



On computing boundary functional sums

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Abstract

A method for solving enumeration problems is suggested. We consider the enumeration problems which are reducible to estimation of the sums of type $T(X, f) = \sum_A f(A)$ where f is so called boundary functional (BF) on X , and the summation is over all subsets of X (or over some special subfamily of 2^X). An evolution of the n -cube, the percolation problem, the problem of computation of the matchings number and the independent sets number, the monotone Boolean functions number, the binary codes number and so on are among such problems. We show how to obtain asymptotics for $T(X, f)$. In conclusion we give an example of application of the BF method to finding the number of independent sets in the bipartite graphs, induced by neighboring levels of the n -cube. © 2000 Elsevier Science B.V. All rights reserved.

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1. Main notions results and examples

We consider the enumeration problems which are reducible to estimate sums of the type $T(X, f) = \sum_A f(A)$ where f is the so-called boundary functional on X and the summation is over all subsets of X or over some subfamily of 2^X . An evolution of the n -cube [1], the percolation problem [2], the problem of computation of the matchings number and the independent sets number, the monotone Boolean functions number, the binary codes number and so on (see [4,5] and examples below) are among such problems. The goal of the paper is to obtain asymptotics for $T(X, f)$. In conclusion, we give an example of the application of the BF method in finding the number of independent sets in special bipartite graphs.

Let X be a finite set. A mapping $f : 2^X \rightarrow (0, 1]$, is called a *boundary functional* (abbreviated, BF) if the following properties hold:

- (i) $f(A) = 1$ if and only if $A = \emptyset$,
- (ii) $f(A \cup B) \geq f(A)f(B)$,

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$$(iii) f(A \cup B) > f(A)f(B) \Rightarrow \exists u \in A \exists v \in B f(\{u, v\}) > f(\{u\})f(\{v\}).$$

Example 1. Let $G = (X, Y; E)$ be a bipartite graph without isolated vertices in the part X . A *boundary* $\vartheta(A)$ of $A \subseteq X$ is defined by $\vartheta(A) = \{v \in Y: \exists u \in A(u, v) \in E\}$. Then f such that $f(A) = 2^{-|\vartheta(A)|}$ is a BF, and $2^{|X|} \cdot T(X, f)$ is the number of independent sets of G (see [4], and also Lemma 3 below).

Example 2. Let B^n be the n -cube and r the Hamming distance. An *edge boundary* $e(A)$ of $A \subseteq B^n$ is defined as follows:

$$e(A) = \{(u, v) \in B^n: v \in A, u \in B^n \setminus A, r(u, v) = 1\}.$$

Then f such that $f(A) = p^{|e(A)|}$ with $0 < p < 1$ is a boundary functional, and $\sum_A f(A)$ where the summation is over all connected sets $A \subseteq B^n$ is the expectation of the number of components in a random subgraph of the n -cube under random choice of edges with the probability p (see [1]).

Example 3. Let P be the plane integer grid and A some set of vertices of P . Denote by $g(A)$ the set $\{v \in P: r(v, A) = 1\}$. For any $0 < p < 1$, a mapping f s.t. $f(A) = p^{|A|}(1 - p)^{|g(A)|}$ for each $A \subseteq P$ is a BF. Note that $1 - \sum f(A)$, where summation is over all connected sets A with $(0, 0) \in A$, is the probability of the percolation in the Boolean model (see [2]).

Example 4. Let B^n be the n -cube and $B_k^n = \{(a_1, \dots, a_n) \in B^n: a_1 + \dots + a_n = k\}$ the k th level of B^n . Given $A \subseteq B^n$, the set $S_k(A) = \{v \in B_k^n: \exists u \in A u < v \text{ or } \exists u \in A v \leq u\}$ will be called a k -shadow of A . We consider B^n as a poset with the usual order: $(a_1, \dots, a_n) \leq (b_1, \dots, b_n)$ iff $a_i \leq b_i$; for $i = 1, \dots, n$. A set $A \subseteq B^n$ is called an *antichain* if $u \not\leq v$ and $v \not\leq u$ (i.e. u and v are incomparable) for any two distinct elements u and v from A . For $B \in B_k^n$ let $Q_K^-(B)$ ($Q_K^+(B)$) be the number of antichains $A \subseteq \bigcup_{j \leq k} B_j^n$ ($A \subseteq \bigcup_{j \geq k} B_j^n$) with $S_k(A) = B$. Let n be even and $k = n/2$. Then $f_{k-1}^-(C) = Q_{k-1}^-(C)2^{-|S_k(C)|}$ and $f_{k+1}^+(C) = Q_{k+1}^+(C)2^{-|S_k(C)|}$ are BFs and

