Super learner for tabular synthetic data generation

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Introduction

Introduction : Sensitive Medical Data

Privacy and Medical Data

- **In health dataset medical information are sensitives**, data breaches.
- **General regulations** (e.g., adoption of GDPR by the EU in 2018, HIPAA in USA), data cannot be kept after a certain delay and can be shared under strict conditions.

Introduction : Current Solutions

Pseudonymisation and Anonymisation

- **Pseudonymisation** (replacing directly identifiable data, e.g. names with codes). Pseudonymisation remains vulnerable to linkage attacks.
- **Anonymisation** : irreversible removal of data identifiability. Fully anonymized data are the goal, can be shared according to GPDR but can lose utility - See Supplementary Material.

Federated learning with Differential Privacy (DP)

Promising approach but have some drawbacks

- **Federated learning** requires specific architectural configurations,
- **Differential Privacy** [1] considered the gold standard for privacy protection, necessitates a DP-compliant version of each ML or stat. algorithm used.

Synthetic data

- The goal is to enable data sharing with a better utility than anonymization, especially for educational or open science purposes.

1. Dwork, "Differential privacy." In *Proceedings of the International Colloquium on Automata, Languages, and Programming*, pages 1–12, 2006. Springer.

Synthetic Data Challenge

- Synthetic data is "*a promising alternative to address the **trade-off** between **broad data access** and **disclosure protection***" [2]

- Synthetic data is an old subject **attributed to Rubin** [3] in 1993 (one of the fathers of missing data literature and causal inference).
  - He proposed multiple synthetic generation datasets.
  - Inferential methods for multiple synthetic generation were developed by Raghunathan et al. [4] and Reiter [5].

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2. Drechsler, J. (2024). *Synthetic Data for Official Statistics : State of the Art and Challenges*. Journal of Official Statistics, 40(1), 30–52.
3. Rubin, D. B. (1993). *Statistical disclosure limitation*. Journal of Official Statistics, 9(2), 461–468.
4. Raghunathan, T. E., Reiter, J. P., and Rubin, D. B. (2003). *Multiple imputation for statistical disclosure limitation*. Journal of Official Statistics, 19(1), 1–16.
5. Reiter, J. P. (2003). *Inference for partially synthetic, public use microdata sets*. Survey Methodology, 29(2), 181–188.

Privacy versus Utility

Privacy has a cost on the utility of the analysis, ideally it should not destroy it.

Utility

Utility is a measure of how well synthetic data retains the statistical properties and practical usefulness of real data :

- Statistical utility : Synthetic data should preserve all the statistical properties of the original data (marginal and joint distribution).
- Task-based utility : regression's coefficients, supervised learning, etc.

Privacy

- Privacy can be defined as "the ability of an individual to withhold information about themselves".
- The goal is to preserve the right of individuals to control how their personal data is shared and to ensure that it is kept secure and only accessed by authorized parties.

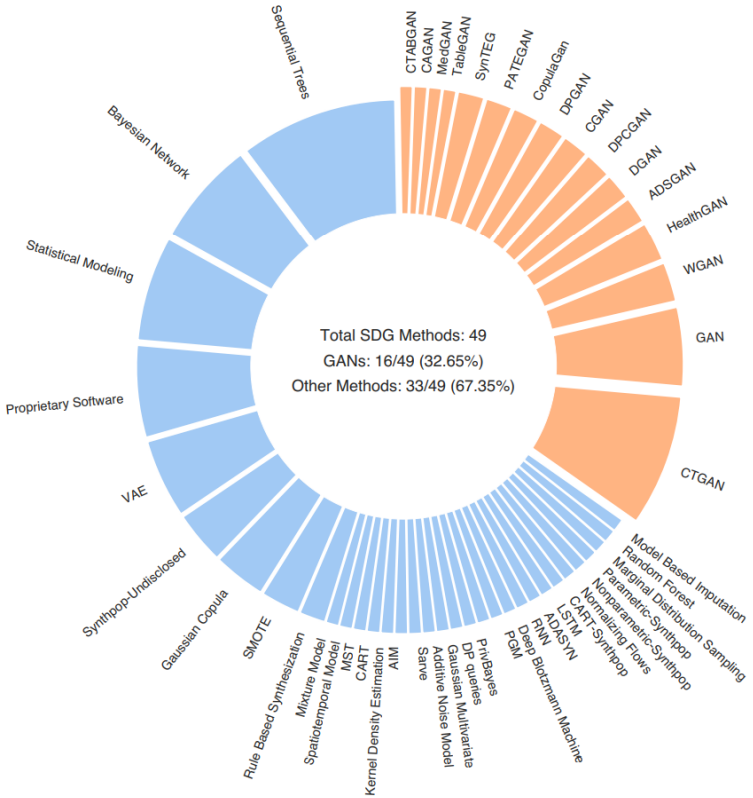
Overview of the Presentation

We will cover the following topics :

- Commonly used methods for synthetic data generation.
- Approaches for evaluating privacy and utility metrics.
- Superlearner-based frameworks : several methods tested on simulated datasets.
- Open challenges and future directions for superlearner-based synthetic data generation.

Existing methods

The Rise of Synthetic Data Generation with GANs



Synthetic data generation methods [6]

49 different synthetic data generation methods : GANs (32.65 % of the total) and other techniques reports in that figure in a review based on 92 studies. They founded 48 utility metrics and 9 methods to evaluate privacy.

6. Kaabachi, Bayrem, et al. "A scoping review of privacy and utility metrics in medical synthetic data." NPJ digital medicine 8.1 (2025)

Concurrent Methods

In our analysis, we further categorize these into :

- **Synthpop** : One of the first packages available (in R) since 2016 [7].
- **Avatar** : A SMOTE-like method based on k-nearest neighbors [8]. Octopize startup, not free, re-implemented using custom Python code.
- **Conditional Tabular Generative Adversarial Network (CTGAN)** : A more recent approach, available in several Python libraries, with support for various data structures (longitudinal, survival, etc.).
  - CTGAN from Synthcity [9].
  - Synthetic Data Vault [10].
  - TabGAN [11]

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7. Nowok et al., "synthpop : Bespoke creation of synthetic data in R." *Journal of Statistical Software*, 74 :1–26, 2016.
8. Guillaudeux et al., "Patient-centric synthetic data generation, no reason to risk re-identification in biomedical data analysis." *NPJ Digital Medicine*, 6(1) :37, 2023. Nature Publishing Group UK, London.
9. Qian et al., "Synthcity : a benchmark framework for diverse use cases of tabular synthetic data." *Advances in Neural Information Processing Systems*, 36 :3173–3188, 2023.
10. Patki et al., "The Synthetic Data Vault." In *Proceedings of the IEEE International Conference on Data Science and Advanced Analytics (DSAA)*, pages 399–410, October 2016. doi : 10.1109/DSAA.2016.49.
11. Ashrapov, I. (2020). Tabular GANs for uneven distribution. arXiv preprint arXiv :2010.00638. ; https ://github.com/Diyago/Tabular-data-generation/tree/master

Synthpop Method [12]

The **Synthpop** approach models the joint distribution of variables and then samples from it sequentially.

Let $\{X^{(1)}, X^{(2)}, \ldots, X^{(p)}\}$ be a set of p variables. The joint distribution is factorized as :

$$P(X) = \prod_{k=1}^{p} P(X^{(k)} \mid X^{(1)}, \ldots, X^{(k-1)})$$

Each conditional distribution is estimated (e.g., via GLMs or CART) and used to simulate synthetic values in order.

Algorithm : Synthpop Generation of a Sample

1: Draw $x_{\text{syn}}^{(1)}$ from the empirical distribution of $\{x_{\text{true},1}^{(1)}, \ldots, x_{\text{true},n}^{(1)}\}$
2: **for** $k = 2$ to p **do**
3: Draw $x_{\text{syn}}^{(k)} \sim \widehat{P}\left(X^{(k)} \mid x_{\text{syn}}^{(1)}, \ldots, x_{\text{syn}}^{(k-1)}\right)$
4: **end for**

12. Nowok et al., "synthpop : Bespoke creation of synthetic data in R." *Journal of Statistical Software*, 74 :1–26, 2016.

Synthpop's Properties

Models and Flexibility :

- **CART** is the default model. Although it is not inherently distributional, it approximates draws from a conditional distribution by sampling from the leaves [13].
- **Alternatives** : Logistic, multinomial, and Poisson regression models are also supported.
- **Custom models** can be defined for specific data types.

Pros and Cons :

- **+ Flexible** : Allows different models per variable and supports known data structure.
- **– Sensitive to variable order** : The generation process depends on variable sequencing, which may affect synthetic data quality.

13. Future work may explore distributional tree models such as DRF : Cevid, Domagoj, et al. "Distributional random forests : Heterogeneity adjustment and multivariate distributional regression." *Journal of Machine Learning Research* 23.333 (2022) : 1-79.

Avatar [14]

1. **Normalization** and projection using **Principal Component Analysis (PCA)** to reduce the dimensionality of the dataset.
2. Apply the k-**nearest neighbors algorithm** to the PCA-transformed dataset to select the k neighbors $x_i^1, \ldots, x_i^k$ of each original sample x_i.
3. Generate synthetic data in the latent space using :

$$\tilde{x}_i = \frac{\sum_{j=1}^{k} P_i^j x_i^j}{\sum_{j=1}^{k} P_i^j},$$

   where P_i^j is the weight attributed to neighbor x_i^j of the original sample x_i.
4. The weight is computed as :

$$P_i^j = \frac{1}{d_i} \times R_i^j \times C_i^j,$$

   where :
   - $d_i = d(x_i, x_i^j)$ is the distance between x_i and its neighbor x_i^j,
   - $R_i^j \sim \mathcal{E}xp(1)$ is a random weight following an exponential distribution,
   - $C_i^j = \left(\frac{1}{2}\right)^{\sigma(j)}$ is a contribution term, where σ is a random permutation in $\mathcal{S}_k$, the space of bijections over $\{1, \ldots, k\}$.
5. Return to the original space and reverse the normalization.

14. Guillaudeux et al., "Patient-centric synthetic data generation, no reason to risk re-identification in biomedical data analysis." *NPJ Digital Medicine*, 6(1) :37, 2023. Nature Publishing Group UK, London.

Avatar's illustration and properties

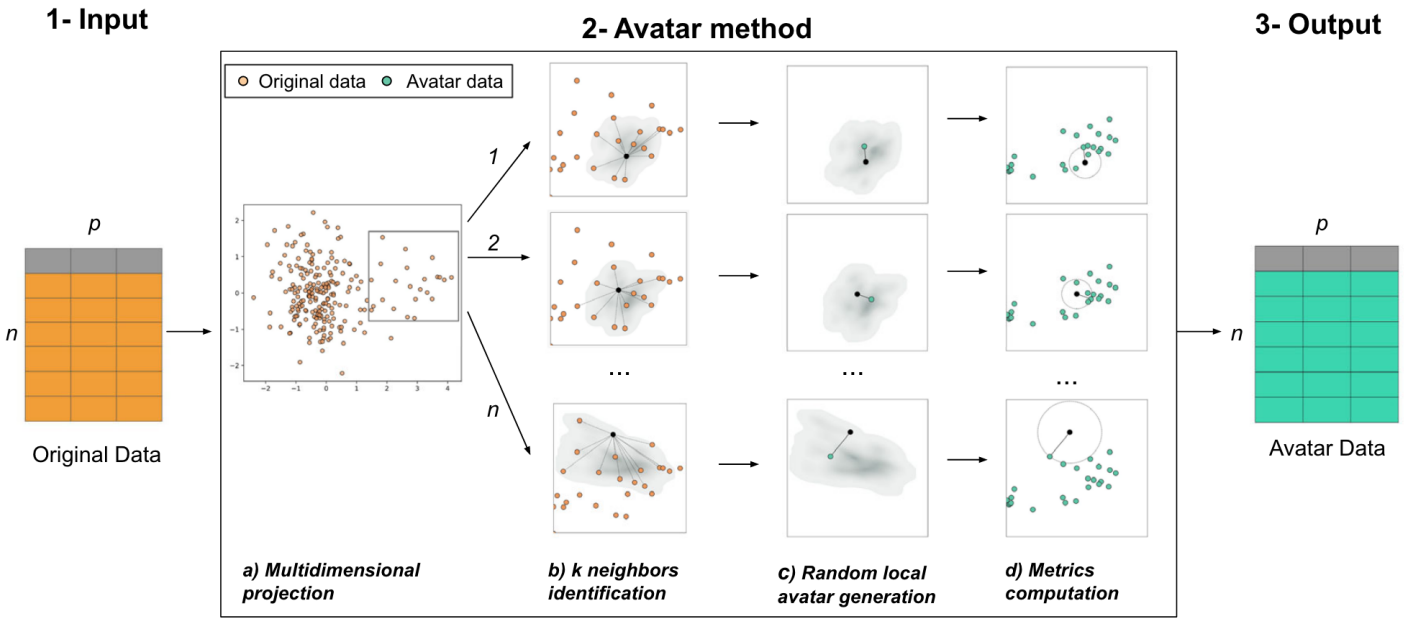


Figure 1 – Guillaudeux, et al. NPJ Digital Medicine, 6(1) :37, 2023.

