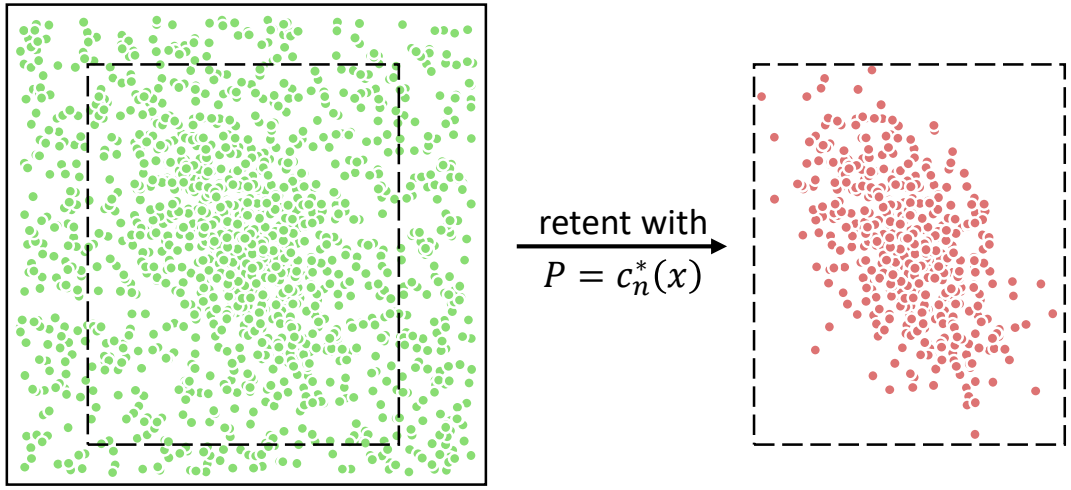
A consistent method for generating synthetic tabular data with a fully connected neural network



Interactive
perceptron visualizer



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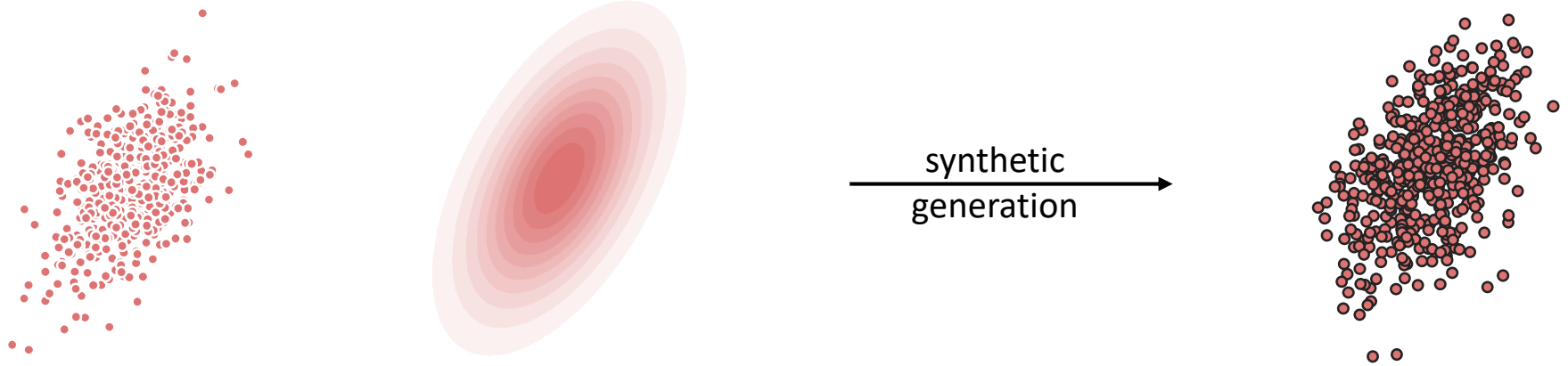
ИСП РАН

Synthetic tabular data generation

- $X = \{x_1, x_2, \ldots, x_n\} \subset [0,1]^d$ – dataset from unknown probability distribution with uniform continuously density function $f(x)$;
- $\bar{X} = \{\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_m\}$ – synthetic dataset.

Goal: construct new dataset $\bar{X}$, that approximates the statistical and structure properties of X while maintaining privacy constraints.

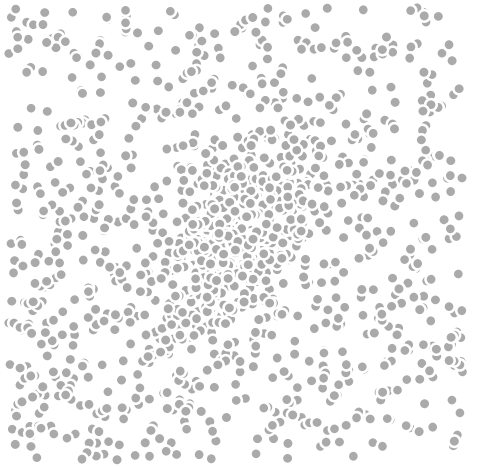


X $f(x)$ $\bar{X}$

Density estimation: approaches

Common approach:

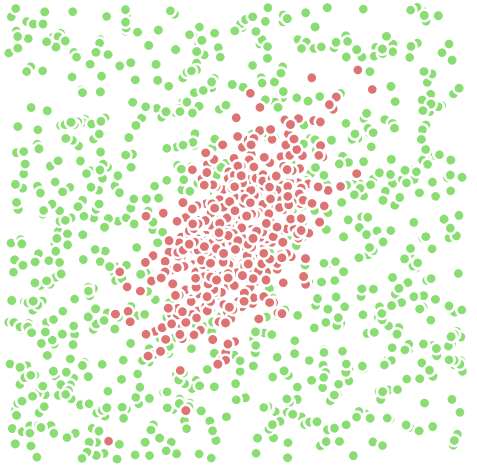
- Nonparametric estimator $\hat{f}(x)$ of $f(x)$: histogram, k-nearest neighbors (kNN), …



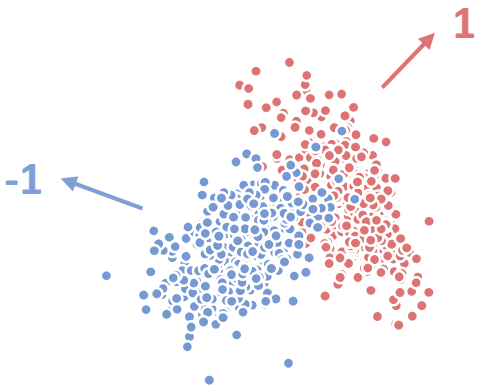
unary classification

Our approach:

- Based on **unary classification**;
- Dense neural network trained to distinguish support of the real data from a background distribution.



Bayesian binary classifier (classic)



- $D = (X, Y)$ – random vector with a certain distribution P;
- $X \subset [0,1]^d$, $Y \in \{\pm 1\}$;
- $f: [0,1]^d \to \{\pm 1\}$ – discriminant function;
- S – support of distribution of vector X.

