Probabilistic Graphical Models & Applications

Pseudo Boolean Optimization I/III

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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 Roof Dual
    - Reduction of Complementation to Maximum st-Flow
    - Strong persistency
- Submodularity

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**.
- For any A and any $B \subseteq A$, let $B^c := A - B$ denote the **complement** of B in A.
- 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

$$\forall a \in A \; \exists b \in B \quad ab \in f$$
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Definition 1

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

Definition 2

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

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

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 $c \in C_{nd}$, $f_c : \{0,1\}^n \to \mathbb{R}$ such that

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

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

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

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

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Lemma 1

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

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

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

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

Explicitly,

$$\begin{aligned}
f(0,0) &= c_\emptyset \\
f(1,0) &= c_\emptyset + c_{\{1\}} \\
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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,

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

is written equivalently as

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

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Proof.

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

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

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Definition 4

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

$$F_{nd} := \{f : \{0,1\}^n \to \mathbb{R} \mid \exists c \in C_{nd} : \; f = f_c\} \tag{4}$$

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 $f : \{0,1\}^n \to \mathbb{R}$,

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

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

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

- 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*

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

Lemma 2

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

$$z = xy \quad \Leftrightarrow \quad xy - 2xz - 2yz + 3z = 0 \ , \tag{8}$$

$$z \neq xy \quad \Leftrightarrow \quad xy - 2xz - 2yz + 3z > 0 \ . \tag{9}$$

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* $c^m_J \neq 0$
    Choose $j, k \in J$ *such that* $j \neq k$
    $c^{m+1} := c^m$
    $c^{m+1}_{\{j,k\}} := c^{m+1}_{\{j,k\}} + M$
    $c^{m+1}_{\{j,m+1\}} := -2M$
    $c^{m+1}_{\{k,m+1\}} := -2M$
    $c^{m+1}_{\{m+1\}} := 3M$
    for all $\{j,k\} \subseteq J' \subseteq [n]$ *such that* $c^{m+1}_{J'} \neq 0$
        $c^{m+1}_{J' - \{j,k\} \cup \{m+1\}} := c^{m+1}_{J'}$
        $c^{m+1}_{J'} := 0$
    $m := m + 1$
$c' := c^m$

Theorem 1

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

$$\begin{aligned} & \hat{x} \in \operatorname*{argmin}_{x \in \{0,1\}^n} f_c(x) \\ \Leftrightarrow \quad & \exists \hat{x}' \in \mathbb{R}^m \left(\hat{x}'_{[n]} = \hat{x}_{[n]} \wedge \hat{x}' \in \operatorname*{argmin}_{x' \in \{0,1\}^m} f_{c'}(x') \right) \quad . \end{aligned} \tag{10}$$

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 $x_{m+1} = x_j x_k$,

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

  - If $x_{m+1} \neq x_j x_k$,

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

(by Lemma 2 and by definition of M).

- For every iteration m,

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

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* $d \in \{0, \ldots, n\}$, *let*

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

$$J^+_{nm} := \bigcup_{m=0}^{d} K^+_{nm}$$

$$C^+_{nm} := \{c : J^+_{nm} \to \mathbb{R} \mid \forall j \in J^+_{nm} - \{(\emptyset, \emptyset)\} : \ 0 \leq c_j\}$$

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 $c \in C^+_{nd}$, $f_c : \{0,1\}^n \to \mathbb{R}$ such that

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

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

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

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

Definition 7

For any $n \in \mathbb{N}$, any $d \in \{0, \ldots, n\}$ and any $c \in C^+_{nd}$, $f_c : \{0,1\}^n \to \mathbb{R}$ such that

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

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

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Definition 8

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

$$\forall x \in \{0,1\}^n \quad K_x^1 := \{j \in [n] | x_j = 1\}$$
$$K_x^0 := \{j \in [n] | x_j = 0\}$$

and

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

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

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

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

Lemma 3

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

Corollary 1

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

Lemma 3

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

Corollary 1

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Proof of Lemma 3.

- Let $n \in \mathbb{N}$ and $f : \{0,1\}^n \to \mathbb{R}$. Moreover, let $c : J \to \mathbb{R}$ the min-term posiform of f.
- c is a posiform (by definition).
- Let $g : \{0,1\}^n \to \mathbb{R}$ 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,

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

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

Definition 9

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

$$C^+_{nd}(f) := \left\{ c \in C^+_{nd} \mid f_c = f \right\} \quad . \tag{12}$$

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

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Lemma 4

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

Proof.

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

$$f(x) = \sum_{m=0}^{d} \sum_{(K^1,K^0) \in K^+_{nm}} c_{K^1K^0} \prod_{j \in K^1} x_j \prod_{j' \in K^0} (1 - x'_j)$$

$$= c_{\emptyset\emptyset} + \sum_{m=1}^{d} \sum_{(K^1,K^0) \in K^+_{nm}} c_{K^1K^0} \prod_{j \in K^1} x_j \prod_{j' \in K^0} (1 - x'_j) \ ,$$

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

$$\forall x \in \{0,1\}^n \qquad f(x) \geq c_{\emptyset\emptyset} \ .$$

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- Thus,

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Definition 10

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

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

Lemma 5

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

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

holds

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

Corollary 2 (weak persistency)

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

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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,

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

- Furthermore,

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

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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