Probabilistic Graphical Models & Applications

Pseudo Boolean Optimization II/III

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For any $n \in \mathbb{N}$, consider n-variate **quadratic** forms:

- any **multi-linear polynomial form** $c \in C_{n2}$ and $f_c : \{0,1\}^2 \to \mathbb{R}$, i.e., for all $x \in \{0,1\}^n$,

$$f_c(x) = c_\emptyset + \sum_{j \in [n]} c_{\{j\}} x_j + \sum_{\{j,k\} \in \binom{[n]}{2}} c_{\{j,k\}} x_j x_k$$

- any **posiform** $c' \in C^+_{n2}$ and $f'_c : \{0,1\}^2 \to \mathbb{R}$, i.e., for all $x \in \{0,1\}^n$,

$$\begin{aligned} f'_{c'}(x) = c'_{\emptyset\emptyset} &+ \sum_{j \in [n]} \Big(c'_{\{j\}\emptyset} x_j + c'_{\emptyset\{j\}} (1 - x_j) \Big) \\ &+ \sum_{\{j,k\} \in \binom{[n]}{2}} \big(c'_{\{j,k\}\emptyset} x_j x_k + c'_{\{j\}\{k\}} x_j (1 - x_k) \\ &\qquad + c'_{\{k\}\{j\}} x_k (1 - x_j) + c'_{\emptyset\{j,k\}} (1 - x_j)(1 - x_k) \big) \end{aligned}$$

Lemma 1

For any $n \in \mathbb{N}$, any QPBF $f : \{0,1\}^n \to \mathbb{R}$, the $c \in C_{n2}$ such that $f_c = f$ and any $c' \in C^+_{n2}(f)$ holds

$$c_\emptyset = c'_{\emptyset\emptyset} + \sum_{j=1}^{n} c'_{\emptyset\{j\}} + \sum_{\{j,k\} \in \binom{[n]}{2}} c'_{\emptyset\{j,k\}}$$

$$\forall j \in [n] \quad c_{\{j\}} = c'_{\{j\}\emptyset} - c'_{\emptyset\{j\}} + \sum_{k \in [n]-\{j\}} \left(c'_{\{j\}\{k\}} - c'_{\emptyset\{j,k\}} \right)$$

$$\forall \{j,k\} \in \binom{[n]}{2} \quad c_{\{j,k\}} = c'_{\{j,k\}\emptyset} + c'_{\emptyset\{j,k\}} - c'_{\{j\}\{k\}} - c'_{\{k\}\{j\}}$$

Proof.

- Expansion of the posiform c' yields a quadratic multi-linear polynomial form.
- Comparison with c yields the conditions stated in the Lemma.

Definition 1 (Complementation)

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

$$r_f := \max_{c' \in C^+_{n2}(f)} c'_{\emptyset\emptyset} \tag{1}$$

is called the **floor dual** *of* f.

Lemma 2

For any $n \in \mathbb{N}$ and any QPBF $f : \{0,1\}^n \to \mathbb{R}$, the floor dual can be computed in polynomial time.

Proof. For the multi-linear polynomial form $c \in C_{n2}$ such that $f_c = f$, r_f is the solution of the linear programming problem below (by Lemma 1).

$$\begin{aligned}
\max_{c' : J_{n2}^+ \to \mathbb{R}} \quad & c_\emptyset - \sum_{j=1}^{n} c'_{\emptyset\{j\}} - \sum_{\{j,k\} \in \binom{[n]}{2}} c'_{\emptyset\{j,k\}} \\
\text{subject to} \quad & \forall j \in [n] \quad c_{\{j\}} = c'_{\{j\}\emptyset} - c'_{\emptyset\{j\}} + \sum_{k \in [n]-\{j\}} \left(c'_{\{j\}\{k\}} - c'_{\emptyset\{j,k\}} \right) \\
& \forall \{j,k\} \in \binom{[n]}{2} \quad c_{\{j,k\}} = c'_{\{j,k\}\emptyset} + c'_{\emptyset\{j,k\}} - c'_{\{j\}\{k\}} - c'_{\{k\}\{j\}} \\
& \forall J \in J_{n2}^+ - \{(\emptyset, \emptyset)\} \quad 0 \leq c'_J \enspace .
\end{aligned}$$

Can the floor dual be computed more efficiently than by an algorithm for general LPs?

