Binary Classification Using Some Notions of Kernelized Data Depths

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Data depth

Data depth is a non-parametric approach that measures the relative position of a point with respect to the given data cloud (or, a probability distribution). A simple example is

$$D(x, F_n) = \min\{F_n(x), 1 - F_n(x)\}.$$

$F_n(x)$ is the proportion of data points that are on the left of x (the empirical distribution function). Note: $\max\limits_{x \in \mathbb{R}} D(x, F_n) = \frac{1}{2}$.

$D(x, F_n) = \min\{\frac{6}{10}, \frac{4}{10}\} = \frac{2}{5}$; $D(x, F_n) = \min\{\frac{2}{10}, \frac{8}{10}\} = \frac{1}{5}$

Red point is more close to the centre as compared to green point.

Desirable properties of a depth function

Let $D(.,.) : \mathbb{R}^d \times \mathcal{F} \to [0,1]$ be a bounded, non-negative depth function. Ideally, D should satisfy:

- **Affine invariant**: $D(A\mathbf{x} + \mathbf{b}, F_{A\mathbf{X}+\mathbf{b}}) = D(\mathbf{x}, F_{\mathbf{X}})$.
- **Maximality at center**: $D(\boldsymbol{\theta}, F) = \sup_{\mathbf{x} \in \mathbb{R}^d} D(\mathbf{x}, F)$ for any F with center $\boldsymbol{\theta} \in \mathbb{R}^d$.
- **Monotonicity relative to deepest point**: For symmetric F (with centre at $\boldsymbol{\theta}$), $D(\mathbf{x}, F) \leq D(\alpha \cdot \mathbf{x} + (1-\alpha) \cdot \boldsymbol{\theta}, F)$, for $\alpha \in [0,1]$.
- **Vanishing at infinity**: $D(\mathbf{x}, F) \to 0$ as $\|\mathbf{x}\|_2 \to \infty$.

Half-space depth (HD)

Half-space depth at $\mathbf{x} \in \mathbb{R}^d$ w.r.t the distribution F is defined to be

$$HD(\mathbf{x}; F) = \inf_{H}\{P(H) : \text{H is a closed half-space in } \mathbb{R}^d \text{ and } \mathbf{x} \in H\}. \quad (1)$$

Alternatively,

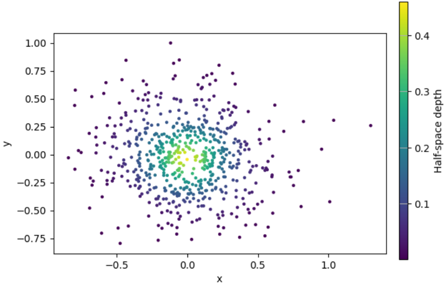
$$HD(\mathbf{x}; F) = \inf_{\mathbf{u} \in \mathbb{S}(0,1)} \mathbb{P}(\langle \mathbf{u}, \mathbf{X} \rangle \geq \langle \mathbf{u}, \mathbf{x} \rangle) \text{ for } \mathbf{X} \sim F. \quad (2)$$

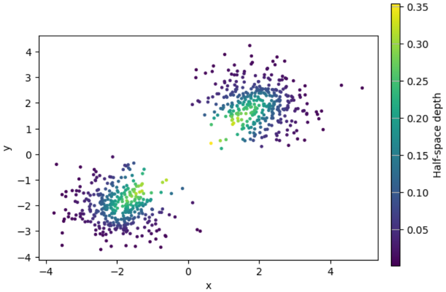
A sample version of HD is given by:

$$HD(\mathbf{x}; F_n) = \inf_{\mathbf{u} \in \mathbb{S}(0,1)} \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}\left(\langle \mathbf{u}, \mathbf{x_i} \rangle \geq \langle \mathbf{u}, \mathbf{x} \rangle\right), \quad (3)$$

where $\mathbb{I}$ is the indicator function.

HD for data with convex and non-convex support





Left: Data is simulated from $N_2((0,0)^T, I_2)$ (convex support).

Right: Data is simulated from $\frac{1}{2}N_2((2,2)^T, I_2) + \frac{1}{2}N_2((-2,-2)^T, I_2)$ (non-convex support).

