Redukált nemlineáris optimális paraméterbecslés

Vizsgálat és implementáció Sparse Grid módszerekkel

Matszangosz Ákos

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Konzulensek:
Dr. Moireau Philippe
Dr. Chapelle Dominique
INRIA-MACS *csoport*

Dr. Kiss Bálint
Irányítástechnika és Informatika Tanszék (IIT)

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Notations

- $x(\cdot)$, $x_\xi(\cdot)$ state trajectory
- $x_\vartheta(\cdot)$ reduced state/parameter trajectory
- ξ state
- ϑ reduced state/parameter
- ζ state final condition
- η state/parameter initial uncertainty
- $u(\cdot)$ control
- $\omega(\cdot)$ model noise
- p adjoint variable
- $L(\cdot,\cdot)$ trajectory error
- $D(\cdot,\cdot)$ innovation
- $J(\cdot,\cdot,\cdot)$ cost function
- $V(\cdot,\cdot)$ value function
- $\tilde{V}(\cdot,\cdot)$ Lyapunov function

0 Absztrakt

A dolgozat témája nagy[1] dimenziójú nemlineáris rendszerek optimális identifikációja. A probléma általános; nem feladatspecifikusan vizsgáljuk a dolgozatban, azonban röviden szót ejtünk arról is, hogy előreláthatólag hogyan kerül majd alkalmazásra az itt ismertetett módszer.

A probléma egy mondatban összefoglalható a következőképpen: egy valós fizikai rendszert leíró modell ismeretlen paramétereit szeretnénk optimális módon meghatározni. Pontosabban a következő mondható: Adott egy parciális differenciálegyenletek által leírt rendszer (pl. egy flexibilis mechanikai rendszer, esetünkben a szív), melynek valamilyen ismeretlen állapotait vagy paramétereit (összehúzódási képesség, idegen szóval kontraktilitás) szeretnénk meghatározni. Ehhez rendelkezésre állnak valamilyen jellegű mérési adatok (a szív esetében MR képek, vagy újabban címkézett-MR képek: Tagged-MRI). A (végtelen dimenziós) rendszert diszkretizálva valamilyen választott numerikus eljárással (pl. végeselemmódszerrel) egy véges, de rendkívül nagy dimenziójú rendszert kapunk, melyet már közönséges differenciálegyenletek írnak le; ezt a numerikusan már kezelhető modellt szeretnénk a valós mérési adatokhoz illeszteni. Ehhez pedig állapotbecslési/szűrési[2] eljárásokat alkalmazunk. Megjegyzendő, hogy mivel az itt szereplő szűrők közönséges differenciálegyenletek által meghatározott rendszerekre alkalmazhatók, ezért a „klasszikus" identifikációs feladatokra (robotika, repüléstechnika, folyamatszabályozás...) is alkalmasak.

A fő cél az ilyen szűrési eljárásokkal beteg-specifikus modelleket készíteni a szívről, melyeket egyaránt diagnosztika, és prognosztika (előrejelzés) céljából fejlesztenek. A szív ugyanis különböző régiókra osztható, és infarktus esetén a szívnek az elektromos impulzusra való összehúzódási képessége (az említett kontraktilitási tényező) megváltozik. A célunk ennek a kontraktilitási tényezőnek a meghatározása a különböző régiókban. Infarktust követően ugyanis a szív struktúrális átalakulásokon is átmegy, a szív fala néhol elvékonyodik, ami a szív falának átszakadását is eredményezheti, ez halálos. Ezért az ilyen átalakulások pontos előrejelzése életmentő lehet. Kísérleti eredmények is rendelkezésre állnak; egy házi sertésnél infarktust idéztek elő, majd a modellt mérési adatokhoz illesztve, valóban a modell által előrejelzett módon változott a szív állapota a továbbiakban. Azért esett a választás házi sertésre, ugyanis fiziológiailag ennek az állatnak hasonlít a szíve a legjobban az emberére. A további részletekért ld. [8].

Ilyen szűrési eljárások (redukált kiterjesztett Kalman-szűrő – ROEKF, redukált 'Unscented' Kalman-szűrő – ROUKF) már kerültek megvalósításra [32], azonban nem elég jó kezdeti

[1] A nagy úgy értendő, hogy a rendszer dimenziója egy végtelen dimenziós rendszer véges közelítésből származik. Természetesen a 'nagy' jelző alsó korlátot nem jelent a rendszer dimenziójára vonatkozóan.

[2] Az állapotbecslés *általában* nem tételez fel zajt a méréseken; amikor zaj van a mért adatokon, akkor inkább szűrésről beszélünk. A szóhasználat leginkább a szakterülettől függ, de bővebb fejtegetés olvasható erről a dolgozat első fejezetében. A dolgozatban leginkább a szűrő szóhasználatot részesítjük előnyben.

becslés (*a priori*) esetén nem konvergáltak a valós[3] érték felé [31], ezért tehát valós alkalmazásokban minél pontosabb szűrési eljárásokra van szükség.

A dolgozatban egy *optimális* szűrési eljárást vizsgálunk meg, mely természeténél fogva kevésbé könnyen megvalósítható és számításigényesebb mint a legtöbbet használt szuboptimális társai (kiterjesztett Kalman-szűrő – EKF, 'Unscented' Kalman-szűrő – UKF), azonban ahogyan a szimulációs eredmények is mutatják, jelentősen jobb eredményeket produkál. A módszert Mortensen [36] javasolta egy cikkében, azonban a dolgozat szerzőjének tudomása szerint ennek megvalósítása még váratott magára. A jelen dolgozatban található megvalósítás C++-ban íródott, az INRIA-ban fejlesztett Verdandi [1] programcsomag keretében, mely egy generikus adatasszimilációs[4] eljárásokat tartalmazó programcsomag. A dolgozat főbb eredményei a következők:

- Megvizsgáltam a probléma formulációját, valamint redukált alakra hoztam az egyenleteket, mely ilyen alakban már szóbajön (a fenti értelemben vett) nagy dimenziójú rendszerek bizonyos paramétereinek meghatározására is.

