Chapter 1

Dynamic measurement

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In metrology, a given measurement technique has fundamental speed and accuracy limitations imposed by physical laws. Data processing allows us to overcome these limitations by using prior knowledge about the sensor dynamics. The prior knowledge considered in this paper is a model class to which the sensor dynamics belongs. We present methods that are applicable to linear time-invariant processes and are suitable for real-time implementation on a digital signal processor. The uncertainty of the estimates are quantified by their covariance matrices.

1.1 Introduction

The accuracy of measurement devices is reduced by measurement noise and transient response. The transient response of the measurement device decays exponentially, so that measuring longer has the effect of (eventually) reducing this source of error. Measuring longer also yields more data, which when used effectively reduces the error due to the measurement noise. The objective, however, is to achieve faster as well as more accurate measurement: there is a trade-off between speed and accuracy determined by the physical properties of the measurement device.

Our goal is to design methods that bring the performance of the measurement device to the theoretically optimal one. To do this, we take into account the dynamical properties of the sensor and reduce the measurement time needed for a specified measurement accuracy. Instead of waiting for the sensor's natural transient response to die out, the methods proposed *predict* the steady state value. The prediction is possible thanks to the assumption that the sensor is a low-order linear time-invariant system. At the same time as reducing the effect of the transient, the methods take into account the measurement noise, reducing also its effect.

How realistic is the low-order linear time-invariance assumption? The answer depends on the application. For example, in temperature and mass measurement the assumptions are satisfied. In more complicated measurement processes, such as the ones in bio-chemical reactors, they are not.

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The sub-field of metrology that takes into account the dynamical properties of the measurement devices is called *dynamic measurement*. A system theoretic way of viewing the dynamic measurements problem is as a problem of designing a *compensator* that reduces the transient process of the sensor. Then, the procedure is: 1) design off-line a dynamical system—the compensator—so that the series connection of the measurement process with the compensator behaves as close as possible to a static gain, 2) process on-line the measurements of the sensor by the compensator.

Note 1 (Link to deadbeat control). *The question of making the transient response as short as possible occurs also in control. It turns out that a reachable discrete-time system can be steered to a steady-state in a finite number of samples. Moreover, the number of samples is less than or equal to the order of the system. The corresponding control is called* deadbeat. *The equivalent of the reference signal in control is the measured value in metrology and the equivalent of the controller is a compensator that implements the prediction method.*

Despite the apparent similarity between deadbeat control and dynamic measurement, however, there are important differences: 1) the reference signal is known, while the measured value is not, 2) the controller is typically implemented in feedback, while the compensator can be applied only in open-loop, 3) in control, the plant's dynamics is typically assumed known, while in metrology it is often unknown. These differences suggest that if deadbeat control methods are used in metrology, they have to be open-loop and adaptive.

Literature review

Most authors assume that a linear time-invariant model of the measurement process is a priori given. In this case, the problem of designing a compensator reduces to the classical problem of designing an inverse system [1]. In the presence of noise, however, compensators that take into account the noise are needed. A theoretically optimal solution in the case of Gaussian noise is given in [2]. It is shown that in this case, the problem reduces to a state estimation problem for a suitably defined autonomous linear time-invariant system. As a consequence the maximum likelihood solution is given by the Kalman filter.

The design problem is more complicated in the case of unknown measurement process dynamics. In this case, adaptive filtering methods are used [3, 4], *i.e.*, the compensator is tuned on-line by a parameter estimation algorithm. The solutions proposed in [3, 4], however, are tailored to the mass measurement problem, which is a second order process.

In this paper, we present two methods that bypass the real-time model identification step done in adaptive filtering methods. The first method is a maximum-likelihood method that requires nonconvex optimization. The second one belongs to the class of the subspace methods [5] and is computationally simple to implement, however, it is not statistically optimal in the maximum-likelihood sense.

