Orthogonal Least Squares Regression: An Efficient Approach for Parsimonious Modelling from Large Data

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Outline

1. Orthogonal Forward Selection
   - Motivations
   - Previous Enhancements
   - Unified Data Modelling
2. Grey-Box Modelling
   - Incorporating Prior knowledge
   - Symmetric RBF Modelling
   - BVC RBF Modelling
3. Branch and Bound
   - Branch and Bound for Efficiency
   - Branch and Bound Aided OLS
4. Recent Extensions
   - New Enhancements

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Nonlinear Identification

- In 80s, NARMAX identification of unknown **nonlinear** system

  $$\begin{aligned} y(k) &= f(u(k-1),\cdots,u(k-n_u),y(k-1),\cdots,y(k-n_y))+\epsilon(k) \\ &= f(\mathbf{x}(k))+\epsilon(k) \end{aligned}$$

  $y(k)$, $u(k)$ and $\epsilon(k)$: output, input and noise; system input vector with $m = n_u + n_y$:

  $$\begin{aligned} \mathbf{x}(k) &= [x_1(k)\cdots x_m(k)]^T \\ &= [u(k-1)\cdots u(k-n_u)\ y(k-1)\cdots y(k-n_y)]^T \end{aligned}$$

- Use **linear-in-the-parameters** nonlinear model

  $$\hat{y}(k) = \sum_{i=1}^{M} \theta_i p_i(k)$$

  $\{\theta_i\}$: unknown model weights; $\{p_i(k)\}$: fixed model bases, e.g. polynomial expansion, radial basis function, etc

- Utilise well-developed **linear** identification techniques

Parsimonious Principle

- Select subset of $M_s \ll M$ significantly model terms to overcome curse of dimensionality, overfitting, and poor generalisation
- Optimal subset selection intractable: candidate bases $M = 500$, subset size $M_s = 40 \Longrightarrow$ possible models to select from

$$\frac{M!}{M_s!(M - M_s)!} = \mathbf{2.2443 \times 10^{59}}$$

- Greedy-type forward subset selection

$$\left[\quad \overbrace{\mathbf{w}_1\ \mathbf{w}_2\ \cdots\ \mathbf{w}_{n-1}}^{\textbf{selected model terms}} \quad \middle| \quad \overbrace{\mathbf{p}_n\ \mathbf{p}_{n+1}\ \cdots\ \mathbf{p}_M}^{\textbf{candidate pool}} \right]$$

- Each time choose one term from candidate pool to add to subset model to maximally improve modelling performance

  $M = 500$ and $M_s = 40 \Longrightarrow$ candidate models to evaluate are:

$$\sum_{n=1}^{M_s} (M - n + 1) < M_s \times M = \mathbf{2 \times 10^4}$$

Orthogonal Decomposition

- Orthogonal decomposition of regression matrix: $\mathbf{P} = \mathbf{W}\mathbf{A}$ with

$$\mathbf{A} = \begin{bmatrix} 1 & \alpha_{1,2} & \cdots & \alpha_{1,M} \\ 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \alpha_{M-1,M} \\ 0 & \cdots & 0 & 1 \end{bmatrix}$$

orthogonal $\mathbf{W} = [\mathbf{w}_1 \ \mathbf{w}_2 \cdots \mathbf{w}_M]$, $\mathbf{A}\theta = \mathbf{g}$ and equivalent model

$$\mathbf{y} = \mathbf{P}\theta + \epsilon \Leftrightarrow \mathbf{y} = \mathbf{W}\mathbf{g} + \epsilon$$

- Training error reduction ratio due to n-th model term

$$[\text{err}]_n = g_n^2 \mathbf{w}_n^T \mathbf{w}_n / \mathbf{y}^T \mathbf{y}$$

and training mean square error of n-term model

$$J^{(n)} = J^{(n-1)} - g_n^2 \mathbf{w}_n^T \mathbf{w}_n$$

Early Orthogonal Least Squares

- Orthogonal least squares methods and their application to non-linear system identification – S. Chen, S. A. Billings and W. Luo – International Journal of Control, 1989
  Google scholar citations: 645 ISI citations: 468 (July 2011) ECS EPrints downloads: average **1.5** per day

- Orthogonal least squares learning algorithm for radial basis function networks – S. Chen, C. F. N. Cowan and P. M. Grant – IEEE Transactions on Neural Networks, 1991
  Google scholar citations: 2166 ISI citations: 1555 (July 2011) ECS EPrints downloads: average **6** per day

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2-Norm Local Regularisation

- Instead of training error $\epsilon^T\epsilon$, consider regularised error criterion

$$J_R(\mathbf{g},\boldsymbol{\lambda}) = \epsilon^T\epsilon + \mathbf{g}^T\boldsymbol{\Lambda}\mathbf{g}$$

where $\boldsymbol{\Lambda} = \mathrm{diag}\{\lambda_1, \lambda_2, \cdots, \lambda_M\}$

- Regularised error reduction ratio

$$[\mathrm{rerr}]_n = g_n^2 \left(\mathbf{w}_n^T\mathbf{w}_n + \lambda_n\right) / \mathbf{y}^T\mathbf{y}$$

