Aalto University

Compressive Extreme Learning Machines

Improved Models Through Exploiting Time-Accuracy Trade-offs

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Outline

- Motivation
- Extreme Learning Machines
- Compressive Extreme Learning Machine
- Experiments
- Conclusions

Outline

Motivation

Extreme Learning Machines

Compressive Extreme Learning Machine

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Trade-offs in Training Neural Networks

- Ideally:
  - training results in *best possible test accuracy*
  - training is *fast*
  - the model is *efficient to evaluate at test time*
- However, in practice, in training of neural networks there exists a trade-off between:
  - testing accuracy
  - training time
  - testing time
- Furthermore, the optimal trade-off depends on the user's requirements

Contributions

- The paper explores time-accuracy trade-offs in various Extreme Learning Machines (ELMs)
- **Compressive Extreme Learning Machine** is introduced:
  - allows for a flexible time-accuracy trade-off by training the model in a reduced space
  - experiments indicate that this trade-off is efficient in the sense that it may yield better models in less time

Outline

Standard ELM

Given a training set $(\mathbf{x}_i, y_i), \mathbf{x}_i \in \mathbb{R}^d, y_i \in \mathbb{R}$, an activation function $f : \mathbb{R} \mapsto \mathbb{R}$ and M the number of hidden nodes:

1: - Randomly assign input weights $\mathbf{w}_i$ and biases b_i, $i \in [1, M]$;
2: - Calculate the hidden layer output matrix $\mathbf{H}$;
3: - Calculate output weights matrix $\beta = \mathbf{H}^\dagger \mathbf{Y}$.

where

$$\mathbf{H} = \begin{pmatrix} f(\mathbf{w}_1 \cdot \mathbf{x}_1 + b_1) & \cdots & f(\mathbf{w}_M \cdot \mathbf{x}_1 + b_M) \\ \vdots & \ddots & \vdots \\ f(\mathbf{w}_1 \cdot \mathbf{x}_N + b_1) & \cdots & f(\mathbf{w}_M \cdot \mathbf{x}_N + b_M) \end{pmatrix}$$

ELM Theory vs Practice

- In theory, ELM is universal approximator
- In practice, limited number of samples; risk of overfitting
- Therefore:
  - the functional approximation should use as limited number of neurons as possible
  - the hidden layer should extract and retain as much useful information as possible from the input samples

ELM Theory vs Practice

Weight considerations:

- weight range determines typical activation of the transfer function (remember $\langle \mathbf{w_i}, \mathbf{x} \rangle = |\mathbf{w_i}||\mathbf{x}| \cos\theta,$)
- therefore, normalize or tune the length of the weights vectors somehow

Linear vs non-linear:

- since sigmoid neurons operate in nonlinear regime, add *d* linear neurons for the ELM to work better on (almost) linear problems

Avoiding overfitting:

- use efficient L2 regularization

Ternary Weight Scheme

$$
\begin{array}{c|cccc|}
 & +\mathbf{1} & 0 & 0 & 0 \\
 & -\mathbf{1} & 0 & 0 & 0 \\
1\ \textit{var} & 0 & +\mathbf{1} & 0 & 0 \\
 & 0 & -\mathbf{1} & 0 & 0 \\
\hline
 & +\mathbf{1} & +\mathbf{1} & 0 & 0 \\
 & +\mathbf{1} & -\mathbf{1} & 0 & 0 \\
 & -\mathbf{1} & +\mathbf{1} & 0 & 0 \\
2\ \textit{vars} & -\mathbf{1} & -\mathbf{1} & 0 & 0 \\
 & & & & \\
 & 0 & 0 & -\mathbf{1} & -\mathbf{1} \\
\hline
3\ \textit{vars} & & & & \\
\end{array}
$$

until enough neurons [vanHeeswijk2014]:

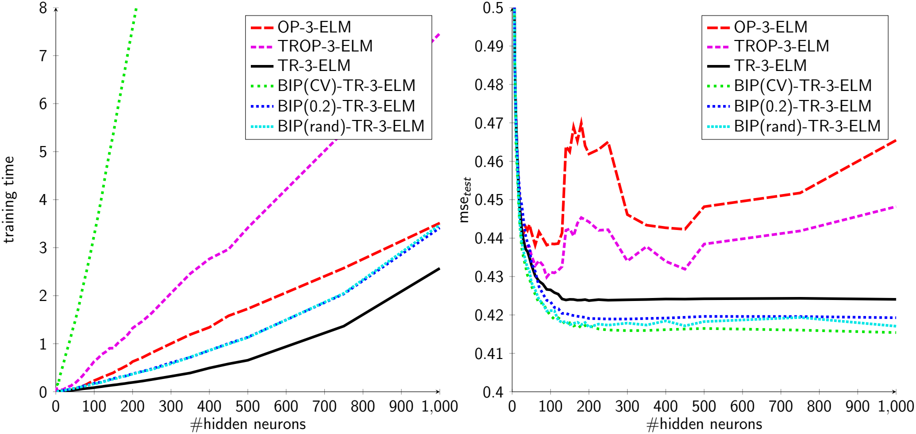
- add $\mathbf{w} \in \{-1, 0, 1\}^d$ with 1 var $(3^1 \times \binom{d}{1})$
- add $\mathbf{w} \in \{-1, 0, 1\}^d$ with 2 vars $(3^2 \times \binom{d}{2})$
- add $\mathbf{w} \in \{-1, 0, 1\}^d$ with 3 vars $(3^3 \times \binom{d}{3})$
- ...

For each subspace, weights are added in random order to avoid bias toward particular variables

Time-accuracy Trade-offs for Several ELMs

- **ELM**
- **OP-ELM**: Optimally Pruned ELM with neurons ranked by relevance, and then pruned to optimize the leave-one-out error
- **TR-ELM:** Tikhonov-regularized ELM, with efficient optimization of regularization parameter λ, using the SVD approach to computing $\mathbf{H}^\dagger$
- **TROP-ELM:** Tikhonov regularized OP-ELM
- **BIP(0.2), BIP(rand), BIP(CV)**:
  - ELMs pretrained using Batch Intrinsic Plasticity mechanism, adapting the hidden layer weights and biases, such that they retain as much information as possible
  - BIP parameter is either fixed, randomized, or cross-validated over 20 possible values

ELM Time-accuracy Trade-offs (Abalone UCI)



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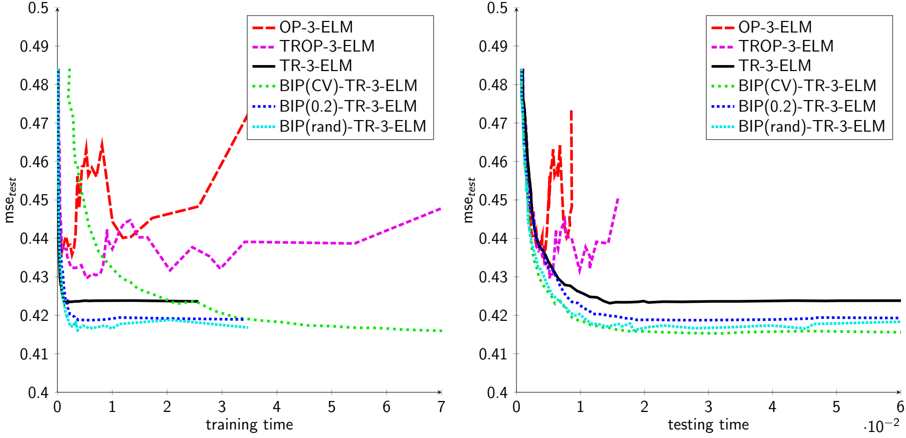

ELM Time-accuracy Trade-offs (Abalone UCI)

Depending on the user's criteria, these results suggest:

- *training time* most important: BIP(rand)-TR-3-ELM
  (almost optimal performance, while keeping training time low)
- if *test error* is most important: BIP(CV)-TR-3-ELM
  (slightly better accuracy, but training time is 20 times as high)
- if *testing time* is most important: BIP(rand)-TR-3-ELM (surprisingly)
  (OP-ELM and TROP-ELM tend to be faster in test, but suffer from slight overfitting)

Since TR-3-ELM offers attractive trade-offs between speed and accuracy, this model will be central in the rest of the paper.

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Two approaches for improving models

Time-accuracy trade-offs suggest **two possible strategies** to obtain models that are preferable over other models:

- **reducing test error**, using a better algorithm
  (“in terms of training time-accuracy plot: “pushing the curve down”)
- **reducing computational time**, while retaining as much accuracy as possible
  (“in terms of training time-accuracy plot: “pushing the curve to the left”)

Compressive ELM focuses on **reducing computational time by performing the training in a reduced space**, and then projecting back the solution back to the original space.