1.2   Problem setup

The sensor is a dynamical system with input the unknown to-be-measured value and output the sensor's reading, corrupted by additive noise. We assume that

1. the sensor dynamics is linear time-invariant;
2. the order n is known;
3. the input u is a step function $u = \bar{u}s$, where $\bar{u}$ is the to-be-measured value;
4. the measurement noise is zero mean, white, Gaussian, with variance σ^2; and
5. in steady-state, $\bar{u}$ can be determined from y.

The linear time-invariance assumption, is essential for the methods considered. The know order assumption can be relaxed. Order selection can be done, for example, by the methods presented in [6]. The assumption that the input is a step function implies that after an initial moment of time (start of the measurement process), the to-be-measured value is constant. This is a common assumption in metrology that is satisfied in many practical situations due to a "short" measurement time and the fact that the measurement process does not affect "significantly" the environment. The assumption that the output is corrupted by additive noise that is zero mean, white, Gaussian (output error setup) is appropriate for applications in metrology, where the mismatch between the observed data and the model is due to measurement noise rather than process noise and model uncertainty. Finally, assumption 5. implies that the DC-gain G of the sensor is known. The known DC-gain assumption means in practice that the sensor is calibrated.

Under the assumption that the input is a step function, the corresponding output is of the form

$$y_d = y + e = G\bar{u} + y_0 + e. \tag{1.1}$$

Here y_d is the observed noisy output, y is the noise-free output signal, e is the measurement noise,

$G\bar{u}$ is the steady-state value of y, and

y_0 is the transient response of the sensor that we aim to eliminate by the compensator.

The assumption that the process is linear time-invariant implies that there are matrices $A \in \mathbb{R}^{n \times n}$, $c \in \mathbb{R}^{1 \times n}$, and a vector $x_0 \in \mathbb{R}^n$, such that

$$\begin{aligned} x(t+1) &= Ax(t), \qquad x(0) = x_0 \\ y_0(t) &= cx(t). \end{aligned} \tag{1.2}$$

Therefore, the sensor's output is given by

$$\underbrace{\begin{bmatrix} y_d(1) \\ y_d(2) \\ \vdots \\ y_d(T) \end{bmatrix}}_{y_d} = \underbrace{\begin{bmatrix} G \\ G \\ \vdots \\ G \end{bmatrix}}_{\mathcal{G}} \bar{u} + \underbrace{\begin{bmatrix} c \\ cA \\ \vdots \\ cA^{T-1} \end{bmatrix}}_{\mathcal{O}} x_0 + \underbrace{\begin{bmatrix} e(1) \\ e(2) \\ \vdots \\ e(T) \end{bmatrix}}_{e}. \tag{1.3}$$

1.3   Model-based vs data-driven approaches

The model-based estimation procedure requires solving approximately the over de-
termined system of equations

$$
\begin{bmatrix} \mathscr{G} & \mathscr{O} \end{bmatrix} \begin{bmatrix} \widehat{u} \\ \widehat{x}_0 \end{bmatrix} \approx y_{\mathrm{d}}.
$$

Under assumption 4., the maximum-likelihood estimator for $\bar{u}$ in (1.3) is defined by
the standard least-squares problem

$$
\begin{aligned}
\text{minimize} \quad &\text{over } \widehat{y}, \widehat{u}, \widehat{x}_0 \quad \|y_{\mathrm{d}} - \widehat{y}\| \\
\text{subject to} \quad &\begin{bmatrix} \mathscr{G} & \mathscr{O} \end{bmatrix} \begin{bmatrix} \widehat{u} \\ \widehat{x}_0 \end{bmatrix} = \widehat{y},
\end{aligned}
\tag{1.4}
$$

where $\| \cdot \|$ is the 2-norm. Correspondingly, $\operatorname{cov}(\widehat{u}) = \sigma^2 V_{11}$, where

$$
V = \left(\begin{bmatrix} \mathscr{G} & \mathscr{O} \end{bmatrix}^\top \begin{bmatrix} \mathscr{G} & \mathscr{O} \end{bmatrix} \right)^{-1}.
$$

