Analysis and Design of Deep Neural Networks

Chapter 2

Complexity Indices and Data analysis

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2 Complexity Indices and Data analysis

2.1. Complexity Indices

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2.2.2 Supervised Feature Selection
2.2.4 Data Connectivity Matrix (Smi Table)
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2.2.3 Unsupervised Feature Selection

2.1 Complexity Indices

Supervised Indices: 1- Separation Index (Classification Prob.), 2-Smoothness Index(Regression Prob.)

2.1.1 Separation index(SI)

- First order SI
- High order SI
- High order soft SI
- Center Based SI
- Cross SI
- Anti SI
- Self Supervised SI

2.1.2 Smoothness index(SmI)

- First order SmI
- High order SmI
- High order soft SmI
- Cross SmI
- Global SmI
- Data Connectivity SmI

Complexity measures

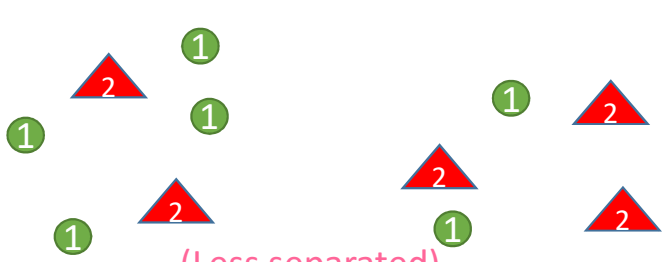
Complexity measures	Overall evaluating approach
√ Feature-based	Discovering informative features by evaluating each feature independently (Orriols-Puig et al., 2010; Cummins, 2013))
√ Linearity separation	Evaluating the linearly separation of different classes (Bottou & Lin, 2007)
√ Neighborhood	Evaluating the shape of the decision boundary to distinguish different classes overlap (Lorena et al., 2012; Leyva et al., 2014)
√ Network	Evaluating the data dataset structure and relationships by representing it as a graph (Garcia et al., 2015)
√ Dimensionality	Evaluating the sparsity of the data and the average number of features at each dimension (Lorena et al., 2012; Basu & Ho, 2006)
√ Class imbalanced	Evaluating the proportion of dataset number between different classes (Lorena et al., 2012)

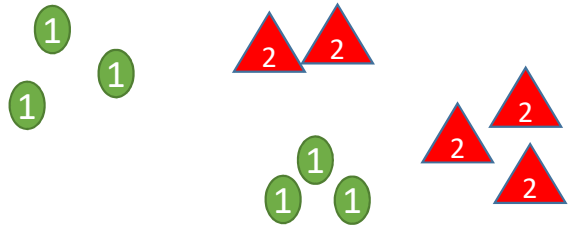
Table 1. Some complexity measures and their evaluating approaches in a classification problem

Two Supervised Complexity measures

1. A separation measure (in classification problems)

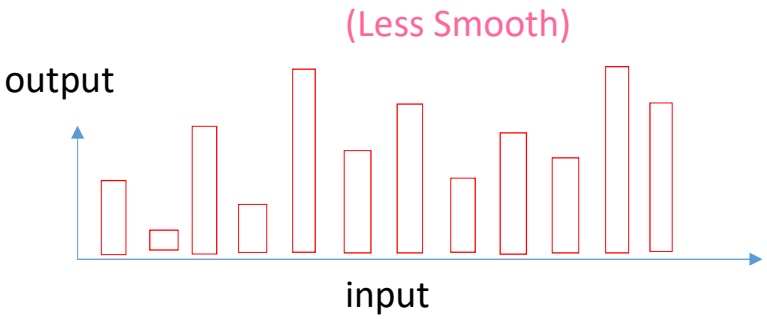
   It shows that how much input data points separate the labels from each others.

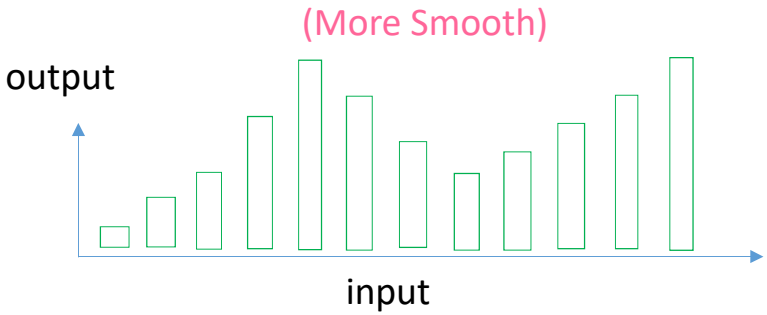




2. An smoothness measure (in regression problems)

   It shows that how much input data points make the output targets smooth





Separation index (SI)

"SI" measures that how much input data points(the feature space) separate different class labels from each others.

"SI" is a variant of similarity measure between feature space(input distribution) and the label space(output distribution)

2.1. Separation index (SI)

1. First order SI

$Data = \{(\boldsymbol{x}_i, l_i)\}_{i=1}^{m} \forall i: \boldsymbol{x}^i \epsilon R^{n\times 1}$ $l_i \epsilon \{1,2,\dots,n_C\}$ n_C:number of classes

*it is assumed that "Data" is a measured sample from a domain with high enough diversity.

*$\boldsymbol{x}_i$may have any format (video, image, time series, etc.) ; however, to compute SI, it must be reshaped as a vector.

$$\mathrm{SI}(Data) = \frac{1}{m}\sum_{i=1}^{m} \delta(l_i, l_{i^*})$$

$$i^* = \underset{\forall q \neq i}{\arg\, min} \left\| \boldsymbol{x}_i - \boldsymbol{x}_q \right\| \qquad \delta(l_i, l_{i^*}) = \begin{cases} 1 & if\ l_i = l_{i^*} \\ 0 & else \end{cases}$$

kronecker delta

*$\|\cdot\|$ denotes Euclidian distance (L_2 norm) but it may be another distance definition such as L_p norm:

$$\left\| \boldsymbol{x}_i - \boldsymbol{x}_j \right\|_{L_p} = \sqrt[p]{\sum_{k=1}^{n} \left| \boldsymbol{x}_i(k) - \boldsymbol{x}_j(k) \right|^p}$$

** It is assumed that the input data is normalized at each dimension just before computing separation index.

Some notes

1. "SI" is a normalized index between zero and one: $\mathrm{SI} \in [0,1]$
2. $SI \to 1$ $(Sepration\ is\ maximmum)$ and $SI \to 0 (Sepration\ is\ minimmum)$
3. "SI" counts (average of) all data points whose nearest neighbors have the same label
4. "SI" is equal to the accuracy of the nearest neighbor classifier as a non-parametric model. Hence, SI is an informative index having strong correlation with the best accuracy one can access by a model without filter process.
5. SI does not change against shift and scales of data points.

$$\forall \beta \neq 0, \forall \alpha \neq 0, \forall \boldsymbol{x}_0, \forall l_0 \qquad SI(\{(\boldsymbol{x}^i, l^i)\}_{i=1}^m) = SI(\{(\beta x_i + \boldsymbol{x}_0, \alpha l_i + l_0)\}_{i=1}^m)$$

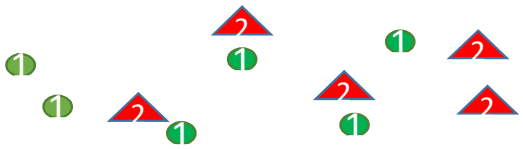
6. Separatin index of $the\ target\ labels\ with\ themselves\ is\ maximum$: $SI(\{(l_i, l_i)\}_{i=1}^m)$=1;

it means that how input data become more similar to labels the separation index will increase.

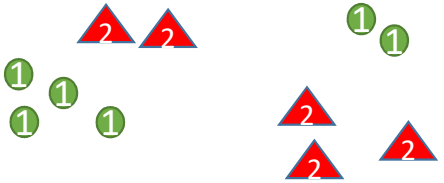
Two dimensional examples (binary classification)

SI=6/11

SI=11/11=1



SI=4/11



SI=11/11=1

Some notes

- To have a high SI, It is enough that examples of each class become near and near together in some regions
- The number of regions is not important but each region must have at least two members.
- The shape of each region is not important.

The distance matrix

- To achieve SI, matrix distance of all data points must be computed (to get nearest neighbor for each data point)

$$Data = \{(\boldsymbol{x}_i, l_i)\}_{i=1}^{m} \qquad \boldsymbol{x}^i \epsilon R^{n\times 1}$$

Distance matrix: $D = [d_{ij}] \quad d_{ij} = \|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2$

Steps

1- Provide data Matrix: $\mathrm{X} = [\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_m]^T, \quad \mathrm{X}\epsilon R^{m\times n}$

2- $\mathrm{M} = \mathrm{X}\mathrm{X}^{\mathrm{T}}, \quad \mathrm{M}\epsilon R^{m\times m}$

3- $\mathrm{d} = \mathrm{diag}(\mathrm{M}), \quad \mathrm{d}\epsilon R^{m\times 1}$

4- $\mathrm{W} = [\mathrm{d}, \mathrm{d}, \dots, \mathrm{d}], \quad \mathrm{W}\epsilon R^{m\times m}$

5- Distance matrix is computed as follows:

$$\mathrm{D} = \mathrm{W} + \mathrm{W}^{\mathrm{T}} - 2\mathrm{M}$$

Separation index of Each data point

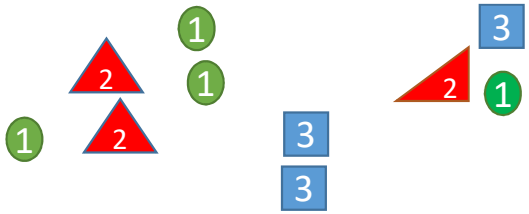
* $SI(Data) = \frac{1}{m}\sum_i si(x_i, l_i)$,$si(x_i, l_i) = \delta(l_i, l_{i^*})$

SI definition with data distribution: $SI(Data) = Exp_{p(x,y)}(si(x, l))$

Challenge: to compute$si(x_i, l_i)$it is required to have x^*as the nearest neighbor of x.

