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Introduction to Smoothing spline ANOVA models (metamodelling)

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Introduction to ANOVA Models

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Consider the mapping $Y = f(x)$

where x is a vector of input variables $x = (x_1, x_2, \ldots, x_k)$

and Y is the output.

x_i is the i-th element of x varying in $0 \le x_i \le 1$

Specification of the input factors

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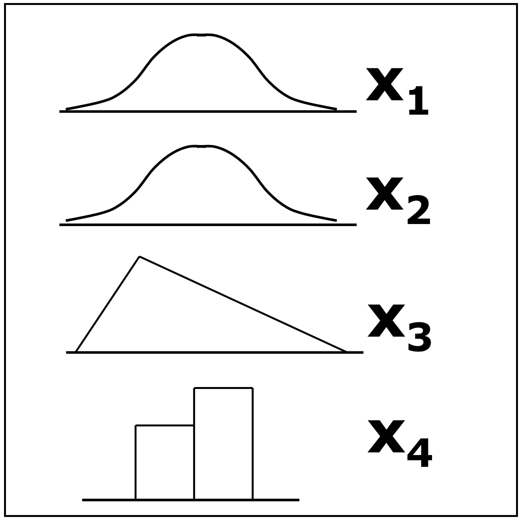
$$X \in \Omega$$

Marginal p.d.f. $p(\vec{x}) = \prod p_i(x_i)$



Marginal p.d.f. + correlation structure

Rank correlation, Dependence-trees, diagonal band, copulas

Joint p.d.f. $p(x_1, x_2, \ldots, x_k)$

MCMC (Gibbs, Metropolis, …)

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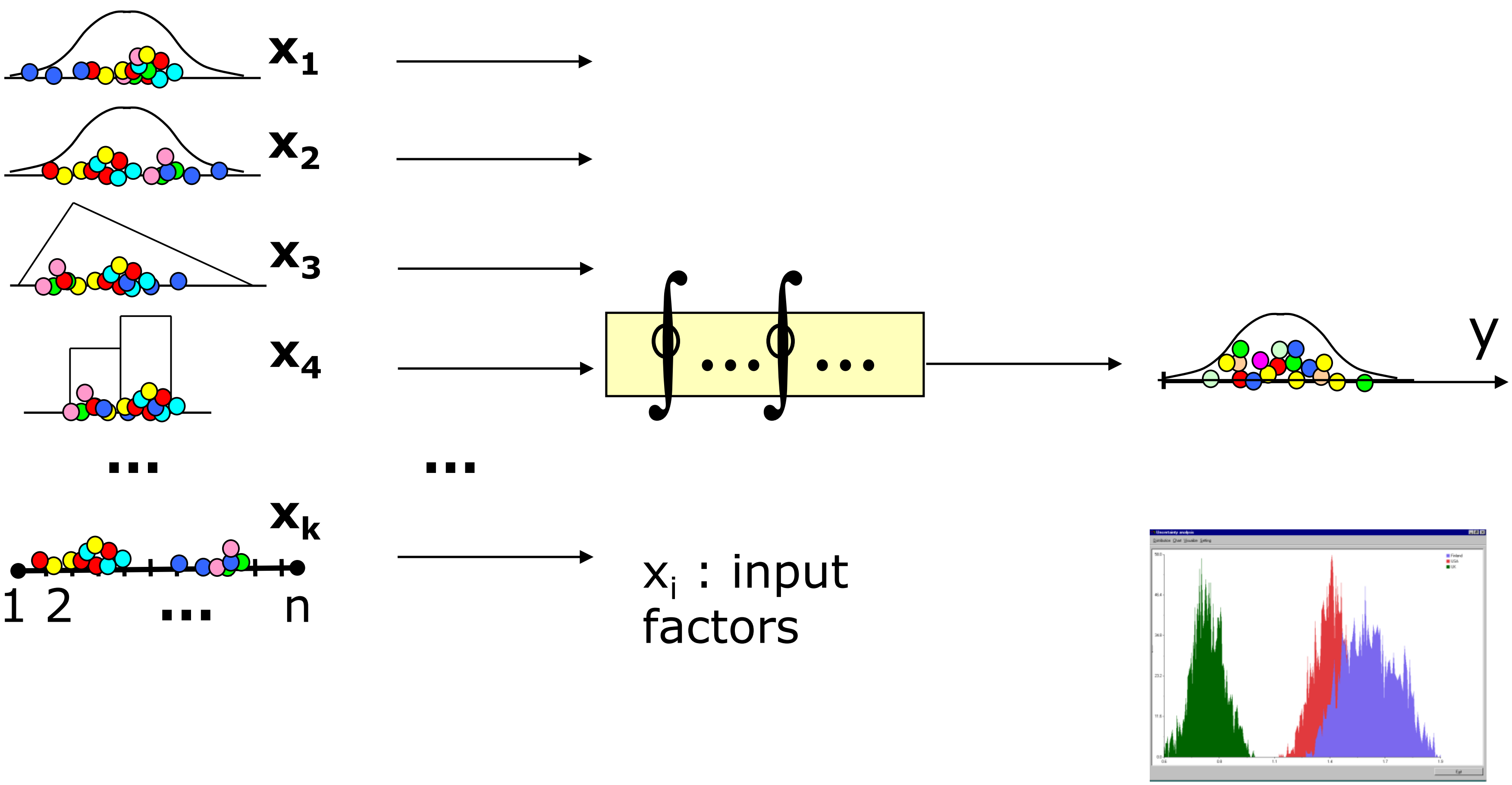
Propagation of uncertainty

Input	*Model*	*Output*
$p(\vec{x})$	$Y = f(\vec{x})$	$p(Y)$



Model approximation (meta-modelling)

$$x \in \Omega \longrightarrow \boxed{f(\mathbf{x})} \longrightarrow Y$$

Realistic Computer models are very costly in terms of run time. We need a way to characterize uncertainty and perform SA based on a limited number of model runs.