- Evidence procedure for updating regularisation parameters

$$\lambda_n^{\mathrm{new}} = \frac{\gamma_n^{\mathrm{old}}}{K - \gamma^{\mathrm{old}}} \frac{\epsilon^T\epsilon}{g_n^2}, \quad 1 \le n \le M$$

$$\gamma_n = \frac{\mathbf{w}_n^T\mathbf{w}_n}{\lambda_n + \mathbf{w}_n^T\mathbf{w}_n} \quad \gamma = \sum_{n=1}^{M} \gamma_n$$

which has a Bayesian interpretation

An Illustrative Example

- Very sparse, and enhance performance
- Additionally help to determine appropriate subset model size

selection stage l	weight θ_l	regulariser λ_l
1	1.87494e+00	2.53227e-01
2	-1.70014e+00	1.81540e-01
3	-1.00970e+00	2.01490e-01
4	5.67310e-01	8.64601e-01
5	4.17979e-01	1.36357e+00
6	-1.51352e-01	6.93984e-01
7	**-9.49873e-10**	**5.67623e+07**
8	**-2.79967e-10**	**1.11770e+08**
9	**7.14157e-11**	**1.03860e+07**
10	**-2.05313e-12**	**1.92708e+08**
	⋮	

Optimal Experiment Designs

- LS estimate $\boldsymbol{\theta}_{\mathrm{LS}} = \left(\mathbf{P}^T\mathbf{P}\right)^{-1}\mathbf{P}^T\mathbf{y}$ of true parameter vector $\boldsymbol{\theta}$:

$$E\left[\boldsymbol{\theta}_{\mathrm{LS}}\right] = \boldsymbol{\theta}, \quad \mathrm{Cov}\left[\boldsymbol{\theta}_{\mathrm{LS}}\right] \propto \left(\mathbf{P}^T\mathbf{P}\right)^{-1}$$

- Optimal experiment designs prevent selection of oversized ill-posed model and overcome problem of high parameter estimate variances
- *A*-optimal design minimises trace of the covariance matrix $\mathrm{Cov}\left[\boldsymbol{\theta}_{\mathrm{LS}}\right]$, which in orthogonal decomposition space is

$$\mathrm{tr}\left[\left(\mathbf{W}^T\mathbf{W}\right)^{-1}\right] = \sum_{n=1}^{M} \frac{1}{\mathbf{w}_n^T\mathbf{w}_n}$$

- *D*-optimal design maximises determinant of design matrix

$$\det\left[\mathbf{W}^T\mathbf{W}\right] = \prod_{n=1}^{M} \mathbf{w}_n^T\mathbf{w}_n$$

Combined LROLS and *D*-Optimality

- Combined LROLS and *D*-optimality criterion

$$J_{CR}(\mathbf{g},\boldsymbol{\lambda},\beta) = J_R(\mathbf{g},\boldsymbol{\lambda}) + \beta \sum_{n=1}^{M} -\log\left(\mathbf{w}_n^T \mathbf{w}_n\right)$$

- Combined regularised error reduction and *D*-optimality ratio

$$[\mathrm{crerr}]_n = \left(g_n^2\left(\mathbf{w}_n^T\mathbf{w}_n + \lambda_n\right) + \beta \log\left(\mathbf{w}_n^T\mathbf{w}_n\right)\right)/\mathbf{y}^T\mathbf{y}$$

- Or selecting *n*-th model term by minimising combined criterion

$$J^{(n)} = J^{(n-1)} - g_n^2\left(\mathbf{w}_n^T\mathbf{w}_n + \lambda_n\right) - \beta \log\left(\mathbf{w}_n^T\mathbf{w}_n\right)$$

- S. Chen, X. Hong and C. J. Harris, “Sparse kernel regression modelling using combined locally regularized orthogonal least squares and *D*-optimality experimental design,” *IEEE Trans. Automatic Control*, Vol.48, No.6, 1029–1036, June 2003

Leave-One-Out Cross Validation

- Highly desirable to select model terms by directly optimising model generalisation performance, instead of training MSE
- Model generalisation can be evaluated by test performance on data not used in training, and leave-one-out cross validation:
- "Remove" kth data from training set $D_K = \{\mathbf{x}(k), y(k)\}_{k=1}^{K}$, identify model $\hat{y}^{(n,-k)}$, and test error on data point not in training

$$\epsilon^{(n,-k)}(k) = y(k) - \hat{y}^{(n,-k)}(k)$$

- "Repeating" for each k leads to LOO MSE

$$J^{(n)} = \frac{1}{K} \sum_{k=1}^{K} \left(\epsilon^{(n,-k)}(k) \right)^2$$

a generalisation measure for model $\hat{y}^{(n)}$ identified with whole D_K

OLS-LOO Algorithm

- All above LOO cross validation steps are *virtual*, and orthogonal decomposition makes everything simple
- Leave-one-out error

$$\epsilon^{(n,-k)}(k) = \frac{\epsilon^{(n)}(k)}{\eta^{(n)}(k)}$$

- Modelling error of n-term model $\hat{y}^{(n)}$

$$\epsilon^{(n)}(k) = \epsilon^{(n-1)}(k) - w_n(k)g_n$$

$\epsilon^{(n-1)}(k)$ is modelling error of $(n-1)$-term model $\hat{y}^{(n-1)}$

- Leave-one-out weighting

$$\eta^{(n)}(k) = \eta^{(n-1)}(k) - \frac{w_n^2(k)}{\mathbf{w}_n^T\mathbf{w}_n + \lambda_n}$$

