Appendix A. DRO reformulation via the MILP in Naderi et al. (2014)

In this section, the DRO model transformation based on the MILP formulation proposed in Naderi et al. (2014) is demonstrated. And as the DRO model is a min-max-min form, we also prove that the dual of the inner max problem with mixed integer variables is essentially a linear programming problem, based on the totally unimodularity. However, we also show that the DRO version of the underlined model could not be reformulated as a MILP, as the inner min-max structure of the DRO problem is difficult, if not impossible, to process.

To construct the DRO model based on the MILP formulation mentioned in Naderi et al. (2014), the related symbols are listed in Table A.1.

Table A.1: Notations of decision variables and parameters

Symbol	Notation
$C_{s,j}$	continuous variable which indicates the completion time of job j at stage s.
$X_{s,j,k}$	binary variable equals 1 if job k is processed before job j at stage s, and 0 otherwise.
$Y_{s,l,j}$	binary variable equals 1 if job j is processed at stage s on machine l, and 0 otherwise.
C_{max}	continuous variable which indicates the makespan.
$p_{s,j}$	continuous variable which indicates processing time of job j at stage s.

As it is shown below, a MILP model is built in (A.1) for the two-stage hybrid flow shop scheduling problem, which is characterized by having only one machine in the first stage and m machines in the second stage.

$$\min \quad C_{max} \tag{A.1a}$$

$$\text{s.t.} \quad Y_{1,1,j} = 1 \quad j = 1, \ldots, n \tag{A.1b}$$

$$\sum_{l=1}^{m} Y_{2,l,j} = 1 \quad j = 1, \ldots, n \tag{A.1c}$$

$$C_{s,j} - C_{s-1,j} \geq p_{s,j} \quad s = 1, 2; j = 1, \ldots, n \tag{A.1d}$$

$$C_{1,j} \geq C_{1,k} + p_{1,j} - M(1 - x_{1,j,k}) \quad j = 1, \ldots, n-1; k = j+1, \ldots, n \tag{A.1e}$$

$$C_{2,j} \geq C_{2,k} + p_{2,j} - M(3 - X_{2,j,k} - Y_{2,l,j} - Y_{2,l,k})$$
$$l = 1, \ldots, m; j = 1, \ldots, n-1; k = j+1, \ldots, n \tag{A.1f}$$
$$C_{1,k} \geq C_{1,j} + p_{1,k} - MX_{1,j,k} \quad j = 1, \ldots, n-1; k = j+1, \ldots, n \tag{A.1g}$$
$$C_{2,k} \geq C_{2,j} + p_{2,k} - MX_{2,j,k} - M(2 - Y_{2,l,j} - Y_{2,l,k})$$
$$l = 1, \ldots, m; j = 1, \ldots, n-1; k = j+1, \ldots, n \tag{A.1h}$$
$$C_{max} \geq C_{2,j} \quad j = 1, \ldots, n \tag{A.1i}$$
$$C_{1,j}, C_{2,j} \geq 0 \quad j = 1, \ldots, n \tag{A.1j}$$
$$C_{0,j} = 0 \quad j = 1, \ldots, n. \tag{A.1k}$$

where the objective function (A.1a) aims to minimize the makespan. Constraints (A.1b) and (A.1c) guarantee that each job can only be processed on one machine in each stage. Constraint (A.1d) ensures that the processing of jobs in the second stage can only be carried out after the processing in the first stage is completed. Constraints (A.1e), (A.1f), (A.1g), and (A.1h) collectively determine that two jobs cannot be processed simultaneously on the same machine, and jobs processed on the same machine should wait for the previous job's completion. M represents an arbitrarily large number. Constraint (A.1i) defines the completion time. And constraints (A.1j) and (A.1k) define the variables.