We aim to identify a 'simple' relationship between Xi's and Y that fits well the original model and is less computationally demanding.

Model approximation (meta-modelling)

A Meta-model is a simpler model that mimics the larger computational model.

Evaluations of Meta-Models are much faster.

Model approximation (meta-modelling)

Local approximation methods take f and its derivatives at a base point X_0 and construct a function that matches the properties of *f* in the nearby region (Taylor series).

Model approximation (meta-modelling)

1. Linear Regression
2. Quadratic Response Surface Regression
– Options 1 and 2 work pretty well in some cases. However many realistic models are highly nonlinear and/or periodic and these methods fail.
3. Gaussian Process or Spatial Models
4. Nonparametric Regression Models
– Both 3 and 4 work fairly well for a small number of inputs.
– Variable selection is helpful for a modest number of inputs.

ANOVA Models

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ANOVA models define a decomposition of Y=*f(x)* into main effects and interactions

$$Y = f(x) = f_0 + \sum_{i=1}^{k} f_i(x_i) + \sum_i \sum_{j>i} f_{ij}(x_i, x_j) + \ldots + f_{1,2,\ldots,k}(x_1, x_2, \ldots, x_k)$$

This is also called the High Dimensional Model Representation (HDMR)

E.g., if k=3:

$$f(x) = f_0 + f_1(x_1) + f_2(x_2) + f_3(x_3) + f_{12}(x_1, x_2) + f_{13}(x_1, x_3) + f_{23}(x_2, x_3) + f_{123}(x_1, x_2, x_3)$$

This decomposition is non-unique for general joint pdf's of **x.**

The total number of summands in the ANOVA is 2^k

Properties of the ANOVA decomposition (orthogonal case)

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$$Y = f(x) = f_0 + \sum_{i=1}^{k} f_i(x_i) + \sum_i \sum_{j>i} f_{ij}(x_i, x_j) + \ldots + f_{1,2,\ldots,k}(x_1, x_2, \ldots, x_k)$$

If each term is chosen with zero mean ...

$$\int_0^1 f_i(x_i) \quad dp(x_i) = 0, \quad \forall x_i \quad i = 1, 2, \ldots, k$$

$$\int_0^1 \int_0^1 f_{ij}(x_i, x_j) \quad dp(x_i) dp(x_j) = 0, \quad \forall x_i, x_j \quad i < j$$

....

$$\int_\Omega f_{12\ldots k}(x_1, x_2, \ldots, x_k) \quad dp(x_1) dp(x_2) \ldots dp(x_k) = 0.$$

Properties of the ANOVA decomposition (orthogonal case)

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$$Y = f(x) = f_0 + \sum_{i=1}^{k} f_i(x_i) + \sum_i \sum_{j>i} f_{ij}(x_i, x_j) + \ldots + f_{1,2,\ldots,k}(x_1, x_2, \ldots, x_k)$$

… then the ANOVA decomposition has TWO properties

$$\int_{\Omega} f(x) \; dp(x) = f_0 = E(Y)$$

All the summands are orthogonal:

if $(i_1,\ldots,i_s) \neq (j_1,\ldots,j_l)$ $\quad \int_{\Omega^k} f_{i_1,\ldots,i_s} f_{j_1,\ldots,j_l} dp(x) = 0$

It follows that the ANOVA decomposition is **unique** and each term can be defined as …

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Properties of the ANOVA decomposition

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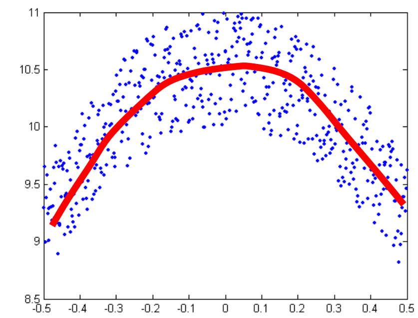
$$Y = f(x) = E(Y) + \sum_{i=1}^{k} f_i(x_i) + \sum_i \sum_{j>i} f_{ij}(x_i, x_j) + \ldots + f_{1,2,\ldots,k}(x_1, x_2, \ldots, x_k)$$

$$\int_{\Omega - x_i} \cdot \int f(x)\, dp(x \mid x_i) = f_0 + f_i(x_i) = E(Y \mid x_i)$$



$$\int_{\Omega - \{x_i, x_j\}} \cdot \int f(x)\, dp(x \mid x_i x_j) = f_0 + f_i(x_i) + f_j(x_j) + f_{ij}(x_i, x_j)$$
$$= E(Y \mid x_i, x_j)$$

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ANOVA

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$$Y - E(Y) = \sum_{i=1}^{k} f_i\left(x_i\right) + \sum_i \sum_{j>i} f_{ij}\left(x_i, x_j\right) + \ldots + f_{1,2,\ldots,k}\left(x_1, x_2, \ldots, x_k\right)$$

Being the terms orthogonal, we can square and integrate the eq above over Ω and decompose the variance of *f(x)* into terms of increasing dimensionality (ANOVA)

$$V(Y) = \sum_{i=1}^{k} V_i + \sum_i \sum_j V_{ij} + \sum_i \sum_j \sum_k V_{ijk} \ldots + V_{1,2,\ldots,k}$$

$$V_i = \int f_i^2(x_i)dx_i$$

$$V_{i_1,i_2,\ldots i_s} = \int f^2{}_{i_1,\ldots,i_s} dx_{i_1} dx_{i_2} \ldots dx_{i_s}$$

$$1 = \sum_{i=1}^{k} S_i + \sum_i \sum_j S_{ij} + \sum_i \sum_j \sum_k S_{ijk} \ldots + S_{1,2,\ldots,k}$$

