'} c(u,v) + \sum_{u \in S'', v \in T'', (u,v) \in \mathcal{E}''} c(u,v)$$

$$= \sum_{u \in S, v \in T, (u,v) \in \mathcal{E}'} c(u,v) = \tilde{E}(x_1, \ldots, x_n).$$

■

## 7.2 Basic lemmas

**Definition 7.1** *The functional $\pi$ will be a mapping from the set of all functions (of binary variables) to the set of real numbers which is defined as follows. For a function $E(x_1, \ldots, x_n)$*

$$\pi(E) = \sum_{x_1 \in \{0,1\}, \ldots, x_n \in \{0,1\}} \left(\Pi_{i=1}^{n} (-1)^{x_i}\right) E(x_1, \ldots, x_n).$$

For example, for a function $E$ of two variables $\pi(E) = E(0,0) - E(0,1) - E(1,0) + E(1,1)$. Note that a function $E$ of two variables is regular if and only if $\pi(E) \le 0$.

It is trivial to check the following properties of $\pi$.

**Lemma 7.2**

- *$\pi$ is linear, i.e. for a scalar $c$ and two functions $E'$, $E''$ of $n$ variables $\pi(E' + E'') = \pi(E') + \pi(E'')$ and $\pi(c \cdot E') = c \cdot \pi(E')$.*

- *If $E$ is a function of $n$ variables that does not depend on at least one of the variables then $\pi(E) = 0$.*

**Lemma 7.3 (equivalence lemma)** *Suppose $E$ and $E'$ are two functions of $n$ variables such that*

$$\forall x_1, \ldots, x_n \qquad E'(x_1, \ldots, x_n) = \begin{cases} E(x_1, \ldots, x_n), & x_k = 0 \\ E(x_1, \ldots, x_n) + C, & x_k = 1, \end{cases}$$

*for some constants $k$ and $C$ ($1 \leq k \leq n$). Then*

- *$E'$ if graph-representable if and only if $E$ is graph-representable;*

- *$E'$ is regular if and only if $E$ is regular.*

Proof: Let us introduce the following function $E^C$:

$$\forall x_1, \ldots, x_n \qquad E^C(x_1, \ldots, x_n) = \begin{cases} 0, & x_k = 0 \\ C, & x_k = 1. \end{cases}$$

We need to show that $E^C$ is graph-representable for any $C$ then the first part of the lemma will follow from the additivity theorem (theorem 6.1) since $E' \equiv E + E^C$ and $E \equiv E' + E^{-C}$.

It is easy to construct a graph which represents $E^C$. The set of nodes in this graph will be $\{v_1, \ldots, v_n, s, t\}$ and the set of edges will include the only edge $(s, v_k)$ with the capacity $C$ (if $C \geq 0$) or the edge $(v_k, t)$ with the capacity $-C$ (if $C < 0$). It is trivial to check that this graph exactly represents $E^C$ (in the former case) or $E^C + C$ (in the latter case).

Now let us assume that one of the functions $E$ and $E'$ is regular, for example, $E$. Consider a projection of $E'$ of two variables:

$$E'[x_{i(1)} = \alpha_{i(1)}, \ldots, x_{i(m)} = \alpha_{i(m)}],$$

where $m = n - 2$ and $\{i(1), \ldots, i(m)\} \subset \{1, \ldots, n\}$. We need to show that this function is regular, i.e. that the functional $\pi(E')$ is nonpositive. Due to the linearity of $\pi$ we can write

$$\pi(E'[x_{i(1)} = \alpha_{i(1)}, \ldots, x_{i(m)} = \alpha_{i(m)}]) =$$
$$= \pi(E[x_{i(1)} = \alpha_{i(1)}, \ldots, x_{i(m)} = \alpha_{i(m)}]) \quad +$$
$$+ \quad \pi(E^C[x_{i(1)} = \alpha_{i(1)}, \ldots, x_{i(m)} = \alpha_{i(m)}]).$$

The first term is nonpositive by assumption, and the second term is 0 by lemma 7.2. ■

### 7.2.1 Properties of the functional $\pi$

While the functional $\pi$ has a form that at first seems counterintuitive, it actually has a close relationship with the classes of energy functions we are concerned with. To see this, let us define the class $\mathcal{F}^k$ to be functions of binary variables that can be written as a sum of functions of up to $k$ variables at a time,

$$E(x_1, \ldots, x_n) = \sum_{i(1)<\ldots<i(k'), k' \leq k} E^{i(1),\ldots,i(k')}(x_{i(1)}, \ldots, x_{i(k')}) \tag{4}$$

(it is an obvious generalization of classes $\mathcal{F}^2$ and $\mathcal{F}^3$).

In this section we will show that the functional $\pi$ can serve as an indicator of the class of a function.

**Theorem 7.4** *Suppose, $E$ is a function of $n$ binary variables ($n \geq 1$). Then $E \in \mathcal{F}^{n-1}$ if and only if $\pi(E) = 0$.*

PROOF: One direction of the theorem is trivial: if $E \in \mathcal{F}^{n-1}$, then $\pi(E) = 0$ by lemma 7.2. Let us prove $\pi(E) = 0$ implies $E \in \mathcal{F}^{n-1}$ by induction on $n$.

Induction base: $n = 1$ ($E$ is a function of one variable). If $\pi(E) = E(0) - E(1) = 0$, then $E(0) = E(1)$, i.e. $E$ is constant and, therefore, is in $\mathcal{F}^0$.