Avatar can handle **categorical features** and **missing data** using Multiple Correspondence Analysis (MCA), Factorial Analysis of Mixed Data (FAMD) and matrix completion methods (iterative SVD) [15].

15. Josse, J. and Husson, F. (2012). Handling missing values in exploratory multivariate data analysis methods. Journal de la société française de statistique, 153(2), 79–99. - Avatar creators are former student of F. Husson.

CTGAN

- **Generator** : Receives a random noise vector and conditional vector. Outputs synthetic data rows.
- **Discriminator** : Takes real and synthetic data as input. Outputs probability of data being real.
- **Conditional Vector** : Ensures that generated data matches the distribution of real data. Helps in handling imbalanced discrete columns.

Training process :

- Sample a batch of real data and corresponding conditional vectors.
- Generate synthetic data using the generator.
- Train the discriminator to distinguish between real and synthetic data.
- Train the generator to fool the discriminator.
- Repeat until convergence.

Which Metrics Are Relevant ?

Metrics

- **In most cases, univariate metrics** [16] are commonly used, including the t-test, Kolmogorov–Smirnov test, and univariate distributional distances such as the Wasserstein and Hellinger distances.

- A common multivariate proxy in the literature is the **comparison of correlation matrices such as pairwise correlation difference** [17].

- In this work, we focus on **multivariate distributional measures** to capture joint dependencies between variables more comprehensively.

16. Kaabachi, Bayrem, et al. "A scoping review of privacy and utility metrics in medical synthetic data." *NPJ Digital Medicine*, 8(1) :60, 2025.
17. Goncalves et al., Generation and evaluation of synthetic patient data. *BMC Med Res Methodol* 20, 108 (2020)

Utility metrics : Multivariate distributional distance

Energy distance [18]

We suppose that your original data X_i are i.i.d copies from $X \sim P$, we generate synthetic data from a distribution H.

$$\begin{aligned} d(H,P) &= 2\mathbb{E}_{Y\sim P, X\sim H}(||Y-X||_2) - \mathbb{E}_{Y\sim P, Y'\sim P}(||Y-Y'||_2) \\ &\quad -\mathbb{E}_{X\sim P, X'\sim P}(||X-X'||_2). \end{aligned}$$

How to estimate this $d(H,P)$, with X_i and Y_j i.d.d. copies of X and Y ?

$$\begin{aligned} \mathcal{E}_{n,n}(X,Y) &= \frac{2}{n^2}\sum_{i=1}^{n}\sum_{m=1}^{n}||X_i - Y_m||_2 - \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}||X_i - X_j||_2 \\ &\quad - \frac{1}{n^2}\sum_{m=1}^{n}\sum_{k=1}^{n}||Y_k - Y_m||_2. \end{aligned}$$

18. Székely, "E-statistics : The energy of statistical samples." *Bowling Green State University, Department of Mathematics and Statistics Technical Report*, 3(05) :1–18, 2003.

Other Utility Metrics

Wasserstein distance

$$W_2(P, H) = \left(\inf_{\gamma \in \Pi(P,H)} \int_{\mathcal{X} \times \mathcal{X}} d(x, y)^2 \, d\gamma(x, y) \right)^{1/2}.$$

Propensity MSE (pMSE) [19] : Can we distinguish the original and the synthetic data ?

- $\widehat{p}_i$ is the estimated probability by a binary classifier for the sample i to be a synthetic data.
- $c = \frac{n_{syn}}{n_{orig}+n_{syn}}$ the probability to draw a synthetic data into the concatenated original and synthetic dataset
- $pMSE = \sum_{i=1}^{n_{orig}+n_{syn}} (\widehat{p}_i - c)^2$
- Sensible to the classifier used (CART, RF, logistic regression). [20]

19. Woo, M.-J., Reiter, J. et al., "Global measures of data utility for microdata masked for disclosure limitation." *Journal of Privacy and Confidentiality*, 1(1), 2009.

20. Snoke, J., Raab, G. M., Nowok, B., Dibben, C., and Slavković, A. "General and specific utility measures for synthetic data." *Journal of the Royal Statistical Society : Series A (Statistics in Society)*, 181(3) :663–688, 2018. Oxford University Press.

Tasked Based / Inferential utility

- Distance from the parameter from the value of the original dataset
- Coverage : Proportion of times that the confidence intervals of the synthetic data include the true values (possible in simulations)
- Overlap of confidence interval of estimators (Drechsler and Reiter , 2009 [21] ; Nowok, 2015 [22])

21. Drechsler, J., and Reiter, J. P. (2009). Disclosure risk and data utility for partially synthetic data : An empirical study using the German IAB Establishment Survey. Journal of Official Statistics, 25(4), 589.
22. Nowok, B. (2015). Utility of synthetic microdata generated using tree-based methods. UNECE Statistical Data Confidentiality Work Session, 1-11.
23. Decruyenaere et al "The real deal behind the artificial appeal : Inferential utility of tabular synthetic data." *arXiv preprint* arXiv :2312.07837, 2023.

Privacy : Metrics based on distances between sample from the original data $\mathcal{X}$ and the synthetic data $\mathcal{S}$

Distance to Closest Record (DCR)

Measures the Euclidean distance between each synthetic record and its closest real record.

$$DCR(s) = \min_{x \in \mathcal{X}} d(s, x)$$

The metric can be 5th percentile of the vector (Zhao et al. (2021) [24], or the mediane Guillaudeux et al. (2023) [25] and Kotelnikov et al. (2022) [26]).

Nearest Neighbor Distance Ratio (NNDR)

Ratio between the distance to the closest and the second closest real record for each synthetic record $s \in \mathcal{S}$.

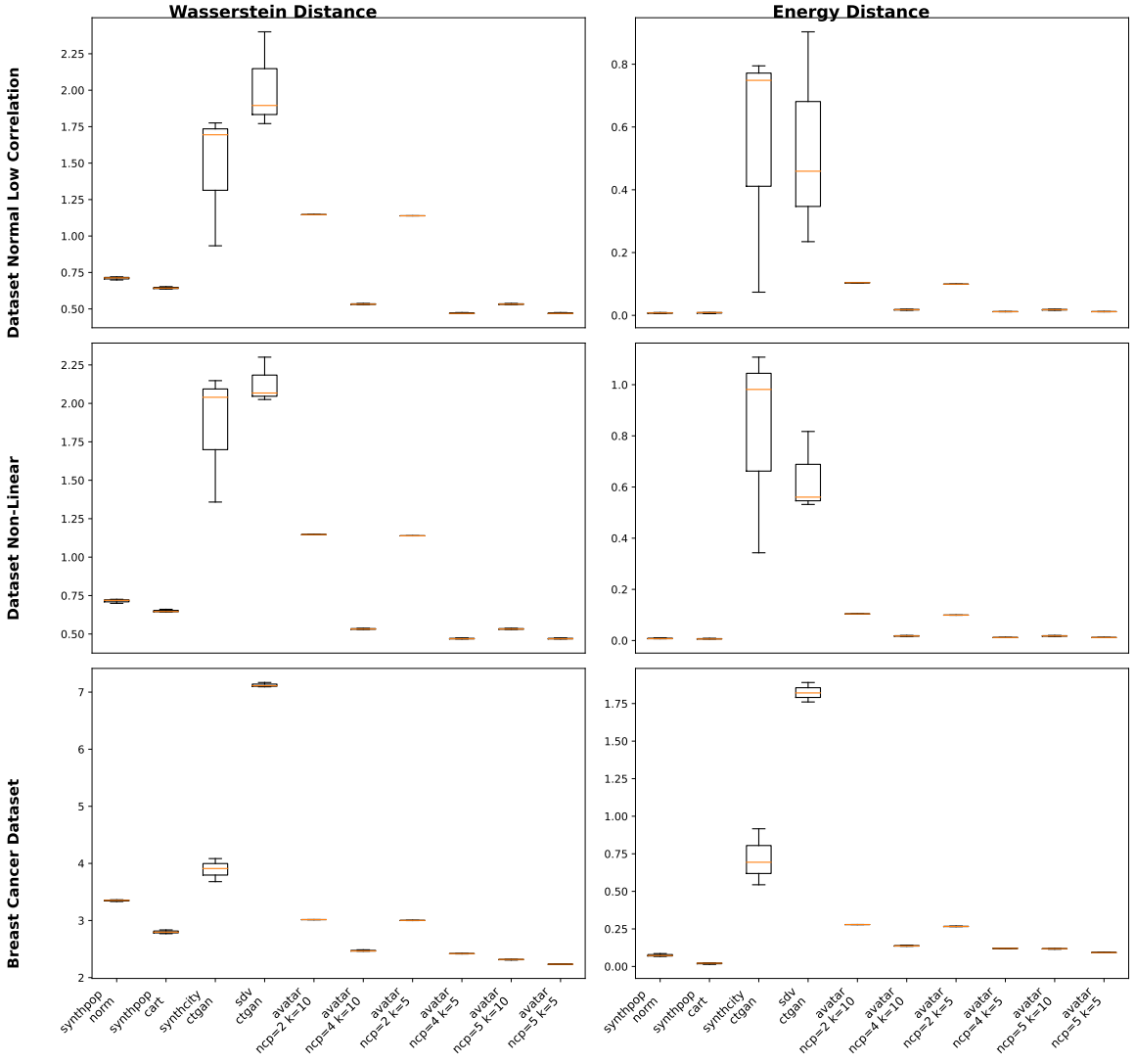
$$\text{NNDR}(s) = \frac{d\left(s, x_{\text{nearest}}\right)}{d\left(s, x_{\text{second-nearest}}\right)}$$

24. Zhao, Z., Kunar, A., Birke, R., Chen, L. Y. (2021, November). Ctab-gan : Effective table data synthesizing. In Asian Conference on Machine Learning (pp. 97-112). PMLR.
25. Guillaudeux et al., "Patient-centric synthetic data generation, no reason to risk re-identification in biomedical data analysis." *NPJ Digital Medicine*, 6(1) :37, 2023. Nature Publishing Group UK, London.
26. Kotelnikov, A., Baranchuk, D., Rubachev, I., Babenko, A. (2023, July). Tabddpm : Modelling tabular data with diffusion models. In International Conference on Machine Learning (pp. 17564-17579). PMLR.

Which methods should we use for the best utility ?

