PCE VS RSM

This example is with known exact solution. Compared with analytical solution, this example hopes to provide surrogate model to create

customer defined loglikelihood to do Bayesian inference

1 - INITIALIZE UQLAB

```
clearvars
rng(100,'twister')
uqlab
```

```
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UQLab is distributed under the BSD 3-clause open source license available at:
C:\NY2023\D_document\UQLab_Rel2.0.0\LICENSE.

To request special permissions, please contact:
  - Stefano Marelli (marelli@ibk.baug.ethz.ch).

Useful commands to get started with UQLab:
uqlab -doc           - Access the available documentation
uqlab -help          - Additional help on how to get started with UQLab
uq_citation help   - Information on how to cite UQLab in publications
uqlab -license       - Display UQLab license information
```

2 - Data for FE realization and measurement

Read measurements for each points along the beam ***Measurement Y*** (dim 10X29): 10 sets of experiments and 29 monitored points ***Z*** along

the beam for each experiement

```
Measurement = xlsread("data.xlsx",'Measurement_for_surrogate','A2:AC11');
```

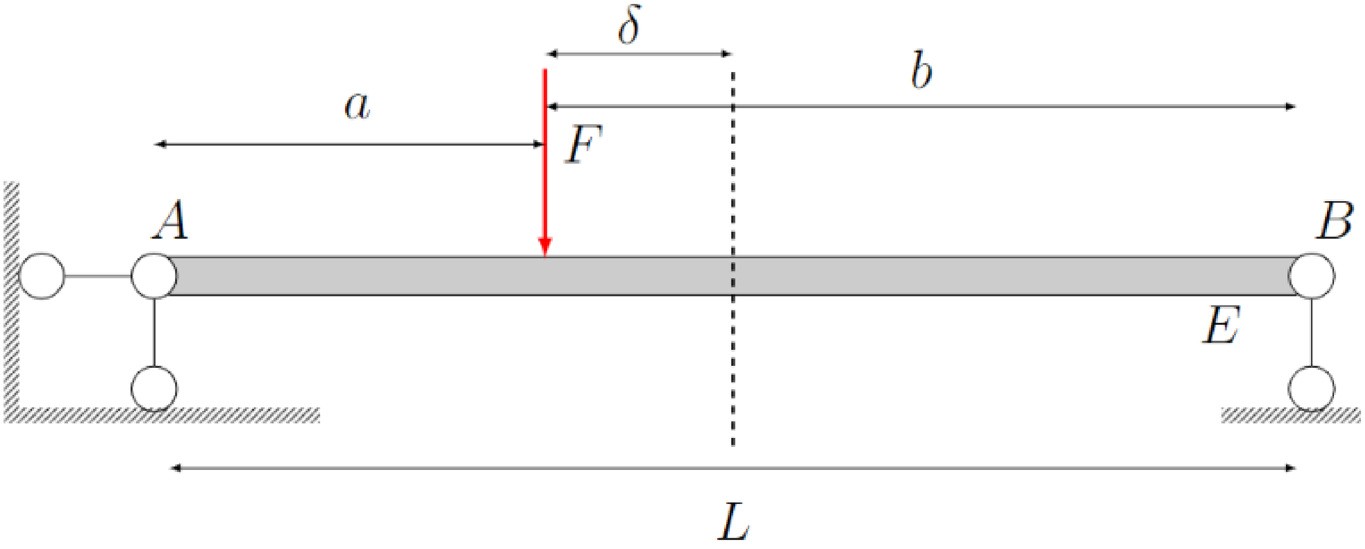
Read FE realization from LHS sampling

$$y = \mathscr{M}(x)$$

Dim (248X3)

```
FE_Realization = xlsread("data.xlsx",'FE_models','A2:AE249');
```

2 - PRIOR DISTRIBUTION for PCE model and Bayesian inference



b_b = 0.15; % beam width (m)

b_h = 0.3; % beam height (m)

a % distance from the point A (m)

b % distance from the point B (m)

L = 30; % beam length (m)