The covariance matrix of $\widehat{u}$ does not depend on the data y_{d}. However, it depends on
the noise variance σ^2, which affects the data. If σ^2 is unknown, it can be estimated as

$$
\widehat{\sigma}^2 = \frac{1}{T} \left\| y_{\mathrm{d}} - \begin{bmatrix} \mathscr{G} & \mathscr{O} \end{bmatrix}^\top \begin{bmatrix} \widehat{u} \\ \widehat{x}_0 \end{bmatrix} \right\|^2.
$$

The matrix $\mathscr{O}$ depends on the model parameters A and c, so that the dynamic
measurement method based on (1.4) requires a priori given model. The data-driven
model-free approach considered next is based on the observation that, in the noise
free case, under an additional assumption (persistency of excitation), the matrix $\mathscr{O}$
can be replaced by a matrix that depends on the observed data only.

The difference signal

$$
\Delta y(t) := y(t) - y(t-1) = y_0(t) - y_0(t-1)
$$

satisfies the same dynamics as y_0, *i.e.*, there is an initial condition $\Delta x \in \mathbb{R}^n$, such that

$$
\begin{aligned}
x(t+1) &= Ax(t), \qquad x(0) = \Delta x \\
\Delta y(t) &= cx(t).
\end{aligned}
$$

Let

$$
\mathscr{H}(\Delta y) := \begin{bmatrix}
\Delta y(1) & \Delta y(2) & \cdots & \Delta y(n) \\
\Delta y(2) & \Delta y(3) & \cdots & \Delta y(n+1) \\
\Delta y(3) & \Delta y(4) & \cdots & \Delta y(n+2) \\
\vdots & \vdots & & \vdots \\
\Delta y(T-n) & \Delta y(T-n) & \cdots & \Delta y(T-1)
\end{bmatrix},
\tag{1.5}
$$

be the Hankel matrix with n columns, constructed from Δy and let

$$
y|_t := \begin{bmatrix} y(1) & \cdots & y(t) \end{bmatrix}^\top.
$$

Under the assumption that Δy is persistently exciting of order $\mathtt{n}$ [7], we have that

$$\text{image}\left(\begin{bmatrix} c \\ cA \\ \vdots \\ cA^{T-n-1} \end{bmatrix}\right) = \text{image}\left(\mathscr{H}(\Delta y)\right).$$

Therefore, for noise free data, there is a vector $\ell \in \mathbb{R}^{\mathtt{n}}$, such that

$$\begin{bmatrix} \mathscr{G} & \mathscr{H}(\Delta y) \end{bmatrix} \begin{bmatrix} \bar{u} \\ \ell \end{bmatrix} = y|_{T-\mathtt{n}}. \tag{1.6}$$

As long as $(1,\ldots,1) \notin \text{image}\left(\mathscr{H}(\Delta y)\right)$, the solution of (1.6) is unique. Therefore, solving (1.2) allows us to estimate $\bar{u}$ directly from the observed exact data y (without knowing the model).

    With noisy data y_{d}, the data-driven estimation procedure aims at an approximate solution of the system of equations

$$\begin{bmatrix} \mathscr{G} & \mathscr{H}(\Delta y_{\mathrm{d}}) \end{bmatrix} \begin{bmatrix} \widehat{u} \\ \ell \end{bmatrix} \approx y_{\mathrm{d}}|_{T-\mathtt{n}}. \tag{1.7}$$

The noise e affects both the left-hand-side of (1.7) (through Δy_{d}) as well as the right-hand-side of (1.7) (through y_{d}), *i.e.*, solving (1.7) is a total least squares problem [8]. Moreover, Δy_{d} enters in a structured way in the left-hand-side of the equation, so that the maximum-likelihood estimator for the parameter $\bar{u}$ is the structured total least-squares problem

$$\begin{aligned} \text{minimize} \quad &\text{over } \widehat{y}, \widehat{u}, \widehat{x}_0 \quad \|y_{\mathrm{d}} - \widehat{y}\| \\ \text{subject to} \quad &\begin{bmatrix} \mathscr{G} & \mathscr{H}(\Delta\widehat{y}) \end{bmatrix} \begin{bmatrix} \widehat{u} \\ \widehat{\ell} \end{bmatrix} = \widehat{y}|_{T-\mathtt{n}}. \end{aligned} \tag{1.8}$$

The uncertainty $\text{cov}(\widehat{u})$ of the estimate $\widehat{u}$ is given by the the Jacobian matrix and the optimal value of the cost function [9]. The Jacobian matrix and the cost function value are computed as byproducts of the local optimization solution method [10].

