Conditional Generative Learning from Invariant Representations in Multi-Source: Robustness and Efficiency

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Outline

- Past: Background and Rethinking
 - Background
 - Motivation
- 2 Now:Exploration and Insights
 - Methodology
 - Statistical Properties
 - Simulation Studies
 - Real Data Analysis
- § Future: Discussion



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Background

- Classical methods: based on Pre-trained Fine-tuning model.
- Transfer Learning, a rapidly growing field in statistics, offers a powerful approach to enhance data analysis, particularly when the target data is limited:
 - Generative Model[Damodaran et al., 2018]
 - Graph Model[Ren et al., 2023]
 - Linear Regression[Tian et al., 2023]
 - Semiparametric Regression[He et al., 2024]

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 - Linear Regression[Tian et al., 2023]
 - Semiparametric Regression[He et al., 2024]
- Theoretical Insights for GAN. More and more statisticians exploring the learning theory from diverse perspectives:
 - Approximation Error & Statistical Error Framwork [Huang et al., 2022]
 - WGAN for Regression [Song et al., 2023]
 - Adaptive WGAN Architecture [Tan et al., 2024]

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The Pre-trained Fine-tuning model has limitations in terms of theoretical guarantees and tabular medical data.

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 - Additionally, there is a lack of large-scale datasets for pre-training.
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 The complex adjustments required to align the generator and discriminator make it difficult to derive rigorous theoretical guarantees.

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We need to establish a new method that does not rely on pre-trained fine-tuning models!

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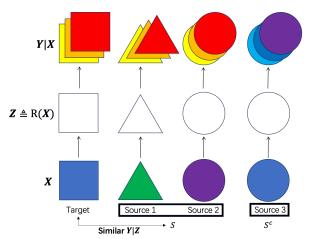
Motivation

Can we learn the "good" representation to effectively utilize the source data?

- What is the "good" representation?
 - **Domain Invariance.** To reduce the distribution discrepancy between the source and target domains.
 - Dimension Reduction. To retain all the necessary information for learning the conditional distribution

Motivation

• Why we need the "good" representation?



Motivation

• How to learn the "good" representation?

Domain Adaptation. Similar challenges have been addressed with a number of well-developed and effective methods in classification task.

- Asymmetric. Transform the features of the source domain to match those of the target domain.[Hoffman et al., 2014, Courty et al., 2017]
- **Symmetric.** Project both domains into a shared latent space, aligning their distributions.[Damodaran et al., 2018, Shen et al., 2018]

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Data and Modeling Framework

- ullet Data. T Sources $\left\{m{x}_i^{(t)},m{y}_i^{(t)}
 ight\}_{i=1}^t$ and Target $\left\{m{x}_i^{(0)},m{y}_i^{(0)}
 ight\}_{i=1}^{(0)}$
- Idea. Find Domain Invariant representation $R: \mathcal{X} \mapsto Z$
- Similarity Measure. Based on the IPM metric,

$$d_{\mathcal{F}_{B}^{1}}\left(P_{Y|Z}^{(t)}, P_{Y|Z}^{(0)}\right) = \sup_{f \in \mathcal{F}_{B}^{1}} \left\{ \mathbb{E}_{P_{Y|Z}^{(t)}} f(\boldsymbol{y}) - \mathbb{E}_{P_{Y|Z}^{(0)}} f(\boldsymbol{y}) \right\},$$



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ullet Reliable Source S. To keep robustness, we consider the threshold h,

$$\forall t \in S, \mathbb{E}_{P_Z^{(t)}} d_{\mathcal{F}_B^1} \left(P_{Y|Z}^{(t)}, P_{Y|Z}^{(0)} \right) \le h.$$

• Goal. Finding a generation function $G(\eta, z)$, such that

$$G(\eta, \mathbf{z}) \sim P_{Y|Z=\mathbf{z}}^{(0)}, \mathbf{z} \in Z.$$

ullet Question. How to estimate reliable source S and make full use of them?

