Efficient Determination of Gibbs Estimators with Submodular Energy Functions

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3rd February 2022

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Abstract

Now the Gibbs estimators are used to solve many problems in computer vision, optimal control, Bayesian statistics etc. Their determination is equivalent to minimization of corresponding energy functions. Therefore, the real use of the estimators is restricted by opportunity to compute or evaluate satisfactory values of the energy functions. New combinatorial techniques that have been developed for the last years allowed efficient employment of high dimensional Ising models with Boolean and rational valued variables. In addition, graph cut methods were proposed to minimize energy functions $U = \sum g_{\mu}(x_{\mu}) + \sum g_{\mu,\nu}(x_{\mu}, x_{\nu}) + \sum g_{\mu,\nu,\kappa}(x_{\mu}, x_{\nu}, x_{\kappa})$ of Boolean variables $x_{\mu}$ and $U = \sum h(i_{\mu}) + \sum g(|i_{\mu} - j_{\nu}|)$ of integer variables $i_{\mu}$ with submodular functions $g$.

In the paper energy functions that often occur in applications (for instance, in estimating of images) are considered. They are suppose to be depended on variables taking values in totally ordered finite sets (finite sets of arbitrary numbers are among them). The representation of functions by Boolean polynomials are described. Fast methods of minimization of submodular Boolean polynomials that correspond to the energy functions are developed. For that the Modified algorithm of minimization of submodular functions (MSFM) is proposed. Also the minimum graph cut technique is presented for submodular Boolean polynomials that satisfy some additional condition. Among such polynomials are, for instance, those with all coefficients before nonlinear monomials negative as well as submodular Boolean polynomials, which have all coefficients before monomials of order more than two positive.

Mathematics Subject Classification 2000: 90C27, 62N, 62H, 68W

Key words and phrases: Gibbs estimators, minimization, submodular functions, SFM-algorithm, Boolean polynomials, representation by graphs

*The research was supported by ISTC B-517 grant.
1 Introduction

Nowadays Gibbs models are successfully employed in mathematical statistics, statistical physics, image processing etc. Often these models allow to get satisfactory solutions of various problems but usually they turn out very hard to be solved efficiently. Finding of Gibbs estimates is equivalent to the problem of identification of minima of corresponding energy functions. In this paper we present fast methods of finding the Gibbs estimates for some models that occur in application (for instance, in image processing).

The Simulated annealing \([2, 4, 5, 10]\) was one of the first method that was used to find the Gibbs estimates. In spite of its slowness, it remains a very popular tool to evaluate the estimates as well as other problems of general global optimization. To speed up computation of the estimator of the Ising model Grieg, Porteous and Seheult \([3]\) in 1989 described the network flow technique that allowed the exact Boolean minimizing the Ising energy function. In the last few years several new approaches, which enable efficient estimation \([1]\) or even efficient minimizing some wide classes of functions of many Boolean or integer variables, have been developed \([6, 8, 11]\). These approaches, which are based on the graph cut technique, demonstrate possibility to solve real practical problems including handling of 3D data for acceptable time (for instance, segmentation of 3D \(200 \times 200 \times 300\) gray-scale image by the such type method took 14 min. of Pentium 4 1.6GH CPU).

Recently the combinatorial algorithm of minimization of submodular functions (SFM) have been developed \([7]\). To minimize a submodular function of \(n\) variables it needs either \(O(n^5 \log M)\) (where \(M\) is some number depending on the function considered) or \(O(n^8)\) operations. Therefore, the SFM can not be immediately used for finding of high dimensional Gibbs estimates for its comparatively high computational expenses. We present a modification of the SFM that can be useful for minimization of submodular Boolean representations of energy functions, which occur in applications, for instance, in image processing.

In order to use the SFM algorithm and the graph cut technique for energy functions, which depend on variables taking values in finite totally ordered sets, we represent the functions by Boolean polynomials. Then we develop methods that allow efficient minimization of submodular Boolean polynomials of special structure. Some Boolean polynomials admit finding parts of Boolean vectors, which minimize these polynomials, by use only parts of their monomials. We illustrate this property with image processing terminology. It means colours of far points of images estimates are independent, i.e. a change of colours of some image pixels in the estimate does not affect colours of other far pixels. Therefore, the modified SFM (MSFM) operates, first, not with an original Boolean polynomial but with separated its parts, trying to find part of coordinates of a solution of the original problem. Then the values found are set in the original polynomial and the procedure are repeated either with other parts of the residual polynomial or with the entire residual polynomial. At worst, it takes as many operations as the usual SFM and, at best, the number of operations is even \(O(n)\), where \(n\) is a number of Boolean variables.

As we mentioned above, new graph cut methods \([8, 11]\) are now an efficient tool to determine Gibbs estimators with energy functions \(U = \sum g_\mu(x_\mu) + \sum g_{\mu,\nu}(x_\mu, x_\nu) + \sum g_{\mu,\nu,\kappa}(x_\mu, x_\nu, x_\kappa)\) that are Boolean polynomials of the third order. We failed to represent an arbitrary submodular Boolean polynomial by a graph but we made it for submodular Boolean polynomials of the special structure that can be met in applications. The set of
those polynomials contains, for instance, Boolean polynomials with all nonlinear monomials negative (of course, such polynomials are submodular) and submodular Boolean polynomials with monomials of order three and higher positive.

2 Representation of Functions by Boolean Polynomials

Below the function $U(x)$, $x = (x_1, \ldots, x_n)$ is supposed to be dependent on variables that take values in an arbitrary finite totally ordered set $\mathcal{R} = \{r_0, r_1, \ldots, r_k\}$, $r_0 \leq r_1 \leq \ldots \leq r_k$. The multiindex $\mathbf{j} = (j_1, j_2, \ldots, j_n)$ is with coordinates $j_i \in \{0, 1, \ldots, k\} = \mathbb{N}_k$. The function of integer variables $V(\mathbf{j}) = U(r_{j_1}, r_{j_2}, \ldots, r_{j_n})$ is considered instead of the initial $U(x)$.

To exploit the MSF and graph cut technique we, first, represent the integer variables $j_i$ as the sum of ordered Boolean ones $j_i = \sum_{l=1}^{k} x_i(l)$, where $x_i(l) \in \{0, 1\}$, $x_i(1) \geq x_i(2) \geq \ldots \geq x_i(k)$. By other words, we establish one-to-one correspondence between each variable $j_i$ and the ordered sequence of Boolean variables $x_i(1) \geq x_i(2) \geq \ldots \geq x_i(k)$. After we represent the function $V(\mathbf{j})$ by a Boolean polynomial and then minimize the polynomial.