Probabilistic Graphical Models & Applications

Excursus: Maximum st-Flow and Minimum st-Cut

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Outline

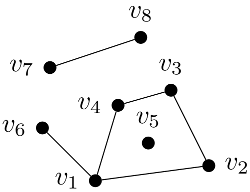
- Definitions: Flux, preflow, flow, network, st-preflow and st-flow
- Maximum st-Flow Problem
- Residual network and augmenting paths
- st-cut
- Minimum st-Cut Problem
- Maximum st-Flow/Minimum st-Cut Theorem
- Algorithms

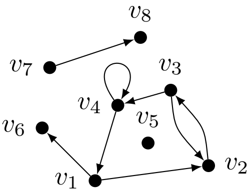
Definition 2

A pair (V, E) is called

- *an* **undirected graph** *iff* $E \subseteq \binom{V}{2}$
- *a* **directed graph** *iff* $E \subseteq V^2$.

The elements of V *are called* **nodes**. *The elements of* E *are called* **edges**.





Definition 3

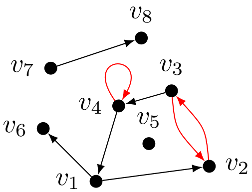
In any directed graph (V, E),

- *an edge $e \in E$ is called a* **self-edge** *iff*

$$\exists v \in V \quad e = vv \ .$$

- *a pair $ee' \in E^2$ of edges is called a* **digon** *iff*

$$\exists v, v' \in V \quad v \neq v' \wedge e = vv' \wedge e' = v'v \ .$$

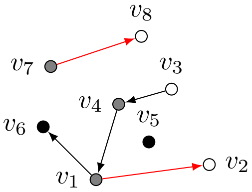


Below, the term **directed graph** shall always mean directed graph **without self-edges** and **without digons**, i.e., a pair (V, E) such that $E \subseteq V^2$ and

$$\forall vw \in V^2 \quad vw \notin E \vee wv \notin E \quad .$$

For any directed graph (V, E), any $U \subseteq V$ and any $W \subseteq V$ let

$$UW := \{uv \in E | u \in U \wedge w \in W\} \ .$$



$U = \{v_1, v_4, v_7\} \quad W = \{v_2, v_3, v_8\} \quad UW = \{v_1 v_2, v_7 v_8\}$

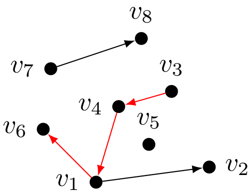
Definition 4

For any directed graph (V, E) and any $n \in \mathbb{N}$, a map $p \in E^{[n]}$ is called a **path** *in (V, E) of* **length** *n iff*

$$\begin{aligned} \forall j, k \in [n] \quad & j = k \vee p_j \neq p_k \\ \forall j \in [n-1]\ \exists v, w, x \in V \quad & p_j = vw \wedge p_{j+1} = wx \ . \end{aligned}$$

A path is called **simple** *iff the nodes along the path are pairwise distinct, except for, possibliy, the first and the last node.*

Below, **path** shall always mean **simple path**.



$p = (v_3v_4, v_4v_1, v_1v_6)$

Definition 5

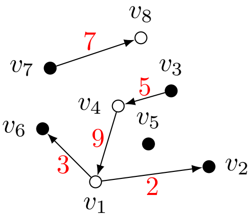
For any directed graph (V, E) *and any* $f \in \mathbb{N}_0^E$, *the maps* $\varphi^+, \varphi^-, \varphi : 2^V \to \mathbb{Z}$ *such that*

$$\forall U \in 2^V \quad \varphi_U^+ = \sum_{uv \in UU^c} f_{uv} \tag{2}$$

$$\varphi_U^- = \sum_{vu \in U^cU} f_{vu} \tag{3}$$

$$\varphi_U = \varphi_U^+ - \varphi_U^- \tag{4}$$

are called the **outflux**, **influx** *and* **flux** *in* (V, E) *w.r.t.* f.

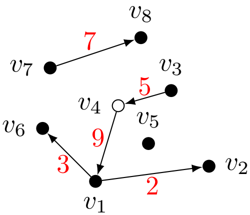


$$U = \{v_1, v_4, v_8\}$$
$$\varphi_U^+ = 3 + 2$$
$$\varphi_U^- = 7 + 5$$
$$\varphi_U = -7$$

For any $u \in V$,

$$\varphi_u^+ := \varphi_{\{u\}}^+$$
$$\varphi_u^- := \varphi_{\{u\}}^-$$
$$\varphi_u := \varphi_{\{u\}}$$

are called the **outflux**, **influx** and **flux** of u in (V, E) w.r.t. f.

