Part3

3. Layer-wise Analysis and Design of Deep Neural Networks

3.1 Two Data Complexity measures

- Separation index (SI)
- Smoothness index(SmI)

3.2 Layer-wise Analysis by Separation and Smoothness indices

- Dataset evaluation, ranking and dividing (SI, SmI)
- Subset Selection (SI, SmI)
- Layer-wise Model evaluation (SI, SmI)
- Pre-train Model ranking (SI, SmI)
- Model Confidence and Guarantee (SI, SmI)
- Causal relationship between two variables(SmI)

3.3 Layer-wise Design by Separation and Smoothness indices

- Model Compressing(SI, SmI)
- Forward learning in the first layer(SI, SmI)
- Layer-wise forward learning(SI, SmI)
- Layer-wise Forward Auto Encoder Learning(SmI)
- Layer-wise branching(SI, SmI)
- Layer-wise Fusion(SI, SmI)
- Forward Design(SI, SmI)
- Forward Multi-Task Design(SI, SmI)
- Artificial Brain Design(SI, SmI)

3.4 Related works in local Layer-wise learning

Indicator	Research (state)	
SI	Initial studies have been done	
SmI	Initial studies have been done	
SI	There are some prepared/under-review works	
SmI	There are some prepared/under-review works	
SI	New idea	
SmI	New idea	

3.1 Two Data Complexity measures

3.1.1 Separation index

- First order SI
- High order SI
- High order soft SI
- Center Based SI

3.1.2 Smoothness index

- First order SmI
- High order SmI
- High order soft SmI

Data Complexity measures

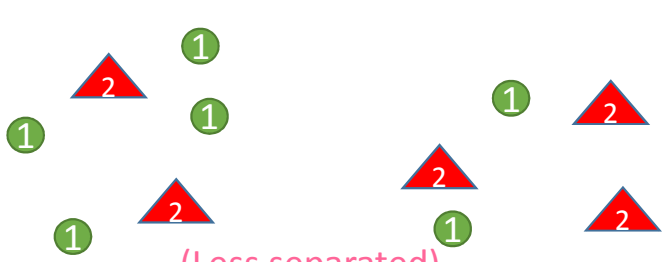
Complexity measures	Overall evaluating approach
√ Feature-based	Discovering informative features by evaluating each feature independently (Orriols-Puig et al., 2010; Cummins, 2013))
√ Linearity separation	Evaluating the linearly separation of different classes (Bottou & Lin, 2007)
√ Neighborhood	Evaluating 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

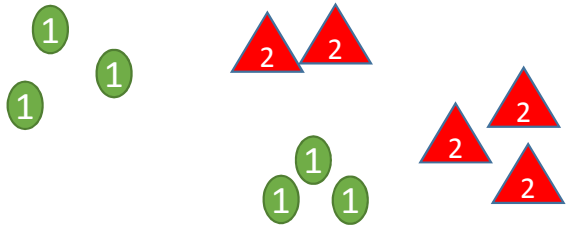
Two Complexity measures

1. A separation measure (in classification problems)

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



(Less separated)

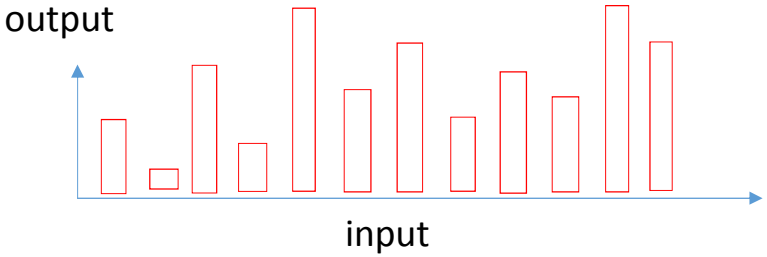


(More separated)

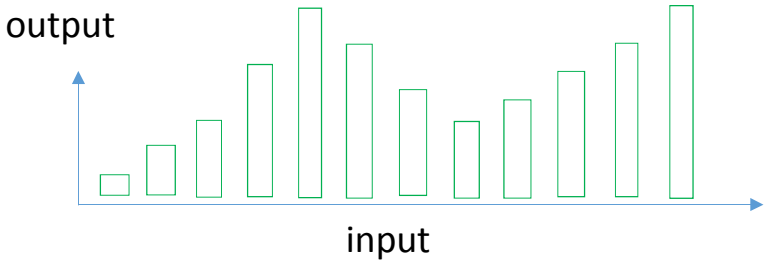
2. An smoothness measure (in regression problems)

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

(Less Smooth)



(More Smooth)



Separation index (SI)

"SI" measures that how much input data points separate class labels from each others.

3.1.1 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: $\mathrm{SmI} \in [0,1]$
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.

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

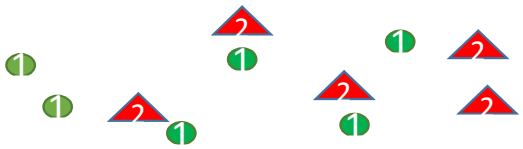
6. Separatin index of $the\ target\ labels\ with\ themselves\ is\ maximum$: $SI(\{(l_i, l_i)\}_{i=1}^m)$=1;

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

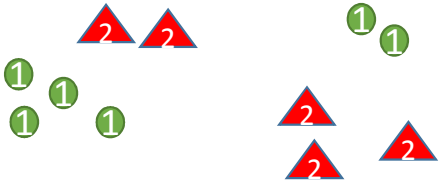
Two dimensional examples (binary classification)

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

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

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

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

5- Distance matrix is computed as follows:

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

Separation index for Each Class

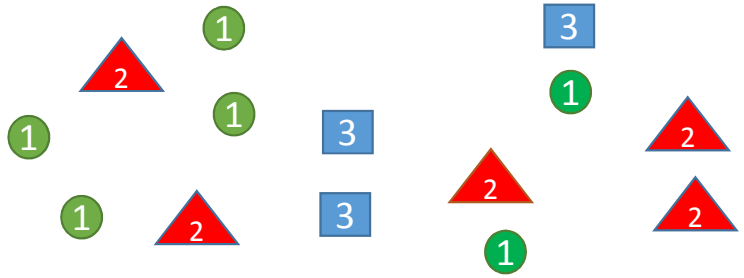
$\mathrm{SI}_c(Data) = \frac{1}{m_c}\sum_i \delta(l_i, c)\delta(l_i, l_{i^*})$ $c=1,2,..,n_C$

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

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

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

A two dimensional illustrative example



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

$SI_1(Data) = 4/6$
$SI_2(Data) = 2/5$
$SI_3(Data) = 2/3$
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

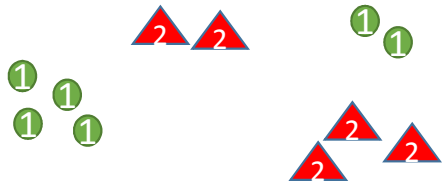
$$\mathrm{SI}^{\mathrm{r}}(Data) = \frac{1}{m}\sum_{i=1}^{m}\prod_{j=1}^{r}\delta\left(l_i, l_{i_j^*}\right) \qquad \text{r: the order of "SI"}$$

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

- "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: $\mathrm{SI}^{\mathrm{r}} \leq \mathrm{SI}^{\mathrm{r}-1} \leq \cdots \leq \mathrm{SI}^{1}$ $\qquad \mathrm{SI}^{1} = \mathrm{SI}$

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

- 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.

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

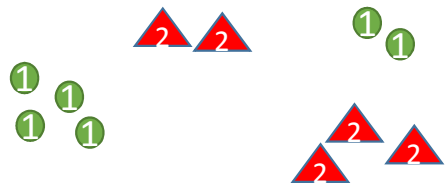
$$\mathrm{SI}^{\mathrm{r}}_{\mathrm{soft}}(Data) = \frac{1}{m\times r}\sum_{i=1}^{m}\sum_{j=1}^{r}\delta(l_i,,l_{i_j^*})$$

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

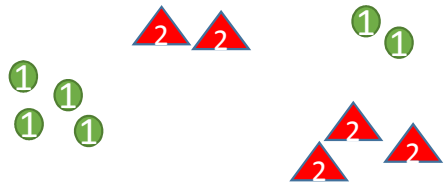
- $\mathrm{SI}^{\mathrm{r}}_{\mathrm{soft}}$ considers less restricted condition of separation than SI^{r}

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

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:

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

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

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

- 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 that examples of each class have all exclusive features of that class and do not have any common feature with examples of other classes.

Smoothens index (SmI)

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

3.1.2 Smoothness index (SI)

A smoothness measure for regression problem

1. First order SI

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

*** to avoid the effect of outliers, it is assumed that all outlier of data points are not considered in computing SmI.

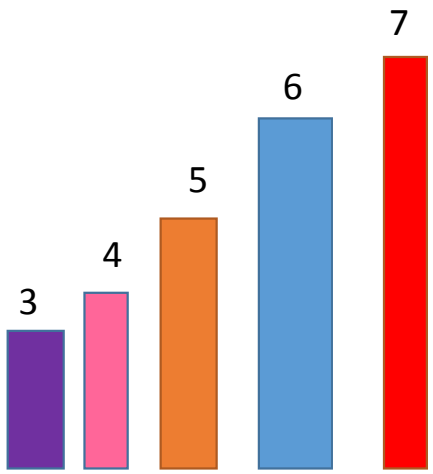
Some notes

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

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

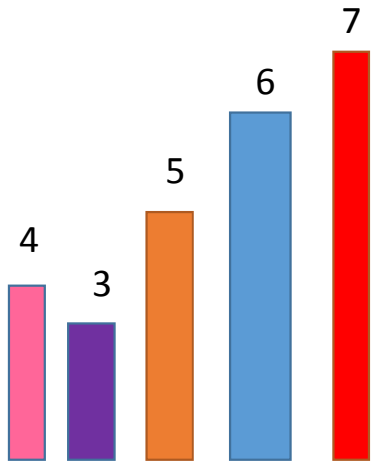
7. Smoothness index of target outputs $with\ themselves\ is$ $maximum$: $SmI(\{(\boldsymbol{y}_i, \boldsymbol{y}_i)\}_{i=1}^m)$=1; it means that how input data become more similar to output the smoothness index will increase.

One-dimensional illustrative examples



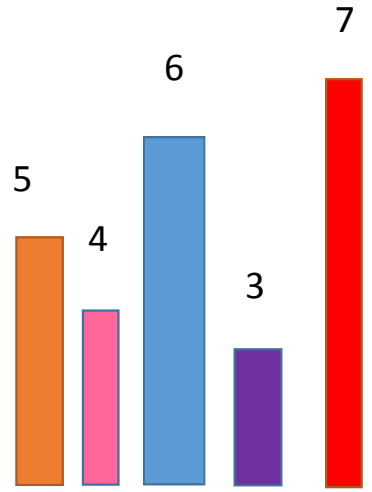
$$SmI = \frac{1}{5}\left(\frac{7-4}{7-4}+\frac{7-3}{7-3}+\frac{7-4}{7-4}+\frac{5-3}{5-3}+\frac{6-3}{6-3}\right)$$

$SmI = 1$



$$SmI = \frac{1}{5}\left(\frac{7-4}{7-4}+\frac{7-3}{7-3}+\frac{7-4}{7-3}+\frac{5-3}{5-3}+\frac{6-3}{6-3}\right)$$

SmI=0.95



$$SmI = \frac{1}{5}\left(\frac{7-4}{7-4}+\frac{7-5}{7-3}+\frac{4-3}{5-3}+\frac{7-6}{7-4}+\frac{3-3}{6-3}\right)$$

SmI=.466

2. High order SmI

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

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

r: the order of "SmI"

$$i_j^* = \underset{\forall q\neq i, i_1^*,\cdots,i_{j-1}^*}{\arg} min\|\boldsymbol{x}_i - \boldsymbol{x}_q\| \qquad imin_j = \underset{\forall q\neq i, imin_1,\cdots,imin_{j-1}}{\arg} min\|\boldsymbol{y}_i - \boldsymbol{y}_q\|$$

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

- $\mathrm{SmI}^r \in [0,1]$
- 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

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

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

r: the order of "SmI"

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

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

3.2 Analysis by Separation and Smoothness indices

3.2.1 Dataset evaluation, ranking and dividing

3.2.2 Subset Selection

3.2.3 Layer-wise Model evaluation

3.2.4 Pre-train Model ranking

3.2.5 Model Confidence and Guarantee

3.2.6 Causal relationship between two variables

3.2.1 Dataset evaluation, ranking and dividing

Here, based on “SI”, some methods are proposed for dataset evaluation, ranking and dividing in classification and regression problems.

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

TABLE II
Evaluation of some known classification datasets by using the separation index.

Dataset	Number of Classes	Separation Index	SI_w *,**
MNIST Digits	10	0.97372	0.10
MNIST Fashion	10	0.54423	0.10
Cifar-10	10	0.2636	0.10
Cifar-100	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)

$$SI_n = SI - 1/n_C$$

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) .

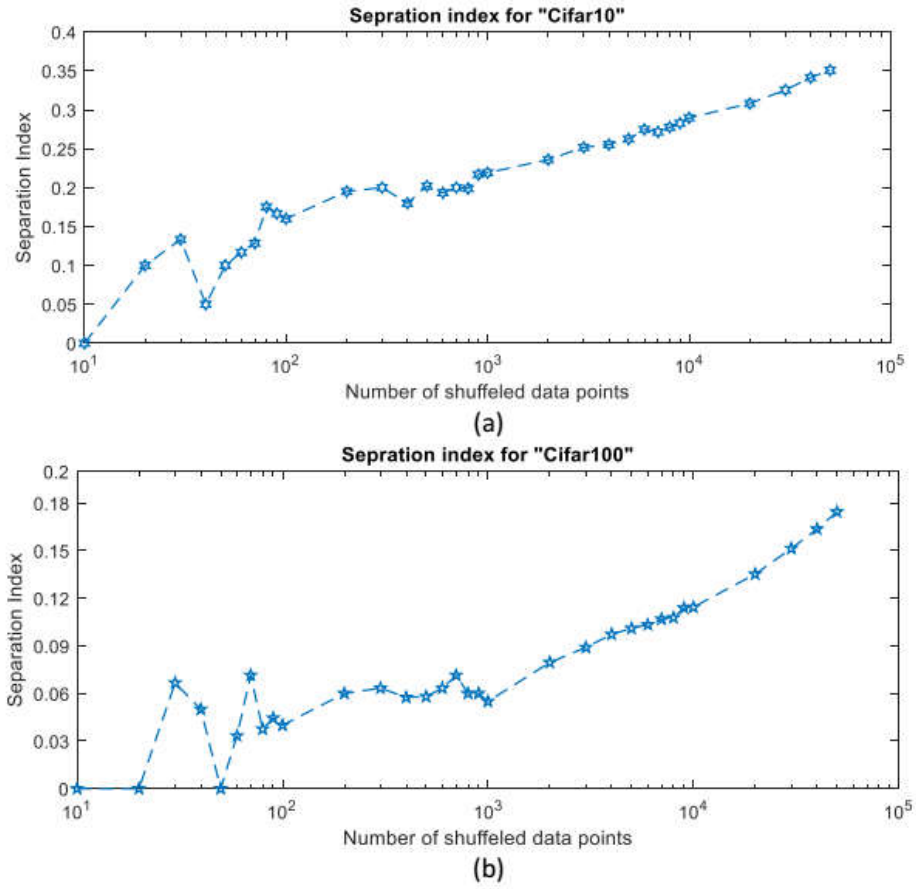


Fig. 6. The plot of separation index versus different number of shuffled data points in both "cifar10" (a) and "cifar100" (b).

Dataset ranking

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

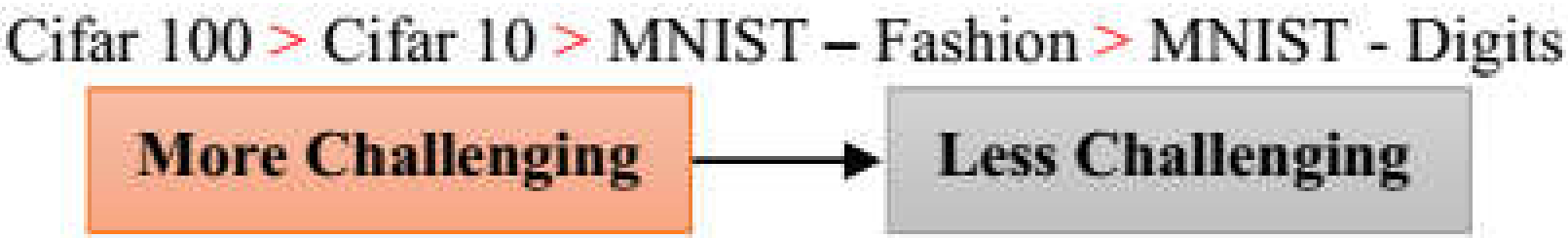


Fig. 4. The ordered classification data sets from more challenging to less challenging.

Cross domain dataset evaluation

1. Classification Problems

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

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

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

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

2. Regression Problems

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

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

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

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

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

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

3.2.2 Subset Selection

Among available inputs, which ones should be selected?

Among different observations which ones should be integrated?

Subset Selection among distinct inputs

- Assume there is $x_{available} = \{x_1, \dots, x_{ne}\}$ with m_e inputs.
- 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 that all non-relevant, redundancies and noise inputs, which decrease the SI(SmI) (or do not increase it significantly), should be removed.
- "Forward selection", "backward elimination" or any other "step-wise selection" algorithms can be used for this purpose.

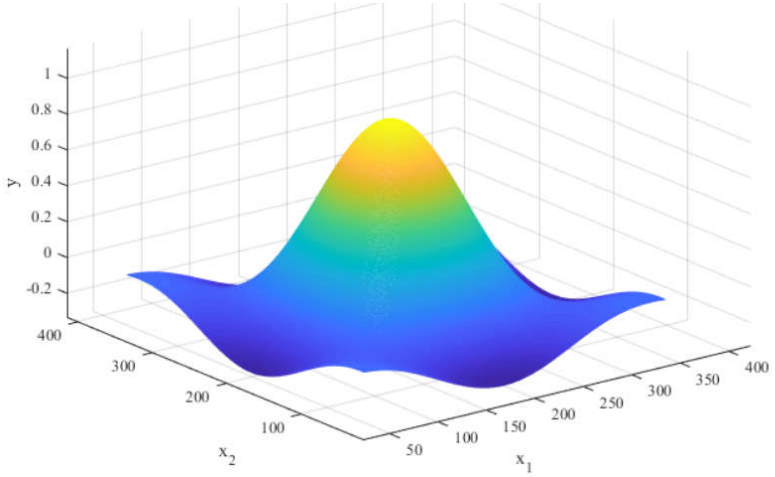
Choosing effective inputs by Smoothness Index
Example1 (illustrative)

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)

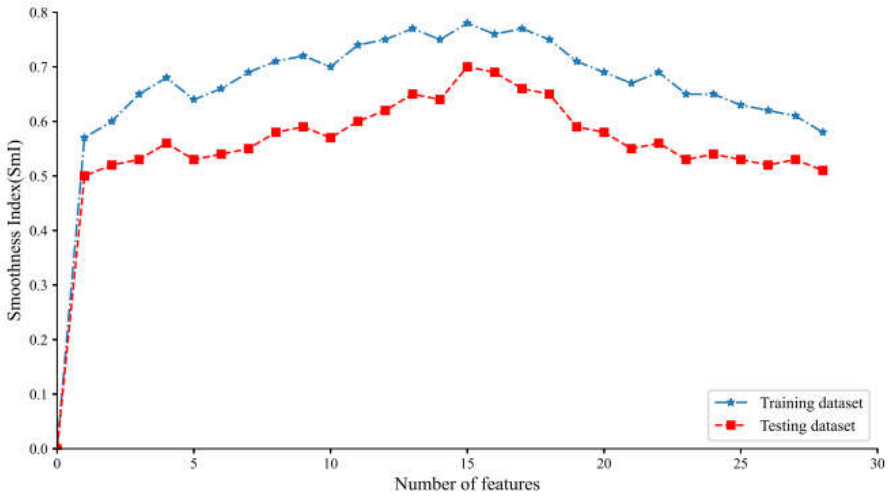
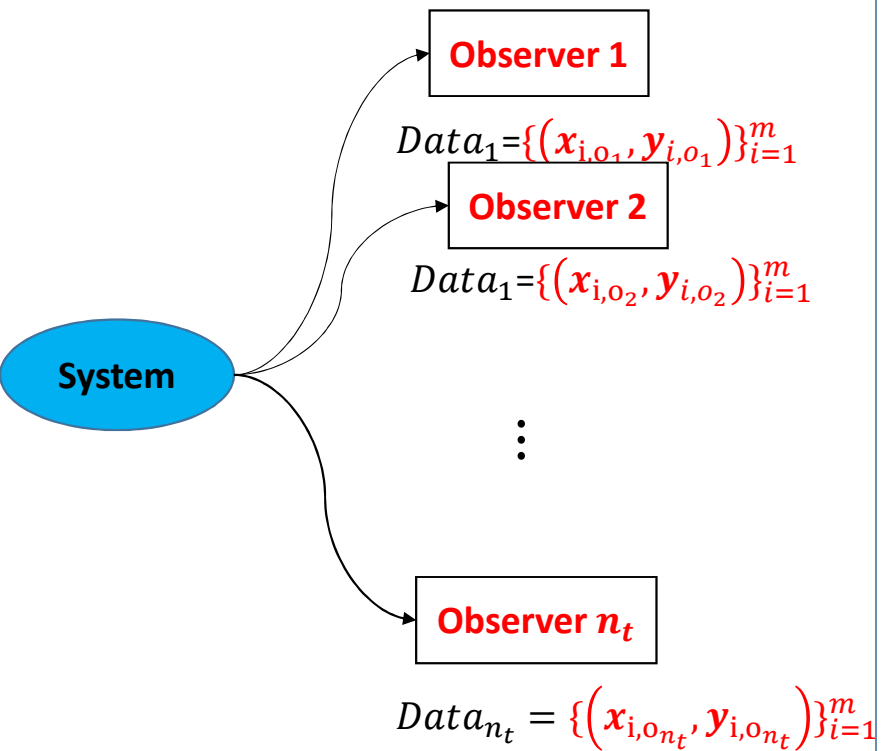


Fig. 5. Smoothness Index (SmI) based on number of features. There is a good correlation between the smoothness charts of training and test datasets, i.e., the selected features based on the absent data are the same as those that give the highest SmI in the training dataset.

