SAND2014-3134P

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# Dakota Sensitivity Analysis and Uncertainty Quantification, with Examples



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#### SAND2014-3134P

#### Dakota Sensitivity Analysis (SA)



- SA goals and examples
- Global SA approaches and metrics available in Dakota
- Select Dakota examples for parameter studies and global SA

#### Why Perform Sensitivity Analysis?



- What? Understand code output variations as input factors vary
- Why? Identify most important variables and their interactions
  - Identify key model characteristics: smoothness, nonlinear trends, robustness
  - Provide a focus for resources
    - Data gathering and model development
    - Code development
    - Uncertainty characterization
  - Screening: Identity the most important variables, down-select for further UQ or optimization analysis
  - Can have the side effect of identifying code and model issues
  - Data can be used to construct surrogate models
- Dakota SA formalizes and generalizes one-off sensitivity studies you're likely already doing
- Provides richer global sensitivity analysis methods

# Sensitivity Analysis: Influence of Inputs on Outputs





#### Assess variations in f(x1) due to (small or large) perturbations in x1.

- Local sensitivities
  - Partial derivatives at a specific point in input space.
  - Given a specific x1, what is the slope at that point?
  - Can be estimated with finite differences
- Global sensitivities
  - Found via sampling and regression.
  - What is the general trend of the function over all values of x1?
  - Typically consider inputs uniformly over their whole range

many already do basic SA; perturb from nominal, see effect

# Global Sensitivity Analysis Example: Earth Penetrator





12 parameters describing target & threat uncertainty, including... threat: width, length



Notional model for illustration purposes only (http://www.sandia.gov/ASC/library/fullsize/penetrator.html)

- Underground target with external threat: assess sensitivity in target response to target construction and threat characteristics
- Response: angular rotation (φ) of target roof at mid-span
- Analysis: CTH Eulerian shock physics code; JMP stats
- Revealed most sensitive input parameters and nonlinear relationships



# Global SA Example: Nuclear Reactor Thermal-Hydraulics Model

- Assess parameter influence on boiling rate, a key crud predictor
- Dakota correlation coefficients: strong influence of core operating parameters (pressure more important than previously thought)
- Dittus-Bolter correlation model may dominate model form sensitivities (also nonlinear effects of ExpPBM)
- Scatter plots help visualize trend in input/output relationships



sensitivity of mass evaporation rate (max) to operating parameters



#### parameter influence on number of boiling sites



# Group Discussion Questions: Your Sensitivity Analysis Practice



- Do you currently perform sensitivity analysis or parameter perturbations?
- What are example SA questions you (could) ask in your domain?
- How do (would) you answer them?
- What measures of sensitivity, ranking, or importance are you most familiar with?
- What are the key challenges you face?

#### **Cantilever Beam Model**





#### **Parameters:**

- L: length (in)
  w: width (in)
  t: thickness (in.)
  ρ: density (lb/ft<sup>3</sup>)
  E: Young's modulus (lb/in<sup>2</sup>)
  X: horizontal load (lb)
  Y: vertical load (lb)
- Posponsos:

#### **Responses:**

M: mass (lb) S: stress (lb/in<sup>2</sup>) D: displacement (in)

$$M = \rho * wt * \frac{L}{12^3}$$

$$S = \frac{600}{wt^2}Y + \frac{600}{w^2t}X$$

$$D = \frac{4L^3}{Ewt} \sqrt{\left(\frac{Y}{t^2}\right)^2 + \left(\frac{X}{w^2}\right)^2}$$

### Global Sensitivity Analysis in Dakota

- Assess effect of input variables considered jointly over their whole range. Dakota process:
  - Specify variables: lower and upper bounds
  - Specify method: e.g., uniform random sampling
  - Specify responses: compute response value at each sample point
  - Run Dakota and analyze input/output relationships
- Sample designs (methods) available:
  - Parameter studies: list, centered, grid, vector, user
  - Random sampling: Monte Carlo, Latin hypercube, Quasi-MC, CVT
  - DOE/DACE: Full-factorial, orthogonal arrays, Box-Behnken, CCD
  - Morris one-at-a-time
  - Sobol indices via variance-based decomposition, polynomial chaos
- Metrics: trends, correlations, main/interaction effects, Sobol indices, importance factors/local sensitivities





# Basic Dakota SA for Cantilever: Centered and Grid Parameter Studies





- Start at nominal values, perturb up and down in each coordinate direction
- Specify the parameter variations, which responses to study
- See Dakota input and output (following slides)

- What changes to Dakota input will instead perform the grid parameter study at left?
- Dakota Reference Manual helps with keyword choice...
- What are benefits/drawbacks of these methods?