Spatial depth (SPD)

Spatial depth at $\mathbf{x} \in \mathbb{R}^d$ w.r.t the distribution F is defined as:

$$SPD(\mathbf{x}; F) = 1 - \|E_F[S(\mathbf{Y} - \mathbf{x})]\|_2 \text{ for } \mathbf{Y} \sim F \ , \tag{4}$$

where

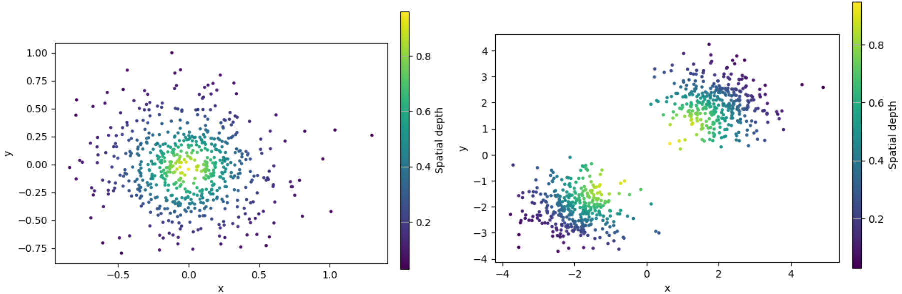
$$S(\mathbf{x}) = \begin{cases} \frac{\mathbf{x}}{\|\mathbf{x}\|_2} & \text{if } \mathbf{x} \neq \mathbf{0} \\ \mathbf{0} & \text{if } \mathbf{x} = \mathbf{0} \ . \end{cases}$$

The sample version is:

$$SPD(\mathbf{x}; F_n) = 1 - \frac{1}{|\mathscr{X} \cup \mathbf{x}| - 1} \left\| \sum_{\mathbf{y} \in \mathscr{X}} S(\mathbf{y} - \mathbf{x}) \right\|_2 \ , \tag{5}$$

where $\mathscr{X} = \{\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_n}\}$ is the sample and $|\mathscr{X} \cup \mathbf{x}|$ denotes cardinality of the union $\mathscr{X} \cup \mathbf{x}$.

SPD for data with convex and non-convex support



Left: Data is simulated from $N_2((0,0)^T, I_2)$ (convex support).

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HD and SPD for non-convex support

HD and SPD cannot adapt to non-convex supports.

This is because they are based on Euclidean scalar products i.e. linear projections.

Note that,

$$HD(\mathbf{x}; F_n) = \inf_{\mathbf{u} \in \mathbb{S}(0,1)} \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}\left(\langle \mathbf{u}, \mathbf{x_i} - \mathbf{x} \rangle \geq 0\right) \text{ and}$$

$$SPD(\mathbf{x}; F_n) = 1 - \frac{1}{|\mathscr{X} \cup \mathbf{x}| - 1} \left\| \sum_{\mathbf{y} \in \mathscr{X}} S(\mathbf{y} - \mathbf{x}) \right\|_2 \text{ where}$$

$$\left\| \sum_{\mathbf{y} \in \mathscr{X}} S(\mathbf{y} - \mathbf{x}) \right\|_2 = \Big(\sum_{\mathbf{z}, \mathbf{y} \in \mathscr{X}} \frac{\langle \mathbf{x}, \mathbf{x} \rangle + \langle \mathbf{y}, \mathbf{z} \rangle - \langle \mathbf{x}, \mathbf{y} \rangle - \langle \mathbf{x}, \mathbf{z} \rangle}{\delta_\kappa(\mathbf{x}, \mathbf{y}) \times \delta_\kappa(\mathbf{x}, \mathbf{z})} \Big)^{\frac{1}{2}} ,$$

$$\delta_\kappa(\mathbf{x}, \mathbf{y}) = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle + \langle \mathbf{y}, \mathbf{y} \rangle - 2 \times \langle \mathbf{x}, \mathbf{y} \rangle} \ .$$

Kernel trick

Let $\kappa : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^+$ be a positive definite kernel ,i.e.,

$$\sum_{i,j=1}^{n} c_i c_j \kappa(\mathbf{x_i}, \mathbf{x_j}) \geq 0 \ \forall \ c_i \in \mathbb{R} \text{ and } \mathbf{x_i} \in \mathbb{R}^d \text{ for } 1 \leq i \leq n \ .$$