$w_n(k)$ is kth element of nth model column $\mathbf{w}_n$

OLS-LOO Procedure

- Thus, leave-one-out mean square error $J^{(n)}$ can be evaluated efficiently
- Moreover $J^{(n)}$ is "locally convex" with respect to model size n, and there exists an "optimal" model size M_s such that
  - For $n \leq M_s$: $J^{(n)}$ decreases as n increases
  - while $J^{(M_s)} \leq J^{(M_s+1)}$
- Regularised OLS algorithm can readily used, but selection of nth model term is based on minimisation of $J^{(n)}$
- S. Chen, X. Hong, C. J. Harris and P. M. Sharkey, "Sparse modelling using orthogonal forward regression with PRESS statistic and regularization," *IEEE Trans. Systems, Man and Cybernetics, Part B*, Vol.34, No.2, 898–911, 2004

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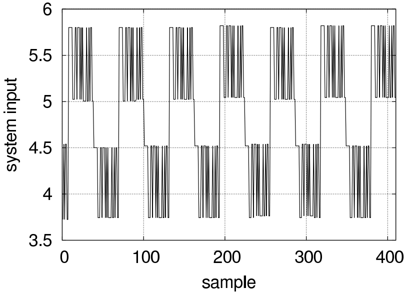
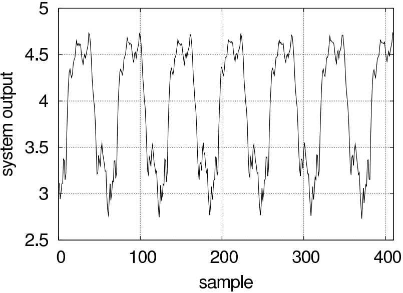
Unified Regression Framework

- Originally derived for regression, all algorithms can be applied to classification and density estimation as well
  - Regression and classification are supervised learning, while density estimation is unsupervised learning
- Two-class classification: give training set $D_K = \{\mathbf{x}(k), y(k)\}_{k=1}^{K}$, where $y(k) \in \{-1, +1\}$, OLS forward selection based on
  - Fisher ratio of interclass difference to intraclass spread
  - Leave-one-out misclassification rate
- Probability density function estimation: give training set $D_K = \{\mathbf{x}(k)\}_{k=1}^{K}$, construct Parzen window estimate on D_K
  - Use PW estimate at $\mathbf{x}(k)$ as $y(k) \rightarrow$ regression problem
  - Weights must be nonnegative and add up to unity

Engine Data Set

- Data collected from a Leyland TL11 turbocharged, direct injection diesel engine operated at low engine speed
- System input $u(k)$ is fuel rack position, and system output $y(k)$ is engine speed





- First 210 data points for training, and last 200 data for testing

Engine Data Results

- Training data $\{\mathbf{x}(k), y(k)\}_{k=1}^{K}$ with $K = 210$, and

$$\mathbf{x}(k) = [y(k-1)\ u(k-1)\ u(k-2)]^T$$

- LROLS-LOO: Gaussian RBF, RBF variance σ^2 determined separately by cross validation
- SVM: Gaussian kernel, kernel variance σ^2, regularisation parameter and error band determined separately by cross validation
- Experimental results:

algorithm	model size	training MSE	test MSE
LROLS-LOO	22	0.000453	0.000490
SVM	92	0.000447	0.000498

Boston Housing Data

- Regression benchmark, comprised 506 data points with 14 variables
  - Predict median house value from remaining 13 attributes
  - 456 data points were randomly selected for training and remaining 50 data points for testing
  - Average results were given over 100 repetitions
  - Gaussian kernel was used
- Experimental results:

algorithm	LROLS-LOO	SVM
model size	58.6 ± 11.3	243.2 ± 5.3
training MSE	12.9690 ± 2.6628	6.7986 ± 0.4444
test MSE	17.4157 ± 4.6670	23.1750 ± 9.0459

The SVM model is overfitted, due to the difficulties in finding near optimal values for three hyperparameters, kernel variance, regularisation parameter and error band

Diabetes Data Set

- Two-class, feature space dimension $m = 8$; 100 realisations, each having 468 training patterns and 300 test patterns
- Experimental results:

algorithm	test error rate %	model size
RBF-Network	24.29 ± 1.88	15
AdaBoost RBF-Network	26.47 ± 2.29	15
LP-Reg-AdaBoost	24.11 ± 1.90	15
QP-Reg-AdaBoost	25.39 ± 2.20	15
AdaBoost-Reg	23.79 ± 1.80	15
SVM	23.53 ± 1.73	not available
Kernel Fisher Discriminant	23.21 ± 1.63	468
ROLS-LOO	23.00 ± 1.70	6.0 ± 1.0

Data and first 7 results from:

`http://ida.first.fhg.de/projects/bench/benchmarks.htm`

Thyroid Data Set

- Two-class, feature space dimension $m = 5$; 100 realisations, each having 140 training patterns and 75 test patterns
- Experimental results:

algorithm	test error rate %	model size
RBF-Network	4.52 ± 2.12	8
AdaBoost RBF-Network	4.40 ± 2.18	8
LP-Reg-AdaBoost	4.59 ± 2.22	8
QP-Reg-AdaBoost	4.35 ± 2.18	8
AdaBoost-Reg	4.55 ± 2.19	8
SVM	4.80 ± 2.19	not available
Kernel Fisher Discriminant	4.20 ± 2.07	140
ROLS-LOO	4.80 ± 2.20	4.6 ± 1.0

