Finite Sample System Identification

Exact, Distribution-Free Confidence Regions

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Dynamical Systems

Mathematical models of dynamical systems are widely used in science and engineering, e.g., for prediction and control purposes.

Dynamical System (Markov)

$$x_t \triangleq f(x_{t-1}, u_t, w_t)$$

where

- t — time (discrete)
- x_t — output (state)
- u_t — input (external)
- w_t — noise (innovation)
- f — transition function

Point Estimation

Consider the parametric identification problem of the system

$$x_t \triangleq f_{\theta^*}(x_{t-1}, u_t, w_t),$$

parametrized with $\theta^* \in \Theta \subseteq \mathbb{R}^d$

Given: a finite sample, $\mathcal{Z}$, of outputs $\{x_t\}$ and inputs $\{u_t\}$

Point Estimate (Parametric)

$$\widehat{\theta}_{\mathcal{Z}} \triangleq \arg\min_{\theta \in \Theta} \mathcal{V}(\theta \mid \mathcal{Z})$$

where $\mathcal{V}$ is a criterion function.

Confidence Regions

In practice often some quality tag is needed to judge the estimate.

Safety, stability, or quality requirements? $\Rightarrow$ confidence regions

Confidence Region (Level μ)

$$\mathbb{P}\big(\theta^* \in \widehat{\Theta}_{\mathcal{Z},\mu}\big) \geq \mu$$

for some $\mu \in (0,1)$, where θ^* is the "true" parameter, $\widehat{\Theta}_{\mathcal{Z},\mu} \subseteq \Theta$.

Typically the level sets of the (scaled) limiting distribution is used.

Issues: only approximately correct for finite samples,
requires the existence of a (known) limiting distribution.

Main Objectives

- We aim at building confidence regions for dynamical systems.
- With non-asymptotic guarantees ("finite sample" method).
- Which are distribution-free: namely, do not make strong statistical assumption on the innovations of the process.
- They should be built around specific point estimates.
- The Sign-Perturbed Sums (SPS) method is presented.
- Its main assumption is that the noise terms are symmetric.
- Under which it can even provide exact confidence sets.
- Main models: linear regression, general linear dynamical systems, volatility models (not covered by this talk).

Linear Regression

Consider a standard linear regression problem:

Linear Regression

$$x_t \triangleq \varphi_t^{\mathrm{T}} \theta^* + w_t$$

where

x_t — output (for time $t = 1, \ldots, n$)

φ_t — regressor (deterministic, d dimensional)

w_t — noise (zero mean, uncorrelated)

σ^2 — variance of the noise (homoscedastic)

θ^* — true parameter (deterministic, d dimensional)

$\Phi_n = [\varphi_1, \ldots, \varphi_n]^{\mathrm{T}}$ — skinny and full rank

Least Squares

Given: a sample, $\mathcal{Z}$, of size n of outputs $\{x_t\}$ and regressors $\{\varphi_t\}$

A classical approach is the least squares criterion, namely

$$\mathcal{V}(\theta \mid \mathcal{Z}) \triangleq \sum_{t=1}^{n} (x_t - \varphi_t^{\mathrm{T}}\theta)^2.$$

The least squares estimate (LSE) can be found by solving

Normal Equation

$$\nabla_\theta \mathcal{V}(\hat{\theta}_n \mid \mathcal{Z}) = \sum_{t=1}^{n} \varphi_t (x_t - \varphi_t^{\mathrm{T}}\hat{\theta}_n) = 0$$

Asymptotic Normality

LSE can be explicitly formulated as

$$\hat{\theta}_n = \left(\sum_{t=1}^{n} \varphi_t \varphi_t^{\mathrm{T}} \right)^{-1} \left(\sum_{t=1}^{n} \varphi_t x_t \right).$$

LSE is asymptotically normal

Limiting Distribution

$$\sqrt{n}\,(\hat{\theta}_n - \theta^*) \xrightarrow{d} \mathcal{N}(0, \sigma^2 R^{-1}) \quad \text{as} \quad n \to \infty$$

where R is the limit of $R_n = \frac{1}{n} \sum_{t=1}^{n} \varphi_t \varphi_t^{\mathrm{T}}$ as $n \to \infty$ (if exists).

Confidence Ellipsoids

The standard confidence region construction is then

Confidence Ellipsoid

$$\widetilde{\Theta}_{n,\mu} \triangleq \left\{ \theta \in \mathbb{R}^d \,:\, (\theta - \hat{\theta}_n)^{\mathrm{T}} R_n (\theta - \hat{\theta}_n) \leq \frac{\mu\, \hat{\sigma}_n^2}{n} \right\}$$

where $\mathbb{P}(\theta^* \in \widetilde{\Theta}_{n,\mu}) \approx F_{\chi^2(d)}(\mu)$, where $F_{\chi^2(d)}$ is the CDF of $\chi^2(d)$,

$$\hat{\sigma}_n^2 \triangleq \frac{1}{n-d} \sum_{t=1}^{n} (x_t - \varphi_t^{\mathrm{T}} \hat{\theta}_n)^2,$$

is an estimate of σ^2 based on the sample.