Now suppose that the theorem is true for $n \geq 1$. Let us consider a function $E(x_1, \ldots, x_{n+1})$ of $n+1$ binary variables such that $\pi(E) = 0$.

Let $E_0 = E[x_{n+1} = 0]$, $E_1 = E[x_{n+1} = 1]$ be functions of $n$ variables $x_1, \ldots, x_n$. It is easy to check that $\pi(E) = \pi(E_0) - \pi(E_1)$. Thus, $\pi(E_0) = \pi(E_1) = C$.

Let $R[C]$ be a function of $n$ variables $x_1, \ldots, x_n$ such that $\pi(R[C]) = C$. (For example, we can define it as $R[C](x_1, \ldots, x_n) = C$, if $x_1 = 0, \ldots, x_n = 0$, and $R[C](x_1, \ldots, x_n) = 0$ otherwise.)

Let

$$E'(x_1, \ldots, x_{n+1}) = E(x_1, \ldots, x_{n+1}) - R[C](x_1, \ldots, x_n)$$

$$E'_0(x_1, \ldots, x_n) = E_0(x_1, \ldots, x_n) - R[C](x_1, \ldots, x_n)$$

$$E'_1(x_1, \ldots, x_n) = E_1(x_1, \ldots, x_n) - R[C](x_1, \ldots, x_n)$$

$E'$ is a function of $n+1$ variables, $E'_0$, $E'_1$ are functions of $n$ variables. Clearly, $E'_0 = E'[x_{n+1} = 0]$, $E'_1 = E'[x_{n+1} = 1]$, $\pi(E'_1) = \pi(E'_0) = \pi(E_0) - \pi(R[C]) = C - C = 0$.

By the induction hypothesis, $E'_0, E'_1 \in \mathcal{F}^{n-1}$:

$$E'_0(x_1,\ldots,x_n) = \sum_\alpha E_0^\alpha(x_1,\ldots,x_n)$$
$$E'_1(x_1,\ldots,x_n) = \sum_\beta E_1^\beta(x_1,\ldots,x_n)$$

where all terms $E_0^\alpha$, $E_1^\beta$ depend on at most $n-1$ variables.

Let $\tilde{E}_0^\alpha$, $\tilde{E}_1^\beta$, $\tilde{E}$ be functions of $n+1$ variables defined as follows:

$$\tilde{E}_0^\alpha(x_1,\ldots,x_{n+1}) = \begin{cases} E_0^\alpha(x_1,\ldots,x_n), & x_{n+1}=0 \\ 0, & x_{n+1}=1 \end{cases}$$

$$\tilde{E}_1^\beta(x_1,\ldots,x_{n+1}) = \begin{cases} 0, & x_{n+1}=0 \\ E_1^\beta(x_1,\ldots,x_n), & x_{n+1}=1 \end{cases}$$

$$\tilde{E} \equiv \sum_\alpha \tilde{E}_0^\alpha + \sum_\beta \tilde{E}_1^\beta$$

We can write

$$\tilde{E}[x_{n+1}=0] \equiv \sum_\alpha \tilde{E}_0^\alpha[x_{n+1}=0] + \sum_\beta \tilde{E}_1^\beta[x_{n+1}=0] \equiv \sum_\alpha E_0^\alpha + 0 \equiv E'[x_{n+1}=0]$$

$$\tilde{E}[x_{n+1}=1] \equiv \sum_\alpha \tilde{E}_0^\alpha[x_{n+1}=1] + \sum_\beta \tilde{E}_1^\beta[x_{n+1}=1] \equiv 0 + \sum_\alpha E_1^\beta \equiv E'[x_{n+1}=1]$$

Thus, $E' \equiv \tilde{E}$. All terms $\tilde{E}_0^\alpha$, $\tilde{E}_1^\beta$ depend on at most $n$ variables, therefore, $E' \in \mathcal{F}^n$ and $E \in \mathcal{F}^n$ (since $E$ is a sum of $E'$ and $R[C]$, and $R[C]$ depends on $n$ variables).

**Theorem 7.5** *Suppose, $E$ is a function of $m$ binary variables ($m \geq n \geq 1$). Then $E \in \mathcal{F}^{n-1}$ if and only if $\pi(E') = 0$ for all functions $E'$ that are projections of $E$ of at least $n$ variables (i.e. at most $m-n$ variables are fixed).*

PROOF: One direction of the theorem is trivial: if $E \in \mathcal{F}^{n-1}$, then all projections $E'$ of $E$ are also in $\mathcal{F}^{n-1}$, therefore $\pi(E') = 0$ by lemma 7.2. Let us prove the opposite direction by induction on $m$.

Induction base (the case $m = n$) follows from theorem 7.4.

Now suppose that it is true for $m \geq n$. Let us consider a function $E(x_1,\ldots,x_{m+1})$ of $m+1$ binary variables such that $\pi(E') = 0$ for all projections $E'$ of $E$ of at least $n$ binary variables.

Any projection of $E[x_{m+1} = 0]$ is also a projection of $E$. Thus, $\pi(E') = 0$ for all projections $E'$ of $E[x_{m+1} = 0]$ of at least $n$ binary variables. $E[x_{m+1} = 0]$ is a function of $m$ variables; by the induction hypothesis, $E[x_{m+1} = 0] \in \mathcal{F}^{n-1}$. Similarly, $E[x_{m+1} = 1] \in \mathcal{F}^{n-1}$.