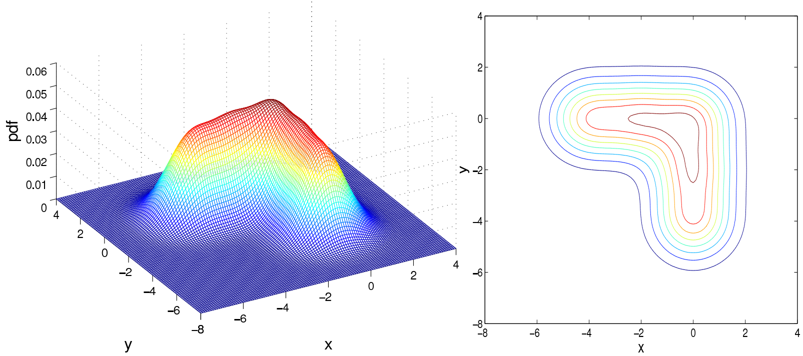
Data and first 7 results from:

`http://ida.first.fhg.de/projects/bench/benchmarks.htm`

2-D Density Example

$$p(x_1,x_2)=\sum_{i=1}^{5}\frac{1}{10\pi}e^{-\frac{(x_1-\mu_{i,1})^2}{2}}e^{-\frac{(x_2-\mu_{i,2})^2}{2}}$$

Means of 5 Gaussians: $[0.0\ -4.0]$, $[0.0\ -2.0]$, $[0.0\ 0.0]$, $[-2.0\ 0.0]$, $[-4.0\ 0.0]$



- Estimation set $K=500$, and experiment repeated 100 times

2-D Density Example Results

- Kernel width was obtained separately via cross validation
- L_1 test error and numerical approximation of Kullback-Leibler divergence are used to assess an estimator
- Average kernel number obtained by OLS with D-optimality is 8
- GMM: Gaussian mixture model estimate, number of mixture componenets set to 8
- RSDE: reduced set density estimate (Girolami & He, 2003)
- Experimental results:

estimator	PW	OLS D-opt	RSDE	GMM
$L_1 \times 10^3$	3.62 ± 0.44	3.24 ± 0.56	3.63 ± 0.36	3.68 ± 0.67
KLC $\times 10^2$	3.42 ± 0.55	3.47 ± 1.30	3.54 ± 0.49	3.39 ± 0.87
kernel no.	500	7.9 ± 0.8	13.2 ± 3.0	8
maximum	500	9	21	8
minimum	500	6	6	8

6-D Density Example

- True density was mixture of three Gaussian distributions

$$p(\mathbf{x}) = \frac{1}{3}\sum_{i=1}^{3}\frac{1}{(2\pi)^{6/2}}\frac{1}{\det^{1/2}|\bar{\boldsymbol{\Gamma}}_i|}e^{-\frac{1}{2}(\mathbf{x}-\bar{\boldsymbol{\mu}}_i)^T\bar{\boldsymbol{\Gamma}}_i^{-1}(\mathbf{x}-\bar{\boldsymbol{\mu}}_i)}$$

- with

$$\begin{aligned}\bar{\boldsymbol{\mu}}_1 &= [1.0\ 1.0\ 1.0\ 1.0\ 1.0\ 1.0]^T,\\ \bar{\boldsymbol{\Gamma}}_1 &= \text{diag}\{1.0, 2.0, 1.0, 2.0, 1.0, 2.0\}\end{aligned}$$

$$\begin{aligned}\bar{\boldsymbol{\mu}}_2 &= [-1.0\ -1.0\ -1.0\ -1.0\ -1.0\ -1.0]^T,\\ \bar{\boldsymbol{\Gamma}}_2 &= \text{diag}\{2.0, 1.0, 2.0, 1.0, 2.0, 1.0\}\end{aligned}$$

$$\begin{aligned}\bar{\boldsymbol{\mu}}_3 &= [0.0\ 0.0\ 0.0\ 0.0\ 0.0\ 0.0]^T,\\ \bar{\boldsymbol{\Gamma}}_3 &= \text{diag}\{2.0, 1.0, 2.0, 1.0, 2.0, 1.0\}\end{aligned}$$

- Estimation set $K = 600$, while experiment is repeated 100 times

6-D Density Example Results

- Kernel width was obtained separately via cross validation
- Average kernel number obtained by OLS with *D*-optimality design is 8.4
- GMM: number of mixture componenets set to 8
- RSDE: reduced set density estimate (Girolami & He, 2003)
- Experimental results:

estimator	PW	OLS *D*-opt	RSDE	GMM
L_1 $\times 10^5$	3.52 ± 0.16	2.78 ± 0.23	2.74 ± 0.50	1.74 ± 0.29
kernel no.	600	8.4 ± 0.9	14.2 ± 3.6	8
maximum	600	10	25	8
minimum	600	6	8	8

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Motivations

- Like many existing data modelling methods, the approach discussed so far is a black-box model, which is appropriate
  - if no *a priori* information exists regarding underlying data generating mechanism
- Known prior knowledge concerning underlying process should be incorporated into model structure explicitly
- How to incorporate prior knowledge to form grey-box model is highly problem dependent, and is really an *art*
- Two types of prior information are considered
  - Underlying process exhibits known symmetry property
  - Underlying process obeys set of boundary value constraints
- Existing learning algorithms can be applied to resulting grey-box models without any modification and added complexity

