Parameter Estimation in a Moving Horizon Perspective

State and Parameter Estimation in Dynamical Systems

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OUTLINE

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**Model**

\[
\begin{align*}
    x(t + 1) &= f(x(t), u(t), w(t), \theta) \\
    y(t) &= h(x(t), u(t), \theta) + e(t)
\end{align*}
\]

**Problem**

Measure \( y(t) \) and \( u(t), t = 1, \ldots, N \). Find \( x(t) \) and \( \theta \)

**Linear Case**

\[
\begin{align*}
    f(x(t), u(t), w(t), \theta) &= A(\theta)x(t) + B(\theta)u(t) + w(t) \\
    h(x(t), u(t), \theta) &= C(\theta)x(t)
\end{align*}
\]

**Known System Case**

\( \theta \) is a known vector
View $\Theta = [\theta, x(t), t = 1, \ldots, N]$ as unknown parameters. Assume $e(t) \in N(0, I)$. Then the negative log-likelihood function is

$$V(\theta, x(\cdot)) = \sum_{t=1}^{N} \|y(t) - h(x(t), u(t), \theta)\|^2$$

Too many parameters! $\Rightarrow$ Regularize!
Do a (nonlinear) change of parameters:
View $\tilde{\Theta} = [\theta, x(1), w(1), \ldots, w(N - 1)] = [\theta, w(\cdot)]$ as the new set of parameters,

$[x(k) = f(x(k - 1), u(k - 1), w(k - 1), \theta) = x(k, \tilde{\Theta})]$ 

[The ML-estimate is unaffected by change of parameters!]

The negative log-likelihood function for $\tilde{\Theta}$ is

$$V(\tilde{\Theta}) = \sum_{t=1}^{N} \| y(t) - h(x(t, \tilde{\Theta}), u(t), \theta) \|^2$$

This to be minimized wrt $\tilde{\Theta} = [\theta, w(\cdot)]$. 
Regularization

With regularization:

\[ W(\tilde{\Theta}) = \sum_{t=1}^{N} \| y(t) - h(x(t, \tilde{\Theta}), u(t), \theta) \|^2 + \lambda R(\tilde{\Theta}) \]

Choices of regularization:

\[ R(\tilde{\Theta}) = \sum_{t=1}^{N} \| w(t) \|^2 \quad \text{[Tichonov]} \]

or

\[ R(\tilde{\Theta}) = \sum_{t=1}^{N} \| w(t) \| \quad \text{[sum-of-norms]} \]
Regularization curbs the flexibility of (large) model sets by pulling the parameters toward the origin.

- Tichonov: Regularization for Bias-Variance Trade-off
- Sum-of-norms: Regularization for Sparsity:
  Solutions with “many” $\|w(t)\| = 0$ are favored
Bayesian Interpretation

Suppose \( w(t) \in N(0, I) \) and \( \theta \) is a random vector with \( \theta \in N(0, cI) \) (dim = \( d \)). Then the joint pdf of \( \theta, y(\cdot), w(\cdot) \) is

\[
-2 \log P(y(\cdot), w(\cdot), \theta) \sim \sum_{t=1}^{N} \left[ \| y(t) - h(x(t, w(\cdot)), u(t), \theta) \|^2 + \| w(t) \|^2 \right] + \| \theta \|^2 / c + \text{const}
\]

\[
x(t, w(\cdot)) = f(x(t - 1, w(\cdot)), u(t - 1), w(t - 1), \theta)
\]

so the MAP estimate of \( \tilde{\Theta} \) is

\[
\hat{\Theta} = \arg \min W(\tilde{\Theta}) + \| \theta \|^2 / c
\]

which for \( c \to \infty \) is the same as the Tichonov-regularized ML estimate of \( \tilde{\Theta} \).
2
State Estimation with Sparse Process Disturbances in Linear Systems

3
Parameter and State Estimation in Unknown (Linear) Systems
Linear System with Sparse Process Disturbances

\[
x(t + 1) = Ax(t) + Bu(t) + w(t)
\]

\[
y(t) = Cx(t) + e(t).
\]

Here, \(e\) is white measurement noise and \(w\) is a process disturbance. In many applications, \(w\) is mostly zero, and strikes, \(w(t^*) \neq 0\), only occasionally. Examples of applications:

- Control: Load disturbance
- Tracking: Sudden maneuvers
- FDI: Additive system faults
- Recursive Identification (\(x=\)parameters): model segmentation
Approaches

- Find the jump times $t$ ($w(t) \neq 0$) and/or the smoothed state estimates $\hat{x}_s(t|N)$, $t = 1, \ldots, N$.