Reference and Sign-Perturbed Sums

Let us introduce a reference sum and $m-1$ sign-perturbed sums.

Reference Sum

$$S_0(\theta) \triangleq R_n^{-\frac{1}{2}} \sum_{t=1}^{n} \varphi_t (x_t - \varphi_t^{\mathrm{T}} \theta)$$

Sign-Perturbed Sums

$$S_i(\theta) \triangleq R_n^{-\frac{1}{2}} \sum_{t=1}^{n} \varphi_t \, \alpha_{i,t} (x_t - \varphi_t^{\mathrm{T}} \theta)$$

for $i = 1, \ldots, m-1$, where $\alpha_{i,t}$ $(t = 1, \ldots, n)$ are i.i.d. random signs, that is $\alpha_{i,t} = \pm 1$ with probability $1/2$ each (Rademacher).

Intuitive Idea: Distributional Invariance

Assume $\{w_t\}$ are independent and each w_t is symmetric about zero.

Observe that, if $\theta = \theta^*$, we have $(i = 1, \ldots, m-1)$

Distributional Invariance

$$S_0(\theta^*) = R_n^{-\frac{1}{2}} \sum_{t=1}^{n} \varphi_t w_t$$

$$S_i(\theta^*) = R_n^{-\frac{1}{2}} \sum_{t=1}^{n} \varphi_t \alpha_{i,t} w_t$$

Consider the ordering $\|S_{(0)}(\theta^*)\|^2 \prec \cdots \prec \|S_{(m-1)}(\theta^*)\|^2$

Note: relation "$\prec$" is the canonical "$<$" with random tie-breaking

$\boxed{\text{All orderings are equally probable!}}$ (they are conditionally i.i.d.)

Intuitive Idea: Reference Dominance

What if $\theta \neq \theta^*$?

In fact, the reference paraboloid $\|S_0(\theta)\|^2$ increases faster than $\{\|S_i(\theta)\|^2\}$, thus will eventually dominate the ordering.

Intuitively, for "large enough" $\|\tilde{\theta}\|$, where $\tilde{\theta} \triangleq \theta^* - \theta$

Eventual Dominance of the Reference Paraboloid

$$\left\| \sum_{t=1}^{n} \varphi_t \varphi_t^{\mathrm{T}} \tilde{\theta} + \sum_{t=1}^{n} \varphi_t w_t \right\|_{R_n^{-1}}^2 > \left\| \sum_{t=1}^{n} \pm \varphi_t \varphi_t^{\mathrm{T}} \tilde{\theta} + \sum_{t=1}^{n} \pm \varphi_t w_t \right\|_{R_n^{-1}}^2$$

with "high probability" (for simplicity $\pm$ is used instead of $\{\alpha_{i,t}\}$).

Non-Asymptotic Confidence Regions

The rank of $\|S_0(\theta)\|^2$ in the ordering of $\{\|S_i(\theta)\|^2\}$ w.r.t. $\prec$ is

$$\mathcal{R}(\theta) = 1 + \sum_{i=1}^{m-1} \mathbb{I}(\|S_i(\theta)\|^2 \prec \|S_0(\theta)\|^2),$$