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Symmetric RBF Network

- Unknown system $f(\bullet)$ possesses odd symmetry $f(-\mathbf{x}) = -f(\mathbf{x})$
  - e.g. from physics, underlying optimal discriminant function for BPSK digital signals has old symmetry
- RBF model with standard node

$$p_i(k) = \varphi\left(\|\mathbf{x}(k) - \mathbf{c}_i\|/\sigma\right)$$

cannot guarantee to have odd symmetry

- Symmetric RBF model with symmetric RBF node

$$p_i(k) = \varphi\left(\|\mathbf{x}(k) - \mathbf{c}_i\|/\sigma\right) - \varphi\left(\|\mathbf{x}(k) + \mathbf{c}_i\|/\sigma\right)$$

guarantees to obey same odd symmetry as underlying process

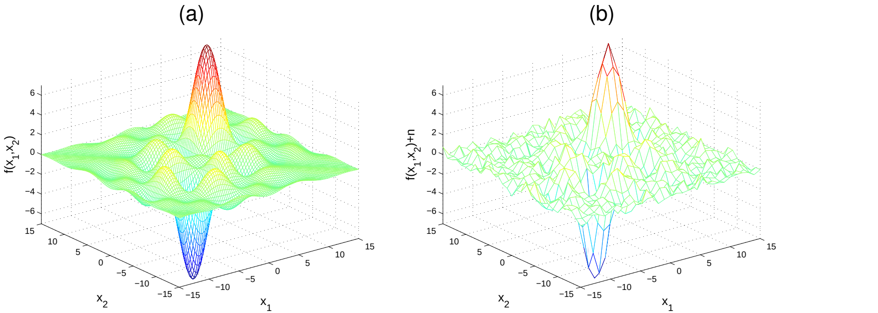
  - incorporate prior information naturally into model structure
  - all RBF learning methods are readily applicable

Symmetric Function Modelling

(a) Underlying function

$$f(x_1, x_2) = 10\left(\frac{\sin(x_1 - 5)\sin(x_2 - 5)}{(x_1 - 5)(x_2 - 5)} - \frac{\sin(x_1 + 5)\sin(x_2 + 5)}{(x_1 + 5)(x_2 + 5)}\right)$$

shown on the grid of 90601 points, and (b) 961 noisy training data points $y = f(x_1, x_2) + \epsilon$, where ϵ is Gaussian noise of zero mean and variance 0.16



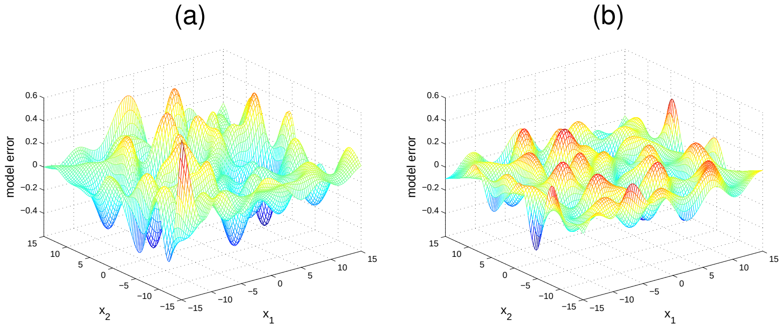
Symmetric Modelling Results

- Every training data used as a RBF centre with $M = K = 961$, RBF variance $\sigma^2 = 8.0$ was determined separately using cross validation
- Local regularisation assisted OLS algorithm with LOO MSE was used to automatically select sparse RBF / SRBF model
- Mean square error MSE $= E[(y - \hat{y})^2]$ was calculated over noisy training set and a separate noisy test set
- Mean modelling error MME $= E[(f(x_1, x_2) - \hat{f}(x_1, x_2))^2]$ was defined over grid of 90601 points noise-free $f(x_1, x_2)$, with $\hat{f}$ denoting estimated mapping

	model size	training MSE	test MSE	test MME
RBF	105	0.1543	0.2047	0.0294
SRBF	68	0.1566	0.1839	0.0093

Symmetric Modelling (continue)

(a) modelling error $f(x_1, x_2) - \hat{f}(x_1, x_2)$ of standard RBF model, and
(b) modelling error $f(x_1, x_2) - \hat{f}(x_1, x_2)$ of symmetric RBF model



Results Analysis

- By incorporating prior information, SRBF offers significantly better generalisation performance than standard RBF
  - Mean modelling error is three times smaller
- OLS algorithm selecting M_s model terms from K-term candidate set, where $M_s \ll K$, has complexity

  $$C = \big(M_s + 1\big) \times K \times \mathcal{O}(K)$$

  For SRBF, $M_s = 68$, while for standard RBF, $M_s = 105$
  - Thus, complexity of SRBF model construction is about half of complexity for constructing standard RBF model
- Computational requirements of a symmetric node is more than that of standard one, but SRBF has few RBF units
  - Prediction complexity of two models are similar

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Boundary Value Constraints

- Underlying system satisfies a set of boundary value constraints

$$f(\mathbf{x}_j) = d_j, \ 1 \leq j \leq L$$

  $\mathbf{x}_j$ and d_j, $1 \leq j \leq L$, are known

  - These BVCs may represent the fact that at some critical regions, there is a complete knowledge about system

- Any identified model $\hat{f}$ is required to strictly meet these BVCs

$$\hat{f}(\mathbf{x}_j) = d_j, \ 1 \leq j \leq L$$

  - RBF model with standard node $p_i(k) = \varphi\left(\|\mathbf{x}(k) - \mathbf{c}_i\|/\sigma\right)$ cannot meet these BVCs

- Using BVCs as constraints dramatically complicates learning

  - Efficient state-of-the-art learning methods cannot be applied directly

BVC-RBF Network

- Boundary value constraint-RBF model takes the form

$$\hat{y}(k) = \hat{f}(\mathbf{x}(k)) = \sum_{i=1}^{M} p_i(\mathbf{x}(k))\theta_i + g(\mathbf{x}(k))$$