❖For a sample of data with high enough diversity SI can be approximated by equation *

A two dimensional illustrative example



i=1,2,….,10

$si(x_i, l_i) = 0, \quad i$=1,8,9,10
$si(x_i, l_i) = 1, \quad i = 2,3,4,5,6,7$

$SI(Data)$ =0.6

Separation index of Each Class

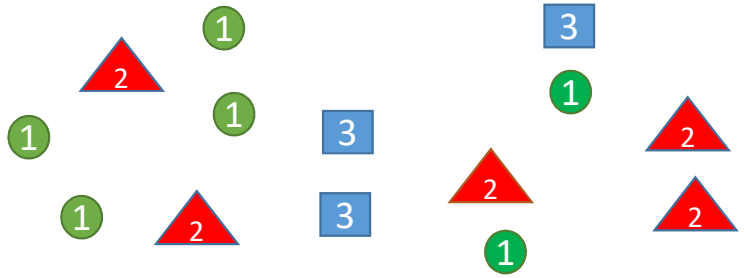
$\mathrm{SI}_c^{class}(Data) = \frac{1}{m_c}\sum_i \delta(l_i, c)\delta(l_i, l_{i^*})$ $c=1,2,..,n_C$

$m_c=\sum_i \delta(l_i, c)$ m_c: number of all data points x^i which $l^i = c$

Relation between "total SI" and "SI of classes"

$$SI(Data) = \frac{1}{m}\sum_{c=1}^{n_C} m_c SI_c^{class}(Data) \qquad \sum_{c=1}^{n_C} m_c = m$$

A two dimensional illustrative example



$n_C = 3, \qquad c = 1,2,3$

$SI_1^{class}(Data) = \frac{4}{6}$

$SI_2^{class}(Data) = 2/5$

$SI_3^{class}(Data) = 2/3$

SI=(4+2+2)/(6+5+3)=8/14

* For when for each class c: $m_c = \frac{m}{n_C}$ and a sufficient high number of data points are distributed with a *uniformly distributed random* variable then it is expected that $SI \to 1/n_C$

2. High order SI

$Data = \{(\boldsymbol{x}_i, l_i)\}_{i=1}^{m}$ $\forall i$: $\boldsymbol{x}_i \epsilon R^{n\times 1}$ $l_i \epsilon \{1,2,\dots,n_C\}$ n_C:number of classes

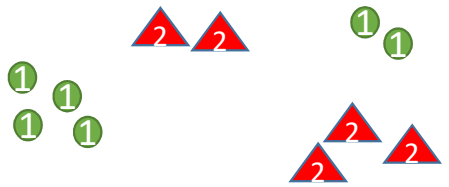
$$\mathrm{SI}^{\mathrm{r}}(Data) = \frac{1}{m}\sum_{i=1}^{m}\prod_{j=1}^{r}\delta\left(l_i, l_{i_j^*}\right)$$ r: the order of "SI"

$$i_j^* = \underset{\forall q \neq i, i_1^*, \cdots, i_{j-1}^*}{\arg} min\left\|\boldsymbol{x}_i - \boldsymbol{x}_q\right\| \qquad \mathrm{SI}^{\mathrm{r}} \in [0,1]$$

- "SI^{r}" counts (average of) all data points whose all "r" nearest neighbors have the same label
- SI^{r} considers more restricted condition of separation than SI^{j} $(j < r)$.
- For each "Data" we have: $\mathrm{SI}^{\mathrm{r}} \leq \mathrm{SI}^{\mathrm{r}-1} \leq \cdots \leq \mathrm{SI}^{1}$ $\mathrm{SI}^{1} = \mathrm{SI}$

Two illustrative Examples

SI^1 =11/11
SI^2 =11/11
SI^3 =11/11
SI^4 =11/11



SI^1 =11/11
SI^2 =7/11
SI^3 =4/11
SI^4 =0

Some notes

1. To increase high order SI, different regions of data points with the same label should merge together and make a hyper-circle shape distribution. In a such case, we will have n_C hyper-circle shape which can separated, linearly from each other.
2. If in a classification problem, the high order SI $\mathrm{SI}^{\mathrm{r}}(r \to \infty) \to 1$, the data points of any pair of classes become more linearly separable.
3. If in a classification problem, the high order SI $\mathrm{SI}^{\mathrm{r}}(r \to \infty) \to 1$, then there is a global separation index (gsi).

3. High order soft SI

$Data = \{(\boldsymbol{x}_i, l_i)\}_{i=1}^{m} \forall i: \boldsymbol{x}_i \epsilon R^{n\times 1}$ $l_i \epsilon \{1,2,\dots,n_C\}$ n_C:number of classes

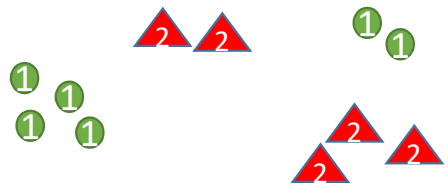
$$\mathrm{SI}^{\mathrm{r}}_{\mathrm{soft}}(Data) = \frac{1}{m\times r}\sum_{i=1}^{m}\sum_{j=1}^{r}\delta(l_i,,l_{i_j^*})$$

r: the order of SI $\quad i_j^* = \underset{\forall q\neq i, i_1^*,\cdots,i_{j-1}^*}{\arg} min\left\|\boldsymbol{x}_i - \boldsymbol{x}_q\right\|$ $\quad \mathrm{SI}^{\mathrm{r}}_{\mathrm{soft}} \in [0,1]$

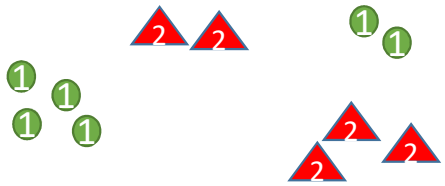
- $\mathrm{SI}^{\mathrm{r}}_{\mathrm{soft}}$ considers less restricted condition of separation than SI^{r}

$$\mathrm{SI}^{\mathrm{r}}_{\mathrm{soft}} \geq \mathrm{SI}^{\mathrm{r}} \quad \text{and} \quad \mathrm{SI}^{1}_{\mathrm{soft}} = \mathrm{SI}^{1}$$

Two illustrative Examples



SI^1 =11/11
SI^2 =7/11
SI^3 =4/11
SI^4 =0



SI^1_{soft} =11/11
SI^2_{soft}=(4+3+0.5+0.5)/11=8/11
SI^3_{soft}=(4+3(2/3)+4*(1/3)/11=8.33/11
SI^4_{soft}=(4*(3/4)+2*(1/4)+2*(1/4)+3*(2/4))/11
=6.5/11

4. Center based Separation Index (CSI)

$Data = \{(\boldsymbol{x}_i, l_i)\}_{i=1}^{m} \forall i: \boldsymbol{x}^i \epsilon R^{n\times 1}$ $l_i \epsilon \{1,2,\dots,n_C\}$ n_C:number of classes

Center of each class is the mean of all input data points having the label of that class:

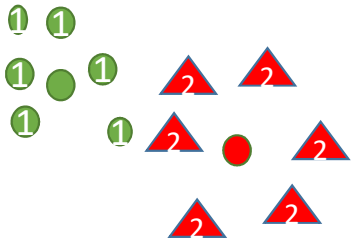
$$\boldsymbol{\mu}_c = \frac{1}{m_c}\sum_{i=1}^{m} \boldsymbol{x}_i \delta(l_i, c), \quad c = 1,2,..,n_C \qquad m_c = \sum_{i=1}^{m} \delta(l_i, c)$$

$$\mathrm{CSI}(Data) = \frac{1}{m}\sum_{i=1}^{m} \delta(l_i, c^*)$$

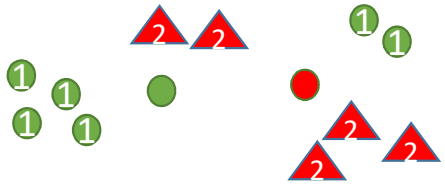
$$c^* = \underset{\forall c}{\arg min} \|\boldsymbol{x}_i - \boldsymbol{\mu}_c\|$$

- CSI is computed much faster than SI because $n_C \ll m$ and you only need to compute the distance matrix of input data points to center of classes.
- It is suggested to compute CSI instead of SI in cases where examples of each class has an indpendent unimodal distribution over a focal point.
- In such cases, each example of a class has most of the exclusive features of that class and has less common features with examples of other classes.

An illustrative Examples



SI =9/11
CSI=11/11



$SI = 1$
CSI=7/11

5. **Self** supervised SI (SSSI)

- $Data = \{(\boldsymbol{x}_i, ?)\}_{i=1}^{m} \forall i: \boldsymbol{x}_i \epsilon R^{n\times 1}$ *Labels are unknown*
- For each $\boldsymbol{x}_i$ we generate some augmented data points: $x_{i_h}, h \in \{1,2,..,n_i\}$
- It is assumed that each x_{i_h} inherits at least an exclusive feature of $\boldsymbol{x}_i$
- An exclusive feature of x_{i_h} is a feature that is sufficient to reveal the label of $\boldsymbol{x}_i$.

$$Data_{\text{aug}} = \{\overbrace{\{(\boldsymbol{x}_{i_h}, i)\}_{h=1}^{n_i}}^{i\text{th (self) class}}\}_{i=1}^{m}$$

$$\text{SSSI}^{\text{r}}(Data) = \text{SI}^{\text{r}}(Data_{\text{aug}}),\ n_C = m,\ m_{aug} = \sum_{i=1}^{m} n_i$$

Cross SI

$Data = \{(\boldsymbol{x}_i, l_i)\}_{i=1}^{m}$ $D_{test} = \{(\breve{\boldsymbol{x}}_i, \breve{l}_i)\}_{i=1}^{m_{test}}$

$$SI_{cross}(D_{test}, Data) = \frac{1}{m_{test}} \sum_{i=1}^{m_{test}} \delta(\breve{l}_i, l_{i^{\#}})$$

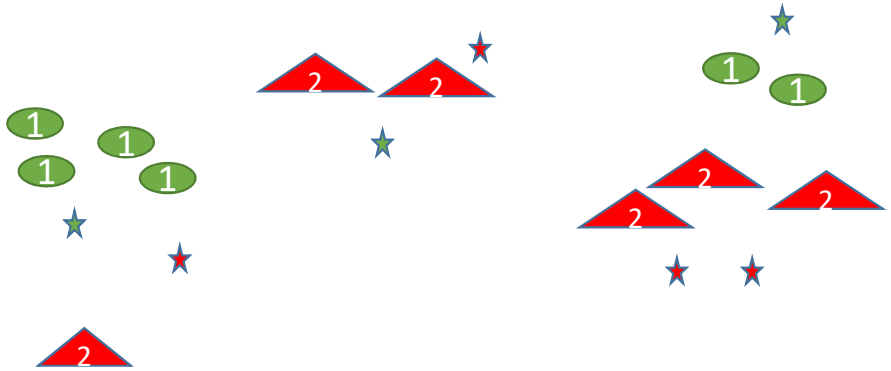
$i^{\#} = \underset{\forall q}{\arg min} \|\breve{\boldsymbol{x}}_i - \boldsymbol{x}_q\|$

Cross SI measures the separation index of a test domain of dataset D_{test} based on the main domain of dataset $Data$.