Simulation on 3 differents dataset :

- Gaussian samples, $Y = \beta X + \epsilon$; Non linear dataset ; Breast cancer dataset [27]



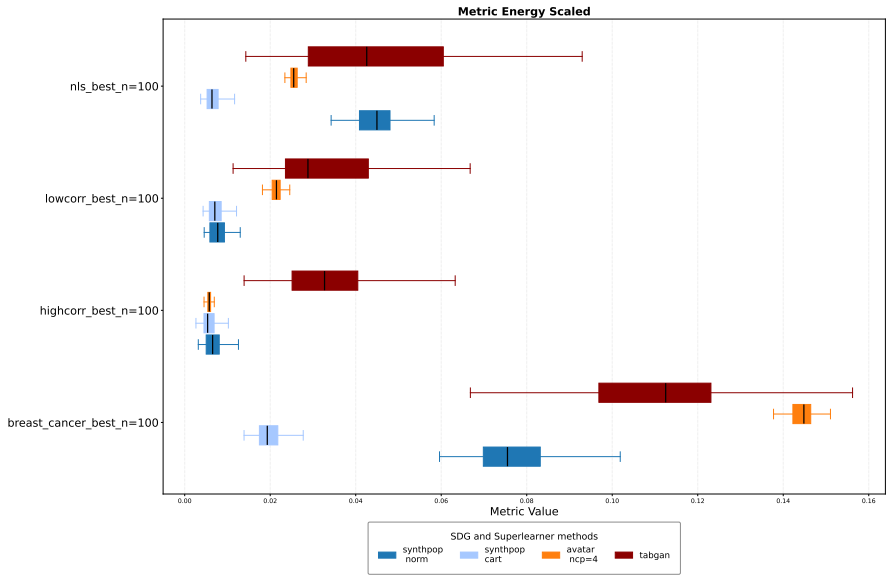


Figure 3 – Utility measure on the 3 differents dataset - best SDG methods, n=100

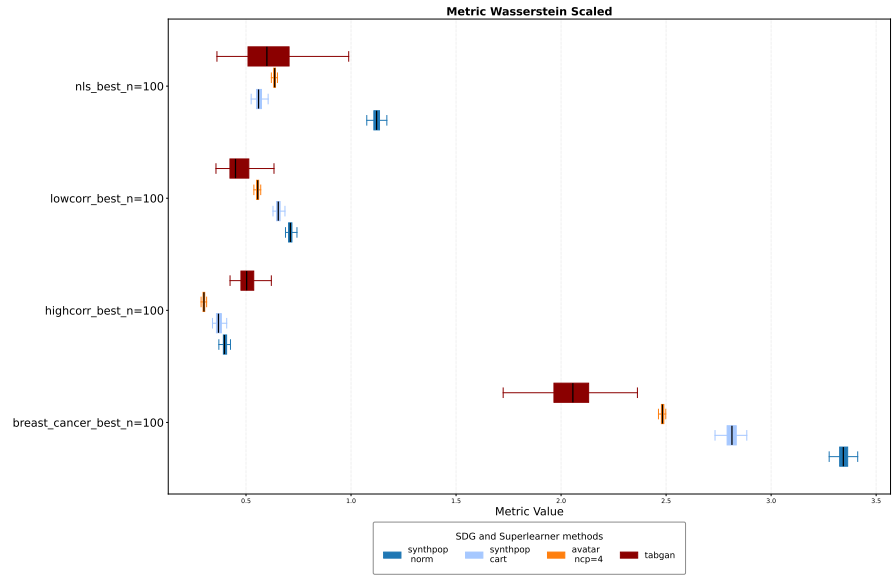


Figure 4 – Utility measure on the 4 differents dataset - best SDG methods, n=100

Which methods should we use for the best privacy ?

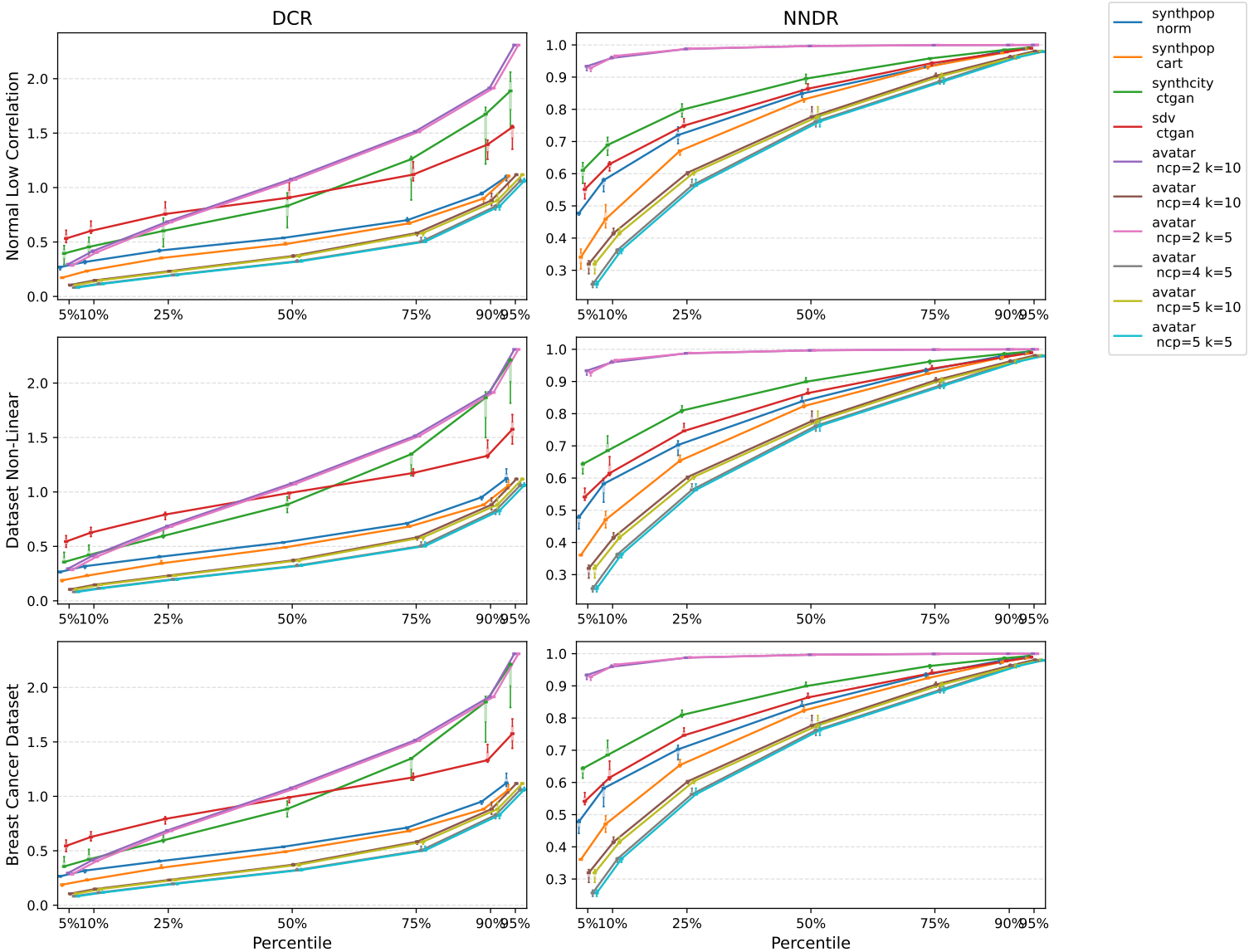


Figure 5 – DCR and NNDR metrics for different percentiles for n=100 simulations

Which Methods Should We Use ?

- **CTGAN (SynthCity / SDV)** :
  - Poor performance and high computational cost.
- **Synthpop (Gaussian regression)** :
  - Effective on normally distributed datasets.
- **Synthpop (CART)** :
  - Also yields good results with more flexibility.
- **Synthpop :** shows the best balance overall in terms of Privacy-Utility
- **Avatar :**
  - Performs well *if* dimensionality reduction is suited to the dataset.
  - May require prior knowledge.

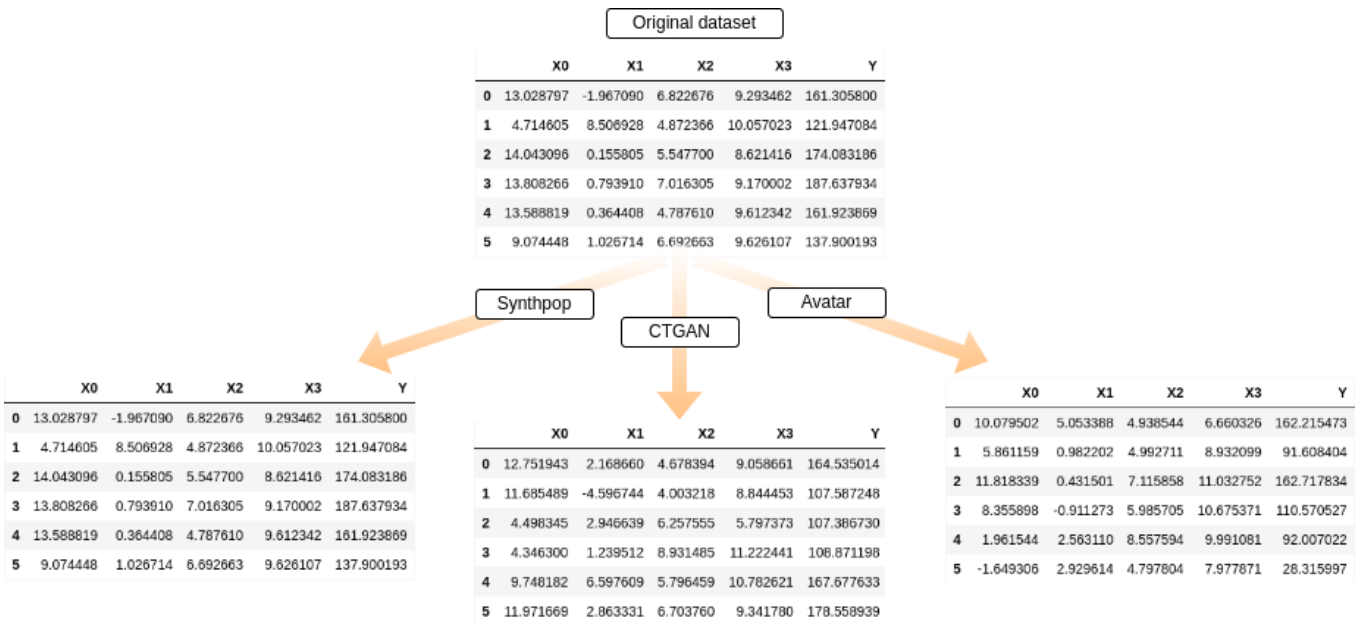
Superlearner ideas

Purpose of a Superlearner

Motivation :

- Different synthetic data generation methods perform better on different types of data structures.
- Combining them can potentially improve both utility and privacy.

Goal : Leverage multiple synthetic datasets to build a more robust and privacy-preserving synthetic dataset.



Original dataset

	X0	X1	X2	X3	Y
0	13.028797	-1.967090	6.822676	9.293462	161.305800
1	4.714605	8.506928	4.872366	10.057023	121.947084
2	14.043096	0.155805	5.547700	8.621416	174.083186
3	13.808266	0.793910	7.016305	9.170002	187.637934
4	13.588819	0.364408	4.787610	9.612342	161.923869
5	9.074448	1.026714	6.692663	9.626107	137.900193

Synthpop

	X0	X1	X2	X3	Y
0	13.028797	-1.967090	6.822676	9.293462	161.305800
1	4.714605	8.506928	4.872366	10.057023	121.947084
2	14.043096	0.155805	5.547700	8.621416	174.083186
3	13.808266	0.793910	7.016305	9.170002	187.637934
4	13.588819	0.364408	4.787610	9.612342	161.923869
5	9.074448	1.026714	6.692663	9.626107	137.900193

CTGAN

	X0	X1	X2	X3	Y
0	12.751943	2.168660	4.678394	9.058661	164.535014
1	11.685489	-4.596744	4.003218	8.844453	107.587248
2	4.498345	2.946639	6.257555	5.797373	107.386730
3	4.346300	1.239512	8.931485	11.222441	108.871198
4	9.748182	6.597609	5.796459	10.782621	167.677633
5	11.971669	2.863331	6.703760	9.341780	178.558939

Avatar

	X0	X1	X2	X3	Y
0	10.079502	5.053388	4.938544	6.660326	162.215473
1	5.861159	0.982202	4.992711	8.932099	91.608404
2	11.818339	0.431501	7.115858	11.032752	162.717834
3	8.355898	-0.911273	5.985705	10.675371	110.570527
4	1.961544	2.563110	8.557594	9.991081	92.007022
5	-1.649306	2.929614	4.797804	7.977871	28.315997

Figure 6 – Superlearner idea

Superlearner ideas

Aggregation Combination Strategies :

- **STATIS-based Approaches :**
  - Dual STATIS
- **Barycenter Methods :**
  - **Wasserstein Barycenter** : based on Wasserstein distance
  - **MMD Barycenter** : based on maximum mean discrepancy in kernel space

Superlearner ideas

- **Original Dataset** :
  - $\mathcal{X} = \{x_1, x_2, \ldots, x_n\}$, with n samples from $\mathbb{R}^p$.
  - The data table is denoted as $\boldsymbol{X}$.