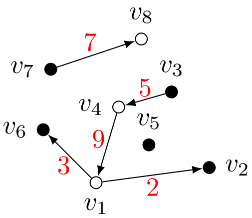


$$\varphi_{v_4}^+ = 9$$
$$\varphi_{v_4}^- = 5$$
$$\varphi_{v_4} = 4$$

Lemma 3

For any directed graph (V, E), any $f \in \mathbb{N}_0^E$ and any $U \subseteq V$

$$\varphi_U = \sum_{u \in U} \varphi_u \quad . \tag{5}$$



Proof.

$$\begin{aligned}
\varphi_U &= \sum_{uv \in UU^c} f_{uv} - \sum_{vu \in U^c U} f_{vu} \\
&= \left(\sum_{uv \in UV} f_{uv} - \sum_{uu' \in UU} f_{uu'} \right) - \left(\sum_{vu \in VU} f_{vu} - \sum_{u'u \in UU} f_{uu'} \right) \\
&= \sum_{uv \in UV} f_{uv} - \sum_{vu \in VU} f_{vu} \\
&= \sum_{u \in U} \left(\sum_{vw \in \{u\}\{u\}^c} f_{vw} - \sum_{vw \in \{u\}^c\{u\}} f_{vw} \right) \\
&= \sum_{u \in U} \varphi_u \quad .
\end{aligned}$$

$\square$

Definition 6

A 5-tuple $N = (V, E, s, t, c)$ is called a **network** *iff (V, E) is a directed graph and $s \in V$ and $t \in V$ and $s \neq t$ and $c \in \mathbb{N}^E$.*

The nodes s and t are called the **source** *and the* **sink** *of N, respectively.*

For any edge $e \in E$, c_e is called the **capacity** *of e in N.*

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For any edge $e \in E$, c_e *is called the* **capacity** *of* e *in* N.

Definition 7

A map $f \in \mathbb{N}_0^E$ *is called an* st-**preflow** *in a network* $N = (V, E, s, t, c)$ *iff*

$$\forall e \in E \quad 0 \le f_e \le c_e \tag{6}$$

$$\forall v \in V - \{s\} \quad \varphi_v \le 0 \ . \tag{7}$$

An st*-preflow* f *in* N *is called an* st-**flow** *in* N *iff, in addition,*

$$\forall v \in V - \{s, t\} \quad \varphi_v = 0 \ . \tag{8}$$

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Definition 8

The instance of the **Maximum** st**-Flow Problem** *w.r.t. a network* $N = (V, E, s, t, c)$ *is to*

$$\max_{f \in \mathbb{N}_0^E} \quad \sum_{sv \in E} f_{sv} \; - \sum_{vs \in E} f_{vs} \tag{9}$$

$$\text{subject to} \quad \forall e \in E \quad 0 \leq f_e \leq c_e \tag{10}$$

$$\forall v \in V - \{s, t\} \quad \sum_{vw \in E} f_{vw} = \sum_{uv \in E} f_{uv} \; . \tag{11}$$

Note:

$$\sum_{sv \in E} f_{sv} \; - \sum_{vs \in E} f_{vs} \quad = \quad \varphi_s$$

Definition 9

For any network $N = (V, E, s, t, c)$ *and any* st*-preflow* f *in* N*, the* **residual network** *of* N *w.r.t.* f *is the network* $N' = (V, E', s, t, c')$ *such that*

$$E' = E^+ \cup E^-$$
$$E^+ = \{vw \in E \mid c_{vw} - f_{vw} > 0\}$$
$$E^- = \{vw \in V^2 \mid wv \in E \wedge f_{wv} > 0\}$$

and

$$\forall vw \in E' \quad c'_{vw} = \begin{cases} c_{vw} - f_{vw} & \text{if } vw \in E^+ \\ f_{wv} & \text{if } vw \in E^- \end{cases} . \tag{12}$$

For any $e \in E'$, c'_e *is called the* **residual capacity** *of* e *w.r.t.* f.

Any path in (V, E') *from* s *to* t *(if such a path exists) is called an* **augmenting path** *of* f.