- A szűrő megvalósíthatóságához valamilyen megoldást kellett találni az ún. dimenziók átkára (Curse of Dimensionality – COD). Ez alatt azt a jelenséget értik, amikor egy rácson való diszkretizáláskor a dimenziók emelkedő számával exponenciálisan növekszik a rácspontszám. Ennek a hatásnak a csillapítására a viszonylag újkeletű 'Sparse Grid' (ritka rács) eljárást alkalmaztam. Ez egy diszkretizációs és interpolációs eljárás, éppen ennek a jelenségnek az enyhítésére. A dolgozatban megvalósítottam egy ilyen Sparse Grid könyvtárat, mely generikus és C++-ban íródott. Mivel jelenleg a szerző tudomása szerint két ilyen könyvtár hozzáférhető, egyik MATLAB-ban (spinterp), másik Pythonban (SPARSE_GRID), ezért nem lenne érdektelen a jövőben valamilyen publikus licensz alatt hozzáférhetővé tenni a könyvtárat.

- A szűrőt megvalósítottam, és a hagyományos diszkretizációs eljárásokhoz képest jelentősen sikerült növelni a dimenziószámot.

- Szimulációkkal validáltam a szűrőt, és más, ismert szűrési eljárásokkal összevetettem. A szimulációhoz modellként egy merev rudat választottunk, ugyanis ugyanazon típusú parciális differenciálegyenletek írják le, mint a szív mechanikai működését. A modell kifejlesztésében is közreműködtem, a modell a Verdandi programcsomagban hozzáférhető.

Klinikai alkalmazhatóság szempontjából azonban a fő célkitűzés megvalósítása még hátravan, ugyanis a szűrőt tartalmazó Verdandi programcsomag C++-ban íródott, és jelenleg a szív végeselemmodellje MATLAB-ban áll csak rendelkezésre. Azonban a szimulációk nagy

[3] A szív modelljén tesztelve, annak pár paraméterét ismeretlennek tételezve fel.

[4] Más szóval identifikációs, állapotbecslési, szűrési. A terminológiát illetően ld. a dolgozat első fejezetét.

számításigénye miatt a szív végeselemmodellje C++-ban is megvalósításra fog kerülni hatékonyság céljából, ezért a szűrő ilyen jellegű valós alkalmazáson még nem lett tesztelve. Ahogyan azt már hangsúlyoztuk, a szűrő megvalósítása modellfüggetlen[5], ezért amint rendelkezésre áll a szív modellje, a szűrőt már csak a hangolás választja el valós alkalmazhatóságától.

A dolgozat felépítése a következő:

A dolgozat első fejezetében ismertetem a vizsgált probléma történeti hátterét, a dolgozatot megelőző vizsgálatok eredményét, a probémakör előfordulását különböző területeken, valamint jelen dolgozat célkitűzéseit. A második fejezetben ismertetem az állapotbecslési feladatot, és stabilitási kérdésekről is szót ejtek. A harmadik fejezet új eredményeket tartalmaz; a Fleming által javasolt állapotbecslő redukált formulációját mutatom be benne. A negyedik fejezetben az implementációs kérdéseket tárgyalom, valamint részletesen bemutatásra kerülnek a numerikus megvalósításban alkalmazott módszerek. Az ötödik fejezetben a numerikus szimulációk eredményei kerülnek ismertetésre, végül pedig konklúzióval és kitekintéssel zárom a dolgozatot. A függelékben sort kerítek érdekes és a munkám szempontjából kevésbé centrális kérdésekre. Bemutatom a mára már klasszikussá vált optimális irányítási eredményeket, hasznosnak és érdekesnek találtam ugyanis a duális szűrési feladattal való összevetés céljából. A későbbi alkalmazás céljából fontos Luenberger szűrőket is ismertetem röviden, és egy redukált variációs módszer is ismertetésre kerül. Ez utóbbi két eljárás is megvalósításra került, azonban részletes bemutatásuk nem célja a dolgozatnak.

Jelen dolgozat nagyrészt 2011 március és augusztus közötti munkám eredményeit foglalja össze, mely nagyrészt az INRIA-Rocquencourt[6] francia kutatóintézet MACS[7] csoportjában készült. A dolgozat nyelve a továbbiakban angol.

[5] Közönséges differenciálegyenletek által leírt rendszerre alkalmas.

[6] Az INRIA az „Institut Nationale de Recherche en Informatique et Automatique” rövidítése. Az ERCIM csoport tagja, melyhez a magyar SZTAKI is tartozik.

[7] Modeling, Analysis and Control in computational Structural dynamics

1 Introduction

Context One of the research fields of the MACS team at INRIA-Rocquencourt is modeling and estimation problems in biomechanics. More specifically, the goal is to formulate a complete continuum mechanics model of the beating heart and coupling it with actual clinical measurements, such as tagged MRI images. The interest in such a model would lie in developing new diagnostical and prognostical methods. See [34], [31] and [7] for details. The team in collaboration with the CLIME team of INRIA-Rocquencourt is currently developing a generic Data Assimilation Library called Verdandi [1]. It is in this context that the following work is presented.