# Dakota Input File: Cantilever Centered Parameter Study





- Catalog variable/response sets to tabular file
- Algorithm configuration: steps in each variable
- Center point: initial point / initial state

- How parameters are mapped to responses
- Responses from simulation

#### **Results: Centered Parameter Study**





 Univariate effects of parameters on each response

mass vs. X

50

Х

55

60

What do you observe?

6.1

6.0

5.9

5.8 seu 5.7

5.6

5.5

5.4

40

45

What are benefits/drawbacks?



# Exercise: Multi-dimensional Parameter Study



- Goal: understand how responses area, stress, and displacement vary with respect to the inputs w and t on a grid of points.
- Exercise: change previous input file to run the mod\_cantilever computational model at a grid of points over [1.0, 4.0] using the multidim\_parameter\_study method
- Try 9 points in one dimension, 6 in the other
- See method and variable commands in Dakota reference manual
- What parts of the file did you have to change?



#### Dakota Input File and Results: Cantilever Multi-dimensional Parameter Study

ı.



environment
tabular_data output_precision 1e-16
method
multidim_parameter_study
partitions = 2 2 2 2 2 2 2 2
vaniah] oc
active all
$conclinuous\_uesign = 5$
$upper_bounds = 1.2 1.2 6.0$
doccnintons "w" "t" "L"
continuous state = 4
$\frac{1}{10000000000000000000000000000000000$
lower bounds = 400 23 F+6 40 80
descriptors 'p' 'E' 'X' 'Y'
interface.
fork
analysis driver = 'driver.sh'
responses,
num objective functions = $3$
response descriptors = 'mass' 'stress' 'displacement
no gradients
no hessians
-



#### Dakota tabular data plotted with Minitab

What are benefits/drawbacks?

#### Dakota Input File and Results: Cantilever Multi-dimensional Parameter Study

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#### Workhorse SA Method: Random Sampling

- Generate space filling design (typically Monte Carlo or Latin hypercube with samples = 2x or 10x number of variables)
- Run model at each point
- Analyze input/output relationships with
  - Correlation coefficients
    - Simple correlation: strength and direction of a linear relationship between variables
    - Partial correlation: like simple correlation but adjusts for the effects of the other variables
    - Rank correlations: simple and partial correlations performed on "rank" of data
  - Regression and resulting coefficients
  - Variance-based decomposition
  - Importance factors



Two-dimensional projections of LHD for Cantilever (plotted with Minitab)



#### Dakota Input File: Cantilever LHS Study

```
method
  sampling
  sample type lhs
 samples = 70
 seed = 3845
variables
  active all
  continuous_design = 3
    upper bounds = 1.2 \ 1.2 \ 6.0
    lower bounds = 0.8 \ 0.8 \ 4.0
                   "w"
    descriptors
                           "+"
                                   "|"
  continuous state = 4
    upper bounds = 600. 35.E+6 60. 120.
    lower bounds = 400. 23.E+6 40. 80.
                   'p' 'E'
                               'X' 'Y'
    descriptors
interface
 fork
    analysis driver = 'driver.sh'
responses
 response functions = 3
 descriptors = 'mass' 'stress''displacement'
 no gradients no hessians
```

#### **Global Sampling Results for Cantilever**

Partial Correlation Matrix for Cantilever					
	mass	stress	displacement		
w	0.95	-0.96	-0.78		
t	0.95	-0.97	-0.90		
L	0.96	-0.17	0.91		
р	0.95	0.11	0.14		
E	-0.08	-0.13	-0.68		
X	-0.03	0.54	0.05		
Y	0.12	0.82	0.44		

correlation coefficients from Dakota console output (colored w/ Excel)



(plotted with Matlab)

Dakota tabular data plotted in Minitab (can use Matlab, JMP, Excel, etc.)