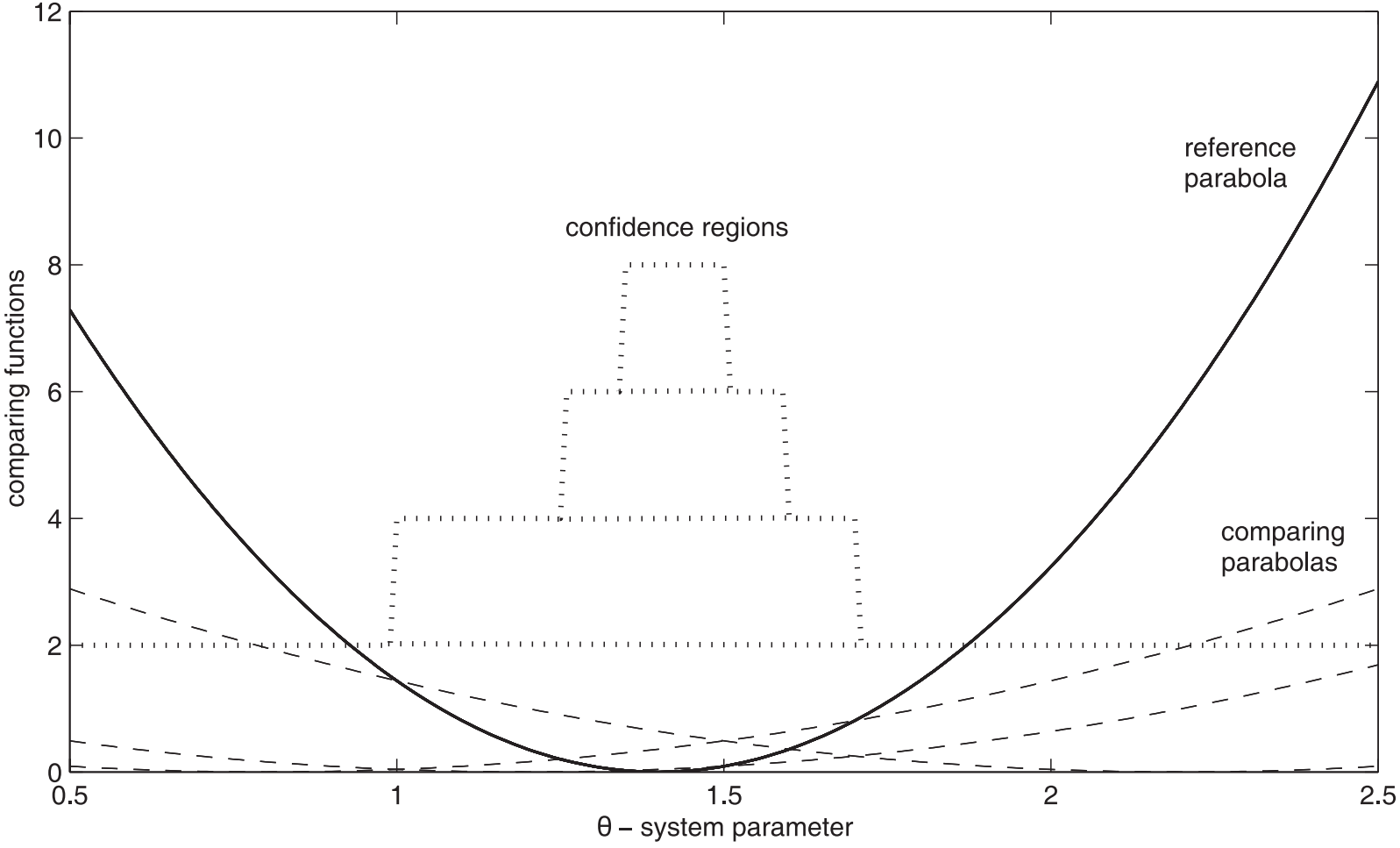
where $\mathbb{I}(\cdot)$ is an indicator function.

Sign-Perturbed Sums (SPS) Confidence Regions

$$\widehat{\Theta}_n \triangleq \left\{ \theta \in \mathbb{R}^d \, : \, \mathcal{R}(\,\theta\,) \leq m - q \right\}$$

where $m > q > 0$ are user-chosen integers (design parameters).

Simple Illustration, Constant in Noise, $n = 3$, $m = 4$



Exact Confidence

(A1) $\{w_t\}$ is a sequence of independent random variables.
Each w_t has a symmetric probability distribution about zero.

(A2) The outer product of regressors is invertible, $\det(R_n) \neq 0$.

Exact Confidence of SPS

$$\mathbb{P}\big(\theta^* \in \widehat{\Theta}_n\big) = 1 - \frac{q}{m}$$

for finite samples. Parameters m and q are under our control.

Note that $\|S_0(\hat{\theta}_n)\|^2 = 0$, thus $\hat{\theta}_n \in \widehat{\Theta}_n$, assuming it is non-empty.

Star Convexity

Set $\mathcal{X} \subseteq \mathbb{R}^d$ is star convex if there is a star center $c \in \mathbb{R}^d$ with

$$\forall x \in \mathcal{X}, \forall \beta \in [0,1] \,:\, \beta\, x + (1-\beta)\, c \in \mathcal{X}.$$

Star Convexity of SPS

$\widehat{\Theta}_n$ is star convex with the LSE, $\hat{\theta}_n$, as a star center

Hint $\widehat{\Theta}_n$ is the union and intersection of ellipsoids containing LSE.

Strong Consistency

(A1) independence, symmetricity: $\{w_t\}$ are independent, symmetric

(A2) invertibility: $R_n \triangleq \frac{1}{n}\sum_{t=1}^{n} \varphi_t \varphi_t^{\mathrm{T}}$ is invertible

(A3) regressor growth rate: $\sum_{t=1}^{\infty} \|\varphi_t\|^4 / t^2 < \infty$

(A4) noise moment growth rate: $\sum_{t=1}^{\infty} \left(\mathbb{E}[w_t^2]\right)^2 / t^2 < \infty$

(A5) Cesàro summability: $\lim_{n\to\infty} R_n = R$, which is positive definite

Strong Consistency of SPS

$$\forall\, \varepsilon > 0 : \exists\, (\text{a.s.})\, N : \forall\, n > N : \widehat{\Theta}_n \subseteq B_\varepsilon(\theta^*)$$

where $B_\varepsilon(\theta^*) \triangleq \{\, \theta \in \mathbb{R}^d : \|\theta - \theta^*\| \leq \varepsilon \,\}$ is a norm ball.

