ARESLab

Adaptive Regression Splines toolbox for Matlab

ver. 1.3

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Reference manual

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1. INTRODUCTION

What is ARESLab

ARESLab is a Matlab toolbox for working with piecewise-linear and piecewise-cubic regression models built using the Multivariate Adaptive Regression Splines technique (also known as MARS). (The term "MARS" is a registered trademark and thus not used in the name of the toolbox.) The original author of MARS technique is Jerome Friedman (Friedman 1991, Friedman 1993).

The toolbox allows building models (referred to as ARES models) using different settings, testing them on a separate test set or using k-fold Cross-Validation, using them for prediction, outputting equations for deployment, plotting the models etc. The built models can also be used as metamodels (also known as surrogate models) for design optimization tasks (e.g. see Chen et al. 2006, Kalnins et al. 2008, Kalnins et al. 2009, Jekabsons 2009b).

This reference manual provides overview of the functions available in the ARESLab.

ARESLab can be downloaded at http://www.cs.rtu.lv/jekabsons/.

The toolbox code is licensed under the GNU GPL ver. 2 or any later version.

Some parts of aresbuild and createList functions are derived from ENTOOL toolbox (Merkwirth & Wichard 2003, Norgaard 2000) which also falls under the GPL licence.

For any feedback on the toolbox including bug reports feel free to contact me (gints D-O-T jekabsons A-T rtu D-O-T lv).

Details

The ARESLab toolbox is written entirely in Matlab. I tried to implement the main functionality of the MARS technique for regression as close to the description in the Friedman's original paper (Friedman 1991) as possible. While implementing the knot placement part (see remarks about minSpan and endSpan in Section 2), I also took a look at the source code of the R Earth package (Milborrow 2009) and implemented it very similarly to Earth version 2.4-0. The only major difference at the moment I think is that the model building is not accelerated using "Fast MARS" queuing (Friedman 1993) together with the "fast least-squares update technique" (Friedman 1991). This difference however affects more the speed of the algorithm execution rather than the predictive performance of resulting models.

The absence of "Fast MARS" queuing means that the code might be rather slow for large data sets (however see the function descriptions on how to make it faster by setting more conservative values for algorithm parameters). Note that a much faster version of Multivariate Adaptive Regression Splines is included in VariReg software tool (Jekabsons 2009a, available at http://www.cs.rtu.lv/jekabsons/) which also can be put to work from within the Matlab environment (although with much less functionality). Another alternative is to use the Earth package for R which is very sophisticated however lacks the ability to create piecewise-cubic models.

Possible future updates for the toolbox (depending on the popularity of the toolbox):

- optional complete re-training of an existing model;
- automatic variable scaling;
- setting the upper limit of interactivity for each input variable separately;
- "Fast MARS" queuing;
- modelling for classification problems (although for two classes, one can code the output as 0/1, treat the problem as a regression, and use the current version of ARESLab).

Some further aspects of MARS mentioned in Friedman's papers but not implemented in ARESLab:

- automatic handling of missing values;
- automatic handling of categorical input variables (with the current version of ARESLab, the user must create a number of dummy variables in the usual way before building the model);
- model slicing.

Citing the ARESLab toolbox

Please give a reference to the software webpage in any publication describing research performed using the toolbox, e.g. like this:

Jekabsons G., ARESLab: Adaptive Regression Splines toolbox for Matlab, 2009, available at http://www.cs.rtu.lv/jekabsons/

2. AVAILABLE FUNCTIONS

ARESLab toolbox provides the following list of functions:

- aresbuild builds an ARES model;
- aresparams creates a configuration for ARES model building algorithm for further use with aresbuild, aresev, or areseve functions;
- arespredict makes predictions using an ARES model;
- arestest tests an ARES model on a test data set;
- aresev tests ARES performance using k-fold Cross-Validation;
- areseve finds the "best" value for penalty *c* (Generalized Cross-Validation penalty per knot) from a set of candidate values using k-fold Cross-Validation and MSE;
- aresplot plots surface of an ARES model;
- areseq outputs an ARES model in an explicit mathematical form.

2.1. Function are sbuild

Purpose:

Builds a regression model using the Multivariate Adaptive Regression Splines technique.

Call:

```
[model, time] = aresbuild(Xtr, Ytr, trainParams, weights, modelOld, verbose)
```

All the arguments, except the first two, of this function are optional. Empty values are also accepted (the corresponding default values will be used).