Let $E_0$, $E_1$ be functions of $m+1$ variables $x_1, \ldots, x_{m+1}$ defined as follows:

$$E_0(x_1, \ldots, x_{m+1}) = \begin{cases} E[x_{m+1} = 0](x_1, \ldots, x_m), & x_{m+1} = 0 \\ 0, & x_{m+1} = 1 \end{cases}$$

$$E_1(x_1, \ldots, x_{m+1}) = \begin{cases} 0, & x_{m+1} = 0 \\ E[x_{m+1} = 1](x_1, \ldots, x_m), & x_{m+1} = 1 \end{cases}$$

It is easy to see that $E_0$ and $E_1$ are in $\mathcal{F}^n$ since $E[x_{m+1} = 0]$ and $E[x_{m+1} = 1]$ are in $\mathcal{F}^{n-1}$. Therefore, $E \equiv E_0 + E_1$ is in $\mathcal{F}^n$ as well.

Thus, $E$ can be written as

$$E(x_1, \ldots, x_{m+1}) = \sum_{i(1) < \ldots < i(n)} \tilde{E}^{i(1), \ldots, i(n)}(x_{i(1)}, \ldots, x_{i(n)}) =$$

$$= \sum_{i(1) < \ldots < i(n)} E^{i(1), \ldots, i(n)}(x_1, \ldots, x_{m+1})$$

where

$$E^{i(1), \ldots, i(n)}(x_1, \ldots, x_{m+1}) = \tilde{E}^{i(1), \ldots, i(n)}(x_{i(1)}, \ldots, x_{i(n)})$$

Let us a take a projection of $E$ of $n$ variables where the variables that are not fixed are $x_{i(1)}, \ldots, x_{i(n)}$ ($i(1) < \ldots < i(n)$), and apply the functional $\pi$ to this projection. Let us denote this operation as $\pi'$.

Let us consider the result of this operation on a single term $E^{i'(1), \ldots, i'(n)}$, $i'(1) < \ldots < i'(n)$. If $(i'(1), \ldots, i'(n))$ coincides with $(i(1), \ldots, i(n))$ then $\pi'(E^{i'(1), \ldots, i'(n)}) = \pi(\tilde{E}^{i'(1), \ldots, i'(n)})$. Suppose that these indeces do not coincide, then $i(k)$ is not in $\{i'(1), \ldots, i'(n)\}$ for some $k$. $E^{i'(1), \ldots, i'(n)}$ does not depend on $x_{i(k)}$. Therefore, any projection of this function where $x_{i(k)}$ is not fixed also does not depend on $x_{i(k)}$, so the functional $\pi$ of such projection is 0 by lemma 7.2. Thus, $\pi'(E^{i'(1), \ldots, i'(n)}) = 0$.

Therefore, $\pi'(E) = \pi'(E^{i(1), \ldots, i(n)}) = \pi(\tilde{E}^{i(1), \ldots, i(n)})$. By assumption $\pi'(E) = 0$, so $\tilde{E}^{i(1), \ldots, i(n)} \in \mathcal{F}^{n-1}$ by theorem 7.4.

$E$ is a sum of terms which lie in $\mathcal{F}^{n-1}$, therefore $E$ is in $\mathcal{F}^{n-1}$ as well.

We can also show that $\pi$ is unique (up to a constant multiplicative factor) among the linear functionals that are indicator variables for the class of an energy function.

**Theorem 7.6** *Suppose, $\pi'$ is a linear functional mapping the set of functions $E$ of $n$ binary variables to the set of real numbers with the property that $E \in \mathcal{F}^{n-1}$ if and only if $\pi'(E) = 0$. Then there exists a constant $c \neq 0$ such that $\pi'(E) = c\pi(E)$ for any function $E$.*

PROOF: $\pi'$ can be written as

$$\pi'(E) = \sum_{x_1 \in \{0,1\}, \ldots, x_n \in \{0,1\}} c(x_1, \ldots, x_n) \cdot E(x_1, \ldots, x_n)$$

where $c(x_1, \ldots, x_n)$ are some constants.

Let $c = c(0, \ldots, 0)$. Let us prove that $c(x_1, \ldots, x_n) = (\Pi_{i=1}^n (-1)^{x_i})\, c$ by induction on $d = x_1 + \ldots + x_n$.

Induction base: if $d = x_1 + \ldots + x_n = 0$, then $x_1 = \ldots = x_n = 0$, so $c(x_1, \ldots, x_n) = c$.

Suppose that it is true for all configurations $x_1, \ldots, x_n$ such that $x_1 + \ldots + x_n = d$ ($d \geq 0$). Let us consider a configuration $x_1, \ldots, x_n$ such that $x_1 + \ldots + x_n = d+1$. At least one of the variables is 1 since $d+1 \geq 1$. Let us assume that this is the first variable (we can ensure it by renaming indeces): $x_1 = 1$. Let us consider the function $E(x'_1, \ldots, x'_n)$ which is 1 if $(x'_2, \ldots, x'_n) = (x_2, \ldots, x_n)$, and 0 otherwise. Clearly,

$$\pi'(E) = c(0, x_2, \ldots, x_n) + c(1, x_2, \ldots, x_n)$$

$0 + x_2 + \ldots + x_n = d$, therefore $c(0, x_2, \ldots, x_n) = (\Pi_{i=2}^n (-1)^{x_i})\, c$ by the induction hypothesis. $E$ is in $\mathcal{F}^{n-1}$ since it does not depend on $x_1$. Thus, $\pi'(E)$ must be 0, so

$$c(1, x_2, \ldots, x_n) = -c(0, x_2, \ldots, x_n) = (\Pi_{i=1}^n (-1)^{x_i})\, c$$

We proved that $\pi'(E) = c\pi(E)$ for any function $E$. $c$ cannot be 0 since otherwise $\pi'(E)$ would always be 0, and there are functions $E$ of $n$ variables which are not in $\mathcal{F}^{n-1}$.