Denote the Boolean vector $x(l) = (x_1(l), x_2(l), \ldots, x_n(l))$, and for two vectors $x, z$ say $x \geq z$, if $x_i \geq z_i$, $i = 1 \div n$ (respectively, $x \not\geq z$, if there is a couple of indexes $i, j$ such that $x_i < z_i$ and $x_j > z_j$). Then

$$V(\mathbf{j}) = V \left( \sum_{l=1}^{k} x(l) \right), \quad x(1) \geq x(2) \ldots \geq x(k).$$

For simplicity let us start with the function of two variables $V(j_1, j_2)$. It is not hard to check the equality

$$V(j_1, j_2) = V(0, j_2) + \sum_{\mu=1}^{k} (V(\mu, j_2) - V(\mu - 1, j_2))x_1(\mu),$$

where ordered Boolean variables $x_1(\mu)$ satisfy the equality $[1]$. Now the expansion

$$V(j_1, j_2)$$

$$= V(0, 0) + \sum_{\mu=1}^{k} (V(\mu, 0) - V(\mu - 1, 0))x_1(\mu) + \sum_{\nu=1}^{k} (V(0, \nu) - V(0, \nu - 1))x_2(\nu)$$

$$+ \sum_{\mu, \nu=1}^{k} (V(\mu, \nu) - V(\mu - 1, \nu) - V(\mu, \nu - 1) + V(\mu - 1, \nu - 1))x_1(\mu)x_2(\nu),$$

(3)
can be constructed by use of equality (2) for the second variable \( j_2 \) of each difference \( V(\mu, j_2) - V(\mu - 1, j_2) \).

In general case, for \( j \in \mathbb{N}_n \) we say

\[
\Delta_i V(j) = V(j) - V(j - e_i), \quad e_i = (0, \ldots, 0, 1, 0, \ldots, 0)
\]

is difference derivative of the first order, and define the mixed difference derivative of higher orders by the recursion

\[
\Delta_{j_1, j_2, \ldots, j_{l+1}} V(j) = \Delta_{j_1, j_2, \ldots, j_l} V(j) - \Delta_{j_1, j_2, \ldots, j_l} V(j - e_{j_{l+1}}).
\]

Note that for any permutation of indices \( \pi(j_1, j_2, \ldots, j_n) \)

\[
\Delta_{\pi(j_1, j_2, \ldots, j_l+1)} = \Delta_{j_1, j_2, \ldots, j_l+1}.
\]

By analogy with 2D case

\[
V(j) = U(0, j_2, \ldots, j_n) + \sum_{\mu=1}^k \Delta_1 V(\mu, j_2, \ldots, j_n) x_1(\mu).
\]

Let the \( G_m \) be the projection operator onto the space of last \( n - m \) coordinate, i.e.

\[
G_m j = (0, \ldots, 0, j_{m+1}, j_{m+2}, \ldots, j_n).
\]

Applying formula (4) recursively \( m \) times to each its item we get the equality

\[
V(j) = V(G_m j) + \sum_{1 \leq l \leq m} \sum_{\mu=1}^k \Delta_l V(G_m j + \mu e_l) x_l(\mu)
\]

\[
+ \sum_{1 \leq l_1 < l_2 \leq m \mu_1, \mu_2 = 1} \Delta_{l_1, l_2} V(G_m j + \mu_1 e_{l_1} + \mu_2 e_{l_2}) x_{l_1}(\mu_1) x_{l_2}(\mu_2) + \ldots
\]

\[
+ \sum_{\mu_1, \ldots, \mu_m = 1} \Delta_{1, 2, \ldots, m} V(G_m j + \mu_1 e_1 + \mu_2 e_2 + \ldots + \mu_m e_m) x_1(\mu_1) x_2(\mu_2) \ldots x_m(\mu_m)
\]

Therefore, the following statement is valid.

**Proposition 1.** The expansion of \( V(j) \) into a polynomial in ordered Boolean variables \( x(1) \geq x(2) \geq \ldots \geq x(k) \) is of the form

\[
V(j) = \tilde{P}_V(x(1), x(2), \ldots, x(k))
\]

\[
= V(0) + \sum_{m=1}^n \sum_{1 \leq l_1 < \ldots < l_m \leq n} \sum_{\mu_1, \ldots, \mu_m = 1} \Delta_{l_1, \ldots, l_m} V \left( \sum_{\kappa=1}^m \mu_\kappa e_{l_\kappa} \right) \prod_{\kappa=1}^m x_{l_\kappa}(\mu_\kappa).
\]
The expansion (5) does not allow to turn immediately to the problem of the Boolean minimization because of ordered variables. To avoid this disadvantage we will use another polynomial

\[ P_V(x(1), x(2), \ldots, x(k)) = \tilde{P}_V(x(1), x(2), \ldots, x(k)) + C \sum_{\mu=1}^{n} \sum_{l=2}^{k} (x_\mu(l) - x_\mu(l - 1))x_\mu(l), \]

for sufficiently large constant \( C > 0 \). This polynomial satisfy the following properties.

**Proposition 2.** The inequality \( \tilde{P}_V \leq P_V \) holds true. Any collection of Boolean vectors \( u^* = (x^*(1), x^*(2), \ldots, x^*(k)) \) that minimizes \( P_V \)

\[ u^* = \arg\min_{x(1), x(2), \ldots, x(k)} P_V(x(1), x(2), \ldots, x(k)) \]

turns to be ordered (non-increasing). This collection minimizes the polynomial \( \tilde{P}_V \), and, therefore, the integer vector \( j^* = \sum_{l=1}^{k} x^*(l) \) minimizes the original function \( V(j) \).

Therefore, instead of minimization of \( V(j) \) we can consider the problem of Boolean minimization of the polynomial

\[ P_V(u) = a_0 + \sum_{m=1}^{n} \sum_{1 \leq l_1 < \ldots < l_m \leq n} a_{l_1, l_2, \ldots, l_m} \prod_{i=1}^{m} u_{l_i}, \quad \dim(u) = kn. \]

Because of the representation of functions \( V(j) \) by Boolean polynomials developed we consider the problem of minimization of general Boolean polynomials \( P(x) \).