1.4   Maximum-likelihood data-driven estimation method

As shown in Section 1.3, the maximum-likelihood model based estimation problem (1.4) is an ordinary least squares problem. A special feature of the problem however is the "shift structure" of the matrix $\begin{bmatrix} \mathscr{G} & \mathscr{O} \end{bmatrix}$. Taking into account this structure in an efficient real-time algorithm leads to the Kalman filter [11].

    The maximum-likelihood model based estimation problem (1.8) is a nonconvex optimization problem. Existing solution methods [8, 12] use local optimization algorithms. Such algorithms require an initial approximation and are susceptible to convergence to a local minimum.

    The initial approximation for the local optimization method can be computed by a convex relaxation of (1.8). This yields a method that is of independent interest. One approach of "convexifying" the problem is to ignore the structure of the matrix

$\begin{bmatrix} \mathscr{G} & \mathscr{H}(\Delta\widehat{y}) \end{bmatrix}$, which turns the structured total least squares problem into an ordinary total linear squares problem. The latter admits an analytical solution in terms of the singular value decomposition. Moreover, there are algorithms that recursively update the singular value decomposition [13, 14]. These algorithms allows real-time implementation of the data-driven input estimation method.

Another approach of relaxing the structured total least squares problem (1.8) is to substitute the optimization variable $\widehat{y}$ in $\begin{bmatrix} \mathscr{G} & \mathscr{H}(\Delta\widehat{y}) \end{bmatrix}$ with the observed data y_d, which results in an ordinary least squares problem (similar to the maximum-likelihood model based estimation problem (1.4)). This solution approach leads to the subspace method of [2, 15].

Independent of the approach being used to compute the initial approximation, the initial estimate can be improved by local optimization. The methods developed in [16, 17] can be used for this purpose, however, they operate off-line. Development of recursive methods, suitable for online solution of the maximum-likelihood model based estimation problem (1.8) is a topic of current research.

1.5   Examples

As an illustration of the methods presented in the paper, we consider temperature and mass measurement, where the process dynamics is linear time-invariant first and second order, respectively. The data is simulated and the methods are implemented in Matlab. We show the actual code used to generate the numerical results in a literate programming style [18], using the no-web syntax [19] and the org-babel system [20]. This makes the results reproducible in the sense of [21]. The code is available from

http://homepages.vub.ac.be/~imarkovs/software/sensor-uncer.tar

Methods and evaluation criterion

The methods compared are:

- y_d/G — the estimate obtained directly from the scaled raw measurements,
- `stepid_kf` — model-based maximum-likelihood method, solving (1.4) using the Kalman filter [2],
- `stepid_ml` — data-driven maximum-likelihood method, solving (1.8) using the SLRA package [17],
- `stepid_dd` — data-driven subspace method, using recursive least squares [15].

The estimates are computed for `ne` repetitions of the experiment with independent noise realizations (Monte-Carlo simulation):

```
% mc simulation
ne = 1000;
G = dcgain(sys);
[a, b, c, d] = ssdata(sys);
n = size(sys, 'order');
for i = 1:ne
    <<noisy-output>>
    uh_nv(:, i)        = yd / G;
    [uh_dd(:, i), V_dd] = stepid_dd(yd, G, n);
```

```
        [uh_ml(i),     V_ml] = stepid_ml(yd, G, n);
        [uh_kf(:, i), V_kf] = stepid_kf(yd, a, b, c, d, sigma^2);
end
```

