Gaussian Process Regression and Emulation

STAT8810, Fall 2017

M.T. Pratola

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Today

Experimental Design;
Sensitivity Analysis

Designing Your Experiment

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- Usually this is defined by a criterion.
    - For example, minimize the prediction error of your statistical emulator.
- This is a large and complex subject, so we will limit ourselves to designs which are more generally useful for predicting "black-box" simulators.

Optimal Design

- Assume a statistical emulator model for $f(\mathbf{x})$ - say $Z(\mathbf{x}) \sim GP(\boldsymbol{\mu}, \sigma^2\mathbf{R})$ with known mean μ, variance σ^2 and correlation function parameters $\boldsymbol{\rho}$.

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- The design is the collection of best settings at which to collect our data,

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- The general form of the problem is

$$\mathbf{D}^* = \arg\min_{\mathbf{D}} \mathcal{J}(\mathbf{D})$$

where $\mathbf{D}$ is searched over all possible n-run designs. Typically this optimization is done over a discretization of χ rather than the continuous version.

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- Typically we will plug-in estimates of $\boldsymbol{\mu}, \sigma^2, \boldsymbol{\rho}$ as taking into account their uncertainty makes the computational cost much worse.
- We are trying to optimize $n \times p$ parameters in this problem - a high-dimensional optimization problem.

Optimal Design

- For our purpose, we will most often be interested in prediction/emulation so an appropriate design criterion is the *Integrated Mean Squared Error* criterion†,

$\hat{Z}(x) = E[Z(x) \mid \underbrace{Z_1, \ldots, Z_n}]$

$Z(x_1^*)$
$\vdots$
$Z(x_n^*)$

$$\mathcal{J}(\mathbf{D}) = \frac{1}{\sigma^2} \int_{\chi} E\left[\left(Z(\mathbf{x}) - \hat{Z}(\mathbf{x})\right)^2\right] d\mathbf{x}$$

where in our usual assumed simple setup ($\boldsymbol{\mu} = 0$) we have

$D = \{x_i^*\}_{i=1}^n$

$$\widehat{Z}(\mathbf{x}) = \mathbf{r}(\mathbf{x})^T \mathbf{R}^{-1} \mathbf{Z}$$

or in the general setup

$$\widehat{Z}(\mathbf{x}) = \mathbf{f}^T \beta + \mathbf{r}(\mathbf{x})^T \mathbf{R}^{-1} (\mathbf{Z} - \mathbf{F}\beta).$$

† A convenient closed-form expression is available in Sacks, Welch, Mitchell and Wynn: *Design and Analysis of Computer Experiments*, Statistical Science, vol.4, pp.409–423 (1989).

Space-Filling Designs

- In order to simplify the criterion, so-called “space-filling” designs were proposed.

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- These involve a distance metric $\delta(\mathbf{x}_i, \mathbf{x}_j)$ with the properties

$$\delta(\mathbf{x}_i, \mathbf{x}_j) = \delta(\mathbf{x}_j, \mathbf{x}_i)$$

$$\delta(\mathbf{x}_i, \mathbf{x}_j) \geq 0 \text{ with equality iff } \mathbf{x}_i = \mathbf{x}_j$$

$$\delta(\mathbf{x}_i, \mathbf{x}_j) \leq \delta(\mathbf{x}_i) + \delta(\mathbf{x}_j).$$

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- $\mathbf{D}^*$ is a minimax distance design if

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where $\delta(\mathbf{x}, \mathbf{D}) = \min_{\mathbf{x}'\in\mathcal{D}} \delta(\mathbf{x}, \mathbf{x}')$.

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  where $\delta(\mathbf{x}, \mathbf{D}) = \min_{\mathbf{x}' \in \mathcal{D}} \delta(\mathbf{x}, \mathbf{x}')$.
- Idea: cover the design space at n points with spheres of minimum radius – ensures design points are never too far away from points *not* in the design.

Maximin Distance Designs

- $\mathbf{D}^*$ is a maximin distance design if

$$\max_{\mathbf{D}} \min_{\mathbf{x},\mathbf{x}' \in \mathbf{D}} \delta(\mathbf{x}, \mathbf{x}') = \min_{\mathbf{x},\mathbf{x}' \in \mathbf{D}^*} \delta(\mathbf{x}, \mathbf{x}') \equiv \delta^*.$$

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- Idea: cover the deisgn space at *n* points with spheres of maximum radius – ensures no two design points are too close to one another, so each one has a larger area of "coverage".
- Generally preferred from a computational perspective since it only involves distances amongst points in the design rather than distances between design and non-design points as in minimax.

Minimax/Maximin Distance Designs

- Johnson et al.† relate these distance-based criteria with model-based critera for GP models when the correlation goes to zero - i.e. the response behaves like it is independent at far-way input settings.

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- The connection is interesting but beyond our scope.
- The idea is that in initial phases of data collection, our relatively few input settings where we will collect data will be remote from one another and this construction mimics this behaviour and gives us a criterion to optimize in selecting such input settings.

† Johnson, Moore and Ylvisaker: *Minimax and Maximin Distance Designs*, Journal of Statistical Planning and Inference, vol. 26, pp. 131–148 (1990).