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 (for equal events) or append (for different events), which can maximize SI (SmI).

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

Appending $\boldsymbol{x}_i^* = \begin{bmatrix} \boldsymbol{x}_{i,o_1^*} \\ \vdots \\ \boldsymbol{x}_{i,o_{n_s}^*} \end{bmatrix}$

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 or appending from available n_t different observations.

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

3.2.3 Layer-wise Model evaluation

The concept of dataflow or information-flow

- By applying the input data, $\boldsymbol{x}$ ($\boldsymbol{x} \equiv \boldsymbol{x}^1$) to a deep neural network with N_L layers, the data will be transformed layer by layer.
- Dataflow (information-flow) denotes the data which transform by layers of a deep neural network :

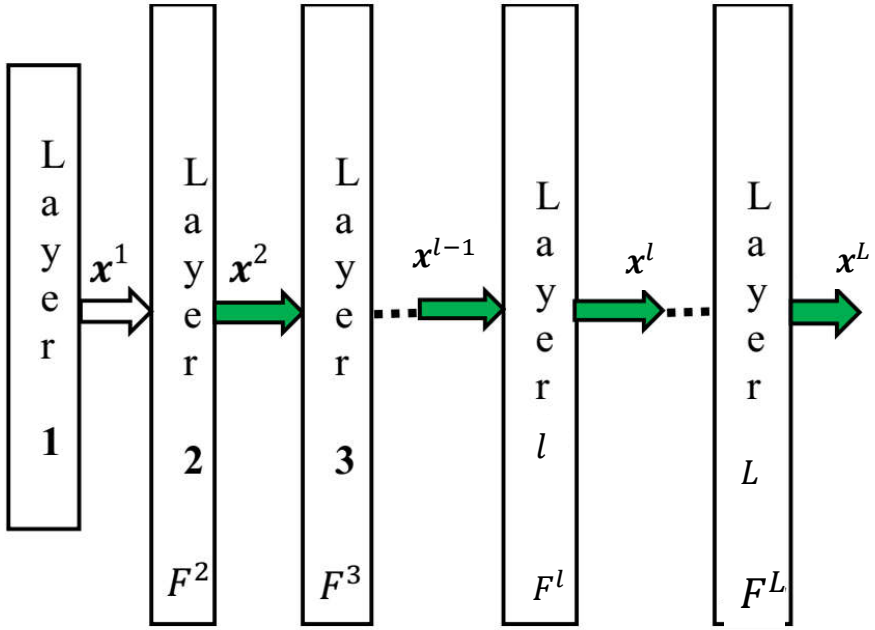
$$\boldsymbol{x}^1 \rightarrow \cdots \boldsymbol{x}^{l-1} \rightarrow \boldsymbol{x}^l \rightarrow \cdots \rightarrow x^L$$

- L: number of layers in the model
- $\boldsymbol{x}^l$ denotes the dataflow at layer l, which is reshaped as a vector and its length is n_L.

$$\boldsymbol{x}^l \boldsymbol{\epsilon} \boldsymbol{R}^{\boldsymbol{n_l} \times \boldsymbol{1}}$$

- One can compute SI(SmI) for dataflow at layer $\boldsymbol{l}$:

$Data^l = \{(\boldsymbol{x}_i^l, l_i)\}_{i=1}^m$ $\quad\quad$ $\boldsymbol{l}$=1,2, … , L



It seems the above DNN is a feedforward network.
However, each layer can be a RNN or a LSTM module, too.
In the case of RNN or LSTM, it is assumed that the hidden state is within the layer.

The complexity measure SI (SmI) in DNNs

Some definitions

- Disturbance: non relevant information which disturb the feature space
- Distortion: Uncertainties due to (1) inherent appearances of the features, (2)the environment constraints on the measuring process, and (3) different measuring parameters.
- Common features: In classification problems, features which are common between examples of different classes they avoid discrimination between different classes.
- Exclusive features: Features which discriminate different classes in a classification problem or maximize smoothness in regression problems.

Two important notes:

1. In a DNN, it is expected that after a certain number of filter layers, a feature space with negligible disturbance, distortion, and common features is appeared.
2. Geometrically, it is proved that by intensifying exclusive features and weakening disturbances, distortions, and common features (complexity), the SI(SmI) of dataflow will increase gradually through layers of a DNN.

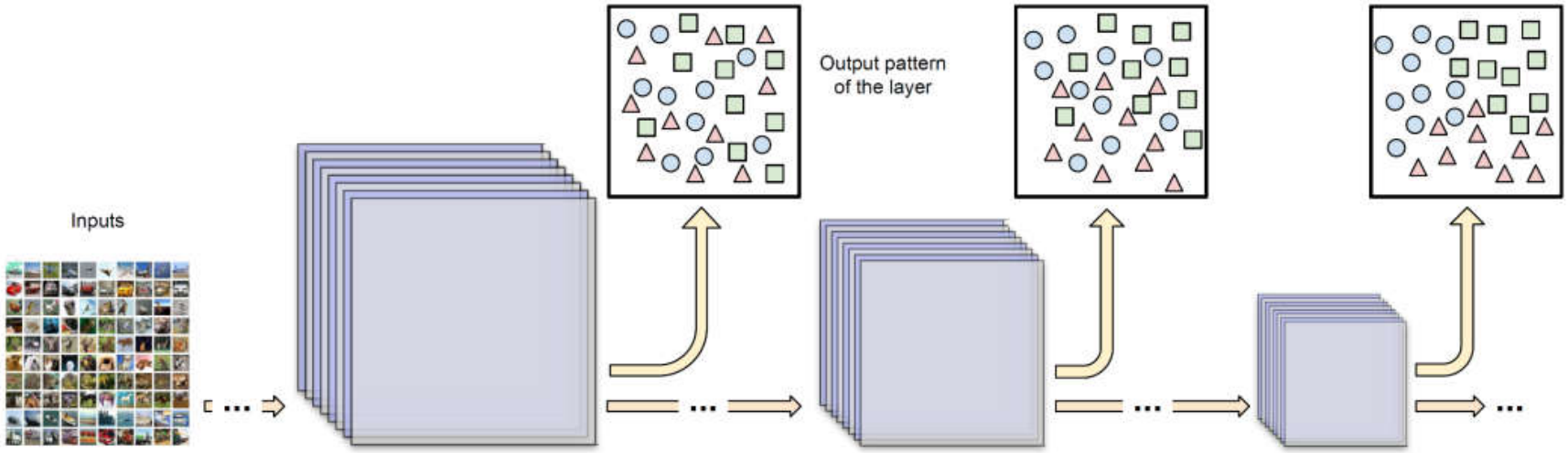
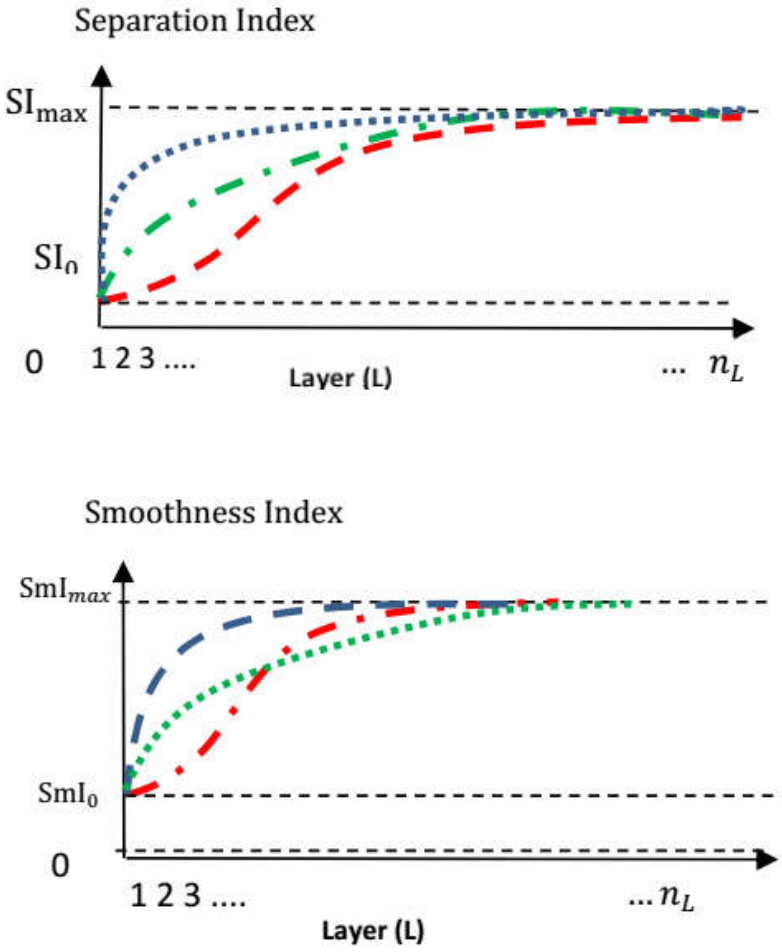


Figure 1. Output pattern of each layer through the network.

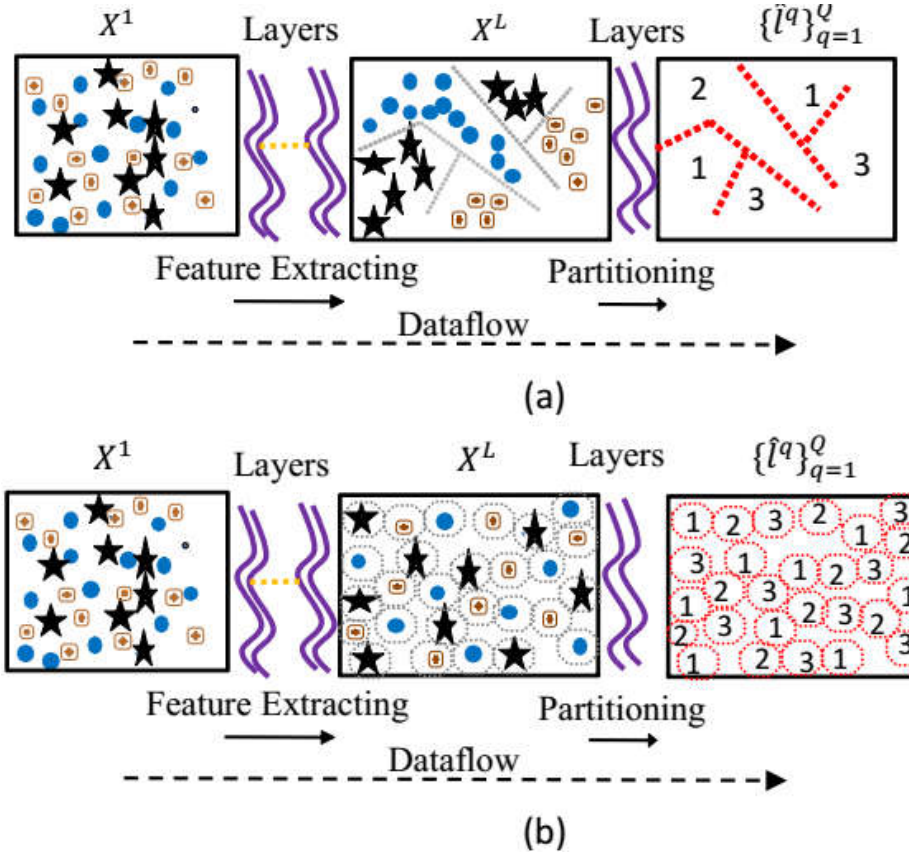
It is expected that the complexity of data decreases layer by layer in a deep neural network.

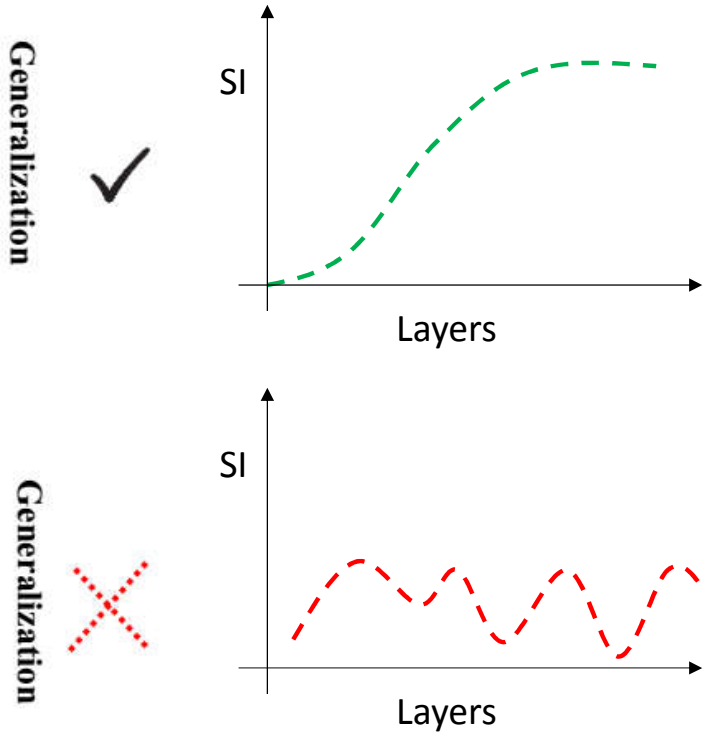
Some important notes

1. In fact, by decreasing the complexity of dataflow through “filter” layers, the SI(SmI) will increase.
2. The SI(SmI) may increase by different trends: different rises, different settling, with smooth or oscillatory changes.
3. Increasing SI(SmI) by Fully Connected (FC) layers is not desired. FC layers due to its redundancies make overfitting and avoid generalization.

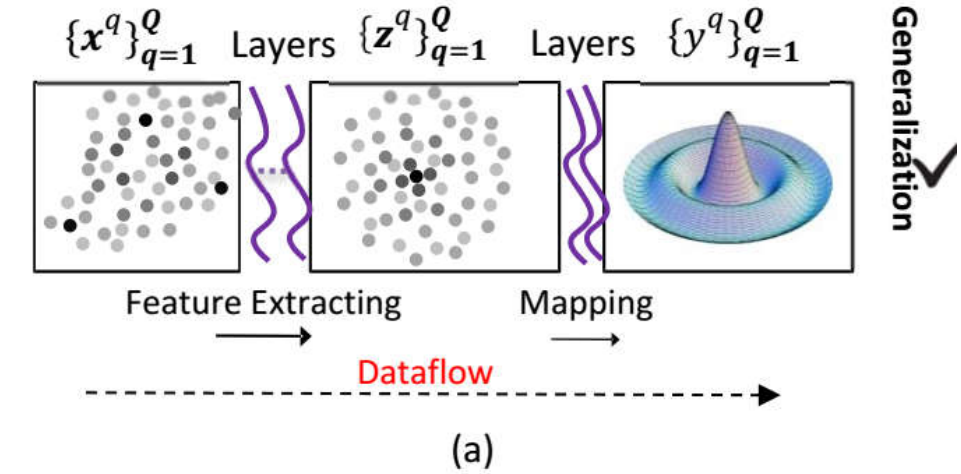


Generalization and Separation index

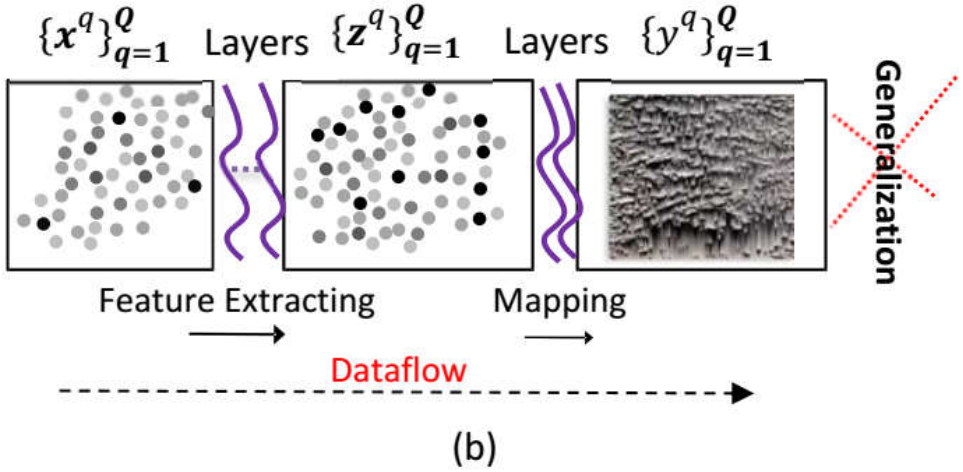




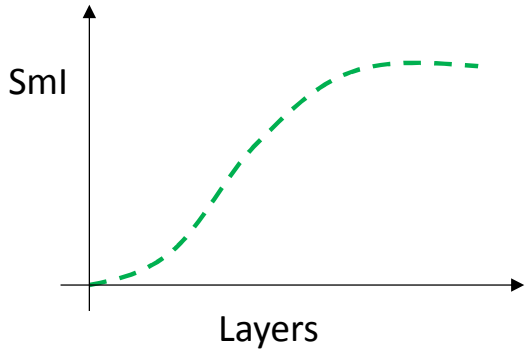
Generalization and Smoothness index

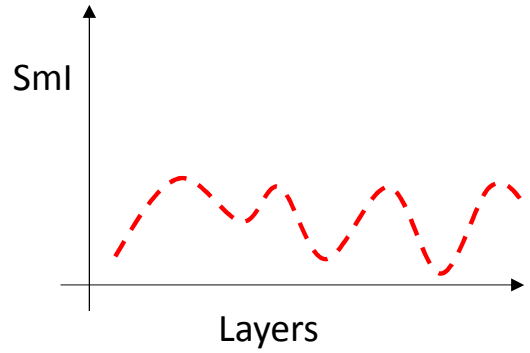


(a)



(b)





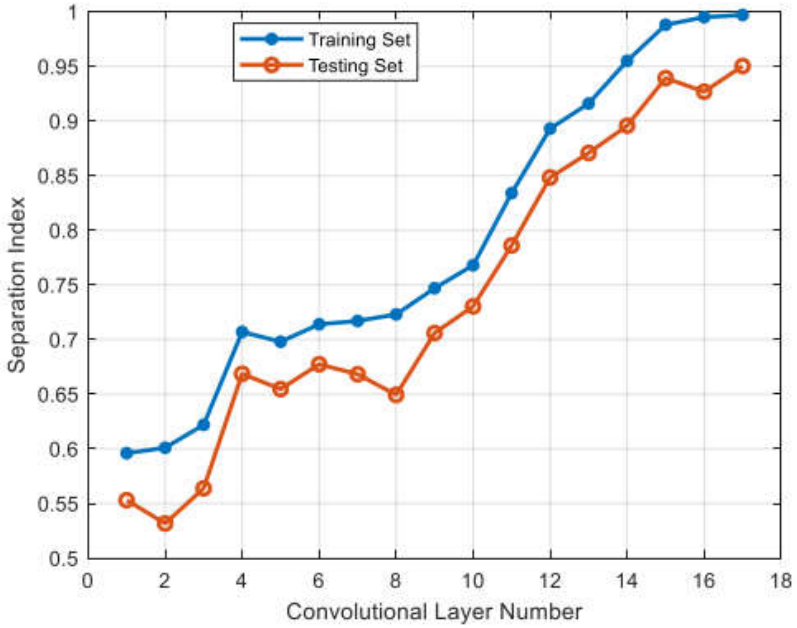
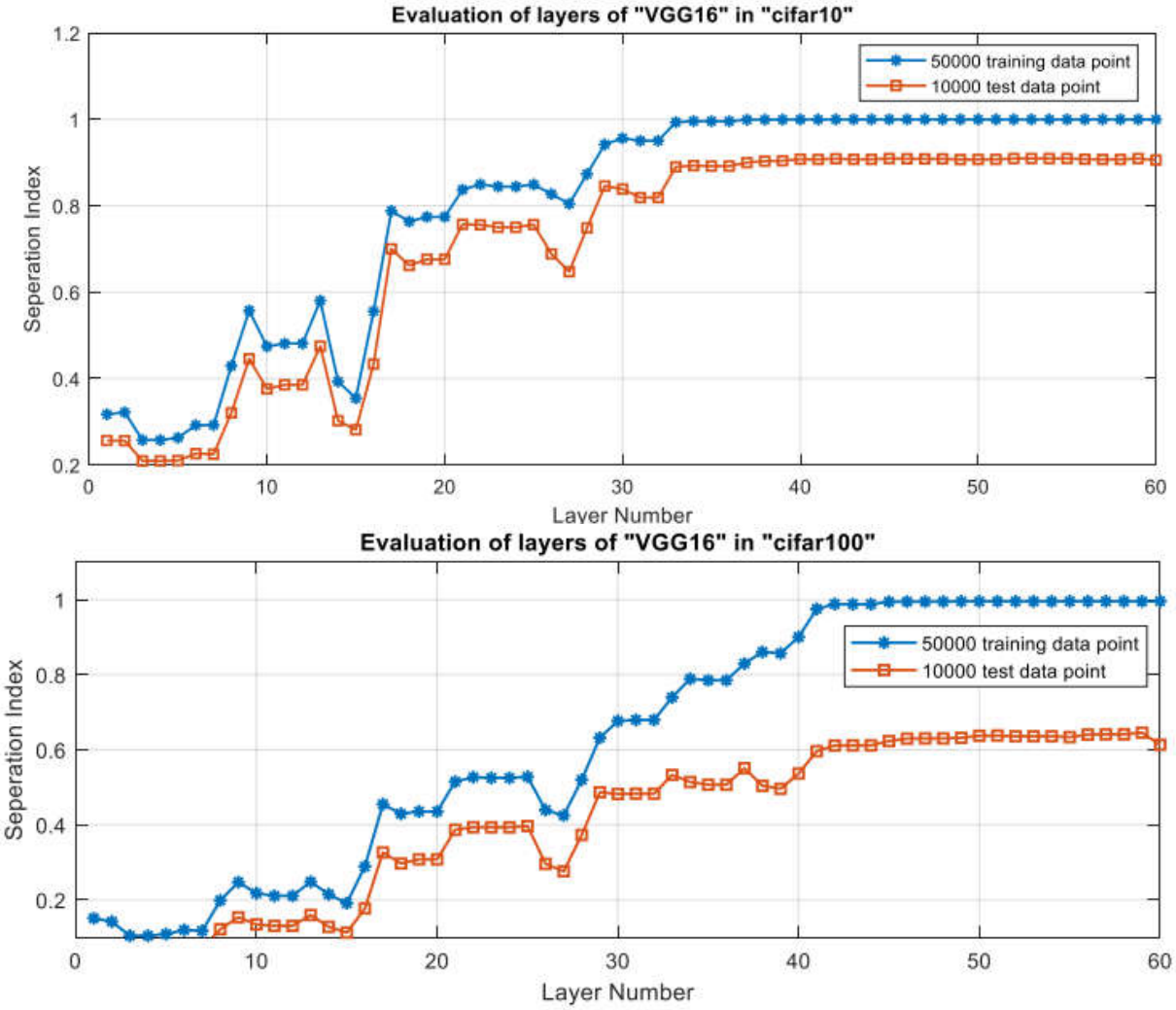


Fig. 10. Evaluation of dataflow through layers of the "Resnet18" network in the classification of Fashion-MNIST.



