Minimal Learning Machine for datasets with missing values

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Today

Summary

- Problem and notation
- The Minimal Learning Machine
    - Formulation
    - ESD for missing data
- Experiments
- Conclusions

Goals and contributions

- Introduce the Minimal Learning Machine (MLM) [a]
- Propose a MLM for missing valued datasets using ESD

[a] A. H. Souza Junior, F. Corona, Y. Miche, A. Lendasse, G. Barreto, and O. Simula, "Minimal learning machine: A new distance-based method for supervised learning", in IWANN'13, LNCS 7902, pp. 408-416, 2013.

The regression problem and notation

We are given

- Set of input points $X = \{\mathbf{x}_i\}_{i=1}^{N}, \quad \mathbf{x}_i \in \mathbb{R}^D$
- Set of output points $Y = \{\mathbf{y}_i\}_{i=1}^{N}, \quad \mathbf{y}_i \in \mathbb{R}^S$

We assume

- A continuous mapping between the input and the output space ($f : \mathcal{X} \to \mathcal{Y}$)

We want to estimate such a mapping using

$$\mathbf{Y} = f(\mathbf{X}) + \mathbf{R},$$

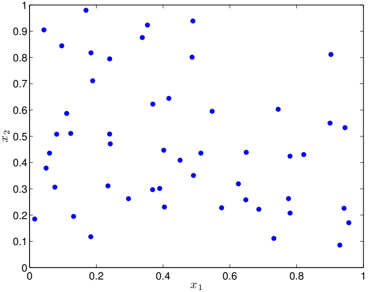
where rows of $\mathbf{X}$ and $\mathbf{Y}$ correspond to observations in the input and output space, and the matrix $\mathbf{R}$ contains the residual vectors.

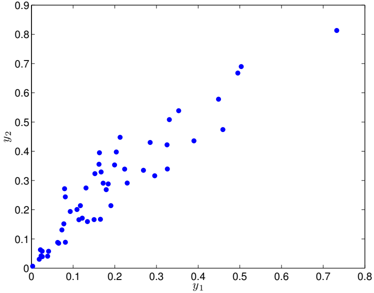
The Minimal Learning Machine

The Minimal Learning Machine algorithm can be decomposed into two main steps:

- Distance regression
- Output estimation

The Minimal Learning Machine





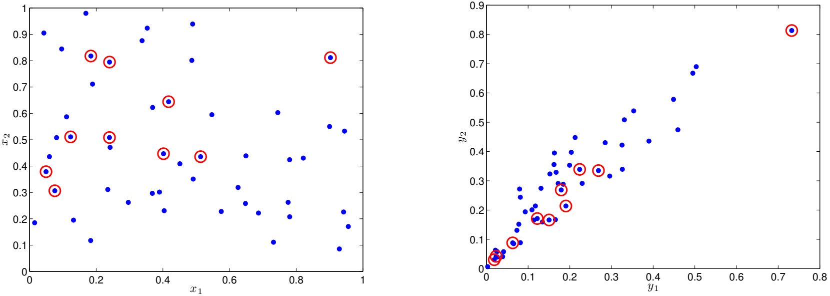
$\mathcal{X}$-space

- $X = \{\mathbf{x}_i\}_{i=1}^N$

$\mathcal{Y}$-space

- $Y = \{\mathbf{y}_i\}_{i=1}^N$

The Minimal Learning Machine



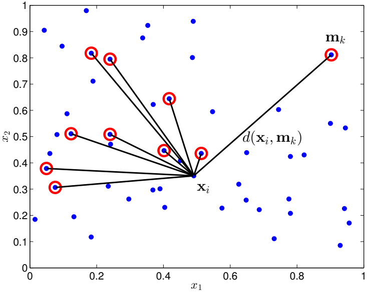
$\mathcal{X}$-space

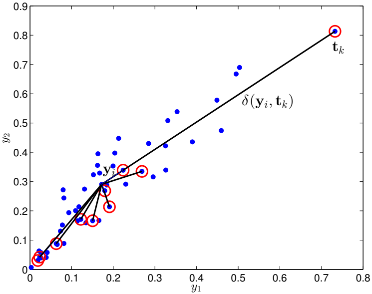
- $X = \{\mathbf{x}_i\}_{i=1}^{N}$
- $R = \{\mathbf{m}_k\}_{k=1}^{K}$