The uncertain job processing time $\tilde{\boldsymbol{p}}$ is defined in the ambiguity set $\mathbb{F}$ in the manuscript with known statistical features. And the DRO model is formulated as the following min-max problem,

$$(DRO) \qquad \min_{\substack{\boldsymbol{X} \in \mathbb{X} \\ \boldsymbol{Y} \in \mathbb{Y}}} \sup_{\mathbb{P} \in \mathbb{F}} \mathbb{E}_{\mathbb{P}}[H(\boldsymbol{X}, \boldsymbol{Y}, \tilde{\boldsymbol{p}})] \tag{A.2}$$

For fixed $\boldsymbol{X}$ and $\boldsymbol{Y}$, the inner problem $\sup_{\mathbb{P} \in \mathbb{F}} \mathbb{E}_{\mathbb{P}}[H(\boldsymbol{X}, \boldsymbol{Y}, \tilde{\boldsymbol{p}})]$ of the DRO model is a maximization problem with $\mathbb{P}$ as the decision variable. And the maximization problem is formulated as the following LP model,

$$\sup \int_{\mathcal{D}_{\tilde{\boldsymbol{p}}}} H(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{p}) d\mathbb{P} \tag{A.3a}$$
$$\text{s.t.} \int_{\mathcal{D}_{\tilde{\boldsymbol{p}}}} p_{1,j} d\mathbb{P} = \mu_{1,j}, \qquad j = 1, \ldots, n \tag{A.3b}$$

$$\int_{\mathcal{D}_{\tilde{\boldsymbol{p}}}} p_{2,j} d\mathbb{P} = \mu_{2,j}, \qquad j = 1, \dots, n \tag{A.3c}$$

$$\int_{\mathcal{D}_{\tilde{\boldsymbol{p}}}} d\mathbb{P} = 1 \tag{A.3d}$$

$$d\mathbb{P} \geq 0 \tag{A.3e}$$

Let $v_{1,j}$, $v_{2,j}$ and ν_0 be the dual variables associated with constraints (A.3b), (A.3c) and (A.3d), respectively. The dual model of problem (A.3) is shown as below,

$$\inf_{\boldsymbol{v},\boldsymbol{\nu}} \sum_{j=1}^{n} v_{1,j}\mu_{1,j} + \sum_{j=1}^{n} v_{2,j}\mu_{2,j} + \nu_0 \tag{A.4a}$$

$$\text{s.t. } \sum_{j=1}^{n} v_{1,j}p_{1,j} + \sum_{j=1}^{n} v_{2,j}p_{2,j} + \nu_0 \geq H(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{p}), \forall \boldsymbol{p} \in \mathcal{D}_{\tilde{\boldsymbol{p}}} \tag{A.4b}$$

Furthermore, for fixed $v_{1,j}$ and $v_{2,j}$, constraint (A.4b) is equivalent to,

$$\nu_0 \geq \max_{\boldsymbol{p}\in\mathcal{D}_{\tilde{\boldsymbol{p}}}} \left\{ H(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{p}) - \sum_{j=1}^{n} v_{1,j}p_{1,j} + \sum_{j=1}^{n} v_{2,j}p_{2,j} \right\} \tag{A.5}$$

Note that the right hand side of inequality (A.5) is a max-min problem, since $H(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{p})$ is a minimization problem. Then with given $\boldsymbol{X}$, $\boldsymbol{Y}$ and $\boldsymbol{p}$, its dual form is presented in Proposition A.1.

Proposition A.1. *For the fixed sequences $\boldsymbol{X}$, $\boldsymbol{Y}$ and $\boldsymbol{p} \in \mathcal{D}_{\tilde{p}}$, the optimal value of $H(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{p})$ in problem* (A.1) *is equivalent to*

$$\begin{aligned} \max_{\boldsymbol{\vartheta},\boldsymbol{\psi},\boldsymbol{\omega},\boldsymbol{\sigma},\boldsymbol{\zeta},\boldsymbol{\tau}} & \sum_{j=1}^{n} (p_{1,j}\vartheta_{1,j} + p_{2,j}\vartheta_{2,j}) + \sum_{j=1}^{n-1} \sum_{k=j+1}^{n} \psi_{j,k}[p_{1,j} - M(1 - X_{1,j,k})] \\ & + \sum_{j=1}^{n-1} \sum_{k=j+1}^{n} \sum_{l=1}^{m} \omega_{j,k,l}[p_{2,j} - M(3 - X_{2,j,k} - Y_{2,l,j} - Y_{2,l,k})] + \sum_{j=1}^{n-1} \sum_{k=j+1}^{n} \sigma_{j,k}(p_{1,k} - MX_{1,j,k}) \\ & + \sum_{j=1}^{n-1} \sum_{k=j+1}^{n} \sum_{l=1}^{m} \zeta_{j,k,l}[p_{2,k} - MX_{2,j,k} - M(2 - Y_{2,l,j} - Y_{2,l,k})] \end{aligned} \tag{A.6a}$$