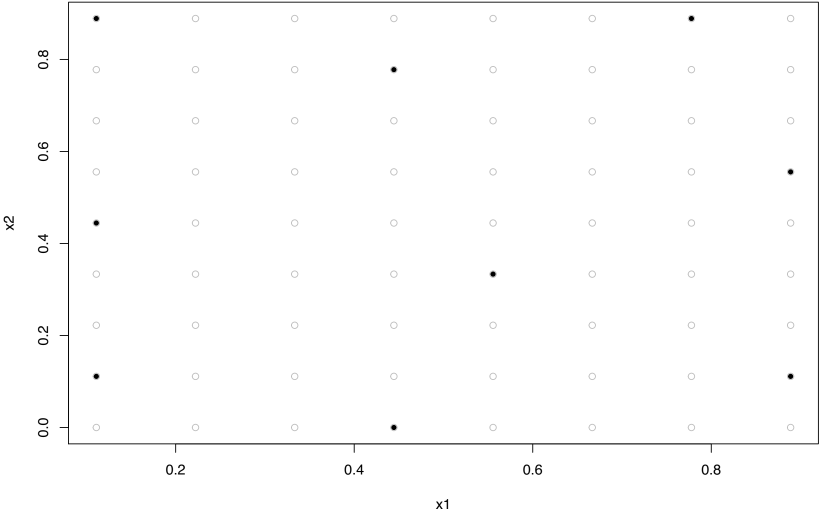
Example - Minimax Distance Design

```
library(fields)
cands=as.matrix(expand.grid(seq(0,1,length=10),seq(0,1,leng
nd=9
design=cover.design(cands,nd,nruns=10)$design
```

```
## Warning in cover.design(cands, nd, nruns = 10): Number c
## (nn) reduced to the actual number of candidates
```

```
plot(design,pch=20,xlab="x1",ylab="x2")
points(cands,col="grey")
```

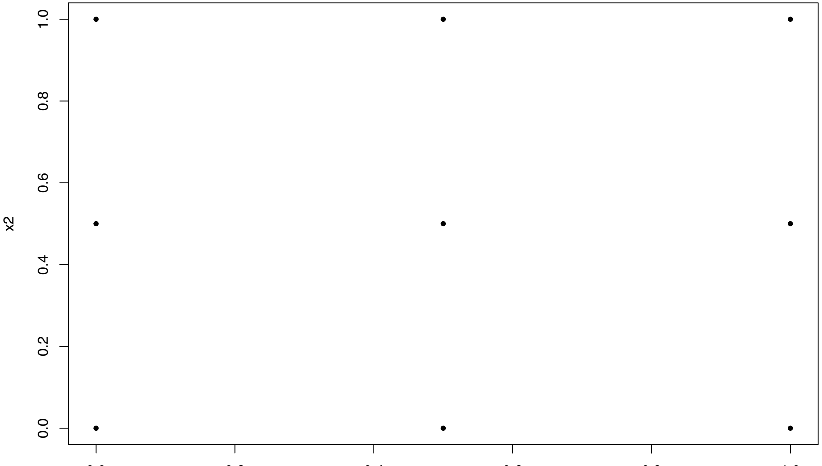
Example - Minimax Distance Design



Grids

Why not just a grid of points?

```
design=as.matrix(expand.grid(seq(0,1,length=3),seq(0,1,leng
plot(design,pch=20,xlab="x1",ylab="x2")
```



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- Lower-dimensional projections are also poor.
- So we would like space-fillingness *and* non-collapsingness.

Latin Hypercube Designs (LHS)

- In a Latin Hypercube Design, the p input axes are stratified into n partitions:

$$[0, \frac{1}{n}), \ldots, [\frac{n-1}{n}, 1]$$

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$$x_i^j = (\pi^j(i) - 0.5)/n$$

for $j = 1, \ldots, p$ and $i = 1, \ldots, n$ where $\pi^j(i)$ are independent random permutations of the integers $1, \ldots, n$.

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- Idea is to place the integers $1, 2, \ldots, n$ into cells defined by the partitions so that each integer appears exactly once in each of the strata for the p dimensions.

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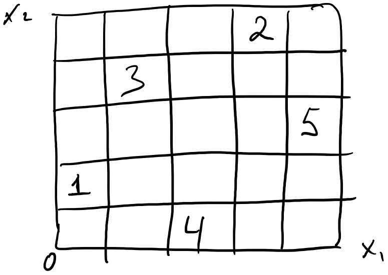
- Idea is to place the integers $1, 2, \ldots, n$ into cells defined by the partitions so that each integer appears exactly once in each of the strata for the p dimensions.
- So in 2D, LHS designs have the property that each row/column of the design has only 1 design point.

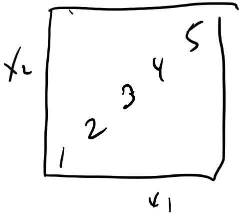
LHS Example

$n=5$

$$\pi^1(1) = 1 \qquad \pi^2(1) = 2$$
$$\pi^1(2) = 4 \qquad \pi^2(2) = 5$$
$$\pi^1(3) = 2 \qquad \pi^2(3) = 4$$
$$\pi^1(4) = 3 \qquad \pi^2(4) = 1$$
$$\pi^1(5) = 5 \qquad \pi^2(5) = 3$$



- Gives design settings for $p = 1$ as $X^1 = \left(\frac{1-0.5}{5}, \frac{4-0.5}{5}, \ldots\right) = (0.1, 0.7, 0.3, 0.5, 0.9)$ and for $p = 2$ as $X^2 = (0.3, 0.9, 0.7, 0.1, 0.5)$



LHS Example

$$\begin{array}{ll}
\pi^1(1) = 1 & \pi^2(1) = 2 \\
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\pi^1(3) = 2 & \pi^2(3) = 4 \\
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- Overall design given by $X = \left[{X^1}^T, {X^2}^T\right]$

Latin Hypercube Designs

- McKay et al. (1979)† showed for a function of the form

$$Y = h(X_1, \ldots, X_k)$$

monotonic in each X_j and a monotonic transformation of Y given by $g(Y)$ then for estimators of the form

$$T(Y) = \sum_{i=1}^{n} g(Y_i),$$

the variance of the estimator using LHS is reduced compared to simple random sampling and stratified sampling.

† McKay, Conover and Beckman: *A comparison of three methods for selecting values of input variables in the analysis of output from a computer code*, Technometrics, vol.21, pp.239–245 (1979).