Ellipsoidal Outer Approximation

The reference paraboloid can be rewritten as

$$\|S_0(\theta)\|^2 = (\theta - \hat{\theta}_n)^{\mathrm{T}} R_n (\theta - \hat{\theta}_n).$$

From which an alternative description of the confidence region is

$$\widehat{\Theta}_n \subseteq \left\{ \theta \in \mathbb{R}^d \,:\, (\theta - \hat{\theta}_n)^{\mathrm{T}} R_n (\theta - \hat{\theta}_n) \leq r(\theta) \right\},$$

where $r(\theta)$ is the qth largest value of $\{\|S_i(\theta)\|^2\}_{i \neq 0}$.

Ellipsoidal Outer Approximation

$$\widehat{\Theta}_n \subseteq \left\{ \theta \in \mathbb{R}^d \,:\, (\theta - \hat{\theta}_n)^{\mathrm{T}} R_n (\theta - \hat{\theta}_n) \leq r^* \right\}$$

The question is of course how to find such an r^* efficiently.

Quadratically Constrained Quadratic Program

$\max\{\|S_i(\theta)\|^2 : \|S_0(\theta)\|^2 \leq \|S_i(\theta)\|^2\}$ can be obtained by

$$\begin{aligned} \text{maximize} \quad & \|z\|^2 \\ \text{subject to} \quad & z^{\mathrm{T}} A_i z + 2 z^{\mathrm{T}} b_i + c_i \leq 0 \end{aligned}$$

$$\begin{aligned} A_i &\triangleq I - R_n^{-\frac{1}{2}} Q_i R_n^{-1} Q_i R_n^{-\frac{1}{2}\mathrm{T}}, \\ b_i &\triangleq R_n^{-\frac{1}{2}} Q_i R_n^{-1} (\psi_i - Q_i \hat{\theta}_n), \\ c_i &\triangleq -\psi_i^{\mathrm{T}} R_n^{-1} \psi_i + 2\hat{\theta}_n^{\mathrm{T}} Q_i R_n^{-1} \psi_i - \hat{\theta}_n^{\mathrm{T}} Q_i R_n^{-1} Q_i \hat{\theta}_n. \end{aligned}$$

$$Q_i \triangleq \sum_{t=1}^{n} \alpha_{i,t} \varphi_t \varphi_t^{\mathrm{T}}, \qquad \psi_i \triangleq \sum_{t=1}^{n} \alpha_{i,t} \varphi_t x_t.$$

Semi-Definite Program

Problem: the previous QCQP is not convex.

Fortunately, strong duality holds and its dual can be written as:

Dual Problem

$$\begin{aligned} \text{minimize} \quad & \gamma \\ \text{subject to} \quad & \lambda \geq 0 \\ & \begin{bmatrix} -I + \lambda A_i & \lambda b_i \\ \lambda b_i^{\mathrm{T}} & \lambda c_i + \gamma \end{bmatrix} \succeq 0 \end{aligned}$$

where "$\succeq 0$" denotes that a matrix is positive semidefinite.

Radius r^* can then be found by solving $m-1$ such convex problems, obtaining $\{\gamma_i^*\}$, and defining r^* the qth largest one.

Simulation Experiment

Finite Impulse Response (FIR) System (2nd order)

$$x_t = 0.7\, u_{t-1} + 0.3\, u_{t-2} + w_t$$

where $\{w_t\}$ are i.i.d. zero mean Laplacian, with variance 0.1.