## 7.3 Construction for regular functions of two variables

Let $E(x_1, x_2)$ be a regular function of two variables represented by a table

$E =$

| | |
|---|---|
| $E(0,0)$ | $E(0,1)$ |
| $E(1,0)$ | $E(1,1)$ |

The equivalence lemma (lemma 7.3) tells us that we can add a constant to any column or row without affecting the $\mathcal{F}^3$ theorem (theorem 5.3). Thus, without loss of generality we can consider only functions $E$ of the form

$$E = \begin{array}{|c|c|} \hline 0 & A \\ \hline 0 & 0 \\ \hline \end{array}$$

(we subtracted a constant from the first row to make the upper left element zero, then we subtracted a constant from the second row to make the bottom left element zero, and finally we subtracted a constant from the second column to make the bottom right element zero).

$\pi(E) = -A \leq 0$ since we assumed that $E$ is regular; hence, $A$ is non-negative. Now we can easily construct a graph $\mathcal{G}$ which represents this function. It will have four vertices $\mathcal{V} = \{v_1, v_2, s, t\}$ and one edge $\mathcal{E} = \{(v_1, v_2)\}$ with the cost $c(v_1, v_2) = A$. It is easy to see that $\mathcal{G}$, $\mathcal{V}_0 = \{v_1, v_2\}$ represent $E$ since the only case when the edge $(v_1, v_2)$ is cut (yielding a cost $A$) is when $v_1 \in S$, $v_2 \in T$, i.e. when $x_1 = 0$, $x_2 = 1$.

Note that we did not introduce any additional nodes for representing binary interactions of binary variables. This is in contrast to the construction in [8] which added auxiliary nodes for representing energies that we just considered. Our construction yields a smaller graph and, thus, the minimum cut can potentially be computed faster.

### 7.4 Regular functions of three variables

Now let us consider a regular function $E$ of three variables. Let us represent it as a table

$$E = \begin{array}{|c|c|} \hline E(0,0,0) & E(0,0,1) \\ \hline E(0,1,0) & E(0,1,1) \\ \hline E(1,0,0) & E(1,0,1) \\ \hline E(1,1,0) & E(1,1,1) \\ \hline \end{array}$$

Two cases are possible:

Case 1. $\pi(E) \geq 0$. We can apply transformations described in the equivalence lemma (lemma 7.3) and get the following function:

$$E = \begin{array}{|c|c|} \hline 0 & 0 \\ \hline 0 & A_1 \\ \hline 0 & A_2 \\ \hline A_3 & A_0 \\ \hline \end{array}$$

It is easy to check that these transformations preserve the functional $\pi$. Hence, $A = A_0 - (A_1 + A_2 + A_3) = -\pi(E) \leq 0$. By applying the regularity constraint to the projections $E[x_1 = 0]$, $E[x_2 = 0]$, $E[x_3 = 0]$ we also get $A_1 \leq 0$, $A_2 \leq 0$, $A_3 \leq 0$.

We can represent $E$ as the sum of functions

$$E = \begin{array}{|c|c|}\hline 0 & 0 \\ \hline 0 & A_1 \\ \hline 0 & 0 \\ \hline 0 & A_1 \\ \hline \end{array} + \begin{array}{|c|c|}\hline 0 & 0 \\ \hline 0 & 0 \\ \hline 0 & A_2 \\ \hline 0 & A_2 \\ \hline \end{array} + \begin{array}{|c|c|}\hline 0 & 0 \\ \hline 0 & 0 \\ \hline 0 & 0 \\ \hline A_3 & A_3 \\ \hline \end{array} + \begin{array}{|c|c|}\hline 0 & 0 \\ \hline 0 & 0 \\ \hline 0 & 0 \\ \hline 0 & A \\ \hline \end{array}$$

We need to show that all terms here are graph-representable, then the additivity theorem (theorem 6.1) will imply that $E$ is graph-representable as well.

The first three terms are regular functions depending only on two variables and thus are graph-representable as was shown in the previous section. Let us consider the last term.

