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Supplementary Materials of Manuscript Entitled “Domain Generalization Study of Empirical Risk Minimization from Causal Perspectives”

VIII. PROOFS OF THEORIES

In this section, the proofs of theories in the paper are offered. Note that equations, tables, and figures, etc., in the Supplementary Materials are all numbered consecutively to those in the paper, while notations and references are consistent with those in the paper.

A. Proof of Lemma 1

First, it is known that the information flow is non-negative, i.e., $\mathcal{I}(A \mapsto B | do(C)) \geq 0$, since the relative entropy is non-negative [38].

Then, we are going to prove the lemma by contradiction. Assume that, given a DAG and its three disjoint sets of nodes A , B , and C , if there is a directed path from A to B unblocked by C , then $\mathcal{I}(A \mapsto B | do(C)) = 0$. By Proposition 1, it implies that $A \perp_{ud} B | C$, which means C blocks all directed paths from A to B . Thus, it contradicts that there is a directed path from A to B unblocked by C . \square

B. Proof of Proposition 2

1) Proof of P1

When C is a null set, we can reformulate (5) as follows.

$$\begin{aligned} A \perp_{ud} B &\Leftrightarrow A \perp_{do} B \Leftrightarrow \\ p(b | do(a)) &= \sum_{a \in A} p(a) p(b | do(a)), \end{aligned} \quad (14)$$

$$\forall a \in A, \forall b \in B$$

In addition, we can also rewrite the information flow in (6) as the full information flow as follows.

$$\begin{aligned} \mathcal{I}(A \mapsto B) &= \sum_{a \in A} p(a) \sum_{b \in B} p(b | do(a)) \\ &\log \frac{p(b | do(a))}{\sum_{a \in A} p(a) p(b | do(a))} \end{aligned} \quad (15)$$

Thus, by the equality condition of relative entropy [38], we have

$$\mathcal{I}(A \mapsto B) = 0 \Leftrightarrow A \perp_{do} B \Leftrightarrow A \perp_{ud} B \quad (16)$$

Then, by the definition of ud -separation, there are no directed paths from A to B , which is equivalent to removing all directed paths from A to B without changing the causal graph. Hence, the Markov condition of the causal graph is intact. \square

2) Proof of P2

We will employ Rule 2 of do Calculus (Theorem 3.4.1 of [15]). Hence, we summarize Rule 2 as follows. Given a DAG G and two disjoint sets of nodes A and B , we denote $G(\underline{B})$ as a DAG by deleting all the arrows emitting from

nodes of B . The Rule 2 says that if A is d -separated from B in $G(\underline{B})$, **which we denote it as** $(A \perp_d B) \odot G(\underline{B})$, then

$$p(A | do(B)) = p(A | B) \quad (17)$$

Thus, if the causal graph is $a \rightarrow b$, then $(b \perp_d a) \odot G(\underline{a})$. Let a' and b' denote all possible values of nodes a and b , respectively. It follows that

$$\begin{aligned} \mathcal{I}(a \mapsto b) &= \sum_{a'} p(a) \sum_{b'} p(b | do(a)) \\ &\log \frac{p(b | do(a))}{\sum_{a'} p(a) p(b | do(a))} \\ &= \sum_{a'} p(a) \sum_{b'} p(b | a) \\ &\log \frac{p(b | a)}{\sum_{a'} p(a) p(b | a)} \\ &= \mathcal{I}(a : b) \end{aligned} \quad (18)$$

\square

3) Proof of P3

It is obvious that a has no ancestors and b has no descendants since a is the root and b is the sink. $\mathcal{I}(a \mapsto b)$ is only dependent on a and b . Hence, this condition is trivially satisfied. \square

4) Proof of P4

First, the setting is that A are roots connected via directed paths with sinks B . In addition, $a \in A$ and $b \in B$. The setting implies the followings:

- (i) $a \perp_d Pa(b \setminus a \mapsto b)$ due to colliders formed with $b \Rightarrow \mathcal{I}(a : b) = \mathcal{I}(a : b | Pa(b \setminus a \mapsto b))$.
- (ii) If there are directed paths from a to b , then $(b \perp_d a) \odot G(\underline{a})$. Thus, by (18), we have $\mathcal{I}(a \mapsto b) = \mathcal{I}(a : b)$. \square