- **Synthetic Datasets** :
  - K methods generate K datasets : $\mathcal{S}_i = \{s_1^{(i)}, \ldots, s_n^{(i)}\}$
  - Each dataset has p variables (columns).
  - Each synthetic dataset has n samples same as the original [28].
  - Samples $s_j^{(i)}$ are not necessarily derived from x_j.
  - Synthetic datasets : $\boldsymbol{S^{(1)}}, \ldots, \boldsymbol{S^{(K)}}$.

28.

Dual Statis [29]

- Find a trade-off table that "summarizes" the synthetic data tables $\boldsymbol{S}^{(1)}, \ldots, \boldsymbol{S}^{(K)}$ represent the data tables.
- For each table l, compute the scalar product matrix :

$$V^{(l)} = (S^{(l)})^\top S^{(l)} \in \mathbb{R}^{p \times p}, \quad V^{(l)}_{ij} = \langle C^{(l)}_i, C^{(l)}_j \rangle$$

- $V^{(l)}$ is a symetric matrix $p \times p$, $V^{(l)}_{i,j} = V^{(l)}_{j,i} = corr(\text{variable i}, \text{variable j})$ (because we center, scale datatable)
- Δ is a $K \times K$ diagonal matrix of weights for each table.
- $$\bar{V} = \underset{V^\star = \underset{\|\gamma\|^2_\Delta = 1}{\text{argmax}} \sum_k^K \gamma_k V^{(k)}}{\text{argmax}} \sum_{k=1}^{K} < V^\star, V^{(k)} >^2_{\text{HS}}$$

29. Lavit, C., Escoufier, Y., Sabatier, R., Traissac, P. (1994). The act (statis method). Computational Statistics Data Analysis, 18(1), 97-119.

Dual Statis

- Matrix of Hilbert-Schmidt scalar products $\Omega_{k,l} =< V^{(k)}, V^{(l)} >_{HS} = \text{trace}(V^{(k)} V^{(l)})$.
- τ_1 : first normalized eigenvector of $\Omega\Delta$ (in decreasing order of the eigenvalues), with all coordinates positive [30].
- The tables can then be represented along the axes defined by the eigenvectors.
- Different way to define a "trade-off table"
  - Mean : $\bar{V} = \frac{1}{K} \sum_{i=1}^{K} V_i$
  - Weighted mean : $\bar{V} = \frac{1}{K} \sum_{i=1}^{K} \delta_i V_i$
  - Weighted mean with eigenvector τ : $\bar{V} = \frac{1}{K} \sum_{i=1}^{K} [\tau_1]_i V_i$

30. This eigenvalue always exists according to Frobenius theorem

How to Reconstruct the Table $\bar{S}$

Singular Value Decomposition

- For each data table $S^{(l)}$, we assume the decomposition :

$$S^{(l)} = Q^{(l)} \Sigma^{(l)} P^{(l)\top}$$

where $\Sigma^{(l)}$ is diagonal.

- Then, define matrix :

$$V^{(l)} = S^{(l)\top} S^{(l)} = P^{(l)} \Lambda^{(l)} P^{(l)\top}$$

$$W^{(l)} = S^{(l)} S^{(l)\top} = Q^{(l)} \Gamma^{(l)} Q^{(l)\top}$$ [31]

where $\Lambda^{(l)} = \Sigma^{(l)\top} \Sigma^{(l)}$ $\Gamma^{(l)} = \Sigma^{(l)} \Sigma^{(l)\top}$ and is diagonal.

- Our goal is to reconstruct the matrix $\bar{S}$ such that :

$$\begin{aligned} \bar{V} &= \bar{S}^\top \bar{S} \\ \bar{S} &= \bar{Q} \bar{\Sigma} \bar{P}^\top \end{aligned}$$

We can then find $\bar{P}$ and $\bar{\Sigma}$ from its eigendecomposition.

31. The original STATIS method interprets the W matrix as being tailored for multiple data tables comprising the same set of individuals, each characterized by different variables.

Constructing $\bar{S}$ and Basis Alignment

- We need to find a matrix $\bar{Q}$, so for that we use the SVD from the best synthetic datatable $S^{(l^*)}$:

$$W^{(l^*)} = S^{(l^*)} S^{(l^*)\top} = Q \Lambda Q^\top$$ [32]

- Define :

$$\bar{\Sigma} = \begin{bmatrix} \sqrt{\lambda_1} & 0 & \dots & 0 \\ 0 & \sqrt{\lambda_2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sqrt{\lambda_p} \\ 0 & 0 & \dots & 0 \end{bmatrix} \in \mathbb{R}^{n \times p}$$

- Final trade-off matrix :

$$\bar{S} = Q \bar{\Sigma} \bar{P}^\top$$

32. An alternative is to use the trade-off matrix $\bar{W}$, capturing correlations between individuals as in the original STATIS framework. However, this assumes that individual i in a synthetic dataset represents the same real individual i, which generally does not hold except in the Avatar scenario. This approach remains feasible if synthetic datasets are appropriately paired

Orthogonal Procrustes Alignment

A basis mismatch remains, as illustrated in Figure 7. To address this, we need to change the basis and identify the optimal orthogonal transformation that aligns the synthetic data table $\bar{\boldsymbol{S}}$ as closely as possible with $\bar{\boldsymbol{X}}$.

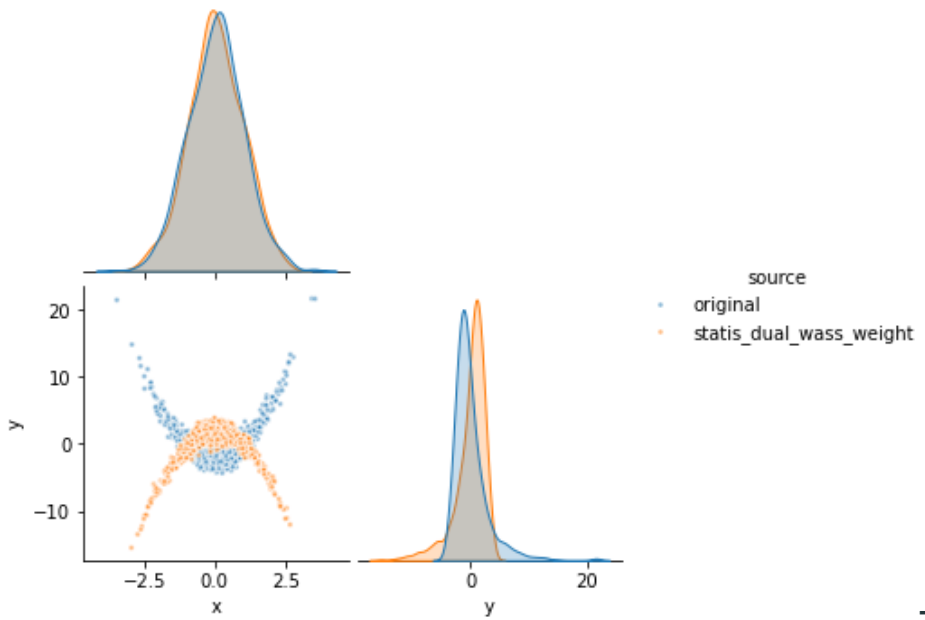


Figure 7 – Example of STATIS

Orthogonal Procrustes Problem

- Given $\boldsymbol{X}, \bar{S} \in \mathbb{R}^{n \times p}$, find $T \in \mathcal{O}(p)$ that minimizes :

$$\min_{T \in \mathcal{O}(p)} \| T\bar{S} - \boldsymbol{X} \|_F$$

- **Solution (Schönemann, 1966) :**
  1. Compute $A = \boldsymbol{X}\bar{\boldsymbol{S}}^\top$.
  2. Perform SVD : $A = U\Sigma V^\top$.
  3. The optimal T is $T = UV^\top$.

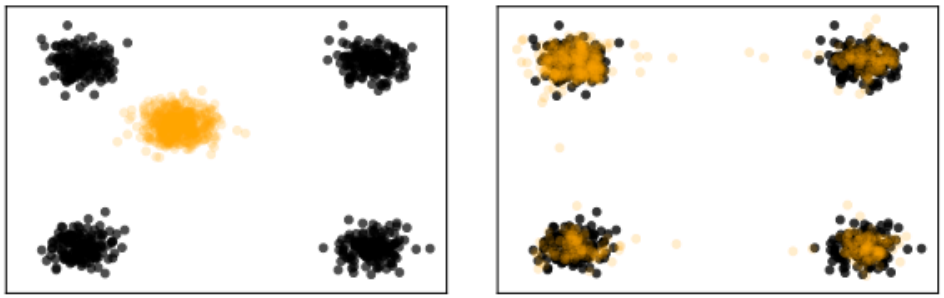
This T is the best orthogonal matrix (in Frobenius norm) aligning $\boldsymbol{X}$ with $\bar{\boldsymbol{S}}$.

Barycenter of Distributions

Definition : The *Fréchet mean* (or barycenter) of a set of probability distributions $\{\mu_1, \ldots, \mu_K\}$ with weights $\beta = (\beta_1, \ldots, \beta_K)$ is the distribution $\bar{\mu}$ minimizing the weighted sum of squared distances :

$$\bar{\mu} \in \arg\min_{\mu} \sum_{i=1}^{K} \beta_i \, d^2(\mu, \mu_i)$$

where d is a distance between probability distributions (e.g., Wasserstein or MMD).



(a) Wasserstein (b) MMD

Figure 8 – Barycenter (orange) of four Gaussians (black) with respect to (a) W ; (b) MMD. Best-left Gaussian has three times the weight of the others : $\beta = [3/6, 1/6, 1/6, 1/6]$.. [33]

33. Cohen et al., "Estimating barycenters of measures in high dimensions." *arXiv preprint arXiv :2007.07105*, 2020.

Super Learner with MMD Barycenter

Proposition (MMD Barycenter) [34] **:**
Let $\mu_1, \ldots, \mu_P \in \mathcal{M}_1^+(\mathcal{X})$ be probability measures and let $\beta \in \Delta_P$ be a weight vector (i.e., $\beta_p \geq 0, \sum_p \beta_p = 1$). If the discrepancy $D = \text{MMD}^2$, then the barycenter μ^* is given by :

$$\mu^* = \sum_{p=1}^{P} \beta_p \mu_p \in \mathcal{M}_1^+(\mathcal{X})$$

The MMD barycenter is simply the weighted *mixture* of the input measures.

Sampling Procedure :

1. Sample index $z \sim \text{Categorical}(\beta)$
2. Draw a sample $x \sim \mu_z$

Implication : Sampling from the MMD barycenter is computationally trivial — no optimization is needed.

34. Cohen et al., "Estimating barycenters of measures in high dimensions." *arXiv preprint arXiv :2007.07105*, 2020.

Super Learner with Wasserstein Barycenter

Goal : Aggregate datasets by computing the barycenter of their empirical distributions.

Wasserstein Barycenter :

$$\hat{\mu}^* = \arg\min_{\mu} \sum_{k=1}^{K} w_k W_2^2(\mu, \mu_k)$$

- $W_p(\mu, \nu)$: Wasserstein distance of order 2

$$W_2(\mu, \nu) = \left(\inf_{\gamma \in \Pi(\mu,\nu)} \int d(x,y)^2 \, d\gamma(x,y) \right)^{1/2}$$

- $w_k > 0$, $\sum w_k = 1$: weights for each empirical distribution

Empirical Measure Construction :

- Datasets : $\mathcal{D}^{(k)} = \{x_i^{(k)}\}_{i=1}^{n_k}$, $x_i^{(k)} \in \mathbb{R}^d$
- Partition space $\mathcal{X}$ into hypercubes I_i

$$\tilde{\mu}_k = \sum_{i=1}^{N} \left(\frac{1}{n_k} \sum_{x \in \mathcal{D}^{(k)}} \mathbb{I}_{\{x \in I_i\}} \right) \delta_{a_i}$$

Computation :

$$\tilde{\mu}^* = \arg\min_{\mu} \sum_{k=1}^{K} w_k W_2^2(\mu, \tilde{\mu}_k) \quad \text{(using OTT-JAX)}\,^{35}$$

Sampling : $\tilde{\mu}^*$ is defined on the same partition space of $\mathcal{X}$. This distribution is defined by the probability of each hypercube, so it becomes easy to sample in it. Flatten the barycenter distribution and sample from it using discrete probabilities.