It can be shown that:

$$SI_{cross}(D_{test}, Data) = \frac{1}{m_{test}} \sum_{i=1}^{m_{test}} SI_{cross}\left((\breve{\boldsymbol{x}}_i, \breve{l}_i), Data\right)$$

An illustrative Examples



$$SI = \frac{12}{13} \qquad Corss\ SI = \frac{5}{7}$$

Anti SI

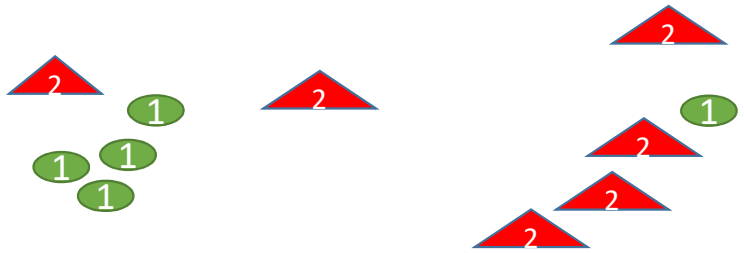
$Data = \{(\boldsymbol{x}_i, l_i)\}_{i=1}^{m}$ $\forall i:\ \boldsymbol{x}_i \epsilon R^{n\times 1}$ $l_i \epsilon \{1,2,\dots,n_C\}$ n_C:number of classes

$$\text{anti\_SI}^{\text{r}}(Data) = \frac{1}{m}\sum_{i=1}^{m}\prod_{j=1}^{r}\left(1-\delta\left(l_i, l_{i_j^*}\right)\right)$$ r: the order of "anti_SI"

$$i_j^* = \underset{\forall q \neq i, i_1^*, \cdots, i_{j-1}^*}{\arg} min\left\|\boldsymbol{x}_i - \boldsymbol{x}_q\right\| \qquad \text{anti\_SI}^{\text{r}} \in [0,1]$$

- "anti SI^{r}" counts (average of) all data points whose all "r" nearest neighbors have different labels with those data points
- Actually data points having higher anti si make hard examples in a data set
- They may be risky examples that experts have labeled them incorrectly. In such a case they should be removed in a "data cleaning process"
- For when data points are images and other spatial or temporal formats, before to score them by "SI" or "anti SI", one must encode them.

An illustrative Examples



$SI^1 = 7/11$
$anti\_SI^1 = 1 - SI^1 = 4/11$

$SI^2 = 5/11$
$anti\_SI^2 = 2/11$

Smoothens index (SmI)

SmI measures how much input data points make the output targets smooth

"SmI" is a variant of similarity measure between feature space(input distribution) and the target space(output distribution)

2.2 Smoothness index (SmI)

A (linear) smoothness measure for regression problem

1. First order SmI

$Data = \{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^{m}$ $\forall i: \boldsymbol{x}_i \epsilon R^{n\times 1}, \boldsymbol{y}_i \epsilon R^{o\times 1}$ o :number of outputs

*it is assumed that Data is a measured sample with high enough diversity.

*$\boldsymbol{x}_i$ and $\boldsymbol{y}_i$ may have any format (video, image, time series, etc.) ; however, to compute SmI, it must be reshaped as a vector.

$$\mathrm{SmI}(Data) = \frac{1}{m}\sum_{i=1}^{m}\left(\frac{\boldsymbol{d}_{imax} - \boldsymbol{d}_{i^*}}{\boldsymbol{d}_{imax} - \boldsymbol{d}_{imin}}\right)$$

$$i^* = \underset{\forall q \neq i}{\arg min}\left\|\boldsymbol{x}_i - \boldsymbol{x}_q\right\| \qquad \boldsymbol{d}_{imax} = \max_{\forall q}\left\|\boldsymbol{y}_i - \boldsymbol{y}_q\right\| \qquad \boldsymbol{d}_{imin} = \min_{\forall q \neq i}\left\|\boldsymbol{y}_i - \boldsymbol{y}_q\right\|$$

$$\boldsymbol{d}_{i^*} = \left\|\boldsymbol{y}_i - \boldsymbol{y}_{i^*}\right\|$$

*$\|\cdot\|$ denotes Euclidian distance (L_2 norm) but it may be another distance definition such as L_p norm.

** It is assumed that the input and target output data are normalized at each dimension just before computing the smoothness index.

*** the above definition of SmI can be biased by outliers.

A modified “linear SmI”

$$\mathrm{SmI}(Data) = \frac{1}{m}\sum_{i=1}^{m} relu\left(1 - \frac{\boldsymbol{d}_{i^*} - \boldsymbol{d}_{imin}}{\boldsymbol{d}_{imean}}\right)$$

$$i^* = \underset{\forall q \neq i}{\arg\, min} \|\boldsymbol{x}_i - \boldsymbol{x}_q\| \qquad \boldsymbol{d}_{imean} = \frac{1}{m}\sum_{q=1}^{m} \|\boldsymbol{y}_i - \boldsymbol{y}_q\| \qquad \boldsymbol{d}_{imin} = \min_{\forall q \neq i} \|\boldsymbol{y}_i - \boldsymbol{y}_q\|$$

$$\boldsymbol{d}_{i^*} = \|\boldsymbol{y}_i - \boldsymbol{y}_{i^*}\|$$

Some notes:

1. the above definition of SmI is not affected by outliers due to using mean of syance instead of maximum distance.
2. The “relu” function actually assign zero smoothness index to all data points whose their nearest neighbors have far enough targets with them.

A modified Exponential SmI

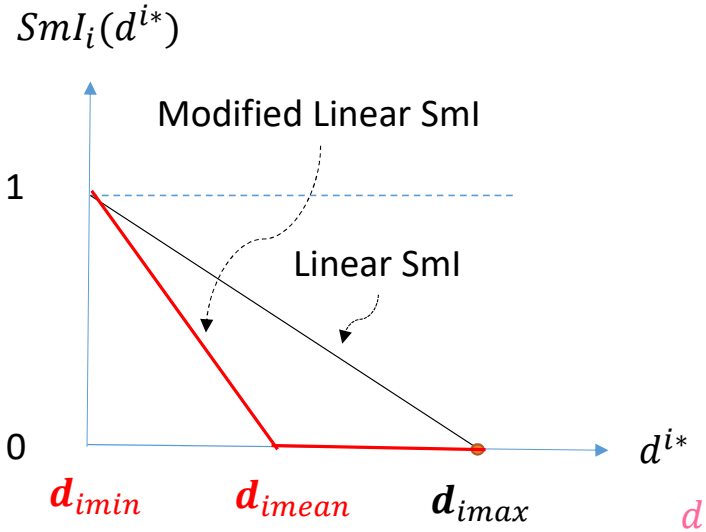
$$\mathrm{SmI}(Data) = \frac{1}{m}\sum_{i=1}^{m} SmI^i \quad SmI^i = \exp\left(-\gamma \frac{\boldsymbol{d}_{i^*} - \boldsymbol{d}_{imin}}{\boldsymbol{d}_{imean}}\right)$$

$$\boldsymbol{d}_{imean} = \frac{1}{m}\sum_{q=1}^{m} \left\| \boldsymbol{y}^i - \boldsymbol{y}^q \right\| \qquad \text{,Smoothness rate } \gamma > 0$$

Some Notes:

1. Exponential SmI is not sensitivity to outliers.
2. For when $\gamma \to \infty$, any distance variation: $\left(\frac{\boldsymbol{d}_{i^*} - \boldsymbol{d}_{imin}}{\boldsymbol{d}_{imean}}\right)$ drops the SmI, significantly.
3. Here we have an exponential smoothness with an optional smoothness rate.
4. To have more restricted definition of SmI, the smoothness rate must be chosen high or $\gamma >> 1$.

SmI Diagrams versus d^{i*}



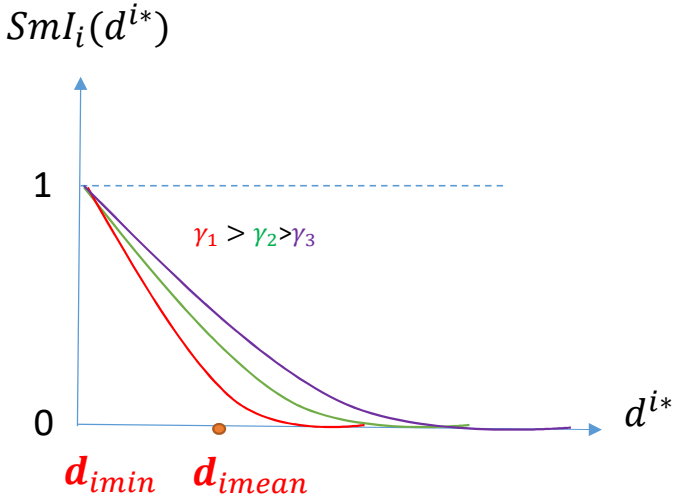
Linear SmI

$$d^{i*} = \|y_i - y_{i^*}\|$$

$$d_{imax} = \max_{\forall q} \|y_i - y_q\|$$

$$d_{imin} = \min_{\forall q \neq i} \|y_i - y_q\|$$

$$d_{imean} = \frac{1}{m} \sum_{q=1}^{m} \|y^i - y^q\|$$



Exponential SmI

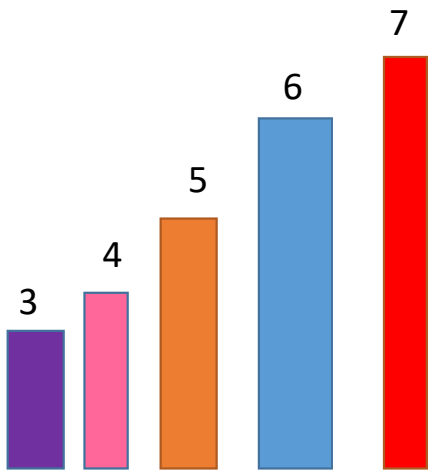
Some notes

1. "SmI" is a normalized index between zero and one: $\mathrm{SmI} \in [0,1]$
2. $SmI \to 1$ $(Smoothness\ is\ maximmum)$ and $SmI \to 0$ $(Smoothness\ is\ minimmum)$
3. "SmI" measures that how nearness of input data leads to nearness of target data.
4. Assuming, the target outputs are outputs of a classification problem in "one-hot" format, SmI is actually measure the separation index: $\mathrm{SmI} = \mathrm{SI}$
5. Increasing the number of classes and considering a nearness among every two classes, SI is interpreted as a smoothness index. Actually, SmI shows in average that how neighboring examples in input space have classes with near distances in output.
6. SmI does not change for arbitrary position shift and (scalar) scale of the data