5) Proof of P5

$\mathcal{I}(A \mapsto B) = 0 \Leftrightarrow A \perp_{do} B \Leftrightarrow A \perp_{ud} B$. Hence, there are no directed paths from A to B . For $a \in A$ and $b \in B$, $\mathcal{I}(a \mapsto b) = 0$. \square

C. Proof of Lemma 2

We continue to follow the same rule in (17). Let G be the DAG shown in Fig. 2. Since $(X_O^e \perp_d Y) \odot G(\underline{Y})$, we have

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$$\begin{aligned}
& \mathcal{I}(Y \mapsto X_O^e | C^e) \\
&= \sum_{c^e \in C^e} p(c^e) \sum_{y \in Y} p(y | c^e) \sum_{x_O^e \in X_O^e} p(x_O^e | do(y), c^e) \\
& \quad \log \frac{p(x_O^e | do(y), c^e)}{\sum_{y \in Y} p(y | c^e) p(x_O^e | do(y), c^e)} \\
&= \sum_{c^e \in C^e} p(c^e) \sum_{y \in Y} p(y | c^e) \sum_{x_O^e \in X_O^e} p(x_O^e | y, c^e) \\
& \quad \log \frac{p(x_O^e | y, c^e)}{\sum_{y \in Y} p(y | c^e) p(x_O^e | y, c^e)} \\
&= \mathcal{I}(Y : X_O^e | C^e)
\end{aligned} \tag{19}$$

□

D. Proof of Corollary 2

Recall Rule 2 of *do* Calculus (Theorem 3.4.1 of [15]), we have $(X_N^e \perp_d Y) \odot G(\underline{Y})$. It then follows similarly as (19).

□

E. Proof of Theorem 1

First, let C be a null set, i.e., $C = \emptyset$, in Lemma 1. Then, we know that both $\mathcal{I}(Y \mapsto X_O^e)$ and $\mathcal{I}(Y \mapsto X_N^e)$ are non-negative, which implies that X_O^e and X_N^e both contain information of Y . However, the causal information X_N^e receives from Y is only mediated by C^e . By Corollary 2,

$$\mathcal{I}(Y \mapsto X_N^e | C^e) = \mathcal{I}(Y : X_N^e | C^e) \tag{20}$$

Since $Y \perp_d X_N^e | C^e$, $\mathcal{I}(Y : X_N^e | C^e) = 0$. Hence,

$$\mathcal{I}(Y \mapsto X_N^e | C^e) = 0 \tag{21}$$

Similarly, since $Y \not\perp_d X_O^e | C^e$, $\mathcal{I}(Y : X_O^e | C^e) > 0$. By Lemma 2, we have

$$\mathcal{I}(Y \mapsto X_O^e | C^e) = \mathcal{I}(Y : X_O^e | C^e) > 0 \tag{22}$$

Therefore,

$$\mathcal{I}(Y \mapsto X_O^e | C^e) > \mathcal{I}(Y \mapsto X_N^e | C^e) \tag{23}$$

From the causal perspective, it implies that, when observing C^e , X_O^e still has more causal information about Y than that X_N^e has about Y . Thus, the model may favor X_O^e rather than X_N^e .

Next, we offer a more formal proof from the information theoretic perspective. From the above, we know that

$$\mathcal{I}(Y : X_O^e | C^e) > \mathcal{I}(Y : X_N^e | C^e) \tag{24}$$

Let X_Z be the feature to be learned by an encoder $X_Z = h_\theta(X^e)$ and then be used to predict labels by a classifier $\hat{Y} = g_\omega(X_Z)$, where X^e is the input data, θ and ω are model parameters, and \hat{Y} is the predicted label.

The mutual information between X_Z and Y given C^e is decomposed as follows.

$$\begin{aligned}
& \mathcal{I}(Y : X_Z | C^e) \\
&= \mathcal{H}(Y | C^e) - \mathcal{H}(Y | X_Z, C^e) \\
&\geq \mathcal{H}(Y | C^e) - \mathcal{H}(Y | X_Z)
\end{aligned} \tag{25}$$

where \mathcal{H} denotes the Shannon's entropy and the inequality comes from the fact that the conditioning reduces entropy.