### 3 Submodular Boolean Polynomials

For two Boolean vectors \( x, y \) let us denote by \( x \lor y \) (respectively, by \( x \land y \)) the vector with coordinates \( \max(x_i, y_i) \) (respectively, with coordinates \( \min(x_i, y_i) \)).

**Definition 3.** A function \( f \) is called submodular if for any Boolean vectors \( x, y \) it satisfies the inequality

\[ f(x \land y) + f(x \lor y) \leq f(x) + f(y). \]

Let the set \( \mathcal{V} = \{1, \ldots, n\} \), and for any \( \mathcal{D} \subset \mathcal{V} \) the set \( \mathcal{D}^c = \mathcal{V} \setminus \mathcal{D} \). Let the vector \( x_\mathcal{D} \) with coordinated \( x_i, \ i \in \mathcal{D} \) be the restriction of \( x \) to the set \( \mathcal{D} \), the abbreviation \( P(x_\mathcal{D}) = P(x_\mathcal{D}, 0_{\mathcal{D}^c}) \).

Below we always suppose \( P(0) = 0 \). Therefore, \( P \) is of the form

\[ P(x) = \sum_{m=1}^{n} \sum_{1 \leq l_1 < \ldots < l_m \leq n} a_{l_1, l_2, \ldots, l_m} \prod_{i=1}^{m} x_{l_i}, \quad (6) \]

For any \( i, j \in \mathcal{V} \) a polynomial \( P(x) \) can be written in the form

\[ P(x) = P(x_{\{i,j\}^c}) + x_i P_i(x_{\{i,j\}^c}) + x_j P_j(x_{\{i,j\}^c}) + x_i x_j P_{i,j}(x_{\{i,j\}^c}) \quad (7) \]
or in the form
\[ P(x) = Q(x) + L(x), \]
where \( Q(x) \) is the polynomial consisting of monomials of degree 2 and higher, and \( L(x) \) is a linear polynomial. It also can be represented as
\[ P(x) = P\{D\}(x) + P(x_{Dc}), \quad D \subset V, \]
where each monomial of \( P\{D\}(x) \) contains at least one variable \( x_i, i \in D \) (and, in general, it depends on \( x_{Dc} \)), and \( P(x_{Dc}) \) is independent of \( x_D \). The following useful properties can be easily verified.

**Proposition 4.** a) A Boolean polynomial \( P(x) \) is submodular if and only if for any vector \( x \) and any couple of indices \( i, j \in N \) the polynomials \( P_{i,j}(x_{i,j}) \leq 0 \).

b) In order to Boolean polynomial \( P(x) \) be submodular it is necessary and sufficient its nonlinear part \( Q(x) \) will be submodular.

c) If \( P(x) \) is submodular, then the polynomial \( Q(x) \) is nonincreasing, in the sense that \( Q(y) \leq Q(x) \) for any ordered pair of vectors \( y \geq x \). Therefore, \( \text{argmin}_x Q(x) = 1_V \).

d) If \( P(x) \) is submodular, then \( P\{D\}(x) \) is submodular polynomial in \( x_D \) for each fixed vector \( x_{Dc} \).

The sentences a), b) and d) are deduced directly from Definition 3. To prove c) let us consider a couple of vectors: \( x \) with \( x_i = 0 \) and \( y = x + e_i \) and inequality
\[ Q(0_V) + Q(y) \leq Q(e_i) + Q(x) \]
that follows from Definition 3. Since \( Q(0_V) = Q(e_i) = 0 \) we have \( Q(y) \leq Q(x) \). To prove c) in general case it is enough to repeat the last inequality successively.

We need two properties of polynomials \( P\{D\}(x) \). The first one is rather clear.

**Proposition 5.** If \( x'_{Dc} \) minimizes the polynomial \( P\{D\}(x) \) for some fixed \( x_{Dc} \), then for any set \( E \subset D \) the restriction \( x'_E \) minimizes the polynomial \( P\{E\}(x_E, x'_{D \setminus E}, x_{Dc}) \) with respect to \( x_E \), and vice versa, if the vector \( x_{Dc} \) minimizes \( P\{E\}(x_E, x'_{D \setminus E}, x_{Dc}) \), then the vector \( \hat{x}_E, x'_{D \setminus E} \) minimizes \( P\{D\}(x_D, x_{Dc}) \) with respect to \( x_D \).

The second property concerns monotonic (in some sense) dependence of the solution \( x'_{Dc} = \text{argmin}_{x_{Dc}} P\{D\}(x_D, x_{Dc}) \) on boundary vector \( x_{Dc} \) for a submodular polynomial \( P \). Let
\[ M(x_{Dc}) = \left\{ \text{argmin}_{x_D} P\{D\}(x_D, x_{Dc}) \right\} \]
be the set of minima of the polynomial \( P\{D\} \) for fixed \( x_{Dc} \). It can be shown that for two ordered boundary vectors \( x'_{Dc} \leq z_{Dc} \) can exist either unordered \( x'_{D} \notin z_{D} \) or non-increasing \( x'_{D} \geq z_{D} \) solutions, but for any \( x'_{D} \) there exists \( z_{D} \) such that \( x'_{D} \leq z_{D} \), and vice versa, for any \( z_{D} \) there is \( x'_{D} \) satisfying the same inequality.
Theorem 6. Let a polynomial $P$ be submodular. Let for $\hat{x}_{DE} \leq \hat{z}_{DE}$ solutions $x' \in M(\hat{x}_{DE})$ and $z' \in M(\hat{z}_{DE})$ do not satisfy the inequality $x'_D \leq z'_D$.

Then for the maximal nonempty set of the inverse order $E = \{i \in D \mid x'_i = 1, z'_i = 0\}$, such that $1_E = x'_E > z'_E = 0_E$, the vector $(z'_E, x'_{D\backslash E}) = (0_E, x'_{D\backslash E}) \in M(\hat{x}_{DE})$ as well as $(x'_E, z'_{D\backslash E}) = (1_E, z'_{D\backslash E}) \in M(\hat{z}_{DE})$ and, therefore, $(z'_E, x'_{D\backslash E}) \leq (x'_E, z'_{D\backslash E})$.

