A Supplementary Material for Interior Point Solving for LP-based prediction+optimisation

A.1 Solution of Newton Equation System of Eq. (11)

Here we discuss how we solve an equation system of Eq (11), for more detail you can refer to[4]. Consider the following system with a generic R.H.S-

$$\begin{bmatrix} -X^{-1}T & A^\top & -c \\ A & 0 & -b \\ -c^\top & b^\top & \kappa/\tau \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} \tag{13}$$

If we write:

$$W \doteq \begin{bmatrix} -X^{-1}T & A^\top \\ A & 0 \end{bmatrix} \tag{14}$$

then, observe W is nonsingular provided A is full row rank. So it is possible to solve the following system of equations-

$$\begin{aligned} W \begin{bmatrix} p \\ q \end{bmatrix} &= \begin{bmatrix} c \\ b \end{bmatrix} \\ W \begin{bmatrix} u \\ v \end{bmatrix} &= \begin{bmatrix} r_1 \\ r_2 \end{bmatrix} \end{aligned} \tag{15}$$

Once we find p, q, u, v finally we compute x_3 as:

$$x_3 = \frac{r_3 + u^\top c - v^\top b}{-c^\top p + b^\top q + \frac{\kappa}{\tau}}; \tag{16}$$

And finally

$$x_1 = u + p x_3 \tag{17}$$

$$x_2 = v + q x_3 \tag{18}$$

To solve equation of the form

$$W \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} -X^{-1}T & A^\top \\ A & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \end{bmatrix}$$

Notice we can reduce it to $Mv = AT^{-1}Xr_1 + r_2$ (where $M = AT^{-1}XA^\top$). As M is positive definite for a full row-rank A, we obtain v by Cholesky decomposition and finally $u = T^{-1}X(A^\top v - r_1)$.

A.2 Differentiation of HSD formulation in Eq. (9)

We differentiate Eq. (9) with respect to c:

$$\begin{aligned} \frac{\partial (Ax)}{\partial c} - \frac{\partial (b\tau)}{\partial c} &= 0 \\ \frac{\partial (A^\top y)}{\partial c} + \frac{\partial t}{\partial c} - \frac{\partial (c\tau)}{\partial c} &= 0 \\ -\frac{\partial (c^\top x)}{\partial c} + \frac{\partial (b^\top y)}{\partial c} - \frac{\partial \kappa}{\partial c} &= 0 \\ \frac{\partial t}{\partial c} &= \frac{\partial (\lambda X^{-1} e)}{\partial c} \\ \frac{\partial \kappa}{\partial c} &= \frac{\partial (\frac{\lambda}{\tau})}{\partial c} \end{aligned} \tag{19}$$

Applying the product rule we can further rewrite this into:

$$\begin{aligned} A\frac{\partial x}{\partial c} - b\frac{\partial \tau}{\partial c} &= 0 \\ A^\top \frac{\partial y}{\partial c} + \frac{\partial t}{\partial c} - (c\frac{\partial \tau}{\partial c} + \tau I) &= 0 \\ -(c^\top \frac{\partial x}{\partial c} + x^\top) + b^\top \frac{\partial y}{\partial c} - \frac{\partial \kappa}{\partial c} &= 0 \\ \frac{\partial t}{\partial c} &= -\lambda X^{-2}\frac{\partial x}{\partial c} \\ \frac{\partial \kappa}{\partial c} &= -\frac{\lambda}{\tau^2}\frac{\partial \tau}{\partial c} \end{aligned} \tag{20}$$