Input:

1		
Xtr, Ytr	: Training data cases ($xtr(i,:)$, $ytr(i)$), $i = 1,, n$. Note that it is recommended to pre-scale xtr values to [0,1] (Friedman 1991) and to standardize ytr values (Milborrow 2009). This is because widely different locations and scales for the input variables can cause instabilities that adversely affect the quality of the final model. The MARS technique is (except for numerics) invariant to the locations and scales of the input variables. It is therefore reasonable to perform a transformation that causes resulting locations and scales to be most favourable from the point of view of numeric stability (Friedman 1991).	
trainParams	: A structure of training parameters for the algorithm. If not provided, default values will be used (see function aresparams for details).	
weights	: A vector of data case weights; if supplied, the algorithm calculates the sum of squared errors multiplying the squared residuals by the supplied weights. The length of weights vector must be the same as the number of data cases (i.e. n). The weights must be nonnegative.	
modelOld	: If here an already built ARES model is provided, no forward phase will be done. Instead this model will be taken directly to the backward phase and pruned. This is useful for fast selection of the "best" penalty trainParams.c value using Cross-Validation e.g. in areseve function.	
verbose	: Set to false for no verbose. (default value = true)	

Output:

model : The built ARES model – a structure with the following elements:

coefs : Coefficient vector of the regression model (for the intercept term and each

basis function).

knotdims : Cell array of indexes of used input variables for each knot in each basis

function.

knotsites : Cell array of knot sites for each knot and used input variable in each basis

function.

knotdirs : Cell array of directions (-1 or 1) of the hinge functions for each used input

variable in each basis function.

experience : Vector of indexes of direct parents for each basis function (0 if there is no

direct parent or it is the intercept term).

trainParams : A structure of training parameters for the algorithm (the same as in the

input).

MSE : Mean Squared Error of the model in the training data set.

GCV : Generalized Cross-Validation (GCV) of the model in the training data set.

The GCV is calculated using trainParams.c argument (for details on GCV calculation, see Friedman 1991). The value may also be Inf if model's effective number of parameters (see Eq. 1) is larger than or equal

to n.

: For piecewise-cubic models only. Matrix of knot sites for the additional

side knots on the left of the central knot.

: For piecewise-cubic models only. Matrix of knot sites for the additional

side knots on the right of the central knot.

minx : Vector of minimums for input variables (used for t1 and t2 placements as

well as for model plotting).

maxx : Vector of maximums for input variables (used for t1 and t2 placements

as well as for model plotting).

endSpan : The used value of endSpan.

time : Algorithm execution time (in seconds)

Remarks:

The model building algorithm builds a model in two phases: forward selection and backward deletion. In the forward phase the algorithm starts with a model consisting of just the intercept term and iteratively adds reflected pairs of basis functions giving the largest reduction of training error. The forward phase is executed until one of the following conditions is met:

- 1) reached maximum number of basis functions (trainParams.maxFuncs);
- 2) the difference between err and newErr is smaller than trainParams.threshold, where newErr is calculated by dividing sum of squared residuals by the variance of Ytr and err is the newErr value from the previous iteration;
- 3) the newErr is smaller than trainParams.threshold;
- 4) the number of model's coefficients (i.e. the number of all the basis functions including the intercept term) in the next iteration is expected to be equal to or larger than n.

At the end of the forward phase we have a large model which typically overfits the data, and so typically a backward deletion phase is engaged. In the backward phase the model is simplified by deleting one least important basis function (according to GCV) at a time until the model again has only the intercept term. At the end of the backward phase, from those "best" models of each size one model of lowest GCV value is selected and outputted as the final one.

GCV for a model is calculated as follows (Hastie et al. 2009, Milborrow 2009):

$$GCV = MSE_{train} / \left(1 - \frac{enp}{n}\right)^2, \tag{1}$$

where MSE_{train} is Mean Squared Error of the evaluated model in the training data, n is the number of data cases in the training data, and enp is the effective number of parameters:

$$enp = k + c \times (k-1)/2, \tag{2}$$

where k is the number of basis functions in the model (including the intercept term) and c is trainParams.c. Note that (k-1)/2 is the number of hinge function knots, so the formula penalizes not only the number of model's basis functions but also the number of knots. Also note that in ARESLab in the situation when $enp \ge n$ the GCV value will be equal to Inf (the model is considered infinitely bad).