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Main effects

If we were to approximate f(x) with a function $g(X_i)$ …

$$L = E[(f(x) - g(x_i))^2]$$

$$g(x_i) = E(Y \mid x_i) \Rightarrow L = L_{\min}$$

$$L_{\min} = E[Var(Y \mid X_i)]$$

… $f_i=E(Y|X_i)$ has the minimum loss L among univariate functions

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Main effects

$$V_i = Var[E(Y \mid x_i)]$$

$$= Var(Y) - E[Var(Y \mid x_i)]$$

$$L = E[(f(x) - g(x))^2]$$

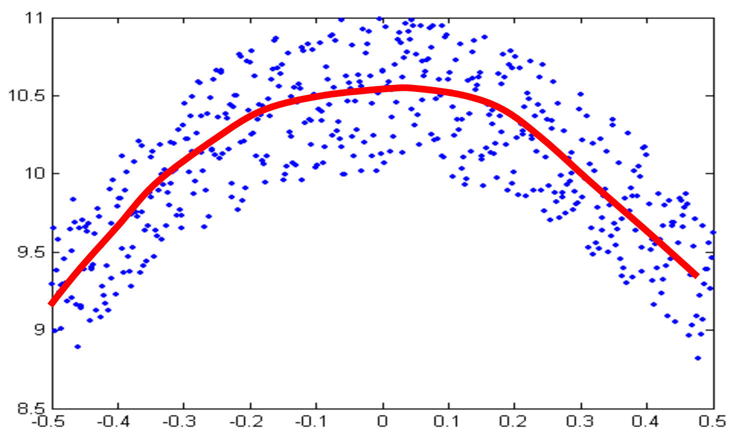
$$g(x) = f_0 \Rightarrow L = V(Y)$$

$$g(x) = f(x) \Rightarrow L = 0$$

$$g(x_i) = E(Y \mid x_i) \Rightarrow L = L_{min}$$

$$L_{min} = E[Var(Y \mid X_i)]$$

when we approximate f(x) with a function $g(x_i)$, $g^* = E(Y|X_i)$ has the minimum loss L



Main effects

… $f_{ij}=E(Y|X_i,X_j)$ has the minimum loss L among bivariate functions …

… and so on …

Var(fi)/var(Y): also called non-parameteric R-squared; Pearson’s correlation ratio; …

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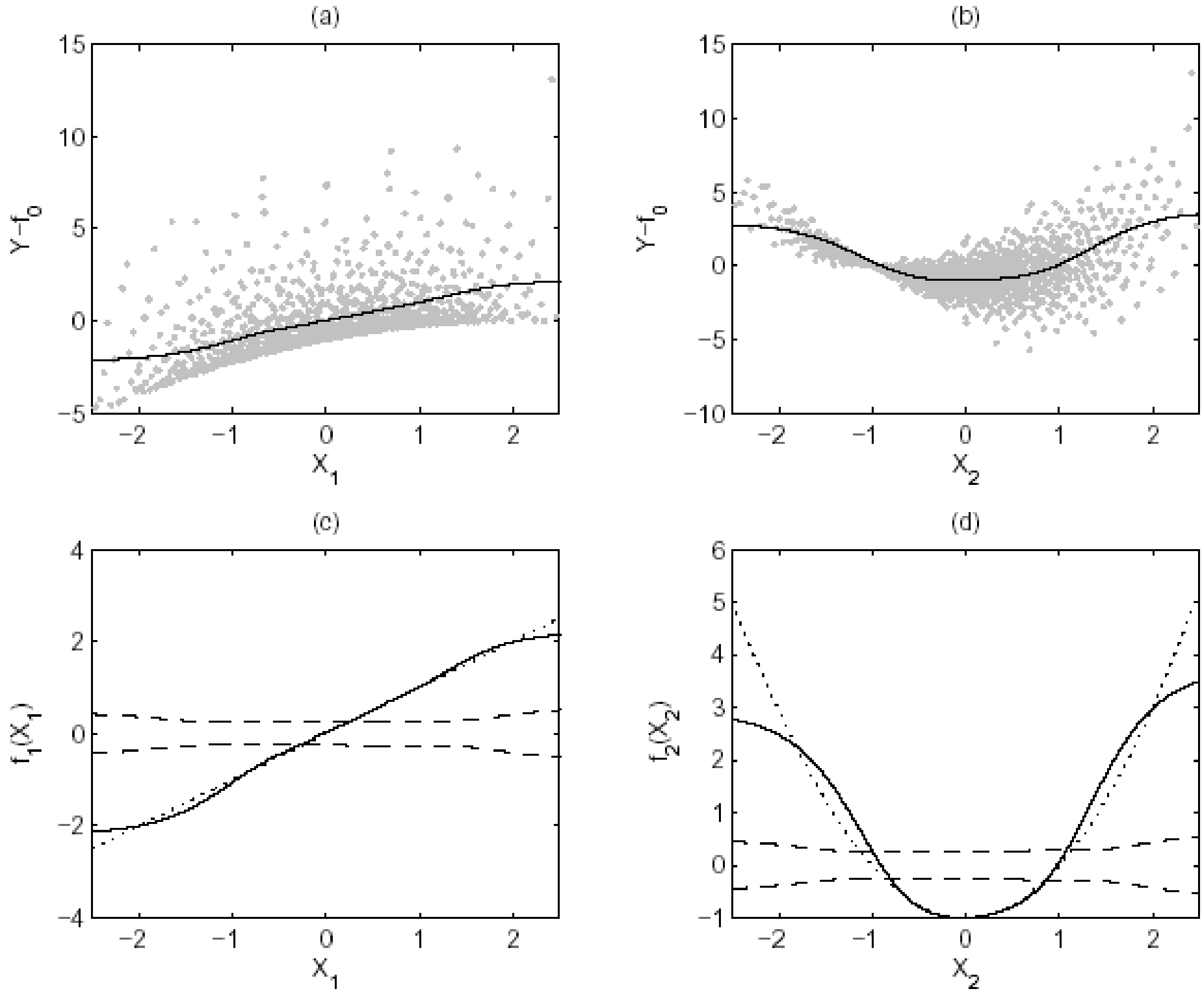
Main effects