Correct Classification rate and SI

To compare correct classification rate and SI:

1. After each convolution layer of a pertained network, two dense layers are added in order to predict the true labels. After two dense layers, a batch normalization layer is utilized and after them, a softmax layer is applied.
2. Considering the sum of squared error as the loss function, the "Adam" optimizer with more than 100 epochs has been utilized.
3. This process is performed on the "cifar10" dataset on pre-trained "VGG-16" and "Fashion-MNIST" dataset on trained "Resnet18" separately.

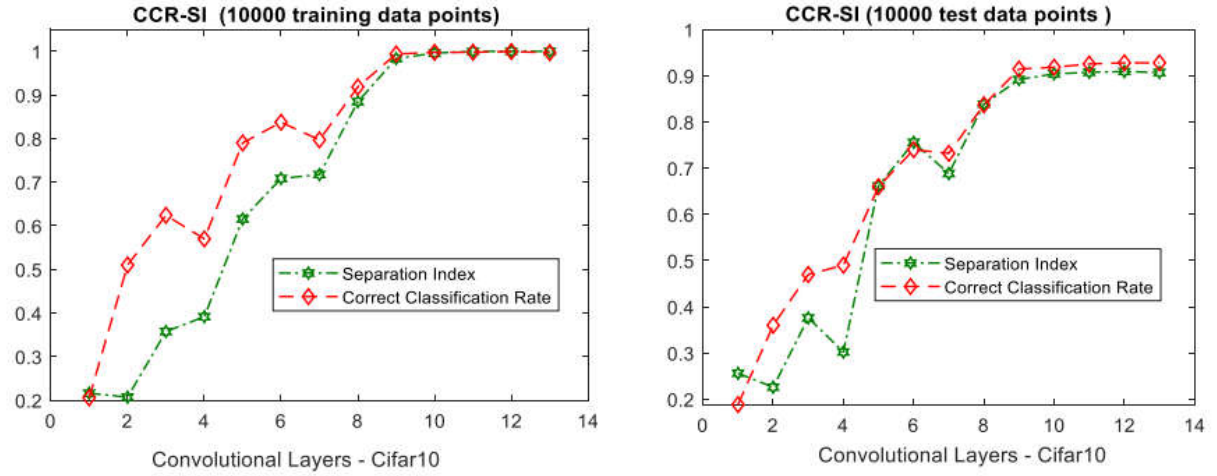


Fig. 11. The plots of separation index and correct classification rates at convolution layers in a pertained "vgg-16" network utilized for classification of "cifar10" for both training and test sets.

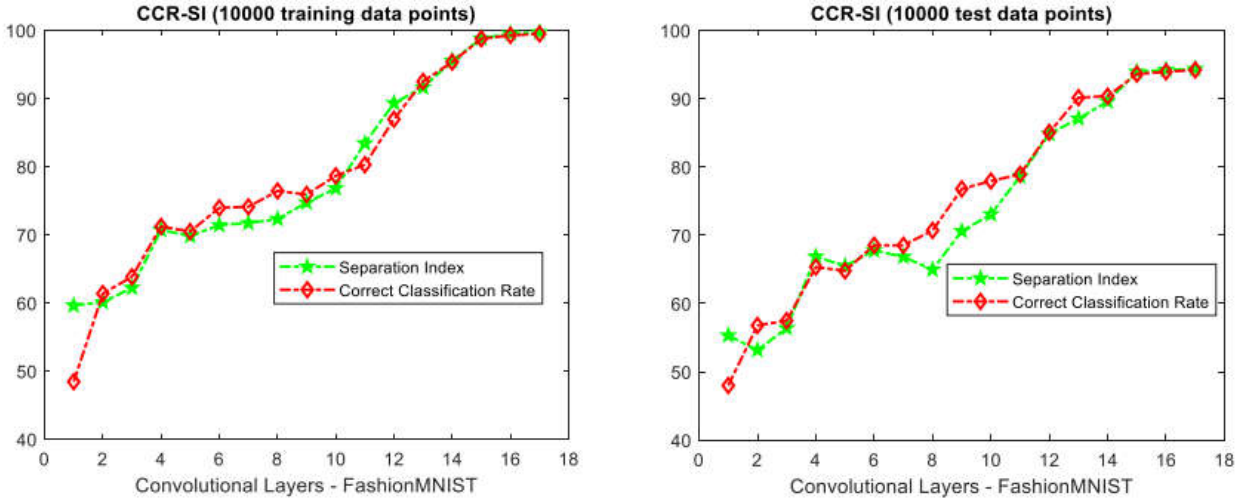


Fig. 12. The plots of separation index and correct classification rates at convolution layers in a trained "Resnet18" network utilized for classification of "Fashion-MNIST" for both training and test sets.

Pre-train Model ranking

- Assume there are M different pre-trained models which are trained by M different source data.
- Assume for j=1,2,…,M, $there\ are\ \ L_j$ layers before fully connected layers .
- Now, we want rank n_{model} pre-trained models to be used in transfer learning for a target data:

$Data$=$\{(x_i, y_i)\}_{i=1}^{m}$ y_i for classification problems denotes the same label l_i

Algortihm2: (To suggest a pre-trained model in transfer learning)

1. Apply the target data to jth pre-trained model and provide following dataflow at the last layer before fully connected layers:

$$Data^{j,L_j}=\left\{\left(x_i^{j,L_j}, y_i\right)\right\}_{i=1}^{m}$$

2. For jth pre-trained model select the best subset of x_i^{j,L_j} as $x_i^{j^*,L_j}$ which maximizes $SI(SmI)$

$$Data^{j^*,L_j}=\left\{\left(x_i^{j^*,L_j}, y_i\right)\right\}_{i=1}^{m} \qquad x_i^{j^*,L_j} \subseteq x_i^{j,L_j}$$

3. Now rank the pre-trained models as best candidates for the target data in transfer learning as follows:

$$Best\_Models = \{j_1 \dots, j_M\} \quad \text{where} \quad SI\left(Data^{j_1^*,L_{j_1}}\right) > SI\left(Data^{j_2^*,L_{j_2}}\right) > \cdots > SI\left(Data^{j_M^*,L_{j_M}}\right)$$

3.2.5 Model Confidence and Guarantee

1. Model Confidence and Guarantee by SI
2. Model Confidence and Guarantee by SmI

Assumptions

1. There is a training dataset $Data = \{(x_i, l_i)\}_{i=1}^{m}$ ($Data = \{(x_i, y_i)\}_{i=1}^{m}$) for a classification(regression) problem.
2. The $SI(Data)$ ($SmI\ (Data)$) is computed for the dataset.
3. There is a test dataset which is homogenous with the training dataset.
4. Based on the Nearest Neighbor (NN) model, we want to predict the target $l\ (\boldsymbol{y})$ of a new test example $\boldsymbol{x}$, as $\hat{l}(\hat{\boldsymbol{y}})$.
5. It is assumed that $\boldsymbol{x}_{i_j^*}$ denotes the jth nearest neighbor of input data to x.
6. There is an "extra" uncertainty in measuring x . It is assumed that x has maximum distance γ with its true value x_{true}: $\|x_{true} - x\| < \gamma$.
7. It is aimed to know that the confidence of the prediction by the NN model.
8. It is aimed to know if there is a guarantee to predict true label in classification problem or to have a limited output error in a regression problem.

Model Confidence and Guarantee by SI (without training data)

Assume dw_{max} denotes the maximum intra distance between examples with the same label and db_{min} denotes the minimum inter distance between examples with different labels .

$Conf(\hat{l}, l^{i_1^*})$ denotes the confidence for prediction of $\hat{l} = l^{i_1^*}$ (by the NN model).

Guar ($\hat{l}, l^{i_1^*}$) denotes the guarantee that prediction of $\hat{l} = l^{i_1^*}$ (by the NN model) is true.

if Guar ($\hat{l}, l^{i_1^*}$) =1 the guarantee exists and otherwise it does not exist.

- $Conf(\hat{l}, l^{i_1^*})$=$SI(Data)$
- $Guar(\hat{l}, l^{i_1^*}) = \delta(SI, 1) * sign(1 - \frac{dw_{max}+\gamma}{db_{min}-\gamma})$

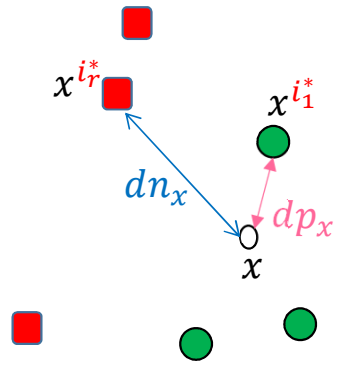
γ: the maximum uncertainty in measuring x :$\|x_{true} - x\| < \gamma$

❖ If $SI(Data) = 1$ and dw_{max}<db_{min}, the true prediction for x $with$ NN $model$ and for $\gamma < 0.5(db_{min} - dw_{max})$ is guaranteed.

Model Confidence and Guarantee by SI (with training data)

$dp_x = \left\| x - x^{i_1^*} \right\|$

$dn_x = \left\| x - x^{i_r^*} \right\|$ $\quad r = \min_{j=1,..,m} j$ subjec to $\delta(l^{i_j^*}, l^{i_1^*}) = 0$



- $Conf(\hat{l}, l^{i_1^*}) = SI$
- $Guar(\hat{l}, l^{i_1^*}) = \delta(SI, 1) * sign(1 - \frac{dp_x + \gamma}{dn_x - \gamma})$

❖ If $SI(Data) = 1$ the true prediction for x $with$ NN $model$ and $\gamma < 0.5(dp_x - dn_x)$ is guaranteed.

- About those cases that we have $SI^r(Data) = 1$ for $r \gg 1$ the guarantee is satisfied for much higher γ than the cases which we have $SI^1(Data) = 1$.

Model Confidence and Guarantee by SmI(with training data)

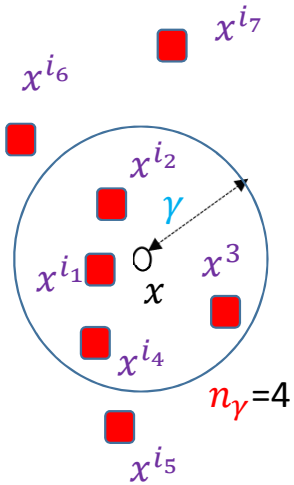
- Assume that for each data point x^i, $\alpha(i^*)=\|y^i - y^{i^*}\|$, where x^{i^*} is the nearest neighbor of x^i.
- Assuming $SmI(Data) = 1$, $\alpha(i^*)$ denotes the distance between the output y^i and its nearest neighbor, y^{imin}.
- In an ideal case a*ssume that the divesity of training dataset is so high* and *for each test data* point x (when there is no measuring uncertainty) $\|y - y^{i_1^*}\| \leq \alpha(i_1^*)$.
- Now assume, γ is the maximum measuring uncertainty of input x.
- Find all training examples: $\{x^{i_j}\}_{j=1}^{n_\gamma}$, which $\|x - x^{i_j}\| \leq \gamma$.

❖ it is guaranteed that if $for\ each\ test\ data\ pint, x, when\ \gamma \geq 0$

$$\|y - y^{i_1^*}\| \leq \bar{e}_y$$

$$\bar{e}_y = \max_{j=1,\dots,n_\gamma} \left(\|y^{i_1^*} - y^{i_j^*}\| + \alpha(i_j^*) \right)$$

- About those cases that we have $SmI^r(Data) = 1$ for $r \gg 1$, $\bar{e}_y$ is much lower than the cases which we have $SmI^1(Data) = 1$.



3.2.6 Causal relationship between two variables

Using SmI it is checked that if one variable has causal relationship with another variable.

Causal relationship between two variables

- A causal relationship exists **when one variable in a data set has a direct influence on another variable**.
- $Assume\ there\ are$"synchronous " $vairables\ x\ and\ y$ (time series, text, image, video) $where\ \{(\mathrm{x}^{\mathrm{i}}, \mathrm{y}^{\mathrm{i}})\}_{i=1}^{m}$ are measured samples through time.

Causal relationship rules by using SmI

1. Assume there are not any uncertainties and redundancies in measuring of $x\ and\ y$ if $SmI\left(\{(\mathrm{x}^{\mathrm{i}}, \mathrm{y}^{\mathrm{i}})\}_{i=1}^{m}\right)$ $\gg SmI\left(\{(\mathrm{y}^{\mathrm{i}}, \mathrm{x}^{\mathrm{i}})\}_{i=1}^{m}\right)$ then x has direct **influence on $\boldsymbol{y}$** and vice versa.
2. Assume there are some uncertainties or redundancies in measuring $x\ and\ y$, applying appropriate encoders to get their latent space if $SmI\left(\{(latent(\mathrm{x}^{\mathrm{i}}), \mathrm{latent}(\mathrm{y}^{\mathrm{i}})\}_{i=1}^{m}\right)$ $\gg SmI\left(\{(latent(\mathrm{y}^{\mathrm{i}}), \mathrm{latent}(\mathrm{x}^{\mathrm{i}}))\}_{i=1}^{m}\right)$, then $\mathrm{latent}(x)$ has direct **influence on $\mathbf{latent}(\boldsymbol{y})$** and vice versa.

3.3 Layer-wise Design by Separation and Smoothness indices

3.3.1 Model Compressing
3.3.2 Forward learning in the first layer
3.3.3 Layer-wise Forward learning
3.3.7 Forward Auto Encoder Learning
3.3.4 Layer-wise branching
3.3.5 Layer-wise Fusion
3.3.6 Forward Design
3.3.8 Forward Multi-Task Design
3.3.9 Artificial Brain Design

3.3.1 Model Compressing

To remove extra layers and units in filter part and then compressing flat layers

Model Compressing

In model compressing some layers and units

Some Definitions:

Filter Part: The layers before fully connected layers which extract features from spatial or temporal inputs. If in some DNNs, one or more than on RNN modules have been used, we assume that they belonged to filter part.

FC Part: one, two, or more than two fully connected layers which are defined after the "Filter Part" and the outputs of the networks.

Algorithm3:

1- Find and remove the last layers of the "Filter Part" which do not increase the SI(SmI), significantly.

2- Find and remove all units of the last layer of the filter part which do not increase the SI(SmI), significantly.

3- Design a new "FC part" with respect the number of units at the last later of the "filter part".

TABLE VIII
Comparison with the prior art of VGG-16 on CIFAR-10.

Compressing method	Retraining needed	FLOPs	Pruned	Accuracy
VGG16-base	-	313.7M (0.0%)	0.0%	94.04%
PFEC **[17]**	Yes	206M (34.3%)	63.3%	93.40%
VP **[45]**	Yes	190M (39.1%)	73.4%	93.18%
SS **[46]**	Yes	183.13M (41.6%)	٧٣,٢%	٩٣,٠٢%
GAL-0.05 **[47]**	No	189.49M (39.6%)	77.2%	92.03%
CP **[48]**	No	107.58M (65.1%)	77.6%	92.03%
HRFM **[49]**	Yes	108.61M (65.3%)	82.1%	92.34%
GAL-0.1 **[47]**	No	171.89M (45.2%)	82.2%	90.73%
Our method	**No**	**75.6M (76.0%)**	**87.5%**	**93.49%**
HRFM **[49]**	Yes	73.70M (76.5%)	88.2%	91.23%

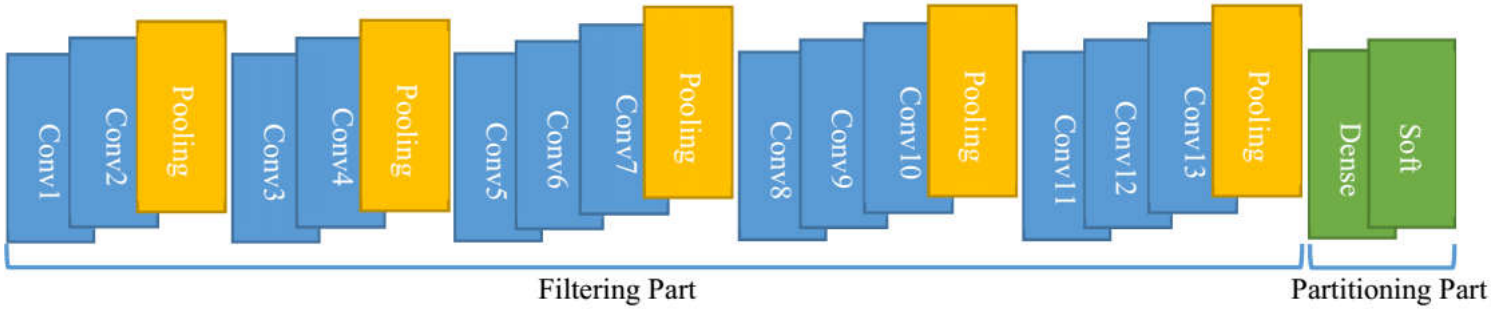


Fig. 5. The architecture of the "VGG-16" network.

TABLE IX
Comparison with the prior art of GoogLeNet on CIFAR-10.

Compressing method	Retraining needed	FLOPS	Pruned	Accuracy
GoogleNet-base	-	1.52B(0.0%)	0.0%	95.05%
PFEC **[17]**	Yes	1.0B(32.9%)	42.9%	94.54%
HRFM **[49]**	Yes	0.69B(54.9%)	55.4%	94.53%
GAL-Apo **[50]**	No	0.76B(50.0%)	53.7%	92.11%
GAL-0.05 **[48]**	No	0.94B(38.2%)	49.3%	93.93%
HRFM **[49]**	Yes	0.45B(70.4%)	69.8%	94.07%
Our method	**No**	**0.39B(74.4%)**	**77.6%**	**95.00%**

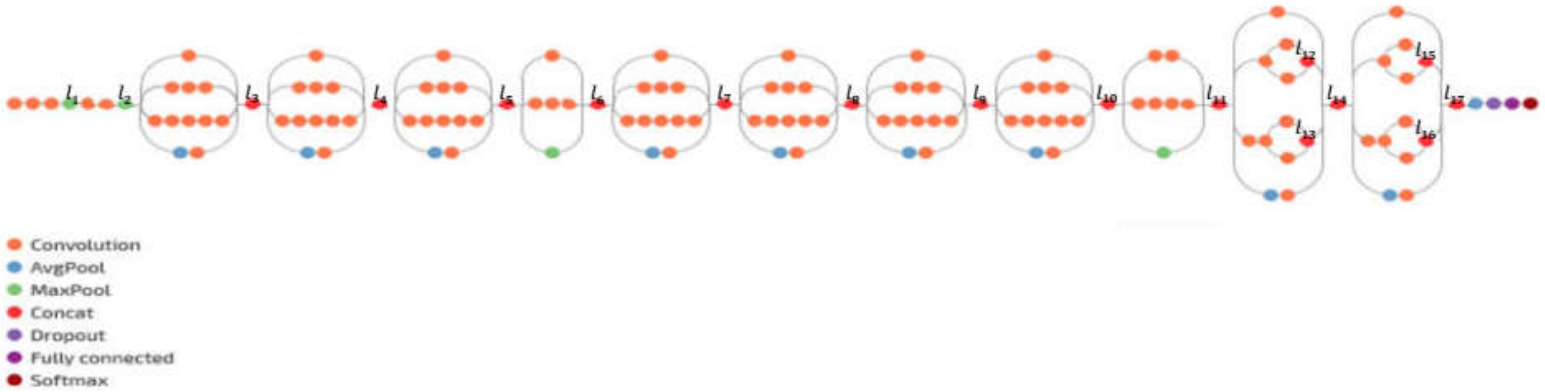


Fig. 7. The architecture of the "Inception V3" network.