The largest possible final model after the pruning has $k = \operatorname{int}((n+c/2)/(1+c/2))$ basis functions for maxInteractions > 1 and $k = \operatorname{int}((n+c/3)/(1+c/3))$ basis functions for maxInteractions = 1. In the forward phase the models may also get larger than this however for such models GCV = Inf as then $enp \ge n$.

2.2. Function aresparams

Purpose:

Creates a structure of ARES configuration parameter values for further use with aresbuild, arescv, or arescvc functions.

Call:

trainParams = aresparams(maxFuncs, c, cubic, cubicFastLevel, selfInteractions,
maxInteractions, threshold, prune, useMinSpan, useEndSpan, maxFinalFuncs)

All the arguments of this function are optional. Empty values are also accepted (the corresponding default values will be used).

Input:

For most applications, it can be expected that the most attention should be paid to the following parameters: maxFuncs, c, cubic, maxInteractions, and maybe threshold.

maxFuncs

: The maximal number of basis functions included in the model in the forward model building phase (before pruning in the backward phase). Includes the intercept term. (default value = 21). The recommended value for this parameter is two times the number of basis functions in the final model (Friedman 1991). While building a model, the number may also not be reached because of some another stopping criterion (see remarks for details).

С

: Generalized Cross-Validation (GCV) penalty per knot. Theory suggests values in the range of about 2 to 4. Larger values will lead to fewer knots being placed (i.e. final models will be simpler). A value of 0 penalizes only terms, not knots (can be useful e.g. with lots of data and low noise). The recommended (and default) value is 3 (Friedman 1991). Note that if $\max[nextions] = 1$ (additive modelling) then function aresbuild will recalculate c so that the actually used value is 2c/3; this is recommended for additive modelling (Friedman 1991).

cubic

: Whether to use piecewise-cubic (true) or piecewise-linear (false) type of modelling (Friedman 1991). It is expected that the piecewise-cubic modelling will give higher predictive performance for smoother and less noisy data. (default value = true)

cubicFastLevel

: In ARESLab, there are three types (levels) of piecewise-cubic modelling implemented. In level 0 cubic modelling for each candidate model is done

in both phases of the technique (slow). In level 1 cubic modelling is done only in the backward phase (much faster). In level 2 cubic modelling is done after both phases only for the final model (fastest). The default and recommended level is 2. Levels 0 and 1 may bring extra precision in the modelling process however the results can actually also be worse. It is expected that the two much slower levels will mostly be not worth the waiting.

selfInteractions: The maximum degree of self interactions for any input variable. In ARESLab, it can be larger than 1 only for piecewise-linear modelling. Usually the self interactions are never allowed. (default value = 1, no self interactions)

maxInteractions

: The maximum degree of interactions between input variables. Set to 1 for additive modelling (i.e. no interaction terms). For maximal interactivity between the variables, set the parameter to $d \times \text{selfInteractions}$, where d is the number of input variables – this way the modelling procedure will have the most freedom building a complex model. Typically only a low degree of interaction is allowed, but higher degrees can be used when the data warrants it. (default value = 1)

threshold

: One of the stopping criteria for the forward phase. The larger the value of threshold the potentially simpler models are generated (see remarks section of aresparams and aresbuild for details). Default value = 1e-4. For noise-free data the value may be lowered.

prune

: Whether to perform the model pruning (the backward phase) or not. (default value = true)

useMinSpan

: In order to lower the local variance of the estimates, a minimum span is imposed that makes the technique resistant to runs of positive or negative error values between knots (by jumping over a (minSpan) number of data cases each time the next potential knot placement is requested) (Friedman 1991). useMinSpan allows to disable (set to 0 or 1) the protection so that all the data cases are considered for knot placement in each dimension (except, see useEndSpan). Disabling minSpan may enable to create a model which is more responsive to local variations in the data however this can lead to an overfitted model even for noise-free data. Setting the useMinSpan to > 1, enables also to manually tune the value. (default and recommended value = -1 which corresponds to the automatic mode)

useEndSpan

: In order to lower the local variance of the estimates near the ends of data intervals, a minimum span is imposed that makes the technique resistant to runs of positive or negative error values between extreme knot locations and the corresponding ends of data intervals (by not allowing to place a knot too near (endSpan) to the end of data interval) (Friedman 1991). useEndSpan allows to disable (set to 0 or 1) the protection so that all the data cases are considered for knot placement in each dimension (except, see useMinSpan). Disabling endSpan may enable to create a model which is more responsive to local variations in the data however this can lead to an overfitted model even for noise-free data. Setting the useMinSpan to > 1, enables also to manually tune the value. (default and recommended value = -1 which corresponds to the automatic mode)

maxFinalFuncs

: Maximum number of basis functions (including the intercept term) in the pruned model. Use this (rather than the maxFuncs parameter) to enforce an upper bound on the final model size. (default value = Inf).