$$s.t. \quad \vartheta_{1,j} - \vartheta_{2,j} - \sum_{a=1}^{j-1} \psi_{a,j} + \sum_{k=j+1}^{n} \psi_{j,k} - \sum_{k=j+1}^{n} \sigma_{j,k} + \sum_{a=1}^{j-1} \sigma_{a,j} \leq 0 \quad j = 1, \dots, n. \tag{A.6b}$$

$$\vartheta_{2,j} - \sum_{a=1}^{j-1}\sum_{l=1}^{m}\omega_{a,j,l} + \sum_{k=j+1}^{n}\sum_{l=1}^{m}\omega_{j,k,l} - \sum_{k=j+1}^{n}\sum_{l=1}^{m}\zeta_{j,k,l} + \sum_{a=1}^{j-1}\sum_{l=1}^{m}\zeta_{a,j,l} - \tau_j \leq 0 \qquad j = 1, \ldots, n. \tag{A.6c}$$

$$\sum_{j=1}^{n} y_j \leq 1 \tag{A.6d}$$

$$\boldsymbol{\vartheta}, \boldsymbol{\psi}, \boldsymbol{\omega}, \boldsymbol{\sigma}, \boldsymbol{\zeta}, \boldsymbol{\tau} \geq 0 \tag{A.6e}$$

Proof. Let $\boldsymbol{\vartheta}, \boldsymbol{\psi}, \boldsymbol{\omega}, \boldsymbol{\sigma}, \boldsymbol{\zeta}, \boldsymbol{\tau}$ be the dual variables of constraints (A.1d), (A.1e), (A.1f), (A.1g), (A.1h), (A.1i) respectively. According to the duality theory, the dual model of (A.1) is shown as (A.6). □

Based on Proposition A.1, the right hand side of inequality (A.5) can be reformulated as below,

$$\max_{\substack{\boldsymbol{\vartheta},\boldsymbol{\psi},\boldsymbol{\omega},\boldsymbol{\sigma},\boldsymbol{\zeta},\boldsymbol{\tau}\\ \boldsymbol{p}}} \left\{ \text{(A.6a)} - \sum_{j=1}^{n} v_{1,j} p_{1,j} + \sum_{j=1}^{n} v_{2,j} p_{2,j} \right\}$$

In order to transform the min-max-min problem into a MILP model, problem (A.6) needs to be reformulated as an unconstrained problem, that is, the pattern of the dual variables should be established. However, it turns out that the exploration might not be always fruitful.

In Proposition A.2, it is proved that problem (A.6) is a LP model with all its dual variables integers.

Proposition A.2. *The dual variables in problem* (A.6) *are all integers.*

Proof. The constraints of problem (A.6), i.e., (A.6b)-(A.6e), can be written in the matrix form as below,

$$\begin{pmatrix} \boldsymbol{I}_{n\times n} & -\boldsymbol{I}_{n\times n} & \boldsymbol{\Psi}_{n\times\frac{n^2-n}{2}} & \boldsymbol{0}_{n\times\frac{m(n^2-n)}{2}} & \boldsymbol{\Sigma}_{n\times\frac{n^2-n}{2}} & \boldsymbol{0}_{n\times\frac{m(n^2-n)}{2}} & \boldsymbol{0}_{n\times n} \\ \boldsymbol{0}_{n\times n} & \boldsymbol{I}_{n\times n} & \boldsymbol{0}_{n\times\frac{n^2-n}{2}} & \boldsymbol{\Omega}_{n\times\frac{m(n^2-n)}{2}} & \boldsymbol{0}_{n\times\frac{n^2-n}{2}} & \boldsymbol{\Delta}_{n\times\frac{m(n^2-n)}{2}} & -\boldsymbol{I}_{n\times n} \end{pmatrix} \begin{pmatrix} \boldsymbol{\vartheta} \\ \boldsymbol{\psi} \\ \boldsymbol{\omega} \\ \boldsymbol{\sigma} \\ \boldsymbol{\zeta} \\ \boldsymbol{\tau} \end{pmatrix} \leq \begin{pmatrix} \boldsymbol{0}_{n\times 1} \\ \boldsymbol{0}_{n\times 1} \end{pmatrix}$$