F = 43000;% Concentrated force (N)

```
%Priors on E and p
PriorOpts.Marginals(1).Name = 'E';                  % Young's modulus
PriorOpts.Marginals(1).Type = 'Gaussian';
PriorOpts.Marginals(1).Moments = [25e9 5e9];    % (N/m^2)
PriorOpts.Marginals(1).Bounds = [25e9 -2*3e9, 25e9 + 2*3e9];

PriorOpts.Marginals(2).Name = 'delta';                  % Concentrated load loading
position
PriorOpts.Marginals(2).Type = 'Gaussian';
PriorOpts.Marginals(2).Moments = [3 5]; % (N/m)
PriorOpts.Marginals(2).Bounds = [-10, 10];

myPriorDist = uq_createInput(PriorOpts);
```

3 - Calculate the residual $r(x,z)$ for surrogate model $\widetilde{\mathscr{M}}$

Calculate the Root-mean-square-error data for surrogate

$$r(\overrightarrow{x}, \overrightarrow{z}) = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(Y_i - \mathscr{M}(\overrightarrow{x}, \overrightarrow{z}))^2}$$

$$\overrightarrow{x} = [E, \delta]; \overrightarrow{z} = [z_1, z_2, ..., z_{28}, z_{29}];$$

r is residual; $\overrightarrow{x}$ is parameters of interests; E is elastic modulus; δ is the loading postion

$\overrightarrow{z}$ is the different measurement points along the beam;

$\mathscr{M}$ is the FE model; Y_i is the measurement data; N is the number of experiment expNum.

```
expNum = size(Measurement,1);% experiment number  N = 10

Nreal = size (FE_Realization,1);% number of FE realization = 248

Npoint = size(Measurement,2);% number of z [z1,z2,...,z28,z29]

Residual = []; % intitail value for Residual

%loop to calculate the ResidualSum
for i  = 1: expNum

        error = ((Measurement(i,:) - FE_Realization(1:Nreal,3:31)) ).^2;

        Residual = [Residual, sum(error,2)];

end

%Divide the number of experiment expNum = 10 and monitored points number along
%the beam Npoint = 29
ResidualSum = sqrt(sum(Residual,2)/expNum/Npoint);
```

4 - Create RSM surrogate $\widetilde{\mathscr{M}}(r)$

RSM:Response surface model

```
%Get the residual data for RSM

RSM_data = [FE_Realization(1:Nreal,1),FE_Realization(1:Nreal,2),ResidualSum];
```