Latin Hypercube Designs

- Stein (1987)† showed that if a function $f(\mathbf{x})$ satisfies $\int f(\mathbf{x})^2 < \infty$ and has the form

$$f(\mathbf{x}) = f_0 + \sum_{j=1}^{p} f_j(\mathbf{x}) + e(\mathbf{x})$$

where $f_0 = \int f(\mathbf{x}) d\mathbf{x}$ and $f_j(\mathbf{x}) = \int (f(\mathbf{x}) - \mu) d\mathbf{x}_{-j}$ then

$$\begin{aligned} \mathrm{Var}_{LHS}\left(\frac{1}{n}\sum_{i=1}^{n} f(\mathbf{x}_i)\right) &= \frac{1}{n}\int e(\mathbf{x})^2 + o\left(\frac{1}{n}\right) \\ &< \frac{1}{n}\int e(\mathbf{x})^2 d\mathbf{x} + \frac{1}{n}\sum_{j=1}^{p}\int f_j(\mathbf{x})^2 d\mathbf{x} \\ &= \mathrm{Var}_{iid} \end{aligned}$$

† Stein: *Large sample properties of simulations using Latin hypercube sampling*, Technometrics, vol.29, pp.143–151 (1987)

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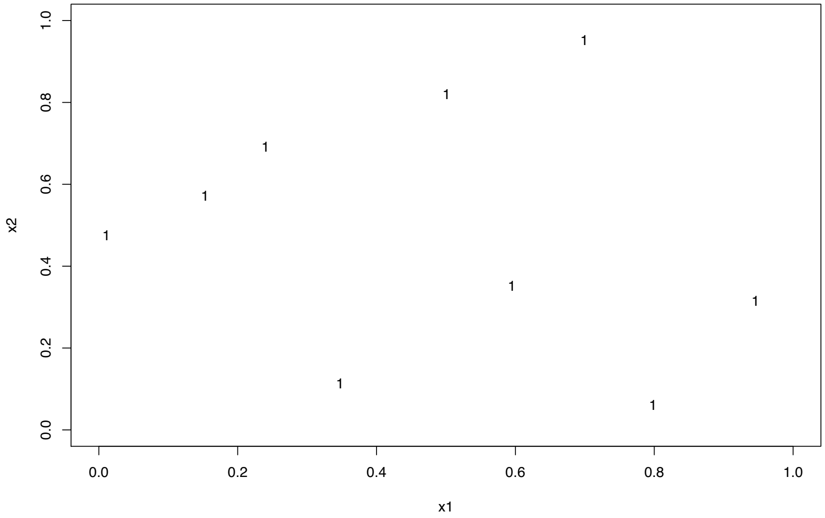
- So typically LHS is combined with another criterion that enforces space-fillingness.
  - e.g. among the LHS designs of size n, choose the LHS that is best from a minimax distance perspective.

LHS Example

- R package lhs offers a few implementations.

```
library(lhs)
set.seed(66) # only to replicate this output
n=9
p=2
design1=randomLHS(n,p)  # default algorithm
set.seed(66)
design2=optimumLHS(n,p) # maximize mean distance
                        # between design points
set.seed(66)
design3=maximinLHS(n,p) # maximize the min distance
                        # between design points
```

LHS Example



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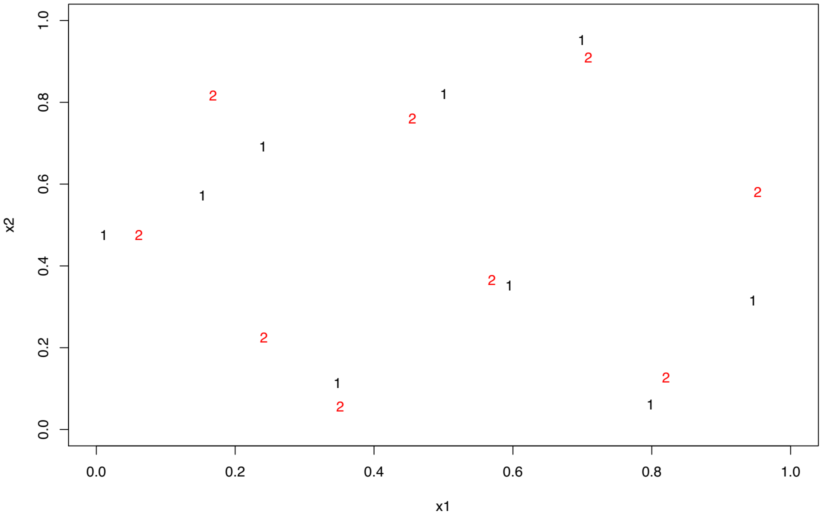

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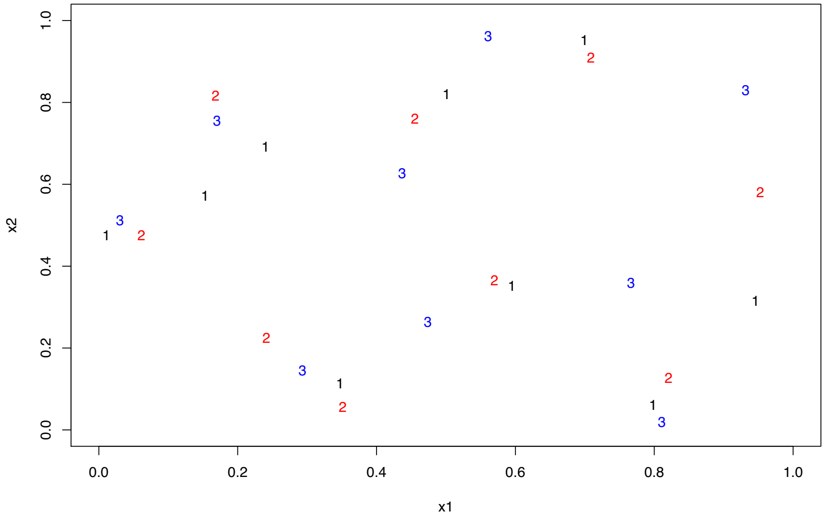

Sequential Designs

- Often we would like to perform a small initial design and then based on the data observed sequentially collect more data to refine our estimate of interest.

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    - a natural sequential design setup in this case is to select points that increasingly refine our estimate of the optimum.