   $\forall \beta \neq 0, \forall \alpha \neq 0, \forall x_0, \forall y_0 \qquad \mathrm{SmI}(\{(x^i, y^i)\}_{i=1}^m) = SmI(\{(\beta \boldsymbol{x}_i + x_0, \alpha \boldsymbol{y}_i + y_0)\}_{i=1}^m)$

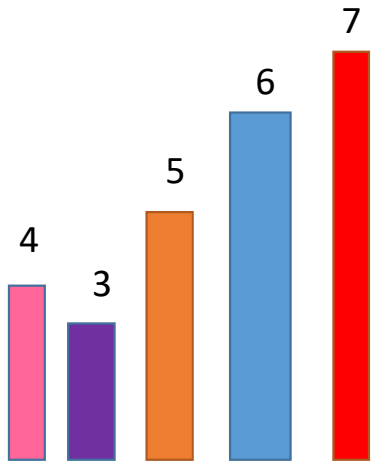
7. Smoothness index of target outputs $with\ themselves\ is$ $maximum$: $SmI(\{(\boldsymbol{y}_i, \boldsymbol{y}_i)\}_{i=1}^m)$=1; it means that how input data become more similar to output the smoothness index will increase.

One-dimensional illustrative examples



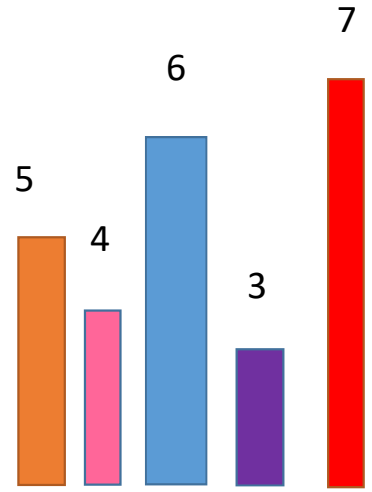
$$SmI = \frac{1}{5}\left(\frac{4-1}{4-1}+\frac{3-1}{3-1}+\frac{2-1}{2-1}+\frac{3-1}{3-1}+\frac{4-1}{4-1}\right)$$

$SmI = 1$



$$SmI = \frac{1}{5}\left(\frac{3-1}{3-1}+\frac{4-1}{4-1}+\frac{2-2}{2-1}+\frac{3-2}{3-1}+\frac{4-1}{4-1}\right)$$

SmI=0.7



$$SmI = \frac{1}{5}\left(\frac{2-1}{2-1}+\frac{3-1}{3-1}+\frac{3-2}{3-1}+\frac{4-3}{4-1}+\frac{4-4}{4-1}\right)$$

SmI=0.566

Smoothness index of Each data point

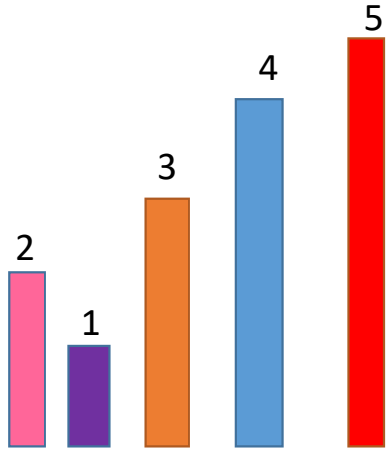
* $SmI(Data) = \frac{1}{m}\sum_i smi(x_i, y_i)$, $smi(x_i, y_i) = \left(\frac{d_{imax} - d_{i^*}}{d_{imax} - d_{imin}}\right)$

SmI definition with data distribution: $SmI(Data) = Exp_{p(x,y)}(smi(x,y))$

Challenge: to compute $\mathrm{smi}(x, y)$ it is required to have x^*as the nearest neighbor of x.

❖ For a sample of data with high enough diversity SI can be approximated by equation *

A one dimensional illustrative example



$$SmI = \frac{1}{5}\left(\frac{3-1}{3-1} + \frac{4-1}{4-1} + \frac{2-2}{2-1} + \frac{3-2}{3-1} + \frac{4-1}{4-1}\right)$$

i=1,2,….,5

$SmI_i^{data} = \frac{3-1}{3-1} = 1$

$SmI_2^{data} = \frac{4-1}{4-1} = 1$

$SmI_3^{data} = \frac{2-2}{2-1} = 0$

$SmI_4^{data} = \frac{3-2}{3-1} = 0.5$

$SmI_5^{data} = \frac{4-1}{4-1} = 1$

2. High order SmI

$Data = \{(x_i, y_i)\}_{i=1}^{m} \forall i: x_i \epsilon R^{n\times 1} \quad y_i \epsilon R^{o\times 1}$

$$\mathrm{SmI}^{r}(Data) = \frac{1}{m}\sum_{i=1}^{m} \min_{\forall j \epsilon \{1,..,r\}} \left(\frac{d_{imax} - d_{i_j^*}}{d_{imax} - d_{imin_j}} \right)$$

r: the order of "SmI"

$$i_j^* = \arg\min_{\forall q \neq i, i_1^*, \cdots, i_{j-1}^*} \|x_i - x_q\| \qquad imin_j = \arg\min_{\forall q \neq i, imin_1, \cdots, imin_{j-1}} \|y_i - y_q\|$$

$$d_{imin_j} = \|y_i - y_{im_j}\| \qquad d_{i^*} = \|y_i - y_{i_j^*}\|$$

- $\mathrm{SmI}^{r} \in [0,1]$
- SmI^{r} considers more restricted condition of smoothness than SmI^{j} $(j < r)$.
- For each "Data" we have: $\mathrm{SmI}^{r} \leq \mathrm{SmI}^{r-1} \leq \cdots \leq \mathrm{SmI}^{1}$ SmI^{1}=SmI

3. High order soft SmI

$Data = \{(\boldsymbol{x}^i, \boldsymbol{y}^i)\}_{i=1}^m \quad \forall i: x^i \epsilon R^{n\times 1} \quad y^i \epsilon R^{o\times 1}$

$$\mathrm{SmI}_{\mathrm{soft}}^{\mathrm{r}}(Data) = \frac{1}{m\times r}\sum_{i=1}^{m}\sum_{j=1}^{r}\left(\frac{\boldsymbol{d}_{imax} - \boldsymbol{d}_{i_j^*}}{\boldsymbol{d}_{imax} - \boldsymbol{d}_{imin_j}}\right) \mathrm{j} = 1,2,\ldots,\mathrm{r}$$

r: the order of "SmI"

- $\mathrm{SmI}_{\mathrm{soft}}^{\mathrm{r}} \in [0,1]$
- $\mathrm{SmI}_{\mathrm{soft}}^{\mathrm{r}}$ considers less restricted condition of smoothness than $\mathrm{SmI}^{\mathrm{r}}$

$$\mathrm{SmI}_{\mathrm{soft}}^{\mathrm{r}} \geq \mathrm{SmI}^{\mathrm{r}} \quad \text{and} \quad \mathrm{SmI}_{\mathrm{soft}}^{1} = \mathrm{SmI}^{1}$$

4. Cross SmI

$Data = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{m}$ $D_{test} = \{(\breve{\boldsymbol{x}}_i, \breve{y}_i)\}_{i=1}^{m_{test}}$

$$SmI_{cross}(D_{test}, Data) = \frac{1}{m_{test}} \sum_{i=1}^{m_{test}} \left(\frac{\boldsymbol{d}_{imax} - \boldsymbol{d}_{i^{\#}}}{\boldsymbol{d}_{imax} - \boldsymbol{d}_{imin_j}} \right)$$

$i^{\#} = \underset{\forall q}{\arg min} \left\| \breve{\boldsymbol{x}}_i - \boldsymbol{x}_q \right\|$

Cross SI measures the separation index of a test domain of dataset D_{test} based on the main domain of dataset $Data$.

It can be shown that:

$$SmI_{cross}(D_{test}, Data) = \frac{1}{m_{test}} \sum_{i=1}^{m_{test}} SmI_{cross}\left((\breve{\boldsymbol{x}}_i, \breve{l}_i), Data \right)$$

Global SmI

- For the Data:$\{(\mathrm{x_i}, y_i)\}_{i=1}^{m}$ we have Global SmI when $SmI^{m-1}(Data) = 1$.
- For Data with Global SmI, One can show that for each example x_i and two other examples x_{i_1} and x_{i_2}:

$$if \ \|x_i - x_{i_1}\| \leq \|x_i - x_{i_2}\| \text{ then } \|y_i - y_{i_1}\| \leq \|y_i - y_{i_2}\|$$

- For Data$(\mathrm{x_i}, y_i)\}_{i=1}^{m}$ where $y_i = \Psi x_i$ and Ψ have orthogonal columns with equal norms, we have global SmI.

Data Node Connectivity Matrix (by SmI)

- $Node^k$:{$(x_i^k)_{i=1}^m$}, k=1,2,...,N, $x_i^k \in R^{n_k}$

Connectivity matrix:

ConMat= $[smI_{k_1,k_2}]_{N\times N}$

smI_{k_1,k_2}=SmI ($Node^{k_1}$, $Node^{k_2}$)

The element indicates how $Node^{k_2}$ is affected by $Node^{k_1}$

when smI_{k_1,k_2}=1, the influence of $Node^{k_1}$ over $Node^{k_2}$ is maximum.

But when smI_{k_1,k_2}=0 the influence of $Node^{k_1}$ over $Node^{k_2}$ is minimum.

Unlike correlation matrix:

1. The matrix is not symmetric
2. The dimensions of different nodes are not necessary equal.
3. The influence is not necessary linear.

Connectivity Matrix

	Node1	Node2	⋯	NodeN
Node1	1	$SmI_{2,1}$	⋯	$SmI_{1,N}$
Node2	$SmI_{1,2}$	1	⋯	$SmI_{2,N}$
⋮	⋮	⋮	⋱	⋮
NodeN	$SmI_{N,1}$	$SmI_{N,2}$	⋯	1

Data Variables Causal Matrix

Non cyclic

var^k :{$\left(x_i^k\right)_{i=1}^m$}, k=1,2,…,N, $x_i^k \in R^1$

Causal Matrix= $\left[ca_{k_1,k_2}\right]_{N\times N}$

$ca_{k_1,k_2} \in \{1,0\}$

	Var1	Var2	⋯	VarN
Var1	0	$ca_{2,1}$	⋯	$ca_{1,N}$
Var2	$ca_{1,2}$	0	⋯	$ca_{2,N}$
⋮	⋮	⋮	⋱	⋮
VarN	$ca_{N,1}$	$ca_{N,2}$	⋯	0

If ca_{k_1,k_2}=1 it means that var^{k_2} is a cause variable for var^{k_1}.