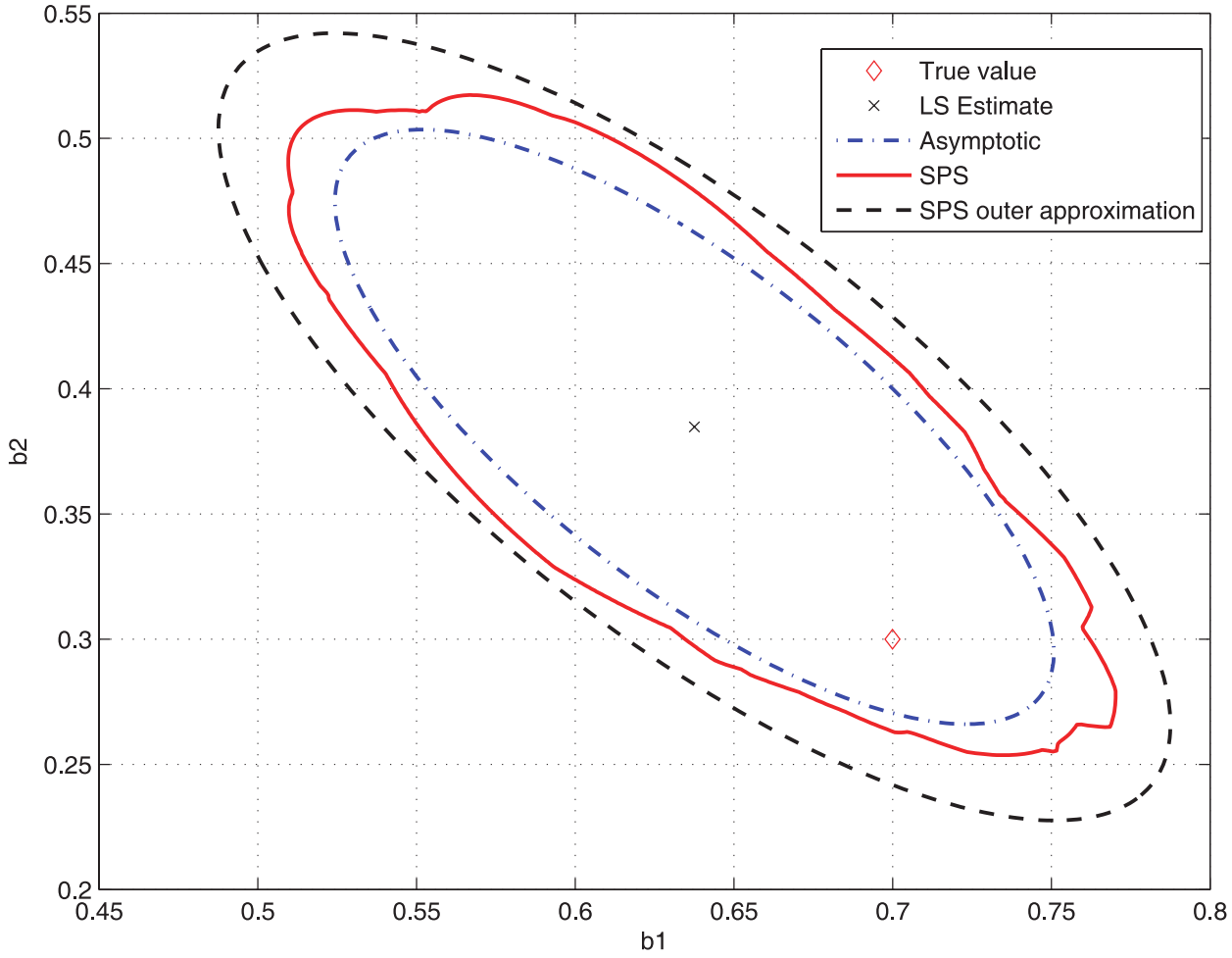
The input signal $\{u_t\}$ is given by the autoregression