$$2^{\binom{n}{k}} \exp \left\{ \sum_{A \subseteq B_{k-1}^n, B \subseteq B_{k+1}^n, r(A, B) > 2} f_{k-1}^-(A) f_{k+1}^+(B) \right\}$$

is the number of monotone Boolean functions depending on n variables (see [4,5]).

The main idea of evaluating sums of the type $T(X, f)$ is to reduce the problem to the computation of some simpler sums of the same type with summation over the family of connected sets $A \subseteq X$. For this purpose, we first introduce a notion of connectivity. Then we obtain some approximate formulas for $T(X, f)$ through the sums over connected sets. These approximate formulas turn out to give asymptotics if some convergency condition holds. The convergency condition consists of the assertion that the sums over the subfamily of connected sets of big size is small enough. This condition is proved only for special type of BFs. At the same time, the above-mentioned approximate

formulas for $T(X, f)$ are valid for arbitrary BF f . The proof of the convergency condition is the hardest part of the method. It requires upper bounds for the number of the sets with a given size of the boundary. These upper bounds are obtained with the help of good coding connected sets (see [3]) and using assertions of the type of the well-known Kruskal–Katona theorem.

Now we introduce some relevant notions. A pair $I = (X, f)$, where X is a finite set and f is a BF of the type $2^X \rightarrow (0, 1]$, is called a *functional pair*. First, we introduce a notion of connectivity. We say that elements u and v of X are *adjacent* (denotation $u\#v$) iff $f(\{u, v\}) > f(\{u\})f(\{v\})$. Otherwise, i.e. if $f(\{u, v\}) = f(\{u\})f(\{v\})$, we say that u and v are *nonadjacent*. For an arbitrary functional pair $I = (X, f)$, we define *graph* $G = (V, E)$ of a *functional pair* I by putting $V = X$ and $E = \{(u, v) : u\#v\}$. We say that a set A is *connected* if the subgraph $H_{G(I)}(A)$ of the graph $G(I)$ induced by A is connected. We say that $B \subseteq A$ is a *component of* A (denotation $B \vdash A$), if B is connected and whereas every C , such that $B \subset C \subseteq A$, is not connected. Let $\mathbf{A} = \mathbf{A}(I)$ be the family of all connected subsets $A \subseteq X$. Note that from the definition it follows that

$$f(A) = \prod_{B \vdash A} f(B).$$

we denote

$$A_k = \{A \in \mathbf{A} : |A| = k\}, \quad A_{\hat{k}} = \bigcup_{i \leq k} A_i, \quad A_{\bar{k}} = A \setminus A_{\hat{k}},$$

and for any $\mathbf{B} \subseteq \mathbf{A}$ and a positive integer v we put

$$\alpha^v(\mathbf{B}) = \sum_{A \in \mathbf{B}} f^v(A).$$

Our purpose is to represent $T(X, f)$ by means of sums of type $\alpha^v(\mathbf{B})$.

Given $\mathbf{B} \subseteq \mathbf{A}$, we denote by $C(\mathbf{B})$ the family of all $A \subseteq X$ representable as a union of components belonging to \mathbf{B} , that is

$$C(\mathbf{B}) = \{A \subseteq X : \text{all the components of } A \text{ are in } \mathbf{B}\}.$$

We put

$$S(\mathbf{B}) = \sum_{A \in C(\mathbf{B})} f(A).$$

Immediately from the definitions, it follows that for any $\mathbf{B} \subseteq \mathbf{A}(I)$

$$S(\mathbf{B}) \leq T(I) = S(\mathbf{A}(I)) \leq S(\mathbf{B})S(\mathbf{A}(I) \setminus \mathbf{B}). \tag{1}$$