$$f(X_1, X_2) =$$
$$X_1 + X_2^2 + X_1 \cdot X_2$$

$$X_i \sim N(0,1)$$

ANOVA model estimation

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Tensor product decomposition (reproducing kernel Hilbert space, RKHS)

$$F = \bigotimes_{j=1}^{k} H_j = \{1\} \oplus \left\{ \bigoplus_{j=1}^{k} \bar{H}_j \right\} \oplus \left\{ \bigoplus_{j<i} (\bar{H}_j \otimes \bar{H}_i) \right\} \oplus \cdots$$

Orthogonal functional decomposition

$$F = \{1\} \oplus \left\{ \bigoplus_{j=1}^{q} F_j \right\}$$

ANOVA model estimation

Smoothing methods to estimate ANOVA decompositions, truncated at the 2nd -3rd order terms:

SMOOTHING SPLINES ANOVA MODELS

Smoothing the y vs x mapping (think of an HP-filter), that provides efficient convergence properties to the true ANOVA decomposition.

[this is one possible methods, other are RBF's, kernel regressions, …]

ANOVA model estimation

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Denote the generic mapping as Y = f(**X**), where $\mathbf{X} \in [0, 1]^k$ and k is the number of parameters.

The simplest example of smoothing spline mapping estimation of z is the additive model:

$$g(\mathbf{X}) = g_0 + \sum_{i=1}^{k} g_i\left(x_i\right)$$

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ANOVA model estimation

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To estimate g we can use a multivariate smoothing spline minimization problem, that is, given λ_j, find the minimizer g(**X**) of:

$$\frac{1}{N}\sum_{n=1}^{N}(y_n - g(\mathbf{X}_n))^2 + \sum_{j=1}^{k}\lambda_j \int_0^1 [g_j''(X_j)]^2 dX_j$$

where a Monte Carlo sample of dimension N is assumed.

This minimization problem requires the estimation of the *k* hyperparameters λ_j (also denoted as smoothing parameters): GCV, GML, etc. (see e.g. Wahba, 1990; Gu, 2002).

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ANOVA model estimation

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We re-formulate the additive model for the general case with interactions as to find the minimizer g(**X**) of:

$$\frac{1}{N}\sum_{n=1}^{N}(y_n - g(\mathbf{X}_n))^2 + \lambda_0 \sum_{j=1}^{q} \frac{1}{\theta_j} \left\| P^j g \right\|_F^2$$

where the q-dimensional vector of θ_j smoothing parameters needs to be optimized ‘somehow’.

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ANOVA model estimation

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Wahba (1990), Gu (2002), Storlie et al. (2007): en-bloc (like HP);

Ratto et al., 2004-2007: based on recursive filtering and smoothing estimation: SDP modelling. (like KF-smoothing version of the HP);

Liu et al. (2002-2006): polynomial basis expansion.

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SDP modelling

SDP modeling is one class of non-parametric smoothing approach first suggested by Young (1993).

The estimation is performed with the help of the `classical' recursive (non-numerical) Kalman filter and associated fixed interval smoothing algorithms and has been applied for sensitivity analysis in Ratto et al. (2004-2007).

Mapping/sensitivity strategies

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OAT (Taylor):
- truncation;
- mapping by knowing all derivatives in a base point
- decomposition with infinite terms

GSA (ANOVA):
- non-parametric regression/smoothing
- mapping on a space-filling MC sample
- decomposition with finite terms

DSGE models

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Let us consider a generic DSGE model:

$$E_t\{g(y_{t+1}, y_t, y_{t-1}, u_t; X)\} = 0$$

y_t endogenous variables,
u_t exogenous shocks
X structural parameters.

X can be characterised by plausible ranges, expressed
in terms of prior distributions, or by a posterior distribution, as a result of an estimation.

DSGE models

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The model behaviour is a function of
the values assumed for X within the prior or posterior space of structural parameters.

Let Y be a generic 'output' of the model: a multiplier, a
measure of fit, an IRF.

Y depends on the values of X

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

f non-linear
analytic form is unknown

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Mapping the reduced form of RE models

Relationship between the reduced form of a rational expectation model and the structural coefficients.

let the reduced form be
$y_t = Ty_{t-1} + Bu_t$,

'outputs' Y of our analysis will be the entries in the transition matrix $T(X_1,\ldots,X_k)$ or in the matrix $B(X_1,\ldots,X_k)$.

Lubik Schorfheide (2005)

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We analyse the reduced form coefficients describing the relationship between

π_t vs $e_{R,t}$

We sample the structural coefficients from posterior ranges obtained after estimating the model using data for Canada.