Filtering and Inverse Problems *Filtering* (or *estimation theory*, or *observer theory* depending on the community) is interested in determining an internal state of a dynamical system (with or without noise). The previous denominations are usually associated with real-time engineering applications, such as electrical, aerospace, mechanical engineering and robotics; even financial applications exist [43]. Filtering implies rather stochastic filtering, from a probabilistic viewpoint, whileas state observers are usually considered from the deterministic viewpoint. The problem of *system identification* (or *data assimilation*, or *inverse problems*) poses basically the same question, (namely determining internal parameters or states) but the data is generally considered to be given "off-line", that is the determination of the internal state must not necessarily be simultaneous with the evolution of the system. The term data assimilation is mostly used in environmental sciences, that is meteorological, hydrological, geophysical, oceanographical and biological systems; it should be associated to high dimensional problems, such as discretization of PDEs. Engineering practice would mostly call this "off-line" process system identification; however system identification considers mostly smaller dimensional systems. Inverse problems is the general framework for these types of parameter estimation problems. Obviously these distinctions are not so sharp, and a lot of work is being done on the boundary of these domains, nevertheless it provides a vague idea of the problematics.

Let us mention some good survey articles. On system identification [3] even if a bit dated, but still proves to be useful reading. On the stochastic approach to nonlinear filtering [10] is rather instructive and gathers some of the most important techniques to date. On the deterministic approach Mitter [30] gives an excellent account, and a more recent survey by Fleming [13] is even more relevant to this report. Robinson and Lermusiaux [38] summarize data assimilation methods with certain filtering aspects also mentioned. Navon gives an excellent and compact review in [37] about the early history of variational methods in meteorology. Misawa and Hedrick [29] give a good overview of nonlinear state estimation methods; [9] and [24] are more recent surveys on the same subject.

A historical overview To our knowledge, the following brief time-line could be given to the history of filtering/state estimation: Wiener in 1942 [44] derives a filter whose purpose is to give the linear Minimum Mean Square Error (MMSE) estimation for a *stationary signal* under Gaussian noise with known covariance functions. Independently Kolmogorov derives in 1941 [23] the discrete time equivalent of Wiener's filter, thus the theory is often called *Wiener-Kolmogorov filtering*. Kalman publishes in 1960 his seminal paper [18] which provides the same result for *non-stationary* signals. This becomes to be known as the *Discrete Kalman Filter*. One year later Kalman and Bucy [19] publish the continuous counterpart of the filter which is nowadays called the *Kalman-Bucy filter*. Then in 1964 Luenberger publishes his paper [27] from which the now popular notion of *Luenberger observer*s emerges. In this article Luenberger considers the state observer as a dynamical system controlled by the observations, and places emphasis on the pole placement of the observer, with the realization that a state observer adds poles to the 'closed-loop' system; in the case of Kalman filtering the pole placement is determined by the statistics of the noise; with no noise, the poles of the filter tend to $-\infty$. In this paper Luenberger also introduces the notion of *reduced observer*s, where only a subspace of the state vector is estimated by the observer. For nonlinear systems so-called *suboptimal* filters appear. These filters take in some sort an approximation of the non-linear system, and apply the Kalman filter on the resulting approximation. The first occurance of the *Extended Kalman Filter* that we have found dates from 1967, due to Larsson, Dressler and Ratner [25] and it is used in a missile defense system. The emergence of the *Unscented Kalman Filter*s is surprisingly recent, Julier and Uhlmann [17] propose the method in 1997. With the exception of the article of Luenberger, the above mentioned filtering methodologies have been derived from the probabilistic/statistical viewpoint. The deterministic viewpoint in filtering is attributed to Mortensen's 1968 article [36]. Actually in modern observer design, a lot of nonlinear and robust control methodologies (H^∞-control, backstepping design, passivity methods, high gain observers, output injection...) have been adapted. We do not attempt to cover these methods.

Inverse problems first appeared in 1929 in an article of Ambarzumian [2], who examined the relationship between the eigenvalues of a differential operator and the parameters appearing in the operator. Basically he was examining an inverse Sturm-Liouville problem. Not much attention was paid to the article, until 1946, when Swedish mathematician Göran discovered [16] and recognized the importance of the article. Variational methods in Data Assimilation have been pioneered by Sasaki [40] in 1955, notably the method now known as the 3-dimensional variational method (3DVAR or 3DDA) is derived in Sasaki's 1958 article [41]. Optimal control methods appearing in data assimilation by the solution of the adjoint equation is due to Marchuk, 1974 [28] and has been further developed in Le-Dimet, Talagrand, 1985 [26]. Nudging (or Newtonian relaxation) was first developed and tested by Kistler in 1974 in his Master's thesis [20]. The *Ensemble Kalman Filter*s emerge in 1994 with the paper of Evensen [11].

Note that this chronology is far from being complete, but it should give an approximate idea of the development of filtering/estimation/data assimilation in engineering practice. Also,

only more relevant methods to this report have been mentioned. It is based on the survey articles mentioned above and personal research.

Objectives The most succesful nonlinear filters application-wise are the so-called suboptimal filters that have been based on their optimal linear counterpart the Kalman Filter. The Extended Kalman Filter traces back the nonlinear problem to a linear one by linearizing around the current position of the filter. The Unscented Kalman Filtering approximates the nonlinearity by averaging in a certain sense; equally distributed particles are generated around the filter's current position, and the nonlinear dynamics is applied to these particles, the average of their image giving the gradient of the filter. Both approaches result in easily implementable and rather robust filters. The primary goal of my internship was to formulate and implement a reduced version of the filter proposed by Mortensen in [36] and later examined by Fleming in [12], as it has been done for the Extended Kalman Filter in [33] and for the Unscented Kalman Filter in [32].

Organization of the report In the first chapter we introduce the optimal control problem. The problem is well-known; however we found it useful to see the duality of the approaches of the optimal control problem and the optimal filtering problem. Then the optimal filtering problem is presented in a deterministic framework. In the next section, the reduced filtering problem is examined. Following this, a numerical strategy for the implementation of the Reduced Mortensen Filter is presented, which relies on Sparse Grid methods. We also present the numerical results that have been obtained. Finally, we conclude the report and present future perspectives of research. In the appendix we shortly present aspects of Luenberger state estimation applied for large dimensional systems. A reduced order variational method is also presented. These also have been implemented and examined to some extent during the internship.