Proof. For boundary vectors $\hat{x}_{DE} \leq \hat{z}_{DE}$ suppose the condition $x'_D \leq z'_D$ is not valid, i.e. either $x'_D \geq z'_D$ or $x'_D \not\leq z'_D$. In this case the set $E = \{i \in D \mid x'_i = 1, z'_i = 0\}$ is nonempty. Let us consider the chain of relations. The inequality

$$P\{(E|z'_E, z'_{D\backslash E}, \hat{z}_{DE}) \leq P\{(E|x'_E, z'_{D\backslash E}, \hat{z}_{DE}) \}

(8)$$

holds true since the vector $z'_E$ minimizes $P\{(E|z'_E, z'_{D\backslash E}, \hat{z}_{DE})$ (see, Proposition 5). The inequality

$$P\{(E|x'_E, z'_{D\backslash E}, \hat{z}_{DE}) \leq P\{(E|z'_E, x'_{D\backslash E}, \hat{z}_{DE}) \}

(9)$$

will be proved later. The relation

$$P\{(E|x'_E, x'_{D\backslash E}, \hat{z}_{DE}) \leq P\{(E|z'_E, x'_{D\backslash E}, \hat{x}_{DE}) \}

(10)$$

is verified the same way as (5). Equalities

$$P\{(E|z'_E, x'_{D\backslash E}, \hat{x}_{DE}) = P\{(E|z'_E, z'_{D\backslash E}, \hat{z}_{DE}) = 0

(11)$$

are valid because $z'_E = 0_E$. Therefore, relations (8)-(11) are, actually, equalities, and the claim of the Theorem can be derived from Proposition 5.

Thus, the Theorem will be proved if we ground the inequality (9). For that we need additional notations. One-element sets $\{j\} \in V$ will be denoted by $j$. Instead of $E \cup \{j\}$ and $E\backslash\{j\}$ we will use abbreviations $E + j$ and $E - j$. For arbitrary sets $A, B, C \subseteq V$ we denote by $P\{(A, B, C)|x\}$ polynomials that consist of monomials of $P(x)$ with variables $x_i, i \in A, x_j, j \in B$ but without $x_k, k \in C$.

First, consider Boolean vectors that for some $j \in E^c$ satisfy the equation $\hat{x}_{E^c} + e_j = \hat{z}_{E^c}$ and the polynomial $P\{E + j\}(x_{E^c+j}, x_{E^c-j})$, which is a submodular function of $x_{E^c+j}$. Let us write the condition of submodularity of the polynomial for vectors $a_{E^c+j} = (0_E, 1_j)$ and $b_{E^c+j} = (x_E, 0_j)$ using the representation

$$P\{E + j\}(x_{E^c+j}, x_{E^c-j}) = P\{E|E^c\}(x_E) + P\{E, j\}(x_{E^c+j}, x_{E^c-j}) + P\{E, E^c - j|E\}(x_{E^c-j}) + a_j x_j.$$

Since $a_{E^c+j} \wedge b_{E^c+j} = 0_{E^c+j}$ and $a_{E^c+j} \vee b_{E^c+j} = (x_E, 1_j)$, it looks as

$$P\{E|E^c\}(x_E) + P\{E, j\}(x_E, 1_j, x_{E^c-j}) + P\{E, E^c - j|E\}(x_{E^c-j}) + a_j x_j.$$
Therefore,
\[ P\{\mathcal{E}, j\}(x_\mathcal{E}, 1, j, x_{\mathcal{E}c-j}) \leq P\{\mathcal{E}, j\}(x_\mathcal{E}, 0, j, x_{\mathcal{E}c-j}) = 0. \] (12)
But
\[ P\{\mathcal{E}\}(x_\mathcal{E}, x_{\mathcal{E}c}) = P\{\mathcal{E}|\mathcal{E}^c\}(x_\mathcal{E}) + P\{\mathcal{E}, j\}(x_\mathcal{E}, x_j, x_{\mathcal{E}c-j}) + P\{\mathcal{E}, \mathcal{E}^c - j|j\}(x_\mathcal{E}, x_{\mathcal{E}c-j}) \] (13)
Inequality (12), equation (13) and condition \( x_{\mathcal{E}c-j} = x_{\mathcal{E}c-j} \) allows to conclude
\[ P\{\mathcal{E}\}(x_\mathcal{E}, x_{\mathcal{E}c}) \geq P\{\mathcal{E}\}(x_\mathcal{E}, z_{\mathcal{E}c}). \] (14)
To prove (14) for an arbitrary pair \( x_{\mathcal{E}c} \leq z_{\mathcal{E}c} \) it is enough to use monotone increasing sequence of boundary vectors \( x_{\mathcal{E}c} < x_{\mathcal{E}c,1} < \ldots < x_{\mathcal{E}c,k} < z_{\mathcal{E}c} \) that differ with one coordinate only. \( \square \)

Theorem 6 allows to describe some properties of the set of solutions
\[ \mathcal{M} = \left\{ \arg \min_{x} P(x) \right\}. \]

Corollary 7. Let \( x_{\mathcal{E}c} \leq z_{\mathcal{E}c} \) be any ordered pair of vectors, then:
(i) for any \( x_D' \in \mathcal{M}(x_{\mathcal{E}c}) \) there exists a solution \( z_D' \in \mathcal{M}(z_{\mathcal{E}c}) \) such that \( x_D' \leq z_D' \).
(ii) For any \( z_D' \in \mathcal{M}(z_{\mathcal{E}c}) \) there exists a solution \( x_D' \in \mathcal{M}(x_{\mathcal{E}c}) \) such that \( x_D' \leq z_D' \).
(iii) The sets \( \mathcal{M}(x_{\mathcal{E}c}) \) and \( \mathcal{M}(z_{\mathcal{E}c}) \) have minimal \( x_D', z_D' \) and maximal \( x_D', z_D' \) elements.
(iv) The minimal and maximal elements are ordered, i.e. \( x_D' \leq z_D' \) and \( x_D' \leq z_D' \).

The sentences (i) and (ii) follow directly from Theorem 6. Sentence (iii) is deduced from Theorem 6 for \( x_{\mathcal{E}c} = z_{\mathcal{E}c} \). And, at last, (iv) can be derived from (i,ii) and definitions of minimal and maximal elements.

