

Discrete Optimization for Image Analysis

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Outline

- ▶ Literature
- ▶ Notation
- ▶ Pseudo-Boolean functions
- ▶ Multi-linear polynomial forms
 - ▶ Existence and uniqueness
 - ▶ Reduction of PBO to QPBO
- ▶ Posiforms
 - ▶ Existence
 - ▶ Bounds
 - ▶ Weak persistency
 - ▶ Complementation and the Floor Dual Bound

This lecture is based on the publications

- ▶ E. Boros, P. L. Hammer, X. Sun: Network flows and minimization of quadratic pseudo-Boolean functions. RUTCOR Research Report 17-1991
- ▶ E. Boros, P. L. Hammer: Pseudo-Boolean optimization. *Discrete Applied Mathematics* 123(1–3): 155–225 (2002)
- ▶ E. Boros, P. L. Hammer, R. Sun, G. Tavares: A max-flow approach to improved lower bounds for quadratic unconstrained binary optimization (QUBO). *Discrete Optimization* 5(2): 501–529 (2008)

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- ▶ For any A and any $k \in \mathbb{N}_0$, $\binom{A}{k}$ denotes the set of all **subsets of A with precisely k elements**.
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- ▶ For any A, B and $(a, b) \in A \times B$, let $ab := (a, b)$, i.e. short-hand for an **ordered pair**.
- ▶ For any $n \in \mathbb{N}$, let $[n] := \{m \in \mathbb{N} | m \leq n\}$.
- ▶ For any A and any B , let B^A denote the set of all **maps from A to B** , i.e., the set of all $f \in 2^{A \times B}$ such that

$$\begin{aligned} \forall a \in A \exists b \in B \quad ab \in f \\ \forall a \in A \forall b, b' \in B \quad (ab \in f \wedge ab' \in f) \Rightarrow (b = b') \end{aligned}$$

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Definition 1

For any $n \in \mathbb{N}$, any $f : \{0, 1\}^n \rightarrow \mathbb{R}$ is called an n -variate **Pseudo-Boolean function (PBF)**.

Definition 2

For any $n \in \mathbb{N}$, any $d \in \{0, \dots, n\}$, let

$$K_{nd} := \binom{[n]}{d} \quad J_{nd} := \bigcup_{m=0}^d K_{nm} \quad C_{nd} := \mathbb{R}^{J_{nd}} \quad (1)$$

and call any $c \in C_{nd}$ an n -variate **multi-linear polynomial form** of degree at most d .

Example. For $n = d = 2$, we have

$$\begin{aligned} J_{22} &= \bigcup_{m=0}^2 \binom{[2]}{m} \\ &= \binom{\{1, 2\}}{0} \cup \binom{\{1, 2\}}{1} \cup \binom{\{1, 2\}}{2} \\ &= \{\emptyset\} \cup \{\{1\}, \{2\}\} \cup \{\{1, 2\}\} \\ &= \{\emptyset, \{1\}, \{2\}, \{1, 2\}\} \end{aligned}$$

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Definition 3

For any $n \in \mathbb{N}$, any $d \in \{0, \dots, n\}$ and any $c \in C_{nd}$, $f_c : \{0, 1\}^n \rightarrow \mathbb{R}$ such that

$$\forall x \in \{0, 1\}^n \quad f_c(x) := \sum_{m=0}^d \sum_{J \in \binom{[n]}{m}} c_J \prod_{j \in J} x_j \quad (2)$$

is called the **PBF defined by c** .

Example. For any $c \in C_{22}$, $f_c : \{0, 1\}^2 \rightarrow \mathbb{R}$ is such that

$$\forall x \in \{0, 1\}^2 \quad f_c(x_1, x_2) = c_{\emptyset} + c_{\{1\}}x_1 + c_{\{2\}}x_2 + c_{\{1,2\}}x_1x_2 .$$

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Lemma 1

Every PBF has a unique multi-linear polynomial form. More precisely,

$$\forall n \in \mathbb{N} \quad \forall f : \{0,1\}^n \rightarrow \mathbb{R} \quad \exists_1 c \in C_{nn} \quad f = f_c . \quad (3)$$

Example. For $n = d = 2$ and any $f : \{0,1\}^2 \rightarrow \mathbb{R}$, the existence of a $c \in C_{22}$ such that $f = f_c$ means

$$\forall x \in \{0,1\}^2 \quad f(x_1, x_2) = c_\emptyset + c_{\{1\}}x_1 + c_{\{2\}}x_2 + c_{\{1,2\}}x_1x_2 .$$

Explicitly,

$$f(0,0) = c_\emptyset$$

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In this example, a suitable c exists and is defined uniquely by f .