The graph $\mathcal{G}$ that represents this term can be constructed as follows. The set of nodes will contain one auxilary node $u$: $\mathcal{V} = \{v_1, v_2, v_3, u, s, t\}$. The set of edges will consist of directed edges $\mathcal{E} = \{(v_1, u), (v_2, u), (v_3, u), (u, t)\}$ with capacities $A' = -A$. Let us prove that $\mathcal{G}$, $\mathcal{V}_0 = \{v_1, v_2, v_3\}$ exactly represent the following function $E'(x_1, x_2, x_3) = E(x_1, x_2, x_3) + A'$:

$$E' = \begin{array}{|c|c|}\hline A' & A' \\ \hline A' & A' \\ \hline A' & A' \\ \hline A' & 0 \\ \hline \end{array}$$

If $x_1 = x_2 = x_3 = 1$ then the cost of the minimum cut is 0 (the minimum cut is $S = \{s\}$, $T = \{v_1, v_2, v_3, u, t\}$. Suppose at least one of the variables $x_1$, $x_2$, $x_3$ is 0; without loss of generality, we can assume that $x_1 = 0$, i.e. $v_1 \in \mathcal{S}$. If $u \in S$ then the edge $(u, t)$ is cut; if $u \in T$ the edge $(v_1, u)$ is cut yielding the cost $A'$. Hence, the cost of the minimum cut is at least $A'$. However, if $u \in S$ the cost of the cut is exactly $A'$ no matter where the nodes $v_1$, $v_2$, $v_3$ are. We proved that $\mathcal{G}$, $\mathcal{V}_0$ exactly represent $E'$.

Case 2. $\pi(E) < 0$. This case is similar to the case 1. We can transform the energy to

$$E = \begin{array}{|c|c|}\hline A_0 & A_3 \\ \hline A_2 & 0 \\ \hline A_1 & 0 \\ \hline 0 & 0 \\ \hline \end{array} = \begin{array}{|c|c|}\hline A_1 & 0 \\ \hline 0 & 0 \\ \hline A_1 & 0 \\ \hline 0 & 0 \\ \hline \end{array} + \begin{array}{|c|c|}\hline A_2 & 0 \\ \hline A_2 & 0 \\ \hline 0 & 0 \\ \hline 0 & 0 \\ \hline \end{array} + \begin{array}{|c|c|}\hline A_3 & A_3 \\ \hline 0 & 0 \\ \hline 0 & 0 \\ \hline 0 & 0 \\ \hline \end{array} + \begin{array}{|c|c|}\hline A & 0 \\ \hline 0 & 0 \\ \hline 0 & 0 \\ \hline 0 & 0 \\ \hline \end{array}$$

where $A = A_0 - (A_1 + A_2 + A_3) = \pi(E) < 0$ and $A_1 \leq 0$, $A_2 \leq 0$, $A_3 \leq 0$ since $E$ is regular. The first three terms are regular functions of two variables and the last term can be represented by the graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ where $\mathcal{V} = \{v_1, v_2, v_3, u, s, t\}$ and $\mathcal{E} = \{(u, v_1), (u, v_2), (u, v_3), (s, u)\}$; capacities of all edges are $-A$.

### 7.5 Constructive proof of the regrouping theorem

Finally let us consider a regular function $E$ which can be written as

$$E(x_1, \ldots, x_n) = \sum_{i<j<k} E^{i,j,k}(x_i, x_j, x_k),$$

where $i$, $j$, $k$ are indices from the set $\{1, \ldots, n\}$ (we omitted terms involving functions of one and two variables since they can be viewed as functions of three variables).

Although $E$ is regular, each term in the sum need not necessarily be regular. However we can "regroup" terms in the sum so that each term will be regular (and, thus, graph-representable). This can be done using the following lemma and a trivial induction argument.

**Definition 7.7** *Let $E^{i,j,k}$ be a function of three variables. The functional $N(E^{i,j,k})$ is defined as the number of projections of two variables of $E^{i,j,k}$ with the positive value of the functional $\pi$.*

Note that $N(E^{i,j,k}) = 0$ exactly when $E^{i,j,k}$ is regular.

**Lemma 7.8** *Suppose the function $E$ of $n$ variables can be written as*

$$E(x_1, \ldots, x_n) = \sum_{i<j<k} E^{i,j,k}(x_i, x_j, x_k),$$

*where some of the terms are not regular. Then it can be written as*

$$E(x_1, \ldots, x_n) = \sum_{i<j<k} \tilde{E}^{i,j,k}(x_i, x_j, x_k),$$

where

$$\sum_{i<j<k} N(\tilde{E}^{i,j,k}) < \sum_{i<j<k} N(E^{i,j,k}).$$

PROOF: For simplicity of notation let us assume that the term $E^{1,2,3}$ is not regular and $\pi(E^{1,2,3}[x_3 = 0]) > 0$ or $\pi(E^{1,2,3}[x_3 = 1]) > 0$ (we can ensure this by renaming indices). Let

$$C_k = \max_{\alpha_k \in \{0,1\}} \pi(E^{1,2,k}[x_k = \alpha_k]) \qquad k \in \{4, \ldots, n\}$$

$$C_3 = -\sum_{k=4}^{n} C_k$$

Now we will modify the terms $E^{1,2,3}$, ..., $E^{1,2,n}$ as follows:

$$\tilde{E}^{1,2,k} \equiv E^{1,2,k} - R[C_k] \qquad k \in \{3, \ldots, n\}$$

where $R[C]$ is the function of two variables $x_1$ and $x_2$ defined by the table

$$R[C] = \begin{array}{|c|c|} \hline 0 & 0 \\ \hline 0 & C \\ \hline \end{array}$$

(other terms are unchanged: $\tilde{E}^{i,j,k} \equiv E^{i,j,k}$, $(i,j) \neq (1,2)$). We have

$$E(x_1, \ldots, x_n) = \sum_{i<j<k} \tilde{E}^{i,j,k}(x_i, x_j, x_k)$$

since $\sum_{k=3}^{n} C_k = 0$ and $\sum_{k=3}^{n} R[C_k] \equiv 0$.