4 Modified SFM Algorithm

The main idea of the Modified SFM algorithm (MSFM) is to determine (if possible) parts of a solution \( x^* = \mathcal{M} \) by use separate parts \( P\{D_i\}(x_{D_i}, x_{D_i}) \), \( (D_i \cup D_j = \emptyset, \bigcap D_i = \mathcal{V}) \) of the original polynomial \( P(x) \). For this purpose monotone dependence of local solutions \( x_{D_i}' \) (in the sense of Corollary 7) on the frontier vector \( x_{\mathcal{E}c} \) can be exploited. If the vector \( x_{D_i}' \in \mathcal{M}(1_{\mathcal{E}c}) \) has some coordinates \( x_j' = 0 \), then there is a solution \( x^* \in \mathcal{M} \) with the same coordinates \( x_j^* = 0 \). Similarly, if the solution \( x_{D_i}' \in \mathcal{M}(0_{\mathcal{E}c}) \) is with coordinates \( x_j^* = 1 \), then there is a solution \( x^* \in \mathcal{M} \) that has \( x_j^* = 1 \).

The strategy developed leads to success not for all Boolean polynomials, but it is useful for polynomials that have local dependence of variables. Such polynomials are quite often used in applications, for instance, in Bayesian estimation or image processing.

Describe the MSFM in details. Partition the set \( \mathcal{V} \) by suitable sets \( D_i(1), \ldots, D_{k_1}(1) \) \( (D_1(1) \cup D_j(1) = \emptyset, \bigcap D_i(1) = \mathcal{V}) \). It follows from Proposition 4 that \( x^*_D(i) \in \mathcal{M}(x^*_D(i)) \),
i.e. $x^*_{D_i(1)}$ minimizes the polynomial $P\{D_i\}(x_{D_i}, x^*_{D_i(1)})$. Corollary 7 substantiates existence of triple of solutions

$$x_{0,D_i(1)} \in \mathcal{M}(0_{D_i^c(1)}), \quad x_{1,D_i(1)} \in \mathcal{M}(1_{D_i^c(1)}) \quad \text{and} \quad x'_{D_i(1)} \in \mathcal{M}(x^*_{D_i(1)})$$

such that $x_{0,D_i(1)} \leq x'_{D_i(1)} \leq x_{1,D_i(1)}$ (the vectors can be found by the usual SFM algorithm).

Therefore, solutions $x'_{D_i(1)}$ have coordinates $x'_{D_i(1),j} = 0$ for sets of indices $B_i(1) = \{j \in D_i(1) \mid x_{1,D_i(1),j} = 0\}$ as well as they have coordinates $x'_{D_i(1),j} = 1$ for sets of indices $\mathcal{W}_i(1) = \{j \in D_i(1) \mid x_{0,D_i(1),j} = 1\}$.

Check the set $\mathcal{R}(1) = \bigcup_{i=1}^k (\mathcal{W}_i(1) \bigcup B_i(1))$. If it is empty we either try another partition or start the standard SFM for the original polynomial $P(x)$.

If $\mathcal{R}(1) \neq \emptyset$, we identified the part of the solution $x^*_{\mathcal{R}(1)} = x'_{\mathcal{R}(1)}$. Set $\mathcal{V}(2) = \mathcal{V} \setminus \mathcal{R}(1)$ and consider the reduced problem of identification of

$$x^*_{\mathcal{V}(2)} = \text{argmin}_{x_{\mathcal{V}(2)}} P(x_{\mathcal{V}(2)}, x^*_{\mathcal{R}(1)}).$$

Partition $\mathcal{V}(2) = \bigcup_{i=1}^{k_2} D_i(2), \quad D_i(2) \bigcap D_j(2) = \emptyset$ and estimate $x^*_{D_i(2)}$ by solutions

$$x_{0,D_i(2)} \in \mathcal{M}(0_{D_i^c(2) \setminus \mathcal{R}(1)}, x^*_{\mathcal{R}(1)}), \quad x_{1,D_i(2)} \in \mathcal{M}(1_{D_i^c(2) \setminus \mathcal{R}(1)}, x^*_{\mathcal{R}(1)}),$$

using sets $B_i(2) = \{j \in D_i(2) \mid x_{1,D_i(2),j} = 0\}$ and $\mathcal{W}_i(2) = \{j \in D_i(2) \mid x_{0,D_i(2,j) = 1}\}$ (Corollary 7 grounds existence of triple of vectors $x_{0,D_i(2)} \leq x^*_{D_i(2)} \leq x_{1,D_i(2)}$). The algorithm is iterated at high levels until the problem will be completely solved or until $\mathcal{R}(l) \neq \emptyset$. In the last case the standard SFM is after applied. Sizes of partitioning sets $D_i(l)$ should be sufficient to have $\mathcal{R}(l)$ nonempty but not very large to have small enough number of operations. It is unlikely possible to estimate them in general case since for some polynomials the MSFM is reduced to the usual SFM for any partition. However, in many applied problems of image processing or Bayesian estimation the finding suitable sizes of $D_i(l)$ is not difficult. In these problems energy functions usually have lack of long distance interactions (or phase transitions). It means solutions $x^*_{D_i(l)}$ for the original image and an image, which coincides with the original on sufficiently large set $D \subset \mathcal{V}$ and differs from it on $D^c$, are approximately equal. By other words, for real applications estimates of image details do not depend on their surrounding objects. In this case the MSFM is preferable to the standard SFM. The number operation required can be here even $O(n)$.

The identification of $x^*_{B_i(l) \bigcup \mathcal{W}_i(l)}$ can be done in concurrent mode. The number of levels depend on the polynomial $P$. Usually, it is enough two or three ones. Formal description of the MSFM is rather simple. It is placed in Fig.1.
MSFM$(P)$:

**Initialization:**

\[ m \leftarrow 1 \quad \text{the enumerator of levels} \]
\[ L \leftarrow \quad \text{a number of levels} \]
\[ \mathcal{V}(1) \leftarrow \quad \mathcal{V} \]
\[ \{\mathcal{D}_i(1)\} \leftarrow \quad \text{a partition of } \mathcal{V} \]
\[ \{x_0, \mathcal{D}_i(1), x_1, \mathcal{D}_i(1)\} \leftarrow \quad \text{such that } x_0, \mathcal{D}_i(1) \leq x_1, \mathcal{D}_i(1), \text{by the SFM} \]
\[ \{\mathcal{B}_i(1), \mathcal{W}_i(1)\} \leftarrow \quad \text{coordinates of the part of the solution found} \]
\[ R(1) \leftarrow \quad \bigcup_{i=1}^{k_1} (\mathcal{W}_i(1) \cup \mathcal{B}_i(1)) \]