Note that $\mathcal{H}(Y | C^e)$ is a constant since Y and C^e are fixed samples in the model learning process [36]. Then, minimizing the objective $\mathcal{H}(Y | X_Z)$ will have the similar effect of maximizing the objective $\mathcal{I}(Y : X_Z | C^e)$ for model learning since both objectives only matter on the conditional value of X_Z and C^e . In addition, C^e represents fixed samples and X_Z varies due to variational functionals in the model learning process. Therefore, if $X_Z = X_O^e$ is a better choice than $X_Z = X_N^e$ in terms of the objective $\mathcal{I}(Y : X_Z | C^e)$, it can be speculated that $X_Z = X_O^e$ is also a better choice than $X_Z = X_N^e$ in terms of the objective $\mathcal{H}(Y | X_Z)$. This reasoning can be also understood by considering the information Venn diagram of three variables Y , X_Z and C^e when two circles of Y and C^e are fixed and the left one varies in position [57].

Note that the cross-entropy used for prediction can be decomposed into two terms as follows.

$$\mathcal{H}(Y; \hat{Y} | X_Z) = \mathcal{H}(Y | X_Z) + D_{KL}(Y \| \hat{Y} | X_Z) \tag{26}$$

Based on the two-step model learning perspective (Lemma 2 of [36]), $\mathcal{H}(Y | X_Z)$ corresponds to the learning of the encoder $h_\theta(\cdot)$, while the KL divergence $D_{KL}(Y \| \hat{Y} | X_Z)$ corresponds to the learning of the classifier $g_\omega(\cdot)$. Note that X_O^e and X_N^e both contain information of Y as stated at the beginning of the proof. Hence, it is possible to make the corresponding KL divergence in (26) similarly approximate to zero given an ideal classifier [36]. Finally, we would expect that X_O^e , compared to X_N^e , will be selected by the encoder and X_O^e also offers lower cross-entropy.

□

F. Proof of Corollary 3

It is known from Theorem 1 that X_O^e will be learned. If C^e and X_O^e is not *ud*-separated, the cross-entropy $\mathcal{H}(Y; \hat{Y} | X_Z = X_O^e)$ will be domain-dependent. It implies that the model fails at DG.

□

G. Proof of Corollary 4

If C^e and X_O^e is *ud*-separated, we can show that X_O (i.e., X_O^e without the domain influence) will be learned. This can be seen as follows.

First, due to the symmetric property of mutual information and the correspondence between X_O and Y assumed in Assumption 1, the mutual information will be equal to the entropy as follows.

$$\mathcal{I}(X_O : Y) = \mathcal{I}(Y : X_O) = \mathcal{I}(Y : L(X_O)) = \mathcal{H}(Y) \tag{27}$$

Then, we consider the mutual information between Y and C^e as follows.

$$\begin{aligned}
& \mathcal{I}(Y : C^e) \\
&= \mathcal{H}(Y) - \mathcal{H}(Y | C^e) \\
&\leq \mathcal{H}(Y)
\end{aligned} \tag{28}$$

where the inequality comes from the fact that the conditional entropy $\mathcal{H}(Y | C^e) \geq 0$.

Note that the path from Y to X_N^e is a Markov chain, by data processing inequality [38], we have

$$I(Y : C^e) \geq I(Y : X_N^e) \tag{29}$$

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TABLE IV

HYPERPARAMETER SEARCH GRIDS USED IN EACH EXPERIMENT

Hyperparameter	Default value	Search grid
Training step	1000	[500, 1000, ..., 5000]
Learning rate	0.001	$10^u, u \sim U(-4.5, -2.5)$
Weight decay	0	$10^u, u \sim U(-8, -4)$
Batch size	64	$\text{int}(10^u), u \sim U(3, 9)$

The $10^u, u \sim U(-4.5, -2.5)$ means drawing u uniformly at random from the range $(-4.5, -2.5)$. $\text{int}()$ means taking the integer value.