2 The deterministic optimal filtering problem

The interest of constructing optimal filters to systems described by differential equations is to propose an alternative to the more or less standard variational approach for determining unknown parameters of such a system. In our applications, the ultimate goal is to determine the contractility of the different heart regions. For small dimensional systems it might be possible to implement the filters presented in this chapter, but for our purposes this formulation is not adequate. It mainly serves as the basis for the reduced formulation, presented in the following chapter.

2.1 Problem formulation

Consider a finite dimensional dynamical system in the general form:

$$\dot{x}_r(t) = A(x_r(t), t) + B(\omega_r(t), t), \tag{2.1}$$
$$x_r(0) = x_0 + \eta_r, \tag{2.2}$$

where $x_r(\cdot) : [0, T] \to \mathcal{X}$ represents the model state, $A(\cdot, \cdot) : \mathcal{X} \times [0, T] \to \mathcal{X}$ is the dynamical operator, $\omega_r(\cdot) : [0, T] \to \Psi$ represents the model noise, $x_0 \in \mathcal{X}$ is an *a priori* estimate of the initial state and $\eta_r \in \mathcal{X}$ is the uncertainty on this initial state.

Remark For a given t, a specific solution of (2.1) with model noise $\omega(\cdot)$ and *final* condition

$$x(t) = \zeta. \tag{2.3}$$

is noted $x_{\zeta,\omega(\cdot)}$. Arbitrary states are noted with ξ. Note also that the differential equation here is to be solved *backwards* as opposed to the control problem.

An observation of the system is given, in the following form:

$$z(t) = H(x_r(t), t), \tag{2.4}$$

with $H : \mathcal{X} \times [0, T] \to \mathcal{Z}$ the observation operator, and $x_r(\cdot)$ solution of the reference system (2.1), (2.2).

Introduce the *innovation* of the system $D(\cdot, \cdot) : \mathcal{X} \times [0, T] \to \mathcal{Z}$:

$$D(\hat{\xi}, t) := z(t) - H(\hat{\xi}, t),$$

that measures the difference between the underlying state of the real system at time t, and an estimated state $\hat{\xi}$ through the observation operator $H(\cdot, \cdot)$, but any other $D(\cdot, \cdot)$ can be considered.

Consider the following, general class of estimators:

$$\dot{\hat{x}}(t) = A(\hat{x}(t), t) + B(KD(\hat{x}(t), t), t), \tag{2.5}$$
$$\hat{x}(0) = x_0, \tag{2.6}$$

where $K : \mathcal{F}(\mathcal{X} \times [0,T], \mathcal{Z}) \to \mathcal{F}(\mathcal{X} \times [0,T], \mathcal{X})$ is a feedback operator of the innovation depending on the estimated state, and on the time. The goal is to find a feedback operator K that is in some sense an optimal solution to this problem. To this end, consider the following *cost functional*:

$$J(\zeta, \omega(\cdot), t) := \frac{1}{2}\|x_{\zeta,\omega(\cdot)}(0) - x_0\|^2_{U_0} + \frac{1}{2}\int_0^t \|D(x_{\zeta,\omega(\cdot)}(s), s)\|^2_M + \|\omega(s)\|^2_S \, \mathrm{d}s. \tag{2.7}$$

Our goal in this section (c.f. (A.7)) is to solve

$$\min_{\zeta,\omega(\cdot)} J(\zeta, \omega(\cdot), T). \tag{2.8}$$

In the same manner using the dynamic programming approach, this problem is embedded in a larger class of problems, notably for $\forall t \in [0,T]$ find $(\bar{\xi}_t, \bar{\omega}_t(\cdot))$:

$$J(\bar{\zeta}_t, \bar{\omega}_t(\cdot), t) = \min_{\zeta,\omega(\cdot)} J(\zeta, \omega(\cdot), t), \tag{2.9}$$

for the moment supposing existence and uniqueness. To facilitate notation introduce:

$$\bar{x}_t(\cdot) := x_{\bar{\zeta}_t,\bar{\omega}_t(\cdot)}(\cdot)$$

defined on $[0,t]$. The optimal *Mortensen filter* (see [36] and [12]) is defined by taking at each time $t \in [0,T]$:

$$\hat{x}(t) = \bar{x}_t(t),$$

that is at each instant t the optimal estimation of ζ and $\omega(\cdot)$ must be found that minimizes $J(\zeta, \omega(\cdot), t)$ - by definition on the window $[0,t]$.

As in the previous section, we use Bellman's *Principle of Optimality*, which states that the optimal trajectory $\bar{x}_t(\cdot)$ associated with the optimal $(\bar{\zeta}_t, \bar{\omega}_t(\cdot))$ satisfies

$$J(\bar{x}_t(s), \bar{\omega}_t(\cdot), s) = \min_{\omega(\cdot)} J(\bar{x}_t(s), \omega(\cdot), s), \qquad \forall s \in [0,t]$$

or in other words an optimal trajectory on $[0,t]$ must be optimal on every subinterval $[0,s]$.

Remark This is a simple consequence of the additivity of the cost function J:

$$J(\zeta, \omega(\cdot), t) = J(x_{\zeta,\omega(\cdot)}(s), \omega(\cdot), s) + \frac{1}{2}\int_s^t \|D(x_{\zeta,\omega(\cdot)}(\tau), \tau)\|^2_M + \|\omega(\tau)\|^2_S \, \mathrm{d}\tau \qquad \forall s \in [0,t]$$

2.2 Optimal filtering law

In this section fix arbitrarily $t \in [0, T]$. In the following to simplify notation subscripts of $x_{\zeta,\omega(\cdot)}(\cdot)$ are only used when necessary.