By using an exploration algorithm for each variable, all possible variables which make maximum possible "SmI" with a certain variable are revealed as cause of that variable and a confidence between 0 and 1 is given for that.

❖A subset of independent variables which provide the largest "SmI" for a certain variable, are indicated as the cause set of that variable.

Similarity transformation in "SI" and "SmI"

- Show that for all possible r

$$SI^r(\{(x_i, l_i)\}_{i=1}^m) = SI^r(\{(\Psi_1 x_i, \Psi_2 l_i)\}_{i=1}^m)$$
$$SmI^r(\{(x_i, y_i)\}_{i=1}^m) = SmI^r(\{(\Psi_1 x_i, \Psi_2 y_i)\}_{i=1}^m)$$

where

Ψ_h (h=1,2) have orthogonal columns with equal norms.

2.1 Complexity Indices
An Unsupervised Index : 3- linear density

Linear Density index (LDI)

LDI measures the average of linear densities of a number of clusters.
(Each cluster has a unimodal distribution around a focal point)

2.1. Linear Density Index (Ldi)

1. Ldi

$Data = \{(\boldsymbol{x}_i)\}_{i=1}^{m} \forall i: \boldsymbol{x}^i \epsilon R^{n\times 1}$

Some notes

1. Assumption: "Data" is a measured sample from a domain with high enough diversity.
2. Data has been clustered as N unimodal shape clusters: $cluster_1$, $cluster_2$, …, $cluster_N$ where:

$$Data = cluster_1 \cup \ldots \cup cluster_N \quad \text{and} \quad \forall k_1 \neq k_2: cluster_{k_1} \cap cluster_{k_2} = 0$$

$$cluster_k = \{(\boldsymbol{x}_i^k)\}_{i=1}^{n_k}, n_k = number\ of\ members\ in\ cluster_k$$

Now, linear density of "Data" is defined as follows:

$$\mathrm{Ldi}(Data) = \frac{1}{n\_clusters}\sum_{k=1}^{n\_clusters} \mathrm{ldi}_k\,, \quad \mathrm{ldi}_k = \frac{n_k}{\bar{\sigma}_k}$$

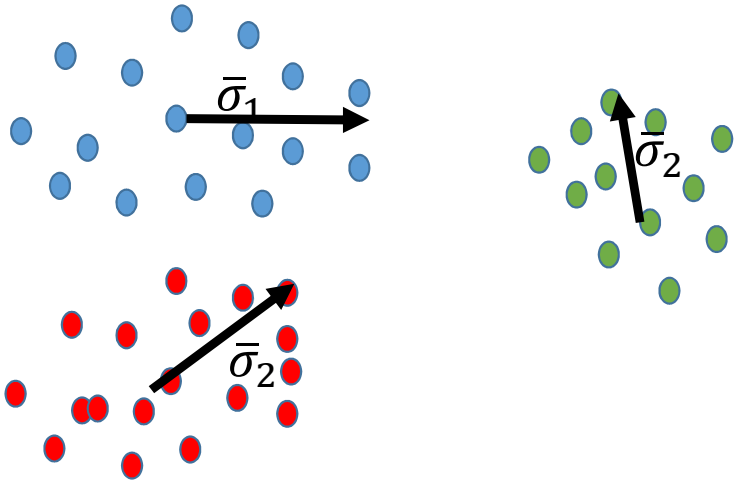
$\bar{\sigma}_k$=Maximum Singular value of the covariance matrix of $cluster_k = \{(\boldsymbol{x}_i^k)\}_{i=1}^{n_k}$

$Cov(cluster_j) = \frac{1}{n_k}\sum_{i=1}^{n_k}(\boldsymbol{x}_i^k - c^k))(\boldsymbol{x}_i^k - c^k)^T \qquad c^k = \frac{1}{n_k}\sum_{i=1}^{n_k}\boldsymbol{x}_i^k$

*It is assumed that the input data is normalized at each dimension just before computing Linear Density Index .

** Each data point such as $\boldsymbol{x}_i$ may have any format (video, image, time series, etc.) ; however, to compute "ldi" for $\boldsymbol{x}_i$, it should be encoded and then being reshaped as a vector.

An illustrative example



$n_{clusters} = N = 3$

$n_1 = 16, \bar{\sigma}_1$=1

$n_2 = 12, \bar{\sigma}_2$=0.9

$n_2 = 20, \bar{\sigma}_3$=1.5

Ldi(Data)=1/3*(16/1+12/0.9+20/1.5)=14.22

What does the density of a distribution tell you?

- Ldi actually computes the density of a data distribution.
- In this sense, the (spatial)density is **the differential probability of observing X∈[x,x+Δx] divided by the length of the interval Δx**. So the density represents a likelihood of observing X∈[x,x+Δx].
- larger densities reflecting a larger likelihood of observing values in that interval.
- Actually, the ldi has a direct relation with Likelihood.
- The clusters with high enough density (hot clusters) are more informative than other regions because they provide larger likelihood for observation.

Ldi and Entropy

- Gibs Entropy Formula: $Entropy = -kB \sum_j p_j \log(p_j)$ s.t. $\sum_j p_j = 1$
  $p_j : microstate$
- In distributions where we have larger ldi, one can say the entropy is decreased and we have more informative data
- Higher densities mean **more deterministic, less randomness and hence more accuracy**.
- Actually, the ldi has an inverse relation with Entropy.

Ldi in classification and regression (problems)

- In a classification problem, it is desired to get feature space that within distances among examples of a class decrease and between distances among examples from different classes increase.
- According to the above property, the examples of each class form one or a few clusters with high ldi.
- The number of clusters must be equal or larger than number of classes.
- However, in a regression problem, it is not expected that the input space become as a number of clusters with high densities.
- The desired distribution of input examples strongly depend to the distribution of target examples.

Relative Density

$Data = \{(\boldsymbol{x}_i)\}_{i=1}^{m}$

1. Cluster Data space by ldi:

$Data = \cup nion(cluster_j) \quad j = 1,2,\dots,J$

$c_j = center\ of\ clustyer\ j$

2. Compute Relative Density

$$RL(Data) = \frac{1}{m}\sum_{i=1}^{m} rd(x_i)$$

$rd(x_i) = 1 - \frac{l_{ij_1}}{l_{ij_2}}$ *(rd: relative density)*

$\mathrm{l_{ij}} = (\|x_i - c_j\|) \qquad l_{ij_1} < l_{ij_2} < l_{ij_3} \dots < l_{ij_J}$

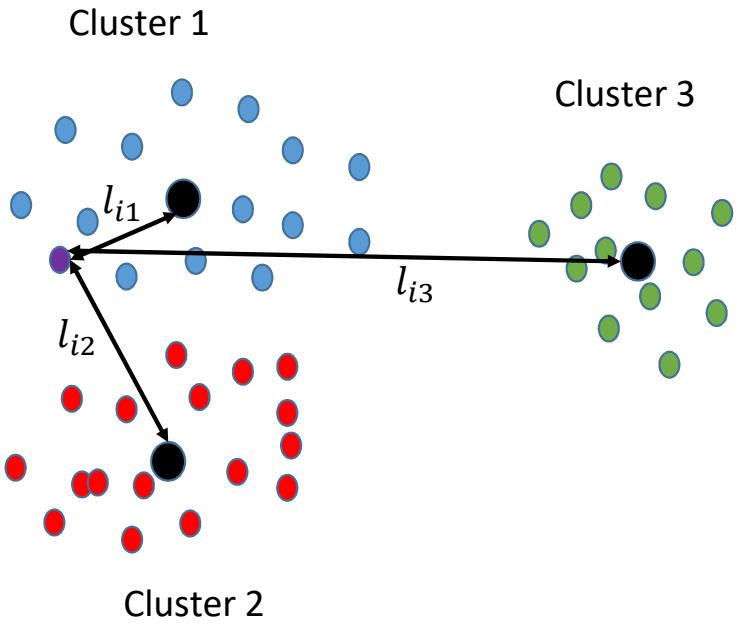
Relative density is an unsupervised normalized index

$$0 \le RL(data) \le 1$$

For when $RL(Data) \to 1$ *we have a data distribution with very dense and separated clusters*

For when $RL(Data) \to 0$ *we have a data distribution with very near clusters.*

-



Cross Relative Density

$Data = \{(\boldsymbol{x}_i)\}_{i=1}^{m}$ $D_{test} = \{(\breve{\boldsymbol{x}}_i)\}_{i=1}^{m_{test}}$

1. Cluster Data space by ldi:

$Data = \cup union(cluster_j)$ $j = 1,2,\dots,J$

$c_j = center\ of\ clustyer\ j$

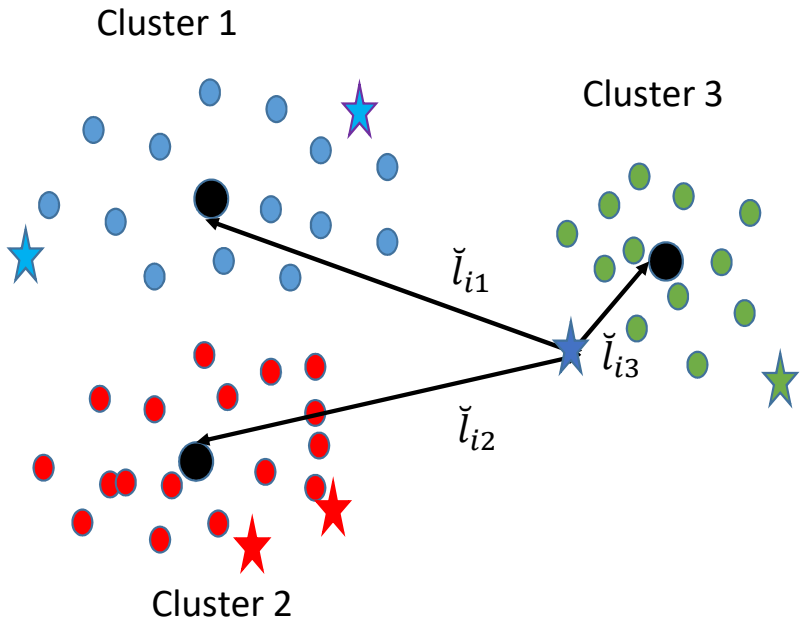
2. Compute Cross Relative Density

$$cross\_RD(Dtest, Data) = \frac{1}{mtest}\sum_{i=1}^{mtes} cross\_rd(\breve{\boldsymbol{x}}_i)$$

$$\text{cross\_rd}(\breve{\boldsymbol{x}}_i) = 1 - \frac{\breve{l}_{i_{j1}}}{\breve{l}_{i_{j2}}}$$