Output:

trainParams : A struc

: A structure of training parameters for aresbuild function containing the provided values of the parameters (or default ones, if not provided).

Remarks:

The knot placement in aresbuild is implemented very similarly to R Earth package version 2.4-0 (Milborrow 2009) with calculations of minSpan and endSpan values using formulas given in Eq. 45 and Eq. 43 of the Friedman's original paper (Friedman 1991) with alpha = 0.05. Note that for a fixed dimensionality of the data, the endSpan value always stays the same but the value of the minSpan is recalculated for each individual parent basis function (including the intercept term) which is used for generation of new basis functions.

If more speed is required, one can try some of the following options:

- 1) decreasing maxFuncs (less iterations in the forward phase);
- 2) increasing value of cubicFastLevel or turning the piecewise-cubic modelling completely off (setting the level below 2 makes the procedure considerably slower; however note that if cubicFastLevel = 2, turning the piecewise-cubic modelling off will give almost no speed gain);
- 3) decreasing selfInteractions (less candidate models in the forward phase);
- 4) decreasing maxInteractions (less candidate models in the forward phase);
- 5) increasing threshold (may result in less iterations in the forward phase);
- 6) manually decreasing values for useMinSpan and useEndSpan (less candidate models in the forward phase).

Note that decreasing the number of iterations or candidate models in the forward phase may also result in underfitted final models.

2.3. Function arespredict

Purpose:

Predicts output values for the given query points using an ARES model.

Call:

```
Yq = arespredict(model, Xq)
```

Input:

model : ARES model

: Inputs of query data points (xq(i,:)), i = 1, ..., nq

Output:

Yq : Predicted outputs of query data points (Yq(i)), i = 1, ..., nq

2.4. Function arestest

Purpose:

Tests an ARES model on a test data set (Xtst, Ytst).

Call:

```
[MSE, RMSE, RRMSE, R2] = arestest(model, Xtst, Ytst)
```

Input:

model : ARES model

Xtst, Ytst : Test data cases (Xtst(i,:), Ytst(i)), i = 1, ..., ntst

Output:

MSE : Mean Squared Error

RMSE : Root Mean Squared Error

RRMSE : Relative Root Mean Squared Error R2 : Coefficient of Determination

2.5. Function arescy

Purpose:

Tests ARES performance using k-fold Cross-Validation.

Call:

```
[avgMSE, avgRMSE, avgRRMSE, avgR2, avgTime] = arescv(X, Y, ... trainParams, weights, k, shuffle, cvc_cTry, cvc_k, verbose)
```

All the arguments, except the first two, of this function are optional. Empty values are also accepted (the corresponding default values will be used).

Input:

x, y: Data cases (x(i,:), y(i)), i = 1, ..., n

trainParams : See function are sbuild. weights : See function are sbuild.

k: Value of k for k-fold Cross-Validation. The typical values are 5 or 10. For

Leave-One-Out Cross-Validation set k equal to n. (default value = 10)

shuffle : Whether to shuffle the order of the data cases before performing Cross-

Validation. Note that the random seed value can be controlled externally

before calling arescv. (default value = true)

cvc_cTry, cvc_k : cTry and k values for arescvc function. Supply these values if you want

to perform another Cross-Validation for finding the "best" penalty c value in each iteration of the outer Cross-Validation loop of aresev. (default

values = [], meaning that a fixed c is used)

verbose : Set to false for no verbose. (default value = true)

Output:

avgmse : Average Mean Squared Error avgrmse : Average Root Mean Squared Error

avgrrmse : Average Relative Root Mean Squared Error

avgR2 : Average Coefficient of Determination

avgTime : Average execution time

2.6. Function arescvc

Purpose:

Finds the "best" value for penalty c from a set of candidate values using k-fold Cross-Validation and MSE.