Compressive ELM

Given $m \times n$ matrix A, compute k-term approximate SVD $A \approx UDV^T$[Halko2009]:

- Form the $n \times (k+p)$ random matrix Ω. (where p is small)
- Form the $m \times (k+p)$ sampling matrix $Y = A\Omega$. (sketch it by applying Ω)
- Form the $m \times (k+p)$ orthonormal matrix Q (such that $range(Q) = range(Y)$)
- Compute $B = Q^* A$.
- Form the SVD of B so that $B = \hat{U}DV^T$
- Compute the matrix $U = Q\hat{U}$

Faster Sketching?

Bottleneck in Algorithm is the time it takes to sketch the matrix. Rather than using Gaussian random matrices for sketching A, use random matrices that are sparse or structured in some way and allow for faster multiplication:

$$\left(\; P \;\right)_{k\times n}\left(\; H \;\right)_{n\times n}\left(\; D \;\right)_{n\times n}$$

- **Fast Johnson Lindenstrauss Transform (FJLT)** introduced in [Ailon2006] for which P is a sparse matrix of random Gaussian variables, and H encodes the Discrete Hadamard Transform
- **Subsampled Randomized Hadamard Transform (SRHT)** for which P is a matrix selecting k random columns from H, and H encodes the Discrete Hadamard Transform

(Experiments did not show substantial difference in terms of computational time. Dataset too small?)

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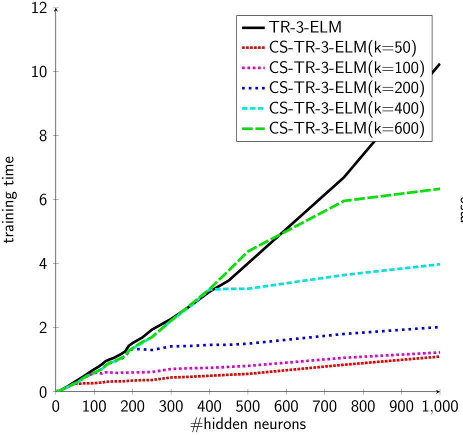
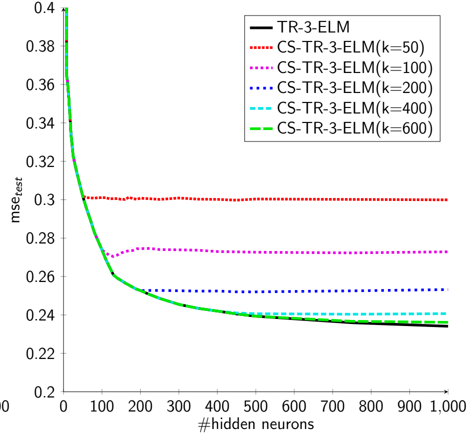
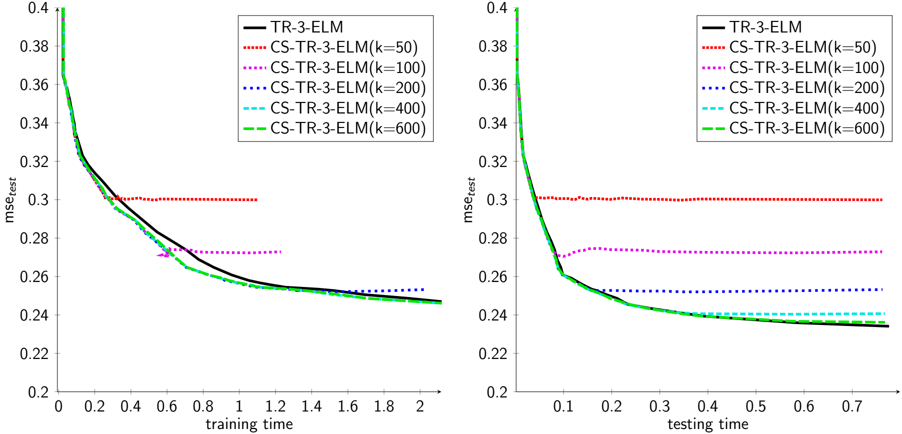
Compressive ELM (CalHousing, FJLT)





Compressive ELM (CalHousing, FJLT)



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Contributions

- Compressive ELM provides **a flexible way to reduce training time** by doing the optimization in a reduced space of k dimensions
- given k large enough, Compressive ELM achieves the **best test error for each computational time**
  (i.e. there are no models that achieve better test error and can be trained in the same or less time).