$$u_t = 0.75\, u_{t-1} + v_t,$$

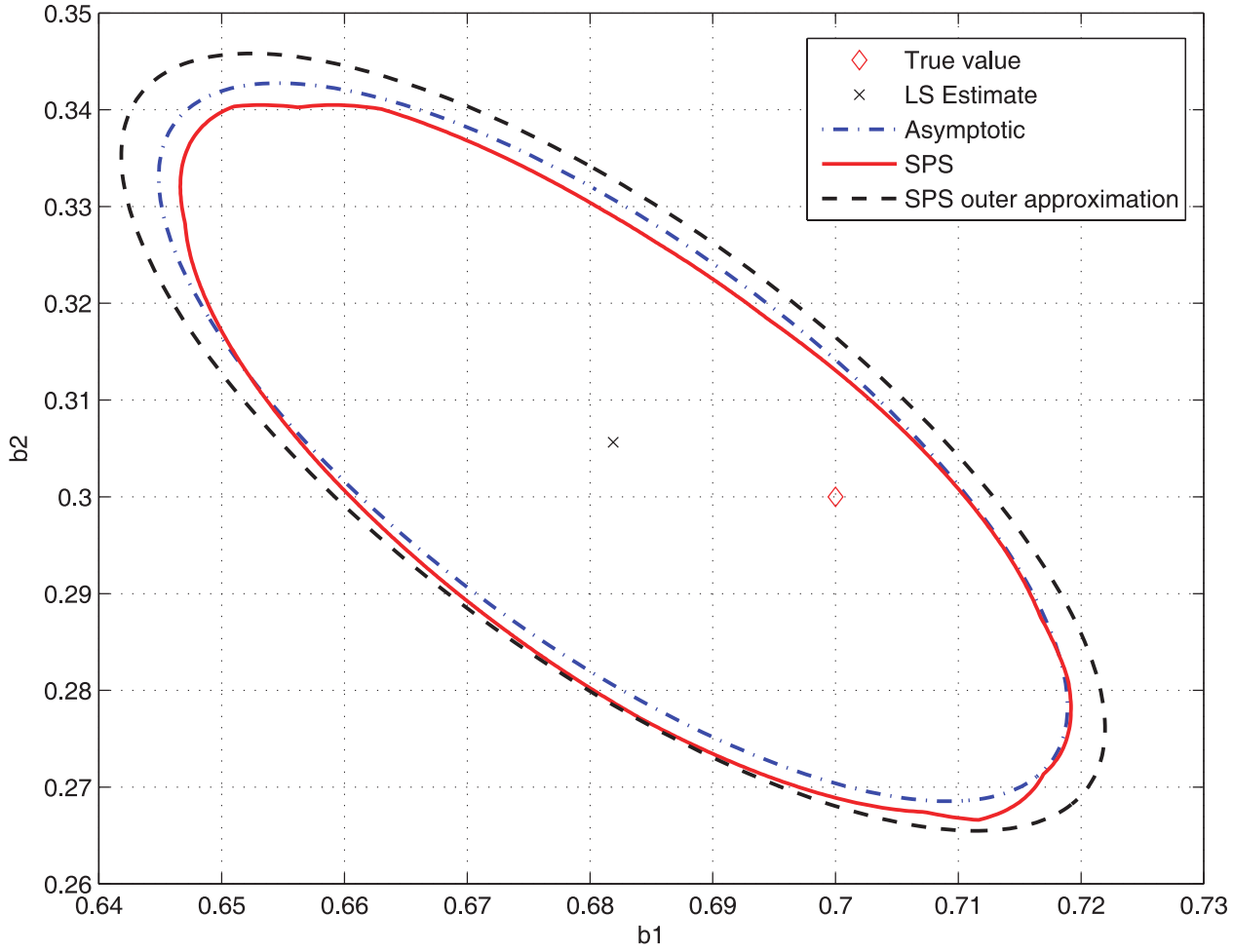
where $\{v_t\}$ is a sequence of i.i.d. standard normal variables.

Confidence regions (level 95 %) of SPS, its outer approximation and the standard asymptotic ellipsoids are compared.

95% Confidence Regions, $n = 25$, $m = 100$, $q = 5$



95% Confidence Regions, $n = 400$, $m = 100$, $q = 5$



Linear Dynamical Systems

Consider systems written using (rational) transfer functions:

General Linear Systems

$$x_t \triangleq G(z^{-1};\theta^*)\, u_t + H(z^{-1};\theta^*)\, w_t$$

(A1) The true system is in the model class, the orders are known.

(A2) The transfer function $H(z^{-1};\theta^*)$ has a (stable) inverse, as well as $G(0;\theta^*) = 0$ and $H(0;\theta^*) = 1$.

(A3) Noises $\{w_t\}$ are independent and symmetrically distributed.

(A4) Inputs $\{u_t\}$ are observed and independent of $\{w_t\}$.

(A5) Initialization: for all $t \leq 0$, we have $x_t = w_t = u_t = 0$.

Prediction Error Estimate

Prediction Error or Residual (for parameter θ)

$$\widehat{\varepsilon}_t(\theta) \triangleq H^{-1}(z^{-1};\theta)\left(x_t - G(z^{-1};\theta)\, u_t\right)$$

Note that $\widehat{\varepsilon}_t(\theta^*) = w_t$, hence, it is accurate for $\theta = \theta^*$.

Prediction Error Estimate (for model class Θ)

$$\hat{\theta}_{\mathrm{PEM}} \triangleq \arg\min_{\theta\in\Theta} \sum_{t=1}^{n} \widehat{\varepsilon}_t^2(\theta)$$

In general, there is no closed-form solution for PEM.

Prediction Error Equation

The PEM estimate can be found, e.g., by using the equation

PEM Equation

$$\nabla_\theta \mathcal{V}(\hat{\theta}_{\mathrm{PEM}} \mid \mathcal{Z}) = \sum_{t=1}^{n} \psi_t(\hat{\theta}_{\mathrm{PEM}})\, \widehat{\varepsilon}_t(\hat{\theta}_{\mathrm{PEM}}) = 0$$

where $\psi_t(\theta)$ is the negative gradient of the prediction error,

$$\psi_t(\theta) \triangleq -\nabla_\theta \widehat{\varepsilon}_t(\theta).$$

These gradients can be directly calculated in terms of the defining polynomials of the rational transfer functions G and H.