Common methods:

- Say $w(t^*) \neq 0$. View $t^*$ and $w(t^*)$ as unknown parameters and estimate them. (Willsky-Jones GLR)
- Set the process noise variance to a small number and use Kalman Smoothing to estimate $x$ (and $w(t)$)
- Branch the KF at each time instant: jump/no jump. Prune/merge trajectories (IMM).
- It is a non-linear filtering problem (linear but not Gaussian noise), so try particle filtering

All methods require some design variables that reflect the trade-off between measurement noise sensitivity and jump alertness.
For one jump at time $t^*$, estimate $t^*$ and $w(t^*)$ as parameters.

\[ x(t + 1) = Ax(t) + Bu(t) + w(t); \quad y(t) = Cx(t) + e(t). \]

- If $t^*$ is known it is a simple LS problem to estimate $w(t^*)$. $x(t)$ is a linear function of $w(t^*)$:

\[
\min_{w(t^*)} \sum \| y(t) - Cx(t) \|^2
\]

- Using the variance of the estimate, the significance of the jump size can be decided in a $\chi^2$ test.

- The time of the most significant jump is the $t^*$ that minimizing

\[
\min_{t^*} \min_{w(t^*)} \sum \| y(t) - Cx(t) \|^2
\]
Willsky-Jones as a Constrained Optimization Problem

- Can be written as

$$\min_{w(k), k=1,...,N-1} \sum_{t=1}^{N} \|y(t) - Cx(t)\|^2$$

subject to

$$\|W\|_0 = 1; \quad W = [\|w(1)\|_2, \ldots, \|w(N-1)\|_2]$$

such that

$$x(t+1) = Ax(t) + Bu(t) + w(t); \quad x(1) = 0.$$ 

- \(k\) jumps: ...

- Adjustable number of jumps:

$$\min_{w(k), k=1,...,N-1} \sum_{t=1}^{N} \|y(t) - Cx(t)\|^2 + \lambda \|W\|_0$$
Do the $\ell_1$ Trick! ($\ell_0 \rightarrow \ell_1$)

This problem is computationally forbidding, so relax the $\ell_0$ norm:

$$\min_{w(k), k=1,...,N-1} \sum_{t=1}^{N} \|y(t) - Cx(t)\|^2 + \lambda \|W\|_1$$

$$= \min_{w(k), k=1,...,N-1} \sum_{t=1}^{N} \|y(t) - Cx(t)\|^2 + \lambda \sum_{t=1}^{N} \|w(t)\|_2$$

[StateSON] This is our Moving Horizon State estimation problem with SON-regularization.

Choice of $\lambda$: ....

DC motor with impulse disturbances at $t = 49, 55$
State RMSE over 500 realizations as a function of time $t : 0 \rightarrow 100$.
Dashed blue: Willsky-Jones, Solid green: StateSON
Varying SNRs

Same system. Jump probability $\mu = 0.015$. Varying SNR: $Q =$ jump size, $R_e =$ measurement noise variance. For each SNR, RMSE averages over 500 MC runs. Many different approaches.

\[ \text{MSE} = \frac{Q}{R_e} \]

**Graph:**

- Clairvoyant
- CUSUM
- STATESON
- WJ
- PF
- Kalman
- IMM

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Parameter Estimation in a Moving Horizon Perspective
Solving the (moving horizon) state estimation problem with Sum-of-Norm ($\ell_1$) regularization is a good way to handle sparse process noise.

Performance is at least as good as for more complicated (hypothesis-testing) routines.
New problem: No longer assume that the parameter vector is known.