Definition 9

For any network $N = (V, E, s, t, c)$ and any st-preflow f in N, the **residual network** *of N w.r.t. f is the network $N' = (V, E', s, t, c')$ such that*

$$\begin{aligned} E' &= E^+ \cup E^- \\ E^+ &= \{vw \in E \mid c_{vw} - f_{vw} > 0\} \\ E^- &= \{vw \in V^2 \mid wv \in E \wedge f_{wv} > 0\} \end{aligned}$$

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For any $e \in E'$, c'_e is called the **residual capacity** *of e w.r.t. f.*

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Any path in (V, E') *from* s *to* t *(if such a path exists) is called an* **augmenting path** *of* f*.*

Lemma 5

Let $N = (V, E, s, t, c)$ *be a network and* f *an* st*-preflow in* N*. Assume that an* $n \in \mathbb{N}$ *and an augmenting path* $p = (v_1 w_1, \ldots, v_n w_n)$ *of* f *exist. Let*

$$\delta := \min_{vw \in p([n])} c'_{vw} \ . \tag{13}$$

Then, $f' \in \mathbb{N}_0^E$ *such that*

$$\forall vw \in E' : \quad f'_{vw} = \begin{cases} f_{vw} + \delta & \text{if } vw \in p([n]) \wedge vw \in E \\ f_{vw} - \delta & \text{if } vw \in p([n]) \wedge wv \in E \\ f_{vw} & \text{otherwise} \end{cases} \tag{14}$$

is an st*-preflow in* N *w.r.t. which*

$$\varphi'_s = \varphi_s + \delta \ . \tag{15}$$

Moreover, if f *is an* st*-flow in* N*, so is* f'*.*

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is an st-preflow in N w.r.t. which

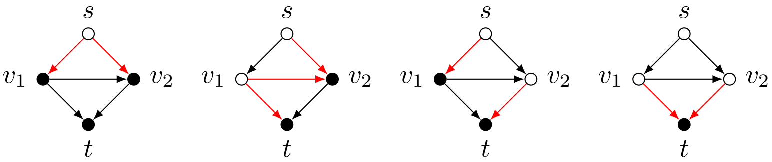
$$\varphi'_s = \varphi_s + \delta \quad . \tag{15}$$

Moreover, if f is an st-flow in N, so is f'.

Definition 10

Let (V, E) be a directed graph. Let $s \in V$ and $t \in V$ and $s \neq t$.

- *$X \subseteq V$ is called an st-**cutset** of (V, E) iff $s \in X$ and $t \notin X$.*
- *$Y \subseteq E$ is called an st-**cut** of (V, E) iff there exists an st-cutset X such that $Y = \{vw \in E | v \in X \wedge w \notin X\}$.*



Definition 11

The instance of the **Minimum** st**-Cut Problem** *w.r.t. a network* $N = (V, E, s, t, c)$ *is to*

$$\min_{x \in \{0,1\}^V} \quad \sum_{vw \in E} x_v(1 - x_w)c_{vw} \tag{16}$$

$$\text{subject to} \quad x_s = 1 \tag{17}$$

$$x_t = 0 \tag{18}$$

Note: With $X := \{v \in V | x_v = 1\}$, we have

$$\sum_{vw \in E} x_v(1 - x_w)c_{vw} = \sum_{vw \in XX^c} c_{vw}$$

Lemma 7

For every network $N = (V, E, s, t, c)$, *every* st*-flow* f *in* N, *and every* st*-cutset* $X \subseteq V$,

$$\varphi_s \leq \sum_{vw \in XX^c} c_{vw} \quad . \tag{19}$$

Theorem 1

For any network $N = (V, E, s, t, c)$, any $s, t \in V$ such that $s \neq t$, and any st-flow f in N, the following three conditions are equivalent

1. *There exists an st-cut whose capacity is equal to φ_s.*
2. *The st-flow f is optimal, i.e., a solution of* (9)–(11)*.*
3. *No augmenting path of f exists.*

Proof.
(1) implies (2) by virtue of Lemma 7.
(2) implies (3) by virtue of Lemma 5.
We prove that (3) implies (1):

- Let f be an st-flow such that no augmenting path exists.
- Let S be the set of all nodes $v \in V$ such that there exists a path in the residual network w.r.t. f from s to v. Let S also include s itself.
- Then, $t \notin S$ (otherwise, the path from s to t in the residual network would be an augmenting path).
- Moreover, ...