Perturbed Samples

Perturbed Output Trajectories

$$\bar{x}_t(\theta, \alpha_i) \triangleq G(z^{-1}; \theta)\, u_t + H(z^{-1}; \theta)\, (\alpha_{i,t}\, \widehat{\varepsilon}_t(\theta))$$

where $\{\alpha_{i,t}\}$ are random signs, as previously.

Recall that $\psi_t(\theta)$ is a linear filtered version of $\{x_t\}$ and $\{u_t\}$,

$$\psi_t(\theta) = W_0(z^{-1}; \theta)\, x_t + W_1(z^{-1}; \theta)\, u_t,$$

where W_0 and W_1 are vector-valued, and $\psi_t(\theta) \in \mathbb{R}^d$.

Perturbed (Negative) Gradients

$$\bar{\psi}_t(\theta, \alpha_i) \triangleq W_0(z^{-1}; \theta)\, \bar{x}_t(\theta, \alpha_i) + W_1(z^{-1}; \theta)\, u_t$$

Sign-Perturbed Sums for General Linear Systems

Reference and Sign-Perturbed Sums

$$S_0(\theta) \triangleq \Psi_n^{-\frac{1}{2}}(\theta) \sum_{t=1}^{n} \psi_t(\theta)\, \widehat{\varepsilon}_t(\theta)$$

$$S_i(\theta) \triangleq \bar{\Psi}_n^{-\frac{1}{2}}(\theta, \alpha_i) \sum_{t=1}^{n} \bar{\psi}_t(\theta, \alpha_i)\, \alpha_{i,t}\, \widehat{\varepsilon}_t(\theta)$$

Reference and Sign-Perturbed Covariances

$$\Psi_n(\theta) \triangleq \frac{1}{n} \sum_{t=1}^{n} \psi_t(\theta) \psi_t^{\mathrm{T}}(\theta)$$

$$\bar{\Psi}_n(\theta, \alpha_i) \triangleq \frac{1}{n} \sum_{t=1}^{n} \bar{\psi}_t(\theta, \alpha_i) \bar{\psi}_t^{\mathrm{T}}(\theta, \alpha_i)$$

Non-Asymptotic Confidence Regions

$\mathcal{R}(\theta)$ is again the rank of $\|S_0(\theta)\|^2$ among $\{\|S_i(\theta)\|^2\}$ w.r.t. $\prec$

SPS Confidence Regions for General Linear Systems

$$\widehat{\Theta}_n \triangleq \left\{ \theta \in \mathbb{R}^d \,:\, \mathcal{R}(\theta) \leq m - q \right\}$$

where $m > q > 0$ are user-chosen (integer) parameters.

We have $S_0(\hat{\theta}_{\mathrm{PEM}}) = 0$, thus, $\hat{\theta}_{\mathrm{PEM}} \in \widehat{\Theta}_n$, if it is non-empty.

Exact Confidence of SPS for General Linear Systems

$$\mathbb{P}\left(\theta^* \in \widehat{\Theta}_n\right) = 1 - \frac{q}{m}$$

Simulation Experiment

Autoregressive Moving Average: ARMA(1,1)

$$x_t + a^* x_{t-1} = w_t + c^* w_{t-1}$$

where $\theta^* = (a^*, c^*)$ and $\{w_t\}$ are i.i.d. standard normal.

The inverse filter of $C(z^{-1};\theta)\, w_t = w_t + c\, w_{t-1}$ is

$$C^{-1}(z^{-1};\theta) = \sum_{k=0}^{\infty} (-1)^k\, c^k\, z^{-k}$$

Can be used to define the prediction errors for $\theta = (a, c)$

$$\widehat{\varepsilon}_t(\theta) = C^{-1}(z^{-1};\theta)\,(x_t + a\, x_{t-1}).$$

Simulation Experiment

Perturbed Output Trajectories

$$\bar{x}_t(\theta, \alpha_i) = -a\,\bar{x}_{t-1}(\theta, \alpha_i) + \alpha_{i,t}\,\widehat{\varepsilon}_t(\theta) + c\,\alpha_{i,t-1}\widehat{\varepsilon}_{t-1}(\theta)$$

for $1 \leq i \leq m$ and $1 \leq t \leq n$, where $\{\alpha_{i,t}\}$ are random signs.

Perturbed (Negative) Gradients

$$\bar{\psi}_t(\theta, \alpha_i) = \begin{bmatrix} -C^{-1}(z^{-1};\theta)\,\bar{x}_t(\theta, \alpha_i) \\ C^{-1}(z^{-1};\theta)\,\alpha_{i,t}\,\widehat{\varepsilon}_t(\theta) \end{bmatrix}$$

which can be used to define the sign-perturbed sums.