Using $t = \lambda X^{-1}e \leftrightarrow \lambda e = XTe$ we can rewrite the fourth equation to $\frac{\partial t}{\partial c} = -X^{-1}T\frac{\partial x}{\partial c}$. Similarly we use $\kappa = \frac{\lambda}{\tau} \leftrightarrow \lambda = \kappa \times \tau$ and rewrite the fifth equation to $\frac{\partial \kappa}{\partial c} = -\frac{\kappa}{\tau}\frac{\partial \tau}{\partial c}$. Substituting these into the first three we obtain:

$$\begin{aligned} A\frac{\partial x}{\partial c} - b\frac{\partial \tau}{\partial c} &= 0 \\ A^\top \frac{\partial y}{\partial c} - X^{-1}T\frac{\partial x}{\partial c} - c\frac{\partial \tau}{\partial c} - \tau I &= 0 \\ -c^\top \frac{\partial x}{\partial c} - x^\top + b^\top \frac{\partial y}{\partial c} + \frac{\kappa}{\tau}\frac{\partial \tau}{\partial c} &= 0 \end{aligned} \tag{21}$$

This formulation is written in matrix form in Eq. (12).

A.3 LP formulation of the Experiments

A.3.1 Details on Knapsack formulation of real estate investments

In this problem, H is the set of housings under consideration. For each housing h, c_h is the known construction cost of the housing and p_h is the (predicted) sales price. With the limited budget B, the constraint is

$$\sum_{h \in H} c_h x_h = B, \; x_h \in 0, 1$$

where x_h is 1 only if the investor invests in housing h. The objective function is to maximize the following profit function

$$\max_{x_h} \sum_{h \in H} p_h x_h$$

A.3.2 Details on Energy-cost aware scheduling

In this problem J is the set of tasks to be scheduled on M number of machines maintaining resource requirement of R resources. The tasks must be scheduled over T set of equal length time periods. Each task j is specified by its duration d_j, earliest start time e_j, latest end time l_j, power usage $p_j.u_{jr}$ is the resource usage of task j for resource r and c_{mr} is the capacity of machine m for resource r. Let x_{jmt} be a binary variable which possesses 1 only if task j starts at time t on machine m. The first constraint ensures each task is scheduled and only once.

$$\sum_{m \in M} \sum_{t \in T} x_{jmt} = 1 \;, \forall_{j \in J}$$

The next constraints ensure the task scheduling abides by earliest start time and latest end time constraints.

$$\begin{aligned} x_{jmt} &= 0 \;\; \forall_{j \in J} \forall_{m \in M} \forall_{t < e_j} \\ x_{jmt} &= 0 \;\; \forall_{j \in J} \forall_{m \in M} \forall_{t + d_j > l_j} \end{aligned}$$

Finally the resource requirement constraint:

$$\sum_{j \in J} \sum_{t - d_j < t' \le t} x_{jmt'} u_{jr} \le c_{mr}, \forall_{m \in M} \forall_{r \in R} \forall_{t \in T}$$

If c_t is the (predicted) energy price at time t, the objective is to minimize the energy cost of running all tasks, given by:

$$\min_{x_{jmt}} \sum_{j \in J} \sum_{m \in M} \sum_{t \in T} x_{jmt} \Big(\sum_{t \leq t' < t + d_j} p_j c_{t'} \Big)$$

A.3.3 Details on Shortest path problem

In this problem, we consider a directed graph specified by node-set N and edge-set E. Let A be the $|N| \times |E|$ incidence matrix, where for an edge e that goes from n_1 to n_2, the $(n_1, e)^{\text{th}}$ entry is 1 and $(n_2, e)^{\text{th}}$ entry is -1 and the rest of entries in column e are 0. In order to, traverse from source node s to destination node d, the following constraint must be satisfied:

$$Ax = b$$

where x is $|E|$ dimensional binary vector whose entries would be 1 only if corresponding edge is selected for traversal and b is $|N|$ dimensional vector whose s^{th} entry is 1 and d^{th} entry is -1; and rest are 0. With respect to the (predicted) cost vector $c \in \mathbb{R}^{|E|}$, the objective is to minimize the cost

$$\min_x c^\top x$$

A.4 Additional Knapsack Experiments

This knapsack experiment is taken from [18], where the knapsack instances are created from the energy price dataset 15. The 48 half-hour slots are considered as 48 knapsack items and a random cost is assigned to each slot. The energy price of a slot is considered as the profit-value and the objective is to select a set of slots which maximizes the profit ensuring the total cost of the selected slots remains below a fixed budget. We also added the approach of Blackbox [25], which also deals with a combinatorial optimization problem with a linear objective.