- Moreover,

$$
\begin{aligned}
\varphi_s &= \sum_{v \in S} \varphi_v && \text{by (8) and } t \notin S \\
&= \varphi_S && \text{by Lemma 3} \\
&= \sum_{vw \in SS^c} f_{vw} - \sum_{vw \in S^c S} f_{vw} && \text{by definition of } \varphi_S \\
&= \sum_{vw \in SS^c} c_{vw} && \text{by the arguments below.}
\end{aligned}
$$

- For any $vw \in SS^c$, we have $f_{vw} = c_{vw}$ (otherwise, the contradiction $w \in S$ follows by construction of S and by definition of the residual network).
- For any $vw \in S^c S$, we have $f_{vw} = 0$ (otherwise, the contradiction $v \in S$ follows by construction of S and by definition of the residual network).

$\square$

Algorithm 1 (Ford and Fulkerson, 1956)

Input: *Network* $N = (V, E, s, t, c)$
Output: $f : E \to \mathbb{N}_0$
for all $vw \in E$
  $f_{vw} := 0$
while $\exists n \in \mathbb{N}$ $\exists$*augmenting path* $p = (v_1w_1, \ldots, v_nw_n)$ *of* f
  $\delta := \min_{vw \in p([n])} c'_{vw}$
  for all $vw \in E$

$$f_{vw} := \begin{cases} f_{vw} + \delta & \text{if } vw \in P \wedge vw \in E \\ f_{vw} - \delta & \text{if } vw \in P \wedge wv \in E \\ f_{vw} & \text{otherwise} \end{cases}$$

Theorem 2

Algorithm 1 terminates. The output f is a maximum st-flow in N.

Proof. Termination.

- For every augmenting path processed, φ_s increases by at least 1.
- Moreover,

$$\varphi_s \leq \sum_{vw \in \{s\}\{s\}^c} c_{vw} \qquad \text{(by Lemma 7)}$$

- Therefore, only finitely many augmenting paths are processed.
- Thus, the algorithm terminates.

Optimality:

- Throughout the execution, f is an st-flow in N.
- When the algorithm terminates, no augmenting path exists.
- Thus, f is a maximum st-flow in N (by Theorem 1).

Note: An implementation with runtime complexity $O(|E|\varphi_s)$ exists.

Ford and Fulkerson (1956) – $O(|E|\hat{\varphi}_s)$

- Dinic (1970) – $O(|V|^2|E|)$
- Edmonds and Karp (1972) – $O(|V||E|^2)$
- Sleator and Tarjan (1983, 1985) – $O(|V||E|\log|V|)$
- $\ldots$

Definition 12

For any network $N = (V, E, s, t, c)$ *and any* st*-preflow* f *in* N*,*
$h : V \to \mathbb{N}_0$ *is said to be* **compatible** *with* f *iff*

1. $h_s = |V|$ *and* $h_t = 0$
2. *For every edge* $vw \in E'$ *in the residual network* (V, E', s, t, c')*,* $h(v) \leq h(w) + 1$*.*

Algorithm 2 (Goldberg and Tarjan, 1986, 1988)

Input: *Network* $N = (V, E, s, t, c)$
Output: $f : E \to \mathbb{N}_0$
for all $vw \in E \quad f_{vw} := \begin{cases} c_{vw} & \text{if } v = s \\ 0 & \text{otherwise} \end{cases}$
for all $v \in V \quad h_v = \begin{cases} |V| & \text{if } v = s \\ 0 & \text{otherwise} \end{cases}$
while $\exists v \in V : \; v \neq t \wedge \varphi_v < 0$
  if $\exists w \in V : \; vw \in E' \wedge h_w < h_v$
    if $vw \in E$
      $f_{vw} := f_{vw} + \min\{-\varphi_v, c_{vw} - f_{vw}\}$
    else
      $f_{vw} := f_{vw} - \min\{-\varphi_v, f_{vw}\}$
  else
    $h_v := h_v + 1.$

Goldberg and Tarjan (1986, 1988) – $O(|V|^2 E)$

- FIFO node selection – $O(|V|^3)$
- highest node selection – $O(|V|^2 \sqrt{|E|})$
- Sleator and Tarjan (1983, 1985) – $O(|V||E| \log(|V|^2/|E|))$
- $\ldots$