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Lubik Schorfheide (2005)

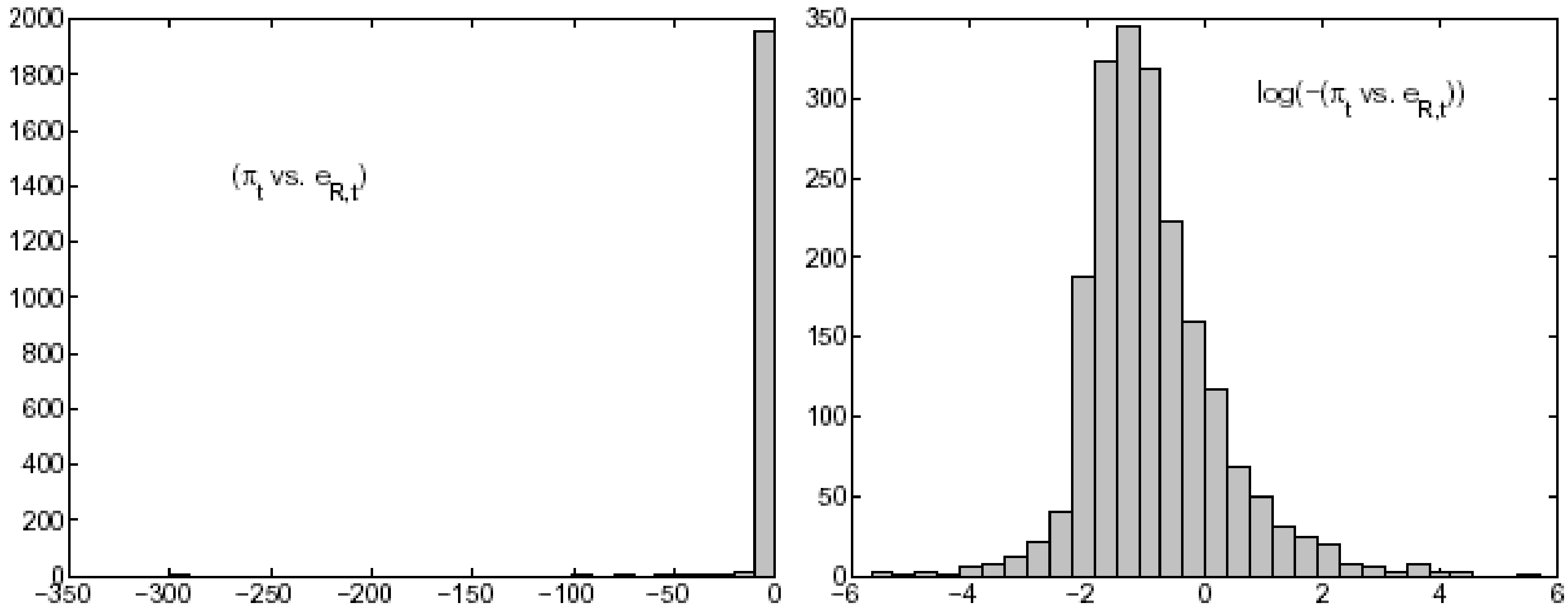

Figure 13: Lubik and Schorfheide model: histograms of the MC sample of the reduced form coefficient $Y = (\pi_t \text{ vs } e_{R,t})$. Left panel: actual values Y; right panel $\log(-Y)$.

Lubik Schorfheide (2005)

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$\log(-(\pi_t \text{ vs } e_{R,t}))$

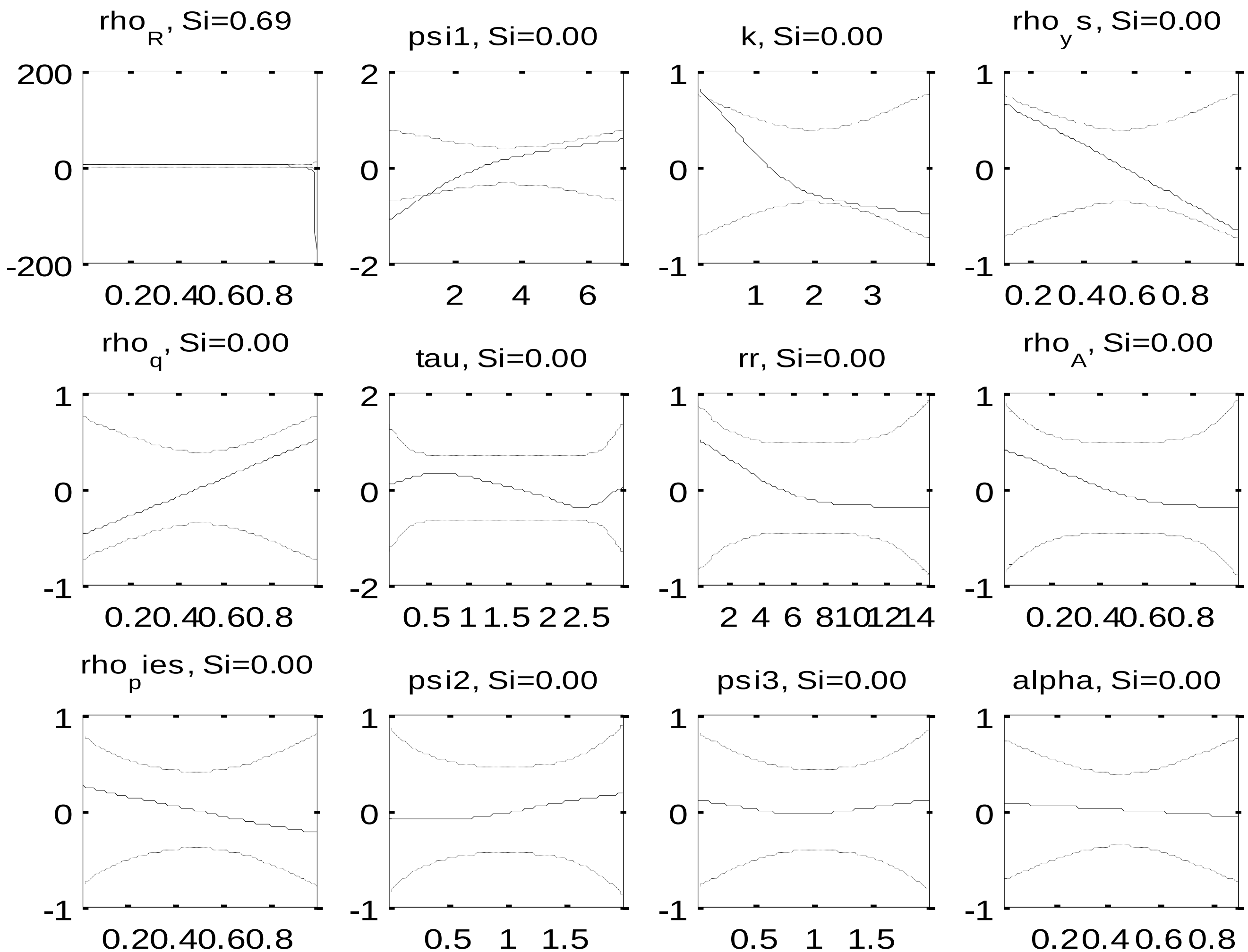
$$Y = -\exp(f_0 + f_1 + \ldots + f_k + e)$$
$$= -\exp(e)\prod_{j=0}^{k}\exp(f_j)$$