Lemma 1. For any $\mathbf{B} \subseteq \mathbf{A}(I)$

$$S(\mathbf{B}) \leq \exp\{\alpha^1(\mathbf{B})\}. \tag{2}$$

Proof. Using the inequality $\ln(1+x) \leq x$ and the denotation $2^{\mathbf{B}}$ for the family of all subsets of \mathbf{B} , we have

$$\begin{aligned} S(\mathbf{B}) &= \sum_{A \in C(\mathbf{B})} \prod_{D \vdash A} f(D) \leq \sum_{F \in 2^{\mathbf{B}}} \prod_{D \in F} f(D) \\ &= \prod_{A \in \mathbf{B}} (1 + f(A)) = \exp \left\{ \sum_{A \in \mathbf{B}} \ln(1 + f(A)) \right\} \leq \exp\{\alpha^1(\mathbf{B})\}, \end{aligned}$$

which proves the Lemma. \square

Definition. A functional pair $I = (X, f)$ is called (Δ, κ, q, c) -ordinary if the following properties hold:

- (1) $f(\{v\}) \leq 2^{-\kappa}$,
- (2) $|X| \leq 2^{(A+1)\kappa - \log_2^2 \kappa}$,
- (3) $f(A \cup \{v\}) \leq f(A)f(\{v\})2^{|A|q}$,
- (4) $|\{A \subseteq X: |A| = m \text{ and } f(A \cup \{v\}) > f(A)f(\{v\})\}| \leq \kappa^{cm}$.

A sequence of functional pairs $\{I_n = (X_n, f_n)\}$ is called Δ -convergent, if

$$\lim_{n \rightarrow \infty} \sum_{A \in A_{\Delta}(I_n)} f_n(A) = 0. \tag{3}$$

Lemma 2. Let $\{I_n = (X_n, f_n)\}$ be a sequence of Δ -convergent functional pairs. Then¹

$$T(I_n) \sim S(A_{\Delta}(I_n)) \tag{4}$$

as $n \rightarrow \infty$.

Proof. The assertion follows from (1) to (3) with $\mathbf{B} = A_{\Delta}(I)$.

Proofs of the following two theorems are contained in [4]. We prove the first one here because the proof is short and gives a notion about the used technique.

Theorem 1. Let a sequence of $(1, \kappa_n, q, c)$ -ordinary pairs $\{I_n = (X_n, f_n)\}$ be 1-convergent and $\lim_{n \rightarrow \infty} \kappa_n = \infty$. Then,

$$T(I_n) \sim \exp\{\alpha^1(A_1(I_n))\} = \exp \left\{ \sum_{B \in A_1(I_n)} f_n(B) \right\} \tag{5}$$

as $n \rightarrow \infty$.

Proof. Upper bound follows from (2) and (4).

Lower bound: Note that

$$\prod_{A \in A_1} (1 + f(A)) \leq \sum_{B \in C(A_1)} f(B) \sum_{D \in C(A_1)} \prod_{v \in D} f(v).$$

¹ $a(n) \sim b(n)$ denotes that $a(n)/b(n) \rightarrow 1$ as $n \rightarrow \infty$.

From this by using (2) and (3) with $\Delta = 1$, and property (ii) of BF, we have

$$\prod_{A \in \mathcal{A}_1} (1 + f(A)) \leq S(\mathcal{A}_1)S(\mathcal{A}_1^c) \leq S(\mathcal{A}_1) \exp \alpha^1(\mathcal{A}_1^c) \leq S(\mathcal{A}_1)(1 + o(1)). \tag{6}$$

On the other hand, with the help of the inequality $\ln(1 + x) \geq x - x^2/2$, we have

$$\prod_{A \in \mathcal{A}_1} (1 + f(A)) \geq \exp \left\{ \alpha^1(\mathcal{A}_1) - \frac{1}{2} \alpha^2(\mathcal{A}_1) \right\}. \tag{7}$$