$\mathcal{Y}$-space

- $Y = \{\mathbf{y}_i\}_{i=1}^{N}$
- $T = \{\mathbf{t}_k\}_{k=1}^{K}$

The Minimal Learning Machine





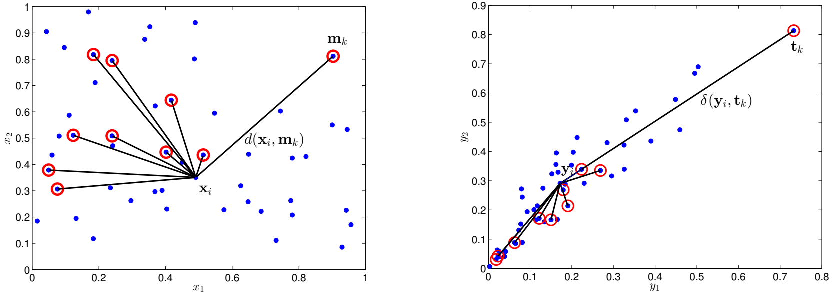
$\mathcal{X}$-space

- $X = \{\mathbf{x}_i\}_{i=1}^{N}$
- $R = \{\mathbf{m}_k\}_{k=1}^{K}$
- $\mathbf{D}_x(i,k) = [d(\mathbf{x}_i, \mathbf{m}_k)]$

$\mathcal{Y}$-space

- $Y = \{\mathbf{y}_i\}_{i=1}^{N}$
- $T = \{\mathbf{t}_k\}_{k=1}^{K}$
- $\mathbf{\Delta}_y(i,k) = [\delta(\mathbf{y}_i, \mathbf{t}_k)]$

The Minimal Learning Machine: Distance regression



We are interested in finding a mapping $g : \mathbb{R}^K \rightarrow \mathbb{R}^K$ such that

$$\mathbf{\Delta}_y = g(\mathbf{D}_x) + \mathbf{E}$$

The Minimal Learning Machine: Distance regression

Let's assume that the mapping g is linear, then

$$\mathbf{\Delta}_y = \mathbf{D}_x \mathbf{B} + \mathbf{E},$$

and the solution is given by $\hat{\mathbf{B}} = (\mathbf{D}_x^T \mathbf{D}_x)^{-1} \mathbf{D}_x^T \mathbf{\Delta}_y$.

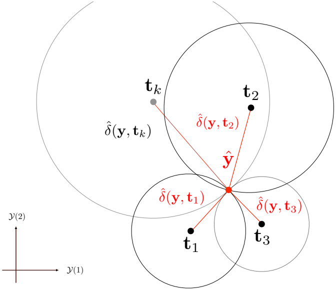
For a test point $\mathbf{x}$:
Collect the distances from the K reference points in the vector $\mathbf{d}(\mathbf{x}, R) = [d(\mathbf{x}, \mathbf{m}_1), \ldots, d(\mathbf{x}, \mathbf{m}_K)]$, then estimate distances in $\mathcal{Y}$

$$\hat{\boldsymbol{\delta}}(\mathbf{y}, T) = \mathbf{d}(\mathbf{x}, R)\hat{\mathbf{B}}.$$

The Minimal Learning Machine: Output estimation

For finding an estimate to the output $\mathbf{y}$, we need to solve

$$(\mathbf{y}-\mathbf{t}_k)^T(\mathbf{y}-\mathbf{t}_k)=\hat{\delta}^2(\mathbf{y},\mathbf{t}_k), \quad \forall k=1,\ldots,K$$