If we consider $R[C]$ as a function of $n$ variables and take a projection of two variables where the two variables that are not fixed are $x_i$ and $x_j$ $(i < j)$, then the functional $\pi$ will be $C$, if $(i,j) = (1,2)$, and 0 otherwise since in the latter case a projection actually depends on at most one variable. Hence, the only projections of two variables that could have changed their value of the functional $\pi$ are $\tilde{E}^{1,2,k}[x_3 = \alpha_3, \ldots, x_n = \alpha_n]$, $k \in \{3, \ldots, n\}$, if we treat $\tilde{E}^{1,2,k}$ as functions of $n$ variables, or $\tilde{E}^{1,2,k}[x_k = \alpha_k]$, if we treat $\tilde{E}^{1,2,k}$ as functions of three variables.

First let us consider terms with $k \in \{4, \ldots, n\}$. We have $\pi(E^{1,2,k}[x_k = \alpha_k]) \leq C_k$, thus

$$\pi(\tilde{E}^{1,2,k}[x_k = \alpha_k]) = \pi(E^{1,2,k}[x_k = \alpha_k]) - \pi(R[C_k][x_k = \alpha_k]) \leq C_k - C_k = 0$$

Therefore we did not introduce any nonregular projections for these terms.

Now let us consider the term $\pi(\tilde{E}^{1,2,3}[x_3 = \alpha_3])$. We can write

$$\pi(\tilde{E}^{1,2,3}[x_3 = \alpha_3]) = \pi(E^{1,2,3}[x_3 = \alpha_3]) - \pi(R[C_3][x_3 = \alpha_3]) =$$
$$= \pi(E^{1,2,3}[x_3 = \alpha_3]) - (-\sum_{k=4}^{n} C_k) = \sum_{k=3}^{n} \pi(E^{1,2,k}[x_k = \alpha_k])$$

where $\alpha_k = \arg\max_{\alpha \in \{0,1\}} \pi(E^{1,2,k}[x_k = \alpha])$, $k \in \{4, \ldots, n\}$. The last expression is just $\pi(E[x_3 = \alpha_3, \ldots, x_n = \alpha_n])$ and is nonpositive since $E$ is regular by assumption. Hence, values $\pi(\tilde{E}^{1,2,3}[x_3 = 0])$ and $\pi(\tilde{E}^{1,2,3}[x_3 = 1])$ are both nonpositive and, therefore, the number of nonregular projections has decreased. ■

### 7.6 Proof of the regularity theorem

In this section we will prove theorem 5.4 (the regularity theorem). This theorem provides a necessary condition for graph representability: if a function of binary variables is graph-representable then it is regular. It will also imply the corresponding directions of the $\mathcal{F}^2$ and $\mathcal{F}^3$ theorems (theorems 4.1 and 5.3).

Note that the $\mathcal{F}^2$ theorem needs a little bit of reasoning, as follows. Let us consider a graph-representable function $E$ from the class $\mathcal{F}^2$:

$$E(x_1, \ldots, x_n) = \sum_i E^i(x_i) + \sum_{i<j} E^{i,j}(x_i, x_j)$$

$E$ is regular as we will prove in this section. This implies that the functional $\pi$ of any projection of $E$ of two variables is nonpositive. Let us consider a projection where the two variables that are not fixed are $x_i$ and $x_j$. By lemma 7.2 the value of the functional $\pi$ of this projection is equal to $\pi(E^{i,j})$ (all other terms yield zero). Hence, all terms $E^{i,j}$ are regular, i.e. they satisfy the condition of the $\mathcal{F}^2$ theorem.

**Definition 7.9** *Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be a graph, $v_1, \ldots, v_k$ be a subset of nodes $\mathcal{V}$ and $\alpha_1, \ldots, \alpha_k$ be binary constants whose values are from $\{0, 1\}$. We will define the graph $\mathcal{G}[x_1 = \alpha_1, \ldots, x_k = \alpha_k]$ as follows. Its nodes will be the same as in $\mathcal{G}$ and its edges will be all edges of $\mathcal{G}$ plus additional edges corresponding to nodes $v_1, \ldots, v_k$: for a node $v_i$, we add the edge $(s, v_i)$, if $\alpha_i = 0$, or $(v_i, t)$, if $\alpha_i = 1$, with an infinite capacity.*

It should be obvious that these edges enforce constraints $f(v_1) = \alpha_1$, $\ldots$, $f(v_k) = \alpha_k$ in the minimum cut on $\mathcal{G}[x_1 = \alpha_1, \ldots, x_k = \alpha_k]$, i.e. if $\alpha_i = 0$ then $v_i \in S$, and if $\alpha_i = 1$ then $v_i \in T$. (If, for example, $\alpha_i = 0$ and $v_i \in T$ then the edge $(s, v_i)$ must be cut yielding an infinite cost, so it would not the minimum cut.)

Now we can give a definition of graph representability which is equivalent to the definition 3.1. This new definition will be more convenient for the proof.