Call:

```
cBest = arescv(X, Y, trainParams, cTry, weights, k, shuffle, verbose)
```

All the arguments, except the first three, of this function are optional. Empty values are also accepted (the corresponding default values will be used).

Input:

x, y: Data cases (x(i,:), y(i)), i = 1, ..., n

trainParams : See function are sbuild.

cTry : A set of candidate values for c. (default = 1:5)

weights : See function are sbuild.

k : Value of k for k-fold Cross-Validation. The typical values are 5 or 10. For

Leave-One-Out Cross-Validation set k equal to n. (default value = 10)

shuffle : Whether to shuffle the order of the data cases before performing Cross-

Validation. Note that the random seed value can be controlled externally

before calling areseve. (default value = true)

verbose : Set to false for no verbose. (default value = true)

Output:

cBest : The "best" value for penalty c.

Remarks:

This function finds the best penalty c value using Cross-Validation in a clever way using function are sbuild, i.e. in each CV iteration the forward phase in are sbuild is done only once while the backward phase is done separately for each cty value. The results will be the same as if each time a full model building process would be performed because in the forward phase the GCV criterion is not used.

2.7. Function aresplot

Purpose:

Plots surface of an ARES model.

Call:

```
aresplot(model, minX, maxX, vals, gridSize)
```

All the arguments, except the first one, of this function are optional. Empty values are also accepted (the corresponding default values will be used).

Input:

model : ARES model

minx, maxx : User defined minimum and maximum values for each input variable (this

is the same type of data as in model.minx and model.maxx). If not supplied,

the model.minx and model.maxx values will be used.

vals : Only used when the number of input variables is larger than 2. This is a

vector of fixed values for all the input variables except the two varied in the plot. The two varied variables are identified in vals using NaN values. By default the two first variables will be varied and all the other will be fixed

at (max - min) / 2.

gridSize : Grid size. (default value = 50)

2.8. Function areseq

Purpose:

Outputs an ARES model in an explicit mathematical form (useful e.g. for deployments of built ARES models in other software).

Call:

```
eq = areseq(model, precision)
eq = areseq(model)
```

Input:

model : ARES model

precision : Number of digits in the model coefficients and knot sites.

Output:

eq : A cell array of equations for individual basis functions and the main

model. Note that the outputted equations will have piecewise-linear form even if the model itself is really piecewise-cubic. The model coefficients

however will be those from the original piecewise-cubic model.

3. EXAMPLES OF USAGE

3.1. Ten-dimensional function with noise

We start by creating a data set using a ten-dimensional function with zero mean unit variance Gaussian noise. The data consists of 200 cases randomly uniformly distributed in a ten-dimensional unit hypercube.

```
clear X = rand([200,10]); Y = 10.*sin(pi.*X(:,1).*X(:,2)) + 20.*(X(:,3)-0.5).^2 + ... 10.*X(:,4) + 5.*X(:,5) + randn(200,1);
```

We define the maximal number of basis functions to be 41 (including the intercept term), and limit maximum interaction level to 2 (only pairwise products of basis functions will be allowed), leaving all the other parameters to their defaults. The model will be of piecewise-cubic type as it is the default.

```
params = aresparams(41, [], [], [], 2);
```

Now the ARES model is built by calling aresbuild.

```
model = aresbuild(X, Y, params)
```

As the model building process ends, we can examine the data structure of the final model. It has 19 basis functions including the intercept term.

We evaluate predictive performance of this ARES configuration on the data using 5-fold Cross-Validation.

```
[avgMSE, avgRMSE, avgRRMSE, avgR2] = arescv(X, Y, params, [], 5)
avgMSE = 1.3324
avgRMSE = 1.1533
avgRRMSE = 0.2264
avgR2 = 0.9484
```

Let's try doing the same but instead of piecewise-cubic modelling we will use piecewise-linear.

```
params = aresparams(41, [], false, [], [], 2);
model = aresbuild(X, Y, params)
```

```
model =
          coefs: [16x1 double]
       knotdims: {15x1 cell}
      knotsites: {15x1 cell}
       knotdirs: {15x1 cell}
        parents: [15x1 double]
    trainParams: [1x1 struct]
            MSE: 0.8912
            GCV: 1.3668
           minX: [1x10 double]
           maxX: [1x10 double]
        endSpan: 10
[avgMSE, avgRMSE, avgRRMSE, avgR2] = arescv(X, Y, params, [], 5)
avgMSE = 2.1058
avgRMSE = 1.4404
avgRRMSE = 0.2760
avgR2 = 0.9232
```

