Online Supplement S1 to "A Computational Framework for Solving Nonlinear Binary Optimization Problems in Robust Causal Inference"

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Appendix 1: Assumptions in Causal Inference

In this paper, we make the following assumptions which are commonly used in causal inference literature and are essential in estimating causal quantity from observational data [1, 2].

Assumption 1. (Conditional Independence) *$\exists$ a measured set of covariates $\mathbf{X} \in \mathcal{X}$ such that conditioning on $\mathbf{X}$, the potential outcomes and treatment status of samples are independent: $(Y_i^1, Y_i^0) \perp\!\!\!\perp T_i|\mathbf{X}_i$, $\forall i \in \mathscr{S}$.*

Assumption 2. (Positivity) *Given a set of measured covariate $\mathbf{X}_i$, each sample $i \in \mathscr{S}$ has a strictly positive probability of receiving treatment: $0 < Pr(T_i = 1|\mathbf{X}) < 1$, $\forall i \in \mathscr{S}$.*

Assumption 3. (SUTVA) *Treatment applied to sample i does not effect the outcome of sample j: $Y_j^1 \perp\!\!\!\perp T_i$ when $i \neq j$ and only one version of treatment exists: $Y_i^{(T_1,T_2,\cdots,T_N)} = Y_i^{T_i}$.*

Assumption 1, also known as *strong ignorability* and *selection on observables*, infers that the treatment assignment process on samples retained after controlling for $\mathbf{X}$ is 'as good as random'. Hence, we can use the untreated samples as the counterfactual. Assumption 2 ensures that the treated and control group samples have overlap in their covariate distributions (i.e., common support) so that we are not extrapolating. Finally, assumption 3 implies that the samples do not interfere with each other's outcomes and every sample in the study receives treatment in the same way so that the way of receiving treatment does not confound its effect on the outcome. These assumptions ensure causal inference made from observational data with the matching method is valid and as unbiased as possible.

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Appendix 2: Feasibility Formulation of the Maximization Problem

In this section, we discuss the feasibility reformulation for the maximization problem and the possible cases.

Cases for Maximization problem

The quadratic constraint in the maximization problem is setup in the following way:

$$\frac{1}{\sqrt{n}}\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j}\geq\gamma\times\sqrt{\frac{1}{n}\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t-y_j^c)a_{i,j}]^2-(\frac{1}{n}\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j})^2} \tag{1}$$

$$\frac{1}{n}(\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j})^2\geq\gamma^2\frac{1}{n}\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t-y_j^c)a_{i,j}]^2-\gamma^2(\frac{1}{n}\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j})^2 \tag{2}$$

We take the square of this inequality and consider additional constraints to validate the action. The resulting cases along with the constraints are presented below. The equivalent feasibility formulation of maximizing the Z-test model can be framed as the following binary-feasibility problem: $\exists$ a set of assignment $a_{i,j}$ so that $Z(\mathbf{a})\geq\gamma$ with constraints (3)-(8).

$$(1+\gamma^2\frac{1}{n})(\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j})^2-\gamma^2\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t-y_j^c)a_{i,j}]^2\geq 0 \tag{3}$$

$$\sum_{i\in\mathscr{T}}a_{ij}\leq 1\quad\forall j \tag{4}$$

$$\sum_{j\in\mathscr{C}}a_{ij}\leq 1\quad\forall i \tag{5}$$

$$\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}a_{ij}=n \tag{6}$$

$$\text{Additional constraints to validate the inequality (3)} \tag{7}$$

$$a_{ij}\in\{0,1\}\quad\forall i,j \tag{8}$$

In the following, we discuss the possible constrints required to validate the square of the inequality in (2). Similar to the minimization cases, we consider $\hat{\sigma}>0$, therefore, will not influence the cases.