Response surface model fitting

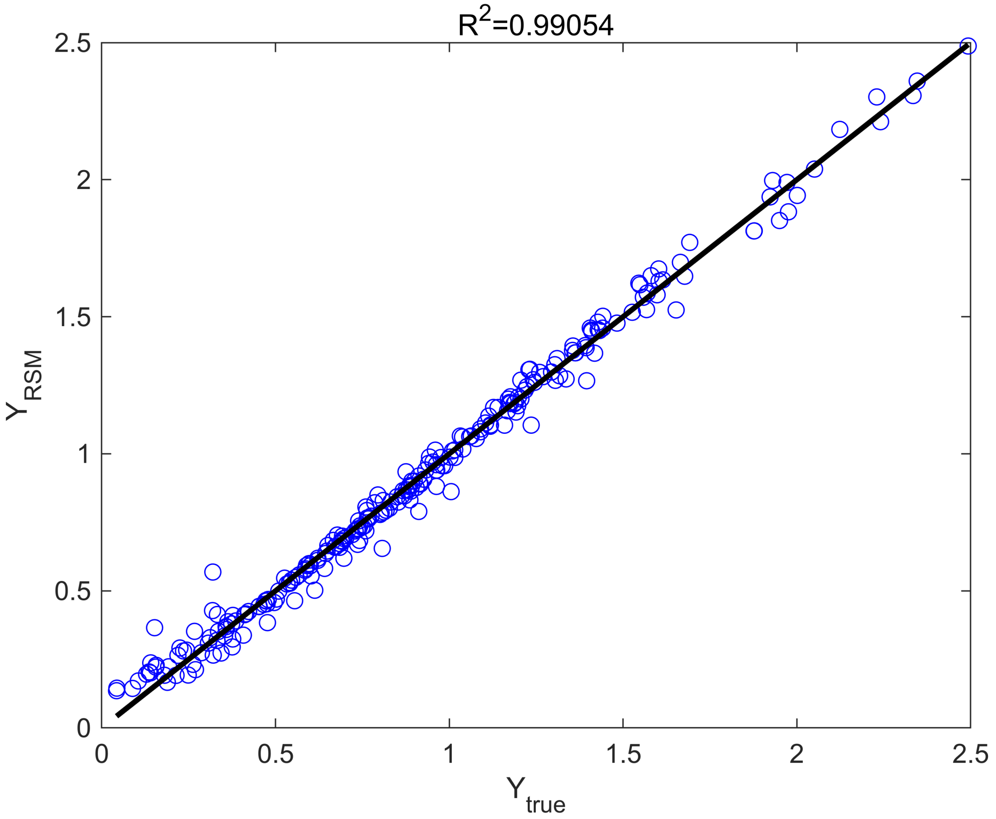
```
x(:,1) = RSM_data(:,1)./10e9;% normlized the E with 10e9Pa, beacuase E is too big
to fit good results
x(:,2) = RSM_data(:,2)./5;% normalized the delta with deviatoin = 5m
y_fit = RSM_data(:,3); % sum error

% response surface model-- Six order polynomial equation

model_fun_RSM = @(p,x) p(1) + ...
p(2) * x(:,1) + ...
p(3) * x(:,2) + ...
p(4) * x(:,1).^2 + ...
p(5) * x(:,2).^2 + ...
p(6) * x(:,1).^3 + ...
p(7) * x(:,2).^3 + ...
p(8) * x(:,1).^4 + ...
p(9) * x(:,2).^4 + ...
p(10) * x(:,1).^3 .* x(:,2) + ...
p(11) * x(:,1).^2 .* x(:,2).^2 + ...
p(12) * x(:,1) .* x(:,2).^3 + ...
p(13) * x(:,1).^4 .* x(:,2) + ...
p(14) * x(:,1) .* x(:,2).^4 + ...
p(15) * x(:,1).^5 + ...
p(16) * x(:,2).^5 + ...
p(17) * x(:,1).^4 .* x(:,2).^2 + ...
p(18) * x(:,1).^3 .* x(:,2).^3 + ...
p(19) * x(:,1).^2 .* x(:,2).^4 + ...
p(20) * x(:,1) .* x(:,2).^5 + ...
p(21) * x(:,1).^6 + ...
p(22) * x(:,2).^6 + ...
p(23) * x(:,1).^5 .* x(:,2) + ...
p(24) * x(:,1).^4 .* x(:,2).^2 + ...
p(25) * x(:,1).^3 .* x(:,2).^3 + ...
p(26) * x(:,1).^2 .* x(:,2).^4 + ...
p(27) * x(:,1) .* x(:,2).^5 + ...
p(28) * x(:,1).^6 .* x(:,2) + ...
p(29) * x(:,1).^5 .* x(:,2).^2 + ...
p(30) * x(:,1).^4 .* x(:,2).^3 + ...
p(31) * x(:,1).^3 .* x(:,2).^4 + ...
p(32) * x(:,1).^2 .* x(:,2).^5 + ...
p(33) * x(:,1) .* x(:,2).^6;


p0 = [1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1  1 1 1 1 1 1 1 1 ];%initial
value for the coeficients

[p,R,J,CovB,MSE,ErrorModelInfo] = nlinfit(x,y_fit,model_fun_RSM,p0);
```

```
警告: 解处的 Jacobian 矩阵为病态，而且某些模型参数的估计值可能不准确(不可识别)。进行预测时要谨慎。
```

```
% coeficient :https://ww2.mathworks.cn/help/stats/nlinfit.html#d124e38841
```