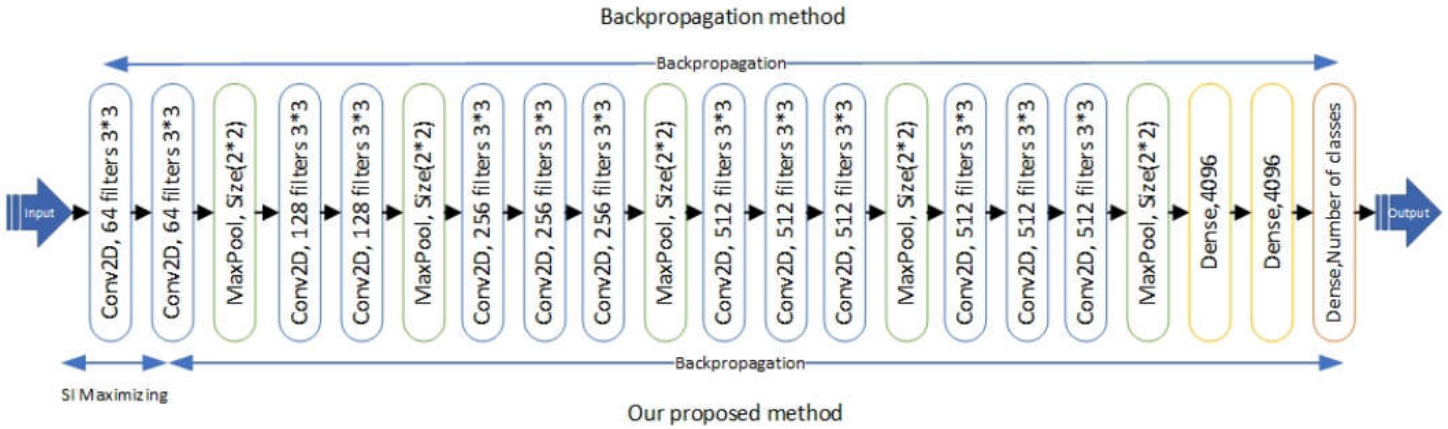
TABLE X
Comparison with the prior art of DenseNet-40 on CIFAR-10.

Compressing method	**Retraining needed**	**FLOPS**	**Pruned**	**Accuracy**
DenseNet-base	-	0.29B(0.0%)	0.0%	94.22%
ECNS **[51]**	Yes	0.12B(58.3%)	67.2%	94.35%
HRFM **[49]**	Yes	0.11B(61.8%)	55.1%	94.53%
GAL-0.05 **[48]**	No	0.13B(55.6%)	57.9%	92.11%
VP **[45]**	No	0.16B(45.8%)	60.7%	93.16%
Our method	**No**	**0.07B(76.1%)**	**78.8%**	**94.17%**

3.3.2 Forward learning in the first layer

For classification problems but the method can be generalized for regression problems

Forward learning in the first layer



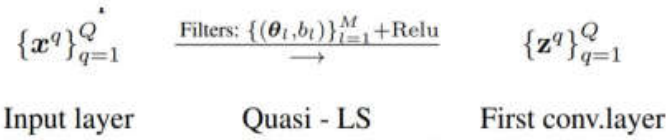


Figure 3: Applying M convolutional filters and biases to the input patterns and then activating the convolved units by Relu function the feature maps are resulted.

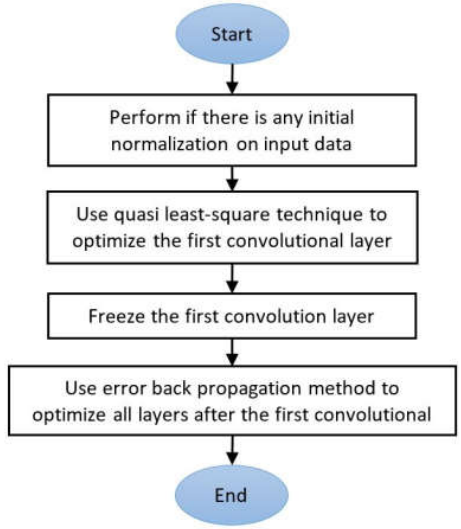


Figure 2: This flowchart indicates the learning method in which the quasi-LS is utilized first convolution layer, and other layers are learned by an error backpropagation method

Algorithm to train the first layer by Quasi Least Square (QLS) technique

1. Define the matrix of patches from the input data: X
2. Subtract the matrix from their mean: $\widetilde{\mathrm{X}} = X - mean(X)$
3. Define Auto-correlation matrix of patches: $\mathrm{W_{np}} = \widetilde{\mathrm{X}}^{\mathrm{T}}\widetilde{\mathrm{X}}$
4. Apply SVD technique to get Eigen values and Eigen vectors: $W = \sum_{i=1}^{n_p} \lambda_i v_i v_i^T$
5. Rank Eigen vectors by their Eigen values and then initiate all filters parameters and the biases by Eigen vectors, their negatives and the mean of patches.

   $\left\{\left\{\boldsymbol{\theta}^j, b^j\right\}\right\}_{j=1}^{n_F}$ n_F:number of filters
6. Based on the filter parameters at the first (convolutional)layer compute the second layer and for each example(anchor) find nearest neighbor for both positive and negative examples and define triplet loss for all data batch.

   $$J_{triplet} = \sum_{i=1}^{m}(\left\|x_i^2 - x_{ipos}^2\right\|^2) - \sum_{i=1}^{m}(\left\|x_i^2 - x_{ineg}^2\right\|^2)$$
7. Use a QLS technique to minimize $J_{triplet}$ and update all filters.

   $\boldsymbol{\theta}^j := \boldsymbol{\theta}^j + \mu\, \widetilde{\boldsymbol{\theta}}^j$ $\quad b^j := b^j + \mu \tilde{b}^j$ $\quad \mu$=learning rate
8. Repeat steps 6 and 7 for several epochs to get maximum possible SI on the second layer.

Now, one can train further layers by Backpropagation Algorithms.

Comparison between our method and backpropagation algorithm

Dataset	Learning Method	**AlexNet**	**VGG16**	**ResNet50**	**InceptionV3**
CIFAR10	Backpropagation	84.61	92.95	93.17	94.20
	Our proposed method	**85.84**	**94.81**	**95.02**	**95.43**
	Percentage of improvement	1.23	1.86	1.85	1.23
CIFAR10 - (plane,truck)	Backpropagation	96.45	97.18	97.64	97.09
	Our proposed method	**97.09**	**98.36**	**98.49**	**97.77**
	Percentage of improvement	0.64	1.18	0.85	0.68
CIFAR10 - (plane,cat,bird)	Backpropagation	96.21	96.80	96.88	96.81
	Our proposed method	**96.62**	**97.63**	**97.16**	**97.14**
	Percentage of improvement	0.41	0.83	0.28	0.33
CIFAR100	Backpropagation	62.22	70.98	75.30	76.31
	Our proposed method	**62.45**	**71.74**	**75.58**	**76.72**
	Percentage of improvement	0.23	0.76	0.28	0.41
FASHION-MNIST	Backpropagation	92.53	94.17	95.24	95.78
	Our proposed method	**92.65**	**94.73**	**95.38**	**95.91**
	Percentage of improvement	0.12	0.56	0.14	0.13

Table 5: Comparing the accuracy of our proposed method in different architectures and datasets with backpropagation method

3.3.3 Layer-wise forward learning

Layer Wise Forward Learning

Algorithm

For L=1:L_{final}

While (SI ($Data^l$) may still increase)

For $l = 1: L$

$$\boldsymbol{g}_{\boldsymbol{p}^l} = \frac{\partial \text{Loss}_{\text{triplet}}(Data^l)}{\boldsymbol{p}^l}$$

$$\boldsymbol{p}^l := \boldsymbol{p}^l - \gamma \boldsymbol{g}_{\boldsymbol{p}^l}$$

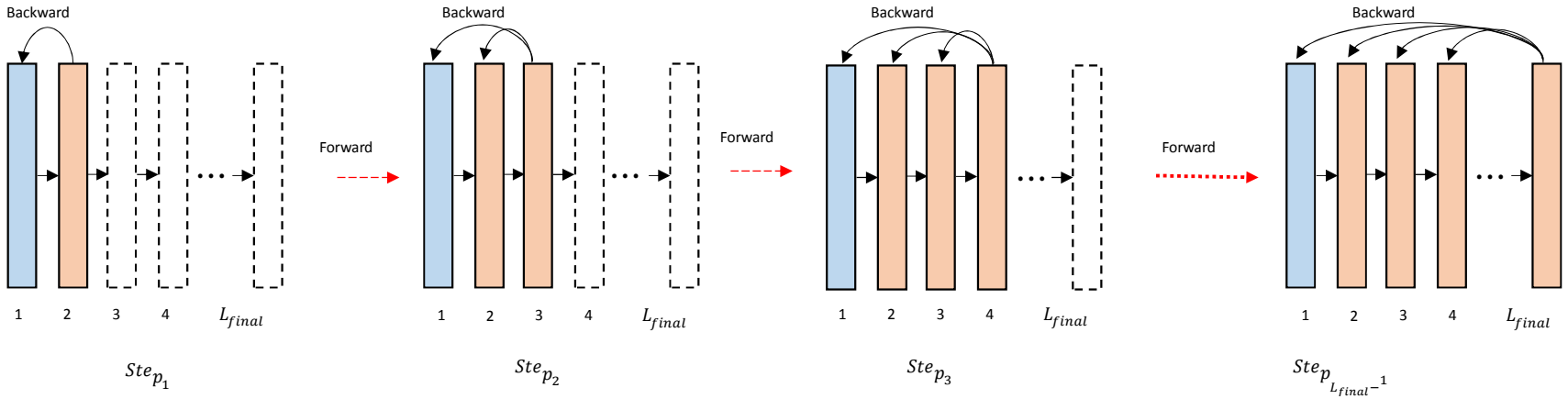
$Data^l = \{(\boldsymbol{x}_i^L, \boldsymbol{y}_i^L)\}$ *Data at layer l*

Triplet Loss

$$\text{Loss}_{\text{triplet}}(Data^L) = \frac{1}{m}\sum_{i=1}^{m}\left(\left\|\boldsymbol{x}_i^L - \boldsymbol{x}_{i_p^*}^L\right\|^2 - \left\|\boldsymbol{x}_i^L - \boldsymbol{x}_{i_n^*}^L\right\|^2\right)$$

$$i_p^* = \underset{\forall q \neq i}{\arg\ min} \frac{1}{\delta(\boldsymbol{y_i}, \boldsymbol{y}_q) + \varepsilon}\left\|\boldsymbol{x}_i^L - \boldsymbol{x}_q^L\right\|^2 \quad \varepsilon \to 0^+$$

$$i_n^* = \underset{\forall q \neq i}{\arg\ min} \frac{1}{1 - \delta(\boldsymbol{y_i}, \boldsymbol{y}_q) + \varepsilon}\left\|\boldsymbol{x}_i^L - \boldsymbol{x}_q^L\right\|^2$$



index is feasible by training the first layers with the Forward learning approach.

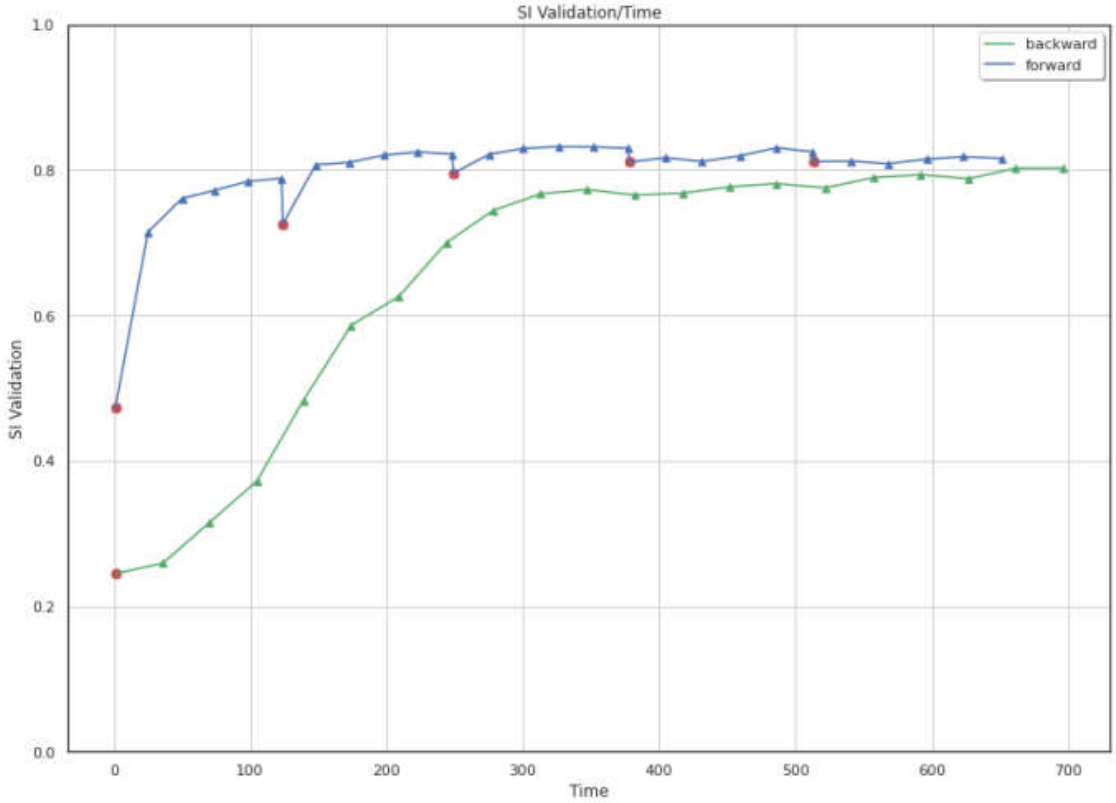


Figure 2. Comparing the separation index of the forward learning and backward learning approaches over time. Each triangle shows a single epoch in the learning process and the red dots in the Forward learning method are convolutional layers.

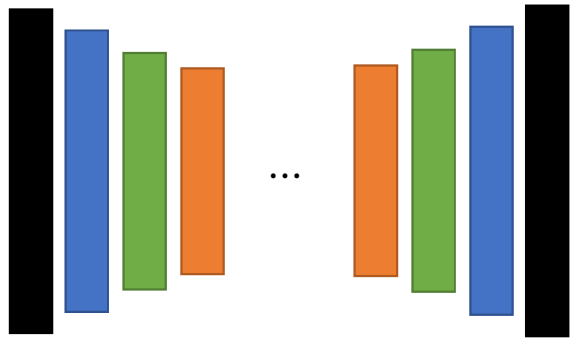
Comparison between our method and backpropagation algorithm

VGG١٦	ResNet٥٩	InceptionV٣	EfficientNetB٠		
٩٢.٩٥	٩٣.١٧	٩٤.٢٠	٩٨.١١	Backpropagation	CIFAR١٠
٩٣.٦٧	**٩٤.٦٥**	**٩٤.٦٣**	**٩٨.٢٤**	Our method	
٧٠.٩٨	٧٥.٣٠	٧٦.٣١	٨٨.١٤	Backpropagation	CIFAR١٠٠
٧١.١٩	**٧٥.٤٧**	**٧٦.٤٩**	**٨٨.١٧**	Our method	
٩٤.١٧	٩٥.٣٨	٩٥.٩١	٩٧.٢٣	Backpropagation	Fashion-MNIST
٩٤.٥٢	**٩٦.٦١**	**٩٦.٢١**	**٩٧.٤١**	Our method	

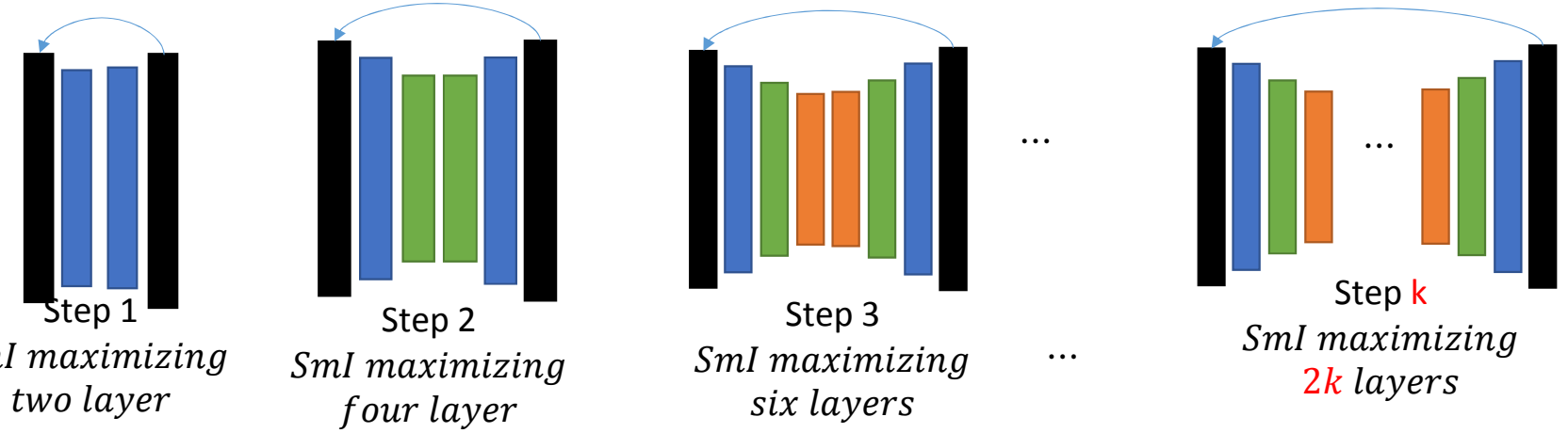
3.3.4 Layer-wise Forward Auto-Encoder Learning

Layer Wise Forward Learning of an Auto-Encoder

- Smoothness index can be used to train an auto-encoder step by step in a forward manner.
- At the first step two hidden layers are trained and then by each further step two new layers are added and trained to the AE.
- At each step, the training procedure is based on "SmI" maximizing.
- In fact, the smoothness index is approximated by a triplet loss and then the loss is minimized.
- Each example at the output layer decreases(increases) its distance to one of its K nearest neighbors that has nearest (furthest) distance at the target(input) space (reconstruction)



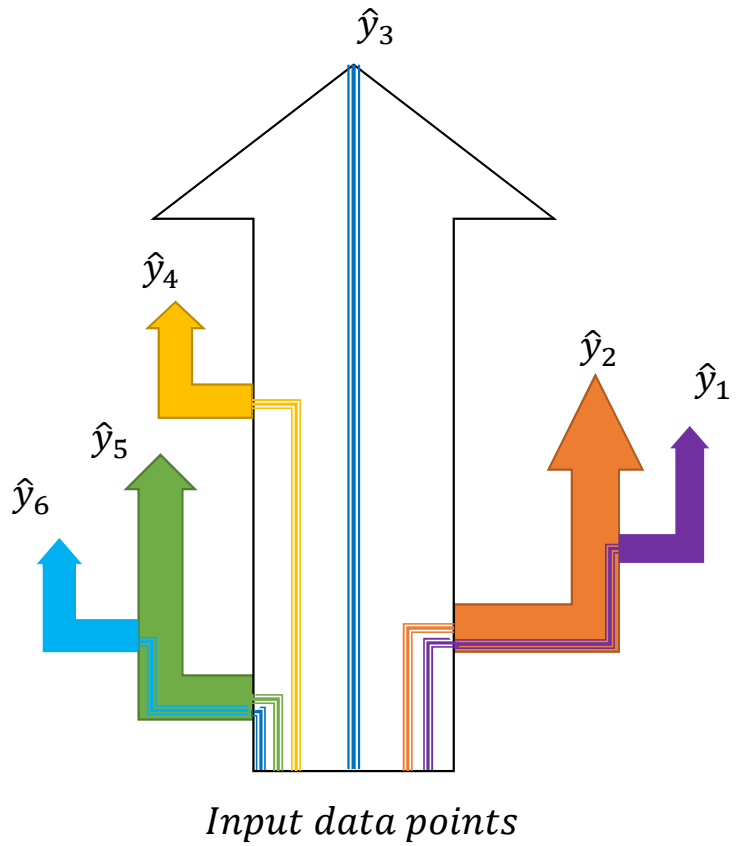
Layer-wise Learning through Smoothness Maximizing