Case 1: For this case, we consider $\gamma\geq 0$ and $\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j}\geq 0$. The inequality (1) can be written as the following:

$$\frac{1}{\sqrt{n}}\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(t_i^t-y_j^c)a_{i,j}\geq\gamma\hat{\sigma} \tag{9}$$

Here, $\gamma \geq 0, \hat{\sigma} > 0$ and $\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j} \geq 0$. So, both sides of the inequality are non-negative. Taking the square will not flip the inequality. Hence, we will have the following constraints.

$$(1+\gamma^2\frac{1}{n})(\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j})^2 - \gamma^2\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t - y_j^c)a_{i,j}]^2 \geq 0 \tag{10}$$

$$\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j} \geq 0 \tag{11}$$

Case 2: For this case, we consider $\gamma \leq 0$ and $\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j} \leq 0$. The inequality (1) can be written as the following:

$$\frac{1}{\sqrt{n}}\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j} \geq \gamma\hat{\sigma} \tag{12}$$

Here, $\gamma \leq 0, \hat{\sigma} > 0$ and $\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j} \leq 0$. As both sides of the inequality are non-positive, the sign of the quadratic constraint will flip and we will have the following constraints.

$$(1+\gamma^2\frac{1}{n})(\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j})^2 - \gamma^2\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t - y_j^c)a_{i,j}]^2 \leq 0 \tag{13}$$

$$\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j} \leq 0 \tag{14}$$

Case 3: For this case, we consider $\gamma \geq 0$ and $\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j} \leq 0$. The inequality (1) can be written as the following:

$$\frac{1}{\sqrt{n}}\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j} \geq \gamma\hat{\sigma} \tag{15}$$

As the left side of the inequality is non-positive and right side is non-negative, the above equation only holds at equality: $\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j} = 0$. However, this is already considered in the other cases.

Case 4: For this case, we consider $\gamma \leq 0$ and $\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j} \geq 0$. The inequality (1) can be written as the following:

$$\frac{1}{\sqrt{n}}\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j} \geq \gamma\hat{\sigma} \tag{16}$$

As $\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j} \geq 0$, left side of the inequality is non-negative but, $\gamma \leq 0$ and $\hat{\sigma} > 0$

which makes the right side non-positive. Science, this is true for all $\gamma \in \mathbb{R}$ and $\gamma \leq 0$, then, we have,

$$\frac{1}{\sqrt{n}} \sum_{i \in \mathscr{T}} \sum_{j \in \mathscr{C}} (y_i^t - y_j^c) a_{i,j} \geq \max_{\gamma \in \mathbb{R}} (\gamma \hat{\sigma}) = 0 \tag{17}$$

Therefore, we will have the following constraints. For this case, our non-linear feasibility problem becomes a linear feasibility problem.

$$\sum_{i \in \mathscr{T}} \sum_{j \in \mathscr{C}} (y_i^t - y_j^c) a_{i,j} \geq 0 \tag{18}$$

Please note that, the case 4 of the maximization problem is similar to the case 3 of the minimization problem. Therefore, to maintain consistency in the discussion, we will refer to the case 4 of the maximization as the case 3. All cases and resulting constraints are summarized in the following table.

Table 1: Cases and resulting constraints for the maximization problem feasibility formulation of robust Z-test.

Case	Case constraints	Quadratic Constraint
1	$\gamma \geq 0$, $\sum_{i \in \mathscr{T}} \sum_{j \in \mathscr{C}} (y_i^t - y_j^c) a_{i,j} \geq 0$	$(1 + \gamma^2 \frac{1}{n})(\sum_{i \in \mathscr{T}} \sum_{j \in \mathscr{C}} (y_i^t - y_j^c) a_{i,j})^2 - \gamma^2 \sum_{i \in \mathscr{T}} \sum_{j \in \mathscr{C}} [(y_i^t - y_j^c) a_{i,j}]^2 \geq 0$
2	$\gamma \leq 0$, $\sum_{i \in \mathscr{T}} \sum_{j \in \mathscr{C}} (y_i^t - y_j^c) a_{i,j} \leq 0$	$(1 + \gamma^2 \frac{1}{n})(\sum_{i \in \mathscr{T}} \sum_{j \in \mathscr{C}} (y_i^t - y_j^c) a_{i,j})^2 - \gamma^2 \sum_{i \in \mathscr{T}} \sum_{j \in \mathscr{C}} [(y_i^t - y_j^c) a_{i,j}]^2 \leq 0$
3	$\gamma \geq 0$, $\sum_{i \in \mathscr{T}} \sum_{j \in \mathscr{C}} (y_i^t - y_j^c) a_{i,j} \leq 0$	No quadratic constraint (Redundant, only true when both inequalities are zero)
4	$\gamma \leq 0$, $\sum_{i \in \mathscr{T}} \sum_{j \in \mathscr{C}} (y_i^t - y_j^c) a_{i,j} \geq 0$	No quadratic constraint