Computation is very long and not suitable in high dimension ($p = 5$)

35. Cuturi, M., Meng-Papaxanthos, L., Tian, Y., Bunne, C., Davis, G., Teboul, O. (2022). Optimal transport tools (ott) : A jax toolbox for all things wasserstein. arXiv preprint arXiv :2201.12324.

Simulations

Simulation Scenarios : Dataset 1 - 2

- Linear dataset with low correlation (called :"lowcorr")
  - The original dataset is simulated as $X_i \overset{\text{iid}}{\sim} \mathcal{N}(m, \Sigma)$.
  - Mean vector and covariance matrix :

$$m = [7,\ 1.9,\ 6,\ 9], \Sigma = \begin{bmatrix} 5 & 0.08 & 0.005 & 0.15 \\ 0.08 & 2.5 & -0.03 & 0.034 \\ 0.005 & -0.03 & 1 & 0.13 \\ 0.15 & 0.034 & 0.13 & 1.5 \end{bmatrix}$$

  - $Y = X\beta + \epsilon$ with $\beta = [10,\ 6,\ 9,\ -2], \quad \epsilon \sim \mathcal{N}(0,\ 0.02)$.

- Linear dataset with high correlation (called :"highcorr")
  - Same process but with different correlation value
  - Mean vector and covariance matrix :

$$m = [7,\ 1.9,\ 6,\ 9], \Sigma = \begin{bmatrix} 0.5 & 0.08 & 2.5 & 0.5 \\ 0.08 & 0.25 & -1.3 & 0.5 \\ 2.5 & -1.3 & 1 & 3 \\ 0.5 & 0.5 & 3 & 0.5 \end{bmatrix}$$

Simulation Scenarios : Dataset 2-3

- Non-linear dataset
  - $X_0 \sim \mathcal{N}(0, 1) \quad (500 \text{ samples})$
  - $X_1 \sim \mathcal{N}(0.9, 0.51^2) \quad (500 \text{ samples})$
  - $X_2 = (X_1 - 0.9)^2 + \epsilon_2, \quad \epsilon_2 \sim \mathcal{N}(0, 0.25^2)$
  - $X_3 \sim \chi^2(6) + \exp(X_0)$
  - $Y = 2.5 \cdot \exp(-1.3X_0 - 2X_1 - 1.2X_2 - 0.03X_3) + \epsilon_y, \quad \epsilon_y \sim \mathcal{N}(0, 0.02^2)$

- Breast Cancer dataset [a]

a. Wolberg, W., Mangasarian, O., Street, N., and Street, W. (1993). Breast Cancer Wisconsin (Diagnostic) [Dataset]. UCI Machine Learning Repository.

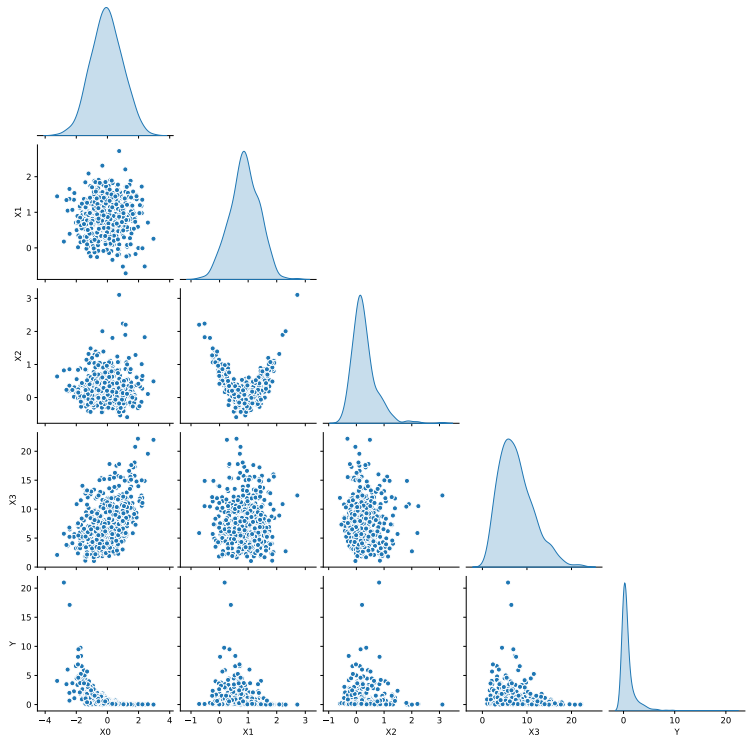


Figure 9 – Pairplot NLS dataset

Evaluating Superlearners Using Best Methods - Wasserstein distance

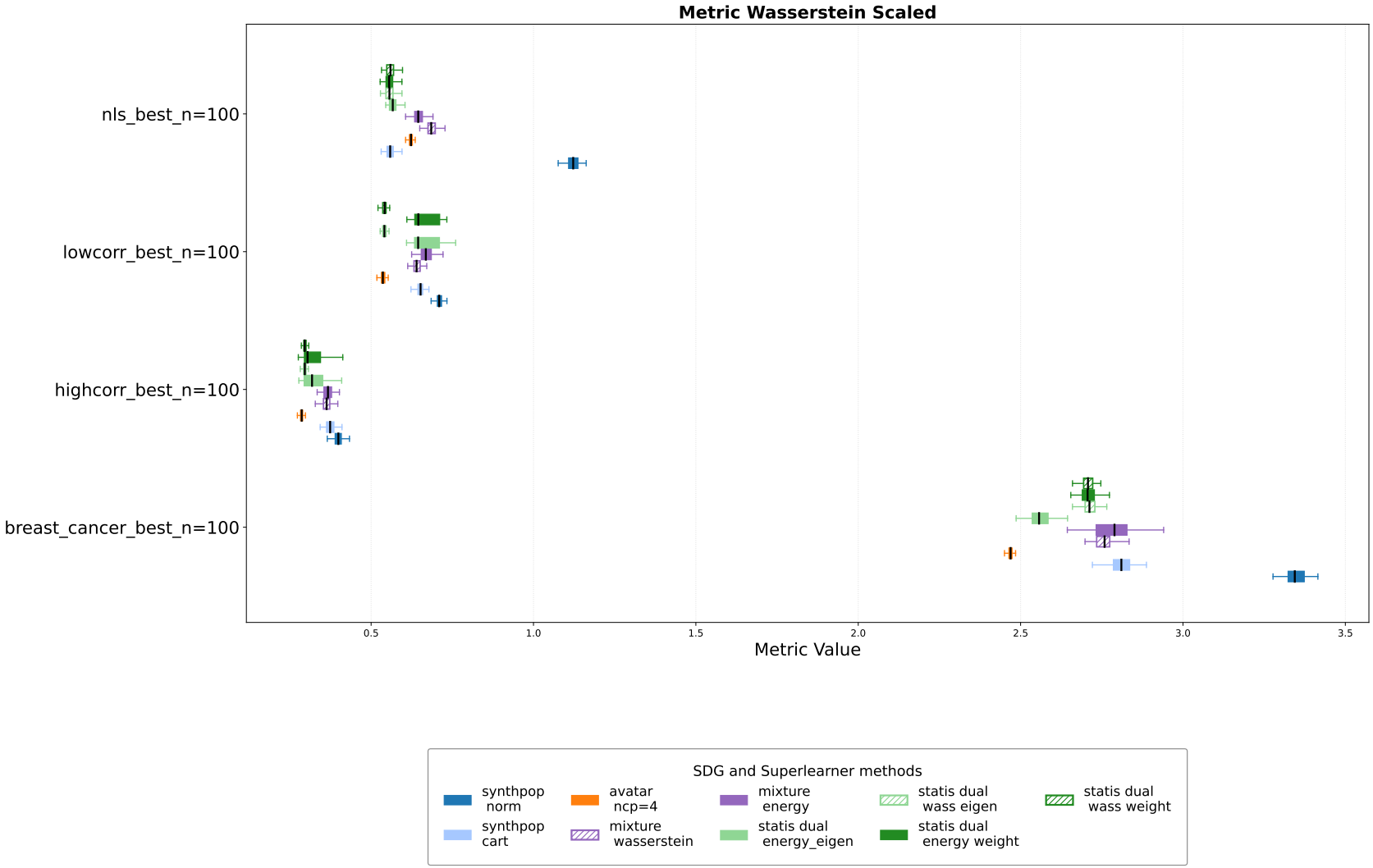


Figure 10 – Results in superlearners with best methods (**Synthpop CART**, **Synthpop norm**, **Avatar**) on different datasets

Evaluating Superlearners Using Best Methods - Energy distance

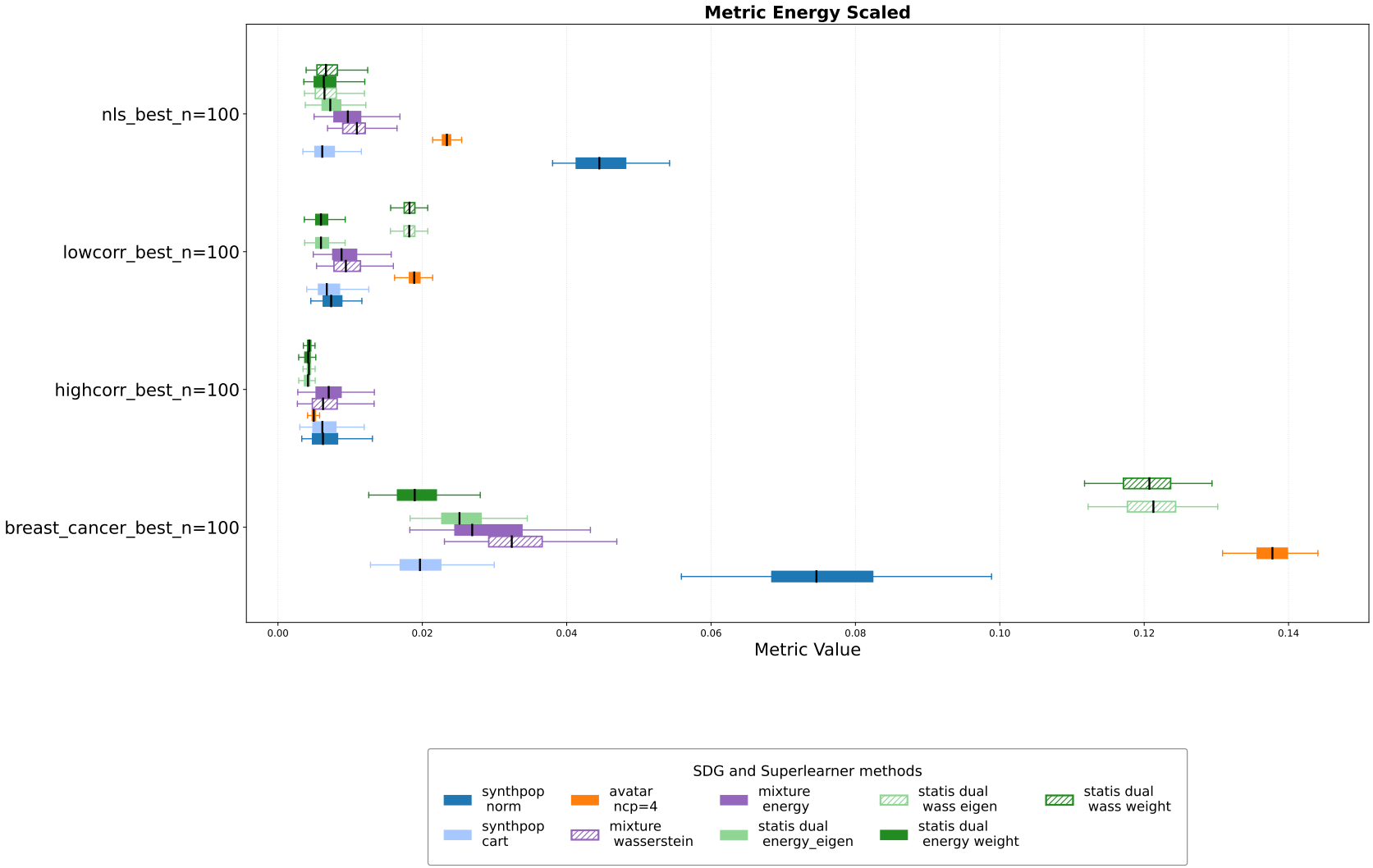


Figure 11 – Wasserstein distance with superlearners with best methods (**Synthpop CART**, **Synthpop norm**, **Avatar**) on different datasets