3.3.4 Layer-wise branching

Layer-wise branching

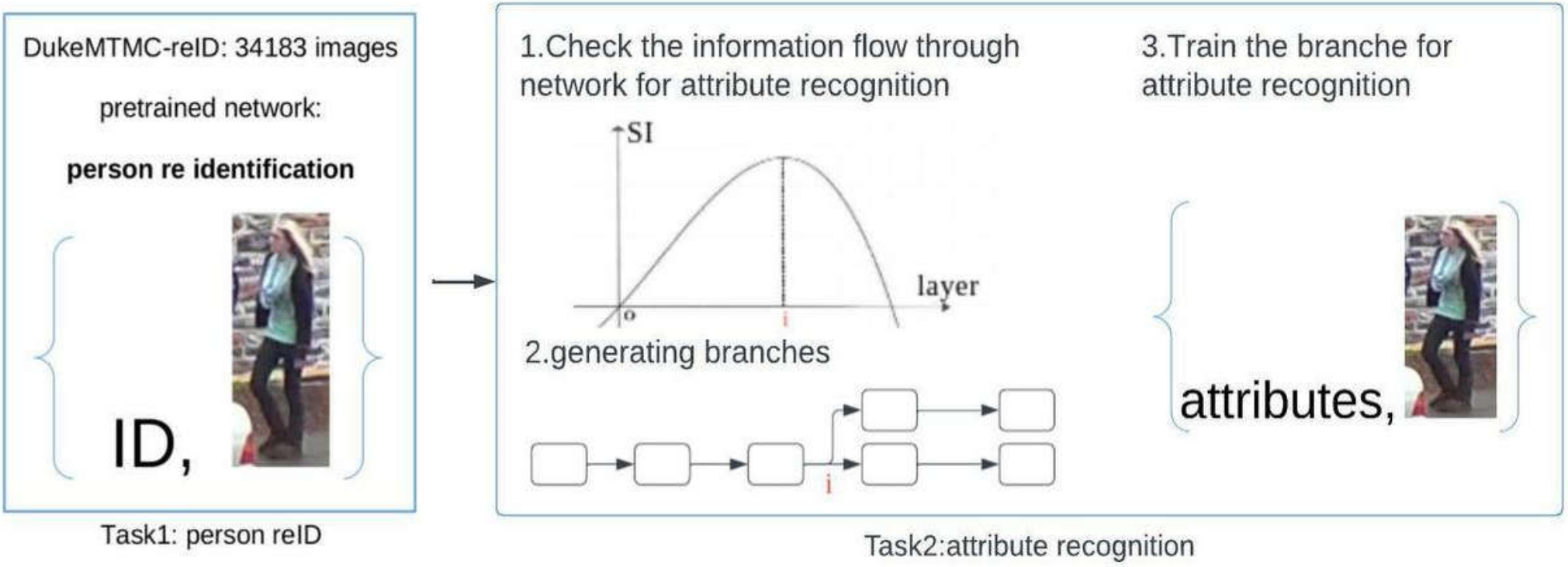
- In a classification (regression) problem, the required features may be extracted earlier or later through layers of a DNN.
- If we design a new architecture of DNN which can conduct earlier features in some independent paths, more compact and more generalized DNNs can be learned.
- In such an architecture, there are a main body and some branches. The main body forms the main flow of data but each branch process a part of data-flow.
- We can use complexity measures like SI(SmI) to distinguish early features from other features and form a new branch for it.
- Each branch like the man body can define some sub-braches, too.
- In such a DNN, the amount of data-flow decreases through the main body just after each branching.



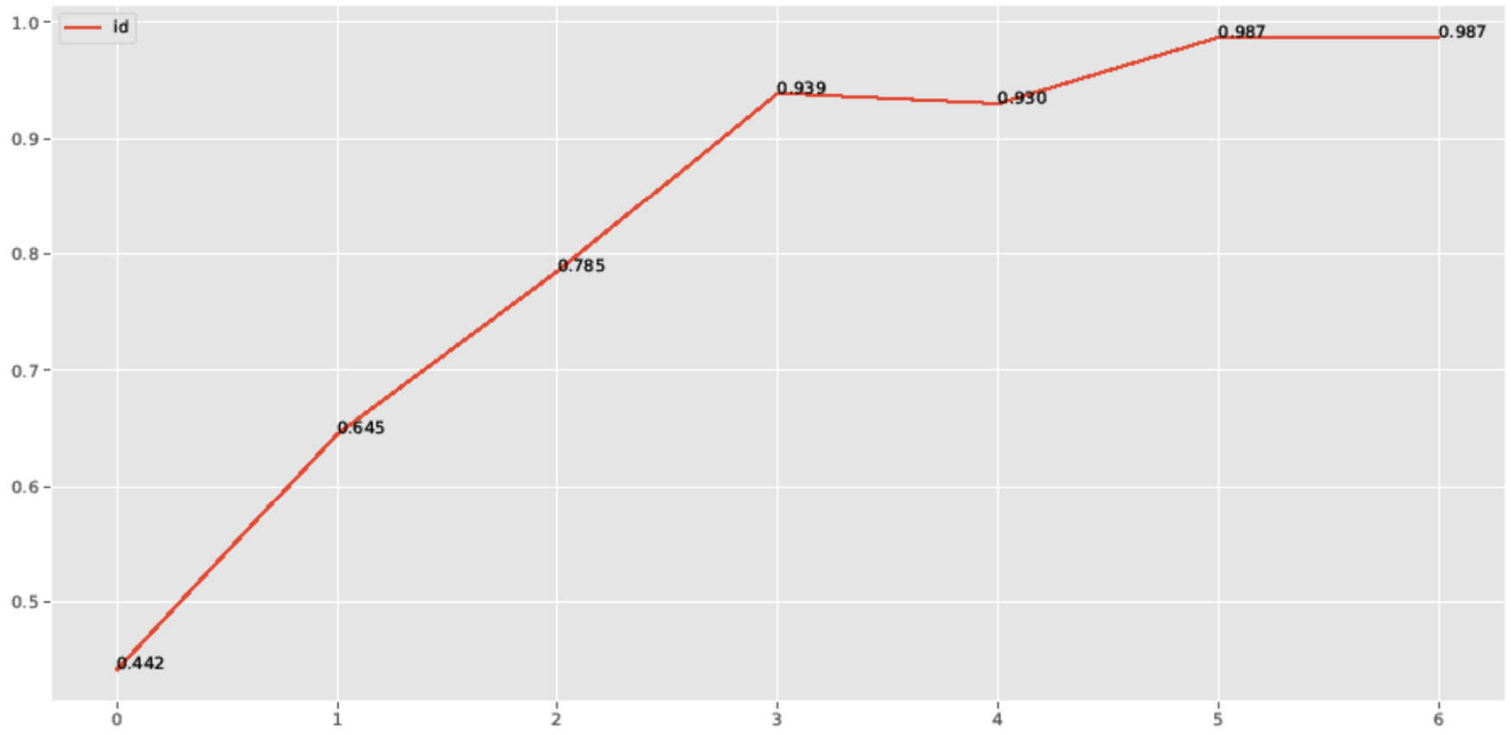
Some notes

- Branch in point where an increasing jump on SI(SmI) is occurred.
- Find the appropriate part of data (class/output/examples) to be branched.
- Branching is done as a forward design operation

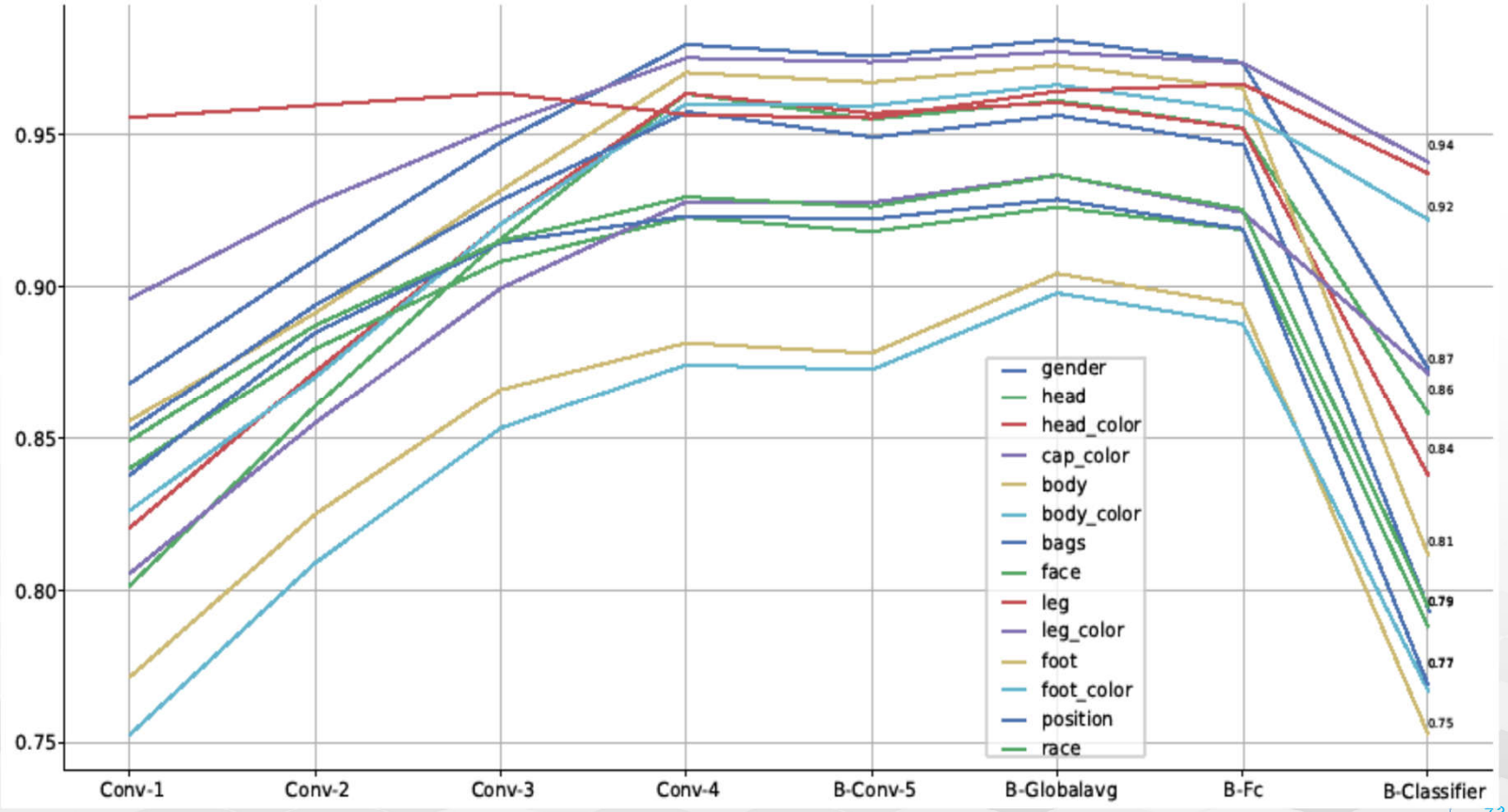
Utilizing SI for Branching

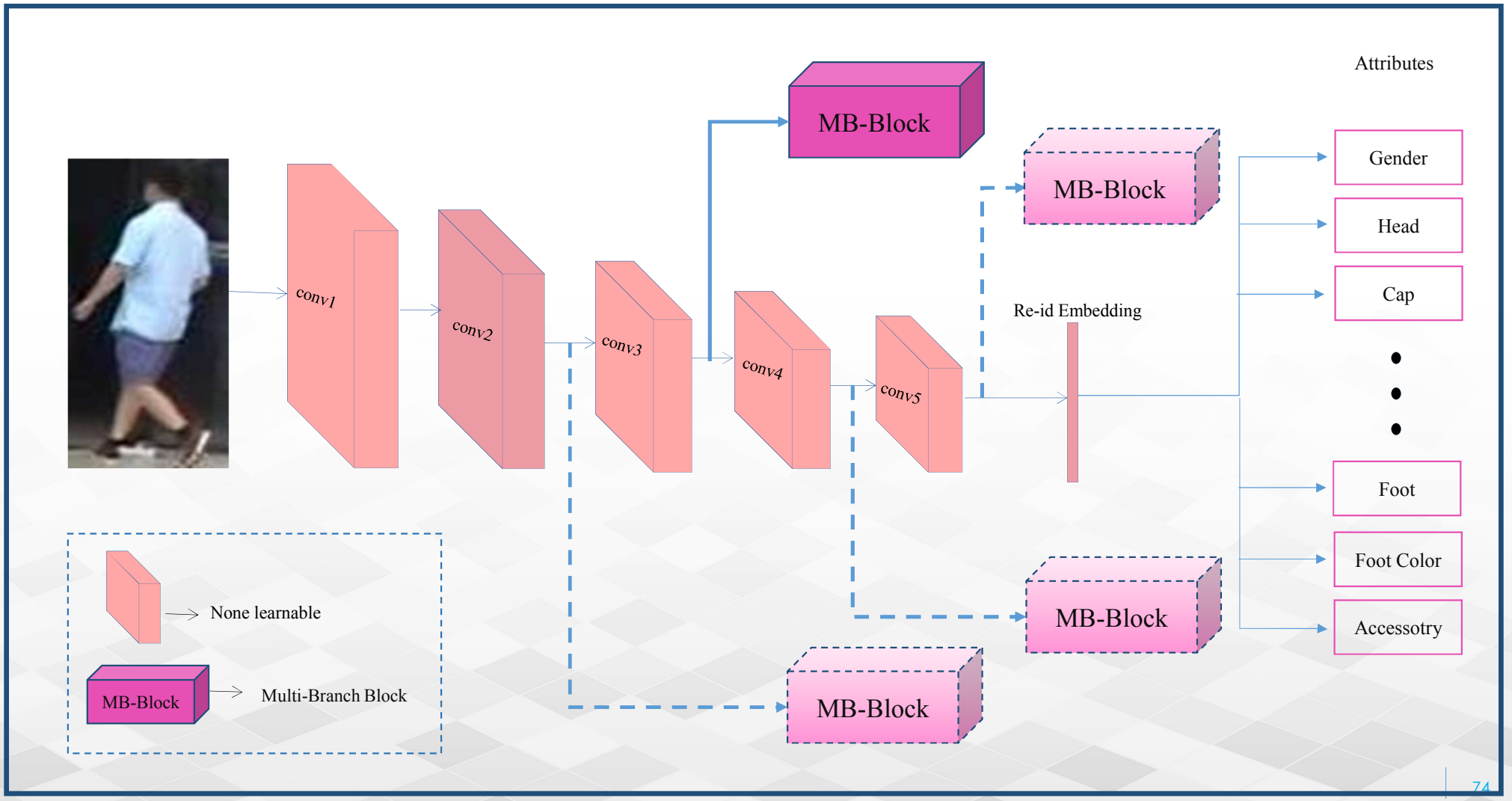


Separation Index for a classification

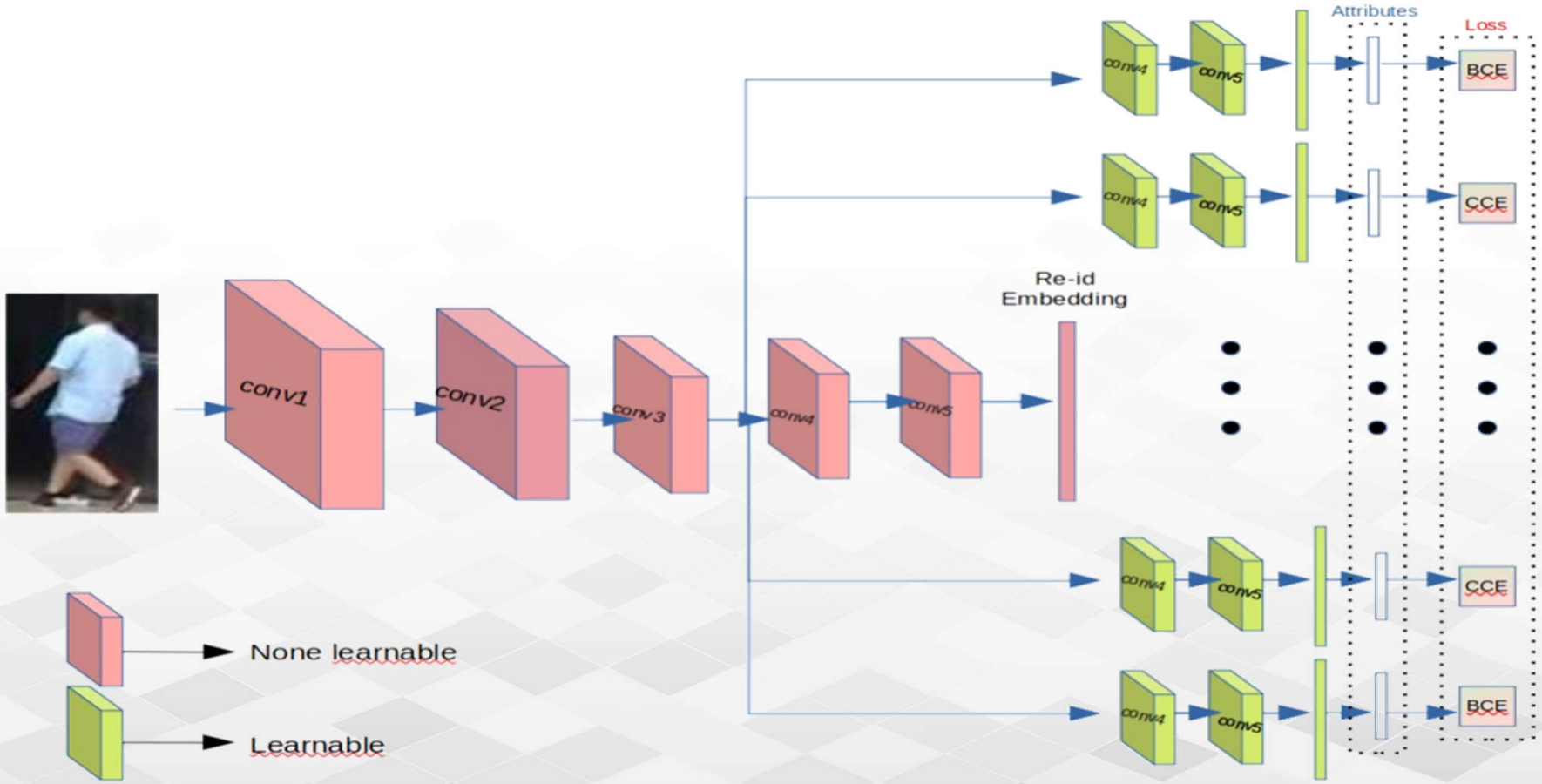


Separation Index for Multi-label Multi classification




Attributes
MB-Block
MB-Block
Gender
Head
Cap
conv1
conv2
conv3
conv4
conv5
Re-id Embedding
Foot
Foot Color
Accessotry
MB-Block
MB-Block
None learnable
MB-Block
Multi-Branch Block

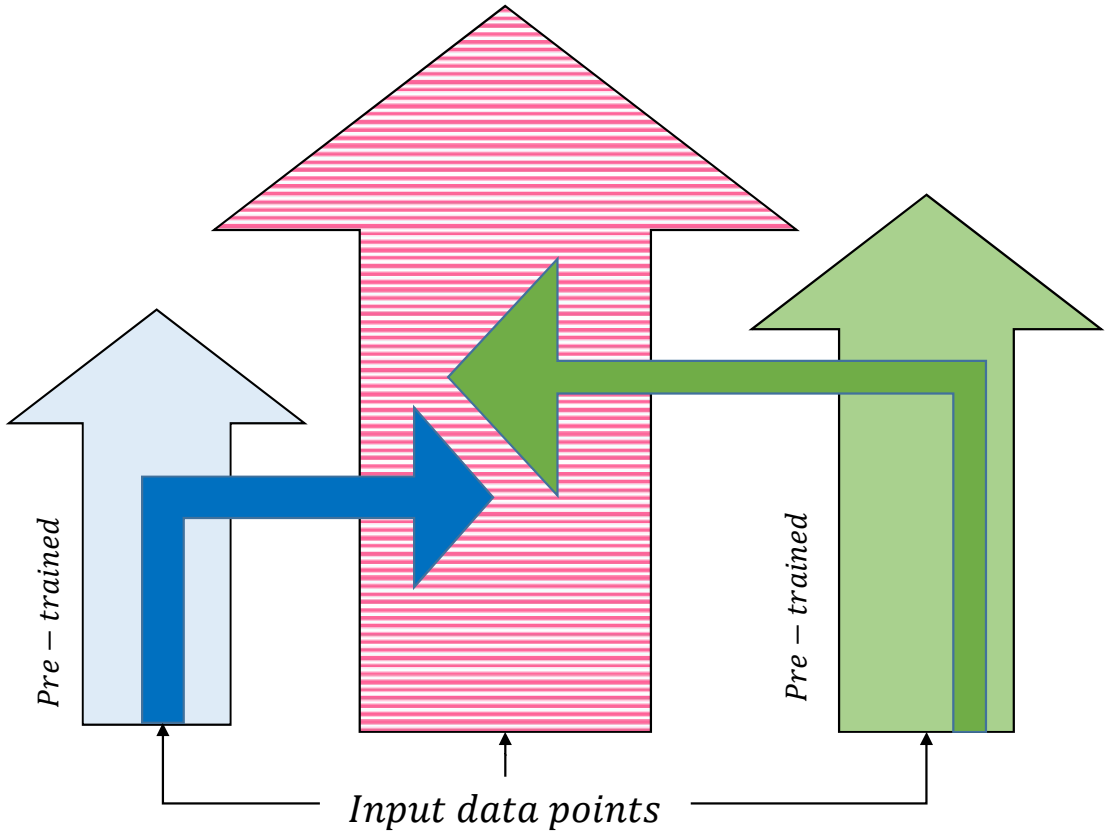
Multi-Branch Network



3.3.6 Layer-wise Fusion

Layer-wise Fusion

- In a classification (regression) problem, the required features may be extracted by fusing some prepared features from some pre-trained models.
- If we design a new architecture of DNN which can combine desired features from some pre-trained DNNs, more generalized DNNs can be learned.
- In such an architecture, there are a main body which is integrated by some branches from other DNNs at different points. The main body forms the main flow of data but each branch insert information-flow.
- We can use complexity measures like SI(SmI) to find some desired features from other pre-trained DDNs.



