

## 486 A Complete Proof

### 487 A.1 Maximum Independent Set

488 In maximum independent set, we use the energy function:

$$f(x) := - \sum_{i=1}^n w_i x_i + \sum_{(i,j) \in E} \beta_{ij} x_i x_j \quad (25)$$

489 We are going to prove the following proposition.

490 **Proposition A.1.** *If  $\beta_{ij} \geq \min\{w_i, w_j\}$  for all  $(i, j) \in E$ , then for any  $x \in \{0, 1\}^n$ , there exists a*  
 491  *$x' \in \{0, 1\}^n$  that satisfies the constraints in (16) and has lower energy:  $f(x') \leq f(x)$ .*

492 *Proof.* For arbitrary  $x \in \{0, 1\}^n$ , if  $x$  satisfies all constraints, we only need to let  $x' = x$ . Else, there  
 493 must exist an edge  $(i, j) \in E$ , such that  $x_i x_j = 1$ . Denote  $k = \arg \min\{w_i, w_j\}$ , we define  $x'_i = x_i$   
 494 if  $i \neq k$  and  $x'_k = 0$ . In this case, we have:

$$f(x') - f(x) = w_k - \sum_{j \in N(k)} \beta_{k,j} x_j \leq w_k (1 - \sum_{j \in N(k)} x_j) \leq 0 \quad (26)$$

495 Thus we show  $f(x') \leq f(x)$ .

496 On the other side, consider a graph  $G = (V = \{1, 2\}, E = \{(1, 2)\})$  and  $\beta_{12} < w_1 < w_2$ . Then the  
 497 maximum independent set is  $\{2\}$ , which can be represented by  $x = (0, 1)$ . However, in this case, let  
 498  $x' = (1, 1)$  is feasible while  $f(x') \leq f(x)$ . This means the condition we just derived is sharp.  $\square$

### 499 A.2 Maximum Clique

500 In maximum independent set, we use the energy function:

$$f(x) := - \sum_{i=1}^n w_i x_i + \sum_{(i,j) \in E^c} \beta_{ij} x_i x_j \quad (27)$$

501 We are going to prove the following proposition.

502 **Proposition A.2.** *If  $\beta_{ij} \geq \min\{w_i, w_j\}$  for all  $(i, j) \in E^c$ , then for any  $x \in \{0, 1\}^n$ , there exists a*  
 503  *$x' \in \{0, 1\}^n$  that satisfies the constraints in (18) and has lower energy:  $f(x') \leq f(x)$ .*

504 *Proof.* For arbitrary  $x \in \{0, 1\}^n$ , if  $x$  satisfies all constraints, we only need to let  $x' = x$ . Else,  
 505 there must exist an edge  $(i, j) \in E^c$ , such that  $x_i x_j = 1$ . Denote  $k = \arg \min\{w_i, w_j\}$ , we define  
 506  $x'_i = x_i$  if  $i \neq k$  and  $x'_k = 0$ . In this case, we have:

$$f(x') - f(x) = w_k - \sum_{j: (k,j) \in E^c} \beta_{k,j} x_j \leq w_k (1 - \sum_{j: (k,j) \in E^c} x_j) \leq 0 \quad (28)$$

507 Thus we show  $f(x') \leq f(x)$ .

508 On the other side, consider a graph  $G = (V = \{1, 2\}, E = \{\})$  and  $\beta_{12} < w_1 < w_2$ . Then the  
 509 maximum clique is  $\{2\}$ , which can be represented by  $x = (0, 1)$ . However, in this case, let  $x' = (1, 1)$   
 510 is feasible while  $f(x') \leq f(x)$ . This means the condition we just derived is sharp.  $\square$

### 511 A.3 Minimum Dominate Set

512 In maximum independent set, we use the energy function:

$$f(x) := \sum_{i=1}^n w_i x_i + \sum_{i=1}^n \beta_i (1 - x_i) \prod_{j \in N(i)} (1 - x_j) \quad (29)$$

513 We are going to prove the following proposition.

514 **Proposition A.3.** *If  $\beta_i \geq \min_k \{w_k : k \in N(i) \text{ or } k = i\}$ , then for any  $x \in \{0, 1\}^n$ , there exists a*  
 515  *$x' \in \{0, 1\}^n$  that satisfies the constraints in (18) and has lower energy:  $f(x') \leq f(x)$ .*

516 *Proof.* For arbitrary  $x \in \{0, 1\}^n$ , if  $x$  satisfies all constraints, we only need to let  $x' = x$ . Else, there  
 517 must exist a node  $t \in V$ , such that  $x_t = 0$  and  $x_j = 0$  for all  $j \in N(t)$ . Let  $k = \arg \min\{w_j : j \in$   
 518  $N(t), \text{ or } j = t\}$ , we define  $x'_i = x_i$  if  $i \neq k$  and  $x'_k = 1$ . In this case, we have:

$$f(x') - f(x) = w_k - \beta_t + \sum_{i \neq t} \beta_i \left[ (1 - x'_i) \prod_{j \in N(i)} (1 - x'_j) - (1 - x_i) \prod_{j \in N(i)} (1 - x_j) \right] \leq 0 \quad (30)$$

519 Thus, we prove  $f(x') \leq f(x)$ .

520 On the other side, consider a graph  $G = (V = \{1\}, E = \{\})$  and  $\beta_1 < w_1$ . Then the maximum  
 521 clique is  $\{1\}$ , which can be represented by  $x = (1)$ . However, in this case, let  $x' = (0)$  is feasible  
 522 while  $f(x') \leq f(x)$ . This means the condition we just derived is sharp.  $\square$

## 523 A.4 Minimum Cut

524 In maximum independent set, we use the energy function:

$$f(x) := \sum_{(i,j) \in E} x_i(1 - x_j)w_{ij} + \beta \left( \sum_{i=1}^n d_i x_i - D_1 \right)_+ + \beta \left( D_0 - \sum_{i=1}^n d_i x_i \right)_+ \quad (31)$$

525 We are going to prove the following proposition.

526 **Proposition A.4.** *If  $\beta \geq \max_i \{\sum_{j \in N(i)} |w_{i,j}|\}$ , then any  $x \in \{0, 1\}^n$ , there exists a  $x' \in \{0, 1\}^n$*   
 527 *that satisfies the constraints in (18) and has lower energy:  $f(x') \leq f(x)$ .*

## 528 B Experiment Details

### 529 B.1 Hardware

530 All methods were run on Intel(R) Xeon(R) Gold 5215 CPU @ 2.50GHz, with 377GB of available  
 531 RAM. The neural networks were executed on a single RTX6000 25GB graphics card. The code was  
 532 executed on version 1.9.0 of PyTorch and version 1.7.2 of PyTorch Geometric.