where $\boldsymbol{\vartheta} = (\vartheta_{s,j})_{s=1,2,j=1,\ldots,n}$, $\boldsymbol{\psi} = (\psi_{j,k})_{j=1,\ldots,n-1,k=j+1,\ldots,n}$, $\boldsymbol{\omega} = (\omega_{j,k,l})_{j=1,\ldots,n-1,k=j+1,\ldots,n,l=1,\ldots,m}$,$\boldsymbol{\sigma} = (\sigma_{j,k})_{j=1,\ldots,n-1,k=j+1,\ldots,n}$, $\boldsymbol{\zeta} = (\zeta_{j,k,l})_{j=1,\ldots,n-1,k=j+1,\ldots,n,l=1,\ldots,m}$, $\boldsymbol{\tau} = (\tau_j)_{j=1,\ldots,n}$.

And, we define

$$\boldsymbol{I}_{n\times n} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}_{n\times n}$$

$$\boldsymbol{\Psi}_{n\times\frac{n^2-n}{2}} = \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 & 0 & 0 & 0 & \cdots & 0 & \cdots & 0 \\ -1 & 0 & 0 & \cdots & 0 & 1 & 1 & 1 & \cdots & 1 & \cdots & 0 \\ 0 & -1 & 0 & \cdots & 0 & -1 & 0 & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \cdots & \vdots \\ \underbrace{0 \quad 0 \quad 0 \quad \cdots \quad -1}_{n\times(n-1)} & & & & & \underbrace{0 \quad 0 \quad 0 \quad \cdots \quad -1}_{n\times(n-1)} & & & & & \underbrace{\cdots}_{n\times\frac{n^2-5n+4}{2}} & -1 \end{pmatrix}_{n\times\frac{n^2-n}{2}}$$

$$\boldsymbol{\Sigma}_{n\times\frac{n^2-n}{2}} = \begin{pmatrix} -1 & -1 & -1 & \cdots & -1 & 0 & 0 & 0 & \cdots & 0 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & 0 & -1 & -1 & -1 & \cdots & -1 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 & 1 & 0 & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \cdots & \vdots \\ \underbrace{0 \quad 0 \quad 0 \quad \cdots \quad 1}_{n\times(n-1)} & & & & & \underbrace{0 \quad 0 \quad 0 \quad \cdots \quad 1}_{n\times(n-2)} & & & & & \underbrace{\cdots}_{n\times\frac{n^2-5n+4}{2}} & 1 \end{pmatrix}_{n\times\frac{n^2-n}{2}}$$

$$
\mathbf{\Omega}_{n\times\frac{m(n^2-n)}{2}} =
$$

$$
\begin{pmatrix}
\mathbf{1}_m & \mathbf{1}_m & \mathbf{1}_m & \cdots & \mathbf{1}_m & \mathbf{0}_m & \mathbf{0}_m & \mathbf{0}_m & \cdots & \mathbf{0}_m & \cdots & \mathbf{0}_m \\
-\mathbf{1}_m & \mathbf{0}_m & \mathbf{0}_m & \cdots & \mathbf{0}_m & \mathbf{1}_m & \mathbf{1}_m & \mathbf{1}_m & \cdots & \mathbf{1}_m & \cdots & \mathbf{0}_m \\
\mathbf{0}_m & -\mathbf{1}_m & \mathbf{0}_m & \cdots & \mathbf{0}_m & -\mathbf{1}_m & \mathbf{0}_m & \mathbf{0}_m & \cdots & \mathbf{0}_m & \cdots & \mathbf{0}_m \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \cdots & \vdots \\
\mathbf{0}_m & \mathbf{0}_m & \mathbf{0}_m & \cdots & -\mathbf{1}_m & \mathbf{0}_m & \mathbf{0}_m & \mathbf{0}_m & \cdots & -\mathbf{1}_m & \cdots & -\mathbf{1}_m \\
 & & \underbrace{\qquad\qquad}_{n\times m(n-1)} & & & & & \underbrace{\qquad\qquad}_{n\times m(n-2)} & & & \underbrace{}_{n\times\frac{m(n^2-5n+4)}{2}} &
\end{pmatrix}_{n\times\frac{m(n^2-n)}{2}}
$$