General **classification** problem:

$$P\big(Y \neq f(X)\big) \to \min_f$$

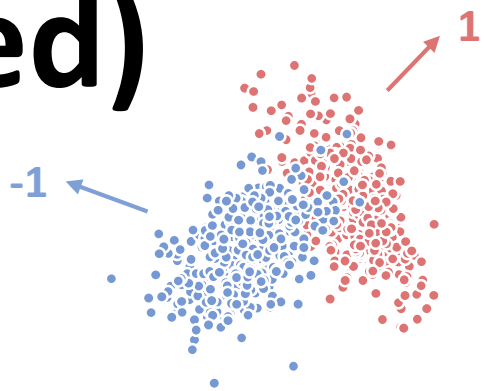
Bayesian classifier $g(x)$ – **optimal discriminant function** of classification problem:

$$s(x) = \begin{cases} 1, & if\ g(x) > 0\ and\ x \in S \\ \boldsymbol{any}\ of\ \pm 1, & if\ g(x) = 0\ or\ x \notin S \\ -1, & if\ g(x) < 0\ and\ x \in S \end{cases}$$

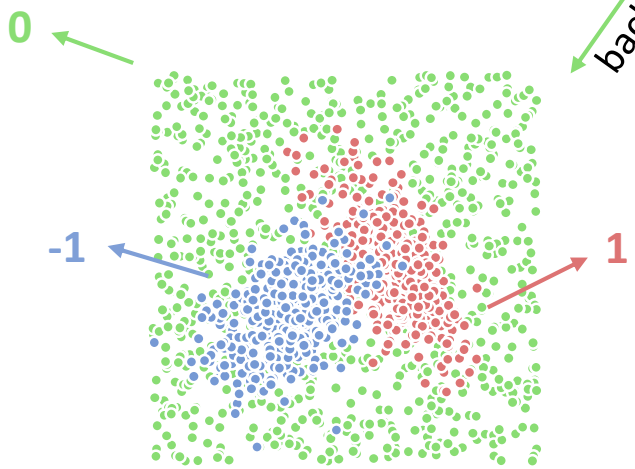
Bayesian binary classifier (modified)

Add m "background" vectors $(\check{X}, \check{Y})$:

- $\check{X} \subset [0,1]^d$ – uniformly distributed noise on the compact domain K;
- $\check{Y} \in \{0\}$ – label of "background" class.



add background



Mixture of two distributions:

- $(X, Y) \in [0,1]^d \times \{\pm 1, 0\}$ – new data-vector;
- $P_\alpha = \alpha P + (1-\alpha)\check{P}, \alpha \in (0,1)$;
- $\check{P}$ – distribution of the background.

Optimal solution $\check{s}(x)$ based on modified dataset **does not worsen** $g(x)$, but $\check{s}(x)$ **equals to 0** if $x \notin S$.

Unary classification: mixture data

- (X, Y) – random variable;
- $X \subset [0,1]^d$ – vector with a mixture density $\alpha f(x) + (1-\alpha)p(x)$;
- $Y = 0$ for background distribution and $Y = 1$ for target class label;
- $f(x)$ – density of target class;
- $p(x)$ – density of the uniform distribution over a compact set K;
- α – weighting coefficient, $\alpha \in [0,1)$;

Posterior probability (or regression function) of Y given X:

$$g(x) = P(Y = 1 | x = x) = E(Y | X = x) = \frac{\alpha f(x)}{\alpha f(x) + (1-\alpha)p(x)}$$

Unary classification: problem solution

- $g(x)$ **known** (wow!):

  x part of distribution if $g(x) > 0$, otherwise reject.

- $g(x)$ **unknown** (typically):

  construct an **approximation** from the given data.

Unary classification: approximation

- $c(x)$ – a continuous function defined on a compact set K;

Mean-squared approximation problem (minimization takes over all $c(x)$):

$$c^*(x) = \operatorname{argmin} \mathrm{E}(\mathrm{c}(\mathrm{x}) - \mathrm{Y})^2 \quad \textbf{(2)}$$

$$E(c(x) - Y)^2 = E(c(x) - g(x) + g(x) - Y)^2$$

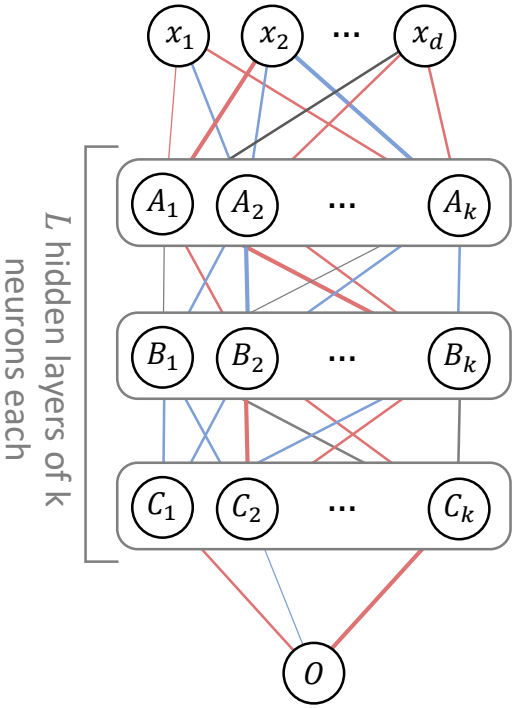
$$E(c(x) - Y)^2 = E\big(c(x) - g(x)\big)^2 + \underbrace{E(g(x) - Y)^2}_{\text{independent of } c(x)}$$

Problem **reduces** to the approximation of the regression function:

$$c^*(x) = \operatorname{argmin} \mathrm{E}(\mathrm{c}(\mathrm{x}) - g(x))^2 \quad \textbf{(4)}$$

Unary classification: perceptron

- $c(x)$ – multilayer **perceptron** with L hidden layers of k neurons each, one neuron in the output layer and piecewise-linear activation function (Abs, $ReLU$, …).



Universal approximation theorem: for any $\epsilon > 0$ there exist values of k and L such that for any $x \in K$:

$$\sup|c(x) - g(x)| < \epsilon$$

Thus, an ϵ-approximated solution of **(2)** **theoretically exists**.

Cybenko G. Approximation by superpositions of a sigmoidal function (1989)

Unary classification: perceptron

- $\{X_i, 1\}_{i=1}^{n}$ – labeled set of n observations from **target** density $f(x)$;
- $\{X_j, 0\}_{j=n+1}^{n+m}$ – m added **background** samples, $m = n \cdot \frac{1-\alpha}{\alpha}$;
- $C(L, k)$ – class of **MLP** with activation function $\boldsymbol{Abs}$ and given $\boldsymbol{L}$, $\boldsymbol{k}$;

Optimization problem (minimization takes over all $c_n(x) \in C(L, k)$):

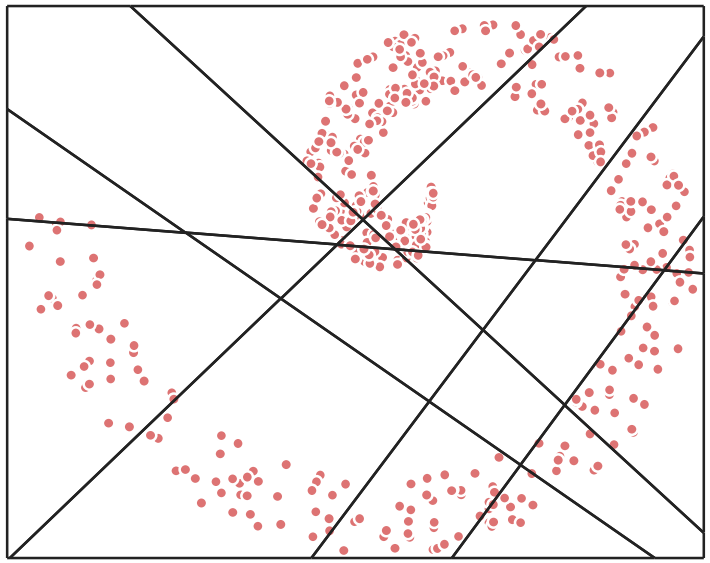
$$\sum_{i=1}^{n+m} (c_n(X_i) - Y_i)^2 \to min \qquad (6)$$

Let $c_n^*(x)$ – is solution of (6), called **neural regression function**.