Budget	Two-stage	QPTL	SPO	Blackbox	IntOpt
60	1042 (3)	579 (3)	624 (3)	533 (40)	570 (58)
120	1098 (5)	380 (2)	425 (4)	383 (14)	406 (71)

A.5 Hyperparameters of the experiments [2]

A.5.1 Knapsack formulation of real estate investments

Model	Hyperaprameters*
Two-stage	• optimizer: optim.Adam; learning rate: 10^{-3}
SPO	• optimizer: optim.Adam; learning rate: 10^{-3}
QPTL	• optimizer: optim.Adam; learning rate: 10^{-3}; τ (quadratic regularizer): 10^{-5}
IntOpt	• optimizer: optim.Adam; learning rate: 10^{-2}; λ-cut-off: 10^{-4}; damping factor α: 10^{-3}

* for all experiments embedding size: 7 number of layers:1,hidden layer size: 2

A.5.2 Energy-cost aware scheduling

Model	Hyperaprameters
Two-stage	• optimizer: optim.SGD; learning rate: 0.1
SPO	• optimizer: optim.Adam; learning rate: 0.7
QPTL	• optimizer: optim.Adam; learning rate: 0.1; τ (quadratic regularizer): 10^{-5}
IntOpt	• optimizer: optim.Adam; learning rate: 0.7; λ-cut-off: 0.1; damping factor α: 10^{-6}

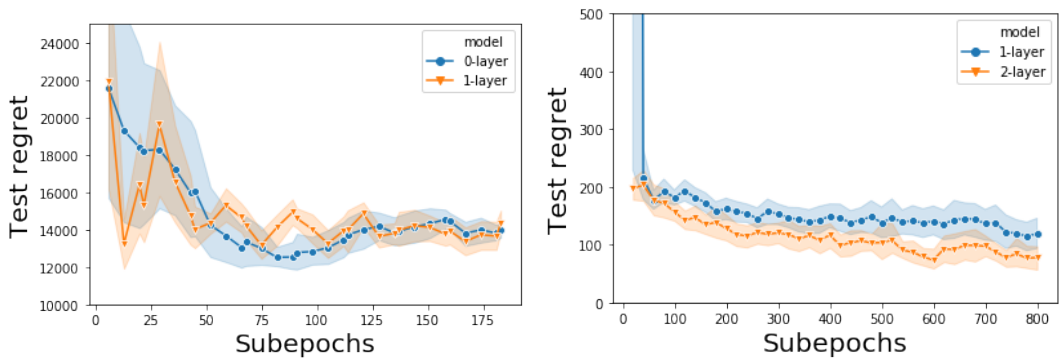
[2]For more details refer to https://github.com/JayMan91/NeurIPSIntopt

A.5.3 Shortest path problem

Model		Hyperaprameters*
Two-stage	1-layer	• optimizer: optim.Adam; learning rate: 0.01
	2-layer	• optimizer: optim.Adam; learning rate: 10^{-4}
SPO	1-layer	• optimizer: optim.Adam; learning rate: 10^{-3}
	2-layer	• optimizer: optim.Adam; learning rate: 10^{-3}
QPTL	1-layer	• optimizer: optim.Adam; learning rate: 0.7; τ (quadratic regularizer): 10^{-1}
	2-layer	• optimizer: optim.Adam; learning rate: 0.7; τ (quadratic regularizer): 10^{-1}
IntOpt	1-layer	• optimizer: optim.Adam; learning rate: 0.7; λ-cut-off: 0.1; damping factor α: 10^{-2}
	2-layer	• optimizer: optim.Adam; learning rate: 0.7; λ-cut-off: 0.1; damping factor α: 10^{-2}

* for all experiments hidden layer size: 100

A.6 Learning Curves



(a) Energy-cost aware scheduling (b) Shortest path problem

Figure 2: IntOpt Learning Curve