$$
\mathbf{\Delta}_{n\times\frac{m(n^2-n)}{2}} =
$$

$$
\begin{pmatrix}
-\mathbf{1}_m & -\mathbf{1}_m & -\mathbf{1}_m & \cdots & -\mathbf{1}_m & \mathbf{0}_m & \mathbf{0}_m & \mathbf{0}_m & \cdots & \mathbf{0}_m & \cdots & \mathbf{0}_m \\
\mathbf{1}_m & \mathbf{0}_m & \mathbf{0}_m & \cdots & \mathbf{0}_m & -\mathbf{1}_m & -\mathbf{1}_m & -\mathbf{1}_m & \cdots & -\mathbf{1}_m & \cdots & \mathbf{0}_m \\
\mathbf{0}_m & \mathbf{1}_m & \mathbf{0}_m & \cdots & \mathbf{0}_m & \mathbf{1}_m & \mathbf{0}_m & \mathbf{0}_m & \cdots & \mathbf{0}_m & \cdots & \mathbf{0}_m \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \cdots & \vdots \\
\mathbf{0}_m & \mathbf{0}_m & \mathbf{0}_m & \cdots & \mathbf{1}_m & \tilde{\mathbf{0}}_m & \mathbf{0}_m & \mathbf{0}_m & \cdots & \mathbf{1}_m & \cdots & \mathbf{1}_m \\
 & & \underbrace{\qquad\qquad}_{n\times m(n-1)} & & & & & \underbrace{\qquad\qquad}_{n\times m(n-2)} & & & \underbrace{}_{n\times\frac{m(n^2-5n+4)}{2}} &
\end{pmatrix}_{n\times\frac{m(n^2-n)}{2}}
$$

where $\boldsymbol{z}_m$ represents a m-dimensional row vector with each element being z.

As it is shown in Hoffman (1979), a (0, 1, -1) matrix A is totally unimodular if it contains no more than one 1 and no more than one -1 in each column. For that reason, it is easy to see that the coefficient matrix consists only of 0, 1, and -1, and each column contains at most one 1 and at most one -1. Therefore, the matrix is totally unimodular, which indicates that the optimal values of the dual variables are integers. $\square$

Through the aforementioned Proposition 1 and Proposition 2, we have demonstrated that the dual variables of the dual problem A.6 are all binary variables, taking values of 0 or 1. Building upon this characteristic, we aim to reformulate the dual problem into an unconstrained problem. This reformulation is essential because only by doing so can we effectively eliminate the maximization problem on the right-hand side of inequality (A.5), thereby converting the min-max problem, i.e., Model (A.4), into a tractable minimization problem.

However, difficulties are encountered while transforming the dual model (A.6) into an unconstrained problem, which is specifically manifested as the difficulty in exploring the pattern among the six dual variables. This conundrum may be attributed to the relatively large number of dual variables, especially with the existence of two three-index dual variables $\boldsymbol{\omega}$ and $\boldsymbol{\zeta}$. Since it is cumbersome, if not impossible, to transform the dual problem (A.6) into an unconstrained model, it directly leads to the dead-end of the DRO model tractable transformation. As for the P2, P3, and P4 models in Fernandez-Viagas et al. (2019), more constraints are involved, for instance, the added scheduling rules. And hence, the corresponding dual variables in the dual model are more difficult to eliminate, which renders these models unsuitable for the equivalent reformulation of their DRO counterparts.

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