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- For example, in uncertainty quantification the goal is often to optimize a complicated response by use of our statistical GP emulator.
  - a natural sequential design setup in this case is to select points that increasingly refine our estimate of the optimum.
- A popular approach is the expected improvement method of Jones et al.†

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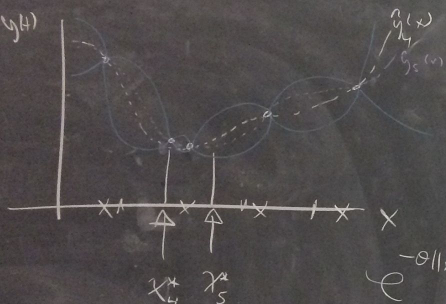
$$I(\mathbf{x}) = \max(f_{min} - Y(\mathbf{x}), 0).$$

- Note that $I(\mathbf{x})$ is a random variable, so one might try to look at the expected improvement as the optimality criteria,

$$\begin{aligned} E[I(\mathbf{x})] &= E[max(f_{min} - Y(\mathbf{x}), 0)] \\ &= (f_{min} - \hat{y}(\mathbf{x}))\Phi\left(\frac{f_{min} - \hat{y}(\mathbf{x})}{\hat{s}(\mathbf{x})}\right) + \hat{s}(\mathbf{x})\phi\left(\frac{f_{min} - \hat{y}(\mathbf{x})}{\hat{s}(\mathbf{x})}\right) \end{aligned}$$

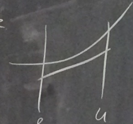
where Φ denotes the standard Normal c.d.f. and ϕ denotes the standard Normal p.d.f.



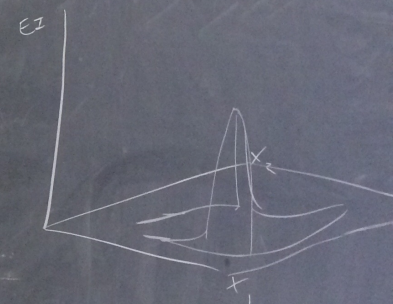
$$E[y(x) \mid y_1, \ldots, y_n] = \hat{y}_n(x) = r^T R^{-1} \underline{y}$$

$$\hat{s}_n^2(x) = \sigma^2 (1 - r^T R^{-1} r)$$

$$e^{-\theta \|x - x\|^2}$$



$$\sim N(\hat{y}_n(x), \hat{s}_n^2(x))$$



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- It turns out:

$$\frac{\partial E[\cancel{(}I(\mathbf{x}))]}{\partial \hat{y}} = -\Phi\left(\frac{f_{min} - \hat{y}(\mathbf{x})}{\hat{s}(\mathbf{x})}\right) < 0$$

$$\frac{\partial E[\cancel{(}I(\mathbf{x}))]}{\partial \hat{s}} = \phi\left(\frac{f_{min} - \hat{y}(\mathbf{x})}{\hat{s}(\mathbf{x})}\right) > 0$$

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- So we can interpret this as meaning the expected improvement increases as $\hat{y}$ decreases and it also increases as $\hat{s}$ increases.
- EI trades-off between choosing a sequential design point that further reduces the minimum value f_{min} or reduces the uncertainty of the response surface.

Example: EI on Branin Test Function

We'll look at applying EI to the Branin test function – see
`https://www.sfu.ca/~ssurjano/branin.html`

```
library(DiceOptim)
library(rgl)

# get our initial starting design
#set.seed(7)
#design=optimumLHS(9,2)
design=as.matrix(expand.grid(seq(0,1,length=3),seq(0,1,leng
colnames(design)=c("x1","x2")
y.branin=apply(design,1,branin)
```

Example: EI on Branin Test Function

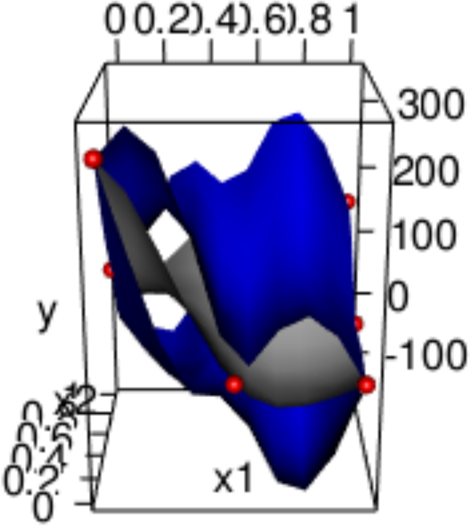
```
# Fit the GP model - built into the DiceOptim package
fit.gp=km(~1, design = data.frame(x = design),
          response = y.branin,covtype = "gauss")
```

```
##
## optimisation start
## -------------------
## * estimation method   : MLE
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~1
## * covariance model :
##   - type :  gauss
##   - nugget : NO
##   - parameters lower bounds :  1e-10 1e-10
##   - parameters upper bounds :  2 2
##   - best initial criterion value(s) :  -53.33026
```

Example: EI on Branin Test Function

```
persp3d(seq(0,1,length=10),seq(0,1,length=10),
        matrix(yhat$mean,10,10),col="grey",
        xlab="x1",ylab="x2",zlab="y")
persp3d(seq(0,1,length=10),seq(0,1,length=10),
        matrix(yhat$lower95),col="blue",add=TRUE)
persp3d(seq(0,1,length=10),seq(0,1,length=10),
        matrix(yhat$upper95),col="blue",add=TRUE)
plot3d(design[,1],design[,2],y.branin,type="s",
        radius=7,col="red",add=TRUE)
```