Surrogate mode: Predicted vs True

```
y_estimate = model_fun_RSM(p,x);
SSR = sum(R.^2);
SST = sum((y_fit - mean(y_fit)).^2);
R2 = 1 - SSR / SST;
str=['R^2=', num2str(R2)];
close all;
plot(y_fit,y_estimate,'bo');
hold on;
plot([min(y_fit),max(y_fit)],[min(y_fit),max(y_fit)],'k-','LineWidth',2);
title(str);
xlabel('Y_{true}')
ylabel('Y_{RSM}')
hold off;
```



5 - Create PCE surrogate $\widetilde{\mathscr{M}}(r)$

PCE: Polynomial Chaos expansion

```
%Get the residual data for PCE

PCE_data = [FE_Realization(1:Nreal,1),FE_Realization(1:Nreal,2),ResidualSum];
```

PCE Fitting

```
myPCE = PCE_create(PCE_data);
```

```
---   Calculating the PCE coefficients by regression.   ---
警告: Warning: numerical instability!! Gamma for LAR iteration 5 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 7 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 8 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 9 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 14 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 11 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 12 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 13 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 19 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 20 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 25 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 27 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 31 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 32 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 33 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 34 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 35 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 34 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 35 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 44 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 10 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 53 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 54 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 16 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 22 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 47 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 51 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 52 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 53 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 54 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 55 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 56 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 58 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 59 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 60 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 61 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 62 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 63 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 64 was set to 0 to prevent crashes.
警告: Warning: numerical instability!! Gamma for LAR iteration 65 was set to 0 to prevent crashes.
The estimation of PCE coefficients stopped at polynomial degree 10 and qNorm 1.00 for output variable 1
Final LOO error estimate: 4.064805e-01
---                Calculation finished!                               ---
```

Print a summary of the resulting PCE metamodel:

```
uq_print(myPCE)
```

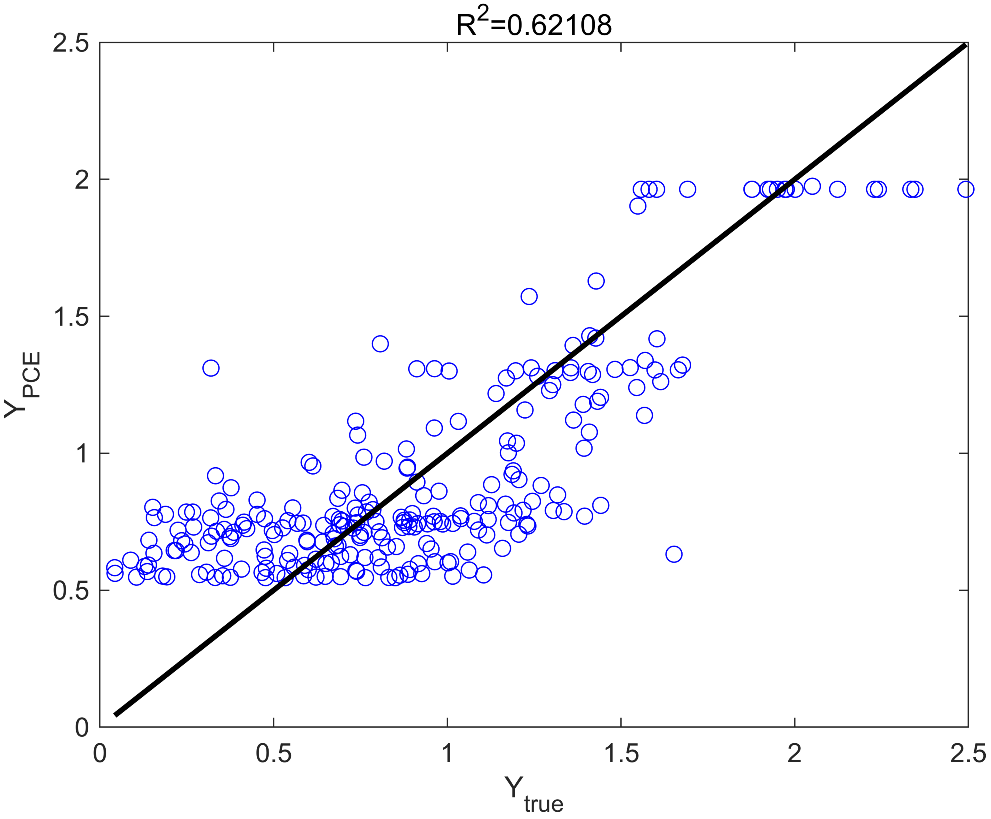
```
%------------ Polynomial chaos output ------------%
   Number of input variables:    2
   Maximal degree:               10
   q-norm:                       1.00
   Size of full basis:           66
   Size of sparse basis:         5
   Full model evaluations:       248
   Leave-one-out error:          3.9285616e-01
   Modified leave-one-out error: 4.0648052e-01
```

```
    Mean value:                      0.8220
    Standard deviation:              0.2572
    Coef. of variation:               31.295%
 %-------------------------------------------------%
```

```
hold on
```