Error Decomposition

• If S is known, we can consider pool-training.

Decompose error
$$d_{\mathcal{F}_B^1}\left(P_{\hat{Z},\hat{G}},P_{\hat{Z},Y}^{(0)}\right)$$
, where $P_{\hat{Z},Y}=\sum_{t\in S\cup\{0\}}\frac{\mathbf{n}_t}{n}P_{\hat{Z},Y}^{(t)}$

- Learning bias. $\mathrm{d}_{\mathcal{F}_{\mathrm{B}}^{1}}\left(P_{\hat{\mathbf{Z}},\hat{\mathbf{G}}},P_{\mathbf{Z},\mathbf{Y}}\right)$, We focus on \hat{R},\hat{G} by Conditional WGAN.
- Transfer bias. $d_{\mathcal{F}_{B}^{1}}\left(P_{\hat{Z},Y},P_{\hat{Z},Y}^{(0)}\right)$ We focus on \hat{R} by Optimal Transport Regularization.
- Combine the two parts, we get the loss:

$$\mathcal{L}_{1}(R, G, D; S) = \mathbb{E}_{P_{X}P_{\eta}}D(X, G(\eta, R(X))) - \mathbb{E}_{P_{X,Y}}D(X, Y) + \sum_{t \in S} \lambda_{t} \inf_{\gamma} \int \left\| \left(R\left(X^{(t)}\right), Y^{(t)}\right) - \left(R\left(X^{(0)}\right), Y^{(0)}\right) \right\|_{1} d\gamma.$$



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$$+ \sum_{t \in S} \lambda_{t} \inf_{\gamma} \int \left\| \left(R\left(X^{(t)}\right), Y^{(t)}\right) - \left(R\left(X^{(0)}\right), Y^{(0)}\right) \right\|_{1} d\gamma.$$

• If S is unknown, can we develop a data-driven selection criterion to estimate the subset S?

Data-driven Selection Criterion

• If S is unknown, can we develop a data-driven selection criterion to estimate the subset S?

Pre-train full model to learn the "rough" domain invariant representation $\tilde{\boldsymbol{Z}}$

$$\hat{S} = \left\{ t : W_1 \left(P_{\tilde{Z}, Y'}^{n_t}, P_{\tilde{Z}, Y}^{n_0} \right) \le C \left(\max \left\{ n^{-1/(r+q)}, n_0^{-1/r} \right\} \right) \right\}$$

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Notations

- $\pmb{x}_i^{(t)} \in \mathcal{X} \subset \mathbb{R}^d$ is drawn according to distribution $P_X^{(t)}$ over \mathcal{X} , and then $\pmb{y}_i^{(t)} \in \mathcal{Y} \subset \mathbb{R}^q$ is drawn according to the conditional distribution $P_{Y|X=\pmb{x}_i^{(t)}}^{(t)}$, $t \in [T]$. Besides, we assume a low-dimensional subspace $\mathcal{Z} \subset \mathbb{R}^r$, r << d.
- The overall architecture of the network is characterized by its width, denoted as $W = \max{\{p_1, \dots, p_H\}}$, and its depth, represented by H. To facilitate discussion, we denote a neural network with input dimension p_0 , output dimension p_{H+1} , a maximum width of W, and a maximum depth of H as $\mathcal{NN}\left(p_0, p_{H+1}, W, H\right)$.

Notations

- For the generator network class G_{θ} : Let $\mathcal{G} \equiv NN \ (r+m,q,W_G,H_G)$ be a class of ReLU-activated FNNs, $G_{\theta}: \mathbb{R}^{d+m} \to \mathbb{R}^q$, with parameter θ , width W_G , and depth H_G .
- For the discriminator network class D_{ϕ} : Let $\mathcal{D} \equiv \mathcal{N} \mathcal{N} \left(r+q,1,W_D,H_D\right) \cap \mathcal{F}^1_{\mathsf{Lip}}$ be a class of ReLU-activated FNNs, $f_{\delta}: \Omega \to \mathbb{R}$, with parameter ϕ , width $W_{\mathcal{D}}$, and depth $H_{\mathcal{D}}$.
- For the representation network class R_{ω} : Let $\mathcal{R} \equiv \mathcal{NN} (d, r, W_R, H_R)$ be a class of ReLU-activated FNNs, $R_{\omega} : \mathbb{R}^d \to \mathbb{R}^r$, with parameter ω , width W_R , and depth H_R .