Finally we output the equation of the model with all the basis functions.

```
areseg(model, 5);
   BF1 = max(0, x4 - 0.40253)
   BF2 = max(0, 0.40253 - x4)
   BF3 = \max(0, x1 - 0.6947)
   BF4 = max(0, 0.6947 -x1)
   BF5 = max(0, x2 - 0.49984)
   BF6 = max(0, 0.49984 - x2)
   BF7 = max(0, x5 - 0.21788)
   BF8 = max(0, 0.21788 -x5)
   BF9 = max(0, 0.56159 -x3)
   BF10 = BF5 * max(0, x1 -0.50511)
   BF11 = BF5 * max(0, 0.50511 -x1)
   BF12 = BF6 * max(0, 0.82122 -x1)
   BF13 = max(0, x3 - 0.17529)
   BF14 = BF5 * max(0, x8 - 0.07177)
   BF15 = BF13 * max(0, x6 -0.63998)
   y = 9.9718 + 10.305*BF1 - 10.39*BF2 + 6.1989*BF3 - 13.962*BF4 + 9.92*BF5 - 20.214*BF6 + 4.8195*BF7
6.8873*BF8 +18.216*BF9 -65.491*BF10 -18.646*BF11 +22.03*BF12 +11.225*BF13 +2.6317*BF14 +4.227*BF15
```

3.2. Noise-free two-dimensional function

We start by creating training and test data using a two-dimensional noise-free function. The training data consists of 121 cases distributed in a regular 11×11 grid. The test data has 10000 cases distributed randomly.

```
clear
[tmpX1,tmpX2] = meshgrid(-1:0.2:1, -1:0.2:1);
X(:,1) = reshape(tmpX1, numel(tmpX1), 1);
X(:,2) = reshape(tmpX2, numel(tmpX2), 1);
clear tmpX1; clear tmpX2;
Y = sin(0.83.*pi.*X(:,1)) .* cos(1.25.*pi.*X(:,2));

Xt = rand([10000,2]);
Yt = sin(0.83.*pi.*Xt(:,1)) .* cos(1.25.*pi.*Xt(:,2));
```

Such noise-free functions can be approximated very precisely. We define the maximal number of basis functions to be 121, no penalty for knots, and maximum interaction level equal to 2 (the

number of input variables), leaving all the other parameters to their defaults. The model will be of piecewise-cubic type as it is the default.

```
params = aresparams(121, 0, [], [], [], 2);
```

Now the ARES model is built by calling aresbuild.

```
model = aresbuild(X, Y, params)
```

As the model building process ends, we can examine the data structure of the new model. The model has 44 basis functions including the intercept term.

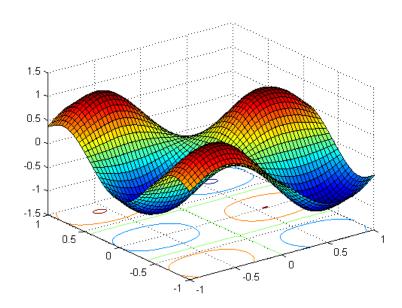
We test the model using test data.

```
[MSE, RMSE, RRMSE, R2] = arestest(model, Xt, Yt)

MSE = 1.9909e-004
RMSE = 0.0141
RRMSE = 0.0244
R2 = 0.9994
```

Plot the surface of the model.

```
aresplot(model);
```

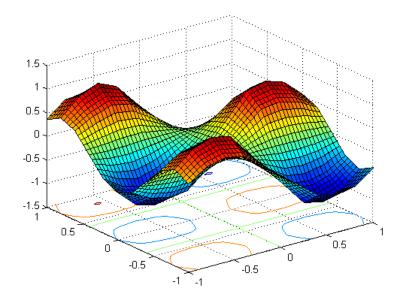


Let's try doing the same but instead of piecewise-cubic modelling we will use piecewise-linear.

```
params = aresparams(100, 0, false, [], [], 2);
model = aresbuild(X, Y, params);
[MSE, RMSE, RRMSE, R2] = arestest(model, Xt, Yt)

MSE = 0.0023
RMSE = 0.0480
RRMSE = 0.0829
R2 = 0.9931

aresplot(model);
```



4. REFERENCES

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