99% Confidence Regions, $n = 500$, $m = 100$, $q = 1$

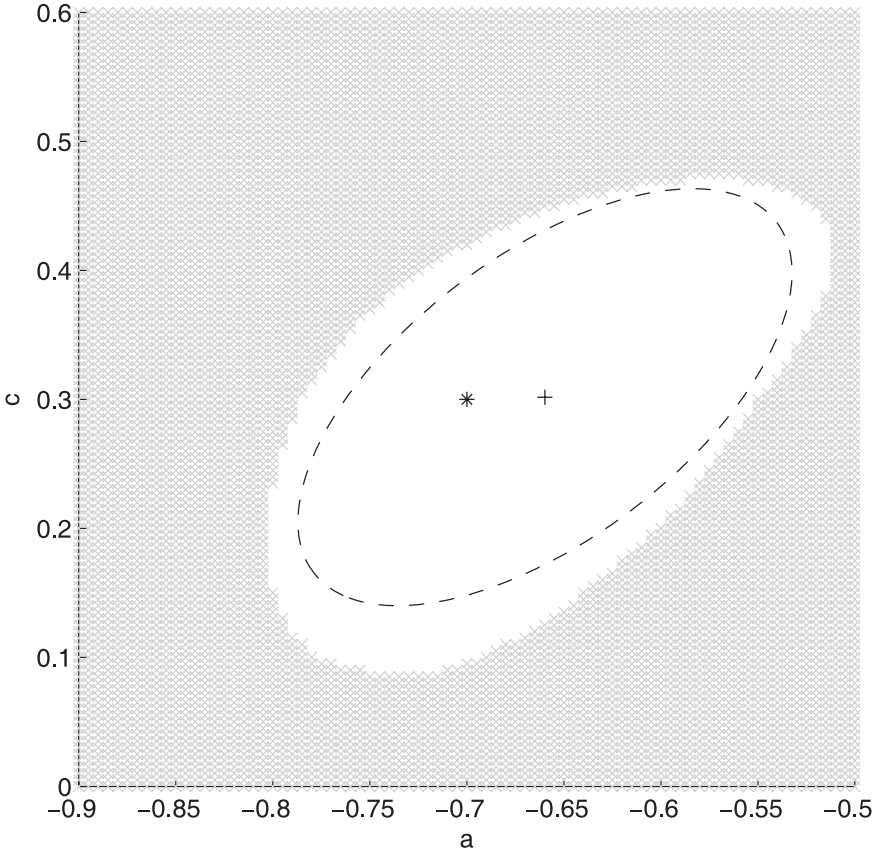
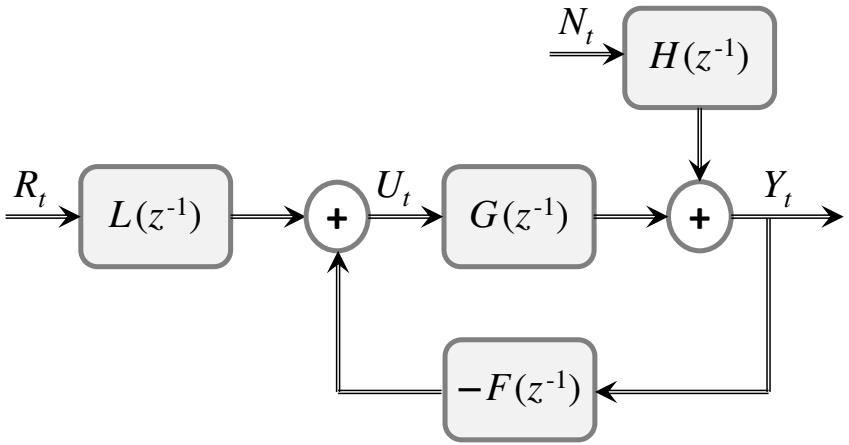


Figure: "$\times$": SPS (compl.); "$*$": θ^*; "$+$": PEM; "--": asymp. ellipsoid

Extensions

- SPS can be modified for instrumental variable estimates, which simplifies to construction, but needs instrumentals.
- SPS can be extended to closed-loop systems, to the direct, indirect and joint input-output approach of PEM.



- The core ideas of SPS can be transferred to volatility models.

Summary

- A new finite sample estimation method (SPS) was presented.
- It builds confidence regions around the least squares estimate.
- Only mild statistical assumptions are needed, e.g., symmetry.
- Not needed: stationarity, moments, particular distributions.
- For (rational) probabilities, exact confidence sets can be built.
- SPS is strongly consistent, i.e., the confidence regions almost surely shrink around the true parameter (for lin.reg.).
- SPS is star convex with the LSE as a center (for lin.reg.).
- Efficient ellipsoidal outer approximation exists (for lin.reg.).
- The algorithm was also presented for general linear systems.
- Its fundamental ideas work for other kinds of systems, as well.

Thank you for your attention.