- with novel RBF node structure

$$p_i(\mathbf{x}) = h(\mathbf{x})\varphi(\|\mathbf{x} - \mathbf{c}_i\|/\sigma)$$

- **Geometric mean** of data sample $\mathbf{x}$ to BVCs $\mathbf{x}_j$, $1 \leq j \leq L$

$$h(\mathbf{x}) = \sqrt[L]{\prod_{j=1}^{L} \|\mathbf{x} - \mathbf{x}_j\|}$$

- Since $h(\mathbf{x}_j) = 0$ at any boundary point $\mathbf{x}_j$, node $p_i(\mathbf{x})$ has property of **zero forcing** at any $\mathbf{x}_j$

BVC-RBF Offset Function

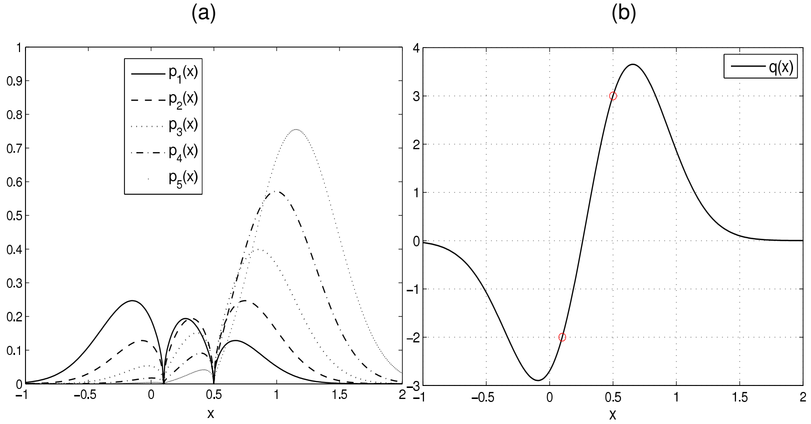
- **Offset function** $$g(\mathbf{x}) = \sum_{j=1}^{L} \alpha_j e^{-\frac{\|\mathbf{x}-\mathbf{x}_j\|^2}{\tau}}$$
- τ is a positive scalar, $\boldsymbol{\alpha} = [\alpha_1 \ \alpha_2 \cdots \alpha_L]^T$ is obtained by solving $g(\mathbf{x}_j) = d_j$, $1 \leq j \leq L$, i.e. $\boldsymbol{\alpha} = \mathbf{G}^{-1}\mathbf{d}$, with $\mathbf{d} = [d_1 \ d_2 \cdots d_L]^T$ and

$$\mathbf{G} = \begin{bmatrix} 1 & e^{-\frac{\|\mathbf{x}_1-\mathbf{x}_2\|^2}{\tau}} & \cdots & e^{-\frac{\|\mathbf{x}_1-\mathbf{x}_L\|^2}{\tau}} \\ e^{-\frac{\|\mathbf{x}_2-\mathbf{x}_1\|^2}{\tau}} & 1 & \ddots & e^{-\frac{\|\mathbf{x}_2-\mathbf{x}_L\|^2}{\tau}} \\ \vdots & \ddots & \ddots & \vdots \\ e^{-\frac{\|\mathbf{x}_L-\mathbf{x}_1\|^2}{\tau}} & e^{-\frac{\|\mathbf{x}_L-\mathbf{x}_2\|^2}{\tau}} & \cdots & 1 \end{bmatrix}$$

- Offset function $g(\mathbf{x})$ passes all predetermined boundary values $f(\mathbf{x}_j) = g(\mathbf{x}_j) = d_j$, $1 \leq j \leq L$, and it is completely determined by BVCs but does not depend on D_K

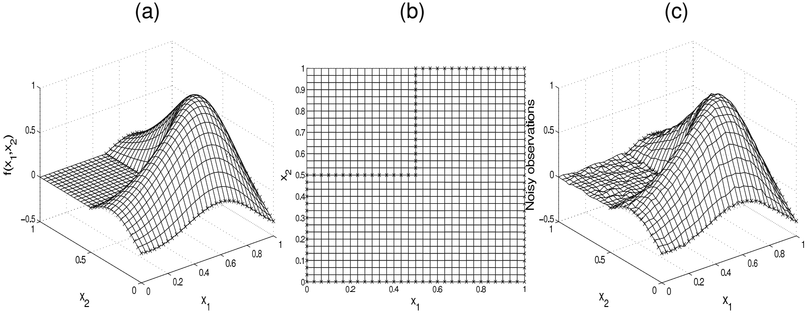
BVC-RBF Illustration

- One-dimensional function $f(x)$ with two BVCs: $f(0.1) = -2$, $f(0.5) = 3$
- Five RBFs with zero forcing at two boundary points (a), and offset passing function $g(x)$ (b)



BVC-Function Modelling

(a) Underlying function $f(x_1, x_2)$ shown on grid of 961 points, (b) $L = 120$ BVCs given by coordinates marked as cross points, and (c) 961 noisy training points, with Gaussian noise of zero mean and variance 0.01^2