Example: EI on Branin Test Function



Example: EI on Branin Test Function

```r
# Calculate EI
ego=apply(as.matrix(X),1,EI,fit.gp,type="UK",
          minimization=TRUE)
persp3d(seq(0,1,length=10),seq(0,1,length=10),
        matrix(ego,10,10),col="grey",
        xlab="x1",ylab="x2",zlab="y")

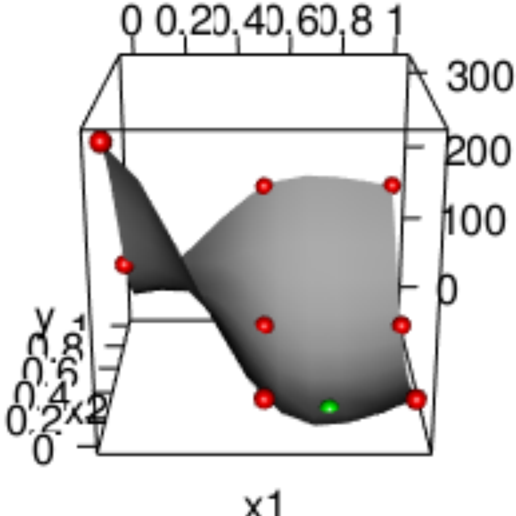

# Get next x that maximizes the EI
x.new=max_EI(fit.gp,lower=rep(0,2),upper=rep(1,2),
             parinit = 0.5,minimization=TRUE)$par
yhat.xnew=predict(fit.gp,newdata=x.new,type="UK")$mean
```

Example: EI on Branin Test Function

```
## Warning in genoud(EI, nvars = d, max = TRUE, pop.size =
## Ignoring 'starting.values' because length(staring.values

##
##
## Mon Sep 25 13:23:43 2017
## Domains:
##  0.000000e+00   <=  X1   <=    1.000000e+00
##  0.000000e+00   <=  X2   <=    1.000000e+00
##
## Data Type: Floating Point
## Operators (code number, name, population)
##  (1) Cloning...........................  2
##  (2) Uniform Mutation..................  1
##  (3) Boundary Mutation.................  1
##  (4) Non-Uniform Mutation..............  1
##  (5) Polytope Crossover................  1
```

Example: EI on Branin Test Function



Example: EI on Branin Test Function

```
# Update by evaluating our expensive function
y.new=apply(x.new,1,branin)
y.branin=c(y.branin,y.new)
design=rbind(design,x.new)

# Refit the GP model
fit.gp=km(~1, design = data.frame(x = design),
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```

```
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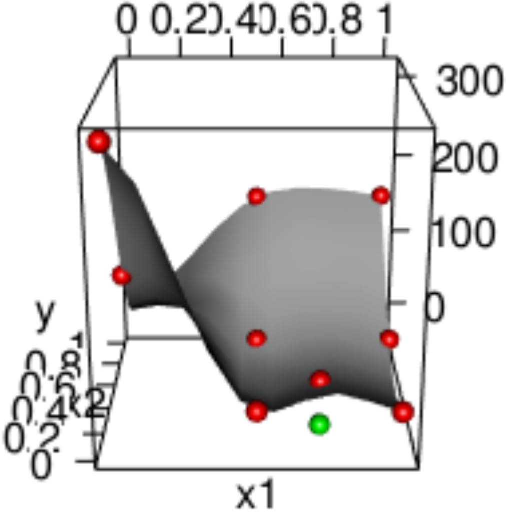

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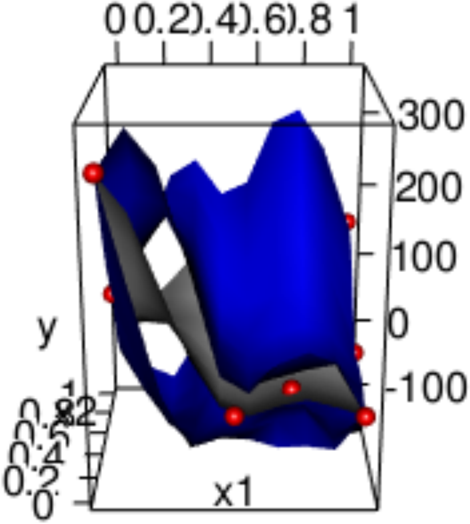

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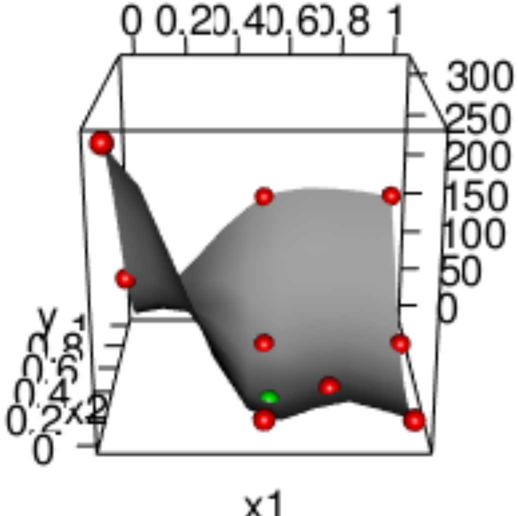

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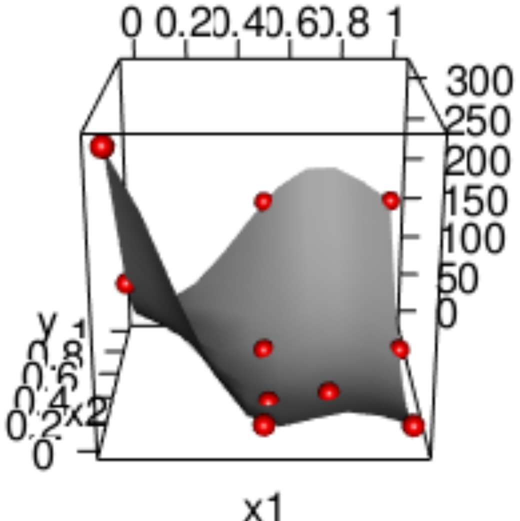

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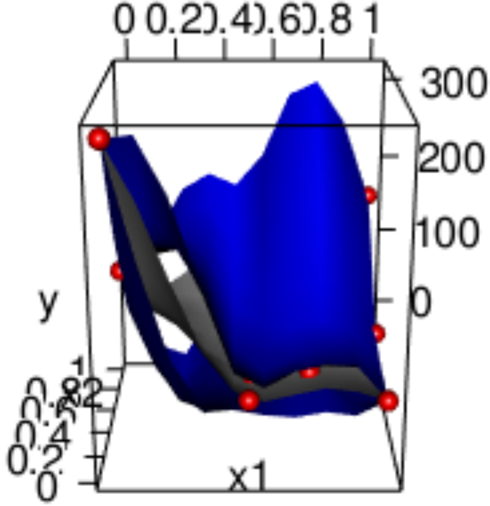