#### Group discussion



- What is expected, limited about this approach?
- What approaches would you take?
- What assumptions are we making? How would changing them affect results?



#### Morris One-at-a-Time (MOAT)



- Sample paths around global space in coordinate directions
- Give good measure of main (linear, first-order) and interaction / nonlinear effect for modest simulation budget
- How would you know how to configure Dakota to do this study?



# Other SA Approaches Require Changing Method



Dakota Reference Manual guides in specifying keywords

method,
sampling
sample\_type lhs
seed =52983
samples = 100

LHS Sampling

method,
sampling
sample_type lhs
seed =52983
samples = 500
<pre>variance_based_decomp</pre>

Variance-based Decomposition using LHS Sampling method,
 dace oas
 main\_effects
 seed =52983
 samples = 500

Main Effects Analysis using Orthogonal Arrays

method,
 psuade\_moat
 partitions = 3
 seed =52983
 samples = 100

Morris One-At-a-Time

# Dakota Sensitivity Analysis Summary

- Sandia National Laboratories
- What? Understand code output variations as input factors vary; main effects and key parameter interactions.
- Why? Identify most important variables and their interactions
- How? What Dakota methods are relevant? What results?

Category	Dakota method names	univariate trends	correlations	modified mean, s.d.	main effects Sobol inds.	importance factors / local sensis	
Parameter	centered, vector, list	Р					
studies	grid		D		Ρ		
Sampling	sampling, dace lhs, dace random, fsu_quasi_mc, fsu_cvt with variance_based_decomp	Ρ	D		D		multi- purpose!
DACE (DOE-like)	dace {oas, oa_lhs, box_behnken, central_composite}		D		D		D: Dakota
MOAT	psuade_moat			D			P: Post-
PCE, SC	polynomial_chaos, stoch_collocation				D	D	(3 <sup>rd</sup> party tools)
Mean value	local_reliability					D	

Also see Dakota Usage Guidelines in User's Manual

#### Common Question: UQ versus SA



#### What distinguishes sensitivity analysis from uncertainty analysis?

- With SA you primarily gain information about variables
  - Rank importance of parameters and characterize in what way they influence responses
  - Sometimes called inverse UQ
  - Secondarily, characterize model properties
- With UQ you primarily gain information about responses
  - Statistical properties of output responses
  - Intervals indicating bounds on response
  - Likelihood (probability of failure)
- Some methods can be used for both, e.g.,
  - LHS is often used for SA (correlations) and UQ (moments, PDFs, CDFs)
  - Polynomial chaos expansions (PCE) thought of as a UQ method, but also efficiently produce Sobol indices for ranking parameter influence

#### Sensitivity Analysis References



- Saltelli A., Ratto M., Andres T., Campolongo, F., et al., Global Sensitivity Analysis: The Primer, Wiley, 2008.
- J. C. Helton and F. J. Davis. Sampling-based methods for uncertainty and sensitivity analysis. Technical Report SAND99-2240, Sandia National Laboratories, Albuquerque, NM, 2000.
- Sacks, J., Welch, W.J., Mitchell, T.J., and Wynn, H.P. Design and analysis of computer experiments. Statistical Science 1989; 4:409–435.
- Oakley, J. and O'Hagan, A. Probabilistic sensitivity analysis of complex models: a Bayesian approach. J Royal Stat Soc B 2004; 66:751–769.
- Dakota User's Manual
  - Parameter Study Capabilities
  - Design of Experiments Capabilities/Sensitivity Analysis
  - Uncertainty Quantification Capabilities (for MC/LHS sampling)
- Corresponding Reference Manual sections



# **BACKUP SA SLIDES**

# Cantilever Beam Analysis Problem



- Example sensitivity analysis goals:
  - Determine influence of beam\_width, beam\_thickness, R (yield stress), E (Young's modulus), X (horizontal load), Y (vertical load) on each of area (weight), stress, and displacement
  - Determine whether these have only a main effect or if parameter interactions and higher order effects figure in

weight (area = w\*t)

stress = 
$$\frac{600}{wt^2}Y + \frac{600}{w^2t}X \leq R$$
  
displaceme  $nt = \frac{4L^3}{Ewt}\sqrt{\left(\frac{Y}{t^2}\right)^2 + \left(\frac{X}{w^2}\right)^2} \leq D_0$ 