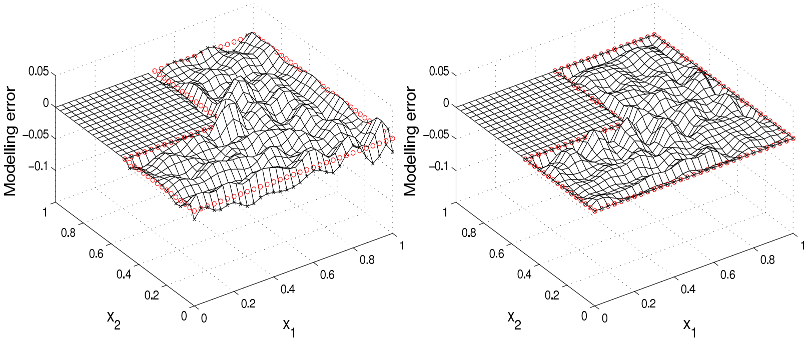


- OLS algorithm with training MSE and *D*-optimality was used to automatically identify standard RBF and BVC-RBF models
- RBF variance $\sigma^2 = 0.01$ was determined by cross validation, $\tau = 0.04$, and *D*-optimality weighting $\beta = 10^{-5}$

BVC-Function Modelling Results

	model size	training MSE (inside D_K)	test MME (inside boundary)	test MME (on boundary)
RBF	91	1.6894×10^{-4}	1.0229×10^{-4}	2.1249×10^{-4}
BVC-RBF	68	1.0736×10^{-4}	4.3787×10^{-5}	7.2598×10^{-11}

Modelling error $f(x_1, x_2) - \hat{f}(x_1, x_2)$ of standard RBF (a) and BVC-RBF (b)


(a)

(b)

Outline

1. Orthogonal Forward Selection
   - Motivations
   - Previous Enhancements
   - Unified Data Modelling
2. Grey-Box Modelling
   - Incorporating Prior knowledge
   - Symmetric RBF Modelling
   - BVC RBF Modelling
3. Branch and Bound
   - Branch and Bound for Efficiency
   - Branch and Bound Aided OLS
4. Recent Extensions
   - New Enhancements

Motivations

*n*th stage of OLS forward subset selection

$$\left[\overbrace{\mathbf{w}_1\ \mathbf{w}_2\ \cdots\ \mathbf{w}_{n-1}}^{\textbf{selected subset model}} \;\middle|\; \overbrace{\mathbf{p}_n\ \mathbf{p}_{n+1}\ \cdots\ \mathbf{p}_M}^{\textbf{candidate set } \mathcal{S}}\right]$$

- choose one term from candidate set $\mathcal{S}$ as $\mathbf{w}_n$ to add to subset model which maximumly improves modelling performance

With Branch and bound, *n*th stage of OLS forward subset selection

$$\left[\overbrace{\mathbf{w}_1\ \mathbf{w}_2\ \cdots\ \mathbf{w}_{n-1}}^{\textbf{selected subset model}} \;\middle|\; \overbrace{\mathbf{p}_n\ \mathbf{p}_{n+1}\ \cdots\ \mathbf{p}_{M_n}}^{\textbf{candidate set } \mathcal{S}} \;\middle|\; \overbrace{\mathbf{p}_{M_n+1}\ \mathbf{p}_{M_n+2}\ \cdots\ \mathbf{p}_M}^{\textbf{infeasible set } \bar{\mathcal{S}}}\right]$$

- choose one term from candidate set $\mathcal{S}$ as $\mathbf{w}_n$ to add to subset model, and check any candidate in $\mathcal{S}$ can be safely removed to infeasible set $\bar{\mathcal{S}}$ (will not be considered in subsequent stages)

What is Branch and Bound

- An evaluation procedure for all candidate solutions by using upper and lower estimated bounds of the quantity optimised, leading to large subsets of fruitless candidates being discarded
  - Branching: successively dividing a candidate solution set into subsets
  - Bounding: computing upper and lower bounds for a given subset
- Let candidate set be divided into two disjoint subsets, $\mathcal{A}$ and $\mathcal{B}$, and a bounding function is based on current best solution
  - If lower bound for $\mathcal{A}$ is greater than current best solution, it is discarded, and search space is reduced to $\mathcal{B}$
- It is often difficult to design a branch and bound strategy for specific problem
  - For OLS algorithm, it can be implemented effectively

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Branch and Bound OLS with *A*-Optimality

- OLS selection based on training MSE and *A*-optimality

$$J^{(n)} = J^{(n-1)} - \frac{1}{K} g_n^2 \mathbf{w}_n^T \mathbf{w}_n + \frac{\beta}{\mathbf{w}_n^T \mathbf{w}_n}$$

β: *A*-optimality weighting, K: the full candidate set size

- nth stage, a candidate from $\mathcal{S}$ is selected as $\mathbf{w}_n$, which has minimum $J^{(n)}$

- **Theorem**. Consider another candidate $\mathbf{p}_j$ in $\mathcal{S}$, let

$$\mathbf{w}^{(-)} = \mathbf{p}_j - \sum_{i=1}^{n-1} \alpha_{i,j}^{(-)} \mathbf{w}_i \text{ with } \alpha_{i,j}^{(-)} = \frac{\mathbf{p}_j^T \mathbf{w}_i}{\mathbf{w}_i^T \mathbf{w}_i}$$

If

$$\left(\mathbf{w}^{(-)}\right)^T \mathbf{w}^{(-)} < \frac{\beta}{J^{(n)}}$$

$\mathbf{p}_j$ can **safely** be removed from $\mathcal{S}$ into $\bar{\mathcal{S}}$