**If** \( R(1) = \emptyset \) **then** use the SFM, **Stop**

\[ x^*_{\mathcal{D}_i(1),j} \leftarrow \quad 0 \quad \text{for } j \in \mathcal{B}_i(1) \]
\[ x^*_{\mathcal{D}_i(1),j} \leftarrow \quad 1 \quad \text{for } j \in \mathcal{W}_i(1) \]

**While** \( m < L \) **do**

\[ m \leftarrow m + 1 \]
\[ \mathcal{V}(m) \leftarrow \quad \mathcal{V}(m - 1) \setminus R(m - 1) \]
\[ \{\mathcal{D}_i(m)\} \leftarrow \quad \text{partition of } \mathcal{V}(m) \]
\[ P_i(x_{\mathcal{V}(m)}) \leftarrow \quad \text{the residual polynomial } P_i(x_{\mathcal{V}(m)}, x^c_{\mathcal{V}(m)}) \]
\[ \{x_0, \mathcal{D}_i(m), x_1, \mathcal{D}_i(m)\} \leftarrow \quad \text{such that } x_0, \mathcal{D}_i(m) \leq x_1, \mathcal{D}_i(m), \text{by the SFM for } P_i(x_{\mathcal{V}(m)}) \]
\[ \{\mathcal{B}_i(m), \mathcal{W}_i(m)\} \leftarrow \quad \text{coordinates of the part of the solution found} \]

**If** \( \bigcup_{i=1}^{km} (\mathcal{W}_i(m) \cup \mathcal{B}_i(m)) = \emptyset \) **then** use the SFM, **Stop**

\[ R(m) \leftarrow \quad R(m - 1) \cup \big( \bigcup_{i=1}^{km} (\mathcal{W}_i(m) \cup \mathcal{B}_i(m)) \big) \]
\[ x^*_{\mathcal{D}_i(m),j} \leftarrow \quad 0 \quad \text{for } j \in \mathcal{B}_i(m) \]
\[ x^*_{\mathcal{D}_i(m),j} \leftarrow \quad 1 \quad \text{for } j \in \mathcal{W}_i(m) \]

**If** \( R(L) \neq \emptyset \) **then** use the SFM

Return \( x^* \)

End

Fig.1
5 Representability of Some Submodular Polynomials by Graphs

Recently Kolmogorov & Zabih have described some class of functions $V(x)$ in Boolean variables $x = (x_1, \ldots, x_n)$ that permit minimization by the graph cut technique. For convenience we reformulate and then use their results in terms of Boolean polynomials. We also represent some submodular Boolean polynomials by graphs to make possible their efficient minimization via graph cut technique (recall that finding the minimum graph cut requires $O(N^3)$ operations on number $N$ of nodes).

Let the network $\Gamma = (S, A)$ consist of $N + 2$ numbered nodes $S = \{0, \ldots, N+1\}$, where $s = 0$ is the source, $t = N + 1$ is the sink and $V' = \{1, \ldots, N\}$ are usual nodes. The set of directed arcs is $A = \{(i, j) : i, j \in S\}$. The capacities of arcs are denoted by $d_{i,j} > 0$.

The cut (we use this term as abbreviation of the term $s$-$t$ cut) is a partition of the set $S$ by two disjoint sets $W, B$ such that $s \in W$ and $t \in B$. For any cut $(W, B)$ nodes $i \in W$ will be labeled by $z_i = 1$ and nodes $i \in B$ - by $z_i = 0$ so that there is one-to-one map between cuts and Boolean vectors $z = (z_1, \ldots, z_N)$.

5.1 Graph representability

In [8] the following definition of graph representability is given.

**Definition 8.** A function $V(x)$ of $n$ Boolean variables is called graph representable if there exists a network $\Gamma = (S, A)$ with number of nodes $N \geq n$ and the cost function $C(z)$ such that for some constant $c$

$$V(x) = \min_{z_{n+1}, \ldots, z_N} C(x_1, \ldots, x_n, z_{n+1}, \ldots, z_N) + c.$$

Costs of the graph cuts $C(z)$ are equal to values of the quadratic Boolean polynomial $p(z)$ of the form (see, [3, 9]).

$$C(z) = p(z) = \sum_{i \in V} d_{s,i}(1 - z_i) + \sum_{i \in V} d_{i,t}z_i + \sum_{i,j \in V} d_{i,j}(z_i - z_j)z_i + c, \quad d_{i,j}, \; c \geq 0. \quad (15)$$

Therefore, we can give an equivalent definition of the graph representability.

**Definition 9.** We say a function $V(x)$ of $n$ Boolean variables can be represented by graph if there exists a quadratic polynomial $p(z)$ of $N$ ($N \geq n$) Boolean variables of the form (15), which satisfies the equality

$$V(x) = \min_{z_{n+1}, \ldots, z_N} p(x_1, \ldots, x_n, z_{n+1}, \ldots, z_N) + c.$$

The class $F^2$ of Boolean functions that are often used in applications and that are, actually, quadratic Boolean polynomials

$$V \in F^2 \iff V(x) = P_V(x) = \sum_{1 \leq l \leq n} a_l x_l + \sum_{1 \leq l_1 < l_2 \leq n} a_{l_1, l_2} x_{l_1} x_{l_2} + c. \quad (16)$$
was considered in \cite{8}. The characterization of the graph representability of $V \in F^2$ in terms of Boolean polynomials has been done. It can be used, in particular, to minimize functions of integer variables.

**Theorem 10.** A function $V \in F^2$ is graph representable if and only if all quadratic coefficients of its polynomial representation $\bar{P}_V(x)$ are nonpositive, i.e. $a_{l_1,l_2} \leq 0$. Therefore, in order to function $V \in F^2$ be graph representable it is necessary an sufficient it will be submodular.

The sufficiency of the Theorem follows immediately from Definition \cite{9} and Proposition \cite{4}a). The necessity will be proven below for more general case. The following result has been proven in \cite{8} by graph cut technique.