Conditions and Assumptions

 Assumption 1. The similarity measure between the outlier sources and the target domain is assumed to be of a much larger order than h,

$$\forall t \in S^c, \mathbb{E}_{P_{\tilde{Z}}^{(t)}} d_{\mathcal{F}_B^1} \left(P_{Y|\tilde{Z}}^{(t)}, P_{Y|\tilde{Z}}^{(0)} \right) = O(h^{\alpha}), \alpha > 1.$$

• Assumption 2. For some $\delta>0, (\hat{Z},Y)$ satisfies the first-order moment tail condition, for any $n\geq 1$,

$$\mathbb{E}\left[\|(\hat{Z},Y)\|\mathbb{I}_{\{\|(\hat{Z},Y)\|>\log n\}}\right] = O\left(n^{-(\log n)^{\delta}/(r+q)}\right).$$

- Assumption 3. The noise distribution P_{η} is absolutely continuous with respect to the Lebesgue measure.
- Assumption 4. The IPM distance between the conditional distributions of reliable source domains and the target domain is bounded in expectation, for some $h = O\left(\max\left\{n^{-1/r+q}, n_0^{-1/r}\right\}\right)$,

$$\forall t \in S \subset [T], \quad \mathbb{E}_{P_{\hat{Z}}^{(t)}} d_{\mathcal{F}_{B}^{1}} \left(P_{Y|\hat{Z}}^{(t)}, P_{Y|\hat{Z}}^{(0)} \right) \leq h.$$

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Conditions and Assumptions

• Assumption 5. The conditional distribution of the target domain satisfies a certain Lipschitz condition under the Total Variation (TV) distance, for some K>1:

$$\forall \hat{\mathbf{z}}_1, \hat{\mathbf{z}}_2, d_{TV} \left(P_{Y|\hat{Z} = \hat{\mathbf{z}}_1}^{(0)}, P_{Y|\hat{Z} = \hat{\mathbf{z}}_2}^{(0)} \right) \leq \frac{K - 1}{2B} \left\| \hat{\mathbf{z}}_1 - \hat{\mathbf{z}}_2 \right\|_1,$$

where $d_{TV}(\cdot, \cdot)$ is the TV distance.

• **Assumption 6.** The conditional distribution of the target domain satisfies a certain Lipschitz condition under the 1-Wasserstein distance, for some K>1:

$$\forall \tilde{\mathbf{z}}_1, \tilde{\mathbf{z}}_2 \in \mathcal{Z}, W_1\left(P_{Y|\tilde{Z}=\tilde{\mathbf{z}}_1}^{(0)}, P_{Y|\tilde{Z}=\tilde{\mathbf{z}}_2}^{(0)}\right) \leq (K-1) \|\tilde{\mathbf{z}}_1 - \tilde{\mathbf{z}}_2\|_1,$$

where $W_1(\cdot,\cdot)$ is the 1-Wasserstein distance.



If S is known

Theorem 1 Suppose Assumptions 2-5 hold. Let (W_D, H_D) of $D_{\phi}, (W_G, H_G)$ of G_{θ} and (W_R, H_R) of R_{ω} be specified such that $W_D H_D = \lceil \sqrt{n} \rceil, W_G^2 H_G = c_1 q n$. and $W_R^2 H_R = c_2$ rn for some constants $12 \le c_1, c_2 \le 384$. Let $n = \sum_{t \in S \cup \{0\}} n_t$, we have:

$$\mathbb{E}_{\hat{G}} d_{\mathcal{F}_{B}^{1}} \left(P_{\hat{Z}, \hat{G}}, P_{\hat{Z}, Y}^{(0)} \right) \lesssim n^{-1/(r+q)} \log n + n_{0}^{-1/r}.$$

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When $P_{Z,Y}$ has a bounded support, we can drop the logarithm factor.