Appendix 3: QIP Formulation

In this section, we discuss the Quadratic Integer Programming (QIP) formulation of feasibility problem. Please note that we introduced the following constraints (19)-(23) in Section 2.4 and later refereed them as assignment constraints.

$$\sum_{i \in \mathscr{T}} a_{ij} \leq 1 \quad \forall j \tag{19}$$

$$\sum_{j \in \mathscr{C}} a_{ij} \leq 1 \quad \forall i \tag{20}$$

$$a_{i,j} \leq d_{i,j} \quad \forall i, j \tag{21}$$

$$\sum_{i \in \mathscr{T}} \sum_{j \in \mathscr{C}} a_{ij} = n \tag{22}$$

$$a_{ij} \in \{0, 1\} \quad \forall i, j \tag{23}$$

In addition, after converting the robust Z-test problem into a feasibility problem, we find the following constraints for cases 1 and 2:

Case 1:

$$(1+\gamma^2\frac{1}{n})(\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j})^2-\gamma^2\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t-y_j^c)a_{i,j}]^2\leq 0 \tag{24}$$

$$\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j}\geq 0 \tag{25}$$

Case 2:

$$(1+\gamma^2\frac{1}{n})(\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j})^2-\gamma^2\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t-y_j^c)a_{i,j}]^2\geq 0 \tag{26}$$

$$\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j}\leq 0 \tag{27}$$

QIP formulation for minimization problems

Here, we develop the quadratic integer programs (QIPs) for the possible cases of the minimization problem by leveraging the structure of the feasibility formulation.

Case 1: $\gamma\geq 0$ and $\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t-y_j^c)a_{i,j}]\geq 0$

Apart from the assignment constraints (19)-(23), we have to satisfy the constraints (24) and (25) to calculate γ^* in the range $\gamma\geq 0$. Simplifying the constraint (24) will result to the following:

$$(\frac{n\gamma^2}{n+\gamma^2})\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}\left[(y_i^t-y_j^c)a_{i,j}\right]^2\geq[\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j}]^2 \tag{28}$$

As our objective is to find an assignment $a_{i,j}$ that produces the smallest value of γ while satisfying the constraints (28) and (25), we can exploit the structure of equation (28). Note that in equation (28), for any number of samples (n) minimum possible value of γ is possible when $\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}\left[(y_i^t-y_j^c)a_{i,j}\right]^2$ is maximum and $\left(\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j}\right)^2$ is minimum. At the same time, the assignment should ensure $\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t-y_j^c)a_{i,j}]\geq 0$. Therefore, we need to solve the following coupled problem simultaneously for a given sample size n:

$$\arg\max_{a_{i,j}\in\mathscr{M}}\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}\left[(y_i^t-y_j^c)a_{i,j}\right]^2\quad \text{S.t.: }\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t-y_j^c)a_{i,j}]\geq 0\text{ and constraints (19)-(23)} \tag{29}$$

$$\arg\min_{a_{i,j}\in\mathscr{M}}[\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j}]^2\quad \text{S.t.: }\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t-y_j^c)a_{i,j}]\geq 0\text{ and constraints (19)-(23)} \tag{30}$$

We can use the following problem to solve the coupling problem (29) and (30):

$$\max_{a_{i,j}\in\mathscr{M}} \sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}\left[(y_i^t-y_j^c)a_{i,j}\right]^2 - [\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j}]^2$$
$$\text{subject to:} \sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t-y_j^c)a_{i,j}] \geq 0 \text{ and constraints (19)-(23)}$$

Case 2: $\gamma \leq 0$ and $\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t-y_j^c)a_{i,j}] \leq 0$

To get γ^* in the range $\gamma \leq 0$, we have to find an assignment of pre-defined number of pairs (n) while satisfying the constraints (26) and (27) along with necessary assignment constraints (19)-(23). Simplifying the equation (26) will result the following:

$$[\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j}]^2 \geq (\frac{n\gamma^2}{n+\gamma^2})\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}\left[(y_i^t-y_j^c)a_{i,j}\right]^2 \tag{31}$$

Using the same mechanism we used for case 1, we get the following coupled optimization problem.