**Theorem 11.** In order to polynomial $P(x)$ of degree $m$ can be represented by a graph it should be submodular.

**Proof.** To prove this sentence we use representation \cite{7} of the polynomial $P(x)$ at page \cite{5}. For arbitrary couple of indices $i, j$ let us fixed the vector $x_{ij}$. Since $P(x)$ is graph representable the quadratic polynomial $x_{ij}P_{ij}(x_{ij})$ of two variables $x_i, x_j$ is graph representable, as well. That is

$$x_{ij}P_{ij}(x_{ij}) = \min_{z_n+1, \ldots, z_N} p(x_1, x_2, z_{n+1}, \ldots, z_N) + c$$

(in general, the quadratic submodular polynomial $p$ and $c$ depend on $x_{ij}$ but it is fixed now). Suppose $P_{ij}(x_{ij}) > 0$. Then $p$ has at least two values of the argument $(x_1, x_2, z_{n+1}, \ldots, z_N)$ that minimize the polynomial globally. One of them is with coordinates $(0,1,\ldots)$, and the other is of the form $(1,0,\ldots)$. Because of submodularity of $p$ it follows from Corollary \cite{4} (i) there exists the third vector, which minimizes $p$ globally. This vector has coordinates $(1,1,\ldots)$. The existence of such the vector contradicts with the assumption $P_{ij}(x_{ij}) > 0$. Therefore, $P_{ij}(x_{ij}) \leq 0$ for any couple of indices $i,j$ and vector $x_{ij}$ and the sentence of the Theorem follows from Corollary \cite{4}a).

\[\Box\]

### 5.2 Graph representability of some subset of submodular polynomials

The submodularity is necessary condition in order to a Boolean polynomial can be represented by a graph. Below we prove representability by graphs of some subset $P_{suf}$ of submodular polynomials. To define this subset we use formula \cite{7} at page \cite{5}. Let $b_{l_1,\ldots,l_m}(i,j) = a_{l_1,\ldots,l_s,i,j}\ldots,l_m$, $(l_1 < \ldots < i < \ldots < j < \ldots < l_m, \ m = 0 \div n - 2)$ be coefficients of $P_{ij}(x_{ij})$ and $b_{l_1,\ldots,l_m}(i,j)$ be the positive ones (note that $b(i,j) = a_{i,j} < 0$). Let the set of polynomials

$$P_{suf} = \left\{ P \left| -a_{i,j} + \sum_{m=1}^{n-2} \sum_{l_1<l_2<\ldots<l_m} b_{l_1,l_2,\ldots,l_m}(i,j) \leq 0, \ \forall i,j \in V \right. \right\}.$$  

This set is a proper subset of all submodular polynomials $P_{submod}$ (see Proposition \cite{4}a). It contains, for instance, the set $F^{n} = \{ P \left| a_{l_1,l_2,\ldots,l_k} \leq 0, \ k = 2 \div m \right. \}$ of Boolean polynomials
with all coefficients of nonlinear monomials nonpositive and the set \( \mathcal{F}_+^m = \{ P \mid P \in \mathcal{P}_{\text{submod}}, a_{1,l_2,\ldots,l_k} \geq 0, k = 3 \div m \} \) of submodular polynomials with all coefficients of order more than two nonnegative.

**Remark 1.** Note the condition

\[-a_{i,j} + \sum_{m=1}^{n-2} \sum_{l_1 < l_2 < \ldots < l_m} b_{1,l_2,\ldots,l_m}^+ (i,j) \leq 0, \ \forall i, j \in \mathcal{V}\]

is necessary and sufficient in order to the polynomial, which has all coefficients of order more than two positive (i.e. \( P \in \mathcal{P}_{\text{submod}} \)), be submodular.

Polynomials of those types can be used, for instance, in image processing for recognition of images or Bayesian estimation. To prove representability of \( P \in \mathcal{P}_{\text{subf}} \) by graphs we need two lemmas, which give a constructive tool to build a corresponding graph as well.

**Lemma 12.** For any natural \( m \) and real \( a < 0 \) the Boolean polynomial \( ax_1 x_2 \ldots x_m \) is graph representable.

The graph that represents \( ax_1 x_2 \ldots x_m \) is drawn in Fig.2. It needs one additional node \( z \). The corresponding polynomial is

\[ p(x_1, x_2, \ldots, x_m, z) = -a \sum_{i=1}^{m} (z - x_i) + az. \]

If at least one \( x_i = 0 \), then \( \min z p(x_1, x_2, \ldots, x_m, z) = 0 \) otherwise \( \min z p(1,1,\ldots,1,z) = a \). Hence, \( ax_1 x_2 \ldots x_m = \min z p(x_1, x_2, \ldots, x_m, z) \).

The monomials of order greater than 2 with positive coefficients can not be represented by graphs directly. To do it we should accompany those positive monomials by quadratic items with large enough negative coefficients. It requires additional nodes in graphs that represent the monomials.

**Lemma 13.** For any natural \( m > 2 \) and \( a > 0 \) the Boolean polynomial \( P(x_1, x_2, \ldots, x_n) = ax_1 x_2 \ldots x_m - a \sum_{1 \leq i < j \leq m} x_i x_j \) is graph representable.

**Proof.** In order to prove the Lemma we construct for each \( m > 2 \) a quadratic Boolean polynomial that specifies graph (the examples of graphs for \( m = 3 \div 6 \) are drawn in Fig.3 at page 17). The number of additional variables of this polynomial is \( l = \frac{m-1}{2} \) if \( m \) is odd and is \( l = \frac{m-2}{2} \) if \( m \) is even. It is of the form

\[ p(x_1, \ldots, x_m, z_1, \ldots, z_l) = \sum_{j=1}^{l} b_j \sum_{i=1}^{m} (z_j - x_i) z_j + \sum_{j=1}^{l} e_j z_j \quad (17) \]
with all \( b_j > 0 \) and \( e_j < 0 \), such that the minimum of \( p \) with respect to \( z_1, \ldots, z_l \) is equal to corresponding values of \( P \). Those values are

\[
P(x_1, x_2, \ldots, x_m) = \begin{cases} 
0, & \text{if all } x_i = 0, \\
0, & \text{if } x_{i_1} = 1 \text{ and } x_{i_2} = \ldots = x_{i_m} = 0 \\
-a\left(\binom{k}{2}\right), & \text{if } x_{i_1} = \ldots = x_{i_k} = 1 \text{ and } x_{i_{k+1}} = \ldots = x_{i_m} = 0 \\
-a\left(\binom{m}{2}\right) + a, & \text{if } x_1 = \ldots = x_m = 1.
\end{cases}
\]