Let $\widehat{u}^k$ be the estimate computed in the k-th repetitions of the experiment. The results reported are the empirical bias $\frac{1}{ne}\sum_{k=1}^{ne}\bar{u}-\widehat{u}^k$, the empirical variance $\frac{1}{ne}\sum_{k=1}^{ne}(\bar{u}-\widehat{u}^k)^2$, and the theoretically computed variance by the methods.

```
% show results
[mean(ub - uh_nv(T, :)) var(uh_nv(T, :)) sigma^2
 mean(ub - uh_dd(T, :)) var(uh_dd(T, :)) sigma^2 * V_dd
 mean(ub - uh_ml(:))    var(uh_ml(:))    sigma^2 * V_ml
 mean(ub - uh_kf(T, :)) var(uh_kf(T, :)) V_kf            ]
```

Example of temperature measurement

The setup of the temperature measurement problem is as follows. A thermometer is placed in an environment with temperature $\bar{u}$. The measured temperature y satisfies the Newton's law of cooling

$$\frac{d}{dt}y = a(y - \bar{u}). \tag{1.9}$$

Here a is a negative constant that depends on the thermometer and the environment. The differential equation (1.9) defines a first order linear time-invariant system with input the environmental temperature $\bar{u}$ and output the thermometer's reading y. The system is described by an input/state/output model

$$\frac{d}{dt}x = Ax + Bu, \qquad y = Cx + Dx,$$

where

$$A = -a, \quad B = a, \quad C = 1, \quad \text{and} \quad D = 0.$$

```
% temperature measurement process parameters
a = 0.4; A = -a; B = a; C = 1; D = 0;
```

The input is a step function $u = \bar{u}s$ and the initial condition is $x(0) = x_{ini}$

```
ub = 1; xini = 0.1;
```

The continuous-time model is discretized using the input zero-order hold method with a sampling period =ts=. The data

$$y_d = (y_d(1), \dots, y_d(T))$$

is generated in the output-error setup, using the discrete-time model and zero-mean, white, Gaussian noise with noise-to-signal ratio s

```
ts = 0.4; T = 10; s = 0.02;
```

```
% true system and true output
sys = c2d(ss(A, B, C, D), ts);
u = ub * ones(T, 1);
y = lsim(sys, u, [], xini);
```

```
% noisy output
yt = randn(T, 1);
sigma = s * norm(y) / norm(yt);
yd = y + sigma * yt;
```

Example of mass measurement

The setup of the mass measurement problem is as follows. An object with mass M is placed on a scale with mass m. At the time of placing the object, the scale is in a specified (in general nonzero) initial condition. The object placement has the effect of a step input as well as a step change of the total mass of the system—scale and object. The sensor is the scale. It is modeled as a mass, spring, damper system

$$(M+m)\frac{d^2}{dt^2}y = -ky - d\frac{d}{dt}y - Mg, \tag{1.10}$$

where y is the scale's reading, g is the gravitational constant, k is the elasticity constant, and d is the damping constant. In this case, the sensor is a second order linear time-invariant dynamical system with input the measured mass M.

```
% mass measurement process parameters
m = 1; M = 5; k = 1; d = 1; g = 9.81;
A = [0, 1; -k / (m + M), -d / (m + M)];
B = [0; -g / (m + M)]; C = [1, 0]; D = 0;
T = 50; ts = 1; s = 0.05; ub = M; xini = 0.1 * [1; 1];
```

Results

From theoretical considerations—use of prior knowledge about the true data generating system and the optimal vs suboptimal nature of the methods—we expect that the model-based maximum likelihood estimation method `stepid_kf` achieves the best performance (smallest bias and variance); the data-driven maximum likelihood estimation method `stepid_ml`, the second best; and the data-driven subspace method `stepid_dd` has the worst performance of the three methods, which, however is still better than the one of the naive estimator `yd / G`. This conjecture is confirmed by the simulation results shown in Table 1.1 for the temperature measurement setup and Table 1.2 for the mass measurement setup.