Future work

- let theory/bounds on low-distortion embeddings inform the choice of k

Questions?

Backup Slides

Batch Intrinsic Plasticity

- suppose $(\mathbf{x}_1, ..., \mathbf{x}_N) \in \mathbb{R}^{N \times d}$, and output of neuron i is $h_i = f(a_i \mathbf{w}_i \cdot \mathbf{x}_k + b_i)$, where f is an invertible transfer function
- for each neuron i
  - from exponential distribution with mean μ_{exp}, draw targets $\mathbf{t} = (t_1, t_2, \ldots, t_N)$ and sort such that $t_1 < t_2 < \ldots < t_N$
  - compute all presynaptic inputs $\mathbf{s}_k = \mathbf{w}_i \cdot \mathbf{x}_k$, and sort such that $s_1 < s_2 < \ldots < s_N$
  - now, find a_i and b_i such that

$$\begin{pmatrix} s_1 & 1 \\ \vdots & 1 \\ s_N & 1 \end{pmatrix} \begin{pmatrix} a_i \\ b_i \end{pmatrix} = \begin{pmatrix} f^{-1}(t_1) \\ \vdots \\ f^{-1}(t_N) \end{pmatrix}$$

Fast leave-one-out cross-validation

The leave-one-out (LOO) error can be computed using the PRESS statistics:

$$E_{loo} = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{y_i - \hat{y}_i}{1 - hat_{ii}}\right)^2$$

where hat_{ii} is the i^{th} value on the diagonal of the HAT-matrix, which can be quickly computed, given $\mathbf{H}^\dagger$:

$$\begin{aligned}\hat{\mathbf{Y}} &= \mathbf{H}\beta = \mathbf{H}\mathbf{H}^\dagger\mathbf{Y}\\ &= \mathrm{HAT}\cdot\mathbf{Y}\end{aligned}$$

Fast leave-one-out cross-validation

Using the SVD decomposition of $\mathbf{H} = \mathbf{U}\mathbf{D}\mathbf{V}^T$, it is possible to obtain all needed information for computing the PRESS statistic without recomputing the pseudo-inverse for every λ:

$$\begin{aligned}
\hat{\mathbf{Y}} &= \mathbf{H}\beta \\
&= \mathbf{H}(\mathbf{H}^T\mathbf{H} + \lambda\mathbf{I})^{-1}\mathbf{H}^T\mathbf{Y} \\
&= \mathbf{H}\mathbf{V}(\mathbf{D}^2 + \lambda\mathbf{I})^{-1}\mathbf{D}\mathbf{U}^T\mathbf{Y} \\
&= \mathbf{U}\mathbf{D}\mathbf{V}^T\mathbf{V}(\mathbf{D}^2 + \lambda\mathbf{I})^{-1}\mathbf{D}\mathbf{U}^T\mathbf{Y} \\
&= \mathbf{U}\mathbf{D}(\mathbf{D}^2 + \lambda\mathbf{I})^{-1}\mathbf{D}\mathbf{U}^T\mathbf{Y} \\
&= \mathrm{HAT} \cdot \mathbf{Y}
\end{aligned}$$

Fast leave-one-out cross-validation

where $\mathbf{D}(\mathbf{D}^2 + \lambda \mathbf{I})^{-1}\mathbf{D}$ is a diagonal matrix with $\frac{d_{ii}^2}{d_{ii}^2+\lambda}$ as the i^{th} diagonal entry. Now:

$$\begin{aligned}
\mathrm{MSE}^{\text{TR-PRESS}} &= \frac{1}{N}\sum_{i=1}^{N}\left(\frac{y_i - \hat{y}_i}{1 - hat_{ii}}\right)^2 \\
&= \frac{1}{N}\sum_{i=1}^{N}\left(\frac{y_i - \hat{y}_i}{1 - \mathbf{h}_{i\cdot}(\mathbf{H}^T\mathbf{H} + \lambda\mathbf{I})^{-1}\mathbf{h}_{i\cdot}^T}\right)^2 \\
&= \frac{1}{N}\sum_{i=1}^{N}\left(\frac{y_i - \hat{y}_i}{1 - \mathbf{u}_{i\cdot}\left(\frac{d_{ii}^2}{d_{ii}^2+\lambda}\right)\mathbf{u}_{i\cdot}^T}\right)^2
\end{aligned}$$