Let the vector \( \mathbf{1}_k = (1, \ldots, 1, 0, \ldots, 0) \). The polynomial \( p \) (as well as \( P \)) is symmetrical with respect to \( x_1, \ldots, x_m \). It has the same value \( p(\mathbf{1}_k) = \sum_{j=1}^{l}(m - k)b_j + e_jz_j \) for all permutations of \( \mathbf{1}_k \). Therefore, the set of inequalities should hold true

\[
\begin{align*}
\sum_{j=1}^{l}(mb_j + e_j)z_j & \geq 0 \\
\sum_{j=1}^{l}((m - 1)b_j + e_j)z_j & \geq 0 \\
\sum_{j=1}^{l}((m - 2)b_j + e_j)z_j & \geq -a \\
\vdots & \\
\sum_{j=1}^{l}((m - k)b_j + e_j)z_j & \geq -a\left(\binom{k}{2}\right) \\
\vdots & \\
\sum_{j=1}^{l}(b_j + e_j)z_j & \geq -a\left(\binom{m-1}{2}\right) \\
\sum_{j=1}^{l}e_jz_j & \geq -a\left(\binom{m}{2}\right) + a
\end{align*}
\] (18)

together with the additional condition:

(M) \text{ There exist vectors } \{z^*_k\} \text{ that turn corresponding inequalities into equality.}

For any odd \( m > 2 \) we propose one of possible collections of variables \( b_i, e_i \) that satisfy (18) for Boolean variables \( (z_1, \ldots, z_m) \) as well as condition (M). The collection is identified
by the following system of equations

\[
\begin{align*}
((m - 2)b_1 + e_1) &= -a(2) \\
((m - 3)b_1 + e_1) &= -a(3) \\
((m - 4)b_1 + e_1) + ((m - 4)b_2 + e_2) &= -a(4) \\
((m - 5)b_1 + e_1) + ((m - 5)b_2 + e_2) &= -a(5) \\
& \vdots \\
\sum_{j=1}^{k} ((m - 2k)b_j + e_j) &= -a\left(\frac{2k}{2}\right) \\
\sum_{j=1}^{k} ((m - 2k - 1)b_j + e_j) &= -a\left(\frac{2k+1}{2}\right) \\
& \vdots \\
\sum_{j=1}^{l} (b_j + e_j) &= -a\left(\frac{m-1}{2}\right) \\
\sum_{j=1}^{l} e_j &= -a\left(\frac{m}{2}\right) + a
\end{align*}
\]

(19)

It is

\[
b_1 = b_2 = \ldots = b_{l-1} = 2a, \quad b_l = a,
\]

(20)

\[
e_j = -(2m - 4j + 1)a, \quad (j = 1 \div l - 1), \quad e_l = -2a.
\]

Since the inequalities

\[
(m - 1)b_j + e_j > 0, \quad j = 1 \div l,
\]

\[
(m - 2k)b_j + e_j < 0, \quad (m - 2k - 1)b_j + e_j < 0, \quad \text{if} \quad j \leq k, \quad k = 1 \div l - 1,
\]

\[
(m - 2k)b_j + e_j > 0, \quad (m - 2k - 1)b_j + e_j > 0, \quad \text{if} \quad j > k, \quad k = 1 \div l - 1,
\]

\[
b_j + e_j < 0, \quad j = 1 \div l,
\]

\[
e_j < 0, \quad j = 1 \div l.
\]

hold true, the solution (20) actually satisfies inequality (18) together with condition (M) for vectors \(z^*_1 = z^*_2 = 0, \quad z^*_3 = z^*_4 = 1_1, \quad \ldots, \quad z^*_{2k+1} = z^*_{2k+2} = 1_k, \quad \ldots, \quad z^*_m = z^*_{m+1} = 1_l\).

For even \(m > 2\) the collection of \(l = \frac{m-2}{2}\) variables \(b_i, e_i\) can be found as a solution of
Again the inequalities that looks similar to (19) but consists of only \( m \) equations, since the equation

\[
\sum_{j=1}^{l} (2b_j + e_j) = -a \binom{m-2}{2}
\]

that follows from the last two ones of system (21). The solution of the system is

\[
b_j = 2a, \quad e_j = -(2m - 4j + 1)a, \quad j = 1 \div l.
\]

Again the inequalities

\[
(m - 1)b_j + e_j > 0, \quad j = 1 \div l,
\]

\[
(m - 2k)b_j + e_j < 0, \quad (m - 2k - 1)b_j + e_j < 0, \quad \text{if} \quad j \leq k, \quad k = 1 \div l,
\]

\[
(m - 2k)b_j + e_j > 0, \quad (m - 2k - 1)b_j + e_j > 0, \quad \text{if} \quad j > k, \quad k = 1 \div l,
\]

hold true and, therefore, (18) together with condition (M) is fulfilled for vectors \( \mathbf{z}^*_1 = \mathbf{z}^*_2 = \mathbf{0}, \quad \mathbf{z}^*_3 = \mathbf{z}^*_4 = \mathbf{1}_1, \quad \ldots, \quad \mathbf{z}^*_{2k+1} = \mathbf{z}^*_{2k+2} = \mathbf{1}_k, \quad \ldots, \quad \mathbf{z}^*_{m-1} = \mathbf{z}^*_m = \mathbf{z}^*_{m+1} = \mathbf{1}_l \).

So, the coefficients of the polynomial \( \mathbf{p} \) (see (17)) that represents \( P \) for odd and even \( m \) are determined by (20) and (22).

Lemmas 12 and 13 allow to prove each \( P \in \mathcal{P}_{\text{suf}} \) can be represented by a graph.
**Theorem 14.** The polynomials $P \in \mathcal{P}_{suf}$ are graph representable.

In order to prove the Theorem it is enough to use Lemma 12 to represent nonlinear items of $P$ with negative coefficients and, then, to exploit Lemma 13 to determine that all items with positive coefficients can be accompanied by quadratic monomials and after be represented by graphs as well.

Let the Boolean polynomial $P(x_1, \ldots, x_n) \in \mathcal{P}_{suf}$ of degree $m$ consists of $L_h$ monomials of degree more than two, then it can be represented by a graph with $\frac{L_h(m-1)}{2} + n$ nodes. The worst case is when $P(x_1, \ldots, x_n) \in \mathcal{F}_m^-$. The polynomial $P(x_1, \ldots, x_n) \in \mathcal{F}_m^+$ can be represented by a graph with $L_h + n$ nodes. Hence, the global minimization of $P(x_1, \ldots, x_n) \in \mathcal{P}_{suf}$ require less than $O\left(\frac{L_h(m-1)}{2} + n\right)^3$ operations, though for some classes of polynomials that occur in applications the number of operations can be reduced even to $O\left(\frac{L_h(m-1)}{2} + n\right)$ (see, [11]).
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