$\breve{l}_{ij} = (\|\breve{\boldsymbol{x}}_i - c_j\|)$ $\breve{l}_{ij_1} < \breve{l}_{ij_2} < \breve{l}_{ij_3} \dots < \breve{l}_{ij_J}$

-



Some applications of using “ldi”

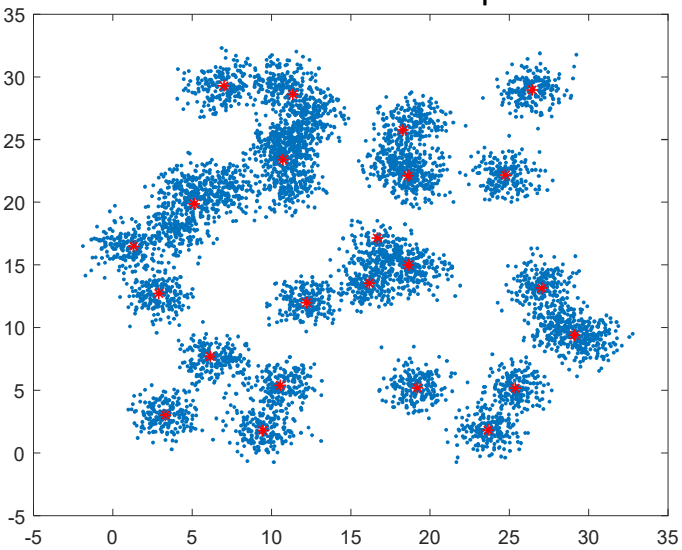
1. Data Clustering

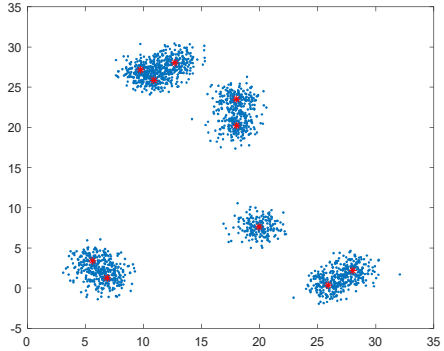
Clustering is an important task in the process of knowledge discovery in data mining.

suppose that a distribution of data is formed as a mixture of Gaussian shape clusters where they have almost the same size and their overlap is pretty low. One can use “ldi” to find all clusters and their members. In fact, the ldi for when the predicted clusters are the same defined clusters, is maximum.

N=30 clusters
with a few overlaps

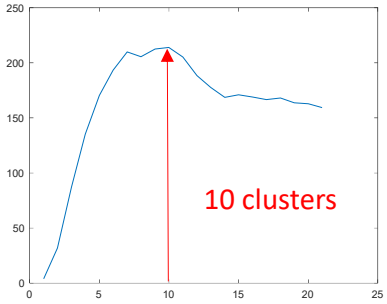
ldi



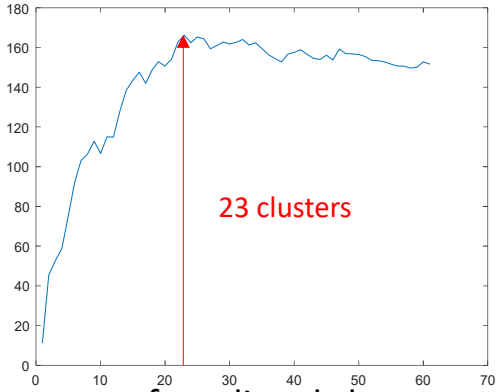


N=10 clusters

ldi



num of predicted clusters



num of predicted clusters

2. Unsupervised Feature Selection

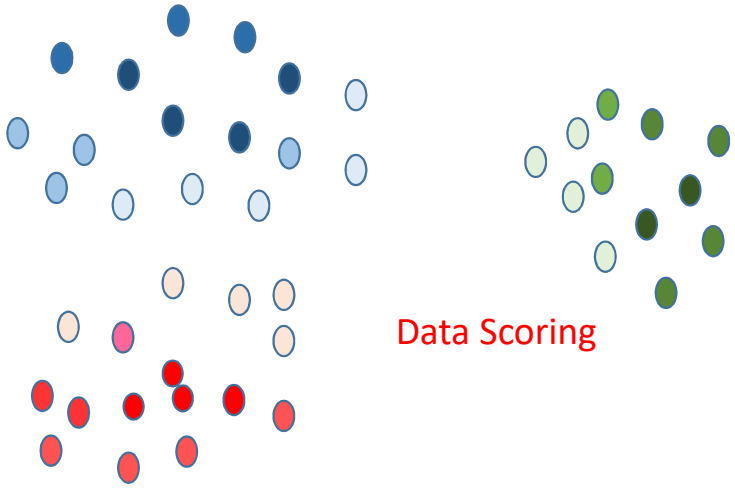
After removing some correlated features by an encoder or using SmI, One can choose a subset of features which provide maximum sum of "Idi" over clusters or equally with (maximum N*Idi) (N= number of clusters).

3. Feature Representation (Self Supervised Learning)

- In self supervised learning process, the space which has more sum of "Idi" over clusters, has more information

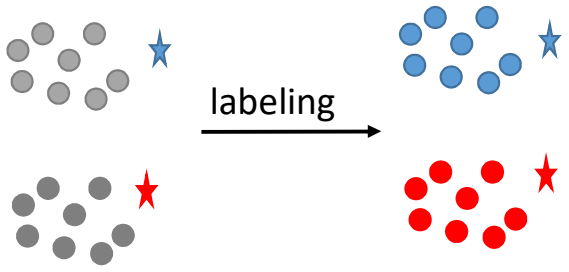
4. Unsupervised Data Scoring

By using the concept of “ldi” one can find the clusters and then score each data point with respect to its nearness to the center of clusters. Data example with high scores are near to center of a cluster and far from centers of other clusters.



5. Data Labeling with a few labeled data

Assume that there are a few data points with known labels (rare labeled data points). After clustering of the unlabeled data points with ldi, assign the labels of all member of each cluster as the label of a rare labeled data point which has minimum distance to its center.



6. Unsupervised (Self-Cross) Data domain scoring

How one can score a domain of data points with respect to its distribution or distribution of another domain of data points. Actually, by using the concept of ldi and clustering the data points one can compute the self or cross score for a domain dataset.

2.2. Data Analysis

2.2.1 Dataset evaluation and Scoring

Dataset Evaluation

- Assume that a dataset: $Data = \{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^{m}$ is provided for training a model in a classification $(\boldsymbol{y}_i \equiv l_i)$ or regression problem.
- We would like to know how such a dataset is challenging and which model is more appropriate for it.

Algortihm1: (To suggest deep or shallow for a classification or regression problem with a given dataset)

1. Compute $SI(Data)$ ($SmI\ (Data)$) of the dataset.
2. If $SI(Data)$ ($SmI\ (Data)$) is nearer to one than to zero, the provided data is less challenging and a shallow model is suggested for the problem.
3. If $SI(Data)$ ($SmI\ (Data)$) is nearer to zero, the provided data is less challenging and a deep learning model with high enough complexity is suggested for the problem.

Fair

SI index for some known datasets

$Data = \{(\boldsymbol{x}_i, l_i)\}_{i=1}^{m} \; m = 50000$

DataSet	N. Of Classes	Sepration Index	SI_random
MNIST Digits	10	0.9722	0.10
Fashion MNIST	10	0.85072	0.10
Cifar10	10	0.35086	0.10
Cifar100	100	0.17446	0.01

*The expected SI is equal to $SI_w = 1/n_C$ for when (1) each class has equal number of examples and (2) all examples are distributed with uniform random variable.

** to have fair comparison among SI of different data set the it is suggested to normalize in number of classes (n_C)

$$A\ sugestion\colon\ SI_n = \frac{SI - 1/n_C}{1 - 1/n_C}$$

The sensitivity of SI to the number of data points in a data-set

- Actually, the SI(SmI) is suggested to be used for a standard data-set with high enough diversity.
- For a data-set with a very low number of data points (insufficient diversity), SI (SmI) changes non-smoothly versus number of data points. In such a state, it does not show the true complexity of the data, and the sensitivity to variation of number of data points is high.
- For a data-set, while the number of data points is high enough (sufficient diversity), the SI (SmI) changes more smoothly versus number of data points (low sensitivity) .

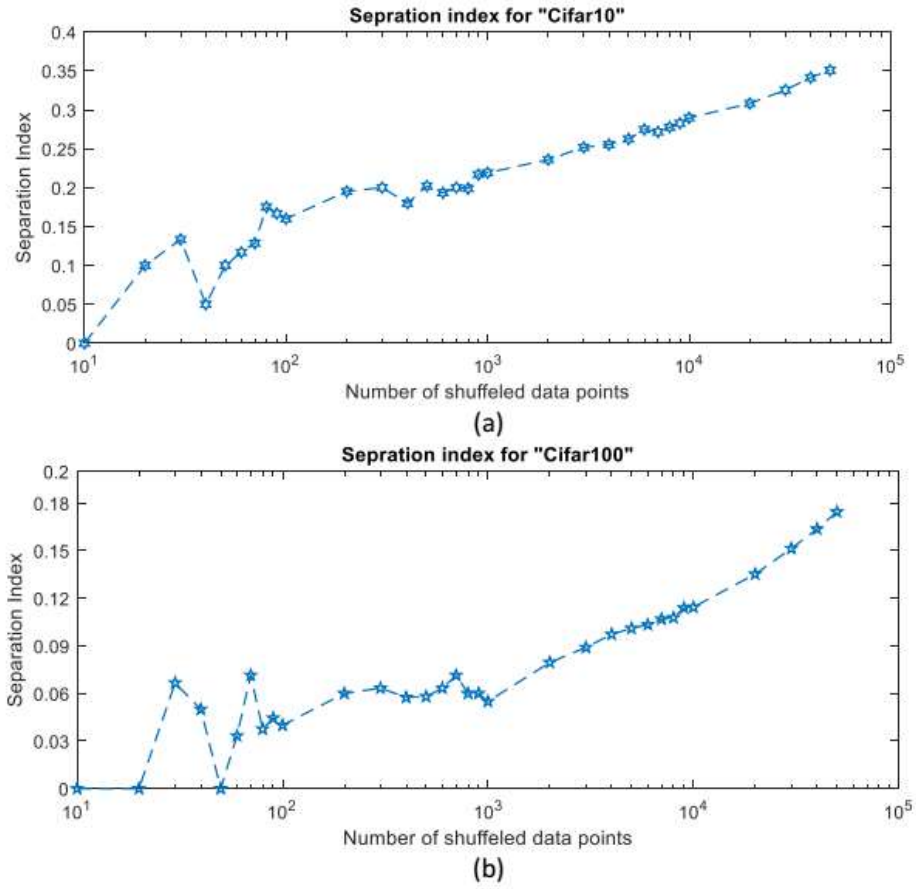


Fig. 6. The plot of separation index versus different number of shuffled data points in both "cifar10" (a) and "cifar100" (b).