A positive definite kernel κ, implicitly defines an embedding map

$$\phi : \mathbf{x} \in \mathbb{R}^d \to \phi(\mathbf{x}) \in \mathbb{F}$$

via an inner product in the feature space $\mathbb{F}$. Thus, we have

$$\kappa(\mathbf{x}, \mathbf{y}) = \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle \ .$$

In HD and SPD, features appear as **inner products**. These inner products are replaced by kernels evaluated on features in the induced space.

Kernelized depths: Sphere depth (SD)

Kernelized version of HD is given by:

$$SD^r(\mathbf{z}, F) \stackrel{\text{def}}{=} \inf_{\mathbf{c} \in \mathbb{S}(\mathbf{z}, r)} \mathbb{P}(\kappa(\mathbf{c}, \mathbf{X}) \geq \kappa(\mathbf{c}, \mathbf{z})) \ , \tag{6}$$

where $\mathbf{X} \sim F$ and $\kappa : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^+$ is a positive definite kernel with $r > 0$.

After some modification, the sphere depth can be expressed as:

$$SD^r_s(\mathbf{z}, F) = \inf_{\mathbf{c} \in \mathbb{S}(\mathbf{z}, r)} \mathbb{E}\left[sig_s(r^2 - \|\mathbf{X} - c\|_2^2)\right] \ . \tag{7}$$

The sample version of sphere depth is given by:

$$SD^r_s(\mathbf{z}, F_n) = \inf_{\mathbf{c} \in \mathbb{S}(\mathbf{z}, r)} \frac{1}{n} \sum_{i=1}^{n} \left[sig_s(r^2 - \|\mathbf{x_i} - c\|_2^2)\right] \text{ where } sig_s : x \to \frac{1}{1 + e^{-x/s}} \ . \tag{8}$$

Kernelized Spatial depth (KSPD)

Kernelized spatial depth is the kernelized version of SD and is defined as:

$$KSPD(\mathbf{x}, F) = 1 - \|E[S(\phi(\mathbf{Y}) - \phi(\mathbf{x}))]\|_2 \ , \tag{9}$$

where $\phi : \mathbf{x} \in \mathbb{R}^d \to \phi(\mathbf{x}) \in \mathbb{F}$ (here, $\mathbb{F}$ is the induced feature space).

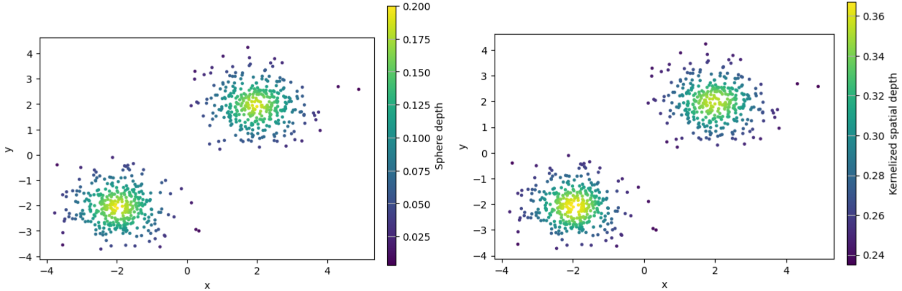
The sample version is given by:

$$KSPD_\kappa(\mathbf{x}, F_n) = 1 - \frac{1}{|\mathscr{X} \cup \mathbf{x}| - 1} \left(\sum_{\mathbf{z},\mathbf{y} \in \mathscr{X}} \frac{\kappa(\mathbf{x},\mathbf{x}) + \kappa(\mathbf{y},\mathbf{z}) - \kappa(\mathbf{x},\mathbf{y}) - \kappa(\mathbf{x},\mathbf{z})}{\delta_\kappa(\mathbf{x},\mathbf{y}) \times \delta_\kappa(\mathbf{x},\mathbf{z})} \right)^{\frac{1}{2}} \ , \tag{10}$$

where $\delta_\kappa(\mathbf{x}, \mathbf{y}) = \sqrt{\kappa(\mathbf{x}, \mathbf{x}) + \kappa(\mathbf{y}, \mathbf{y}) - 2 \times \kappa(\mathbf{x}, \mathbf{y})}$,

$\mathscr{X} = \{\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_n}\}$ and $\kappa(\mathbf{x}, \mathbf{y}) = \exp\left(- \frac{\|\mathbf{x}-\mathbf{y}\|^2}{\sigma^2} \right)$.