**Definition 7.10** *We say that the function $E$ of $n$ binary variables is exactly represented by the graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ and the set $\mathcal{V}_0 \subset \mathcal{V}$ if for any configuration $\alpha_1, \ldots, \alpha_n$ the cost of the minimum cut on $\mathcal{G}[x_1 = \alpha_1, \ldots, x_k = \alpha_k]$ is $E(\alpha_1, \ldots, \alpha_n)$.*

**Lemma 7.11** *Any projection of a graph-representable function is graph-representable.*

PROOF: Let $E$ be a graph-representable function of $n$ variables, and the graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ and the set $\mathcal{V}_0$ represents $E$. Suppose that we fix variables $x_{i(1)}, \ldots, x_{i(m)}$. It is straightforward to check that the graph $\mathcal{G}[x_{i(1)} = \alpha_{i(1)}, \ldots, x_{i(m)} = \alpha_{i(m)}]$ and the set $\mathcal{V}_0' = \mathcal{V}_0 - \{v_{i(1)}, \ldots, v_{i(m)}\}$ represent the function $E' = E[x_{i(1)} = \alpha_{i(1)}, \ldots, x_{i(m)} = \alpha_{i(m)}]$. ■

This lemma implies that it suffices to prove theorem 5.4 only for energies of two variables.

Let $E(x_1, x_2)$ be a graph-representable function of two variables. Let us represent this function as a table:

$$E = \begin{array}{|c|c|} \hline E(0,0) & E(0,1) \\ \hline E(1,0) & E(1,1) \\ \hline \end{array}$$

The equivalence lemma (lemma 7.3) tells us that we can add a constant to any column or row without affecting theorem 5.4. Thus, without loss of generality we can consider only functions $E$ of the form

$$E = \begin{array}{|c|c|} \hline 0 & 0 \\ \hline 0 & A \\ \hline \end{array}$$

(we subtracted a constant from the first row to make the upper left element zero, then we subtracted a constant from the second row to make the bottom left element zero, and finally we subtracted a constant from the second column to make the upper right element zero).

We need to show that $E$ is regular, i.e. that $\pi(E) = A \leq 0$. Suppose this is not true: $A > 0$.

Suppose the graph $\mathcal{G}$ and the set $\mathcal{V}_0 = \{v_1, v_2\}$ represent $E$. It means that there is a constant $K$ such that $\mathcal{G}$, $\mathcal{V}_0$ exactly represent $E'(x_1, x_2) = E(x_1, x_2) + K$:

$$E' = \begin{array}{|c|c|} \hline K & K \\ \hline K & K + A \\ \hline \end{array}$$

The cost of the minimum $s$-$t$-cut on $\mathcal{G}$ is $K$ (since this cost is just the minimum entry in the table for $E'$); hence, $K \geq 0$. Thus the value of the maximum flow from $s$ to $t$ in $\mathcal{G}$ is $K$. Let $\mathcal{G}^0$

be the residual graph obtained from $\mathcal{G}$ after pushing the flow $K$. Let $E^0(x_1, x_2)$ be the function exactly represented by $\mathcal{G}^0, \mathcal{V}_0$.

By the definition of graph representability, $E'(\alpha_1, \alpha_2)$ is equal to the value of the minimum cut (or maximum flow) on the graph $\mathcal{G}[x_1 = \alpha_1, x_2 = \alpha_2]$. The following sequence of operations shows one possible way to push the maximum flow through this graph.

- First we take the original graph $\mathcal{G}$ and push the flow $K$; then we get the residual graph $\mathcal{G}^0$. (It is equivalent to pushing flow through $\mathcal{G}[x_1 = \alpha_1, x_2 = \alpha_2]$ where we do not use edges corresponding to constraints $x_1 = \alpha_1$ and $x_2 = \alpha_2$).

- Then we add edges corresponding to these constraints; then we get the graph $\mathcal{G}^0[x_1 = \alpha_1, x_2 = \alpha_2]$.

- Finally we push the maximum flow possible through the graph $\mathcal{G}^0[x_1 = \alpha_1, x_2 = \alpha_2]$; the amount of this flow is $E^0(\alpha_1, \alpha_2)$ according to the definition of graph representability.

The total amount of flow pushed during all steps is $K + E^0(\alpha_1, \alpha_2)$; thus,

$$E'(\alpha_1, \alpha_2) = K + E^0(\alpha_1, \alpha_2)$$

or

$$E(\alpha_1, \alpha_2) = E^0(\alpha_1, \alpha_2)$$

We proved that $E$ is exactly represented by $\mathcal{G}^0$, $\mathcal{V}_0$.

The value of the minimum cut/maximum flow on $\mathcal{G}^0$ is 0 (it is the minimum entry in the table for $E$); thus, there is no augmenting path from $s$ to $t$ in $\mathcal{G}^0$. However, if we add edges $(v_1, t)$ and $(v_2, t)$ then there will be an augmenting path from $s$ to $t$ in $\mathcal{G}^0[x_1 = \alpha_1, x_2 = \alpha_2]$ since $E(1, 1) = A > 0$. Hence, this augmenting path will contain at least one of these edges and, therefore, either $v_1$ or $v_2$ will be in the path. Let $P$ be the part of this path going from the source until $v_1$ or $v_2$ is first encountered. Without loss of generality we can assume that it will be $v_1$. Thus, $P$ is an augmenting path from $s$ to $v_1$ which does not contain edges that we added, namely $(v_1, t)$ and $(v_2, t)$.