Given values of w, t, R, E, X, Y, Dakota's mod\_cantilever driver computes area, stress-R, displacement-D<sub>0</sub>



# Optional: Additional Sensitivity Analysis Capabilities



- Variance-based decomposition (via sampling or PCE)
  - Goal: Apportion uncertainty in responses to uncertainty in inputs
  - Expensive: K\*(N+2) simulations required, K = # samples, N = # variables, recommended K ≥ 100
  - Exercise: Modify the sensitivity analysis method to perform variancebased decomposition on the cantilever problem
- Main Effects/Analysis of Variance (ANOVA)
  - Goal: Determine effect of a variable on mean behavior
  - Uses design of experiments: Coverage of space (e.g., space filling, interior, boundaries/extremes, etc.) varies by design
  - Exercise: Modify the sensitivity analysis method to perform a main effects analysis using an orthogonal array on the cantilever problem

#### **Results for VBD and Main Effects**



Global sensitivity indices for each response function:						
weight	Sobol	indices:				
	Main	Total				
	0.00	0.00	R			
	0.00	0.00	E			
	0.00	0.00	Х			
	0.00	0.00	Y			
	0.49	0.51	beam_width			
	0.51	0.52	beam_thickness			
stress	Sobol	indices:				
	Main	Total				
	0.16	0.13	R			
	0.00	0.00	E			
	0.37	0.36	X			
	0.39	0.36	Y			
	0.08	0.08	beam_width			
	0.11	0.12	beam_thickness			
displ	Sobol	indices:				
	Main	Total				
	0.00	0.00	R			
	0.90	0.92	E			
	0.02	0.02	X			
	0.07	0.08	Y			
	0.02	0.01	beam_width			
	0.04	0.05	beam thickness			

Variance-based decomposition

#### **Response Function 1**

ANOVA	Table	for	Factor	(Variable)	4	
Source	of	Sum	of	Mean	Sum	
Variation	DoF	Squares	of	Squares	Fdata	
Between	Groups	22	2.18E-03	9.89E-05	3.22E-03	Υ
Within	Groups	506	1.55E+01	3.07E-02		
Total	528	1.55E+01				
ANOVA	Table	for	Factor	(Variable)	5	
Source	of	Sum	of	Mean	Sum	
Variation	DoF	Squares	of	Squares	Fdata	
Between	Groups	22	7.80E+00	3.55E-01	2.32E+01	Beam Width
Within	Groups	506	7.73E+00	1.53E-02		
Total	528	1.55E+01				
ANOVA	Table	for	Factor	(Variable)	6	
Source	of	Sum	of	Mean	Sum	
Variation	DoF	Squares	of	Squares	Fdata	
Between	Groups	22	7.70E+00	3.50E-01	2.26E+01	Beam Thickness
Within	Groups	506	7.84E+00	1.55E-02		
Total	528	1.55E+01				

#### **Main Effects Analysis**

Same relative ranking across methods.

# Sensitivity Analysis with Sampling

- Assume inputs fall within lower and upper bounds
- Generate uniform random samples over these intervals
- Compute response value at each sample point
- Look at correlation results
  - Simple and partial correlations
  - Raw and rank correlations
- Caution: measures the strength and direction of a linear relationship between variables correlation only
- Correlation coefficient near
  - 0 indicates no relationship
  - 1 indicates strong positive relationship (as x increases, y increases)
  - -1 indicates strong negative relationship (as x increases, y decreases)





# Additional Sensitivity Analysis Capabilities



- Variance-based decomposition
  - Goal: Apportion uncertainty in responses to uncertainty in inputs
  - Expensive: K\*(N+2) simulations required, K = # samples, N = # variables, recommended K ≥ 100
  - Exercise: Modify the sensitivity analysis method to perform variancebased decomposition on the "textbook" problem
- Main Effects/Analysis of Variance (ANOVA)
  - Goal: Determine effect of a variable on mean behavior
  - Uses design of experiments: Coverage of space (e.g., space filling, interior, boundaries/extremes, etc.) varies by design
  - Exercise: Modify the sensitivity analysis method to perform a main effects analysis using an orthogonal array on the "textbook" problem