Better Weights

- random layer weights and biases drawn from e.g. uniform / normal distribution with certain range / variance
- typical transfer function $f\left(\langle \mathbf{w_i}, \mathbf{x} \rangle + b_i\right)$
- from $\langle \mathbf{w_i}, \mathbf{x} \rangle = |\mathbf{w_i}||\mathbf{x}| \cos\theta$, it can be seen that the typical activation of f depends on:
  - expected length of $\mathbf{w_i}$
  - expected length of $\mathbf{x}$
  - angles θ between the weights and the samples

Better Weights: Orthogonality?

Idea 1:

- improve the diversity of the weights by taking weights that are mutually orthogonal (e.g. M d-dimensional basis vectors, randomly rotated in the d-dimensional space)
- however, does not give significantly better accuracy
- apparently, for the tested cases, random weight scheme of ELM already covers the possible weight space pretty well

Better Weights: Sparsity!

Idea 2:

- improve the diversity of the weights by having each of them work in a different subspace (e.g. each weight vector has different subset of variables as input)
- spoiler: significantly improves accuracy, at no extra computational cost
- experiments suggest this is due to the weight scheme enabling implicit variable selection

Binary Weight Scheme

$$
\begin{array}{c|c}
 & \mathbf{1} \quad 0 \quad 0 \quad 0 \quad 0 \\
 & 0 \quad \mathbf{1} \quad 0 \quad 0 \quad 0 \\
1\ \textit{var} & 0 \quad 0 \quad \mathbf{1} \quad 0 \quad 0 \\
 & 0 \quad 0 \quad 0 \quad \mathbf{1} \quad 0 \\
 & 0 \quad 0 \quad 0 \quad 0 \quad \mathbf{1} \\
\hline
 & \mathbf{1} \quad \mathbf{1} \quad 0 \quad 0 \quad 0 \\
 & \mathbf{1} \quad 0 \quad \mathbf{1} \quad 0 \quad 0 \\
 & \mathbf{1} \quad 0 \quad 0 \quad \mathbf{1} \quad 0 \\
2\ \textit{vars} & \mathbf{1} \quad 0 \quad 0 \quad 0 \quad \mathbf{1} \\
 & \dots \\
 & \dots \\
 & 0 \quad 0 \quad 0 \quad \mathbf{1} \quad \mathbf{1} \\
\hline
3\ \textit{vars} & \textit{etc.}
\end{array}
$$

until enough neurons:

- add $\mathbf{w} \in \{0,1\}^d$ with 1 var $(\# = 2^1 \times \binom{d}{1})$
- add $\mathbf{w} \in \{0,1\}^d$ with 2 vars $(\# = 2^2 \times \binom{d}{2})$
- add $\mathbf{w} \in \{0,1\}^d$ with 3 vars $(\# = 2^3 \times \binom{d}{3})$
- ...

For each subspace, weights are added in random order to avoid bias toward particular variables

Ternary Weight Scheme

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For each subspace, weights are added in random order to avoid bias toward particular variables

Experimental Settings

Data	Abbreviation	number of variables	# training	# test
Abalone	**Ab**	**8**	**2000**	**2177**
CaliforniaHousing	Ca	8	8000	12640
CensusHouse8L	Ce	8	10000	12784
DeltaElevators	De	6	4000	5517
ComputerActivity	**Co**	**12**	**4000**	**4192**

- BIP(CV)-TR-ELM vs BIP(CV)-TR-2-ELM vs BIP(CV)-TR-3-ELM
- Experiment 1: relative performance
- Experiment 2: robustness against irrelevant vars
- Experiment 3: implicit variable selection
- (all results are averaged over 100 repetitions, each with randomly drawn training/test set)