To derive the filter equations, introduce the *adjoint variable* $p(\cdot) : [0, t] \to \mathcal{X}$ associated with a given trajectory $x(\cdot)$ defined on $[0, t]$:

$$\begin{aligned} \dot{p}(s) + \left.\frac{\partial A}{\partial \xi}\right|_{x(s),s}^{T} p(s) &= \left.\frac{\partial D}{\partial \xi}\right|_{x(s),s}^{T} MD(x(s), s), \qquad s \in [0, t] \quad (2.10) \\ p(0) &= U_0^T (x(0) - x_0) \quad (2.11) \end{aligned}$$

Theorem 2.1 *$\bar{x}_t(\cdot)$ is given by*

$$\begin{aligned} &\dot{\bar{x}}_t(s) = A(\bar{x}_t(s), s) + BS^{-1}B^T \bar{p}_t(s), \qquad \forall s \in [0, t] \\ &\bar{x}_t(0) = x_0 + U_0^{-1} \bar{p}_t(0), \end{aligned} \quad (2.12)$$

where $\bar{p}_t(\cdot)$ denotes the adjoint variable defined on $[0, t]$ associated with the optimal trajectory $\bar{x}_t(\cdot)$.

Proof. The partial derivative of J with respect to ζ writes as:

$$\begin{aligned} \left.\frac{\partial J}{\partial \zeta}\right|_{\zeta,\omega(\cdot),t} \delta\zeta &= (x(0) - x_0)^T U_0 \left.\frac{\partial x}{\partial \zeta}\right|_0 \delta\xi + \int_0^t D(x(s), s)^T M \left.\frac{\partial D}{\partial \xi}\right|_{x(s),s} \left.\frac{\partial x}{\partial \zeta}\right|_s \delta\zeta \, \mathrm{d}s \\ &= (x(0) - x_0)^T U_0 \left.\frac{\partial x}{\partial \zeta}\right|_0 \delta\zeta + \int_0^t \left(\dot{p}(s) + \left.\frac{\partial A}{\partial \xi}\right|_{x(s),s}^{T} p(s)\right)^T \left.\frac{\partial x}{\partial \zeta}\right|_s \delta\zeta \, \mathrm{d}s \\ &= (x(0) - x_0)^T U_0 \left.\frac{\partial x}{\partial \zeta}\right|_0 \delta\zeta + \left[p(s)^T \left.\frac{\partial x}{\partial \zeta}\right|_s \delta\zeta\right]_0^t - \int_0^t p(s)^T \frac{\mathrm{d}}{\mathrm{d}t}\left(\left.\frac{\partial x}{\partial \zeta}\right|_s \delta\zeta\right) \mathrm{d}s \\ &\quad + \int_0^t p(s)^T \left.\frac{\partial A}{\partial \xi}\right|_{x(s),s} \left.\frac{\partial x}{\partial \zeta}\right|_s \delta\zeta \, \mathrm{d}s \\ &= p(t)^T \delta\zeta \end{aligned}$$

since the sensitivity of the state with respect to the initial condition satisfies the differential equation:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\left(\left.\frac{\partial x}{\partial \zeta}\right|_s\right) &= \left.\frac{\partial A}{\partial \xi}\right|_{x(s),s} \left.\frac{\partial x}{\partial \zeta}\right|_s \\ \left.\frac{\partial x}{\partial \zeta}\right|_t &= \mathbb{1} \end{aligned}$$

In the optimum $\left(\bar{\zeta}_t, \bar{\omega}_t(\cdot)\right)$, one must have

$$\left.\frac{\partial J}{\partial \zeta}\right|_{\bar{\zeta}_t, \bar{\omega}_t(\cdot), t} = 0,$$

which leads to

$$\bar{p}_t(t) = 0,$$

where $\bar{p}_t(\cdot)$ is the adjoint variable associated with $\bar{x}_t(\cdot)$. Performing the same calculations for $\omega(\cdot)$:

$$\begin{aligned}
\left.\frac{\partial J}{\partial \omega}\right|_{\zeta, \omega(\cdot), t} \delta\omega(\cdot) &= (x(0) - x_0)^T U_0 \left.\frac{\partial x}{\partial \omega}\right|_0 \delta\omega(\cdot) \\
&\quad + \int_0^t D(x(s), s)^T M \left.\frac{\partial D}{\partial \xi}\right|_{x(s), s} \left.\frac{\partial x}{\partial \omega}\right|_s \delta\omega(\cdot) + \omega(s)^T S\, \delta\omega(\cdot)\, \mathrm{d}s \\
&= (x(0) - x_0)^T U_0 \left.\frac{\partial x}{\partial \omega}\right|_0 \delta\omega(\cdot) \\
&\quad + \int_0^t \left(\dot{p}(s) + \left.\frac{\partial A}{\partial \xi}\right|_{x(s), s}^T p(s)\right)^T \left.\frac{\partial x}{\partial \omega}\right|_s \delta\omega(\cdot) + \omega(s)^T S\, \delta\omega(\cdot)\, \mathrm{d}s \\
&= (x(0) - x_0)^T U_0 \left.\frac{\partial x}{\partial \omega}\right|_0 \delta\omega(\cdot) \\
&\quad + \left[p(s)^T \left.\frac{\partial x}{\partial \omega}\right|_s \delta\omega(\cdot)\right]_0^t - \int_0^t p(s)^T \frac{\mathrm{d}}{\mathrm{d}t}\left(\left.\frac{\partial x}{\partial \omega}\right|_s \delta\omega(\cdot)\right) \mathrm{d}s \\
&\quad + \int_0^t p(s)^T \left.\frac{\partial A}{\partial \xi}\right|_{x(s), s} \left.\frac{\partial x}{\partial \omega}\right|_s \delta\omega(\cdot)\, \mathrm{d}s + \int_0^t \omega(s)^T S\, \delta\omega(\cdot)\, \mathrm{d}s \\
&= \int_0^t \left(\omega(s)^T S - p(s)^T \left.\frac{\partial B}{\partial \omega}\right|_{\omega(s), s}\right) \delta\omega(\cdot)\, \mathrm{d}s
\end{aligned}$$