Some notes

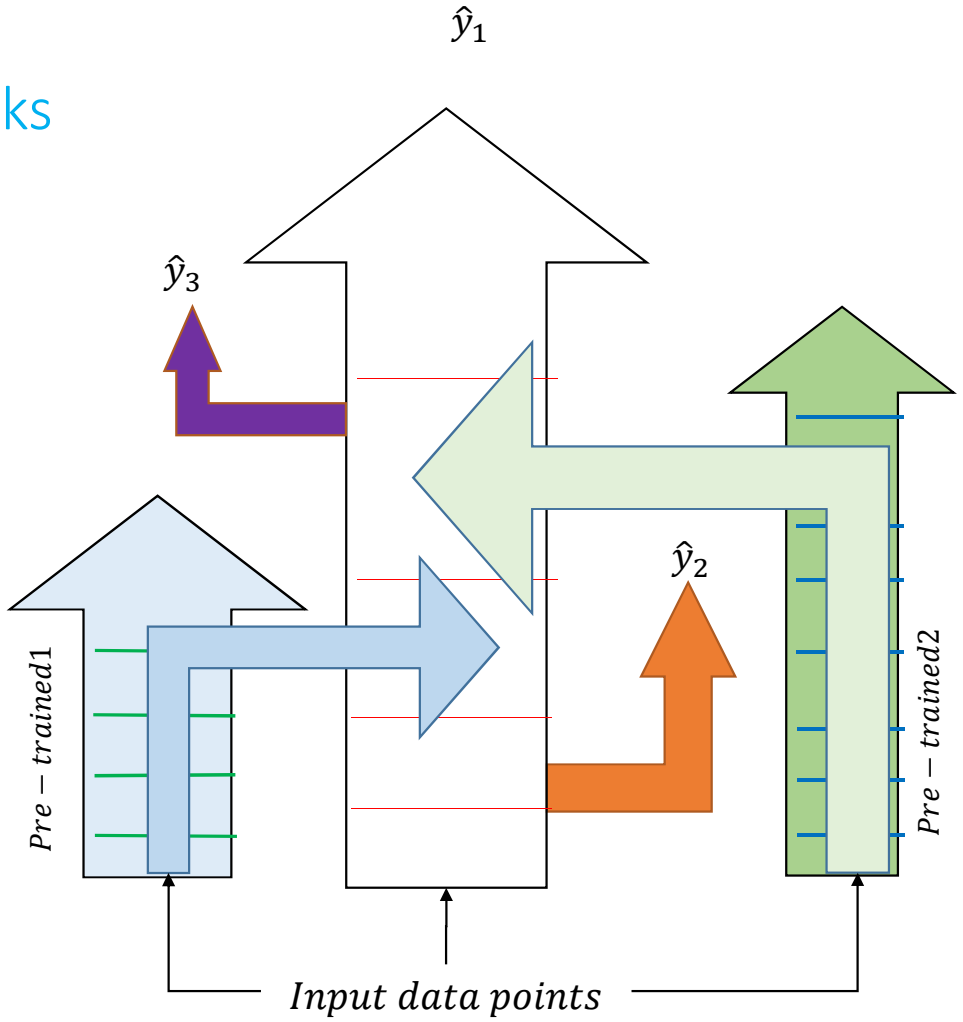
- Fuse at any point where SI(SmI) may increase significantly.
- Fusion is done in as a forward design operation.

3.3.7 Forward Design

Forward Design of Deep Neural Networks

In forward design of deep neural network, flowing tasks are done in a way that SI(SmI) maximizes in a classification(regression) problem.

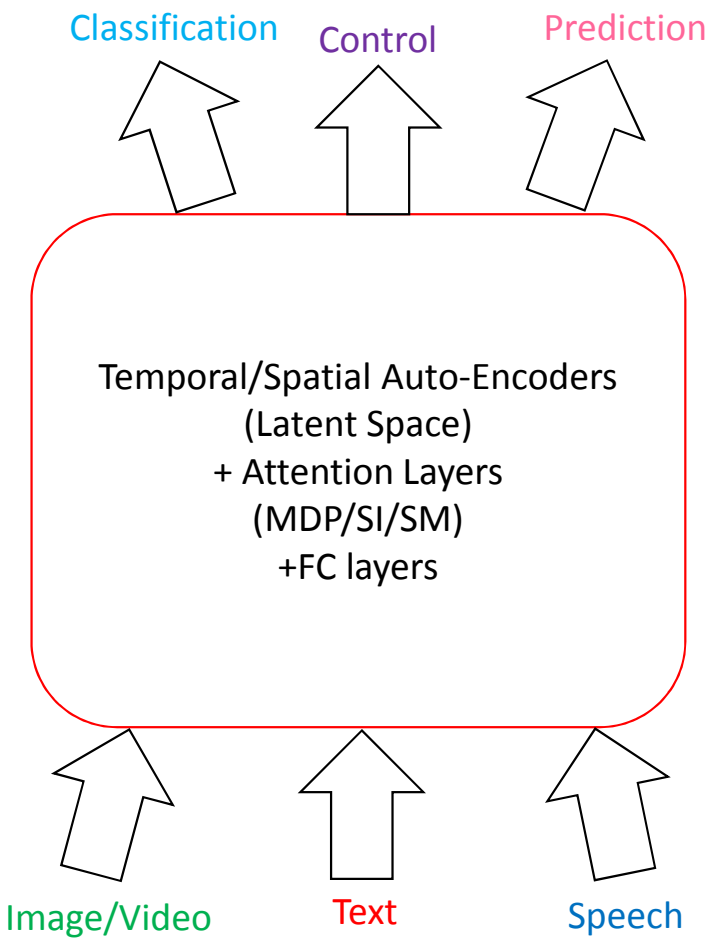
1. Organization of different layers
2. Adjusting the resolution, width, and depth of the network
3. Adding new branches on some layers where SI(SmI) increases significantly.
4. Fusing at some nodes from some other pre-trained networks through which SI(SmI) increases significantly.



3.3.8 Forward Multi-Task Design

A neural network which receives multi-modal data and it is trained to do multi-tasks in a supervised method. Such network works as a generalist AI agent. The key idea is that by appropriate temporal/spatial encoders, different data steams are encoded as the latent space; then the required features for each task are chosen from the latent space by using SmI(SI).

- Language Tasks
  - Speech recognition
  - Speech generating
  - ...
- Vision Tasks
  - Image recognition
  - Action Recognition
  - Text recognition
  - ...
- Physical world tasks
  - Motion tasks
  - Grasping tasks
  - ...



Narrow AI→ General and wide AI

DeepMind Introduces Gato

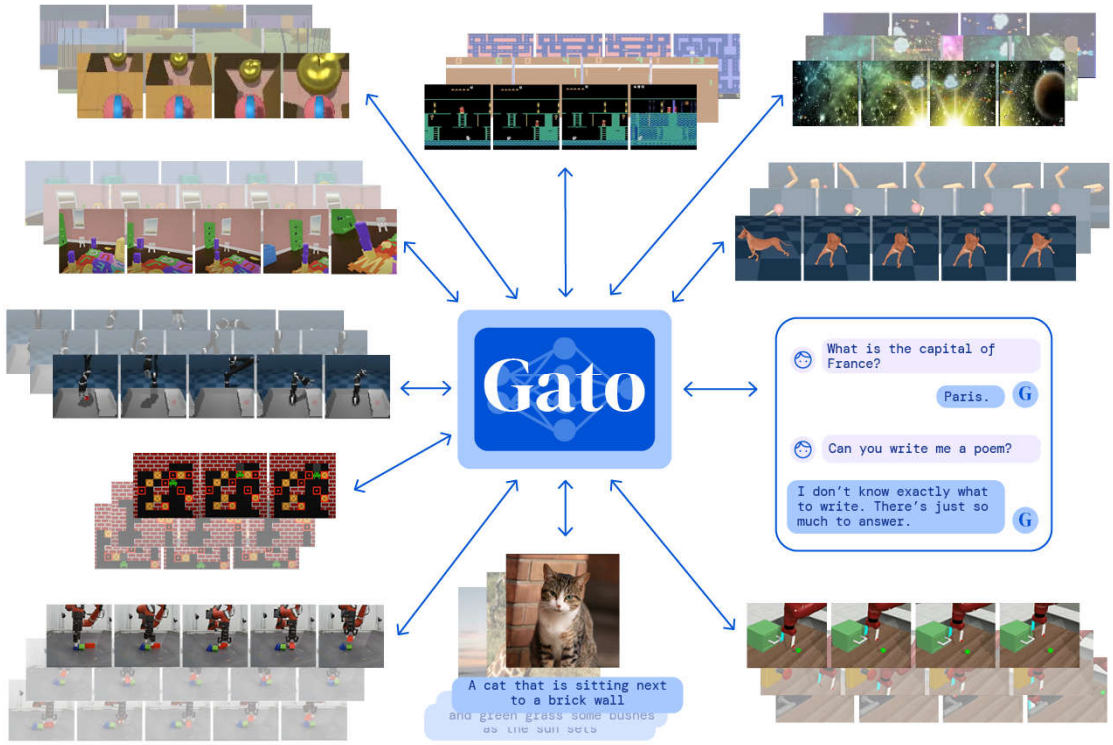
DeepMind Introduces Gato, a New Generalist AI AgentGato, as the agent is known, is DeepMinds's generalist AI that can perform many different tasks that humans can do, without carving a niche for itself as an expert on one task. Gato can perform more than 600 different tasks, such as playing video games, captioning images and moving real-world robotic arms. Gato is a multi-modal, multi-task, multi-embodiment generalist policy.

https://www.youtube.com/watch?v=6fWEHrXN9zo&t=254s

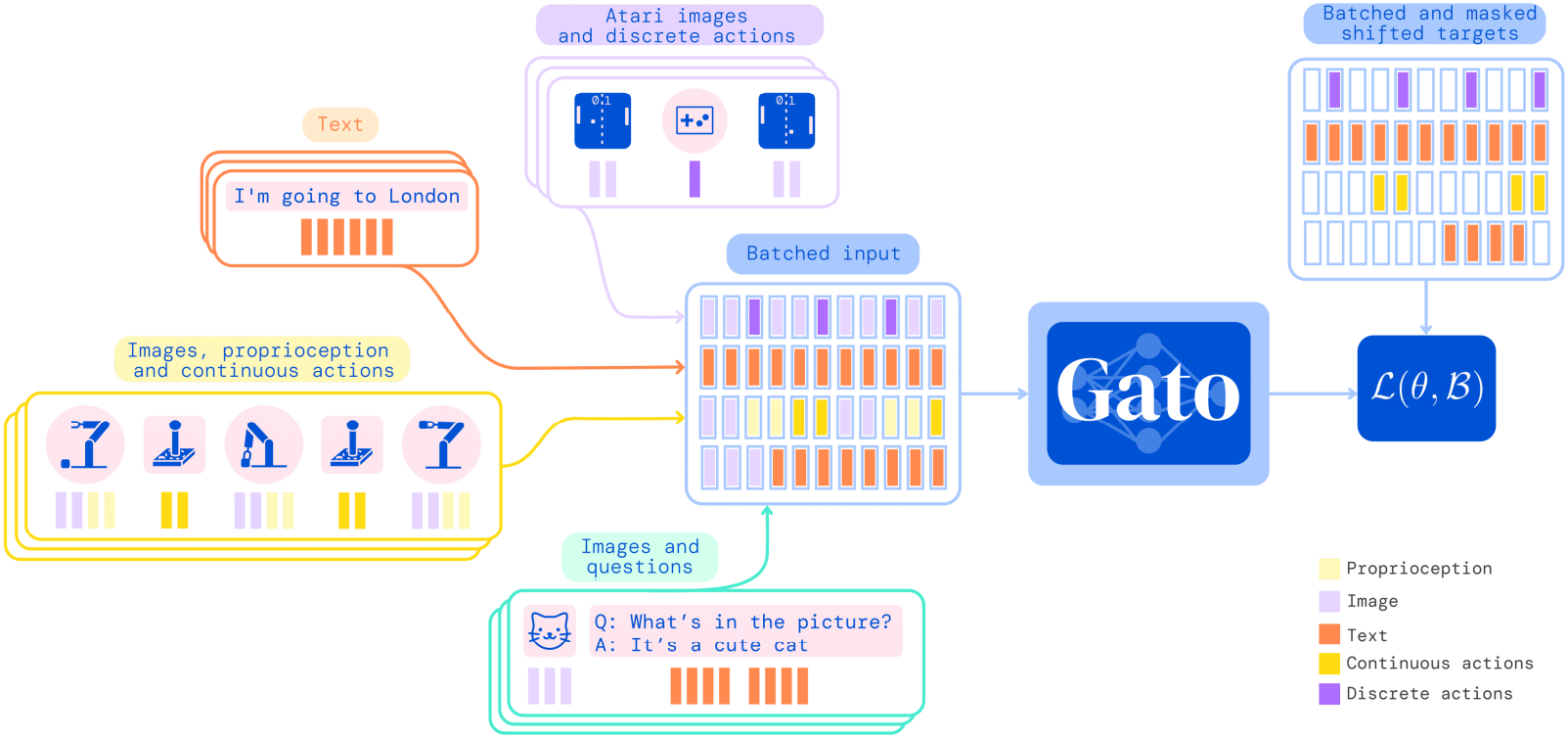
Integrated AI - Gato by DeepMind (May/2022) 1.2B + Asimo, GPT-3, Tesla Optimus, Boston Dynamics

Inspired by progress in large-scale language modelling,... https://www.deepmind.com/publications/a-generalist-agent

Inspired by progress in large-scale language modelling, we apply a similar approach towards building a single generalist agent beyond the realm of text outputs. The agent, which we refer to as Gato, works as a multi-modal, multi-task, multi-embodiment generalist policy. The same network with the same weights can play Atari, caption images, chat, stack blocks with a real robot arm and much more, deciding based on its context whether to output text, joint torques, button presses, or other tokens.



During the training phase of Gato, data from different tasks and modalities are serialised into a flat sequence of tokens, batched, and processed by a transformer neural network similar to a large language model. The loss is masked so that Gato only predicts action and text targets.



Token: something serving to represent or indicate some fact, event, feeling, etc.

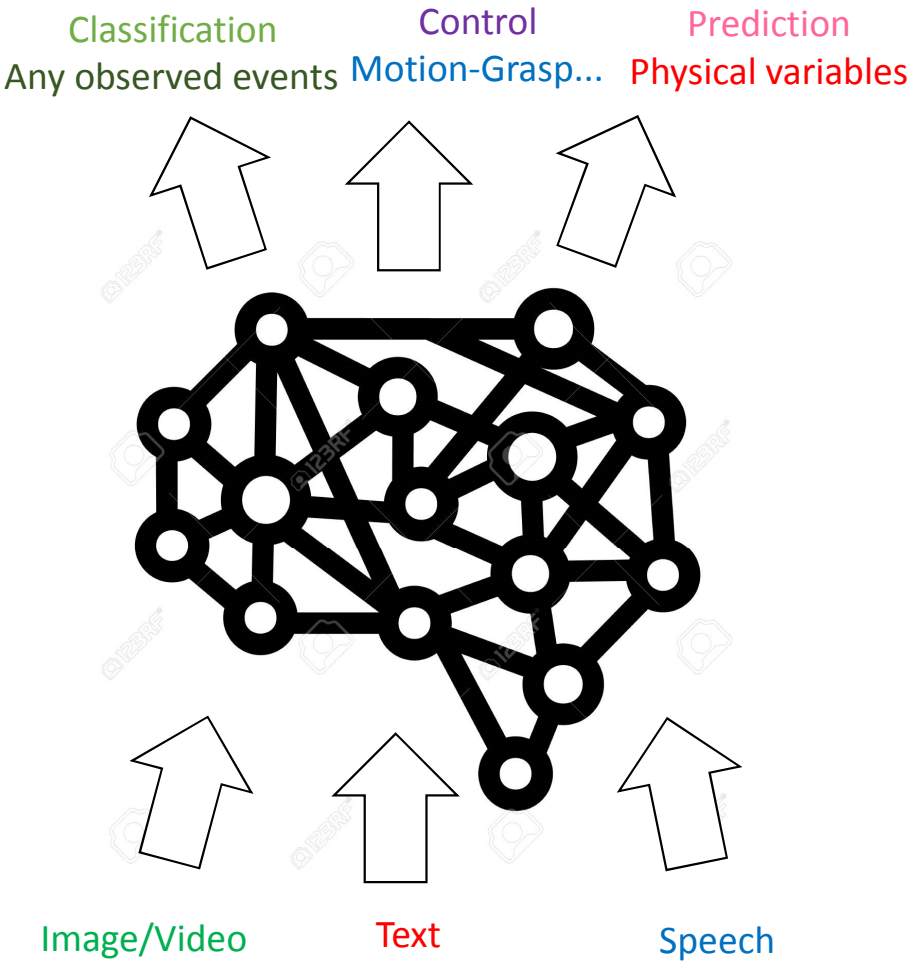
3.3.9 Artificial Brain Design

A neural network which receives multi-modal data and it is trained to do multi-tasks in an un-supervised method.

Such network works as a generalist AI agent which must learn without using labels and targets.

Some Steps

1. Receive all measuring signals: Visual, inertial, force,.....
2. Encode them as latent space by using appropriate spatial, temporal, and recurrent encoders
3. Using some attention layers and mechanisms to reveals some useful features which maximizes the gathered information from the environment
4. Learning to motion in the environment and to label objects .
5. Learning to do the required physical tasks.

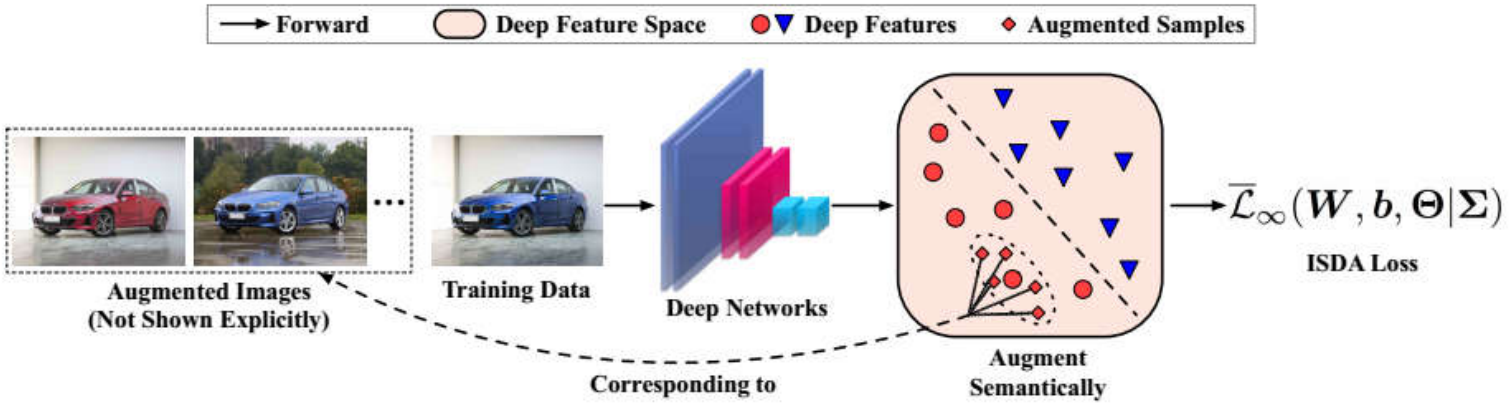


3.4 Related works in local Layer-wise learning

- To introduce a learning approach that is more plausible with the learning in the brain
- To have better learning and design in accuracy, compactness, speed,...
- To increase the generalization and robustness of DNNs

(1) Implicit Semantic Data Augmentation for Deep Networks

Yulin Wang et al. 2020, Department of Automation, Tsinghua University, Beijing, China



The proposed implicit semantic data augmentation (ISDA) has two important components, i.e., (1) online estimation of class-conditional covariance matrices and (2) optimization with a robust loss function.

The first component aims to find a distribution from which we can sample meaningful semantic transformation directions for data augmentation, while the second saves us from explicitly generating a large amount of extra training data, leading to remarkable efficiency compared to existing data augmentation techniques.

Comparison Tables

$Image\ net \rightarrow$

$Cifar10 + Cifar100 \downarrow$

Table 1: Single crop error rates (%) of different deep networks on the validation set of ImageNet. We report the results of our implementation with and without ISDA. The better results are **bold-faced**, while the numbers in brackets denote the performance improvement achieved by ISDA. We also report the theoretical computational overhead and the additional training time introduced by ISDA in the last two columns, which is obtained with 8 Tesla V100 GPUs.