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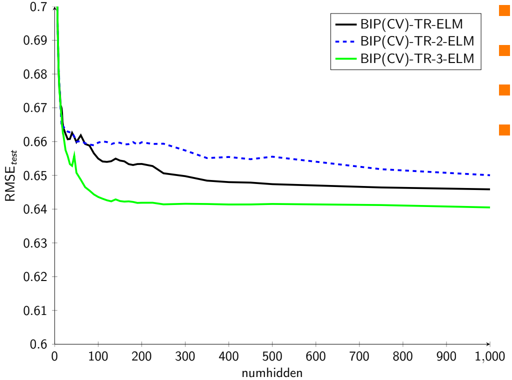
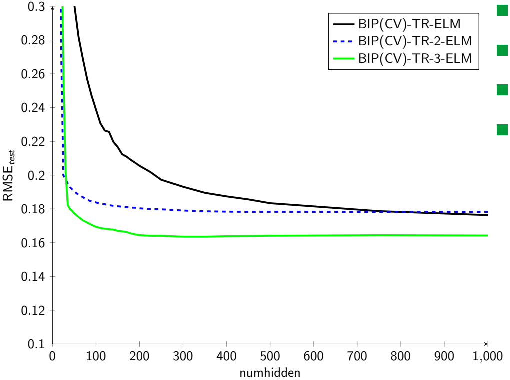
Exp 1: numhidden vs. RMSE (Abalone)



- averages over 100 runs
- gaussian < binary
- ternary < gaussian
- better RMSE with much less neurons

Exp 1: numhidden vs. RMSE (CpuActivity)



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- binary < gaussian
- ternary < gaussian
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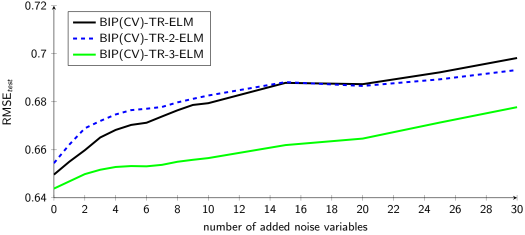
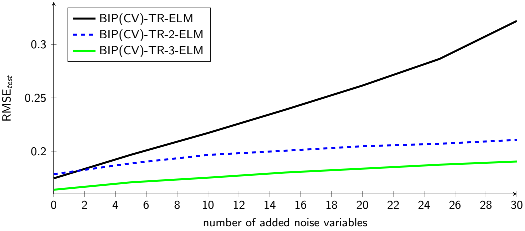
Exp 2: Robustness against irrelevant variables (Abalone)



- 1000 neurons
- binary weight scheme gives similar RMSE
- ternary weight scheme makes ELM more robust against irrelevant vars

Exp 2: Robustness against irrelevant variables (CpuActivity)



- 1000 neurons
- binary and ternary weight scheme makes ELM more robust against irrelevant vars

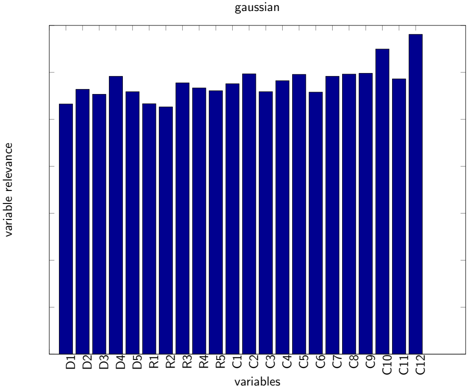
Exp 2: Robustness against irrelevant variables

	Ab			Co		
	gaussian	binary	ternary	gaussian	binary	ternary
RMSE with original variables	0.6497	0.6544	0.6438	0.1746	0.1785	0.1639
RMSE with 30 added irr. vars	0.6982	0.6932	0.6788	0.3221	0.2106	0.1904
RMSE loss	0.0486	**0.0388**	**0.0339**	0.1475	**0.0321**	**0.0265**

Table : Average RMSE loss of ELMs with 1000 hidden neurons, trained on the original data, and the data with 30 added irrelevant variables

Exp 3: Implicit Variable Selection (CpuAct)

- relevance of each input variable quantified as $\sum_{i=1}^{M} |\beta_i \times \mathbf{w}_i|$



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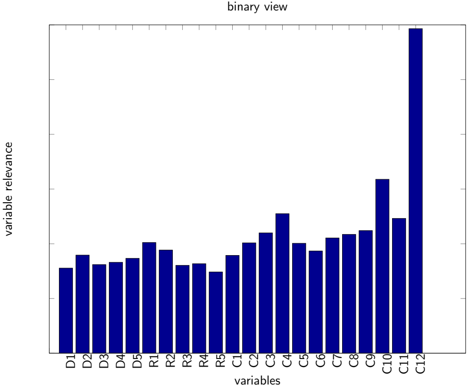

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