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Proof.

- For any $J \subseteq [n]$, let $x^J \in \{0, 1\}^n$ such that

$$\forall j \in [n] \quad x_j^J = \begin{cases} 1 & \text{if } j \in J \\ 0 & \text{otherwise} \end{cases} .$$

- Now,

$$\forall x \in \{0, 1\}^n \quad f(x) = \sum_{J \in 2^{[n]}} c_J \prod_{j \in J} x_j$$

is written equivalently as

$$\begin{aligned} f(x^\emptyset) &= c_\emptyset \\ \forall J \neq \emptyset \quad f(x^J) &= c_J + \sum_{J' \subset J} c_{J'} . \end{aligned}$$

- Thus, c is defined uniquely (by induction over the cardinality of J).

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Definition 4

For any $n \in \mathbb{N}$ and any $d \in \{0, \dots, n\}$, let

$$F_{nd} := \{f : \{0, 1\}^n \rightarrow \mathbb{R} \mid \exists c \in C_{nd} : f = f_c\} \quad (4)$$

and call any $f \in F_{nd}$ an n -variate **PBF of degree at most d** .

In addition, call any $f \in F_{n2}$ a **quadratic PBF (QPBF)**.

Note. For any $n \in \mathbb{N}$, F_{nn} is the set of all n -variate PBFs (by Lemma 1).

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- **Pseudo-Boolean Optimization (PBO):** Given $n \in \mathbb{N}$ and $f : \{0, 1\}^n \rightarrow \mathbb{R}$,

$$\min_{x \in \{0,1\}^n} f(x) . \quad (5)$$

- **Quadratic Pseudo-Boolean Optimization (QPBO):** Given $n \in \mathbb{N}$ and $f \in F_{n2}$,

$$\min_{x \in \{0,1\}^n} f(x) . \quad (6)$$

- Is QPBO less complex than PBO?

Definition 5

For any $n \in \mathbb{N}$ and any $c \in C_{nn}$, define the **size** of c as

$$\text{size}(c) := \sum_{J \subseteq [n]: c_J \neq 0} |J| . \quad (7)$$

Lemma 2

For any $x, y, z \in \{0, 1\}$:

$$z = xy \quad \Leftrightarrow \quad xy - 2xz - 2yz + 3z = 0 \quad , \quad (8)$$

$$z \neq xy \quad \Leftrightarrow \quad xy - 2xz - 2yz + 3z > 0 \quad . \quad (9)$$

Proof. By verifying equivalence for all eight cases.

Algorithm 1 (Boros and Hammer 2001)

Input: $c \in C_{nn}$

Output: $c' \in C_{n2}$

$M := 1 + 2 \sum_{J \subseteq [n]} |c_J|$

$m := n$

$c^m := c$

while there exists a $J \subseteq [n]$ such that $|J| > 2$ and $c_J^m \neq 0$

 Choose $j, k \in J$ such that $j \neq k$

$c^{m+1} := c^m$

$c_{\{j,k\}}^{m+1} := c_{\{j,k\}}^{m+1} + M$

$c_{\{j,m+1\}}^{m+1} := -2M$

$c_{\{k,m+1\}}^{m+1} := -2M$

$c_{\{m+1\}}^{m+1} := 3M$

for all $\{j, k\} \subseteq J' \subseteq [n]$ such that $c_{J'}^{m+1} \neq 0$

$c_{J' - \{j,k\} \cup \{m+1\}}^{m+1} := c_{J'}^{m+1}$

$c_{J'}^{m+1} := 0$

$m := m + 1$

$c' := c^m$

Theorem 1

- ▶ *Algorithm 1 terminates in polynomial time in $\text{size}(c)$.*
- ▶ *$\text{size}(c')$ is polynomially bounded by $\text{size}(c)$.*
- ▶ *The multi-linear quadratic form c' is such that $\forall \hat{x} \in \mathbb{R}^n$:*

$$\hat{x} \in \underset{x \in \{0,1\}^n}{\operatorname{argmin}} f_c(x)$$
$$\Rightarrow \exists \hat{x}' \in \{0,1\}^m \left(\hat{x}'_{[n]} = \hat{x}_{[n]} \wedge \hat{x}' \in \underset{x' \in \{0,1\}^m}{\operatorname{argmin}} f_{c'}(x') \right) . \quad (10)$$

Proof.