Plot the true vs. predicted values:

```
%Obtain the X_val and YPCE/Y_val
X_val(:,1) = PCE_data(1:Nreal,1);
X_val(:,2) = PCE_data(1:Nreal,2);
YPCE = uq_evalModel(myPCE,X_val);
Y_val = PCE_data(1:Nreal,3);
R = Y_val - YPCE;
SSR = sum(R.^2);
SST = sum((Y_val - mean(Y_val)).^2);
R2 = 1 - SSR / SST;
str=['R^2=', num2str(R2)];
close all;
plot(Y_val,YPCE,'bo');
hold on;
plot([min(Y_val),max(Y_val)],[min(Y_val),max(Y_val)],'k-','LineWidth',2);
title(str);
xlabel('Y_{true}')
ylabel('Y_{PCE}')
hold off;
```



Export the PCE strucuture

```
save myPCE
```

6 - Define the priors for discrepancy σ

By default, UQlab assumes an independent and identically distributed discrepancy

$\varepsilon \sim \mathcal{N}(0, \mu_y^2)$, with $\mu_y = \frac{1}{N} \sum_{i=1}^{N} y_i$

```
PriorOpts.Marginals(3).Name = 'sigma2'; % variance
PriorOpts.Marginals(3).Type = 'Uniform';
sigma2 = mean(Measurement(:,:),"all");
PriorOpts.Marginals(3).Parameters = [0 sigma2^2];
myPriorDist = uq_createInput(PriorOpts);
```

7 - Define the custom-loglikelihood and measurement data for UQlab calculation

$$\log \mathscr{L}(\Theta) = \sum_{i=1}^{N} \left(-\frac{1}{2} \left(r_i(\vec{x}, \vec{z}) \right)^T \Sigma(\epsilon)^{-1} \left(r_i(\vec{x}, \vec{z}) \right) \right) - \frac{3N}{2} \log(2\pi) - \frac{N}{2} \log\left(\det(\Sigma(\epsilon))\right)$$

Monitored data Y_i for beam deflection have been used in PCE surrogate model. No measurements available for Bayesian inference: Pass zeros to measurement Y_i just for calculation, which equals:

$$r(\vec{x}, \vec{z}) \sim (0 - r(\vec{x}, \vec{z})) \sim (Y_i - \mathscr{M}(\vec{x}, \vec{z}))$$

$r(\vec{x}, \vec{z})$ dim 248X1 $\sim$ $(Y_i - \mathscr{M}(\vec{x}, \vec{z}))$ dim 248X29

Also, measurement data for Y_{10X29} changed into Y_{10X1}

```
y = zeros(1,1);
myData.y = y;
myData.Name = 'Zeros vector measurement for Bayesian inference';
```

Loglikelihood still follows the Gaussian discrepancy criteria

```
myLogLikeli = @(params,y) myLogLikeli2(params,y);
```

8 - Solver options

```
Solver.Type = 'MCMC';
Solver.MCMC.Visualize.Parameters = [1 2];
Solver.MCMC.Visualize.Interval = 10;
Solver.MCMC.Sampler = 'AIES';
Solver.MCMC.Steps = 500;
Solver.MCMC.NChains = 5;
Solver.MCMC.Proposal.PriorScale = 1e-3;
```