How to estimate also the parameter $\theta$ in the system description?
State and Parameter Estimation

Recall:

$$\hat{\Theta} = [\theta, x(1), w(1), \ldots, w(N-1)] = [\theta, w(\cdot)]$$

$$x(k) = f(x(k-1), u(k-1), w(k-1), \theta) = x(k, \hat{\Theta})$$

$$\min_{\hat{\Theta}} \sum_{t=1}^{N} [\|y(t) - h(x(t, \hat{\Theta}), u(t), \theta)\|^2 + \|w(t)\|^2]$$

This is (a) ML/MAP joint estimate of the states and the parameter vector.

View it as minimization over

$$\Theta = [\theta, x(1), x(2), \ldots, x(N)] = [\theta, x(\cdot)]$$

$$x(k) = f(x(k-1), u(k-1), w(k-1, x(\cdot)), \theta)$$
Joint State and Parameter Estimate

\[
\min_{\Theta} V(\theta, x(\cdot))
\]

\[
V(\theta, x(\cdot)) = \sum_{t=1}^{N} \|y(t) - h(x(t), u(t), \theta)\|^2 + \|w(t, x)\|^2
\]

"\sim P(\mathcal{Y}|\theta, X)"

\[
[\hat{\theta}^l, x^s(t, \hat{\theta}^l)] = \hat{\Theta} = \arg\min_{\Theta} V(\theta, x(\cdot))
\]

\[
x^s(t, \theta^*) = \text{The smoothed states for given parameter } \theta^*
\]

The states are \textit{nuisance parameters} in the estimation of \( \theta \).
Possible Parameter Estimates

\( \hat{\theta}_J \) as above; joint estimate with states

\[
\hat{\theta}^{ML} = \arg \max P(Y|\theta) \sim \arg \max \int P(Y|\theta, X)P(X|\theta)dX
\]

\[
\hat{\theta}^{SEM} = \arg \min_\theta \sum_{t=1}^{N} \|y(t) - h(x^s(t, \theta), u(t), \theta)\|^2 \text{ "smoothing error est"}
\]

- \( \hat{\theta}_J \) is conceptually simple to compute (in line with MPC) - could be a lot of numerical work, though.
- \( \hat{\theta}^{SEM} \) sounds like a good idea: “Smoothing Error minimization should be better than Prediction Error minimization”
- \( \hat{\theta}^{ML} \) has good credentials, but the ML criterion for nonlinear models involves solving the non-linear filtering problem.
- (The marginalization wrt \( x \) above is an extensive task.)
The integration will of course in general affect the maximum:
When the likelihood function is difficult to form, it may be advantageous to extend the problem with latent variables for a well defined likelihood function, and iterate between estimating these variables and the parameters.

This is the EM-algorithm, and in our case the states $x$ can serve as these latent variables.

Take expectation of $V(\theta, x(\cdot))$ under the assumption that $x$ has been generated by the model with the parameter value $\alpha$:

$$Q(\theta, \alpha) = E[V(\theta, x(\cdot))|Y, \theta = \alpha]$$

$$\theta^k = \arg\min_{\theta} Q(\theta, \theta^{k-1})$$

$$\hat{\theta}^{EM} = \lim_{k \to \infty} \theta^k \quad [\approx \theta^{ML}?]$$

How much work is required to form $Q(\theta, \alpha)$?
Linear Models

How are these estimates related - and are they any good?

Parameter and State Estimation in Unknown Linear Systems

Linear Model: (Joint discussions with Thomas Schön and David Törnqvist)

\[ x(t + 1) = A(\theta)x(t) + B(\theta)u(t) + w(t) \]
\[ y(t) = C(\theta)x(t) + e(t) \]
\[ Ew(t)w^T(t) = Q(\theta) \quad Ee(t)e^T(t) = R(\theta) \]

Specialize to (without much loss of generality):

\[ u(t) \equiv 0, \quad Q(\theta) = I, \quad R(\theta) = I \]
Notation

\[ X^T = [x(1)^T \ x(2)^T \ \cdots \ x(N)^T] \]

\( W^T;E^T \), and \( Y^T \) analogously

\[
F_\theta = \begin{bmatrix}
I & 0 & 0 & \cdots & 0 \\
A(\theta) & I & 0 & \cdots & 0 \\
A^2(\theta) & A(\theta) & I & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
A^{N-1}(\theta) & A^{N-2}(\theta) & A^{N-3}(\theta) & \cdots & 0
\end{bmatrix}
\]

\[
H_\theta = \begin{bmatrix}
C(\theta) & 0 & \cdots & 0 \\
0 & C(\theta) & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & C(\theta)
\end{bmatrix}
\]
Matrix Formulation

\[ X = F_\theta W, \quad Y = H_\theta X + E \]