SD and KSPD for data with non-convex support



SD (left) and KSPD (right) are able to capture the bimodal structure.

Using the kernel trick, the data projections are non-linear and can be adapted for distributions with non-convex supports.

Classification problem

Problem of interest: A supervised classification problem with 2 competing classes.

Let $\mathbf{X_1}, \cdots, \mathbf{X_n} \stackrel{i.i.d}{\sim} F_0$ and $\mathbf{Y_1}, \cdots, \mathbf{Y_m} \stackrel{i.i.d}{\sim} F_1$.

Task: To construct a decision rule for classifying an unlabeled observation $\mathbf{X}$ to one of these 2 classes.

We used the idea of data depth for this purpose.

Transformed $d-$dimensional data into $2-$dimensional data ($\mathbb{R}^d \rightarrow [0, 1]^2$) using depth values calculated for each observation with respect to two class subsets.

Trained multiple classifiers on the transformed dataset.

Classifiers

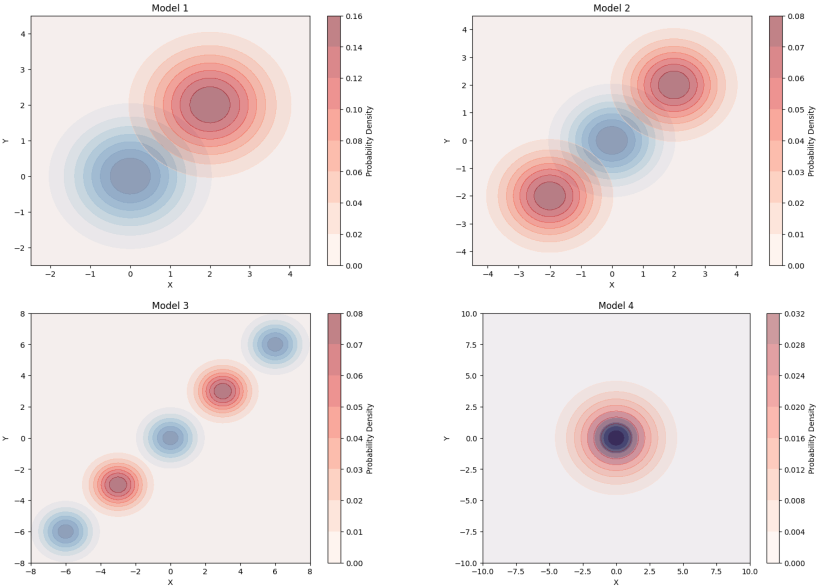
- Support vector machines with Radial Basis Function kernel (SVM-RBF).
- K-nearest neighbors (KNN).
- Generalized additive models (GAM) with logistic link. The model is given by

$$\log\left[\frac{\mu(\mathbf{x})}{1-\mu(\mathbf{x})}\right] = \alpha + f_1(X_1) + \cdots + f_p(X_p) \; ,$$

where $\mu(\mathbf{x}) = Pr(Y = 1|\mathbf{X} = \mathbf{x})$ and each of the functions f_j are unspecified smooth functions for $1 \leq j \leq p$.

Non parametric form of f_j ensures flexibility, while the additive nature ensures interpretability.

Simulation Models



Results-I

Model 1:

dim	Bayes	On $\mathbb{R}^d$	SD	KSPD
5	1.28 (0.59)	1.75 (0.77)	3.47 (0.85)	4.20 (2.70)
10	0.12 (0.13)	3.55 (2.68)	0.48 (0.58)	6.43 (0.12)

Table: 100 $\times$ Mean misclassification (standard error) using SVM-RBF.