$$\arg\max_{a_{i,j}\in\mathscr{M}}[\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j}]^2 \quad \text{S.t.:} \sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t-y_j^c)a_{i,j}] \leq 0 \text{ and constraints (19)-(23)} \tag{32}$$
$$\arg\min_{a_{i,j}\in\mathscr{M}}\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}\left[(y_i^t-y_j^c)a_{i,j}\right]^2 \quad \text{S.t.:} \sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t-y_j^c)a_{i,j}] \leq 0 \text{ and constraints (19)-(23)} \tag{33}$$

Now, for a predefined number of required assignments n, we can solve the following QIP to find optimal γ for case 2.

$$\arg\max_{a_{i,j}\in\mathscr{M}}[\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j}]^2 - \sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}\left[(y_i^t-y_j^c)a_{i,j}\right]^2 \tag{34}$$
$$\text{subject to:} \sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t-y_j^c)a_{i,j}] \leq 0 \text{ and constraints (19)-(23)} \tag{35}$$

QIP formulation for maximization problems

Case 1: $\gamma \geq 0$ and $\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t-y_j^c)a_{i,j}] \geq 0$

The objective of this case is to find the maximum value of γ (i.e.,γ^*) in the range of $\gamma \geq 0$ for a pre-defined number of pairs while satisfying constraints (10) and (11) along with necessary assignment constraints. With further simplification, constraint (10) can be simplified as the following:

$$[\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t-y_j^c)a_{i,j}]^2 \geq (\frac{n\gamma^2}{n+\gamma^2})\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}\left[(y_i^t-y_j^c)a_{i,j}\right]^2 \tag{36}$$

From simplified constraint (36), we can achieve γ^* when $[\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j}]^2$ is maximum and $\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t - y_j^c)a_{i,j}]^2$ is minimum. So, we can solve the case 1 of the maximization problem by solving the following coupled problem simultaneously for a given sample size n:

$$\arg\max_{a_{i,j}\in\mathscr{M}}[\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j}]^2 \quad \text{S.t.: } \sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t - y_j^c)a_{i,j}] \geq 0 \text{ and constraints (19)-(23)} \tag{37}$$

$$\arg\min_{a_{i,j}\in\mathscr{M}}\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}\left[(y_i^t - y_j^c)a_{i,j}\right]^2 \quad \text{S.t.: } \sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t - y_j^c)a_{i,j}] \geq 0 \text{ and constraints (19)-(23)} \tag{38}$$

We can formulate the following QIP by combining the coupling problem (37) and (38).

$$\arg\max_{a_{i,j}\in\mathscr{M}}[\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j}]^2 - \sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}\left[(y_i^t - y_j^c)a_{i,j}\right]^2 \tag{39}$$

$$\text{subject to: } \sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t - y_j^c)a_{i,j}] \geq 0 \text{ and constraints (19)-(23)} \tag{40}$$

Case 2: $\gamma \leq 0$ and $\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t - y_j^c)a_{i,j}] \leq 0$

To get γ^* in the range $\gamma \leq 0$, we have to find an assignment of pre-defined number of pairs (n) while satisfying the constraints (13) and (14) along with necessary assignment constraints. Simplifying the equation (13) will result the following:

$$(\frac{n\gamma^2}{n+\gamma^2})\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}\left[(y_i^t - y_j^c)a_{i,j}\right]^2 \geq [\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j}]^2 \tag{41}$$

Using the same mechanism we used for case 1, we get the following coupled optimization problem.

$$\arg\max_{a_{i,j}\in\mathscr{M}}\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}\left[(y_i^t - y_j^c)a_{i,j}\right]^2 \quad \text{S.t.: } \sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t - y_j^c)a_{i,j}] \leq 0 \text{ and constraints (19)-(23)} \tag{42}$$

$$\arg\min_{a_{i,j}\in\mathscr{M}}[\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j}]^2 \quad \text{S.t.: } \sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t - y_j^c)a_{i,j}] \leq 0 \text{ and constraints (19)-(23)} \tag{43}$$

The problems in (42) and (43) can be combined in the following problem:

$$\arg\max_{a_{i,j}\in\mathscr{M}}\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t - y_j^c)a_{i,j}]^2 - [\sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}(y_i^t - y_j^c)a_{i,j}]^2 \tag{44}$$

$$\text{subject to: } \sum_{i\in\mathscr{T}}\sum_{j\in\mathscr{C}}[(y_i^t - y_j^c)a_{i,j}] \leq 0 \text{ and constraints (19)-(23)} \tag{45}$$

References

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