By properties (1) and (2) of $(1, \kappa_n, q, c)$ -ordinary pair, we obtain that

$$\alpha^2(\mathcal{A}_1) = \sum_{v \in X} f^2(v) \leq |X| 2^{-2\kappa_n} \leq 2^{-\log_2^2 \kappa_n}. \tag{8}$$

Now the lower bound follows from (6) to (8). \square

Theorem 2. *Let a sequence of $(2, \kappa_n, q, c)$ -ordinary pairs $\{I_n = (X_n, f_n)\}$ be 2-convergent and $\lim_{n \rightarrow \infty} \kappa_n = \infty$. Then, for $n \rightarrow \infty$.*

$$T(I_n) \sim \exp\{\mu(I_n)\},$$

where

$$\mu(I) = \alpha^1(\mathcal{A}_1) + \alpha^1(\mathcal{A}_2) - \alpha^2(\mathcal{A}_1)/2 + \beta^1(\mathcal{A}_2)$$

and

$$\alpha^v(\mathcal{A}_k) = \sum_{A \in \mathcal{A}_k} f^v(A), \quad \beta^1(\mathcal{A}_2) = \sum_{A \in \mathcal{A}_2} \prod_{u \in A} f(\{v\}).$$

2. Estimation of the number of independent sets in a special bipartite graph

In this section we demonstrate the application of Theorems 1 and 2 to some concrete enumeration problem. Namely, we obtain the asymptotics for the number of independent sets in the bipartite graph induced by two neighbouring levels of the n -cube.

Let B^n be the n -cube, and $G_{n,k} = (B_k^n, B_{k+1}^n; E)$ the bipartite subgraph of the n -cube, induced by two of its levels B_k^n and B_{k+1}^n . From now we assume that $k < (n - 1)/2$. Denote by $N(G)$ the number of independent sets in a graph G . We shall find the asymptotics of $N(G_{n,k})$ as $n \rightarrow \infty$. For this purpose we define a functional pair $I_{n,k} = (X_{n,k}, f)$ with $X_{n,k} = B_k^n$, and with $f(A) = 2^{-|\vartheta(A)|}$ where $v(A) = \{v \in B_{n+1}^n; \exists u \in A (u, v) \in E\}$.

Lemma 3. *Let $G(X, Z; E)$ be a bipartite graph. Then,*

$$N(G) = 2^{|Z|} \sum_{A \subseteq X} 2^{-|\vartheta(A)|}. \tag{9}$$

Proof. To generate an independent set $A \subseteq X \cup Z$ we choose an arbitrary $C \subseteq X$ as a part of A in X , and then an arbitrary $D \subseteq Z \setminus \vartheta(C)$ as a part of A in Z . It is easy to see that the number of such choices is equal to

$$N(G) = \sum 2^{|\vartheta(C)|} = 2^{|Z|} \sum 2^{-|\vartheta(C)|},$$

where summing is over all subsets $C \subseteq X$. This proves the lemma. \square

As a consequence, we have

$$N(G_{n,k}) = 2^{\binom{n}{k+1}} T(I_{n,k}). \tag{10}$$

Now we should evaluate $T(I_{n,k})$. We assume that n is big enough and $1 \leq k < n/2$. As can be easily checked, a set $A \cap X = B$ is connected relative to f if for any vertices $u, v \in A$ there exists a sequence w_0, w_1, \dots, w_m such that $w_0 = u, w_k = v, r(w_{i-1}, w_i) = 2, i = 1, \dots, m$. Let us check that the functional pair $I_{n,k}$ is (Δ, κ, q, c) -ordinary for $\Delta = 2, \kappa = n - k, q = 1, c = 4$. Note that $|\vartheta(\{v\})| = n - k$ for any $v \in X$. Hence $\kappa = n - k$ and $f(\{v\}) = 2^{-\kappa}$ (property (1) is checked). Note that, due to $k < (n - 1)/2$, we have

$$|X_{n,k}| = \binom{n}{k} < 2^n \leq 2^{2(n-k)}.$$

Hence property (2) holds for $\Delta = 2$. Further, we note that $|\vartheta(A) \cap \vartheta(\{v\})| \leq |A|$ for any $A \subseteq B_k^n$ and $v \in B_k^n$. Therefore,

$$f(A \cup \{v\}) = 2^{-|\vartheta(A \cup \{v\})|} \leq f(A)f(\{v\})2^{|A|}.$$

Hence, property (3) holds with $q = 1$.