Dataset ranking

- Computing $SI(Data)$ ($SmI\ (Data)$) provides a solution to rank and compare standard provided datasets from challenging view point.

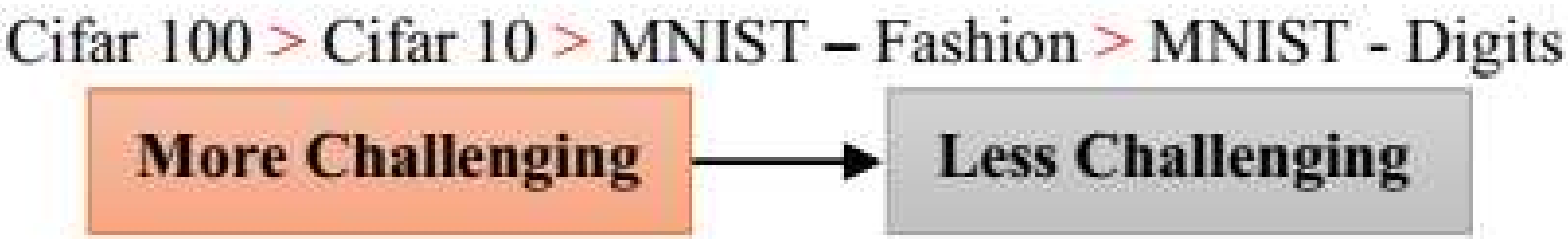


Fig. 4. The ordered classification data sets from more challenging to less challenging.

Cross domain dataset evaluation

1. Classification Problems

$Data = \{(\boldsymbol{x}_i, l_i)\}_{i=1}^{m}$ $D_{test} = \{(\check{\boldsymbol{x}}_i, \check{l}_i)\}_{i=1}^{m_{test}}$

$SI_{cross}(D_{test}, Data) = \frac{1}{m_{test}} \sum_{i=1}^{m_{test}} \delta(\check{l}_i, l_{i^\#})$, $i^\# = \arg\min_{\forall q} \|\check{\boldsymbol{x}}_i - \boldsymbol{x}_q\|$

- if $SI_{cross}(D_{test}, Data) \gg SI(Data)$, then it is expected that $the\ training\ model$ (with "$Data$") will have high $generlization\ for\ D_{test}$.
- if $SI_{cross}(D_{test}, Data) \ll SI(Data)$, then it is expected that $the\ training\ model$ (with "$Data$") will have low $generlization\ for\ D_{test}$.
- The test data set is called homogenous with the training dataset when $SI_{cross}(D_{test}, Data) \approx SI(Data)$

DataSet (m=50000)	N. Of Classes	Sepration Index	Cross Sep. Index
MNIST Digits	10	0.9722	0.9666
Fashion MNIST	10	0.85072	0.844
Cifar10	10	0.35086	0.3539
Cifar100	100	0.17446	0.1755

2. Regression Problems

$Data = \{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^{m}$ $D_{test} = \{(\breve{\boldsymbol{x}}_i, \breve{\boldsymbol{y}}_i)\}_{i=1}^{m_{test}}$

$$SmI_{cross}(D_{test}, Data) = \frac{1}{m_{test}} \sum_{i=1}^{m_{test}} \left(\frac{\boldsymbol{d}_{imax\#} - \boldsymbol{d}_{i^\#}}{\boldsymbol{d}_{imax\#} - \boldsymbol{d}_{imin\#}} \right)$$

$i^{\#} = \arg\min_{\forall q} \left\| \breve{\boldsymbol{x}}_i - \boldsymbol{x}_q \right\|$ $\boldsymbol{d}_{imax\#} = \max_{\forall q} \left\| \breve{\boldsymbol{y}}_i - \boldsymbol{y}_q \right\|$ $\boldsymbol{d}_{imin\#} = \min_{\forall q} \left\| \breve{\boldsymbol{y}}_i - \boldsymbol{y}_q \right\|$ $\boldsymbol{d}_{i^\#} = \left\| \breve{\boldsymbol{y}}_i - \boldsymbol{y}_{i^\#} \right\|$

- if $SmI_{cross}(D_{test}, Data) \gg SmI(Data)$, then it is expected that *the training model* (with "$Data$") will have high $generlization\ for\ D_{test}$.
- if $SmI_{cross}(D_{test}, Data) \ll SmI(Data)$, then it is expected that *the training model* (with "$Data$") will have low $generlization\ for\ D_{test}$.
- The test data set is called homogenous with the training dataset when $SmI_{cross}(D_{test}, Data) \approx SmI(Data)$

Dataset evaluation for some Regression cases

$Data = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{m}$ $D_{test} = \{(\check{\boldsymbol{x}}_i, \check{y}_i)\}_{i=1}^{m_{test}}$

DataSet	N. Of data points	SmI linear	Smi mean
Diabets	(m=353,n=10)	0.7286	0.4230
Car Price	(m=174, n=63)	0.9340	0.7784
California housing	(m=16512,n=8)	0.7303	0.4005
Sinc function	(m=900,n=2)	0.9840	0.8027

California Housing > Diabets > Car price> Sinc-Function

More challenging----------Less Challenging

Cross domain dataset evaluation

1. Regression Problems

$Data = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{m}$ $D_{test} = \{(\breve{\boldsymbol{x}}_i, \breve{y}_i)\}_{i=1}^{m_{test}}$

$SmI_{cross}(D_{test}, Data) = \frac{1}{m_{test}} \sum_{i=1}^{m_{test}} \delta(\breve{l}_i, l_{i^\#})$, $i^\# = \arg\min_{\forall q} \|\breve{\boldsymbol{x}}_i - \boldsymbol{x}_q\|$

- if $SmI_{cross}(D_{test}, Data) \gg SmI(Data)$, then it is expected that $the\ training\ model$ (with "$Data$") will have high $generlization\ for\ D_{test}$.
- if $SmI_{cross}(D_{test}, Data) \ll SmI(Data)$, then it is expected that $the\ training\ model$ (with "$Data$") will have low $generlization\ for\ D_{test}$.
- The test data set is called homogenous with the training dataset when $SmI_{cross}(D_{test}, Data) \approx SmI(Data)$

DataSet	N. Of data points	SmI linear	Smi mean	Cr. Smi linear	Cr. Smi mean
Diabets	(m=353,n=10) (mtest=89,n=10)	0.7286	0.4230	0.7635	0.4739
Car Price	(m=174, n=63),(mtest=31-n=63)	0.9340	0.7784	0.9291	0.7741
California housing	(m=16512,n=8) (m=4128, n=8)	0.7303	0.4005	0.7323	0.4061
Sinc function	(m=900,n=2) (mtest=100,n=2)	0.9840	0.8027	0.9828	0.8295

Data dividing for test and training datasets

- To have high enough generalization, divide an available dataset to test and training sets in order that the $SI_{cross}(SmI\ _{cross})$ of test dataset becomes almost equal to $SI(SmI)$ of the training dataset.

$$Data_{available} \rightarrow \{D_{test}, Data\}$$

1. For classification problems

$$SI_{cross}(D_{test}, Data) \sim SI(Data)$$

2. For regression problems

$$SmI_{cross}(D_{test}, Data) \sim SmI(Data)$$

❖ **Domain Score for train data set= Domain Score for test data set**

Data Point Scoring

1. Classification $Data = \{(\boldsymbol{x}_i, l_i)\}_{i=1}^{m}$

$Score(x_i) = si(x_i)$ (1st order or any variants)

$si(x_i) \in \{0,1\}$

2. Regression $Data = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{m}$

$Score(x_i) = smi(x_i)$ (1st order or any variants)

$smi(x_i) \in [0,1]$

3. Unsupervised $Data = \{(\boldsymbol{x}_i)\}_{i=1}^{m}$

$Score(x_i) = rd(x_i)$

$rd(x_i) \in [0,1]$

Some notes

- Hard Examples are Examples which have lower scores
- One can use score data (1) to determine risky data, (2)to clean data, or (3) to weight data in learning process.
- The score of data domain is the average of scores of all data points (SI, SmI, RD)
- The cross score of test data domain is the average of scores of all test data points in the distribution of the train data domain (cross_SI, cross_SmI, cross_RD)

3.2.2 Supervised Feature Selection

Among available features, which ones should be selected?
Among different observations which ones should be integrated?
How one can make a suitable fusion for some available data sources with different modalities?

Subset Selection among distinct features

- Assume there is $x_{available} = \{x_1, \dots, x_{ne}\}$ with n_e features.
- Among available n_e inputs, select a subset $\boldsymbol{x} \subseteq x_{available}$ and define:

$$Data = \{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^{m}$$

- To decrease the complexity, select $\boldsymbol{x}$ in a way that the $SI(Data)$ $(SmI(Data),)$ becomes maximum.
- It is aimed to remove that all non-relevant, redundancies and noise inputs, which decrease the SI(SmI) or do not increase it.
- "Forward selection", "backward elimination" or any other exploration algorithm can be used for this purpose.