- ▶ The algorithm replaces the occurrence of $x_j x_k$ by x_{m+1} and adds the form $M(x_j x_k - 2x_j x_{m+1} - 2x_k x_{m+1} + 3x_{m+1})$.

- ▶ If $x_{m+1} = x_j x_k$,

$$f^{m+1}(x_1, \dots, x_{m+1}) = f^m(x_1, \dots, x_n) \leq \max_{x' \in \{0,1\}^n} f^m(x') < M/2 .$$

- ▶ If $x_{m+1} \neq x_j x_k$,

$$f^{m+1}(x_1, \dots, x_{m+1}) \geq M/2$$

(by Lemma 2 and by definition of M).

- ▶ For every iteration m ,

$$|\{J \subseteq [n] \mid |J| > 2 \wedge c_J^{m+1} \neq 0\}| < |\{J \subseteq [n] \mid |J| > 2 \wedge c_J^m \neq 0\}|$$

which proves the complexity claims.

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Summary

- ▶ Every PBF has a unique multi-linear polynomial form.
- ▶ PBO is polynomially reducible to QPBO.

Definition 6

For any $n \in \mathbb{N}$ and any $d \in \{0, \dots, n\}$, let

$$K_{nm}^+ := \{(K^1, K^0) \mid K^1, K^0 \subseteq [n] \wedge K^1 \cap K^0 = \emptyset \wedge |K^1| + |K^0| = m\}$$

$$J_{nm}^+ := \bigcup_{m=0}^d K_{nm}^+$$

$$C_{nm}^+ := \{c : J_{nm}^+ \rightarrow \mathbb{R} \mid \forall j \in J_{nm}^+ - \{(\emptyset, \emptyset)\} : 0 \leq c_j\}$$

and call any $c \in C_{nm}^+$ an n -variate **posiform** of degree at most d .

Example. For $n = d = 2$,

$$\begin{aligned} J_{22}^+ = & \{ (\emptyset, \emptyset) \} \\ & \cup \{ (\{1\}, \emptyset), (\emptyset, \{1\}), (\{2\}, \emptyset), (\emptyset, \{2\}) \} \\ & \cup \{ (\{1, 2\}, \emptyset), (\{1\}, \{2\}), (\{2\}, \{1\}), (\emptyset, \{1, 2\}) \} \end{aligned}$$

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Definition 7

For any $n \in \mathbb{N}$, any $d \in \{0, \dots, n\}$ and any $c \in C_{nd}^+$, $f_c : \{0, 1\}^n \rightarrow \mathbb{R}$ such that

$$\forall x \in \{0, 1\}^n \quad f_c(x) := \sum_{(J^1, J^0) \in J_{nd}^+} c_{J^1 J^0} \prod_{j \in J^1} x_j \prod_{j' \in J^0} (1 - x_{j'}) \quad (11)$$

is called the **PBF** defined by c .

Example. For any $c \in C_{22}^+$, $f_c : \{0, 1\}^2 \rightarrow \mathbb{R}$ is such that $\forall x \in \{0, 1\}^2$

$$\begin{aligned} f(x) = & c_{\emptyset\emptyset} \\ & + c_{\{1\}\emptyset} x_1 + c_{\emptyset\{1\}} (1 - x_1) + c_{\{2\}\emptyset} x_2 + c_{\emptyset\{2\}} (1 - x_2) \\ & + c_{\{1,2\}\emptyset} x_1 x_2 + c_{\{1\}\{2\}} x_1 (1 - x_2) + c_{\{2\}\{1\}} (1 - x_1) x_2 \\ & + c_{\emptyset\{1,2\}} (1 - x_1) (1 - x_2) . \end{aligned}$$

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For any $n \in \mathbb{N}$, any $d \in \{0, \dots, n\}$ and any $c \in C_{nd}^+$, $f_c : \{0, 1\}^n \rightarrow \mathbb{R}$ such that

$$\forall x \in \{0, 1\}^n \quad f_c(x) := \sum_{(J^1, J^0) \in J_{nd}^+} c_{J^1 J^0} \prod_{j \in J^1} x_j \prod_{j' \in J^0} (1 - x_{j'}) \quad (11)$$

is called the **PBF** defined by c .