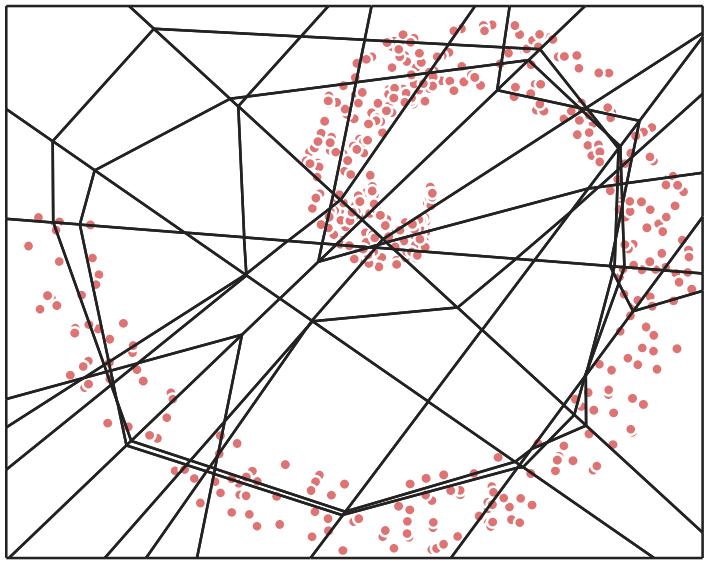
Unary classification: adaptive histogram

- $c_n^*(x)$ constructs a **hierarchical partition** of K into N disjoint cells: $K = \{K_1, K_2, \dots, K_N\}$

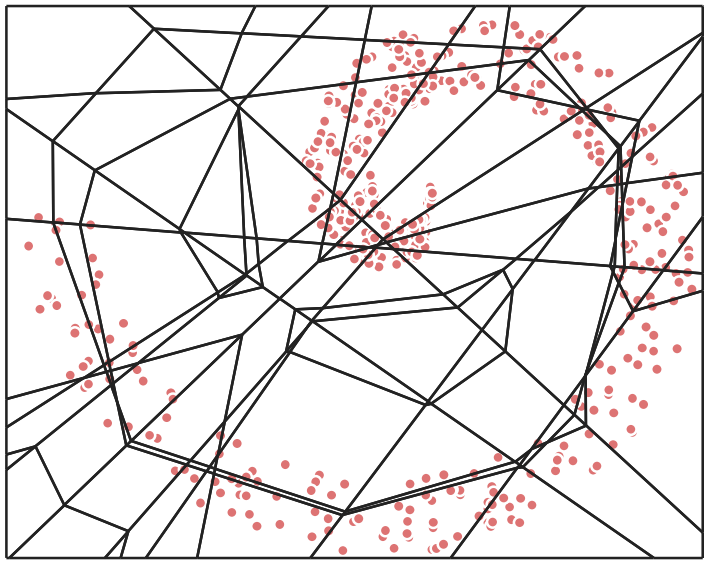
Partition example of some MLP with $L = 2$, $k = 6$ and Abs activation:



Cells after first hidden layer:
18 cells



Cells after second hidden layer:
121 cells



Cells after output neuron:
148 cells

Unary classification: adaptive histogram

- $h_n(x)$ – **piecewise constant** function of histogram regression, defined by minimizing:

$$\sum_{i=1}^{n+m} (h_n(X_i) - Y_i)^2 \to min \qquad (7)$$

Minimization takes over all **piecewise constant** functions defined on cells K_r of K.

- Let $X \in K_r \to$ within each cell K_r the problem **(7)** reduces to

$$n_1(X) \cdot (h_n(X) - 1)^2 + n_0(X) \cdot (h_n(X) - 0)^2 \to min$$

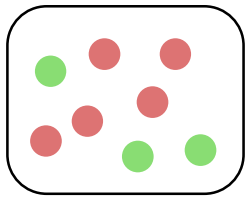
- $n_j(X) = \sum_{i=1}^{n+m} I_{\{X_i \in K_r, Y_i = j\}}$;

Unary classification: adaptive histogram

Differentiating with respect to $h_n(x)$ yields the solution of **(7)**:

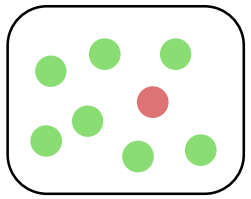
$$h_n^*(x) = \frac{n_1(X)}{n_1(X) + n_0(X)} = \frac{f_n(X)}{f_n(X) + \frac{1-\alpha}{\alpha} p_n(X)}$$

- $f_n(X) = \frac{n_1(X)}{n \cdot V(K_r)}$ – histogram density $f(x)$ estimates at cell K_r;
- $p_n(X) = \frac{n_0(X)}{n \cdot V(K_r)}$ – histogram uniform density $p(x)$ estimates at cell K_r;
- $V(K_r)$ – measure of the cell K_r.



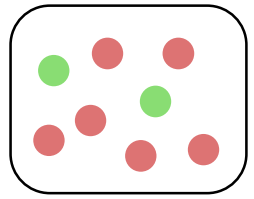
$n_1 = 5, n_0 = 3$

$h_n^*(X) = \frac{5}{5+3} = 0.625$



$n_1 = 1, n_0 = 7$

$h_n^*(X) = \frac{1}{1+7} = 0.125$



$n_1 = 6, n_0 = 2$

$h_n^*(X) = \frac{6}{6+2} = 0.75$

Unary classification: consistency

- **Cell shrinking**: diameter decreases while keeping enough points per cell;
- **Practical**: for $d = 10$, $k = 10$, $L = 2$, $N > 10^4$ – millions of background points are needed;
- **Filled cells** (both target and background points present): $h_n^*(X) \approx c_n^*(X)$;
- **Background-only cells**: $h_n^*(X) = 0$, $c_n^*(X)$ is interpolated (continuity);
- **High-density regions**: $c_n^*(X) \gg 0$;
- **Low-density regions**: $c_n^*(X) \to 0$;

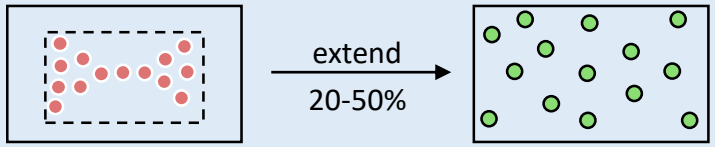
Sufficiently large n and appropriately chosen k and L, the neural regression $c_n^*(X)$ **may be interpreted** as a consistent estimator of $g(X)$.