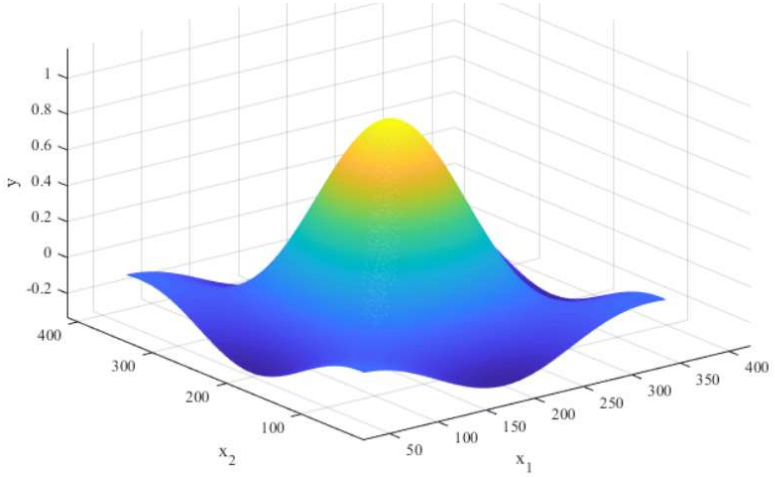
Choosing effective inputs by Smoothness Index
Example1 (illustrative)

Table 4. SmI comparison for different subsets of handmade data

Different subsets of two main inputs and two non-related inputs					Feature Smoothness index	
Subsets / Inputs	x_1	x_2	x_3	x_4	Linear	Exponential
1	×	×			0.9783	0.9788
2	×	×	×		0.9159	0.9249
3	×	×	×	×	0.8314	0.8615
4		×	×		0.4781	0.5972
5		×	×	×	0.4711	0.5888
6				×	0.3464	0.4929

white noise variables with X3, and X4 features have uniform distribution

Two-dimensional synchronous function of 1000 randomly generated data points.



$$y = \frac{sin\,(x_1)\,sin\,(x_2)}{x_1 x_2},$$

$$0 < |x_1| \leq 5, 0 < |x_2| \leq 5, 0 < |x_3| \leq 5, 0 < |x_4| \leq 5$$

While we have relevant inputs the SmI is maximum so the subset selection by SmI reveals the relevant inputs.

Choosing effective inputs by Smoothness Index

Example2

Yearly residential water consumption data, along with climatic characteristics, and socioeconomic factors of rural areas of Isfahan, Iran are aggregated.

Table 8. Performance evaluation using MSE for all models ($\times 10^6$)

	PCA	GUS	RFE	KBS	VT	PCC	MI	FSSmI
MLR	**0.2786**	0.3031	0.2764	0.2726	0.2470	0.2687	0.2655	0.2495
RFR	0.4912	**0.2347**	**0.2306**	0.2714	0.2520	0.3034	0.2901	***0.2301***
SVR	0.2916	0.2600	0.2501	**0.2365**	**0.2301**	**0.2400**	**0.2391**	0.2555
KNN	0.6696	0.5080	0.2576	0.3290	0.3264	0.3100	0.3337	0.2581

Table 7. Performance evaluation using MAE for all models ($\times 10^4$)

	PCA	GUS	RFE	KBS	VT	PCC	MI	FSSmI
MLR	**0.5232**	0.5499	0.5220	0.5219	0.4969	0.5179	0.5105	0.5081
RFR	0.6965	**0.4816**	**0.4796**	0.5203	0.5014	0.5495	0.5351	**0.4986**
SVR	0.5386	0.5066	0.4975	**0.4857**	***0.4781***	**0.4874**	**0.4868**	0.5162
KNN	0.8168	0.7123	0.5381	0.5727	0.5707	0.5555	0.5728	0.5167

Selectin Algorithms

Forward **selection based SmI (FSSmI)**

Principle Component Analysis (PCA)

Recursive feature elimination (RFE)

Generic uni-variant selection (GUS)

Mutual Information (MI)

K-best selection (KBS)

Pearson correlation coefficient (PCC)

Variance threshold (VT)

Models

Support vector regression (SVR)

Multiple linear regression (MLR)

K nearest neighbors (KNN)

Random forest regression (RFR)

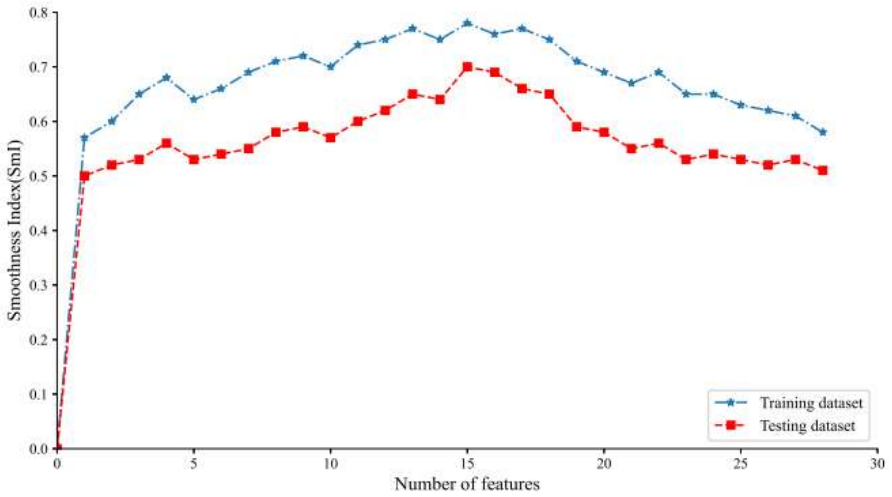
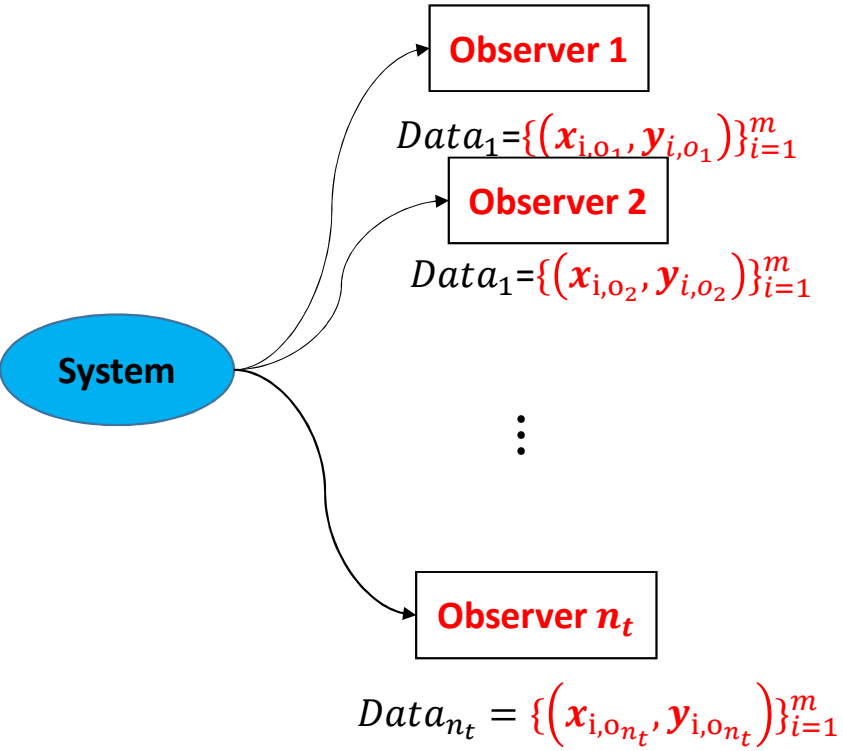


Fig. 5. Smoothness Index (SmI) based on number of features. There is a good correlation between the smoothness charts of training and test datasets, i.e., the selected features based on the absent data are the same as those that give the highest SmI in the training dataset.

Table 5. Selected features. The features, households, subscriptions, and female ratio, are selected by all the feature selection methods that show their influences on regression

Feature	KBS	VT	PCC	MI	GUS	FSSmI	RFE on MLR	RFE on RFR	RFE on SVR	Lasso	Ridge	Elastic
Subscriptions	×	×	×	×	×	×	×	×	×	×	×	×
Households	×	×	×	×	×	×	×	×	×		×	×
Average family size						×		×		×		
Female ratio	×	×	×	×	×	×	×	×	×	×	×	×
Age 0 to 9					×	×	×		×	×		
Age 10 to 19					×		×		×			
Age 20 to 29								×	×			
Age 30 to 39							×	×	×			
Age 40 to 49							×	×	×			
Age 50 to 59							×					
Age 60 to 69					×		×		×	×		
Age 70+					×	×	×	×	×	×		
Literacy rate						×					×	×
Employment rate					×	×						
Owner-occupied housings	×	×	×	×		×	×	×	×	×	×	×
Non-owner-occupied housings	×	×	×	×	×						×	×
Non-apartment housings						×		×			×	×
Area 50- m2		×						×			×	×
Area 51 to 75 m2	×	×	×	×					×		×	×
Area 76 to 80 m2	×	×	×	×				×			×	×
Area 81 to 100 m2	×	×	×	×								×
Area 101 to 150 m2	×	×	×	×			×	×			×	×
Area 151 to 200 m2	×	×	×	×							×	×
Area 201 to 300 m2	×	×	×	×	×					×		×
Area 301 to 500 m2		×	×		×	×				×	×	×
Area 501+		×			×	×						
Max temperature		×	×	×		×	×		×		×	×
Summer temperature		×	×	×	×	×	×	×	×	×	×	×
CDD	×	×	×	×	×	×	×	×	×	×	×	×
Number of features	12	17	15	14	14	15	15	15	15	11	16	18

Subset selection among distinct observations



- It is aimed to select n_s observations from available n_t observations and then concatenate them in order have maximum SI (SmI).

concatenation $\boldsymbol{x}_i^* = [\boldsymbol{x}_{i,o_1^*},\ldots,\boldsymbol{x}_{i,o_{n_s}^*}]$, $\boldsymbol{y}_{i,o_1} = \boldsymbol{y}_{i,o_2} \ldots = \boldsymbol{y}_{i,o_{n_t}}$

For classification problems

$$\mathrm{SI}(\{(\boldsymbol{x}_i^*, l_i)\}_{i=1}^{m}) \geq \mathrm{SI}(\{(\tilde{\boldsymbol{x}}_i, l_i)\}_{i=1}^{m})$$

or for *regression problems*

$$\mathrm{SmI}(\{(\boldsymbol{x}_i^*, \boldsymbol{y}_i)\}_{i=1}^{m}) \geq \mathrm{SmI}(\{(\tilde{\boldsymbol{x}}_i, \boldsymbol{y}_i)\}_{i=1}^{m})$$

where $\tilde{\boldsymbol{x}}$ denotes any other concatenation from available n_t different observations.

- "Forward selection", "backward elimination" or any other exploration algorithms can be used for this purpose.

Thank you