Example. For any $c \in C_{22}^+$, $f_c : \{0, 1\}^2 \rightarrow \mathbb{R}$ is such that $\forall x \in \{0, 1\}^2$

$$\begin{aligned} f(x) = & c_{\emptyset\emptyset} \\ & + c_{\{1\}\emptyset} x_1 + c_{\emptyset\{1\}} (1 - x_1) + c_{\{2\}\emptyset} x_2 + c_{\emptyset\{2\}} (1 - x_2) \\ & + c_{\{1,2\}\emptyset} x_1 x_2 + c_{\{1\}\{2\}} x_1 (1 - x_2) + c_{\{2\}\{1\}} (1 - x_1) x_2 \\ & + c_{\emptyset\{1,2\}} (1 - x_1) (1 - x_2) . \end{aligned}$$

Definition 8

For any $n \in \mathbb{N}$ and any $f : \{0, 1\}^n \rightarrow \mathbb{R}$, the posiform defined by

$$\begin{aligned}\forall x \in \{0, 1\}^n \quad K_x^1 &:= \{j \in [n] \mid x_j = 1\} \\ K_x^0 &:= \{j \in [n] \mid x_j = 0\}\end{aligned}$$

and

$$J := \{(\emptyset, \emptyset)\} \cup \bigcup_{x \in \{0, 1\}^n} \{(K_x^1, K_x^0)\}$$

and $c : J \rightarrow \mathbb{R}$ such that

$$\begin{aligned}c_{\emptyset\emptyset} &:= \min_{x \in \{0, 1\}^n} f(x) \\ \forall x \in \{0, 1\}^n \quad c_{K_x^1 K_x^0} &:= f(x) - c_{\emptyset\emptyset}\end{aligned}$$

is called **min-term posiform** of f .

Lemma 3

For any $n \in \mathbb{N}$ and any $f : \{0, 1\}^n \rightarrow \mathbb{R}$, the min-term posiform c of f holds $f_c = f$.

Corollary 1

For any $n \in \mathbb{N}$ and any $f : \{0, 1\}^n \rightarrow \mathbb{R}$, there exists a posiform $c \in C_{nn}^+$ such that $f_c = f$.

Lemma 3

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Corollary 1

For any $n \in \mathbb{N}$ and any $f : \{0, 1\}^n \rightarrow \mathbb{R}$, there exists a posiform $c \in C_{nn}^+$ such that $f_c = f$.

Proof of Lemma 3.

- ▶ Let $n \in \mathbb{N}$ and $f : \{0, 1\}^n \rightarrow \mathbb{R}$. Moreover, let $c : J \rightarrow \mathbb{R}$ the min-term posiform of f .
- ▶ c is a posiform (by definition).
- ▶ Let $g : \{0, 1\}^n \rightarrow \mathbb{R}$ be the PBF defined by this posiform.
- ▶ Then, for any $x \in \{0, 1\}^n$,

$$(J^1, J^0) \in \{(\emptyset, \emptyset), (K_x^1, K_x^0)\} \subseteq J$$

are the only elements of J for which

$$0 \neq \prod_{j \in J^1} x_j \prod_{j' \in J^0} (1 - x_{j'}) = 1 .$$

- ▶ Thus,

$$\begin{aligned} \forall x \in \{0, 1\}^n \quad g(x) &= c_{\emptyset\emptyset} + c_{K_x^1 K_x^0} \\ &= c_{\emptyset\emptyset} + f(x) - c_{\emptyset\emptyset} \quad (\text{by definition of } c) \\ &= f(x) . \end{aligned}$$

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Note. Unlike multi-linear polynomial forms, posiforms of PBFs need not be unique, e.g., $x_1 = x_1x_2 + x_1(1 - x_2)$.

Definition 9

For any $n \in \mathbb{N}$, any $f : \{0, 1\}^n \rightarrow \mathbb{R}$ and any $d \in \{0, \dots, n\}$, let

$$C_{nd}^+(f) := \{c \in C_{nd}^+ \mid f_c = f\} \quad . \quad (12)$$

Note. For any $n \in \mathbb{N}$ and any $f : \{0, 1\}^n \rightarrow \mathbb{R}$, $C_{nn}^+(f)$ contains at least the min-term posiform of f .