using the initial condition of the adjoint variable, and also that the sensitivity of the state with respect to the model noise satisfies:

$$\begin{aligned}
\left.\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial x}{\partial \omega}\right)\right|_s &= \left.\frac{\partial A}{\partial \xi}\right|_{x(s), s} \left.\frac{\partial x}{\partial \omega}\right|_s + \left.\frac{\partial B}{\partial \omega}\right|_{\omega(s), s} \\
\left.\frac{\partial x}{\partial \omega}\right|_t &= 0
\end{aligned}$$

In the optimum $\left(\bar{\zeta}_t, \bar{\omega}_t(\cdot)\right)$, one must also have

$$\left.\frac{\partial J}{\partial \omega}\right|_{\bar{\zeta}_t, \bar{\omega}_t(\cdot), t} = 0.$$

This leads to the optimum of ω:

$$\bar{\omega}_t(s) = S^{-1} \left.\frac{\partial B}{\partial \omega}\right|^T_{\omega(s),s} \bar{p}_t(s), \qquad \square$$

Let us now introduce the *filter Hamiltonian*

$$\mathcal{H}(\cdot,\cdot,\cdot,\cdot) : \mathcal{X} \times \mathcal{X} \times \Psi \times [0,T] \to \mathbb{R}$$

$$(\xi, p, \omega, t) \mapsto \mathcal{H}(\xi, p, \omega, t) := \frac{1}{2}\|D(\xi,t)\|^2_M + \frac{1}{2}\|\omega\|^2_S - p^T\left(A(\xi,t) + B(\omega,t)\right)$$

For a given trajectory $x(\cdot)$ and the associated $p(\cdot)$ adjoint variable the following relationship holds:

$$\left.\frac{\partial \mathcal{H}}{\partial \xi}\right|^T_{x(s),p(s),\omega,s} = \dot{p}(s) \qquad \forall s \in [0,t],$$

For a given $(\zeta, \omega(\cdot))$ with the resulting trajectory $x(\cdot)$, and the associated $p(\cdot)$ adjoint variable the following relationship holds:

$$\left.\frac{\partial \mathcal{H}}{\partial p}\right|^T_{x(s),p(s),\omega(s),s} = -\dot{x}(s) \qquad \forall s \in [0,t],$$

For the *optimal* $\left(\bar{\zeta}_t, \bar{\omega}_t(\cdot)\right)$ pair, and the associated optimal trajectories $\bar{p}_t(\cdot)$ and $\bar{x}_t(\cdot)$

$$\left.\frac{\partial \mathcal{H}}{\partial \omega}\right|^T_{\bar{x}_t(s),\bar{p}_t(s),\bar{\omega}_t(s),s} = S\,\bar{\omega}_t(s) - \left.\frac{\partial B}{\partial \omega}\right|^T_{\omega(s),s} \bar{p}_t(s) = 0 \qquad \forall s \in [0,t]$$

holds. As in section A, define the *value function* associated with the cost function:

$$V(\zeta, t) := \min_{\omega(\cdot)} J(\zeta, \omega(\cdot), t). \tag{2.13}$$

Theorem 2.2 *Assume that the following minimization problem has a unique solution for* $\forall t \in [0,T]$ *and for* $\forall \xi \in \mathcal{X}$*:*

$$\min_{\omega \in \Psi} \mathcal{H}(\xi, \partial_\xi V(\xi,t), \omega, t)$$

For a given (ξ, t) *pair, note this solution* $\bar{\omega}_{\xi,t}$*. Suppose also that this solution varies continuously with respect to* (ξ, t)*.*

Then $V(\cdot,\cdot)$ *is a solution of the following Hamilton-Jacobi-Bellman equation:*

$$\partial_t V(\xi,t) - \mathcal{H}(\xi, \partial_\xi V(\xi,t)^T, \bar{\omega}_{\xi,t}, t) = 0 \tag{2.14}$$

$$V(\xi, 0) = \frac{1}{2}\|\xi - x_0\|^2_{U_0} \tag{2.15}$$

For a fix t we have the optimal estimation of the model noise:

$$\bar{\omega}_t(s) = \bar{\omega}_{\bar{x}_t(s),s} \qquad \forall s \in [0,t]. \tag{2.16}$$

Proof. Fix $t \in [0, T]$. By introducing $\bar{x}_\xi(\cdot) := x_{\xi,\bar{\omega}_\xi}(\cdot)$ on $[0, t]$, one has by Bellman's principle of optimality:

$$V(\xi, t) = V(\bar{x}_\xi(t - \delta t), t - \delta t) + \frac{1}{2} \int_{t-\delta t}^{t} \|D(\bar{x}_\xi(s), s)\|_M^2 + \|\bar{\omega}_\xi(s)\|_S^2 \, \mathrm{d}s, \qquad \forall\, \delta t \in [0, t]$$

which by using continuity of $D(\cdot, \cdot)$ and $\bar{\omega}_\xi(\cdot)$ leads to