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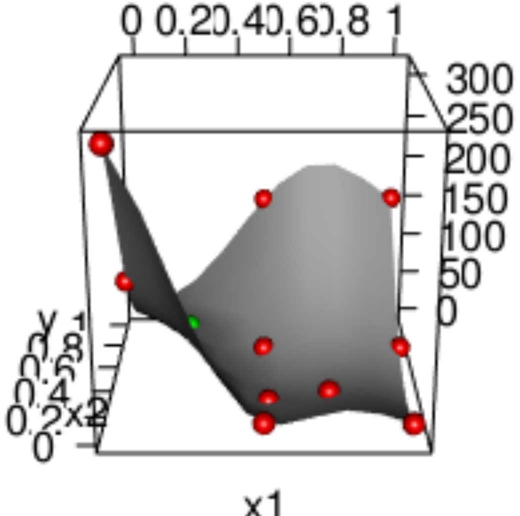

Global Sensitivity Analysis (SA)

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- Total variation of model output is decomposed into terms of increasing dimensionality. Think "functional ANOVA".
- Three main scenarios:
  - Factor screening - identify the influential factors in a system with many factors.
  - Attribute output uncertainty to uncertainty in input factors.
- There is also a local SA where the emphasis is on local impact of factors on the response. Think derivatives.

Sensitivity Analysis

- Assume the input space, $\chi \in \mathbb{R}^k$ is a k-dimensional unit hypercube.

† Sobol': *On sensitivity estimation for nonlinear mathematical models*, Matematicheskoe Modelirovanie, 2.1, pp.112–118 (1990).

Sensitivity Analysis

- Assume the input space, $\chi \in \mathbb{R}^k$ is a k-dimensional unit hypercube.
- The Sobol'† decomposition of $f(\mathbf{x}), \quad \mathbf{x} \in \chi$ is

$$
\begin{aligned}
f(x_1, \ldots, x_k) &= f_0 + \sum_{i=1}^{k} f_i(x_i) + \sum_{1 \le i < j \le k} f_{ij}(x_i, x_j) + \ldots \quad (1) \\
&+ f_{1,2,\ldots,k}(x_1, \ldots, x_k)
\end{aligned}
$$

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- For this decomposition to hold, f_0 must be a constant and

$$\int_0^1 f_{i_1,\ldots,i_s}(x_{i_1}, \ldots, x_{i_s}) dx_{i_j} = 0 \text{ for } 1 \le j \le s. \qquad (2)$$

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Sensitivity Analysis

- A consequence of the constraint (2) is that all summands in (1) are orthogonal, e.g.,

$$\int_{\chi} f_{i_1,\ldots,i_s} f_{j_1,\ldots,j_l} d\mathbf{x} = 0 \quad \text{if } (i_1,\ldots,i_s) \neq (j_1,\ldots,j_l).$$

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- This is because at least one of the indices in $(i_1, \ldots, i_s)$ and $(j_i, \ldots, j_l)$ will not be repeated in both sets of indices, and so the integral vanishes by (2).

Sensitivity Analysis

- Another consequence is that

$$f_0 = \int_{\chi} f(\mathbf{x}) d\mathbf{x}.$$

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Sensitivity Analysis

- Another consequence is that

$$f_0 = \int_{\chi} f(\mathbf{x}) d\mathbf{x}.$$

- Sobol'† showed the decomposition (1) is unique and all the terms can be calculated as

$$f_i(x_i) = -f_0 + \int_0^1 \cdots \int_0^1 f(\mathbf{x}) d\mathbf{x}_{-i}$$

$$f_{ij}(x_i, x_j) = -f_0 - f_i(x_i) - f_j(x_j) + \int_0^1 \cdots \int_0^1 f(\mathbf{x}) d\mathbf{x}_{-(i,j)}$$

and so on.

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Sensitivity Analysis

- Sobol' then defines the *total variance* of $f(\mathbf{x})$ to be

$$\begin{aligned} D &= \int_{\chi} f^2(\mathbf{x}) - f_0^2 \\ &= E\left[f(\mathbf{x})^2\right] - E\left[f(\mathbf{x})\right]^2 \\ &= \mathrm{Var}(f(\mathbf{x})) \end{aligned}$$

where $E[\cdot]$ is taken with respect to a density $\pi(\mathbf{x})$. Usually this is taken to be Uniform on χ.

Sensitivity Analysis

- Similarly, the *partial variances* are

$$D_{i_1,\ldots,i_s} = \int_0^1 \cdots \int_0^1 f^2_{i_1,\ldots,i_s}(x_{i_1},\ldots,x_{i_s})dx_{i_1}\cdots dx_{i_s}$$

where $1 \leq i_1 < \cdots < i_s \leq k$ and $s = 1,\ldots,k$.

Sensitivity Analysis

- Similarly, the *partial variances* are

$$D_{i_1,\ldots,i_s} = \int_0^1 \cdots \int_0^1 f_{i_1,\ldots,i_s}^2(x_{i_1},\ldots,x_{i_s})dx_{i_1}\cdots dx_{i_s}$$

where $1 \leq i_1 < \cdots < i_s \leq k$ and $s = 1,\ldots,k$.

- For example,

$$\begin{aligned}
D_1 &= \int_0^1 f_1^2(x_1)dx_1 \\
&= E\left[f_1^2(x_1)\right] \\
&= E\left[\left(\int \cdots \int f(\mathbf{x})d\mathbf{x}_{-1} - f_0\right)^2\right] \\
&= \mathrm{Var}_{X_1}\left(E\left[f(\mathbf{x})|X_1 = x_1\right]\right)
\end{aligned}$$

Sensitivity Analysis

- In all we have

$$D = \sum_{i=1}^{k} D_i + \sum_{1\le i<j\le k} D_{ij} + \ldots + D_{1,2,\ldots,k}$$

and

$$\begin{aligned}
\mathrm{Var}(f) &= \sum_i \mathrm{Var}_{X_i}\left(E\left[f(\mathbf{x})|X_i = x_i\right]\right) \\
&+ \sum_{1\le i<j\le k} \mathrm{Var}_{X_i,X_j}\left(E\left[f(\mathbf{x})|X_i = x_i, X_j = x_j\right]\right) \\
&+ \ldots + \mathrm{Var}_{X_1,\ldots,X_k}\left(E\left[f(x)|X_1 = x_1, \ldots, X_k = x_k\right]\right)
\end{aligned}$$

where the last term is zero.