Task-based utility on hightcorr and lowcorr datasets

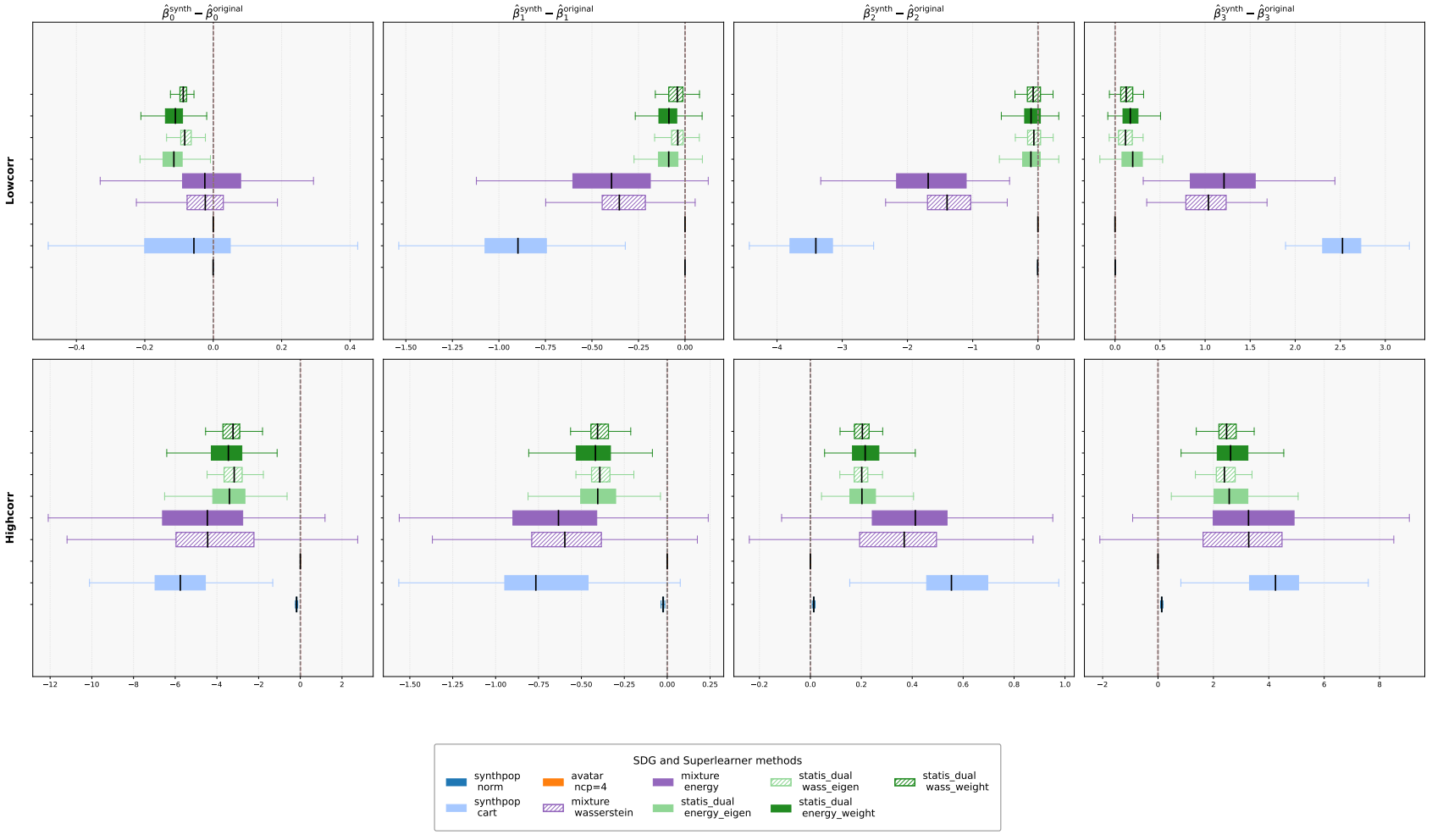


Figure 12 – Result in linear regression $y = \beta X + \epsilon$ for superlearner with **Synthpop norm**, **Synthpop CART** and **Avatar**

Evaluating Privacy Metrics in Superlearners Using Best Methods on Linear Data

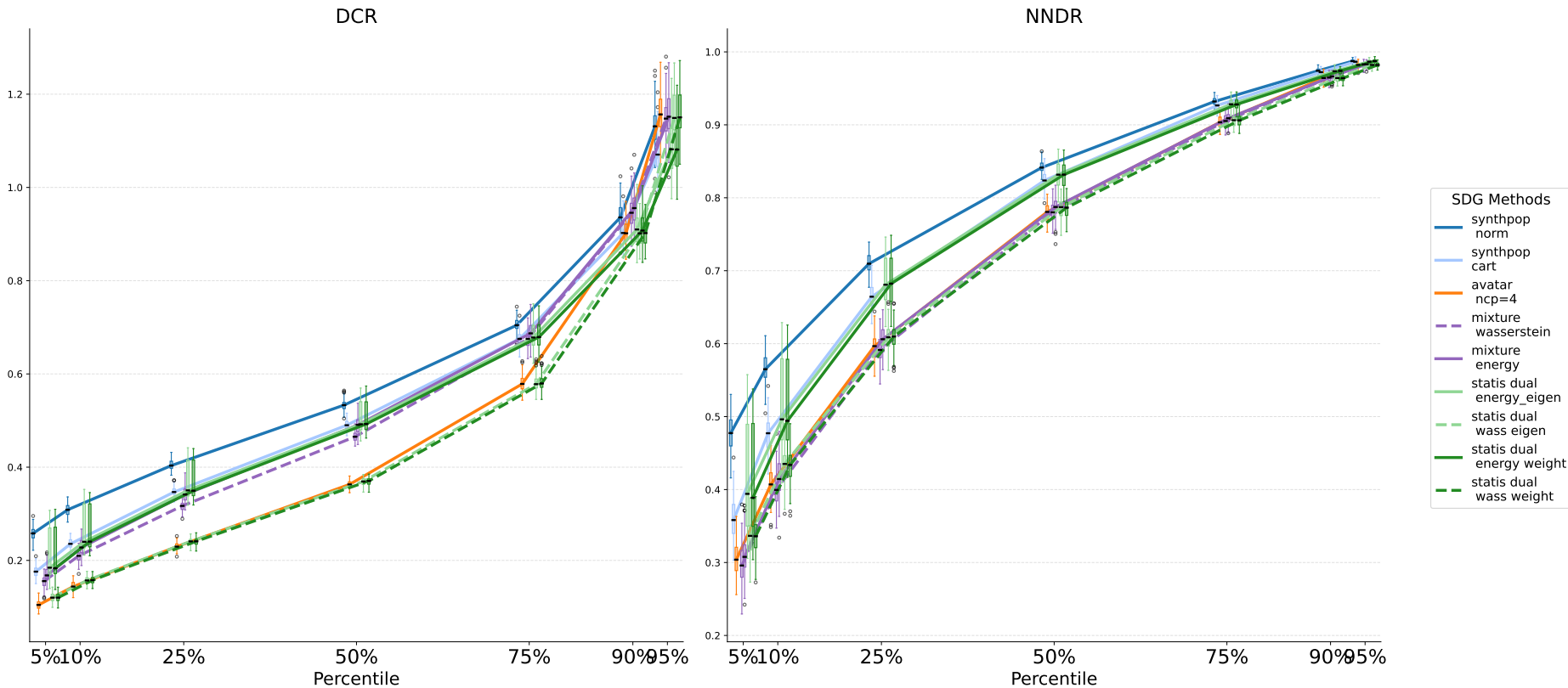


Figure 13 – Privacy results for linear dataset

Evaluating Superlearners Using Best Methods : Synthpop norm and CART and Avartar

- The results differ depending on the evaluation metric used.
- **Avatar** consistently outperforms other methods based on the Wasserstein distance, but in Energy distance it coulbe be the worst method.
- **Statis** with weighted by wasserstein distance (direct weight or by eigen value) seems to **perform well in many case.**
- The **Synthpop CART** method performs poorly on linear regression metrics and appears to negatively impact the superlearner's performance.
- In terms of task-based utility for linear regression, **none of the superlearners demonstrate satisfactory performance**.

Evaluating Task-based Utility in Superlearners Using Best Methods on Linear Data

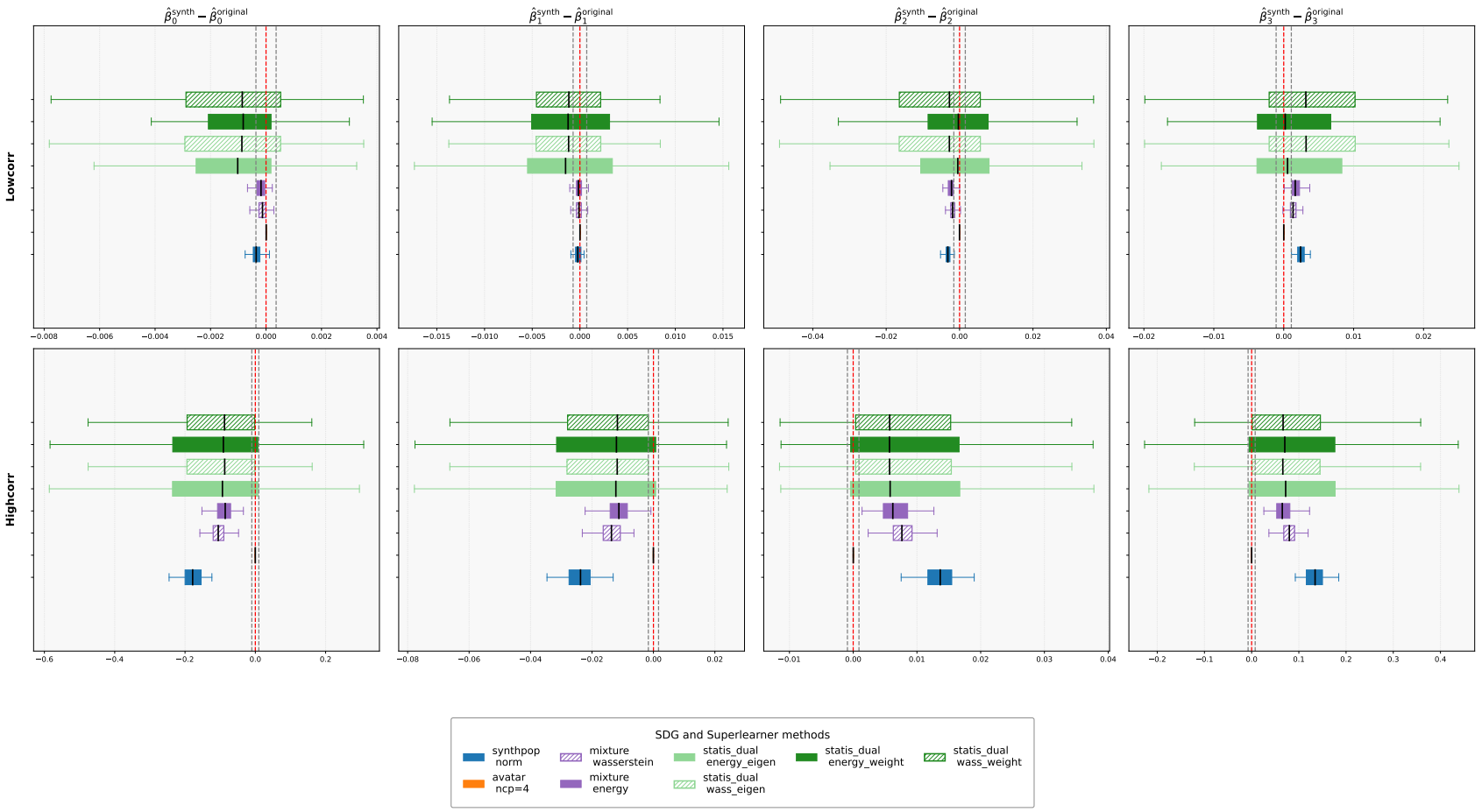


Figure 14 – Result in linear regression $y = \beta X + \epsilon$ for superlearner with **Synthpop norm** and **Avatar**

Evaluating Superlearners Using Best Methods : Synthpop Norm and Avatar

- Results improve significantly when excluding **Synthpop CART** from the superlearner.
- **Avatar** consistently **performs best, exhibiting minimal variance.** Its dispersion is extremely low, resulting in tight confidence intervals with 100% coverage and 100% overlap. However, this reduced variance is notably smaller than that observed in a typical set of bootstrap samples.
- On average, **Mixture** and **Statis** balance the bias between Avatar and Synthpop, but this comes at the cost of greatly increased variance.
- **Statis ranks highest** when evaluated with Wasserstein and Energy distance metrics. However, **regression performance is more variable and dispersed**.