Networks	Params	Top-1 / Top-5 Error Rates (%)		Additional Cost (Theoretical)	Additional Cost (Wall Time)
		Baselines	ISDA		
ResNet-50 [4]	25.6M	23.0 / 6.8	**21.9**$_{(1.1)}$ **/ 6.3**	0.25%	7.6%
ResNet-101 [4]	44.6M	21.7 / 6.1	**20.8**$_{(0.9)}$ **/ 5.7**	0.13%	7.4%
ResNet-152 [4]	60.3M	21.3 / 5.8	**20.3**$_{(1.0)}$ **/ 5.5**	0.09%	5.4%
DenseNet-BC-121 [5]	8.0M	23.7 / 6.8	**23.2**$_{(0.5)}$ **/ 6.6**	0.20%	5.6%
DenseNet-BC-265 [5]	33.3M	21.9 / 6.1	**21.2**$_{(0.7)}$ **/ 6.0**	0.24%	5.4%
ResNeXt-50, 32x4d [33]	25.0M	22.5 / 6.4	**21.3**$_{(1.2)}$ **/ 5.9**	0.24%	6.6%
ResNeXt-101, 32x8d [33]	88.8M	21.1 / 5.9	**20.1**$_{(1.0)}$ **/ 5.4**	0.06%	7.9%

Table 2: Evaluation of ISDA on CIFAR with different models. The average test error over the last 10 epochs is calculated in each experiment, and we report mean values and standard deviations in three independent experiments. The best results are **bold-faced**.

Method	Params	CIFAR-10	CIFAR-100
ResNet-32 [4]	0.5M	7.39 ± 0.10%	31.20 ± 0.41%
ResNet-32 + ISDA	0.5M	**7.09 ± 0.12%**	**30.27 ± 0.34%**
ResNet-110 [4]	1.7M	6.76 ± 0.34%	28.67 ± 0.44%
ResNet-110 + ISDA	1.7M	**6.33 ± 0.19%**	**27.57 ± 0.46%**
SE-ResNet-110 [34]	1.7M	6.14 ± 0.17%	27.30 ± 0.03%
SE-ResNet-110 + ISDA	1.7M	**5.96 ± 0.21%**	**26.63 ± 0.21%**
Wide-ResNet-16-8 [35]	11.0M	4.25 ± 0.18%	20.24 ± 0.27%
Wide-ResNet-16-8 + ISDA	11.0M	**4.04 ± 0.29%**	**19.91 ± 0.21%**
Wide-ResNet-28-10 [35]	36.5M	3.82 ± 0.15%	18.53 ± 0.07%
Wide-ResNet-28-10 + ISDA	36.5M	**3.58 ± 0.15%**	**17.98 ± 0.15%**
ResNeXt-29, 8x64d [33]	34.4M	3.86 ± 0.14%	18.16 ± 0.13%
ResNeXt-29, 8x64d + ISDA	34.4M	**3.67 ± 0.12%**	**17.43 ± 0.25%**
DenseNet-BC-100-12 [5]	0.8M	4.90 ± 0.08%	22.61 ± 0.10%
DenseNet-BC-100-12 + ISDA	0.8M	**4.54 ± 0.07%**	**22.10 ± 0.34%**
DenseNet-BC-190-40 [5]	25.6M	3.52%	17.74%
DenseNet-BC-190-40 + ISDA	25.6M	**3.24%**	**17.42%**

Algorithm 1 The ISDA Algorithm.

Input: $\mathcal{D}$, λ_0
Randomly initialize $\boldsymbol{W}$, $\boldsymbol{b}$ and $\boldsymbol{\Theta}$
for $t = 0$ **to** T **do**
  Sample a mini-batch $\{\boldsymbol{x}_i, y_i\}_{i=1}^{B}$ from $\mathcal{D}$
  Compute $\boldsymbol{a}_i = G(\boldsymbol{x}_i, \boldsymbol{\Theta})$
  Estimate the covariance matrices Σ_1, Σ_2, ..., Σ_C
  Compute $\overline{\mathcal{L}}_\infty$ according to Eq. (4)
  Update $\boldsymbol{W}$, $\boldsymbol{b}$, $\boldsymbol{\Theta}$ with SGD
end for
Output: $\boldsymbol{W}$, $\boldsymbol{b}$ and $\boldsymbol{\Theta}$

$$\mathcal{L}_\infty(W, b, \Theta|\Sigma) \leq \frac{1}{N}\sum_{i=1}^{N} -log\left(\frac{e^{\boldsymbol{w}_{y_i}^T \boldsymbol{a}_i + b_{y_i}}}{\sum_{j=1}^{C} e^{\boldsymbol{w}_j^T \boldsymbol{a}_i + b_j + \frac{\lambda}{2}(\boldsymbol{w}_j^T - \boldsymbol{w}_{y_i}^T)\Sigma_{y_i}(\boldsymbol{w}_j - \boldsymbol{w}_{y_i})}}\right) \triangleq \overline{\mathcal{L}}_\infty.$$

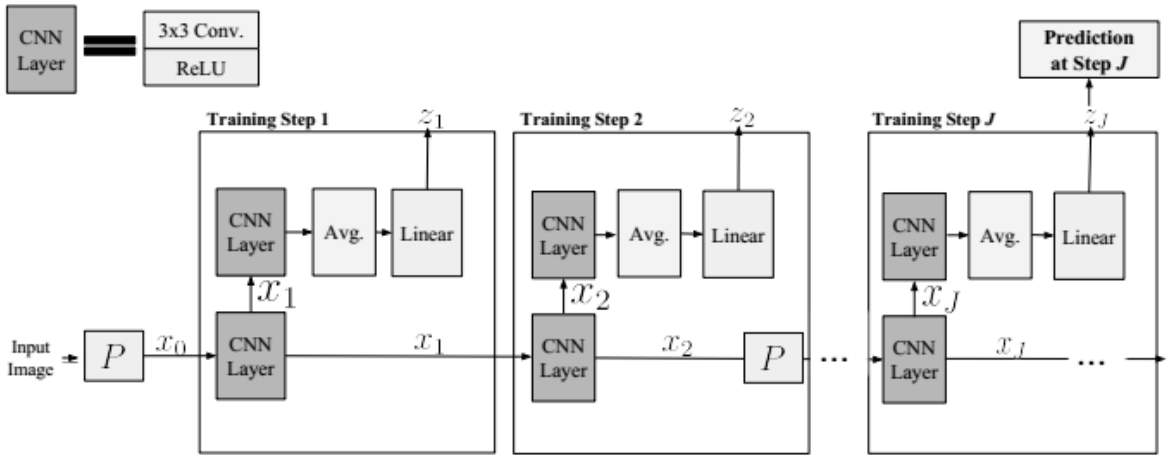
λ is a positive coefficient to control the strength of semantic data augmentation. The strength at initial epochs is chosen low but linearly it increases: $\lambda = (t/T)\times\lambda 0$

(2) Greedy Layerwise Learning Can Scale to ImageNet

Belilovsky et al. (University of Montral)-*Proceedings of the 36 th International Conference on Machine Learning*, Long Beach, California, PMLR 97, 2019.

We find that solving sequential 1-hidden-layer auxiliary problems lead to a CNN that exceeds AlexNet performance on ImageNet.

Extending this training methodology to construct individual layers by solving 2-and-3-hidden layer auxiliary problems, we obtain an 11-layer network that exceeds several members of the VGG model family on ImageNet, and can train a VGG-11 model to the same accuracy as end-to-end learning.



k = 2-hidden layer

Algorithm 1 Layer Wise CNN

Input: Training samples $\{x_0^n, y^n\}_{n \leq N}$
for $j \in 0..J-1$ **do**
  Compute $\{x_j^n\}_{n \leq N}$ (via Eq.(1))
  $(\theta_j^*, \gamma_j^*) = \arg\min_{\theta_j, \gamma_j} \hat{\mathcal{R}}(z_{j+1}; \theta_j, \gamma_j)$
end for

Comparison tables

Layer-wise Trained	Acc. (Ens.)
SimCNN ($k = 1$ train)	88.3 (88.4)
SimCNN ($k = 2$ train)	90.4 (90.7)
SimCNN($k = 3$ train)	91.7 (**92.8**)
BoostResnet (Huang et al., 2017)	82.1
ProvableNN (Malach et al., 2018)	73.4
(Mosca et al., 2017)	81.6
Reference e2e	
AlexNet	89
VGG [1]	92.5
WRN 28-10 (Zagoruyko et al. 2016)	**96.0**
Alternatives	[Ref.]
Scattering + Linear	82.3
FeedbackAlign (Bartunov et al., 2018)	62.6 [67.6]

Table 2. Results on CIFAR-10. Compared to the few existing methods using *only* layerwise training schemes we report much more competitive results to well known benchmark models that like ours do not use skip connnections.In brackets e2e trained version of the model is shown when available.

	Top-1 (Ens.)	Top-5 (Ens.)
SimCNN ($k = 1$ train)	58.1 (59.3)	79.7 (80.8)
SimCNN ($k = 2$ train)	65.7 (67.1)	86.3 (87.0)
SimCNN ($k = 3$ train)	69.7 (71.6)	88.7 (89.8)
VGG-11 ($k = 3$ train)	67.6 (70.1)	88.0 (89.2)
VGG-11 (e2e train)	67.9	88.0
Alternative	[Ref.]	[Ref.]
DTargetProp (Bartunov et al., 2018)	1.6 [28.6]	5.4 [51.0]
FeedbackAlign (Xiao et al., 2019)	6.6 [50.9]	16.7 [75.0]
Scat. + Linear (Oyallon et al., 2018)	17.4	N/A
Random CNN	12.9	N/A
FV + Linear (Sánchez et al., 2013)	54.3	74.3
Reference e2e CNN		
AlexNet	56.5	79.1
VGG-13	69.9	89.3
VGG-19	72.9	90.9
Resnet-152	78.3	94.1

Table 3. Single crop validation acc. on ImageNet. Our SimCNN models use $J = 8$. In parentheses see the ensemble prediction.

k = 1 :the auxiliary classifier consists of only the linear *A* and *L* operators (1-hidden layer NN)
K>1 :K hidden layers for auxiliary classifiers

(3) Hebbian Semi-Supervised Learning in a Sample Efficiency Setting?

Gabriele Lagani, 2021, *Computer Science Department, University of Pisa, Pisa, Italy*

Highlights

1. A semi supervised training strategy that combines Hebbian learning with gradient descent

   Hebbian for internal layers + SGD for the final fully connected layer

2. All internal layers (both convolutional and fully connected) are pre-trained using an unsupervised approach based on Hebbian learning
3. The last fully connected layer (the classification layer) is trained using Stochastic Gradient Descent (SGD)
4. The learning approach has been applied to CIFAR10, CIFAR100, tiny ImageNet
5. In regimes when the number of available labeled samples is low the proposed approach outperforms the other approaches in almost all the cases

Hebian

The classification layer is placed on top of the various internal layers ($L1; : : : ; L5$)

$$\mathbf{w}_{new} = \mathbf{w}_{old} + \Delta\mathbf{w}$$

$$\Delta\mathbf{w} = \eta\, y\, \mathbf{x}$$

"neurons that fire together wire together."

$$\Delta\mathbf{w} = \eta\, y\, \mathbf{x} - \lambda\, \mathbf{w}$$

Adding Stable Term

In particular, the term λ can be chosen in the form $\lambda = \eta y$

$$\Delta\mathbf{w} = \eta\, y\, \mathbf{x} - \eta\, y\, \mathbf{w} = \eta\, y\, (\mathbf{x} - \mathbf{w})$$

In a complex neural network, we need a strategy to prevent neurons from learning redundant information. The Hebbian PCA learning rule is obtained by minimizing the representation error loss function, defined as:

$$L(\mathbf{w_i}) = E[(\mathbf{x} - \sum_{j=1}^{i} y_j\, \mathbf{w_j})^2]$$

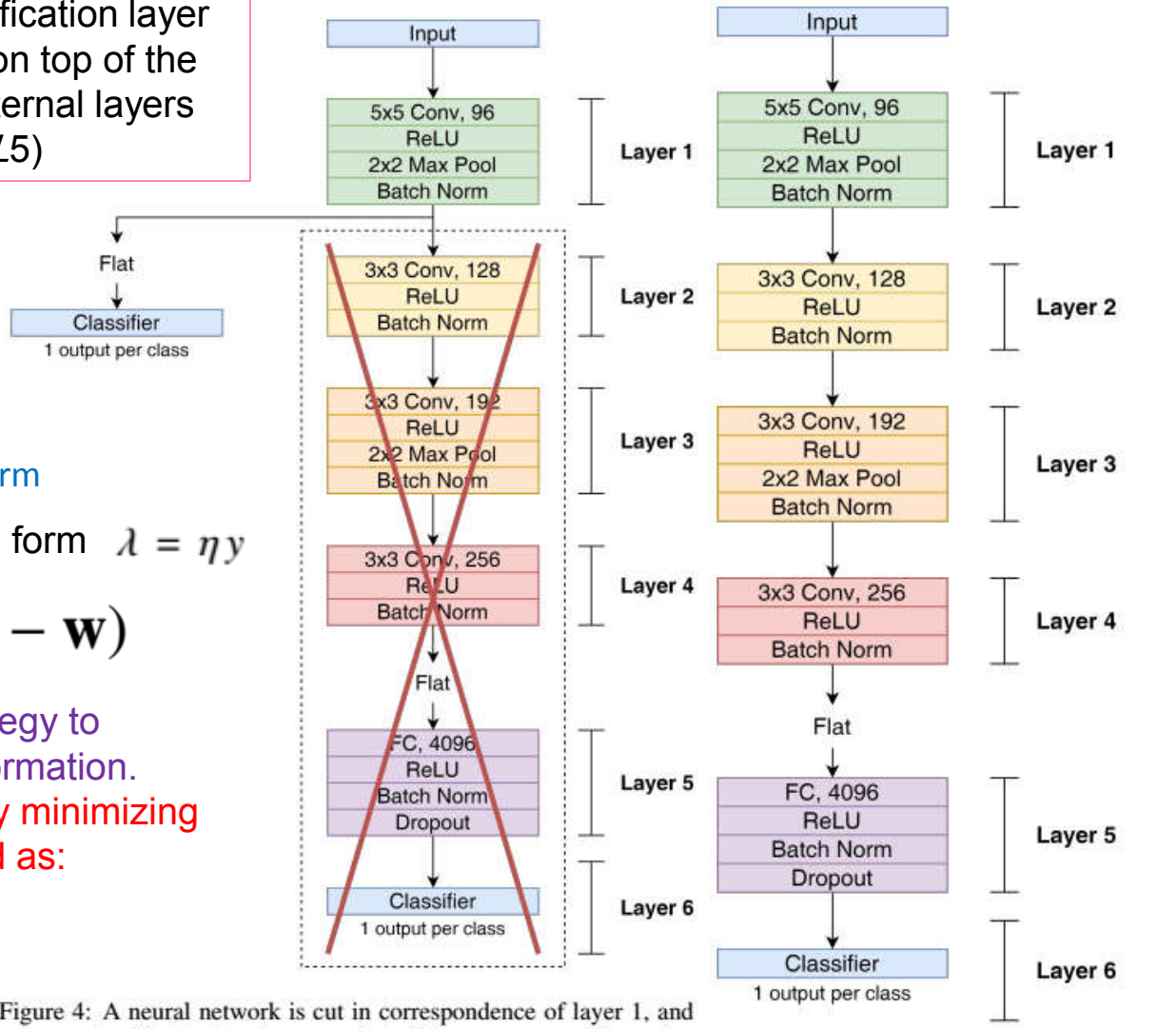


Figure 4: A neural network is cut in correspondence of layer 1, and a linear classifier is placed on top of the features extracted from that layer, in order to evaluate their quality in classification tasks.

1: The neural network used for the experiments.

Comparison Table(CIFAR10)

Table 1: CIFAR10 accuracy (top-1) and 95% confidence intervals, obtained with a linear classifier on top of various layers, for the various sample efficiency regimes. Results obtained with supervised backprop (BP), VAE-based semi-supervised approach(VAE), Hebbian PCA (HPCA), and HPCA plus Fine Tuning (HPCA+FT) are compared. It is possible to observe that, in regimes where the number of available samples is low (roughly between 1% and 5% of the total available samples), HPCA performs better than BP and VAE approaches in almost all the cases, leading to an improvement up to almost 5% (on layer 3, in the 1% regime) w.r.t. non-Hebbian approaches. HPCA+FT helps to further boost accuracy.

Regime: r%- where the percentage of labeled samples is r%

Regimes	Method	L1	L2	L3	L4	L5
1%	BP	33.27 ±0.44	34.56 ±0.34	36.80 ±0.52	35.47 ±0.58	35.18 ±0.57
	VAE	33.54 ±0.27	34.41 ±0.84	29.92 ±1.25	24.91 ±0.66	22.54 ±0.60
	HPCA	36.78 ±0.46	37.26 ±0.14	41.31 ±0.57	39.33 ±0.72	38.46 ±0.44
	HPCA+FT	**37.01** ±0.42	**37.65** ±0.19	**41.88** ±0.53	**40.06** ±0.65	**39.75** ±0.50
2%	BP	37.33 ±0.25	39.01 ±0.19	42.34 ±0.51	41.50 ±0.32	41.10 ±0.39
	VAE	37.65 ±0.35	39.13 ±0.40	36.52 ±0.47	29.39 ±0.32	26.78 ±0.72
	HPCA	41.13 ±0.30	**41.63** ±0.18	45.76 ±0.41	44.70 ±0.45	43.15 ±0.45
	HPCA+FT	**41.60** ±0.28	42.12 ±0.24	**46.56** ±0.38	**45.61** ±0.19	**45.51** ±0.43
3%	BP	40.49 ±0.26	41.90 ±0.40	45.13 ±0.53	45.26 ±0.22	44.52 ±0.24
	VAE	41.22 ±0.27	43.16 ±0.44	42.60 ±0.87	31.91 ±0.44	29.00 ±0.33
	HPCA	44.16 ±0.42	44.84 ±0.08	48.92 ±0.17	47.70 ±0.57	45.60 ±0.27
	HPCA+FT	**44.74** ±0.08	**45.61** ±0.28	**49.75** ±0.41	**48.94** ±0.45	**48.80** ±0.27
4%	BP	43.38 ±0.22	45.43 ±0.18	49.51 ±0.49	48.96 ±0.48	48.80 ±0.24
	VAE	44.39 ±0.30	45.88 ±0.39	46.01 ±0.40	34.26 ±0.21	31.15 ±0.35
	HPCA	46.37 ±0.16	47.16 ±0.28	50.70 ±0.26	49.45 ±0.15	47.75 ±0.54
	HPCA+FT	**47.10** ±0.25	**48.26** ±0.09	**52.00** ±0.16	**51.05** ±0.29	**51.28** ±0.28
5%	BP	45.11 ±0.21	47.57 ±0.29	50.61 ±0.32	50.54 ±0.23	50.42 ±0.14
	VAE	46.31 ±0.39	48.21 ±0.21	48.98 ±0.34	36.32 ±0.35	32.75 ±0.32
	HPCA	47.51 ±0.65	48.69 ±0.37	51.69 ±0.56	50.44 ±0.43	48.51 ±0.32
	HPCA+FT	**48.49** ±0.44	**50.14** ±0.46	**53.33** ±0.52	**52.49** ±0.16	**52.20** ±0.37
10%	BP	51.60 ±0.40	54.60 ±0.31	57.97 ±0.28	**57.63** ±0.23	57.30 ±0.22
	VAE	53.83 ±0.26	**56.33** ±0.22	57.85 ±0.22	52.26 ±1.08	45.67 ±1.15
	HPCA	52.57 ±0.29	53.29 ±0.25	56.09 ±0.38	54.24 ±0.28	52.68 ±0.36
	HPCA+FT	**54.36** ±0.32	56.08 ±0.28	**58.46** ±0.15	56.54 ±0.23	**57.35** ±0.18
25%	BP	60.43 ±0.26	64.96 ±0.18	66.63 ±0.17	68.04 ±0.05	68.04 ±0.20
	VAE	**62.51** ±0.24	**67.26** ±0.32	**68.48** ±0.21	**68.79** ±0.29	**68.70** ±0.15
	HPCA	58.30 ±0.28	59.20 ±0.24	59.98 ±0.20	57.54 ±0.20	56.46 ±0.18
	HPCA+FT	61.45 ±0.26	65.25 ±0.16	64.71 ±0.17	62.43 ±0.13	64.77 ±0.22
100%	BP	61.59 ±0.08	67.67 ±0.11	73.87 ±0.15	83.88 ±0.04	84.71 ±0.02
	VAE	**67.53** ±0.22	**75.83** ±0.31	**80.78** ±0.28	**84.27** ±0.35	**85.23** ±0.26
	HPCA	64.69 ±0.29	65.92 ±0.14	64.43 ±0.21	61.24 ±0.22	61.16 ±0.33
	HPCA+FT	66.76 ±0.13	75.16 ±0.20	79.90 ±0.18	83.55 ±0.33	84.38 ±0.22

(4) Greedy InfoMax for Self-Supervised Representation Learning(GIM)

Sindy Lowe et al. University of Amsterdam

Highlights

1. we propose a novel deep learning method for local self-supervised representation learning that does not require labels nor end-to-end backpropagation but exploits the natural order in data instead.
2. Inspired by the observation that biological neural networks appear to learn without backpropagating a global error signal, we split a deep neural network into a stack of gradient-isolated modules.
3. Each module is trained to maximize the mutual information between its consecutive outputs using the InfoNCE bound from Oord et al.(2018).