Devroye L. Nonparametric density estimates with improved. performance on given sets of densities (1989)

Synthetic data generation: methodology

Background data generation

- **Determine compact**: $K \subset [0,1]^d$ – an axis-aligned hyper rectangle extending 20-50% beyond the real data in each dimension);
- **Margin effect**: ensures enough negative samples for the classifier to distinguish data support and helps push the decision function toward the zero plane.
- **Point set**: $B = \{b_1, b_2, \dots b_n\}$ are sampled uniformly from K with $|B| = |X|$ $(\alpha = 0.5)$



Classifier training

- **Classifier**: MLP $c_n(x)$: $[0,1]^d \rightarrow [0,1]$;
- **Dataset**: $X \cup B$ with binary labels:

$$c_n(x) = \begin{cases} 1, x \in X \\ 0, x \in B \end{cases}$$

- **Loss function**: mean squared error

$$L = \sum_{x \in X} \big(1 - c_n(x)\big)^2 + \sum_{b \in B} \big(0 - c_n(b)\big)^2$$

- **Dynamic background**: points B are generated at each epoch;

Why MSE?

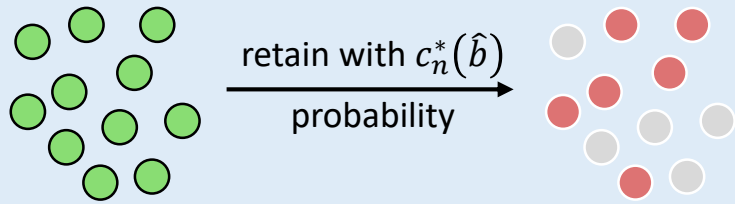
- Smoother approximation of posterior probabilities without requiring sigmoid;
- Supports histogram based interpretation.

Synthetic data sampling

- **Candidate points**: sample points $\hat{B} = \{\hat{b}_1, \hat{b}_2, \dots\}$ uniformly from K.
- **Prediction**: get value of $c_n^*(\hat{b})$ for each point $\hat{b} \in \hat{B}$
- **Retention rule**: point $\hat{b}$ is kept with probability $c_n^*(\hat{b})$:

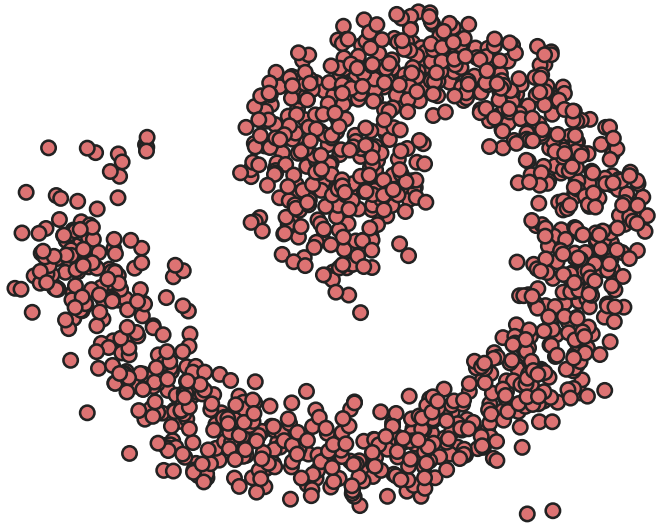
$$\hat{X} = \{\hat{b} \in \hat{B} \mid \xi < c_n^*(\hat{b})\}$$

ξ – is a random variable from uniform distribution $U(0,1)$

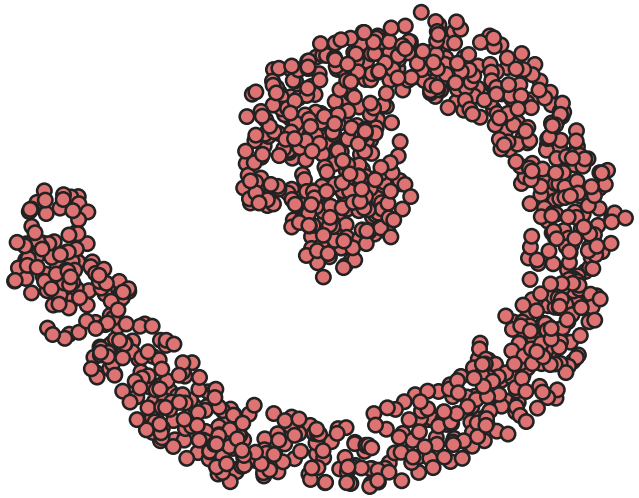


Trust threshold

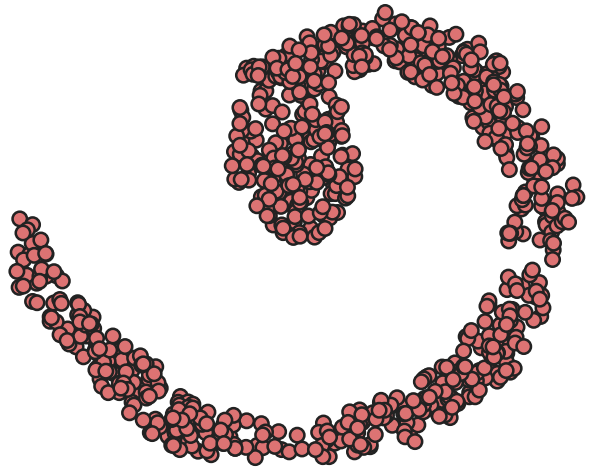
- **Threshold $\boldsymbol{\beta} \in [\mathbf{0}, \mathbf{1})$**: defines regions where the classifier output is unreliable;
- **Smooth decision surface**: $c_n^*(x)$ can not sharply drop to zero outside the data support;
- **Untrusted regions**: occur where $c_n^*(x) < \beta$ (exclude such points from $\hat{X}$);
- **Variance**: increasing the threshold reduces the variance of the synthetic data.