Let us check property (4). We use the following assertion (see the proof of Lemma 2.2 in [3]).

Lemma 4. *Let $G = (V; E)$ be a graph, s the maximum degree of a vertex. Then, for any $v \in V$, the number of connected subsets $A \subseteq V$ with $|A| = a$ and $u \in A$ does not exceed $(4s)^{a-1}$.*

Now consider the graph $G = (V; E)$ with $V = B_k^n, k \geq 1$ and $E = \{(u, v): r(u, v) = 2\}$. It is clear that each vertex of G has a degree equal to $k(n - k) < \kappa^2$. Using Lemma 4, we obtain that for $k \geq 1, n \geq 2$, any $v \in V$, the number of connected sets $A \subseteq V$ with $f(A \cup \{v\}) > f(A)f(\{v\})$ is not more than

$$(1 + k(n - k))(4k(n - k))^{|A|-1} \leq (4\kappa^2)^{|A|}.$$

Since $\kappa > 2$ for big enough n , we obtain property (4) with $c = 4$. Thus, we have checked that $I_{n,k}$ is a $(\Delta, n - k, 1, 4)$ -ordinary functional pair where Δ is 1 or 2 depending on the value of k .

Let us prove that $\{I_{n,k}\}$ is a 2-convergent sequence of functional pairs as $n \rightarrow \infty$. We have to make sure that

$$\lim_{n \rightarrow \infty} \sum_{A \in \mathcal{A}_2} f(A) = 0. \tag{11}$$

Note that from Lemma 4 it follows that

$$|A_m(I_{n,k})| < |B_k^n|(4\kappa^2)^{m-1} \leq \binom{n}{k} (2n)^{2m-2}.$$

On the other hand, from properties (1) and (3) by induction it follows, that $f(A) \leq 2^{-|A|(\kappa - (|A|-1)/2)}$. Hence, for some constant c

$$\begin{aligned} \sum_{2 < m \leq \kappa} \sum_{A \in A_m(I_{n,k})} f(A) &\leq \binom{n}{k} \sum_{2 < m \leq \kappa} (2n)^{2m-2} 2^{-m(\kappa - (m-1)/2)} \\ &\leq \binom{n}{k} (2n)^4 2^{-3\kappa-1} (1 + O(n^4 2^{-\kappa})) \leq c \binom{n}{k} n^4 2^{-3n/2}. \end{aligned} \tag{12}$$

Note that $|\vartheta(A)| > |A|(n-k)/(k+1)$ for any $A \subseteq X_{n,k}$, and $|\vartheta(A)| > |A|(n-k)/(s+1)$ for any $A \subseteq X_{n,k}$ with $|A| \leq \binom{n-k+s-1}{s}$ (see [5, Lemma 17]). As a consequence, we obtain

$$|\vartheta(A)| \geq \binom{n-k+2}{3} = \binom{\kappa+2}{3} =: g_0$$

for all $A \subseteq X_{n,k}$ with $|A| \geq \binom{n-k+2}{2}$ and

$$|\vartheta(A)| \geq |A|\kappa/3$$

for all $A \subseteq X_{n,k}$ with $|A| \geq \binom{n-k+2}{2} = \binom{\kappa+2}{2}$.

Thus, putting $\binom{\kappa+2}{2} = h$, we have

$$\sum_{\kappa < m \leq h} \sum_{A \in A_m(I_{n,k})} f(A) \leq \binom{n}{k} \sum_{\kappa < m \leq h} (2n)^{2m-2} 2^{-m\kappa/3} \leq 2^{-\kappa^2/3 + O(\kappa \log \kappa)}. \tag{13}$$