Factorisation

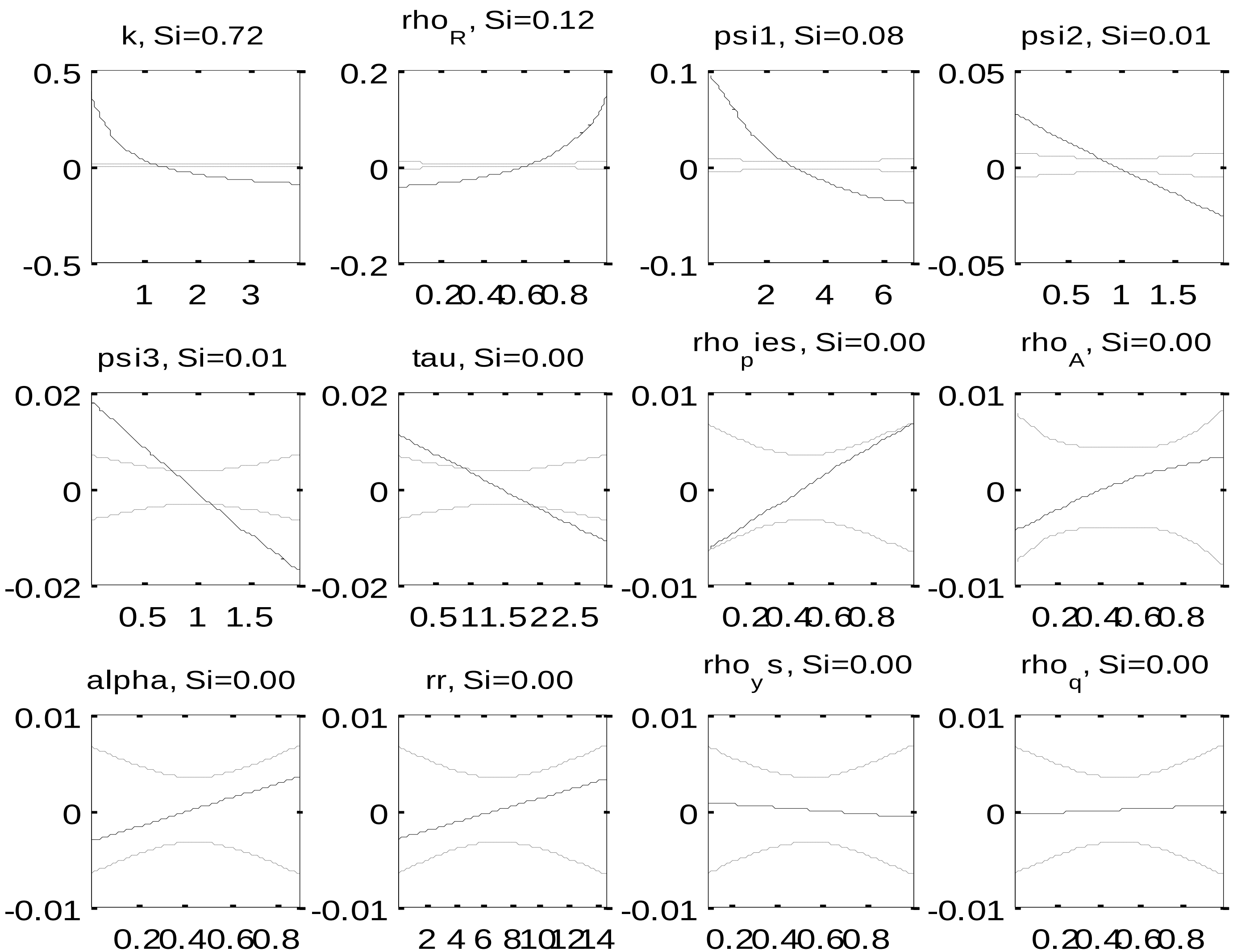
$$Y = -\exp(e)\prod_{j=0}^{k}\exp(f_j) + \sum_{j=0}^{k} g_j + \varepsilon$$

Correction [new in DYNARE 4.5]