$$\begin{aligned} 0 &= \lim_{\delta t \to 0} \left(\frac{1}{2\delta t} \left(\delta t \|D(\bar{x}_\xi(t), t)\|_M^2 + \delta t \|\bar{\omega}_\xi(t)\|_S^2 + o(\delta t) \right) - \frac{V(\bar{x}_\xi(t), t) - V(\bar{x}_\xi(t - \delta t), t - \delta t)}{\delta t} \right) \\ &= \frac{1}{2}\|D(\bar{x}_\xi(t), t)\|_M^2 + \frac{1}{2}\|\bar{\omega}_\xi(t)\|_S^2 - \left. \frac{\mathrm{d}V}{\mathrm{d}t} \right|_{\bar{x}_\xi(t), t} \\ &= \frac{1}{2}\|D(\xi, t)\|_M^2 + \frac{1}{2}\|\bar{\omega}_\xi(t)\|_S^2 - \left. \frac{\partial V}{\partial t} \right|_{\xi,t} - \left. \frac{\partial V}{\partial \xi} \right|_{\xi,t} \left(A(\xi, t) + B(\bar{\omega}_\xi(t), t) \right). \end{aligned}$$

From this, it follows that $\bar{\omega}_\xi(t) = \bar{\omega}_{\xi,t}$, otherwise the value of $V(\xi, t)$ could be decreased by taking $\bar{\omega}_\xi(\cdot) \equiv \bar{\omega}_{\xi,t}$ on a sufficiently short $[t - \delta t, t]$ interval. Expressing this equation by the Hamiltonian function gives the desired result. For the boundary condition

$$V(\xi, 0) = \min_{\omega(\cdot)} J(\xi, \omega(\cdot), 0)$$

with $x_{\xi,\omega}(0) = \xi$ holds. □

Remark $\bar{\omega}_{\xi,t}$ can be expressed as

$$\bar{\omega}_{\xi,t} = S^{-1} \left. \frac{\partial B}{\partial \omega} \right|_{\omega(s),s}^{T} \partial_\xi V(\xi, t)$$

The following theorem helps expressing the optimal filter by means of the value function.

Theorem 2.3 *For all $t \in [0, T]$, the following relationship holds between the optimal $(\bar{x}_t(\cdot), \bar{p}_t(\cdot))$ pair and the value function:*

$$\bar{p}_t(s) = \partial_\xi V(\bar{x}_t(s), s)^T, \qquad \forall s \in [0, t]. \tag{2.17}$$

Proof. On a fix $[0, t]$ interval, for any given $x(\cdot), p(\cdot)$ pair, the initial condition writes as:

$$\partial_\xi V(x(0), 0) = (x(0) - x_0)^T U_0 = p(0)^T.$$

From the HJB equation (2.14) it follows that

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}\xi} \left(\partial_t V(\xi, s) - \mathcal{H}(\xi, \partial_\xi V(\xi, s)^T, \bar{\omega}_{\xi,s}, s) \right) \\ &= \partial_\xi \partial_t V(\xi, s) - \partial_\xi \mathcal{H} \left(\xi, \partial_\xi V(\xi, s)^T, \bar{\omega}_{\xi,s}, s \right) - \partial_p \mathcal{H} \left(\xi, \partial_\xi V(\xi, s)^T, \bar{\omega}_{\xi,s}, s \right) \partial_\xi^2 V(\xi, s) \\ &= \partial_\xi \partial_t V(\xi, s) - D(\xi, s)^T M \partial_\xi D(\xi, s) + \partial_\xi V(\xi, s) \partial_\xi A(\xi, s) + (A(\xi, s) + B\bar{\omega}_{\xi,s})^T \partial_\xi^2 V(\xi, s) = 0, \end{aligned}$$

which gives on the optimal trajectory $\bar{x}_t(\cdot)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\partial_\xi V(\bar{x}_t(s),s)^T\right) = \partial_\xi D(\bar{x}_t(s),s)^T MD(\bar{x}_t(s),s) - \partial_\xi A(\bar{x}_t(s),s)^T \partial_\xi V(\bar{x}_t(s),s)^T$$

Thus $\partial_\xi V(\bar{x}_t(s),s)^T$ and $\bar{p}_t(s)$ satisfy the same dynamics with the same initial condition. □

Now since the optimal filter defined on $[0,T]$ introduced by Mortensen satisfies $\hat{x}(t) = \bar{x}_t(t)$, and since the condition of optimality can be given on the adjoint variable as $\bar{p}_t(t) = 0$, the previous theorem gives

$$\bar{p}_t(t) = \partial_\xi V(\bar{x}_t(t),t)^T = \partial_\xi V(\hat{x}(t),t)^T = 0, \qquad \forall t \in [0,T].$$

Suppose V is C^2 in a neighborhood of $(\bar{x}_t(t),t)$, for $\forall t \in [0,T]$, and that $\partial^2_\xi V(\xi,t) > 0$. Differentiating the previous equation with respect to t, and differentiating the HJB equation (2.14) with respect to ξ, it follows that

$$\begin{aligned}
0 &= \left.\frac{\partial^2 V}{\partial \xi^2}\right|_{\hat{x}(t),t} \dot{\hat{x}}(t) + \left.\frac{\partial^2 V}{\partial \xi \partial t}\right|_{\hat{x}(t),t} \\
&= \left.\frac{\partial^2 V}{\partial \xi^2}\right|_{\hat{x}(t),t} \dot{\hat{x}}(t) + \left.\frac{\partial \mathcal{H}}{\partial \xi}\right|^T_{\hat{x}(t),\partial_\xi V(\hat{x}(t),t)^T,\bar{\omega}_{\hat{x}(t),t},t} + \left.\frac{\partial^2 V}{\partial \xi^2}\right|_{\hat{x}(t),t} \left.\frac{\partial \mathcal{H}}{\partial p}\right|^T_{\hat{x}(t),\partial_\xi V(\hat{x}(t),t)^T,\bar{\omega}_{\hat{x}(t),t},t} \\
&= \left.\frac{\partial^2 V}{\partial \xi^2}\right|_{\hat{x}(t),t} \dot{\hat{x}}(t) + \left.\frac{\partial D}{\partial \xi}\right|^T_{\hat{x}(t),t} MD(\hat{x}(t),t) - \left.\frac{\partial^2 V}{\partial \xi^2}\right|_{\hat{x}(t),t} \left(A(\hat{x}(t),t) + B(S^{-1} \left.\frac{\partial B}{\partial \omega}\right|^T_{\omega(s),s} \bar{p}_t(t),t)\right)
\end{aligned}$$