For an evaluation of the remaining part of sum (3) we need some new notions and assertions. Let $G = (X, Z; E)$ be a bipartite graph, and $A \subseteq X$. Denote by $[A]$ the set $v \in X: \vartheta(v) \subseteq \vartheta(A)$. Given a graph $G = (X, Z; E)$, a set $A \subseteq X$ is called *2-connected* if for any two vertices u and v there exists a sequence w_0, w_1, \dots, w_m of elements in A such that $u = w_0, v = w_k, \tau(w_{i-1}, w_i) = 2, i = 1, 2, \dots, m$. The family of all 2-connected subsets of X will be denoted by $A(X)$. For integer g , and $0 < \delta < 1$, we put

$$F(G, g, \delta) = \{A \in A(X): |\partial(A)| = g, |[A]| \leq g(1 - \delta)\}.$$

Theorem 3 (see [3]). *Let $G(X, Z; E)$ be a bipartite graph with the following properties:*

- (1) $\min |\partial(\{v\})| = \kappa$;
- (2) $\max |\partial(\{u\}) \cap \partial(\{u\})| = q$;
- (3) *There exist constants $p, r \geq 1$ (not depending on κ) such that*

$$r \min_{v \in Z} |\partial(\{v\})| \geq \kappa \geq \max_{v \in Z} |\partial(\{v\})| \geq \max_{v \in X \cup Z} |\partial(\{v\})|/p.$$

Then for all large enough κ and for all $1 > \delta \geq \kappa^{-2} \log_2^9 \kappa$, the following inequality holds:

$$|F(G, g, \delta)| \leq |X| 2^{g(1-\delta)/(6 \log_2 \kappa)}. \tag{14}$$

Now we estimate the rest part of the sum (3). Taking into account that $|\partial(A)| \geq |A|(n-k)/(k+1) \geq |A|(1-(1/\kappa))$, and using (14) with $|X| = \binom{n}{k}$, we obtain

$$\begin{aligned} \sum_{m \geq h} \sum_{A \in \mathcal{A}_m(I_{n,k})} f(A) &\leq \sum_{g \geq g_0} |F(G_{n,k}, g, 1/\kappa)| 2^{-g} \\ &\leq \binom{n}{k} \sum_{g \geq g_0} 2^{-g/(6 \log_2 \kappa)} \leq c \binom{n}{k} \kappa^2 2^{-g_0/(6 \log_2 \kappa)} \\ &\leq 2^{-\kappa^2/36 \log_2 \kappa + O(\kappa)}. \end{aligned} \tag{15}$$

Now (12), (13) and (15) give (3). Thus we may conclude that the sequence $\{I_{n,k}\}$ is 2-convergent.

Let us obtain the asymptotics for $N(G_{n,k})$ by using Theorem 2. We have to calculate $\mu(I_{n,k})$.

$$\begin{aligned} \alpha^v(\mathcal{A}_1) &= \sum_{A \in \mathcal{A}_1} f^v(A) = \sum_{v \in B_k^n} 2^{-v|\vartheta(\{v\})|} = \binom{n}{k} 2^{-v(n-k)}, \\ \alpha^1(\mathcal{A}_2) &= \sum_{A \in \mathcal{A}_2} f(A) = \sum_{\substack{u,v \in B_k^n \\ r(u,v)=2}} 2^{-|\vartheta(\{u,v\})|} = \binom{n}{k} k(n-k) 2^{-2(n-k)}, \\ \beta^1(\mathcal{A}_2) &= \sum_{A \in \mathcal{A}_2} \prod_{v \in A} f(\{v\}) = \sum_{\substack{u,v \in B_k^n \\ r(u,v)=2}} 2^{-|\vartheta(\{u\})| - |\vartheta(\{v\})|} \\ &= \binom{n}{k} k(n-k) 2^{-2(n-k)-1} = \frac{1}{2} \alpha^1(\mathcal{A}_2). \end{aligned}$$

Therefore, we obtain by Theorem 2

$$\mu(I_{n,k}) = \binom{n}{k} (2^{-n+k} + k(n-k) 2^{-2(n-k)} - 1) - 2^{-2(n-k)-1}$$

and

$$N(G_{n,k}) \sim 2^{\binom{n}{k+1}} \exp \left\{ \binom{n}{k} 2^{-n+k} (1 + k(n-k) 2^{-n+k-1}) \right\}. \tag{16}$$

Formula (16) gives the required result.

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