Conclusion

- Superlearners that aggregate well-performing models can offer acceptable utility across multiple evaluation metrics.
- The **Mixture barycenter** achieves solid results in both global and task-based utility.
- However, no superlearner consistently outperforms the best individual method in term of utility (**Avatar**) which remains the top performer across most metrics.

Supplementary Material

Supplementary : Details on Methodology

Anonymization and **Pseudonymization** are solutions to protect sensitive data, enhance its confidentiality during sharing, and limit risks related to data processing and breaches.

Pseudonymization

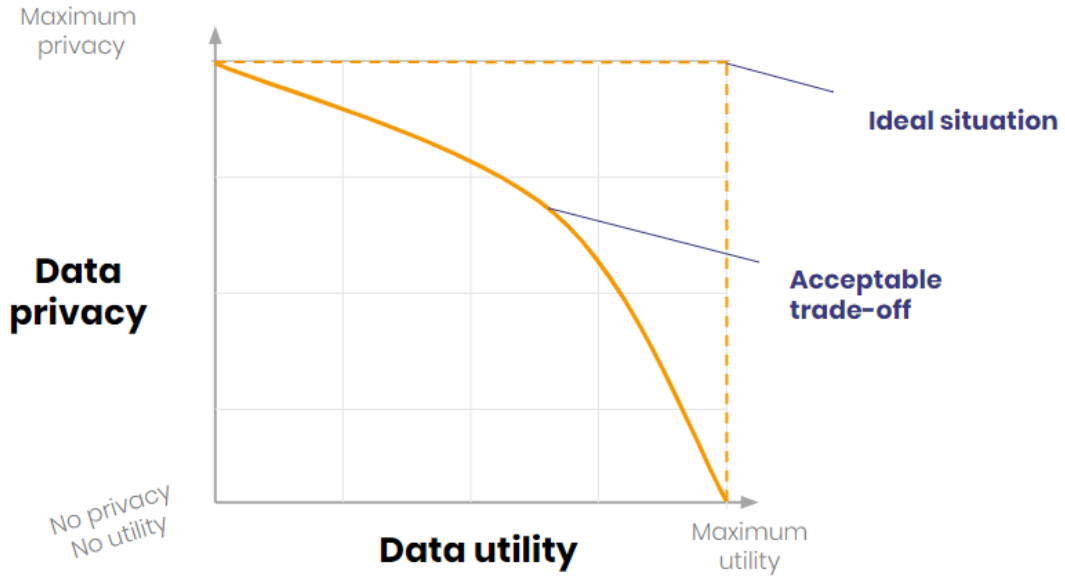
- Replacing directly identifiable data (e.g. first name) with indirectly identifiable data (e.g. code).
- Reversible operation.
- GDPR applies.

Anonymization

- Set of techniques to make impossible to identify the person by any means.
- Complete removal of data identifiability.
- Irreversible operation.
- GDPR does not apply.

Drawbacks of fully anonymized data

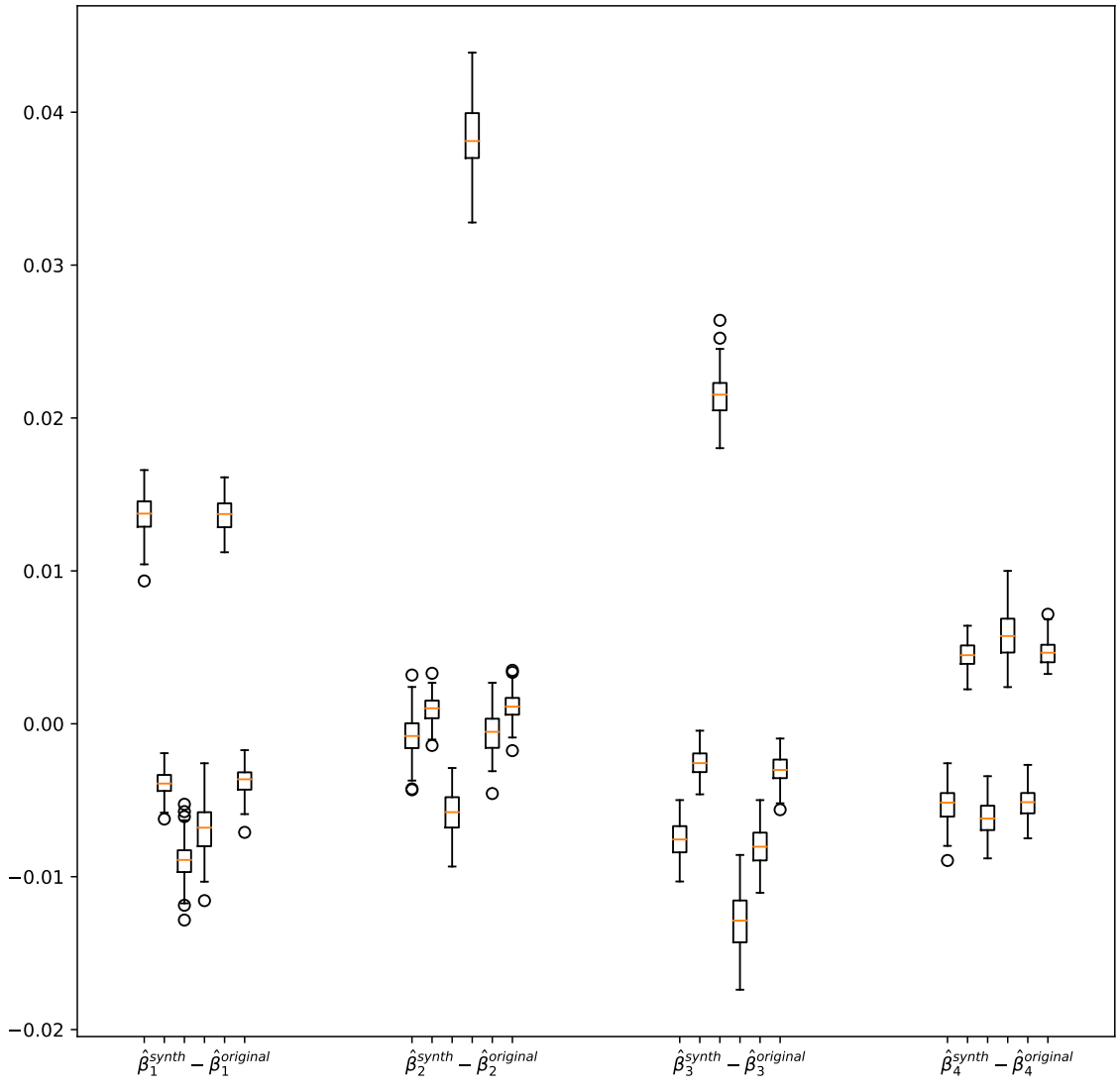
- **Loss of Data Utility :** Fully anonymized data may lose significant value and utility because essential information might be removed to ensure anonymity.



- **Irreversible Process :** Once data is fully anonymized, it cannot be reverted to its original form.
- **Complexity and Cost :** The process of fully anonymizing data can be complex and costly
- **Regulatory Challenges :** Ensuring compliance with diverse and evolving privacy regulations can be challenging when dealing with fully anonymized data.

Synthpop : Sensibility to order

Results for linear regression for unlineary correlated predictors
with data synthesized by synthpop from real data set with different shuffled columns.



More details on pMSE

Propensity MSE (pMSE) [36] **: Can we distinguish the original and the synthetic data ?** :

- $\widehat{p_i}$ is the estimated probability by a binary classifier for the sample i to be a synthetic data.
- $c = \frac{n_{syn}}{n_{orig}+n_{syn}}$ the probability to draw a synthetic data into the concatenated original and synthetic dataset
- $pMSE = \sum_{i=1}^{n_{orig}+n_{syn}} (\widehat{p_i} - c)^2$
- Sensible to the classifier used (CART, RF, logistic regression) [37].
- Theoritical result [38] , under the null hypothesis : Z_{synth} is generated by the true distribution $f(z|\theta)$; $pMSE = aF$ with $F \sim \chi^2(k-1)$.
- Derived pMSE metric :

36. **woo2009global**.
37. Snoke et al., "General and specific utility measures for synthetic data." *Journal of the Royal Statistical Society : Series A (Statistics in Society)*, 181(3) :663–688, 2018. Oxford University Press.
38. Snoke et al., "General and specific utility measures for synthetic data." *Journal of the Royal Statistical Society : Series A (Statistics in Society)*, 181(3) :663–688, 2018. Oxford University Press.

Supplementary simulations results : Evaluating Superlearners Using Best Methods - Breast Cancer Dataset