It can be formulated as an optimization problem

$$\hat{\mathbf{y}}=\underset{\mathbf{y}}{\operatorname{argmin}}\sum_{k=1}^{K}\left((\mathbf{y}-\mathbf{t}_k)^T(\mathbf{y}-\mathbf{t}_k)-\hat{\delta}^2(\mathbf{y},\mathbf{t}_k)\right)^2$$

The Expected Squared Distance (ESD)

- Estimate the squared distance of two vectors in the presence of missing data
- $\alpha, \beta \in \mathbb{R}^D$ drawn from a same multivariate probability distribution, but possibly with deleted entries

$$E[\|\alpha - \beta\|_2^2] = \sum_{i=1}^{D} E[(\alpha_i - \beta_i)^2]$$

The Expected Squared Distance (ESD)

$$E[\|\alpha - \beta\|_2^2] = \sum_{i \notin M_\alpha \cup M_\beta} (\alpha_i - \beta_i)^2 + \sum_{i \in M_\alpha \setminus M_\beta} E[(\alpha_i - \beta_i)^2] + \sum_{i \in M_\beta \setminus M_\alpha} E[(\alpha_i - \beta_i)^2] + \sum_{i \in M_\alpha \cap M_\beta} E[(\alpha_i - \beta_i)^2]$$

For entries $i \in M_\alpha \setminus M_\beta$, we have:

$$\begin{aligned} E[(\alpha_i - \beta_i)^2] &= E[\alpha_i^2 + \beta_i^2 - 2\alpha_i\beta_i] = E[\alpha_i^2] + \beta_i^2 - 2E[\alpha_i]\beta_i \\ &= E[\alpha_i^2] - E[\alpha_i]^2 + E[\alpha_i]^2 + \beta_i^2 - 2E[\alpha_i]\beta_i \\ &= (E[\alpha_i] - \beta_i)^2 + \mathrm{Var}[\alpha_i] \end{aligned}$$

Simulation Methodology

- MLM using different approaches for missing data
  - Drop entries
  - Input sample mean
  - EM
  - ESD

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- MLM using different approaches for missing data
  - Drop entries
  - Input sample mean
  - EM
  - ESD
- Six real-world datasets from UCI
- Varying number of missing data

Datasets

Table: Datasets characteristics

Dataset	attributes	instances
Concrete compression	8	1030
Boston Housing	13	506
Servo	4	167
Stocks	9	950
Breast cancer	30	569
Wine	13	178

Results

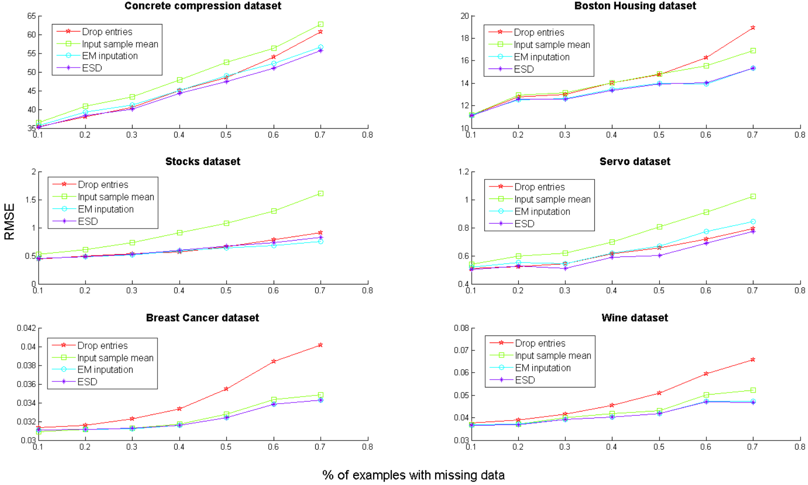

Figure: RMSE for all datasets

Conclusions

- We have introduced a variant of MLM capable of handling missing data

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- We have introduced a variant of MLM capable of handling missing data
- The proposed approach achieved the best results when compared to other strategies for missing data

THANK YOU!!!