Theorem 2 Suppose that $P_{\hat{z}|V}$ is supported on $[-U, U]^{r+q}$ for some U>0and Assumptions 3-5 hold. (W_D, H_D) of D_{ϕ} , (W_G, H_G) of G_{θ} and (W_R, H_R) of R_{ω} be specified such that $W_DH_D=\lceil \sqrt{n}\rceil, W_G^2H_G=c_1qn$ and $W_R^2H_R=c_2rn$ for some constants $12 \le c_1, c_2 \le 384$. Let the output of G_{θ} be on $[-U, U]^q$. Let $n = \sum_{t \in S \cup \{0\}} n_t$, we have:

$$\mathbb{E}_{\hat{G}} d_{\mathcal{F}_{B}^{1}} \left(P_{\hat{Z}, \hat{G}}, P_{\hat{Z}, Y}^{(0)} \right) \lesssim n^{-1/(r+q)} + n_{0}^{-1/r}.$$

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Corollary 3 Under the conditions of Theorem 2 we have

$$\mathbb{E}_{\hat{G}} \mathbb{E}_{P_{\hat{Z}}^{(0)}} d_{\mathcal{F}_{B}^{1}} \left(P_{\hat{G}|\hat{Z}}, P_{Y|\hat{Z}}^{(0)} \right) \lesssim n^{-1/(r+q)} + n_{0}^{-1/r}.$$

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If S is unknown

 $\begin{array}{ll} \underline{\textbf{Theorem 4}} & \text{Suppose that } P_{\tilde{Z},Y}, P_{\hat{Z},Y} \text{ is supported on } [-U,U]^{r+q} \text{ for some } U>0 \text{ and Assumptions 1,3-6 hold. Let } \left(W_{\tilde{D}}, H_{\tilde{D}}\right) \text{ of } D_{\tilde{\phi}}, \left(W_{\tilde{G}}, H_{\tilde{G}}\right) \text{ of } G_{\tilde{\theta}} \text{ and } \left(W_{\tilde{R}}, H_{\tilde{R}}\right) \text{ of } R_{\tilde{\omega}} \text{ be specified such that } W_{\tilde{D}}H_{\tilde{D}} = \lceil \sqrt{n} \rceil, W_{\tilde{G}}^2H_{\tilde{G}} = c_1qn \text{ and } W_{\tilde{R}}^2H_{\tilde{R}} = c_2rn \text{ for some constants } 12 \leq c_1, c_2 \leq 384, \text{ where } n = \sum_{t \in [T] \cup \{0\}} n_t. \\ \text{Let the output of } G_{\tilde{\theta}} \text{ be on } [-U,U]^q \text{ and threshold } C\left(\max\left\{n^{-1/(r+q)}, n_0^{-1/r}\right\}\right) = h, \text{ we have:} \end{array}$

$$\mathbb{E}_{\hat{G}} \mathbb{E}_{P_{\hat{Z}}^{(0)}} d_{\mathcal{F}_{B}^{1}} \left(P_{\hat{G}|\hat{Z}}, P_{Y|\hat{Z}}^{(0)} \right) \lesssim n^{-1/(r+q)} + n_{0}^{-1/(r+q)}.$$

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Simulation data: conditional density estimation

- For methods to compare, consider:
 - Selected Transfer-WGAN(STWGAN): The method we proposed,
 - Target-Only(TO): a method trained exclusively on the target domain without representation learning,
 - **Pool**: an ablation variant where $\lambda_t = 0$,
 - Pre-trained Fine-tuning(PT-FT): pretrained on source data.
- The samples are generated as:
 - Model 1 (M1). A nonlinear model:

$$Y = X_1 + \exp(X_2 + X_3/3) + \sin(X_4 + X_5) + \varepsilon,$$

where $\varepsilon \sim N(0, X_1^2)$.