Sensitivity Analysis

- The *sensitivity indices* are given by

$$S_{i_1,\ldots,i_s} = \frac{D_{i_1,\ldots,i_s}}{D}$$

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- etc.
- Note that $\sum_{i=1}^{k} S_i + \sum_{1 \leq i < j \leq k} S_{ij} + \ldots + S_{1,2,\ldots,k} = 1$.

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- The sum of all sensitivity indices involving factor X_i is called the *total sensitivity index* for factor i, TS_i.

† Homma and Saltelli: *Importance measures in global sensitivity analysis of model output*, Reliability Engineering and Systems Safety, vol.52, pp.1–17 (1996).

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$$TS_1 = S_1 + S_{12} + S_{13} + S_{123}.$$

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- This construction is computationally friendlier since it takes only one Monte Carlo integration (more on this in a moment).
- Here S_{-i} is the sum of all $S_{i_1,\ldots,i_s}$ terms that *do not* involve the index i.

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Sensitivity Analysis

- In other words,

$$TS_i = 1 - \frac{D_{-i}}{D} = \frac{\frac{E_{\mathbf{X}_{-i}}[\mathrm{Var}(f(\mathbf{x})|\mathbf{X}{-i})]}{\mathrm{Var}(f(\mathbf{x}))}}{D}$$

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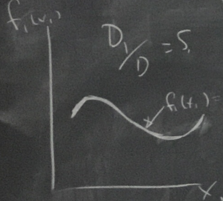
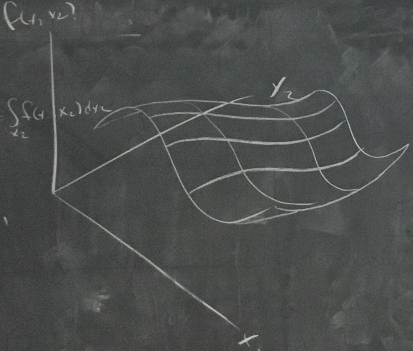
- If S_i and TS_i are similar, it means that factor X_i primarily affects the variance of f through its main effect.
- If S_i and TS_i are different, then the higher-order effects and interactions involving X_i contribute to the variance of f.





$$f_0 + f_1(x_1) + f_2(x_2) + f_{12}(x_1, x_2)$$

$$+ \Big[\underbrace{\int_{x_2} f(x_1, x_2)\,dx_2}_{m_1(x_1)} - f_0\Big] + \Big[\underbrace{\int_{x_1} f(x_1, x_2)\,dx_1}_{m_2(x_2)} - f_0\Big] + \Big[f_{12}(x_1, x_2) - f_0 - \Big(\underbrace{\int_{x_2} f(x_1, x_2)\,dx_2}_{m_1(x_1)} - f_0\Big) - \Big(\underbrace{\int_{x_1} f(x_1, x_2)\,dx_1}_{m_2(x_2)} - f_0\Big)\Big]$$

$n = 25$

$N = 1{,}000$ $\hat{y}(x)$

Computing the Integrals

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- Even better: sample $\mathbf{X}$ using LHS, for instance. This is called Quasi Monte Carlo (QMC).

Computing Sensitivities via Monte Carlo

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- Draw random samples $\mathbf{X}^{(1)}$ and $\mathbf{X}^{(2)}$ both of size N.
- Compute:

$$\widehat{f}_0 = \frac{1}{N} \sum_{m=1}^{N} f(\mathbf{x}_m)$$

$$\widehat{D} = \frac{1}{N} \sum_{m=1}^{N} f^2(\mathbf{x}_m) - \widehat{f}_0^2$$

$$\widehat{D}_i = \frac{1}{N} \sum_{m=1}^{N} f(\mathbf{x}_{-i,m}^{(1)}, x_{i,m}^{(1)}) f(\mathbf{x}_{-i,m}^{(2)}, x_{i,m}^{(1)}) - \widehat{f}_0^2$$

and

$$\widehat{D}_{-i} - \widehat{f}_0^2 = \frac{1}{N} \sum_{m=1}^{N} f(\mathbf{x}_{-i,m}^{(1)}, x_{i,m}^{(1)}) f(\mathbf{x}_{-i,m}^{(1)}, x_{i,m}^{(2)})$$

where $\mathbf{x}_{-i,m} = (\ldots, x_{i-1,m}, x_{i+1,m}, \ldots)$ and superscripts indicate using respective columns from two independent sampling matrices, and $\mathbf{x}$ (no superscript) uses either sample.

Computing Sensitivities via Monte Carlo

- Our sensitivities are then estimated as

$$\widehat{S}_i = \frac{\widehat{D}_i}{\widehat{D}} \text{ and } \widehat{TS}_i = 1 - \frac{\widehat{D}_{-i}}{\widehat{D}}$$

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  - this "plug-in" approach does not propagate uncertainties in $\widehat{f}$ through to $\widehat{S}_i$, $\widehat{TS}_i$. But there are ways of doing this - e.g. Bayesian approach (later).
- So in UQ our sensitivities are subject to two sources of uncertainty: the MC sample size N in approximating the integrals, and the uncertainty of our emulator $\widehat{f}$ since we cannot freely evaluate our model f.

Sensitivity Analysis

- Effectively, SA is based on the following decomposition of the response variance:

$$\mathrm{Var}(f) = \mathrm{Var}_{X_i}(E_{\mathbf{X}_{-i}})(f|X_i)) + E_{X_i}(\mathrm{Var}_{\mathbf{X}_{-i}}(f|X_i))$$

where the first term is the main or first-order effect, and

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Saltelli and Homma: *Sensitivity Analysis of model output: an investigation of new techniques*, Computational Statistics and Data Analysis, vol.15, pp.211–238 (1993).