The equality in (29) holds if and only if $I(Y : C^e | X_N^e) = 0$ i.e., $C^e \rightarrow X_N^e \rightarrow Y$ forms a Markov chain ($Y \perp_d C^e | X_N^e$), which is not true based on the causal graph in Assumption 1. Considering the results in (27), (28), and (29), we obtain

$$\mathcal{I}(Y : X_O) > \mathcal{I}(Y : X_N^e) \quad (30)$$

Then, we can follow the same proof starting from (25) of Theorem 1 without conditioning on C^e , which results in that X_O will be learned and X_N^e will be ignored by the encoder. Therefore, $\mathcal{H}(Y; \hat{Y} | X_Z = X_O)$ is the same across domains. In addition, $\mathcal{H}(Y | X_Z = X_O) = 0$ and $D_{KL}(Y || \hat{Y} | X_Z = X_O) = 0$ since X_O is the casual feature. Hence, $\mathcal{H}(Y; \hat{Y} | X_Z = X_O)$ is the smallest across domains. It implies that the model succeeds at DG. \square

IX. EXPERIMENT DETAIL

A. DomainBed Experiment Principle and Simulation Principle

Our experiments follow the DomainBed experiment principle proposed in [14]. For each model on each task, each hyperparameter is selected based on conducting random searches 20 times over a given search grid. **The search grids of hyperparameters employed in this study are presented in TABLE IV.** Each set of hyperparameters is tested 3 times independently. The model is selected based on the training domain validation and the test domain validation. The training domain validation means that 20% training domain data is reserved as the validation set. The test domain validation means that 20 % test domain data is reserved as the validation set. **The simulation principle is detailed as follows.**

(i) There is a correspondence between the causal feature X_O (i.e., the interested yellow object) and the binary label Y (0 or 1) via the labeling mechanism.

$$Y \doteq L(X_O) \quad (31)$$

(ii) The label then interacts with the domain noise N_1^e to produce spurious influencer C^e .

$$C^e \leftarrow Y \oplus N_1^e \quad (32)$$

$$N_1^e \sim \mathcal{B}(e) \quad (33)$$

where \oplus denotes exclusive OR (i.e., XOR). N_1^e follows a Bernoulli distribution $\mathcal{B}(e)$ with probability e in giving the values of 1s. This process can be regarded as flipping the label with probability e to obtain C^e .

(iii) The spurious influencer C^e is then applied to transform the causal feature X_O and the domain noise N_2^e into the transformed causal feature X_O^e (i.e., the re-colored object) and the transformed spurious feature X_N^e (i.e., the colored noise), respectively.

TABLE V

VARIATIONAL AUTOENCODER-CLASSIFIER FOR MNIST BASED EXPERIMENTS

Subnetwork	Layer	Layer function
Encoder	E1	Flatten()
	E2	Fc_Bn_ReLu($in = x_{dim}$, $out = x_{dim} / 2$)
	E3	Fc_Bn_ReLu($in = x_{dim} / 2$, $out = x_{dim} / 4$)
	E4-1	Fc($in = x_{dim} / 4$, $out = x_{dim} / 8$)
	E4-2	Fc($in = x_{dim} / 4$, $out = x_{dim} / 8$)
Decoder	D1	Reparam()
	D2	Fc_Bn_ReLu($in = x_{dim} / 8$, $out = x_{dim} / 4$)
	D3	Fc_Bn_ReLu($in = x_{dim} / 4$, $out = x_{dim} / 2$)
	D4	Fc($in = x_{dim} / 2$, $out = x_{dim}$)
	D5	Sigmoid(UnFlatten())
Classifier	C1	Fc_Bn_ReLu($in = x_{dim} / 8$, $out = x_{dim} / 16$)
	C2	Fc_Bn_ReLu($in = x_{dim} / 16$, $out = x_{dim} / 32$)
	C3	Fc_Bn_ReLu($in = x_{dim} / 32$, $out = 2$)
	C4	Softmax()

Flatten() is an flattening operator. The reverse is UnFlatten(). Fc_Bn_ReLu() means the composition of a layer of fully connected network Fc(), a batch norm operation, and a relu function. $x_{dim} = 1568$. Sigmoid() is a sigmoid function. Softmax() is the softmax function. E4-1 and E4-2 correspond to the mean and variance latent codes. Reparam() is the reparameterization of the latent codes.

$$X_O^e \leftarrow T(X_O, C^e) \quad (34)$$

$$X_N^e \leftarrow T(N_2^e, C^e) \quad (35)$$

$$N_2^e = (1 - e) \times 10N(0, 1) \quad (36)$$

where $T(\cdot)$ presents a function setting the red channel to zero if $C^e = 1$ and setting the green channel to zero if $C^e = 0$. N_2^e is the Gaussian noise with the domain dependent variance. $N(0, 1)$ denotes the standard Gaussian variable.