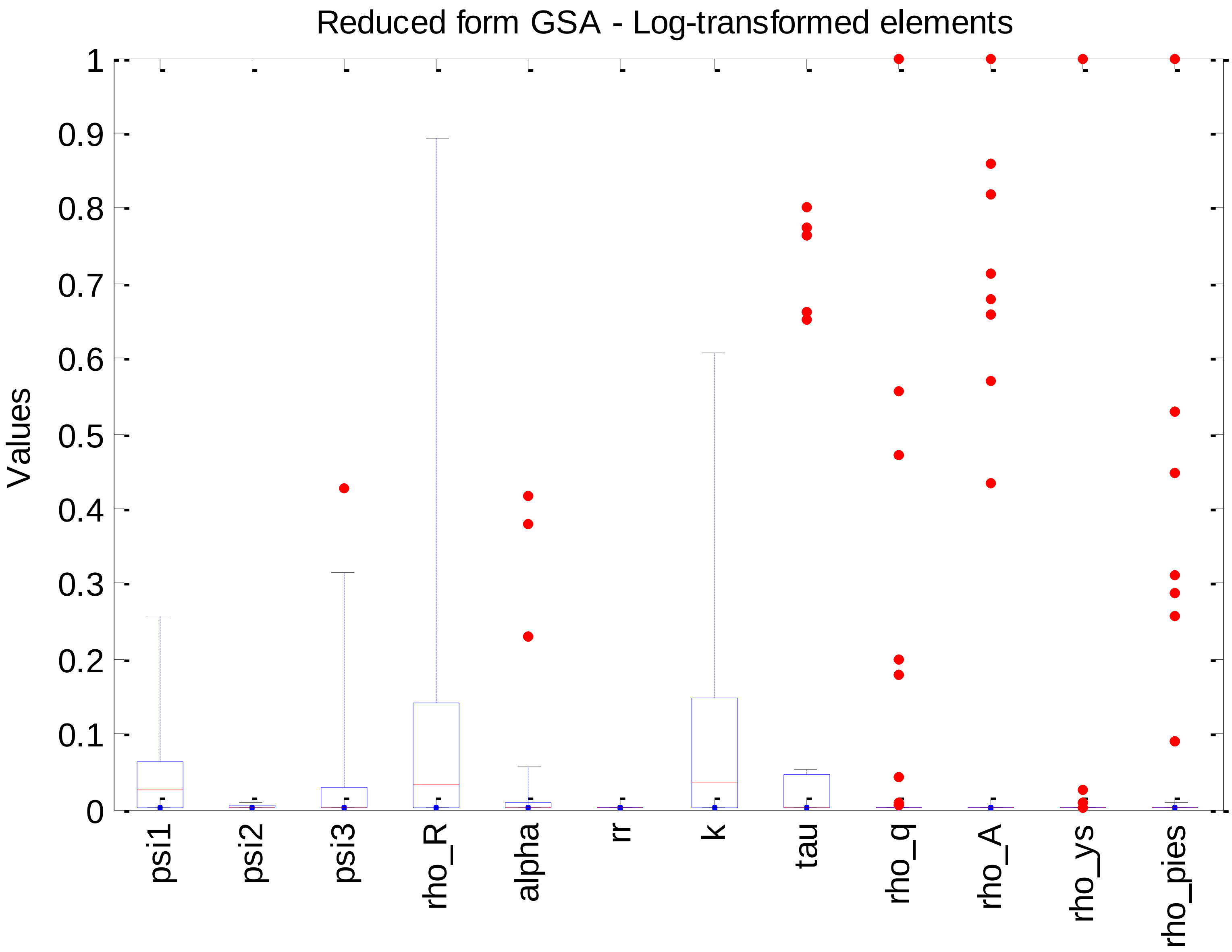
LS2005: pie vs e_R [-log(y)]



LS2005: R vs e_R [-log(y)]



Lubik Schorfheide (2005)



Toolbox documentation

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The mapping of the reduced form soultion forces the use of samples from prior ranges or prior distributions, i.e.:

pprior=1 (default);

ppost=0 (default);

[unless neighbourhood_width is applied]

Toolbox documentation

option name	default	description
`redform`	0	0 = don't prepare MC sample of reduced form matrices 1 = prepare MC sample of reduced form matrices
`load_redform`	0	0 = estimate the mapping of reduced form model 1 = load previously estimated mapping
`logtrans_redform`	0	0 = use raw entries 1 = use log-transformed entries
`threshold_redform`	[]	[] = don't filter MC entries of reduced form coefficients [max max] = analyse filtered entries within the range [max max]
`ksstat_redform`	0.001	critical p-value for Smirnov statistics d when `threshold_redform` is active plot parameters with p-value<`ksstat_redform`
`alpha2_redform`	0.001	critical p-value for correlation ρ when `threshold_redform` is active plot couples of parameters with p-value<`alpha2_redform`
`namendo`	()	list of endogenous variables
	:	jolly character to indicate ALL endogenous
`namlagendo`	()	list of lagged endogenous variables: analyse entries [`namendo`×`namlagendo`]
	:	jolly character to indicate ALL endogenous
`namexo`	()	list of exogenous variables: analyse entries [`namendo`×`namexo`]
	:	jolly character to indicate ALL exogenous

ss_anova Toolbox

Download here the Recursive SS-ANOVA Toolbox for MATLAB.

http://ipsc.jrc.ec.europa.eu/fileadmin/repository/sfa/finepro/software/ss_anova_recurs.zip