$\beta = 0$

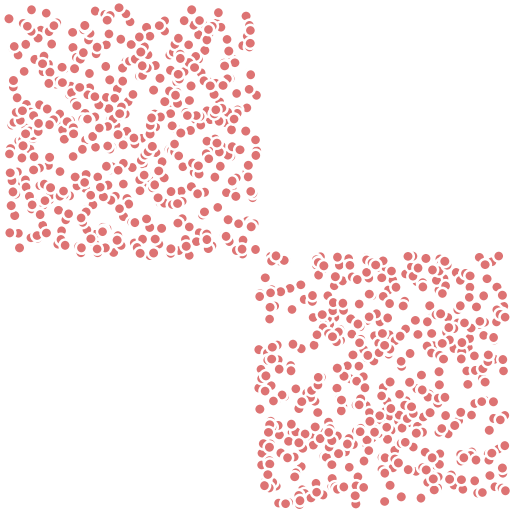


$\beta = 0.3$

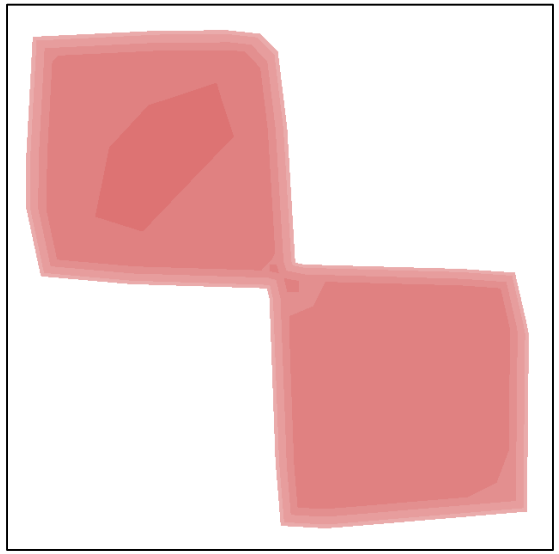


$\beta = 0.6$

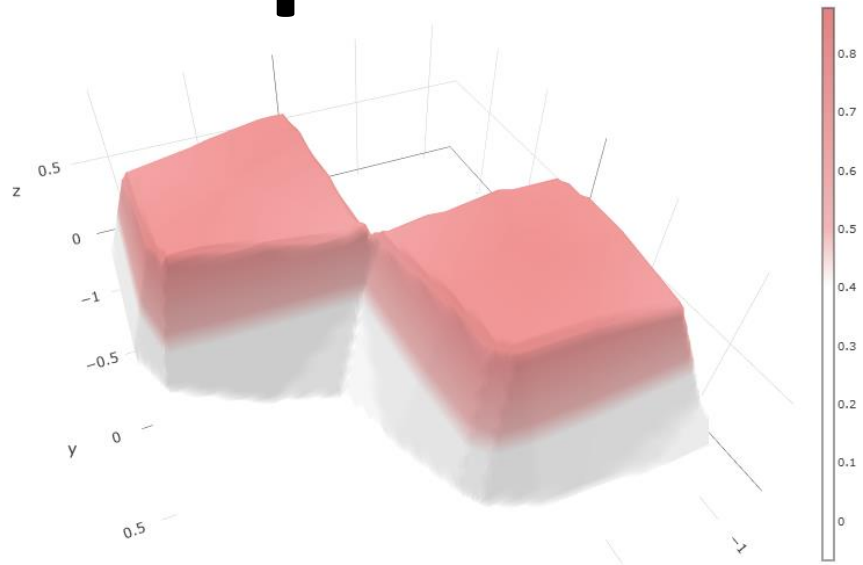
Synthetic data generation: example 1



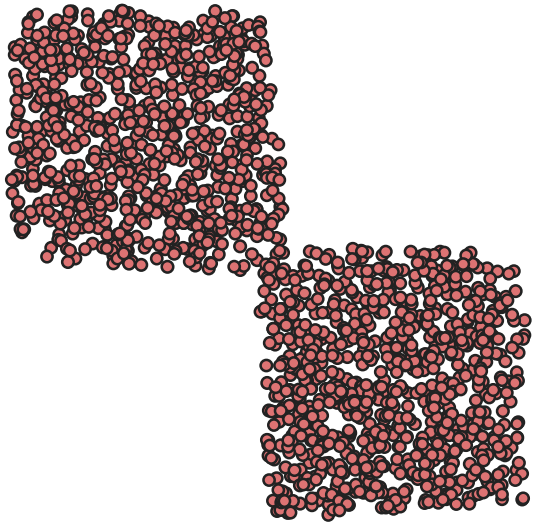
Original (train) dataset



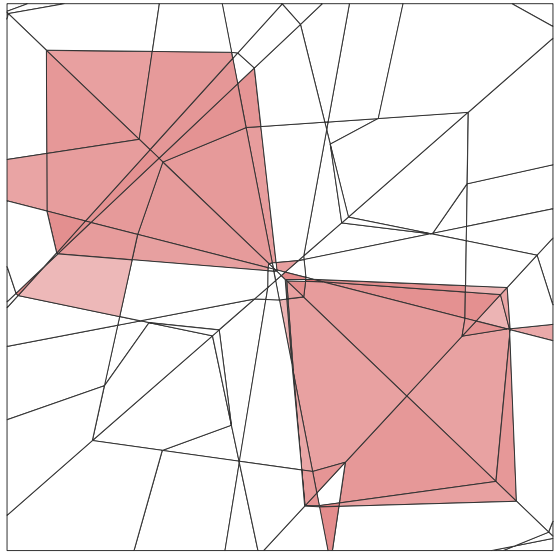
Output of $c_n^*(x)$



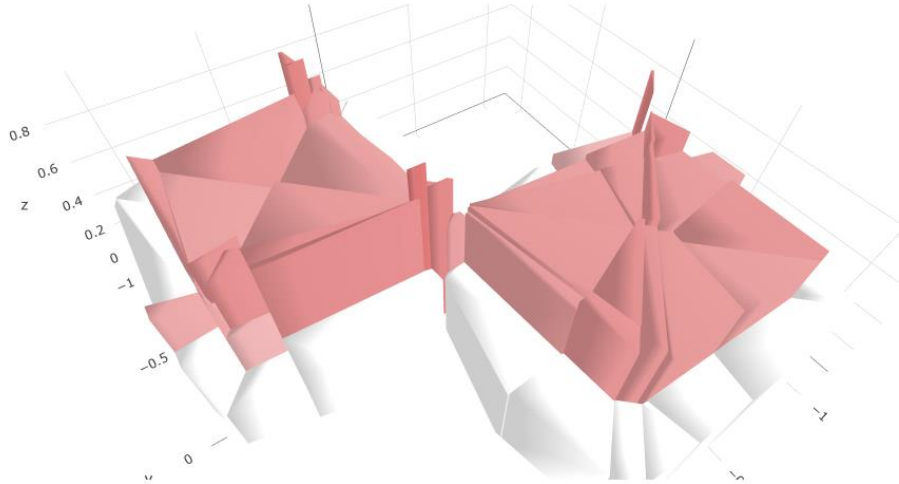
Output of $c_n^*(x)$ in 3D



Reproduced (synthetic) dataset

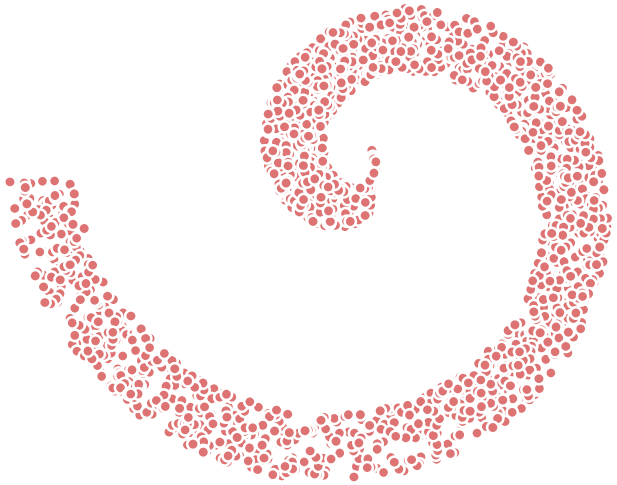


Output of $h_n^*(x)$

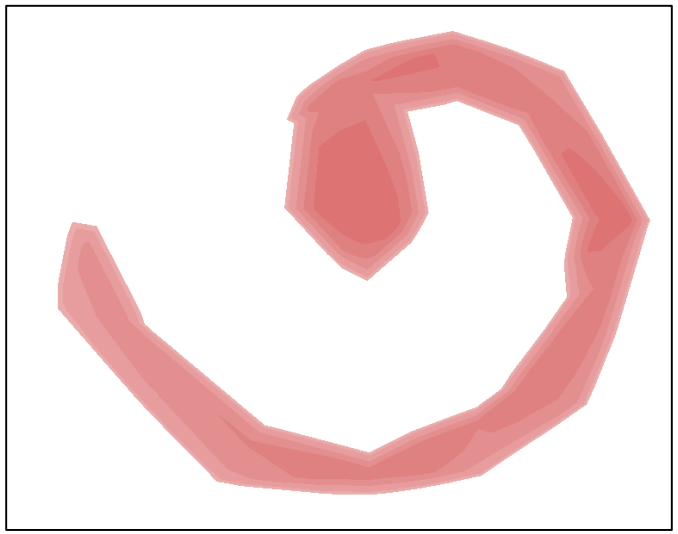


Output of $h_n^*(x)$ in 3D

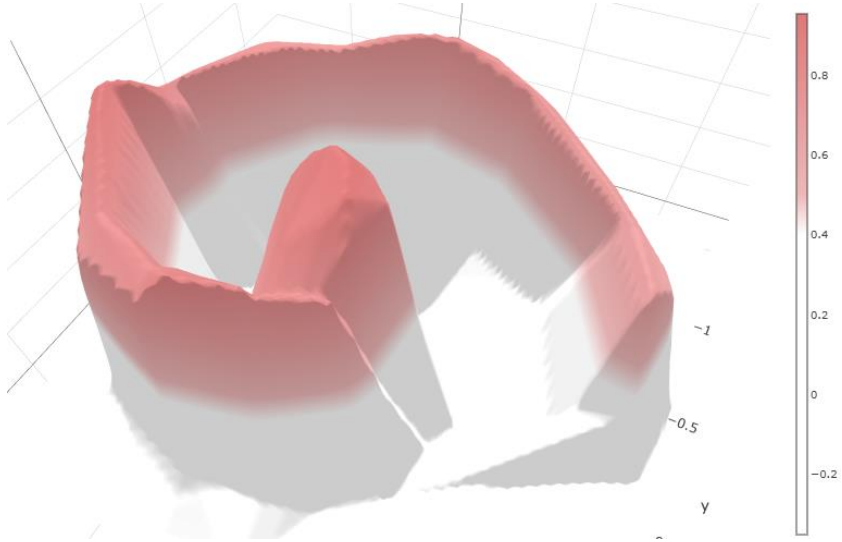
Synthetic data generation: example 2



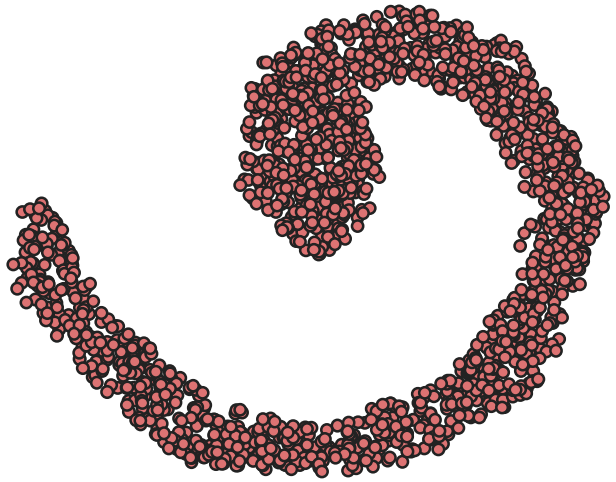