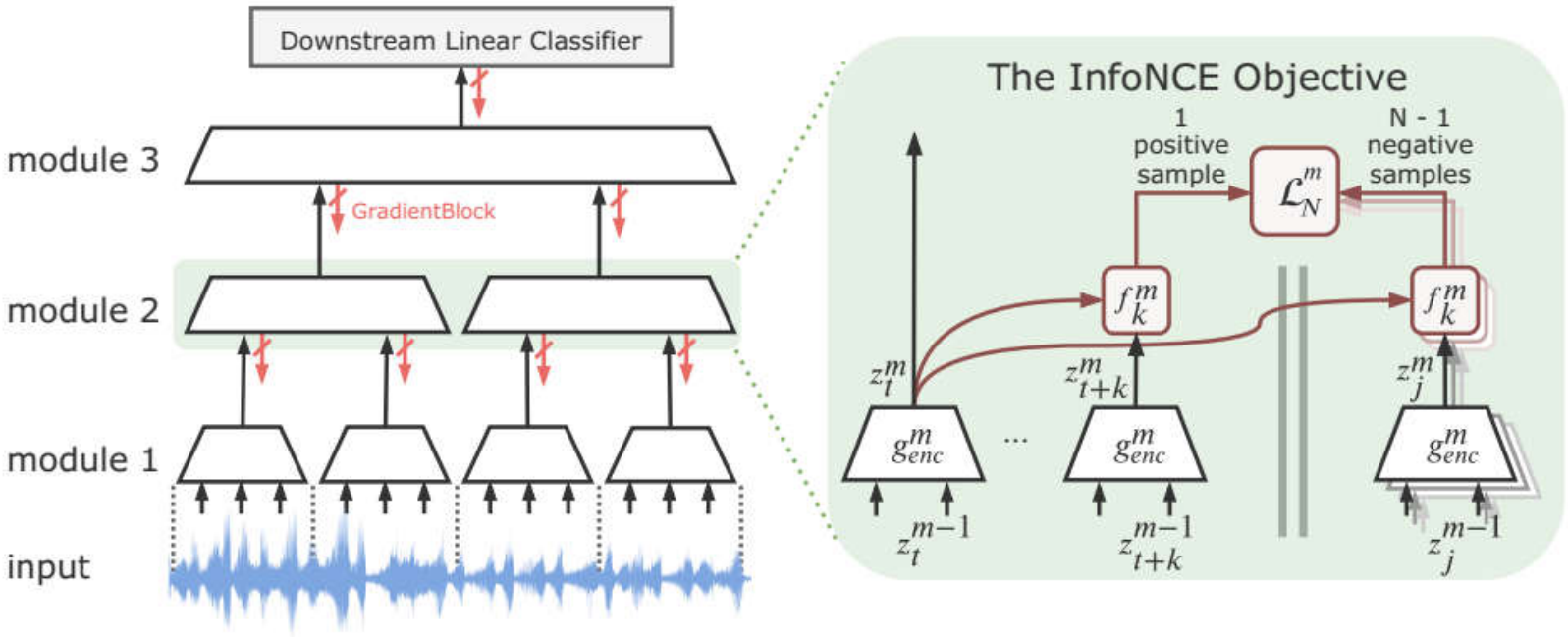


Figure 1. The Greedy InfoMax Learning Approach. **(Left)** For the self-supervised learning of representations, we stack a number of modules through which the input is forward-propagated in the usual way, but gradients do not propagate backwards. Instead, every module is trained greedily using a local loss. **(Right)** Every encoding module maps its inputs z_t^{m-1} at time-step t to $g_{enc}^m(\text{GradientBlock}(z_t^{m-1})) = z_t^m$, which is used as the input for the following module. The InfoNCE objective is used for its greedy optimization. This loss is calculated by contrasting the predictions of a module for its future representations z_{t+k}^m against negative samples z_j^m, which enforces each module to maximally preserve the information of its inputs. We employ an additional autoregressive module g_{ar}, which is not depicted here.

Architecture & Comparison

Table 3. General outline of our architecture

Layer	Output Size (Sequence Length × Channels)	Parameters Kernel	Stride	Padding
Input	20480×1			
Conv1	$4095^2 \times 512$	10	5	2
Conv2	$1023^2 \times 512$	8	4	2
Conv3	$512^2 \times 512$	4	2	2
Conv4	$257^2 \times 512$	4	2	2
Conv5	128×512	1	2	1
GRU	128×256	-	-	-

[2]For applying the InfoNCE objective on these layers, we randomly sample a time-window of size 128 to decrease the dimensionality.

Table 1. Results for classifying speaker identity and phone labels in the LibriSpeech dataset. All models use the same audio input sizes and the same architecture. GIM creates representations that are useful for audio classification tasks despite its greedy training and lack of a global objective.

Method	Phone Classification Accuracy	Speaker Classification Accuracy
MFCC features	39.7%	17.6%
Randomly initialized	27.6%	1.9%
Supervised	74.6%	98.5%
Greedy Supervised	71.1%	84.5%
CPC (Oord et al., 2018)[a]	64.6%	97.4%
Greedy InfoMax (GIM)	60.0%	97.5%

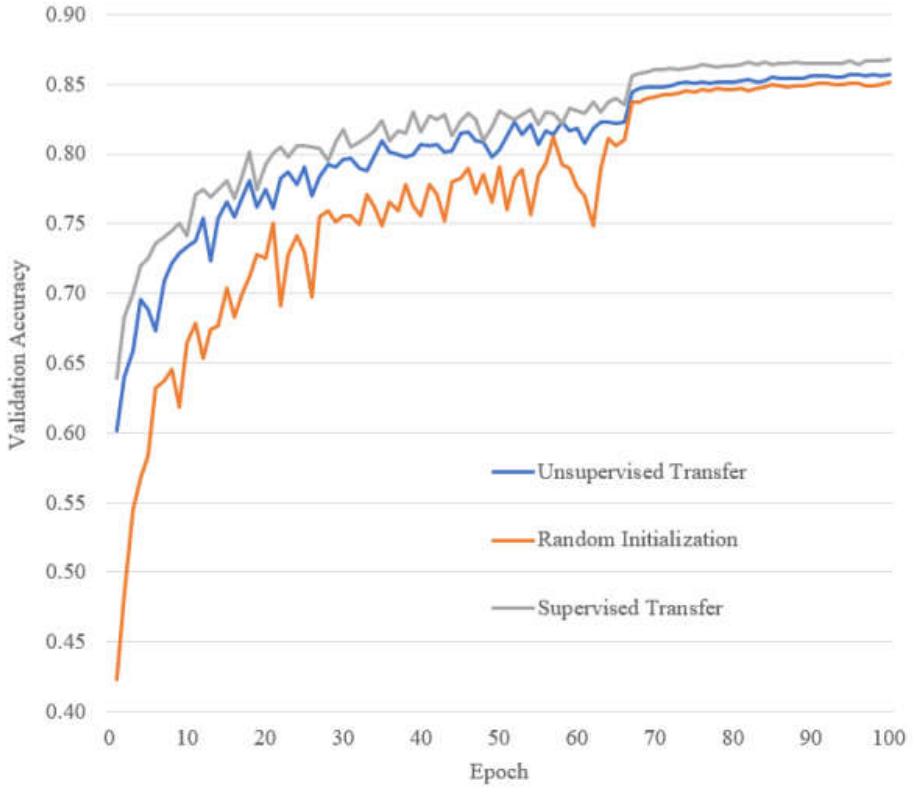
[a]In our reimplementation, we achieved 62.2% for the phone and 98.8% for the speaker classification task.

(5)Layer-Wise Contrastive Unsupervised Representation Learning

Stephen Zhao, 2019

- In this work, we focus on the set of unsupervised learning approaches that Arora et al. (2019) call “contrastive unsupervised representation learning”.
- We use a layer-wise adaptation, starting within the context of images.
- We train feature representations of semantically similar images (i.e. nearby patches within the same image) to be closer than that of unrelated images (e.g. random patches), to learn convolutional neural network filters from unlabeled data.

Figure 3: Performance on CIFAR-10. The learning rate is 0.001 for the first two-thirds of the training, and is 0.0001 afterwards. Results are averaged over 3 independent runs for each line (keeping transferred filters constant across runs, but allowing for fine-tuning).



(6) LoCo: Local Contrastive Representation Learning

Yuwen Xiong et al.

34th Conference on Neural Information Processing Systems (NeurIPS 2020), Vancouver, Canada.

- In this work, we discover that by overlapping local blocks stacking on top of each other, we effectively increase the decoder depth and allow upper blocks to implicitly send feedbacks to lower blocks.
- This simple design closes the performance gap between local learning and end-to-end contrastive learning algorithms for the first time.
- Aside from standard ImageNet experiments, we also show results on complex downstream tasks such as object detection and instance segmentation directly using readout features

LoCo Architecture

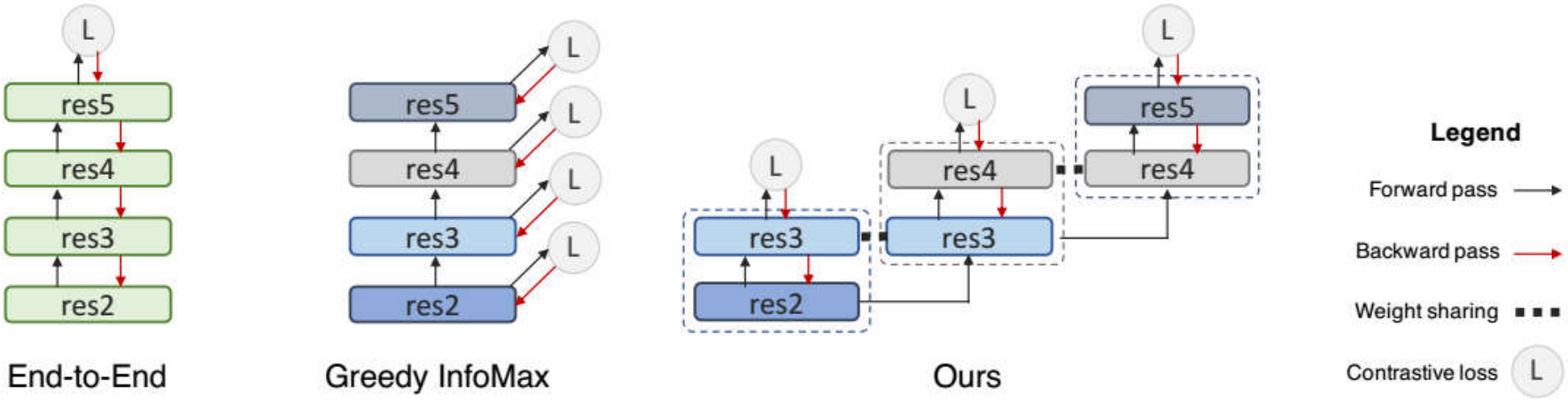


Figure 1: Comparison between End-to-End, Greedy InfoMax (GIM) and LoCo

In this paper, we used SimCLR as our main baseline, since it has superior performance on ImageNet, and we apply the changes proposed in GIM(Greedy Infomax) on top of SimCLR as our local learning baseline.
In our experiments, we find that simply applying GIM on SimCLR results in a significant loss in performance and in the next section we will explain our techniques to bridge the performance gap.

Comparison tables

Greedy InfoMax (GIM)
SimCLR: T. Chen... A simple framework for contrastive learning of visual representations, 2020.

Method	Architecture	Acc.	Local
Local Agg. [62]	ResNet-50	60.2	
MoCo [22]	ResNet-50	60.6	
PIRL [45]	ResNet-50	63.6	
CPC v2 [56]	ResNet-50	63.8	
SimCLR* [11]	ResNet-50	69.3	
SimCLR [11]	ResNet-50	**69.8**	
GIM [39]	ResNet-50	64.7	✓
LoCo (Ours)	ResNet-50	69.5	✓
SimCLR [11]	ShuffleNet v2-50	69.1	
GIM [39]	ShuffleNet v2-50	63.5	✓
LoCo (Ours)	ShuffleNet v2-50	**69.3**	✓

Table 1: ImageNet accuracies of linear classifiers trained on representations learned with different unsupervised methods, SimCLR* is the result from the SimCLR paper with 1000 training epochs.

Method	Arch	COCO		Cityscapes	
		AP^{bb}	AP	AP^{bb}	AP
Supervised	R-50	33.9	31.3	33.2	27.1
Backbone weights with 100 Epochs					
SimCLR	R-50	32.2	29.9	33.2	28.6
GIM	R-50	27.7 (-4.5)	25.7 (-4.2)	30.0 (-3.2)	24.6 (-4.0)
Ours	R-50	32.6 (+0.4)	30.1 (+0.2)	33.2 (+0.0)	28.4 (-0.2)
SimCLR	Sh-50	32.5	30.1	33.3	28.0
GIM	Sh-50	27.3 (-5.2)	25.4 (-4.7)	29.1 (-4.2)	23.9 (-4.1)
Ours	Sh-50	31.8 (-0.7)	29.4 (-0.7)	33.1 (-0.2)	27.7 (-0.3)
Backbone weights with 800 Epochs					
SimCLR	R-50	34.8	32.2	34.8	30.1
GIM	R-50	29.3 (-5.5)	27.0 (-5.2)	30.7 (-4.1)	26.0 (-4.1)
Ours	R-50	34.5 (-0.3)	32.0 (-0.2)	34.2 (-0.6)	29.5 (-0.6)
SimCLR	Sh-50	33.4	30.9	33.9	28.7
GIM	Sh-50	28.9 (-4.5)	26.9 (-4.0)	29.6 (-4.3)	23.9 (-4.8)
Ours	Sh-50	33.6 (+0.2)	31.2 (+0.3)	33.0 (-0.9)	28.1 (-0.6)

Table 2: Mask R-CNN results on COCO and Cityscapes. Backbone networks are frozen. "R-50" denotes ResNet-50 and "Sh-50" denotes ShuffleNet v2-50.

Average Precision (AP)

Average Precision bounding box (APbb)

(7) Progressive Stage-wise Learning for Unsupervised Feature Representation Enhancement

Zefan Li et al., Shanghai Jiao Tong University

In this work, we explore new dimensions of unsupervised learning by proposing the **P**rogressive **S**tage-wise **L**earning (**PSL**) framework.
For a given unsupervised task, we design multilevel tasks and define different learning stages for the deep *network.* *(Each new task has overlap with the former one)*
Early learning stages are forced to focus on low-level tasks while late stages are guided to extract deeper information through harder tasks.
We discover that by progressive stage-wise learning, unsupervised feature representation can be effectively enhanced.
Our extensive experiments show that PSL consistently improves results for the leading unsupervised learning methods.

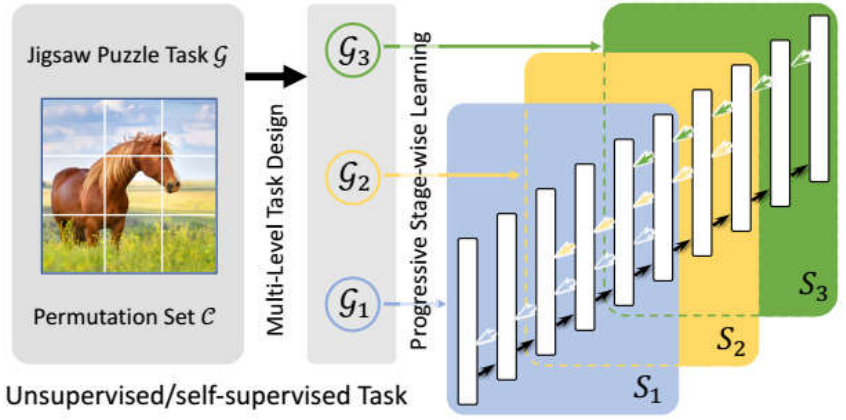


Figure 1. We present the framework of the proposed Progressive Stage-wise Learning (**PSL**) algorithm, aiming for improving unsupervised/self-supervised task. We take the jigsaw puzzle task $\mathcal{G}$ for example. We first do multi-level task partition $\mathcal{G} \rightarrow \{\mathcal{G}_1, \mathcal{G}_2, \mathcal{G}_3\}$ with an increased task complexity and perform progressive stage-wise training for different learning stages of the network. The black arrow denotes forward pass while colored arrow represents the backward pass of each learning stage (i.e., S_1, S_2, and S_3).

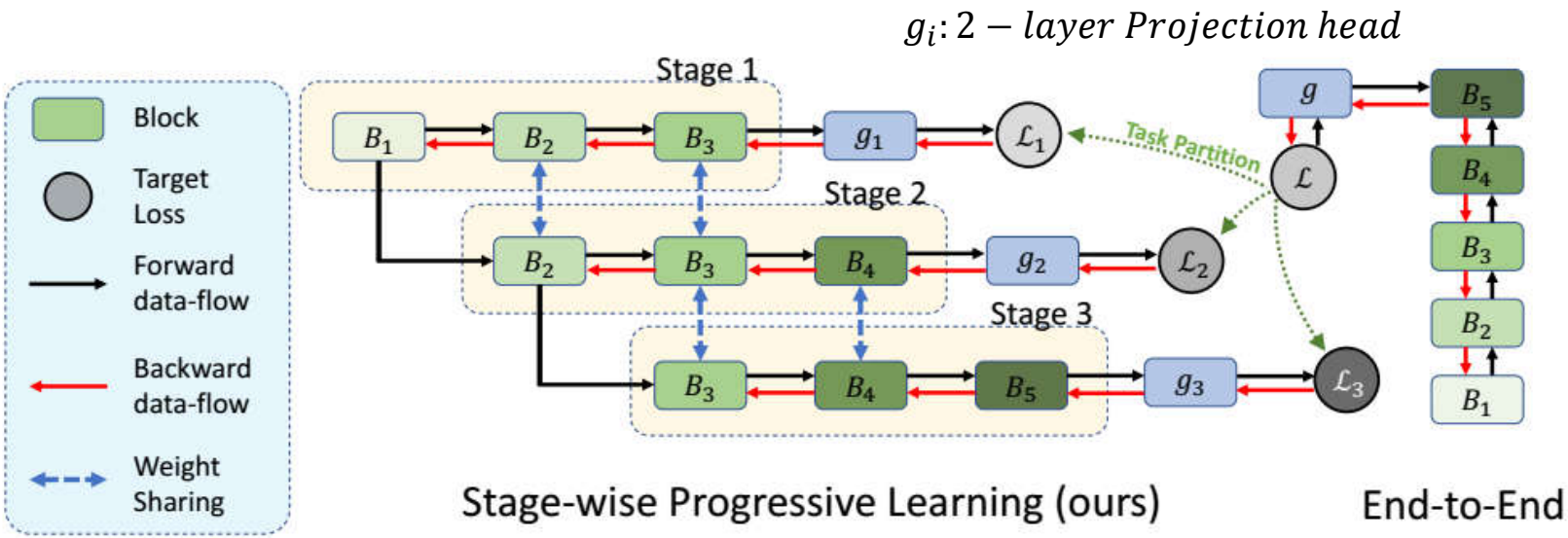


Figure 2. We present the detail of the proposed Stage-wise Progressive Learning framework. In the right is the end-to-end learning scheme while we present PSL in the middle. g and $\{g_i\}_{i=1}^{3}$ are projection heads, mapping the intermediate representation to the target feature space. After the training is completed, we throw away the projection heads and use the backbone network for downstream tasks.

Comparison Tables

Task	1% labels	10% labels
Supervised	48.4	80.4
Jigsaw [38]	45.4	79.6
Jigsaw+PSL	**48.7**	**83.5**
Rotation [21]	52.1	82.5
Rotation+PSL	**54.8**	**83.7**

Table 7. **Semi-supervised learning on ImageNet.** We use ResNet-50 as our backbone networks and report single-crop top-5 accuracy on the ImageNet validation set. All models are self-supervised trained on ImageNet and finetuned on 1% and 10% of the ImageNet training data, following [46, 37]. The supervised results are presented for reference.

Method	Arch	# Param(M)	Top 1
Colorization [49]	R50	24	39.6
BigBiGAN [15]	R50	24	56.6
LA [51]	R50	24	58.8
NPID++ [37]	R50	24	59.0
MoCo [26]	R50	24	60.6
PIRL [37]	R50	24	63.6
CPC v2 [28]	R50	24	63.8
PCL [34]	R50	24	65.9
SwAV [9]	R50	24	75.3
Jigsaw [38]	R50	24	45.7
Jigsaw +PSL	R50	24	**50.9**
Rotation [21]	Rv50w4×	86	47.3
Rotation*	Rv50	24	48.6
Rotation+PSL	Rv50	24	**53.3**
SimCLR [10]	R50	24	61.9
SimCLR+PSL	R50	24	**64.3**
MoCov2 [11]	R50	24	67.5
MoCov2+PSL	R50	24	**68.1**

Table 4. ImageNet accuracy of linear classifiers trained on self-supervised learned representations. All are reported as unsupervised pre-training on ImageNet, followed by supervised linear classification and evaluated on the ImageNet validation set. Note that Rotation [21] uses $\mathcal{R}_2$ as the transformation set while Rotation* uses $\mathcal{R}_3$ as the transformation set. SimCLR results are obtained by 200 training epochs with batchsize 256.

Thank you