Efficient Design Optimization over Mixed-Combinatorial Spaces Enabled by Graph-learning: Supplement Material

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1 *cvxnonsep_psig20* Equation[1]

The objective function for the benchmark problem is defined as:

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\begin{aligned}
&\min_{\mathbf{Z}_{\text{comb}}, \mathbf{X}_{\text{cont}}} \quad f(\mathbf{Z}_{\text{comb}}, \mathbf{X}_{\text{cont}}) \\
&\text{where} \quad f = 20000 \cdot z_1^{-0.32} \cdot z_2^{-0.19} \cdot z_3^{-0.405} \cdot z_4^{-0.265} \cdot z_5^{-0.175} \cdot z_6^{-0.44} \cdot z_7^{-0.275} \cdot z_8^{-0.47} \cdot z_9^{-0.31} \cdot z_{10}^{-0.295} \\
&\qquad \cdot x_1^{-0.105} \cdot x_2^{-0.15} \cdot x_3^{-0.235} \cdot x_4^{-0.115} \cdot x_5^{-0.42} \cdot x_6^{-0.095} \cdot x_7^{-0.115} \cdot x_8^{-0.085} \cdot x_9^{-0.115} \cdot x_{10}^{-0.22} \\
&\qquad + z_1 + z_2 + z_3 + z_4 + z_5 + z_6 + z_7 + z_8 + z_9 + z_{10} \\
&\qquad + x_1 + x_2 + x_3 + x_4 + x_5 + x_6 + x_7 + x_8 + x_9 + x_{10} \\
&\mathbf{Z}_{\text{comb}} = \begin{bmatrix} z_1 & z_2 & \dots & z_{10} \end{bmatrix} \\
&\mathbf{X}_{\text{cont}} = \begin{bmatrix} x_1 & x_2 & \dots & x_{10} \end{bmatrix} \\
&1 \leq x_i \leq 10, \forall\ i = 1, 2, \dots, 10 \\
&\mathbf{Z}_{\text{comb}} \in \mathbb{Z}
\end{aligned}
$$

where f is the objective function, $\mathbf{Z}_{\text{comb}}$ is the combination represented by a vector that contains ten integer variables, $\mathbb{Z}$ is the valid combination set and its content is listed in combination_set_101.csv, $\mathbf{X}_{\text{cont}}$ is the continuous variable vector.

The original problem statement is from the following link: `https://www.minlplib.org/cvxnonsep_psig20.html`

2 GNN-ReCo Structure

Layer	Operation	Output Shape
Input	$\mathbf{Z}_{\text{batch}} = [\mathbf{Z}_1, \mathbf{Z}_2, \dots, \mathbf{Z}_{\text{batch\_size}}]$ $\mathbf{X}_{\text{batch}} = [\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_{\text{batch\_size}}]$	batch_size $\times\ n_{\text{sn}} \times k_{\text{comb}}$ batch_size $\times\ k_{\text{cont}}$
Concatenation	$\mathbf{x} = \text{concat}(\mathbf{Z}_{\text{batch}}, \mathbf{X}_{\text{batche}})$	batch_size $\times\ n_{\text{sn}} \times (k_{\text{comb}} + k_{\text{cont}})$
Conv1	$\mathbf{x} = \text{DenseGCNConv}(\mathbf{x}, \mathbf{E}_{\text{batch}})$	batch_size $\times\ n_{\text{sn}} \times (96)$
ReLU	$\mathbf{x} = \text{ReLU}(\mathbf{x})$	Same as above
Conv2	$\mathbf{x} = \text{DenseGCNConv}(\mathbf{x}, \mathbf{E}_{\text{batch}})$	batch_size $\times\ n_{\text{sn}} \times (48)$
ReLU	$\mathbf{x} = \text{ReLU}(\mathbf{x})$	Same as above
FC	$\mathbf{y} = \text{Linear}(\mathbf{x})$	batch_size $\times\ n_{\text{sn}} \times 1$
Output	$\mathbf{y}$ (reshaped)	batch_size $\times\ n_{\text{sn}}$

The inputs are normalized before sending to the GNN.

Table 1: GNN-ReCo Architecture

References

[1] Jan Kronqvist, Andreas Lundell, and Tapio Westerlund. Convex minlp test problems with non-separable nonlinear functions, 2017. Accessed: 2025-03-17.