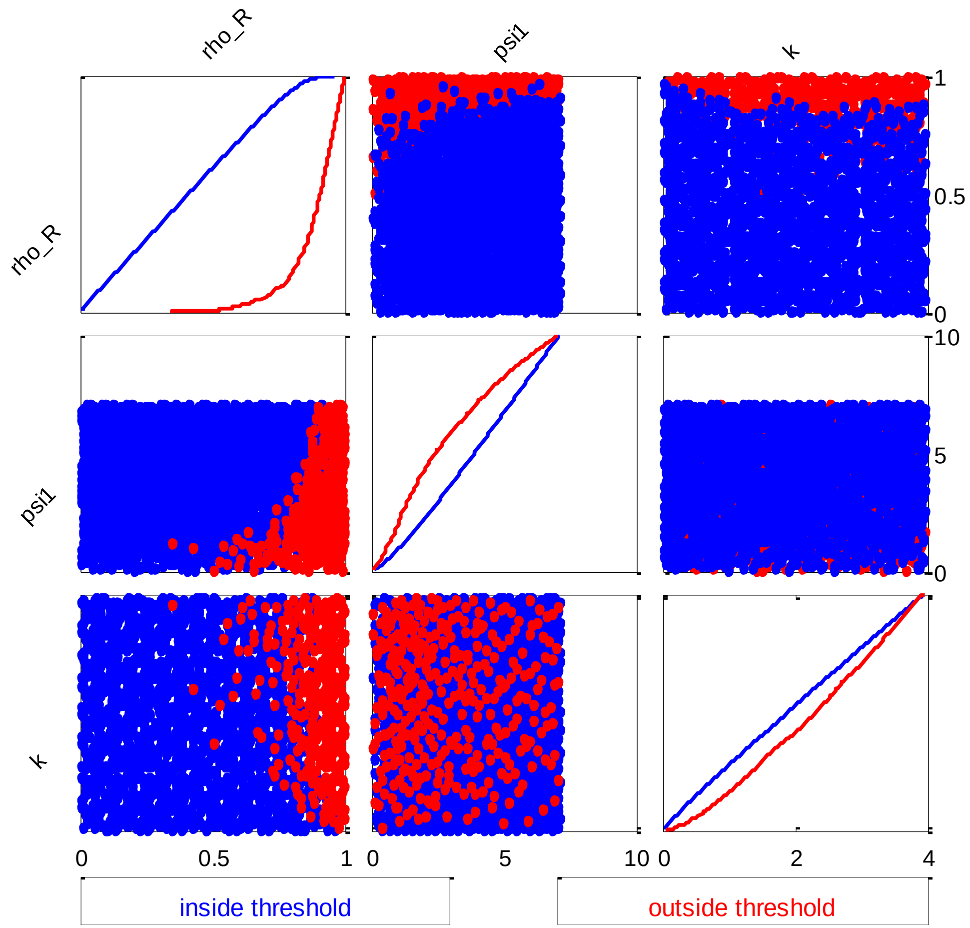
http://ipsc.jrc.ec.europa.eu/fileadmin/repository/sfa/finepro/software/ss_anova_recurs_matlab_ver_less_than_7.5.zip
(MATLAB version < 7.5)

Using Monte Carlo filtering

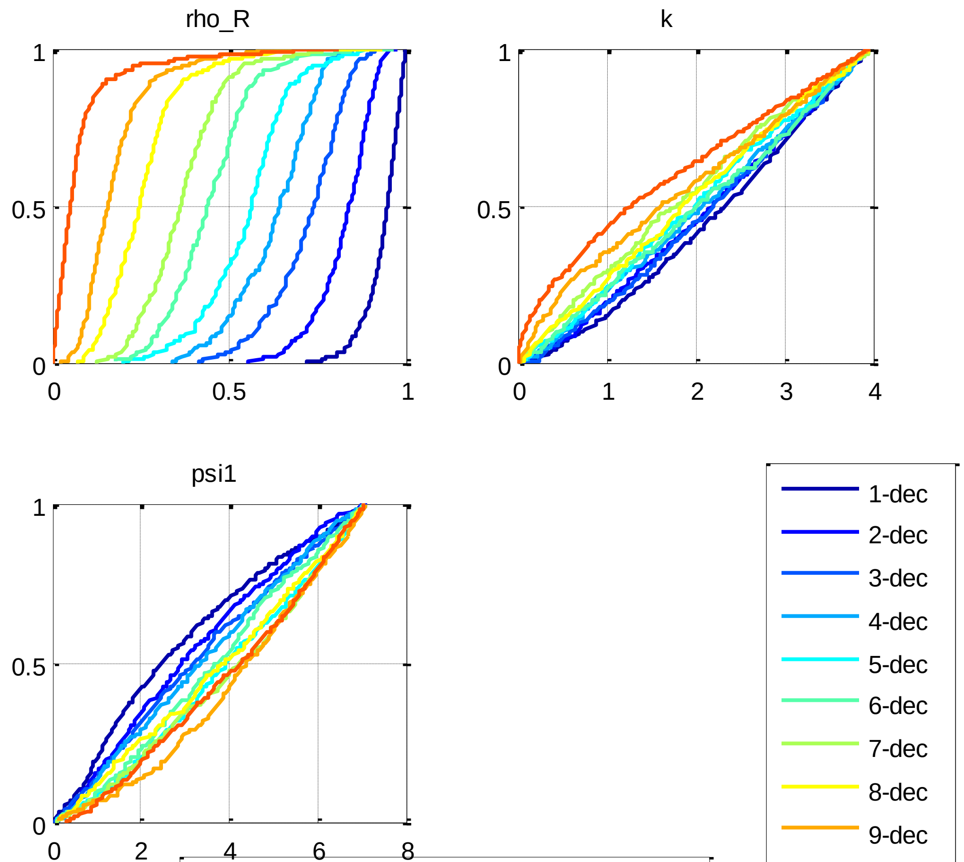
Store the sample of the state space A,B matrices;

For 1-step ahead irf, perform the MCF sensitivity tests for B(i,j) within/outside the specified ranges.

Using Monte Carlo filtering: $y = (\pi_t \text{ vs } R_{t-1}) \in [-1, 0]$



Using Monte Carlo filtering: $y = (\pi_t \text{ vs } R_{t-1}) \in [-\infty, \infty]$



Monte Carlo Filtering for pie vs R

Mapping reduced form solution

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`namendo`	()	list of endogenous variables
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`namexo`	()	list of exogenous variables: analyse entries [`namendo`×`namexo`]
	:	jolly character to indicate ALL exogenous