Complexity Saving

- Number of column orthogonalisations and cost function evaluations for conventional OLS forward selection

$$C_{\mathrm{OLS}} = \sum_{n=1}^{M_s} (K - n + 1)$$

- For branch and bound OLS forward selection, this number is

$$C_{\mathrm{BB-OLS}} = \sum_{n=1}^{M_s} (M_n - n + 1)$$

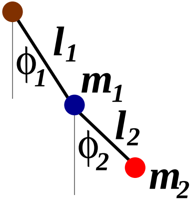
  with $M_{n+1} \le M_n$ and $M_1 = K$

- Empirical results obtained in practice show that typically 20% to 40% saving of computational cost is likely

X. Hong, S. Chen and C.J. Harris, "*A*-optimality orthogonal forward regression algorithm using branch and bound," *IEEE Trans. Neural Networks*, Vol.19, No.11, 1961–1967, 2008

Double Pendulum Results

- Modelling performance for lower pendulum angle ϕ_2
- Integration time span of 200 s at sampling rate of 0.2 s
- First 800 data samples were used in training and last 200 data samples for model testing
- Gaussian RBF variance $\sigma^2 = 3.0$ was set empirically
- Conventional OLS with training MSE and *A*-optimality, and branch and bound aided one



weighting	training MSE		test MSE		model size		BB cost
β	Conv.	BB	Conv.	BB	Conv.	BB	reduction
10^{-11}	0.000127	0.000176	0.000316	0.000515	31	29	**23.02%**
10^{-12}	0.000081	0.000088	0.000196	0.000174	33	35	**20.0%**
10^{-13}	0.000062	0.000078	0.000163	0.000262	42	38	**35.1%**
10^{-14}	0.000046	0.000061	0.000176	0.000162	48	39	**42.8%**

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Elastic-Net OLS

- Elastic net orthogonal forward regression criterion

$$J_{EN}(\mathbf{g}, \lambda_1, \lambda_2) = \epsilon^T \epsilon + \lambda_1 \|\mathbf{g}\|_2 + \lambda_2 \|\mathbf{g}\|_1$$

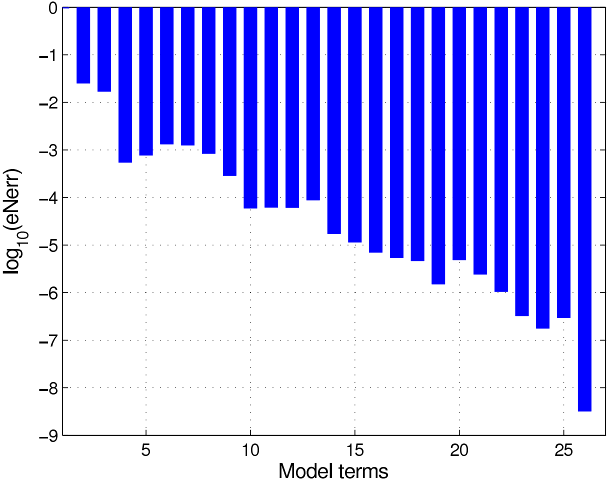
  - Maintain sparsity of LASSO, 1-norm regularisation drives many weights to exactly zero
  - Not as aggressive as LASSO in excluding correlated terms, owing to 2-norm regularisation

- Efficient two level learning
  - At upper level, PSO optimises λ_1 and λ_2 based on LOO MSE values from lower level
  - At lower level, given multiple λ_1 and λ_2 from upper level, perform multiple orthogonal forward selections

- X. Hong and S. Chen, “Automatic kernel regression modeling using elastic net orthogonal forward regression assisted by particle swarm optimization,” submitted to *IEEE Trans. Neural Networks*

Engine Data Set

- Exactly 26 non-zero erro-reduction-ratio (err) terms are selected



- Training MSE: 0.000447, testing MSE: 0.000470

Tunable “Kernel” Modelling

- Tunable “kernel”

$$p_i(k) = \varphi\left(\left(\mathbf{x}(k) - \mathbf{c}_i\right)^T \mathbf{\Sigma}_i^{-1} \left(\mathbf{x}(k) - \mathbf{c}_i\right)\right)$$

  - Centre $\mathbf{c}_i$ and covariance matrix $\mathbf{\Sigma}_i$ are not fixed but parameters to be learnt
- Kernels are optimised by PSO based on LOO criterion one by one in efficient orthogonal forward regression
  - A unified approach for regression, classification and density estimation
- Offer advantages of smaller model size, better generalisation, and less computational complexity in learning, in comparison with “fixed” kernel approach
- S. Chen, X. Hong and C.J. Harris, “Particle swarm optimization aided orthogonal forward regression for unified data modelling,” *IEEE Trans. Evolutionary Computation*, vol.14, no.4, pp.477–499, 2010

Imbalanced Classification

- Highly imbalanced two-class classification problems are widely found in practice
- Construct a Parzen window density estimate based on the positive class training data
- Over-sample the positive class by drawing synthetic samples according to the estimated density
- Apply the PSO aided tunable RBF classifier to the re-balanced data
- M. Gao, X. Hong, S. Chen and C.J Harris, “PDFOS: PDF estimation based over-sampling for imbalanced two class problems,” submitted to *IEEE Trans. Neural Networks*

Conclusions

- The celebrated OLS algorithm has evolved into state-of-the-arts for parsimonious modelling from large data
- Previous enhancements discussed include
  - Local regularisation, optimal experimental design, and leave-one-out cross validation
  - Incorporating prior knowledge naturally for efficient grey-box modelling
  - Implementing branch and bound for further computational efficiency enhancement
- Some very recent extensions have been briefly discussed
- Maintain simplicity and efficiency of original algorithm, which are so appealing to data modelling practitioners