#### **Design of Experiments**



- Design of Experiments (DOE) is sometimes used to help understand variable importance.
- Design and Analysis of Computer Experiments (DACE) refers to DOE for computer models.
- Big difference between physical and computer experiments: many of our codes are deterministic (e.g., same input settings will produce same outputs under replication), whereas physical experiments are usually not.
- DACE can be used to help understand range of outputs and important variables. It is generally NOT an uncertainty propagation method.
- Prototypical method: orthogonal arrays



#### **Orthogonal Arrays**

- For each level of one factor, all levels of the other factors occur an equal number of times: "cancel out" effect.
- Orthogonality: statistical independence between the columns of the experimental design matrix
- Standard analysis involves comparison of main effects: Is the mean of factor 1 at level 1 different than the mean of factor 1 at level 2?
- Large databases of OAs have been compiled by various industry and statistical organizations.
- Example:

Exp. No	Var. 1	Var. 2	Var. 3	Var. 4	Var. 5	Var. 6	Var. 7
1	1	1	1	1	1	1	1
2	1	1	1	2	2	2	2
3	1	2	2	1	1	2	2
4	1	2	2	2	2	1	1
5	2	1	2	1	2	1	2
6	2	1	2	2	1	2	1
7	2	2	1	1	2	2	1
8	2	2	1	2	1	1	2

#### **Textbook Exercise:** SA with Sampling



Statistics based on 100 samples:

Moments for each response function: response\_fn\_1: Mean = 6.3982749478e+00 Std. Dev. = 6.0079987768e+00 Coeff. of Variation = 9.3900290716e-01

95% confidence intervals for each response function: response\_fn\_1: Mean = ( 5.2061576460e+00, 7.5903922496e+00 ) Std Dev = ( 5.2750640532e+00, 6.9793435129e+00 )

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Simple Correlation Matrix among all inputs and outputs:

x1 x2 response\_fn\_1 x1 1.00000e+00 x2 -6.24801e-03 1.00000e+00 response\_fn\_1 1.40254e-01 4.25038e-02 1.00000e+00 Partial Correlation Matrix between input and output:

Partial Correlation Matrix between input and output:

response\_fn\_1

x1 1.40649e-01

x2 4.38140e-02

Simple Rank Correlation Matrix among all inputs and outputs:

x1 x2 response\_fn\_1 x1 1.00000e+00 x2 -3.70837e-03 1.00000e+00

response\_fn\_1 9.11371e-02 -2.59226e-02 1.00000e+00

Partial Rank Correlation Matrix between input and output:

response\_fn\_1

x1 9.10722e-02

x2 -2.56917e-02

#### Sampling Input

#### **Textbook Exercise:**



# SA with Sampling, Tabular Data

method	r			
nond sampling				
sample type	%eval_id	x1	x2	response_fn_1
lhs	1	2.232734001	2.875924025	14.69328591
samples = 100	2	1.793275972	2.311273484	3.352469388
seed = 12345	3	0.9651725828	1.92367612	0.727913444
	4	1.547939246	-0.7228731781	8.900899832
variables	5	2.528758002	-0.239438414	7.821974951
uniform_uncertain = 2	6	1.90385464	0.4789291991	0.7411328243
lower_bounds = -1 -1	7	-0.6187168833	0.6355368689	6.883325151
upper_bounds = 3 3	8	1.596148902	0.5453621751	0.1690276001
descriptors = 'x1' 'x2'	9	2.443838741	2.394096379	8.123060879
	10	2.7503716	2.732582642	18.39793401
interface	11	1.51201481	-0.5424977029	5.729791937
analysis_drivers = 'text_book'	12	2.665546472	1.466315933	7.742610686
direct	13	0.4785859039	2.577518705	6.266871826
	14	0.7086981446	1.228698622	0.009936281628
responses	15	-0.9073449776	0.3829414625	13.37976747
num_response_functions = 1	16	2.392407576	0.0318674671	4.637435939
no_gradients	17	1.029187563	0.6998165904	0.008120552171
no_hessians	18	-0.5761782119	0.3590574848	6.340696728
	19	0.9375857843	2.132517316	1.645066316
strategy	20	-0.7518175888	1.259806897	9.422487756
tabular_graphics_data				
tabular_graphics_file = 'training_sa.dat'	L			
single_method				