(iv) The observational data X^e is the composition of X_O^e and X_N^e , i.e., $X^e = (X_O^e, X_N^e)$. For simulation simplicity, we let $X^e = X_O^e + X_N^e$.

B. Simulated Visualization Experiments

The neural network model applied is the variational autoencoder-classifier. The structure of this model is detailed in TABLE V. The model has three losses, the reconstruction loss, the KL divergence, and the classification loss (cross-entropy), which are assigned with weights 10, 1, and 1, respectively. For the MNIST data, the training step is set to 3000. As for other parameters, they are set to just the default values in TABLE IV.

C. Simulated Numerical Experiments

We follow the same experiment procedure and the similar random search scheme of the DomainBed [14] to train and select the models (the grid search settings used are described in TABLE IV). Regarding the variational autoencoder classifier, the weights of the reconstruction loss, the KL divergence, and the classification loss are selected as 10^{n1} , 10^{n2} , and 10^{n3} , respectively, where $n1 \sim U(0, 2)$, $n2 \sim U(0, 2)$, and $n3 \sim U(0, 3)$ describe values randomly generated from three uniform distributions of respective ranges.

The results of the simulated domain generalization experiment based on the training domain validation are presented in TABLE VI. Essentially, the results are in line with the results based on the test domain validation presented in TABLE I of the paper.

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TABLE VI
TEST RESULTS ON SIMULATION DATASETS FOR THEORY VERIFICATION BASED ON TRAINING DOMAIN VALIDATION

Base	Data settings	TS 1 $e_{\text{test}} = +90\%$	TS 2 $e_{\text{test}} = +80\%$	TS 3 $e_{\text{test}} = -90\%$	DG: Yes/No/N.A.	Δ^*	Avg
Data Base: MNIST	DS 1 $X_o \not\leftarrow X_o$	94.4 +/- 0.5	95.2 +/- 0.4	94.6 +/- 0.4	N.A. (Baseline)	0.8	94.7
	DS 2 $X_N^e \leftarrow C^e \rightarrow X_o^e$	90.7 +/- 1.0	91.3 +/- 0.8	72.6 +/- 1.7	No (Thm.1 & Cllry.3)	18.7	84.8
Model Base: VAEC	DS 3 $X_N^e \not\leftarrow C^e \rightarrow X_o^e$	89.9 +/- 0.4	91.6 +/- 0.8	76.5 +/- 1.9	No (Cllry.3)	15.1	86.0
	DS 4 $X_N^e \leftarrow C^e \not\rightarrow X_o^e$	94.9 +/- 0.6	95.2 +/- 0.2	94.4 +/- 0.2	Yes (Cllry.4)	0.8	94.8
Data Base: Fashion MNIST	DS 1 $X_o \not\leftarrow X_o$	91.9 +/- 0.3	93.4 +/- 0.1	92.2 +/- 0.3	N.A. (Baseline)	1.5	92.5
	DS 2 $X_N^e \leftarrow C^e \rightarrow X_o^e$	93.6 +/- 0.5	93.6 +/- 0.3	79.4 +/- 0.8	No (Thm.1 & Cllry.3)	14.2	88.9
Model Base: MNIST_CNN [14]	DS 3 $X_N^e \not\leftarrow C^e \rightarrow X_o^e$	95.0 +/- 0.2	92.6 +/- 0.2	80.6 +/- 0.3	No (Cllry.3)	14.4	89.4
	DS 4 $X_N^e \leftarrow C^e \not\rightarrow X_o^e$	92.6 +/- 0.3	93.9 +/- 0.2	91.5 +/- 0.6	Yes (Cllry.4)	2.4	92.7
Data Base: CIFAR10	DS 1 $X_o \not\leftarrow X_o$	96.1 +/- 0.4	96.1 +/- 0.4	96.4 +/- 0.2	N.A. (Baseline)	0.3	96.2
	DS 2 $X_N^e \leftarrow C^e \rightarrow X_o^e$	94.2 +/- 0.2	92.9 +/- 0.3	79.6 +/- 0.5	No (Thm.1 & Cllry.3)	14.6	88.9
Model Base: Wide_ResNet [46]	DS 3 $X_N^e \not\leftarrow C^e \rightarrow X_o^e$	94.8 +/- 0.3	92.2 +/- 0.8	79.2 +/- 0.4	No (Cllry.3)	15.6	88.7
	DS 4 $X_N^e \leftarrow C^e \not\rightarrow X_o^e$	94.9 +/- 0.2	94.2 +/- 0.4	94.1 +/- 0.4	Yes (Cllry.4)	0.9	94.4