\( W \) and \( E \) are Gaussian random vectors \( N(0, I) \).

\[ Y = H_\theta F_\theta W + E \]

\[ Y \in N(0, R_\theta), \quad R_\theta = H_\theta F_\theta F_\theta^T H_\theta^T + I \]

\[ -2 \log P(Y|\theta) = Y^T R_\theta^{-1} Y + \log \det R_\theta \]

\[ -2 \log P(Y|\theta, X) = \|Y - H_\theta X\|^2 \]

In a Bayesian setting with \( \theta \in N(0, cI) \)

\[ P(Y, X, \theta) = P(Y|X, \theta)P(X|\theta)P(\theta) \]

\[ V(Y, X, \theta) = -2 \log P(Y, X, \theta) = \|Y - H_\theta X\|^2 + \|F_\theta^{-1} X\|^2 + \|\theta\|^2 / c \]
The Estimates

Joint Criterion:

\[ W(\theta, X) = \|Y - H_\theta X\|^2 + \|F^{-1}_\theta X\|^2 \quad \text{"}(c \to \infty)" \]

Estimates:

State: \[ X^s(\theta) = F_\theta F^T_\theta H^T_\theta R^{-1}_\theta Y \quad (Y - H_\theta X^s(\theta) = \ldots = R^{-1}_\theta Y) \]

Joint: \[ \theta^J = \arg\min \|R^{-1}_\theta Y\|^2 + \|F^{-1}_\theta F_\theta F^T_\theta H^T_\theta R^{-1}_\theta Y\|^2 \]

\[ = \arg\min \gamma^T R^{-1}_\theta Y \]

Smoothed: \[ \hat{\theta}^{SEM} = \arg\min \|R^{-1}_\theta Y\|^2 = \arg\min \gamma^T R^{-2}_\theta Y \]

ML: \[ \hat{\theta}^{ML} = \arg\min \gamma^T R^{-1}_\theta Y + \log \det R_\theta \]

EM: \[ Q(\theta, \alpha) = \ldots \]
Expected Values of the Criteria

Let the true covariance matrix of $Y$ be $R_0 = EYY^T$

ML: $\text{trace} R_0 R_\theta^{-1} + \log \det R_\theta$

J: $\text{trace} R_0 R_\theta^{-1}$

SEM: $\text{trace} R_\theta^{-1} R_0 R_\theta^{-1}$

Note

\[
\text{trace} BA^{-1} + \log \det A \geq \dim B + \log \det B \quad \forall A
\]

equality iff all eigenvalues of $BA^{-1} \equiv 1$

So ML is consistent (but not the others!)
Numerical Illustration

The values that minimize the expected value of the criterion functions (= the limiting estimates as the number of observations tend to infinity) for the system

\[ x(t + 1) = ax(t) + w(t); \quad y(t) = x(t) + e(t); \quad a = 0.7 \]

Figure: The minimizing values of the expected criterion functions as a function of \( N \). Blue solid line: ML, Green dash-dotted line: SEM, Red dashed line: J.
EM-algorithm for this simple case

Figure: The estimates over the first six iterations of the EM-algorithm for different initial guesses
Some Observations

- $J \sim W(\theta, X) \quad \text{ML} \sim " \int W(\theta, X)dX"$
- $J \sim Y^T R_\theta^{-1} Y \quad \text{ML} \sim Y^T R_\theta^{-1} Y + \log \det R_\theta$
- J is not consistent, (but ML is, of course)
- J and ML are different maxima of $W(\theta, X)$
- The marginalization of $W(\theta, X)$ only leads to a data-independent (regularization) term $\log \det R_\theta$
- Is a similar result true also in the non-linear case?
- How would EM work in the non-linear case? (Schön, Wills, Ninness: Automatica 2011.)
Conclusions: State and Parameter Estimation

- Tempting to use MPC-thinking for model estimation using Moving Horizon Estimation - “Just” minimize over $\theta$ as well.
- This however leads to inconsistent estimates.
- Can it be saved by thoughtful regularization?