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- If the model is linear, $\frac{\mathrm{Var}_{X_i}(E_{\mathbf{X}-i}(f|X_i))}{\mathrm{Var}(f)} = \beta^2_{X_i}$.

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Example

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- Because this function is known in closed-form and is rather amenable to hand calculations, we can derive the marginal 1-way effects.
- For instance, recall that $f_i(x_i) = -f_0 + \int_{x_{-i}} f(x) dx_{-i}$
- We calculate the 1-way marginal effects as:

$$f_1(x_1) = -\frac{10}{2\pi x_1} cos(2\pi x_1) + \frac{10}{2\pi x_1} + \frac{13}{12}$$

$$f_2(x_2) = -\frac{10}{2\pi x_2} cos(2\pi x_2) + \frac{10}{2\pi x_2} + \frac{13}{12}$$

$$f_3(x_3) = 3.87964 + (x_3 - 0.5)^2 + 1$$

$$f_4(x_4) = 3.87964 + \frac{7}{12} + x_4$$

$$f_5(x_5) = 3.87964 + \frac{7}{12} + x_5$$

Example

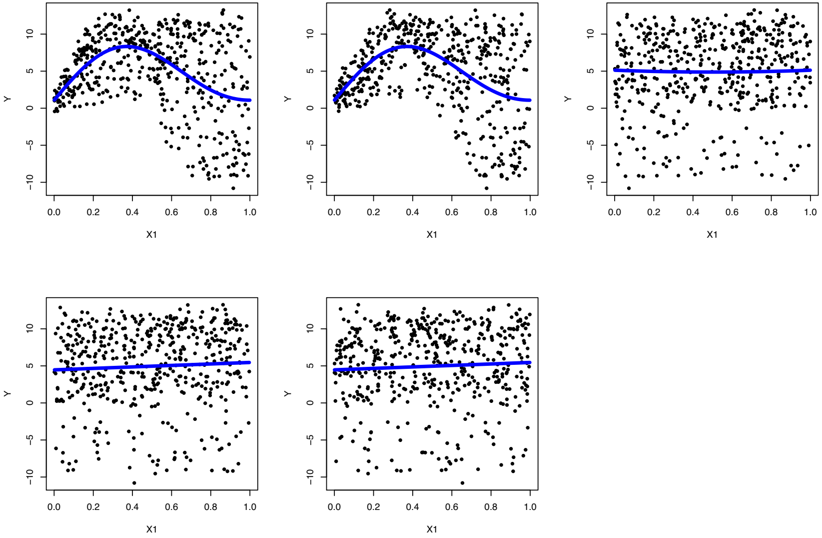
```
# Generate data
set.seed(88) # just to replicate this example
n=500
X=matrix(runif(n*5),ncol=5)
f=10*sin(2*pi*X[,1]*X[,2])+(X[,3]-0.5)^2+X[,4]+X[,5]
y=f+rnorm(n,sd=1)

# true 1-way marginal effects
f1=-10/(2*pi*X[,1])*cos(2*pi*X[,1])+10/(2*pi*X[,1])+13/12
f2=-10/(2*pi*X[,2])*cos(2*pi*X[,2])+10/(2*pi*X[,2])+13/12
f3=3.87964+(X[,3]-0.5)^2+1
f4=3.87964+7/12+X[,4]
f5=3.87964+7/12+X[,5]
```

Example

```
# plot
par(mfrow=c(2,3))
plot(X[,1],y,xlab="X1",ylab="Y",pch=20,xlim=c(0,1))
ix=sort(X[,1],index.return=TRUE)$ix
lines(X[ix,1],f1[ix],lwd=4,col="blue")
plot(X[,2],y,xlab="X1",ylab="Y",pch=20,xlim=c(0,1))
ix=sort(X[,2],index.return=TRUE)$ix
lines(X[ix,2],f2[ix],lwd=4,col="blue")
plot(X[,3],y,xlab="X1",ylab="Y",pch=20,xlim=c(0,1))
ix=sort(X[,3],index.return=TRUE)$ix
lines(X[ix,3],f3[ix],lwd=4,col="blue")
plot(X[,4],y,xlab="X1",ylab="Y",pch=20,xlim=c(0,1))
ix=sort(X[,4],index.return=TRUE)$ix
lines(X[ix,4],f4[ix],lwd=4,col="blue")
plot(X[,5],y,xlab="X1",ylab="Y",pch=20,xlim=c(0,1))
ix=sort(X[,5],index.return=TRUE)$ix
lines(X[ix,5],f5[ix],lwd=4,col="blue")
```

Example



Example

```r
library(sensitivity)
N=10000
X1=data.frame(matrix(runif(N*5),ncol=5))
X2=data.frame(matrix(runif(N*5),ncol=5))
f.test <-function(X) {
    10*sin(2*pi*X[,1]*X[,2])+(X[,3]-0.5)^2+X[,4]+X[,5]
}
si.S=sobolEff(model=f.test,X1=X1,X2=X2,order=1,nboot=0)
si.TS=sobolEff(model=f.test,X1=X1,X2=X2,order=0,nboot=0)
```

Example

First-order sensitivity indices.

```
si.S$S
```

```
##      original std. error min. c.i. max. c.i.
## X1  0.212749   0.011655  0.189907  0.235591
## X2  0.219223   0.011626  0.196437  0.242009
## X3 -0.001839   0.009954 -0.021349  0.017671
## X4 -0.001164   0.009944 -0.020654  0.018326
## X5  0.001597   0.009931 -0.017867  0.021061
```

Example

Total sensitivity indices.

```
si.TS$S
```

```
##    original std. error min. c.i. max. c.i.
## X1 0.776517   0.011585  0.753811  0.799223
## X2 0.782737   0.011602  0.759997  0.805477
## X3 0.000191   0.000004  0.000184  0.000198
## X4 0.002856   0.000055  0.002749  0.002963
## X5 0.002858   0.000054  0.002752  0.002964
```