#### Sampling Input

# Textbook Exercise: SA with Sampling, Different Bounds



method
nond\_sampling
sample\_type
lhs
samples = 100
seed = 12345
variables
uniform\_uncertain = 2
lower\_bounds = 1
upper\_bounds = 3
descriptors = 'x1' 'x2'
interface
analysis\_drivers = 'text\_book'
direct

```
responses
num_response_functions = 1
no_gradients
no_hessians
```

strategy tabular\_graphics\_data tabular\_graphics\_file = 'training\_sa.dat' single\_method Statistics based on 100 samples:

```
Moments for each response function:
response fn 1: Mean = 6.4041210434e+00 Std. Dev. =
6.4508645208e+00
               Coeff. of Variation = 1.0072989684e+00
95% confidence intervals for each response function:
response_fn_1: Mean = (5.1241295700e+00, 7.6841125169e+00)
               Std Dev = ( 5.6639032080e+00, 7.4938096891e+00 )
Simple Correlation Matrix among all inputs and outputs:
                   x1
                                          response fn 1
                                x2
           x1 1.00000e+00
          x2 -6.24801e-03 1.00000e+00
response fn 1 6.40056e-01 5.95030e-01 1.00000e+00
Partial Correlation Matrix between input and output:
         response_fn_1
     x1 8.01025e-01
     x2 7.79668e-01
Simple Rank Correlation Matrix among all inputs and outputs:
                                x2
                                          response_fn_1
                   x1
           x1 1.00000e+00
           x2 -3.70837e-03 1.00000e+00
response fn 1 6.77288e-01 6.06673e-01 1.00000e+00
Partial Rank Correlation Matrix between input and output:
         response fn 1
     x1 8.54822e-01
     x2 8.28019e-01
```

#### Sampling Input

#### Textbook Exercise: SA with Sampling, Scatter Plots

Bounds = [-1, 3]













# Textbook Exercise: Variance-Based Decomposition



#### method nond sampling sample\_type lhs variance\_based\_decomp samples = 100seed = 12345variables uniform uncertain = 2lower\_bounds = 1.1upper bounds = 33descriptors = 'x1' 'x2'interface analysis drivers = 'text book' direct responses num\_response\_functions = 1 no gradients no hessians strategy

tabular\_graphics\_data tabular\_graphics\_file = 'training\_sa.dat' single\_method

Sampling Input

Variance Based Decomposition Sensitivity Indices These indices measure the importance of the uncertain input variables in determining the uncertainty (variance) of the output. Si measures the main effect for variable i itself, while Ti measures the total effect (including the interaction effects of variable i with other uncertain variables.)

response\_fn\_1

```
x1: Si = 4.92001e-01 Ti = 5.81994e-01
```

```
x2: Si = 5.18284e-01 Ti = 5.34544e-01
```

<<<< Function evaluation summary: 400 total (400 new, 0 duplicate)

# Textbook Exercise: Main Effects/ANOVA



method dace oas	Warning: For orthogonal array sampling, the number of samples should be an integer multiple of (num_symbols)^2, and num_symbols should be either 4 or a prime number.
main_effects samples = 100 variables uniform_uncertain = 2 lower_bounds = 1 1 upper_bounds = 3 3 descriptors = 'x1' 'x2'	Adjusting the number of symbols and samples num_variables = 2 OLD num_samples = 100 OLD num_symbols = 0 NEW num_samples = 121 NEW num_symbols = 11 DACE method = oas Samples = 121 Symbols = 11 Seed (system-generated) = 201266
<pre>interface analysis_drivers = 'text_book' direct responses num_response_functions = 1 no_gradients no_hessians</pre>	Main effects for response_fn_1:         ANOVA Table for Factor (Variable) 1         Source of       Sum of         Mean Sum         Variation       DoF         Squares       of Squares         Fdata       p-value         Between Groups       10       2.25672e+03       2.25672e+02       1.08953e+01         ************************************
strategy tabular_graphics_data tabular_graphics_file = 'training_sa.dat' single_method	ANOVA Table for Factor (Variable) 2         Source of       Sum of         Variation       DoF         Squares       of Squares         Fdata       p-value         Between Groups       10       2.21493e+03       2.21493e+02       1.05010e+01
Sampling Input	Total 120 4.53512e+03 Sampling Output