• Model 2 (M2). A model with a multiplicative error:

$$Y = (2 + X_1^2/3 + X_2^2 + X_3^2 + X_4^2 + X_5^2)/3 \times \varepsilon,$$

where $\varepsilon \sim N(X_3, 1)$.

• Model 3 (M3). A mixture model:

$$Y = \mathbb{I}_{\{U \le 1/3\}} N \left(-3 - X_1/3 - X_2^2, 0.25 \right) + \mathbb{I}_{\{U > 1/3\}} N \left(3 + X_1/3 + X_2^2, 1 \right),$$

Simulation data: conditional density estimation

The covariate vector X is generated from $N(\boldsymbol{\mu}^{(t)}, \mathbf{I}_{100})$ in the t-th domain. So the ambient dimension of X is 100, but (M1) and (M2) only depend on the first 5 components of X and (M3) only depends on the first 2 components of X.

Table: The value of $\mu^{(t)}$, where the index (t) represents the domain, with (0) denoting the target domain.

(t)	$oldsymbol{\mu}^{(t)}$	posterior drift
(0)	$(2,1,0,\ldots,0)^{\top}$	-
(1)	$(0,0,0,\ldots,0)^{\top}$	No
(2)	$(5,5,5,\ldots,5)^{\top}$	No
(3)	$(-5,\ldots,-5)^{\top}$	No
(4)	$(2,1,0,\ldots,0)^{\top}$	Yes
(5)	$(2, 1, 0, \dots, 0)^{\top}$	Yes

Simulation data: conditional density estimation

We consider the posterior drift in the fourth and fifth source domains across different data generation models.

- Model 1 (M1). A nonlinear model with an additive error term:
 - (4): $Y = 5X_1 + \exp(X_2 + X_3/3 + 2) + \cos(X_4 + X_5) + \varepsilon + 5$,
 - (5): $Y = X_1/5 + \exp(X_2 + X_3/3 2) + \cos(X_4 + X_5) + \varepsilon 5$,

where $\varepsilon \sim N(0, X_1^2)$.

- Model 2 (M2). A model with a multiplicative Gaussian error term:
 - (4): $Y = (7 + X_1^3/3 + X_2^3 + X_3^3 + X_4^3 + X_5^3) \times \varepsilon + 5,$
 - (5): $Y = (-3 + X_1 + X_2 + X_3 + X_4 + X_5) \times \varepsilon 5$,

where $\varepsilon \sim N(X_3, 1)$

- Model 3 (M3). A mixture of two normal distributions:
 - (4): $Y = \mathbb{I}_{\{U \le 1/3\}} N\left(-8 X_1^3 X_2, 0.25\right) + \mathbb{I}_{\{U > 1/3\}} N\left(8 + X_1^3 + X_2, 1\right),$
 - (5): $Y = \mathbb{I}_{\{U \le 1/3\}} N (2 X_1 X_2, 0.25) + \mathbb{I}_{\{U > 1/3\}} N (-2 + X_1 + X_2, 1),$

where $U \sim \mathrm{Unif}(0,1)$ and is independent of X.

Evaluation

Similar to the experiments conducted by Liu et al. [2021], Zhou et al. [2023], we consider the **mean squared error (MSE)** of the estimated conditional mean $\mathbb{E}(Y\mid X)$ and the estimated conditional standard deviation $\mathrm{SD}(Y\mid X).$ We use a test data set $\{\pmb{x}_1,\ldots,\pmb{x}_K\}$ of size K=2000. For the proposed method, we first generate J=10000 samples $\{\eta_j:j=1,\ldots,J\}$ from the reference distribution P_η and calculate conditional samples $\left\{\hat{G}\left(\eta_j,\pmb{x}_k\right),j\in[J],k\in[K]\right\}.$