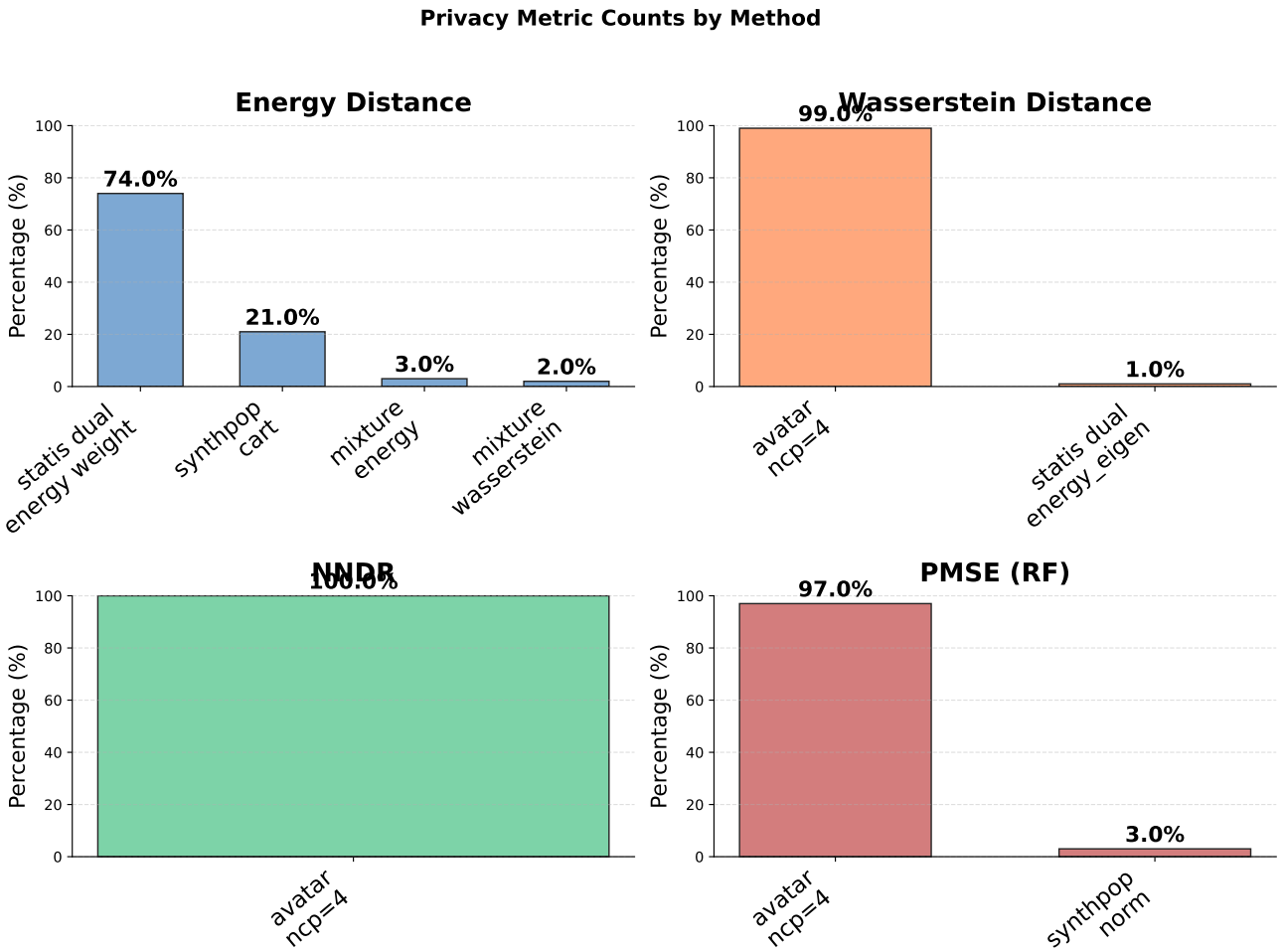
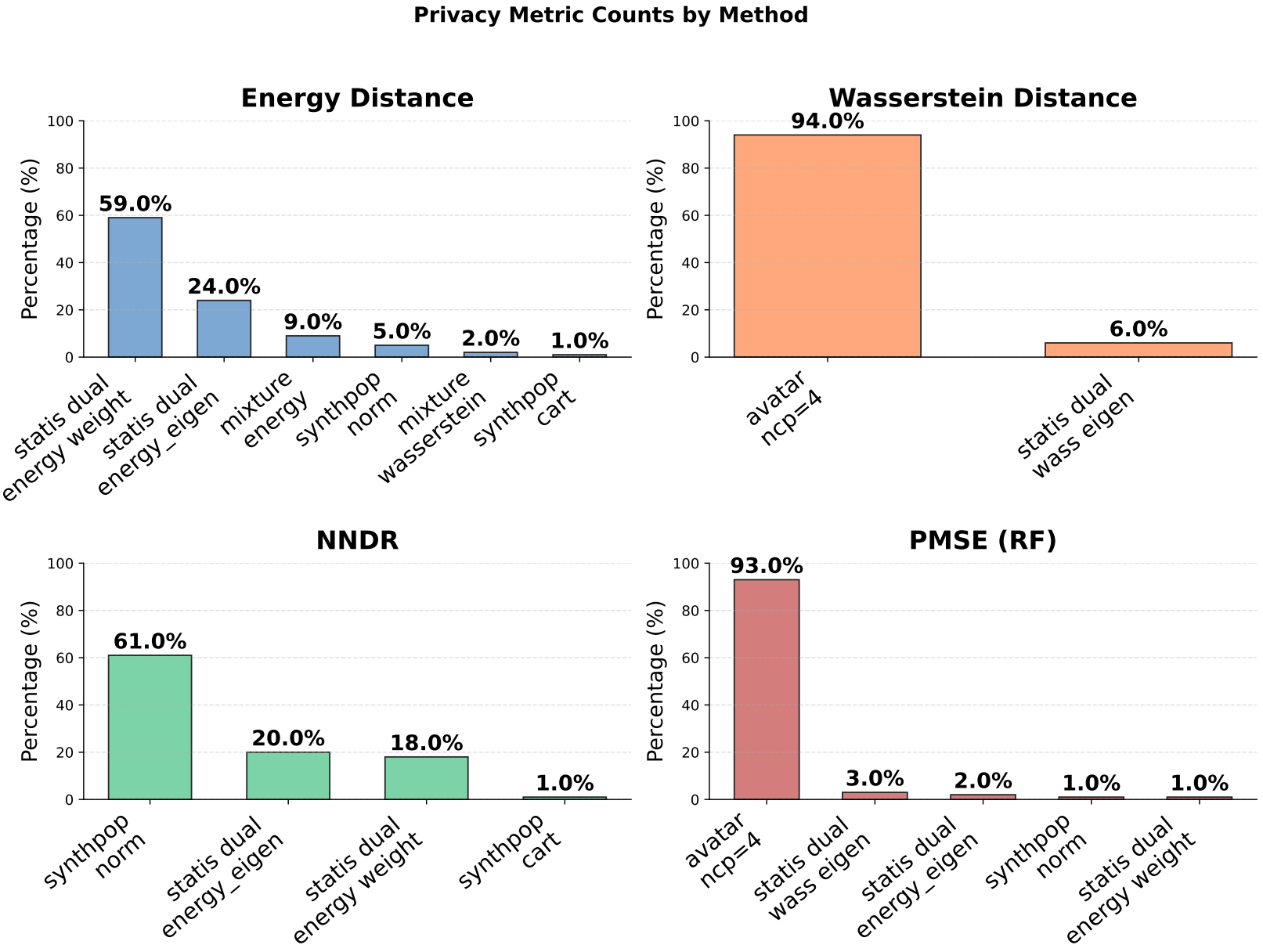
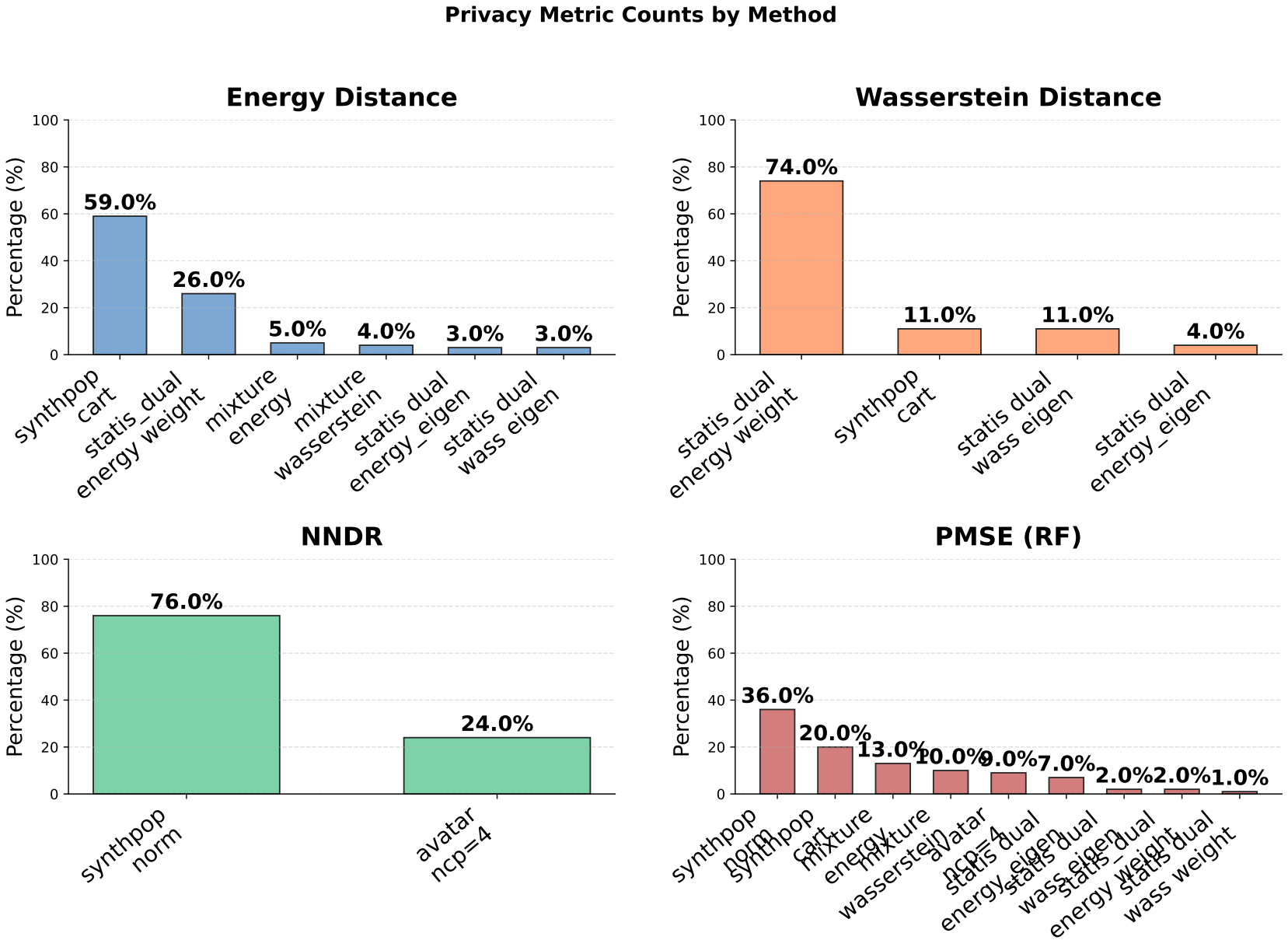


Figure 16 – Privacy and utility result on breast cancer dataset

Supplementary simulations results : Evaluating Superlearners Using Best Methods - Low correlation linear dataset



Supplementary simulations results : Evaluating Superlearners Using Best Methods - NLS dataset



Supplementary simulations results : Breast Cancer Dataset

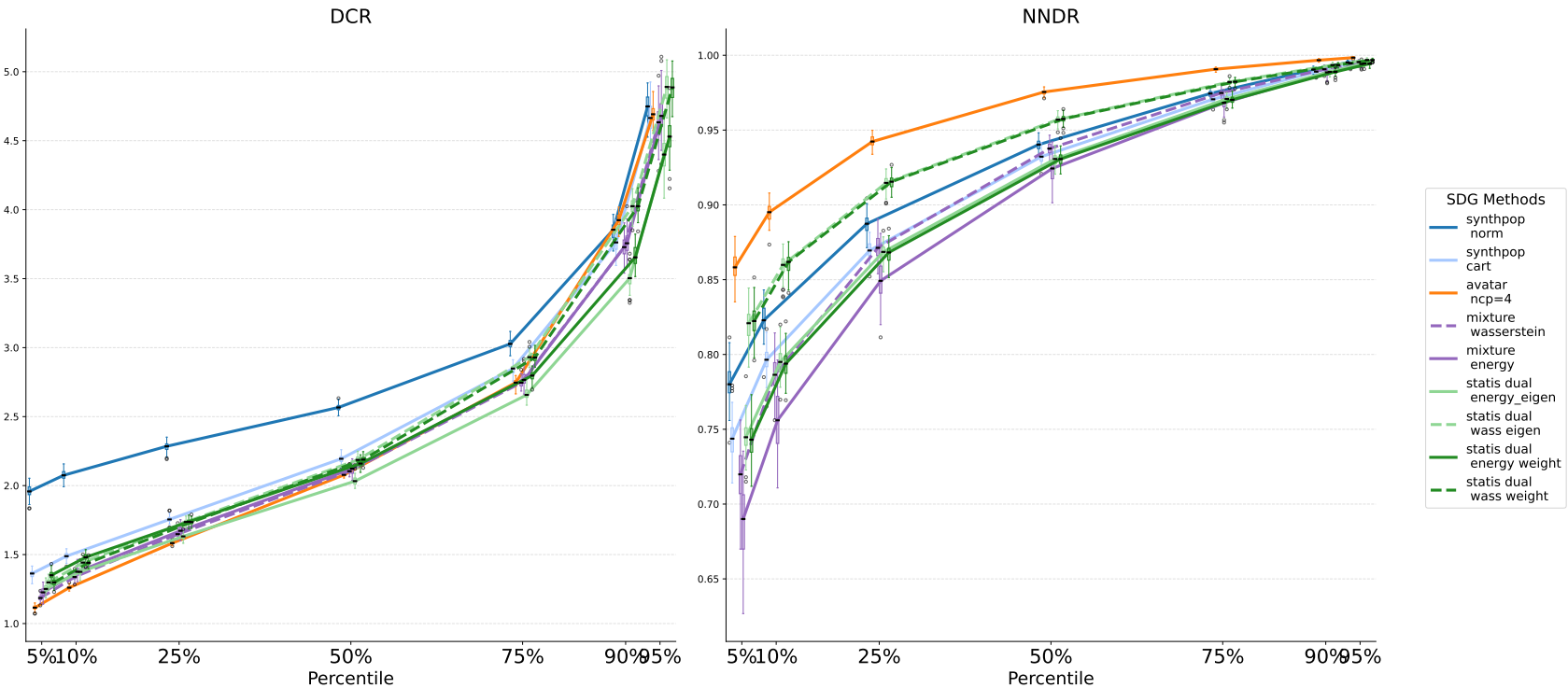


Figure 19 – Privacy results on breast cancer dataset

Supplementary simulations results : Evaluating Superlearners Using Best Methods - NLS dataset