   The theoretical variance of the estimators is based on asymptotic results that are not satisfied in the present measurement setups (transient response with $T = 10$ and $T = 50$ samples respectively). Moreover, the theoretical variance of the `stepid_dd` estimator is based on results for the ordinary least squares method, *i.e.* classical regression, while the actual setup in the application of dynamic measurements leads a structured total least squares problem, *i.e.*, errors-in-variables regression. These considerations put doubt on how useful the theoretical variance formulas will be in practice. The simulation results, however, show that for the maximum-likelihood methods `stepid_kf` and `stepid_ml` the theoretical variance give reasonably good prediction of the empirical variances. For the subspace method `stepid_dd`, the match between the theoretical and empirical variance is good in the case of mass measurement but wrong in the case of temperature measurement. A more rigorous approach to the uncertainty analysis of the subspace method is done in [22].

Table 1.1   *The results for the temperature measurement Monte-Carlo simulation empirically confirm that the model-based maximum likelihood estimation method (`stepid_kf`) gives the best results in the sense of smallest bias and variance. The data-driven maximum likelihood estimation method (`stepid_ml`) leads to some loss of performance due to the weaker prior knowledge used (model class instead of a model). The data-driven subspace method (`stepid_dd`) incurs further loss of performance in comparison with `stepid_ml` due to its heuristic nature (solving the structured total least squares problem as an ordinary least squares problem). The theoretical variances predict of the `stepid_kf` and `stepid_ml` estimators well the empirical variances.*

	bias	empirical variance	theoretical variance
naive	0.2129	0.0001	0.0001
stepid_dd	0.0920	0.0016	0.0001
stepid_ml	-0.0055	0.0017	0.0012
stepid_kf	0.0001	0.0001	0.0001

Table 1.2   *The same observations as the ones for temperature measurement (Table 1.1) hold true for the mass measurement example. In this case, the difference in performance between model-based maximum likelihood estimation method (`stepid_kf`) and the data-driven maximum likelihood estimation method (`stepid_ml`) is less significant. Also, the prediction of the empirical variance of the data-driven subspace estimator (`stepid_dd`) by the theoretical variance is good.*

	bias	empirical variance	theoretical variance
naive	0.0790	0.0636	0.0636
stepid_dd	-0.0265	0.0014	0.0016
stepid_ml	0.0006	0.0013	0.0016
stepid_kf	0.0005	0.0013	0.0015

1.6   Conclusions and discussion

Metrology aims at producing faster and more accurate measurement devices. This can be done by development of new measurement principles and corresponding sensors or by improvement of existing ones with signal processing. In this paper, we considered the latter approach: improvement of existing sensors by building a computational layer, typically implemented in a digital signal processor, which processes the raw signal obtained from the sensor.

The signal processing goal is to improve the given sensor's speed and accuracy characteristics. We presented both model-based and data-driven suboptimal

and optimal in the maximum-likelihood sense methods for dynamic measurements. The model based-method is a classical least-squares problem, which efficient implementation is the Kalman filter. In the data-driven case, the problem is a structured total-least squares, which is a nonconvex optimization problem. Off-line solution methods performing nonlinear optimization exist, however, their recursive real-time implementation is a topic of current research. A computationally cheap alternative to the data-driven maximum likelihood method is a subspace method that can also be viewed as a convex relaxation of the structured total-least squares problem.

The full parameter vectors $(\bar{u}, x_0)$ or $(\bar{u}, \ell)$ of the model-based and data-driven estimation problems, respectively, can not be estimated consistently. This is due to the transient nature of the process (asymptotically decaying true signal). We conjecture that the parameter of interest $\hat{u}$ can nevertheless be estimated consistently, due to the special structure of the regressors matrix: constant block $\mathscr{G}$ corresponding to $\hat{u}$.

The bias of the maximum likelihood estimators, viewed as a function of the number of samples T, is the transient response of the compensated system, *i.e.*, the bias is the remaining transient response. The subspace method introduces an additional bias, which is quantified in [22]. The variance of the maximum likelihood estimators is obtained as a byproduct of the estimation algorithms: Kalman filter in the model-based case and the structured total-least squares algorithm in the data-driven case. The variance of the subspace method is quantified in [22].

Acknowledgements

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