• The MSE of the estimated conditional mean:

$$MSE(mean) = (1/K) \sum_{k=1}^{K} {\{\widehat{\mathbb{E}}(Y \mid X = \mathbf{x}_k) - \mathbb{E}(Y \mid X = \mathbf{x}_k)\}^2},$$

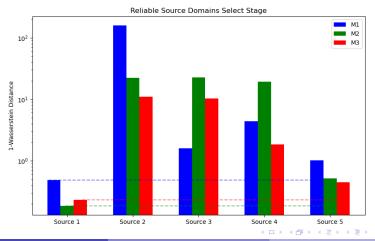
• The MSE of the estimated conditional standard deviation:

$$MSE(sd) = (1/K) \sum_{k=1}^{K} {\{\widehat{SD}(Y \mid X = \boldsymbol{x}_k) - SD(Y \mid X = \boldsymbol{x}_k)\}^2}.$$

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Selection results

In all three data simulated models, the first source domain is considered a reliable source domain, while the others are identified as outlier source domains.



Simulation results

we considered different sample sizes for the source domains while keeping $\,n_0=10,000\,$ fixed, as shown in Table.

			STWGAN	Target enly	Pool	PT-FT
				Target-only		
$n_t = 20,000$	M1	Mean	15.77 (1.29)	21.49(1.24)	16.90(1.63)	77.87(11.27)
		SD	4.43(1.48)	8.21(2.84)	1.89(0.45)	2.17(1.22)
	M2	Mean	4.40(1.10)	9.51(3.63)	6.75(2.35)	3.83(2.82)
		SD	1.95(0.30)	1.39(0.14)	1.84(0.18)	2.08(0.33)
	М3	Mean	2.22 (0.99)	25.75(4.10)	3.07(1.42)	3.07(1.02)
		SD	0.47 (0.10)	10.14(5.20)	0.75(0.10)	9.94(1.69)
$n_t = 40,000$	M1	Mean	10.64 (2.07)	17.06(1.91)	16.94(2.94)	81.76(11.55)
		SD	6.69(4.47)	7.69(3.33)	1.37(0.22)	1.66(0.46)
	M2	Mean	3.12(1.14)	7.10(3.01)	5.15(1.77)	5.01(2.81)
		SD	1.90(0.38)	1.53(0.23)	2.10(0.34)	2.67(1.04)
	М3	Mean	2.09 (1.39)	26.89(7.13)	2.32(1.55)	2.96(0.82)
		SD	0.54 (0.13)	7.72(4.06)	0.61(0.51)	8.09(2.72)
	M1	Mean	10.73 (1.16)	24.40(2.84)	17.56(1.69)	85.43(14.43)
		SD	2.84(1.59)	9.84(2.56)	1.61(0.56)	1.60(0.81)
$n_t = 60,000$	M2	Mean	2.22 (1.30)	7.73(4.01)	6.96(1.42)	5.27(3.10)
		SD	2.37(1.16)	1.51(0.20)	2.05(0.13)	3.46(1.36)
	М3	Mean	1.68(1.34)	20.97(3.40)	2.32(1.55)	2.66(1.03)
		SD	0.56 (0.06)	5.67(2.67)	0.61(0.51)	8.41(2.19)

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Image reconstruction: MNIST dataset

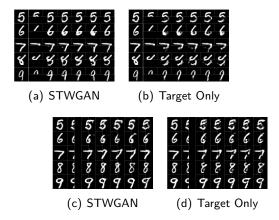


Figure: Comparison of STWGAN and Target Only: (a) and (b) show results of upper2lower, while figures (c) and (d) show results of left2right.

Image-to-Image translation



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Summary and Discussion

We proposed **S**elected **T**ransfer-**WGAN(STWGAN)**, a robust transfer approach designed to address the challenges of multi-source conditional generation models. This is achieved through a two-stage training process that maintains the training stability of WGAN. Our algorithm does not rely on pre-trained models from large datasets and provides both non-asymptotic error bounds and asymptotic guarantees.

Future work will discuss how neural networks can learn complex dimensionality reduction structures and retain useful information.

THANKS!

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