Original (train) dataset



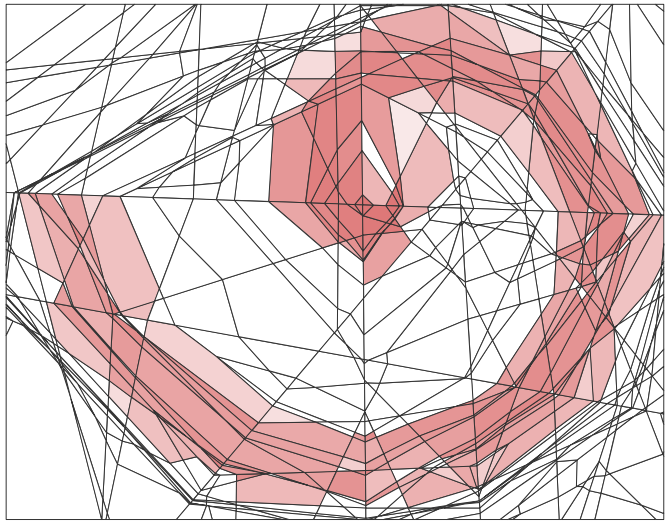
Output of $c_n^*(x)$



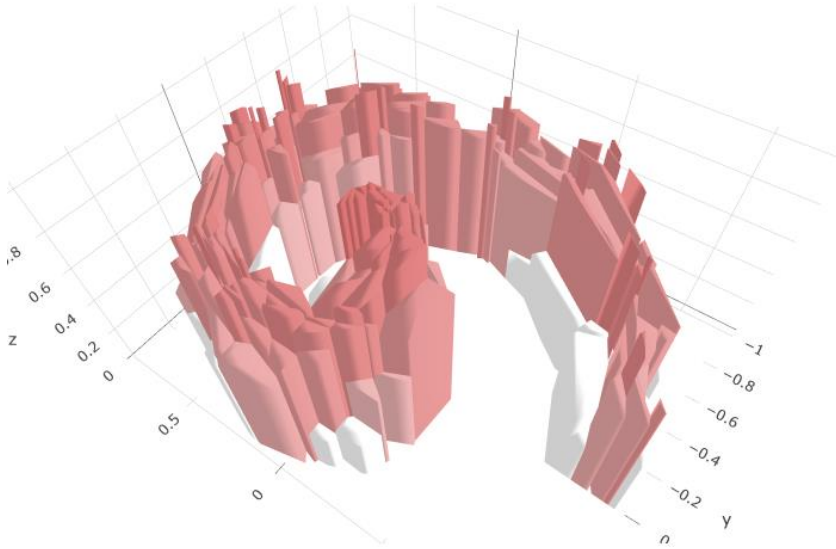
Output of $c_n^*(x)$ in 3D



Reproduced (synthetic) dataset



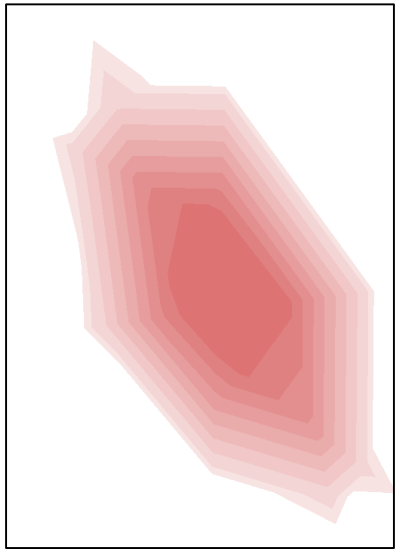
Output of $h_n^*(x)$



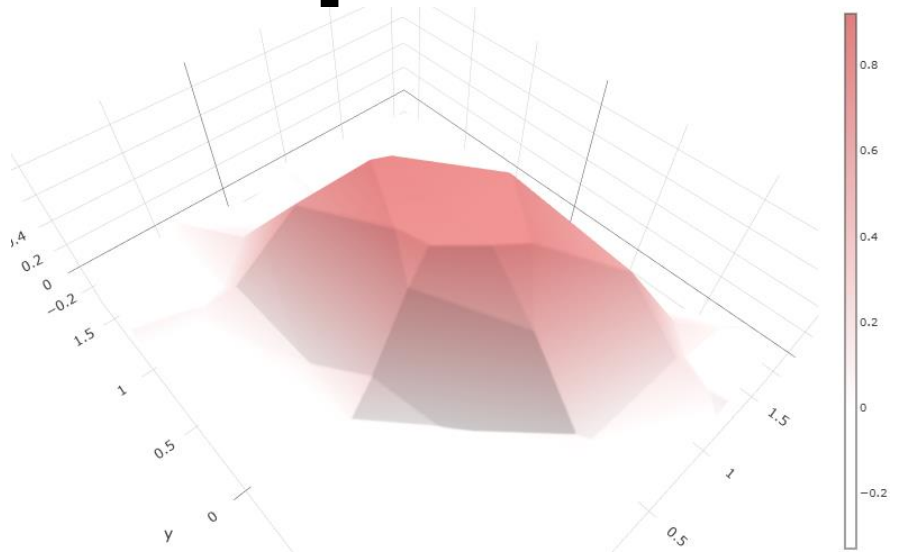
Output of $h_n^*(x)$ in 3D

Synthetic data generation: example 3

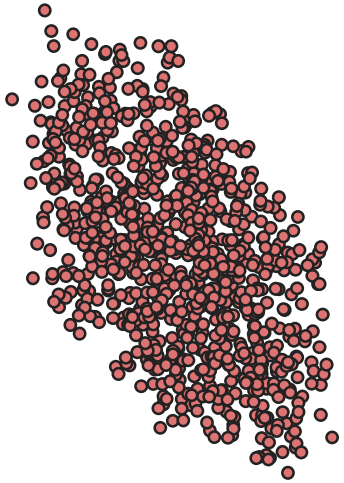
Original (train) dataset



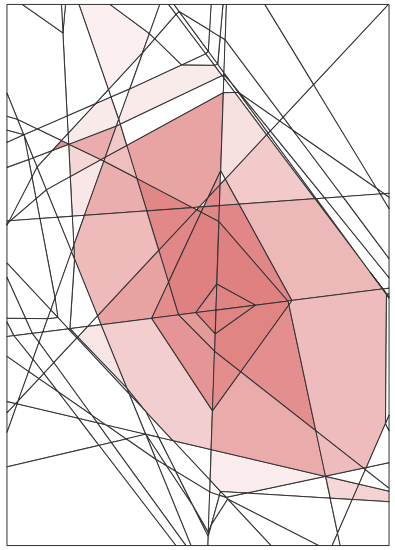
Output of $c_n^*(x)$



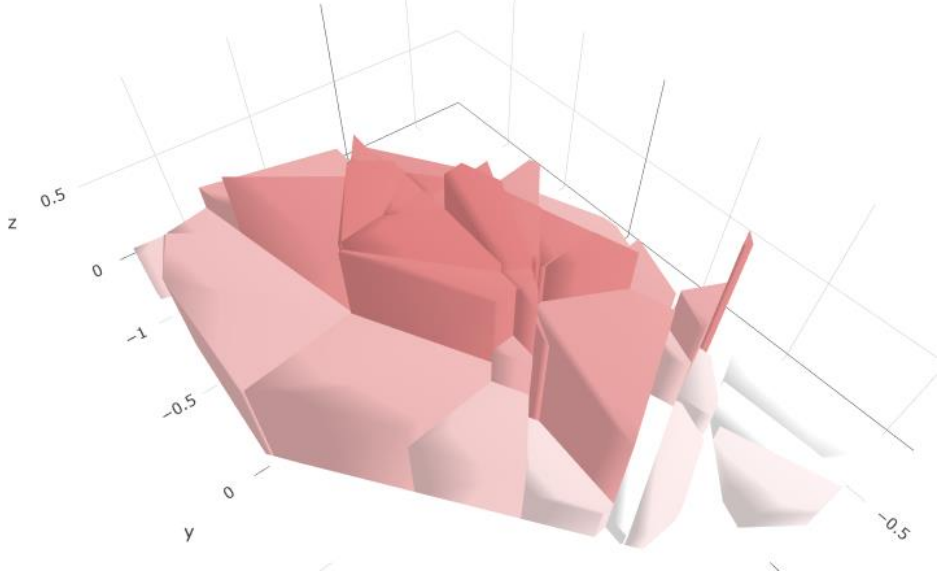
Output of $c_n^*(x)$ in 3D



Reproduced (synthetic) dataset



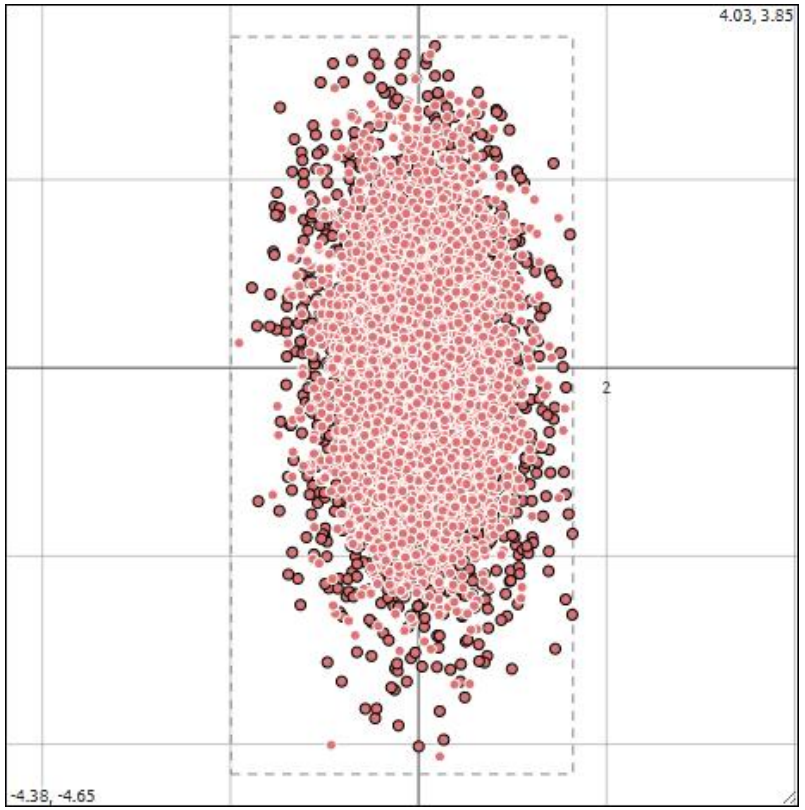
Output of $h_n^*(x)$



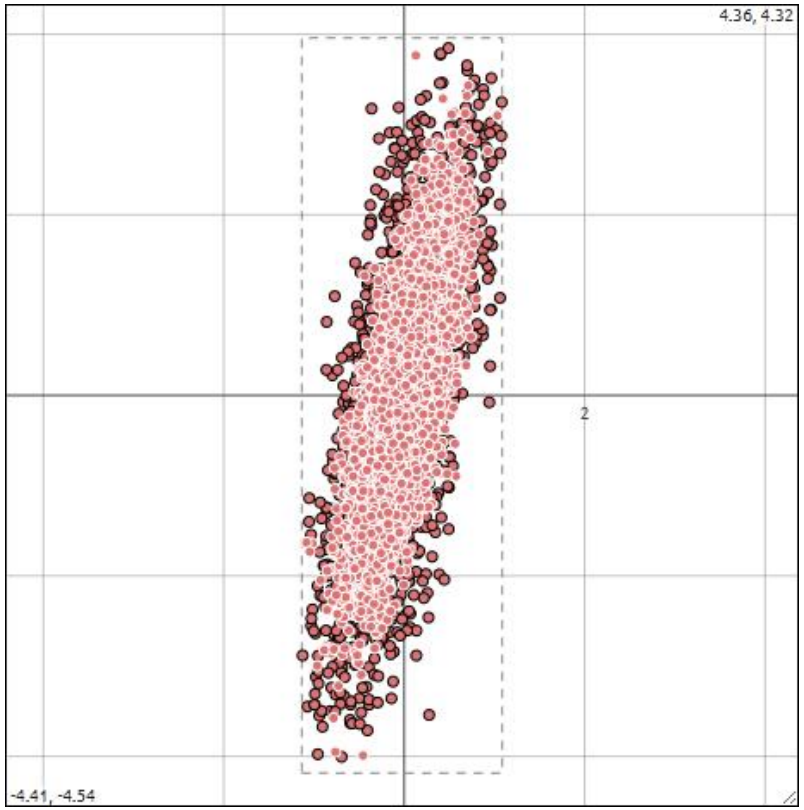