Model 2:

dim	Bayes	On $\mathbb{R}^d$	SD	KSPD
5	2.00 (0.55)	3.05 (0.74)	10.80 (2.93)	12.47 (6.37)
10	0.10 (0.12)	7.80 (3.89)	7.97 (5.20)	6.00 (5.32)

Table: 100 $\times$ Mean misclassification (standard error) using SVM-RBF.

Results-II

Model 3:

dim	Bayes	On $\mathbb{R}^d$	SD	KSPD
5	0.10 (0.12)	0.83 (0.54)	4.43 (4.14)	5.60 (8.46)
10	0.00 (0.00)	0.08 (0.11)	13.93 (6.67)	8.38 (9.00)

Table: 100 $\times$ Mean misclassification (standard error) using GAM.

Model 4:

dim	Bayes	On $\mathbb{R}^d$	SD	KSPD
5	26.15 (2.00)	34.50 (3.26)	36.35 (3.25)	39.75 (4.38)
10	17.80 (1.63)	29.75 (1.82)	36.44 (3.40)	36.44 (3.40)

Table: 100 $\times$ Mean misclassification (standard error) using GAM.

Thank you!

References

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Appendix: Bayes classifier

The Bayes classifier classifies a test point ($\mathbf{x} \in \mathbb{R}^d$) based on the product of the likelihood and the prior probability. It has smallest probability of misclassification.

Let $C(\mathbf{x})$ be the Bayes classifier. Then

$$\begin{aligned} C(\mathbf{x}) &= \arg \max_{r \in \{0,1\}} \mathbb{P}(Y = r | \mathbf{X} = \mathbf{x}) \\ &= \arg \max_{r \in \{0,1\}} \underbrace{\mathbb{P}(\mathbf{X} = \mathbf{x} | Y = r)}_{\text{likelihood}} \cdot \underbrace{\mathbb{P}(Y = r)}_{\text{prior}} \end{aligned}$$

With simulated data the prior and likelihood are known hence the Bayes misclassification rate is used as benchmark for comparison.

SD-I

SD is defined as:

$$SD^r(\mathbf{z}, \mathbf{F}) \stackrel{\text{def}}{=} \inf_{\mathbf{c} \in \mathbb{S}(\mathbf{z}, r)} \mathbb{P}(\kappa(\mathbf{c}, \mathbf{X}) \geq \kappa(\mathbf{c}, \mathbf{z})) \text{ where, } \mathbf{X} \sim F \tag{1}$$

The kernelized depth of equation (1) has two main intuitive advantages:

1. data projections are non-linear and can be adapted for distributions with non-convex support,
2. additional parameter r provides a flexible lever to control the depth's sensitivity depending on the data.

SD-II

If κ is the Gaussian kernel $\kappa(\mathbf{x}, \mathbf{y}) \overset{def}{=} \exp(-\gamma\|\mathbf{x} - \mathbf{y}\|_2^2)$ with $\gamma > 0$, then $SD^r(\mathbf{z}, \mathbf{F})$ can be written as:

$$SD^r(\mathbf{z}, \mathbf{F}) = \inf_{\mathbf{c} \in \mathbb{S}(\mathbf{z}, r)} \mathbb{P}_{\mathbf{X}}(\mathbb{B}(\mathbf{c}, r)) = \inf_{\mathbf{c} \in \mathbb{S}(\mathbf{z}, r)} \mathbb{E}\left[\, \mathbb{I}\{r^2 - \|\mathbf{X} - c\|_2^2 \geq 0\}\right]$$

Justification: For any $\mathbf{x}$, $\mathbf{z} \in \mathbb{R}^d$ and $\mathbf{c} \in \mathbb{S}(\mathbf{z}, r)$:

$\kappa(\mathbf{c}, \mathbf{x}) \geq \kappa(\mathbf{c}, \mathbf{z}) \iff e^{-\gamma\|\mathbf{x}-\mathbf{c}\|_2^2} \geq e^{-\gamma r^2} \iff \|\mathbf{x} - \mathbf{c}\|_2 \leq r$.

Therefore, $\mathbb{P}(\kappa(\mathbf{c}, \mathbf{X}) \geq \kappa(\mathbf{c}, \mathbf{z})) = \mathbb{P}_{\mathbf{X}}(\mathbb{B}(\mathbf{c}, r))$.