Finally let us consider the graph $\mathcal{G}^0[x_1 = 1, x_2 = 0]$ which is obtained from $\mathcal{G}^0$ by adding edges $(v_1, t)$ and $(s, v_2)$ with infinite capacities. There is an augmenting path $\{P, (v_1, t)\}$ from the source to the sink in this graph; hence, the minimum cut/maximum flow on it greater than zero, or $E(1, 0) > 0$. We get a contradiction.

### 7.7 NP-hardness

We now give a proof of the NP-hardness theorem (theorem 5.5), which shows that in the absence of regularity it is intractable to minimize even energy functions in $\mathcal{F}^2$.

Proof: Adding functions of one variable does not change the class of functions that we are considering. Thus, we can assume without loss of generality that $E^2$ has the form

$$E^2 = \begin{array}{|c|c|} \hline 0 & 0 \\ \hline 0 & A \\ \hline \end{array}$$

(We can transform an arbitrary function of two variables to this form as follows: we subtract a constant from the first row to make the upper left element zero, then we subtract a constant from the second row to make the bottom left element zero, and finally we subtract a constant from the second column to make the upper right element zero.)

These transformations preserve the functional $\pi$, so $E^2$ is non-regular, which means that $A > 0$.

We will prove the theorem by reducing the maximum independent set problem, which is known to be NP-hard, to our energy minimization problem.

Let an undirected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be the input to the maximum independent set problem. A subset $\mathcal{U} \subset \mathcal{V}$ is said to be independent if for any two nodes $u, v \in \mathcal{U}$ the edge $(u, v)$ is not in $\mathcal{E}$. The goal is to find an independent subset $\mathcal{U}^* \subset \mathcal{V}$ of maximum cardinality. We construct an instance of the energy minimization problem as follows. There will be $n = |\mathcal{V}|$ binary variables $x_1, \ldots, x_n$ corresponding to the nodes $v_1, \ldots, v_n$ of $\mathcal{V}$. Let us consider the energy

$$E(x_1, \ldots, x_n) = \sum_i E^i(x_i) + \sum_{(i,j) \in \mathcal{N}} E^2(x_i, x_j)$$

where $E^i(x_i) = -\frac{A}{2n} \cdot x_i$ and $\mathcal{N} = \{(i, j) \mid (v_i, v_j) \in \mathcal{E}\}$.

There is a one-to-one correspondence between all configurations $(x_1, \ldots, x_n)$ and subsets $\mathcal{U} \subset \mathcal{V}$: a node $v_i$ is in $\mathcal{U}$ if and only if $x_i = 1$. Moreover, the first term of $E(x_1, \ldots, x_n)$ is $-\frac{A}{2n}$ times the cardinality of $U$ (which cannot be less than $-\frac{A}{2}$), and the second term is 0, if $U$ is independent, and at least $A$ otherwise. Thus, the minimum of the energy yields the independent subset of maximum cardinality.

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## Appendix: Summary of graph constructions

We now summarize the graph constructions used for regular functions. The notation $D(v, c)$ means that we add an edge $(s, v)$ with the weight $c$ if $c > 0$, or an edge $(v, t)$ with the weight $-c$ if $c < 0$.

### Regular functions of one binary variable

Recall that all functions of one variable are regular. For a function $E(x_1)$, we construct a graph $\mathcal{G}$ with three vertices $\mathcal{V} = \{v_1, s, t\}$. There is a single edge $D(v_1, E(1) - E(0))$.

### Regular functions of two binary variables

We now show how to construct a graph $\mathcal{G}$ for a regular function $E(x_1, x_2)$ of two variables. It will contain four vertices: $\mathcal{V} = \{v_1, v_2, s, t\}$. The edges $\mathcal{E}$ are given below.

- $D(v_1, E(1,0) - E(0,0))$;
- $D(v_2, E(1,1) - E(1,0))$;
- $(v_1, v_2)$ with the weight $-\pi(E)$.

### Regular functions of three binary variables

We next show how to construct a graph $\mathcal{G}$ for a regular function $E(x_1, x_2, x_3)$ of three variables. It will contain five vertices: $\mathcal{V} = \{v_1, v_2, v_3, u, s, t\}$. If $\pi(E) \geq 0$ then the edges are

- $D(v_1, E(1,0,1) - E(0,0,1))$;
- $D(v_2, E(1,1,0) - E(1,0,0))$;
- $D(v_3, E(0,1,1) - E(0,1,0))$;

- $(v_2, v_3)$ with the weight $-\pi(E[x_1 = 0])$;
- $(v_3, v_1)$ with the weight $-\pi(E[x_2 = 0])$;
- $(v_1, v_2)$ with the weight $-\pi(E[x_3 = 0])$;
- $(v_1, u)$, $(v_2, u)$, $(v_3, u)$, $(u, t)$ with the weight $\pi(E)$.

If $\pi(E) < 0$ then the edges are

- $D(v_1, E(1,1,0) - E(0,1,0))$;
- $D(v_2, E(0,1,1) - E(0,0,1))$;
- $D(v_3, E(1,0,1) - E(1,0,0))$;
- $(v_3, v_2)$ with the weight $-\pi(E[x_1 = 1])$;
- $(v_1, v_3)$ with the weight $-\pi(E[x_2 = 1])$;
- $(v_2, v_1)$ with the weight $-\pi(E[x_3 = 1])$;
- $(u, v_1)$, $(u, v_2)$, $(u, v_3)$, $(s, u)$ with the weight $-\pi(E)$.

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