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Lemma 4

$$\forall n \in \mathbb{N} \quad \forall f : \{0, 1\}^n \rightarrow \mathbb{R} \quad \forall c \in C_{nn}^+(f) \quad \forall x \in \{0, 1\}^n \quad c_{\emptyset\emptyset} \leq f(x) .$$

Proof.

- ▶ By definition, we have, for all $x \in \{0, 1\}^n$,

$$\begin{aligned} f(x) &= \sum_{m=0}^d \sum_{(K^1, K^0) \in K_{nm}^+} c_{K^1 K^0} \prod_{j \in K^1} x_j \prod_{j' \in K^0} (1 - x_{j'}) \\ &= c_{\emptyset \emptyset} + \sum_{m=1}^d \sum_{(K^1, K^0) \in K_{nm}^+} c_{K^1 K^0} \prod_{j \in K^1} x_j \prod_{j' \in K^0} (1 - x_{j'}) , \end{aligned}$$

and all coefficients $c_{K^1 K^0}$ in the second sum are non-negative.

- ▶ Therefore, the second sum is non-negative.
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$$\forall x \in \{0, 1\}^n \quad f(x) \geq c_{\emptyset \emptyset} .$$

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Definition 10

For any posiform $c : J \rightarrow \mathbb{R}$, a pair (S, y) such that $S \subseteq [n]$ and $y : S \rightarrow \{0, 1\}$ is called a **contractor** of c iff

$$\begin{aligned} \forall (J^1, J^0) \in J \quad & (J^1 \cap S = \emptyset \quad \wedge \quad J^0 \cap S = \emptyset) \\ & \vee (\exists j \in J^1 \cap S \quad y_j = 0) \\ & \vee (\exists j \in J^0 \cap S \quad y_j = 1) . \end{aligned} \tag{13}$$

Lemma 5

For any $n \in \mathbb{N}$, any $f : \{0, 1\}^n \rightarrow \mathbb{R}$, any posiform $c \in C_{nn}^+(f)$, any contractor (S, y) of c and $t_{S,y} : \{0, 1\}^n \rightarrow \{0, 1\}^n$ such that

$$\forall x \in \{0, 1\}^n \quad \forall j \in [n] \quad (t_{S,y}(x))_j = \begin{cases} y_j & \text{if } j \in S \\ x_j & \text{otherwise} \end{cases} \quad (14)$$

holds

$$\forall x \in \{0, 1\}^n \quad f(t_{S,y}(x)) \leq f(x) . \quad (15)$$

Corollary 2 (weak persistency)

$$\hat{x} \in \operatorname{argmin}_{x \in \{0,1\}^n} f(x) \quad \Rightarrow \quad t_{S,y}(\hat{x}) \in \operatorname{argmin}_{x \in \{0,1\}^n} f(x) \quad (16)$$

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Proof of Lemma 5.

► Let $J^{\bar{S}} := \{(J^1, J^0) \in J_{nn}^+ \mid J^1 \cap S = J^0 \cap S = \emptyset\}$ and $J^S := J - J^{\bar{S}}$.

► By definition,

$$\begin{aligned} \forall x \in \{0, 1\}^n \quad f(x) &= \underbrace{\sum_{(J^1, J^0) \in J^S} c_{J^1 J^0} \prod_{j \in J^1} x_j \prod_{j' \in J^0} (1 - x'_{j'})}_{=: f^S(x)} \\ &+ \underbrace{\sum_{(J^1, J^0) \in J^{\bar{S}}} c_{J^1 J^0} \prod_{j \in J^1} x_j \prod_{j' \in J^0} (1 - x'_{j'})}_{=: f^{\bar{S}}(x)}. \end{aligned}$$

► Furthermore,

$$\begin{aligned} \forall x \in \{0, 1\}^n \quad f^S(t_{S,y}(x)) &= 0 && \text{(by definition)} \\ 0 \leq f^S(x) & && \text{(because } (\emptyset, \emptyset) \notin J^S) \\ f^{\bar{S}}(t_{S,y}(x)) &= f^{\bar{S}}(x) && \text{(by definition)} \end{aligned}$$

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Summary

- ▶ Every PBF has a posiform
- ▶ The posiform of a PBF need not be unique
- ▶ For every PBF f and every posiform c of f
 - ▶ $c_{\emptyset\emptyset}$ is a lower bound on the minimum of f
 - ▶ weak persistency holds at any contractor of c