To make the depth function differentiable the indicator function is replaced by the sigmoid function and SD is given by:

$$SD_s^r(\mathbf{z}, F) = \inf_{\mathbf{c} \in \mathbb{S}(\mathbf{z}, r)} \mathbb{E}\left[sig_s(r^2 - \|\mathbf{X} - c\|_2^2)\right] .$$

Algorithm to compute SD

Algorithm 1 Riemannian gradient descent for computing SD

Input: $\mathbf{z}, \mathbf{X_{1:n}}, \mathrm{tol}, \alpha$
Result: $l \stackrel{\mathrm{def}}{=} SD_s^r(\mathbf{z}|\mathbf{X_{1:n}})$
Initialize $\mathbf{u} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x_i}$
$\mathbf{u} \leftarrow \frac{\mathbf{u}}{\|\mathbf{u}\|_2}$
$l \leftarrow L(u)$
for $i = 1$ to n_iter **do**
    $v \leftarrow -\nabla_u \mathbf{L}(u)$
    $v \leftarrow v - \langle v, u \rangle u$
    $v \leftarrow \frac{v}{\|v\|_2}$
    $u \leftarrow \cos(\alpha)u + \sin(\alpha)v$
    $l' \leftarrow \mathbf{L}(u)$
    $\mathrm{dist} \leftarrow |l' - l|$
    if $l' > l$ **then**
        $\alpha \leftarrow \frac{\alpha}{2}$
    else if $\mathrm{dist} < \mathrm{tol}$ **then**
        break
    else
        $l \leftarrow l'$
    end if
end for
Return l

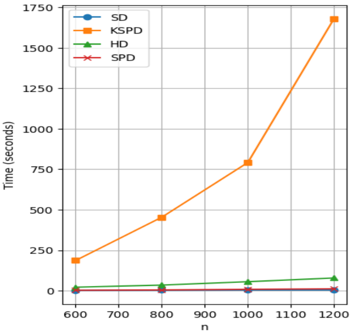
Algorithm to compute KSPD

Algorithm 2 Computation of KSPD

for every pair of $\mathbf{x_i}$ and $\mathbf{x_j}$ in $\mathbf{X}_{1:n}$ **do**
    $K_{ij} = \kappa(\mathbf{x_i}, \mathbf{x_j})$
end for
given input $\mathbf{x}$
for every observation $\mathbf{x_i}$ in $\mathbf{X}_{1:n}$ **do**
    $\zeta_i = \kappa(\mathbf{x}, \mathbf{x_i})$
    $\delta_i = \sqrt{\kappa(\mathbf{x}, \mathbf{x}) + K_{ii} - 2\zeta_i}$
    if $\delta_i = 0$ **then**
        $z_i = 0$
    else
        $z_i = \frac{1}{\delta_i}$
    end if
end for
for every pair of $\mathbf{x_i}$ and $\mathbf{x_j}$ in $\mathbf{X}_{1:n}$ **do**
    $\tilde{K_{ij}} = \kappa(\mathbf{x}, \mathbf{x}) + K_{ij} - \zeta_i - \zeta_j$
end for
$D_\kappa(\mathbf{x}, \mathbf{X}_{1:n}) = 1 - \frac{1}{|\mathcal{X} \cup \{\mathbf{x}\}| - 1} \sqrt{\mathbf{z}^T \tilde{K} \mathbf{z}}$

Computation time for SD and KSPD for varying n

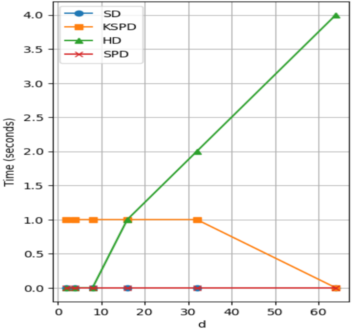
Computation time for varying sample sizes:



The time computation is performed on data simulated from $N_2((0,0)^T, I_2)$.

Computation time for SD and KSPD for varying d

Computation time for varying dimensions:



The time computation is performed on data simulated from $N_2(\mathbf{0}_d, I_d)$. with n = 200.