Output of $h_n^*(x)$ in 3D

Synthetic data generation: example 4

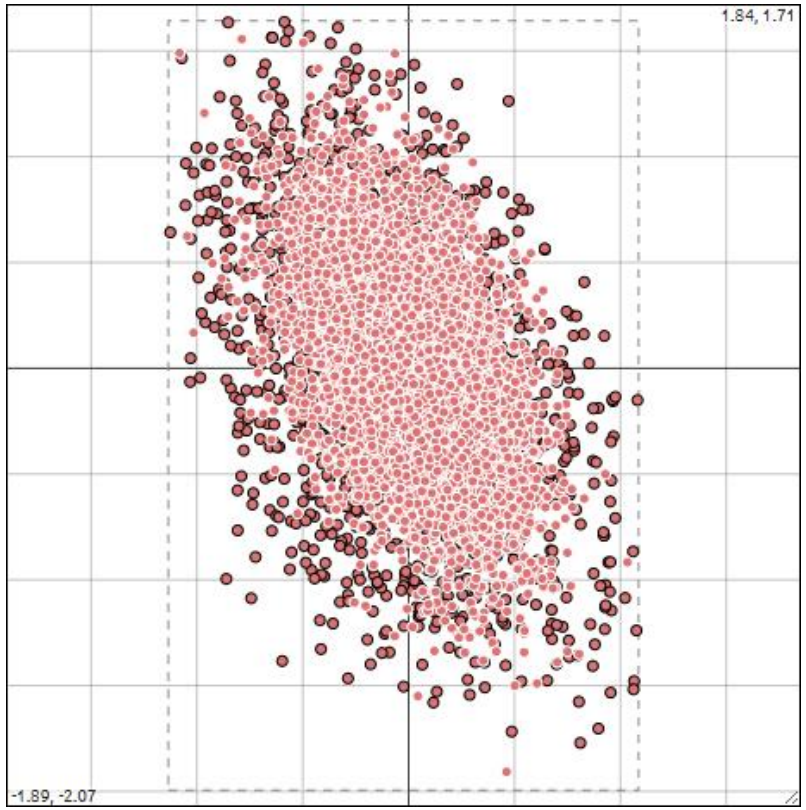
- **Real dataset X**: 10-dimensional Gaussian distribution.
- **Synthetic dataset $\widehat{X}$**: greater dispersion than in the two-dimensional case.



x_1/x_2 projection



x_1/x_3 projection

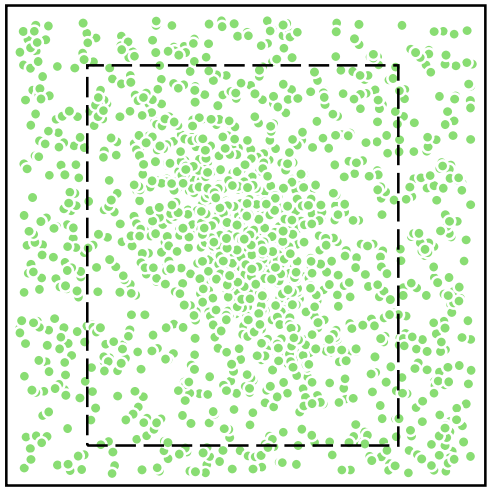


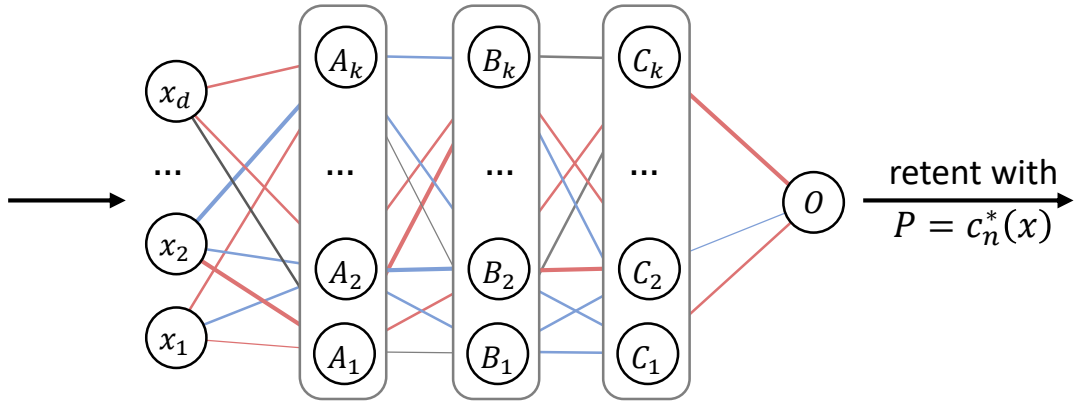
x_2/x_{10} projection

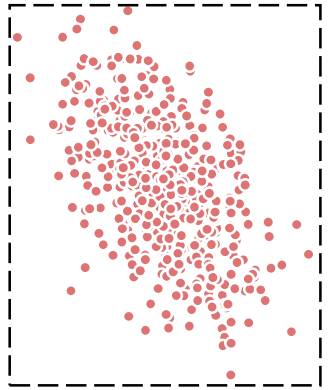
Future work

- **High-dimensional analysis:** studying method behavior in higher dimensions;
- **Training impact:** examining how perceptron training affects final quality;
- **Optimization strategies:** improving stability and efficiency of training;
- **Comparisons:** benchmarking against alternative density estimation methods.

Interactive perceptron visualizer







Conclusion

- **Structured approach**: generates high-fidelity synthetic data while preserving *statistical* and *structured* properties.
- **Adaptive shaping**: classifier output guides the synthetic distribution.
- **Perceptron flexibility**: different architectures capture complex density patterns.
- **Confidence threshold**: balances fidelity and sample sufficiency.

Interactive perceptron visualizer

Challenges

- High-dimensional background sampling remains difficult.
- Perceptron depth / width affects density granularity.
- Over-segmentation risk in complex models.