D. Real-World Datasets for Theory Verification

The experiment procedure also follows the DomainBed experiment principle [14]. The search grids applied are in TABLE IV except for the grid of the batch size, which is set to {8, 16, 32, 64} to obtain a good training efficiency.

Regarding the PU bearing fault dataset [47], at each speed, there are three kinds of data, the normal, the inner race fault, and the outer race fault. Here, we employ data from two speed conditions, 900 rpm and 1500 rpm. In the time domain input setting and the frequency domain input setting, TS 1 is training the model on data of 900 rpm and testing the model on data of 1500 rpm, while TS 2 describes the reverse direction. The baseline training and test data are created from two independent trials of data at 900 rpm.

Regarding the EPdM belt fault dataset [48], at each speed, there are two types of data, the normal and the belt fault. TS 1 is to generalize the model from the data of the lower speed group (speed: 400-900 rpm) to the data of the higher speed group (speed: 1500-2000 rpm). TS 2 is in the opposite direction. The baseline is built by collecting the data of all speeds, randomizing speeds, and splitting data into two datasets.

Regarding the BU human activity dataset [49], the data is collected using the mobile phone vibration sensor when different ages of people (both male and female) are sitting and walking. We know that older people are often less active in movement and have relatively lower speeds than younger people. Thus, the age dependent domain data can be treated as speed dependent domain data. We then divide the data into the younger group (around 20 years old) and older group (around 50 years old) to create two domains of data. TS 1 is generalizing the model from the young group to the old group, while TS 2 considers the reverse direction. Baseline datasets are built by randomizing the ages and then splitting the data into two sets.

Regarding the JUST lung dataset [50], we also segment the data into the younger group (mostly around 30 years old) and the older group (mostly around 60 years old) to obtain two domains of data. TS 1 and TS 2 are similarly defined as the above human activity dataset. However, the change of speed (in terms of frequency shift) in the lung sound is not

significant between the young and the old [51]. Baseline datasets are established by randomizing the ages and splitting the data into two sets.

E. Real-World Datasets for Methodology Verification

Regarding the image segmentation, we employ prostate magnetic resonance imaging (MRI) segmentation data from four different institutions curated in [52]. Hence, different domains correspond to different institutions implementing the MRIs. The encoder model for learning transformed causal features is the U-Net without the last layer [53]. The classifier is a two-layer convolutional neural network. The first layer considers ReLU as the activation function and the second layer does not have activation function to output the logits.

Regarding the image classification, we utilize the PACS dataset, which has seven classes of images in each domain [14]. Different domains have different styles of images, i.e., art, cartoon, real photo, and sketch. The encoder applied is the ResNet18 without the last layer [54]. The classifier is a two-layer dense neural network. The first layer considers the ReLU activation function while the second layer is a linear layer.

Regarding the text classification, we use the multi-domain sentiment datasets originally sourced from [55]. There are four domains of product reviews, books, DVDs, kitchens, and electronics. In each domain, each review of texts was manually labeled as negative or positive. The DistilBERT without the classification layer is selected as the encoder [56]. The classifier is constructed by a two-layer dense network, where the first layer considers ReLU as the activation function and the second layer is a linear layer.

For computation efficiency, we first empirically set the common parameters shared by ERM and FISIP. The learning rate is set as $\gamma = 5 \times 10^{-5}$ for all datasets. The training steps T for image segmentation, image classification, and text classification are 1500, 500, and 1000, respectively. The batch sizes N for image segmentation, image classification, and text classification are 2, 16, and 8, respectively. There are four unique parameters of FISIP. Total 10 random searches are executed for unique parameters of FISIP on each dataset. The search range for each unique parameter is given in step 2 of Algorithm I. Each task is repeated three times to reduce randomness.