using the identities obtained on the derivatives of $\mathcal{H}$. Thus the equations of the optimal filter are given by:

$$\dot{\hat{x}}(t) = A(\hat{x}(t),t) - \left.\frac{\partial^2 V}{\partial \xi^2}\right|^{-1}_{\hat{x}(t),t} \left.\frac{\partial D}{\partial \xi}\right|^T_{\hat{x}(t),t} MD(\hat{x}(t),t) \tag{2.18}$$

$$\hat{x}(0) = x_0. \tag{2.19}$$

Remark Note that in the linear case the filter obtained coincides with the Kalman filter; for a proof, see [31]. In the nonlinear case, usually some sort of approximation of the Kalman filter is used; linearization (EKF) or averaging (UKF). The cost to pay however for the optimal filter, is the necessity to calculate the value function, which is a computationally very demanding task.

2.3 Stability

Let us start by fixing a virtual reference system, with respect to which we wish to show stability:

$$\begin{aligned}
\dot{\breve{x}}_r(t) &= A(\breve{x}_r(t),t) \\
\breve{x}_r(0) &= x_0 + \eta_r,
\end{aligned}$$

such that $D(\check{x}(t), t) \equiv 0$. Now the system error $\tilde{x}$ can be written as

$$\tilde{x}(\cdot) = (x_r(\cdot) - \check{x}(\cdot)) + (\check{x}(\cdot) - \hat{x}(\cdot))$$

Suppose that $\omega_r(\cdot) \in L^2(\mathbb{R}^+)$. Since

$$\mathrm{d}_t V(\hat{x}(t), t) = \partial_\xi V(\hat{x}(t), t)\partial_t \hat{x}(t) + \partial_t V(\hat{x}(t), t) = \partial_t V(\hat{x}(t), t)$$

and $V(\hat{x}(0), 0) = V(x_0, 0) = 0$; $V(\hat{x}(t), t)$ can be expressed as

$$V(\hat{x}(t), t) = \frac{1}{2}\int_0^t \|D(\hat{x}(s), s)\|_M^2 \,\mathrm{d}s$$

Since $\hat{x}(t)$ is a minimizer of $V(\cdot, t)$ at all time instants t, and by the assumption on $\omega_r(\cdot)$, $V(\hat{x}(t), t)$ is bounded:

$$V(\hat{x}(t), t) \leq V(x_r(t), t) = \frac{1}{2}\|x_r(0) - x_0\|_{U_0}^2 + \frac{1}{2}\int_0^t \|\omega_r(s)\|_S^2 \,\mathrm{d}s,$$

Moreover $V(\hat{x}(\cdot), \cdot)$ is monotonically increasing, by using the definition of $\hat{x}(\cdot)$ and $V(\cdot, \cdot)$:

$$V(\hat{x}(t_1), t_1) \leq V(\bar{x}_{t_2}(t_1), t_1) \leq J(\bar{x}_{t_2}(t_1), \bar{\omega}_{t_2}(\cdot), t_1) \leq V(\hat{x}(t_2), t_2) \qquad \text{for } t_1 < t_2.$$

It follows that $\exists c \in \mathbb{R}$:

$$\lim_{t\to\infty} V(\hat{x}(t), t) = \lim_{t\to\infty} \frac{1}{2}\int_0^t \|D(\hat{x}(s), s)\|_M^2 \,\mathrm{d}s \to c$$

Now take as a Lyapunov function candidate:

$$\tilde{V}(\xi, t) := V(\xi + \hat{x}(t), t) - V(\hat{x}(t), t).$$

This is a valid Lyapunov function candidate, since at a given time instant t, $\hat{x}(t)$ is a minimizer of $V(\cdot, t)$ thus $\tilde{V}(\xi, t) \geq 0$, moreover $\tilde{V}(0, t) \equiv 0$. The total time derivative of this Lyapunov function candidate along the error trajectory $\tilde{x}(\cdot) := x_r(\cdot) - \hat{x}(\cdot)$ writes as

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\tilde{V}(\tilde{x}(t), t) &= \frac{\mathrm{d}}{\mathrm{d}t}\left(V(x_r(t), t) - V(\hat{x}(t), t)\right) = \\
&= \partial_\xi V(x_r(t), t)\dot{x}_r(t) + \partial_t V(x_r(t), t) - \partial_\xi V(\hat{x}(t), t)\dot{\hat{x}}(t) - \partial_t V(\hat{x}(t), t) \\
&= \partial_\xi V(x_r(t), t)(\dot{x}_r(t) - A(x_r(t), t) - B\bar{\omega}_{x_r(t)}(t)) \\
&\quad + \frac{1}{2}\|D(x_r(t), t)\|_M^2 + \frac{1}{2}\|\bar{\omega}_{x_r(t)}(t)\|_S^2 - \frac{1}{2}\|D(\hat{x}(t), t)\|_M^2 - \frac{1}{2}\|\bar{\omega}_{\hat{x}(t)}(t)\|_S^2 \\
&= \partial_\xi V(x_r(t), t)B(\omega_r(t) - \bar{\omega}_{x_r(t)}(t)) + \frac{1}{2}\|\chi\|_M^2 + \frac{1}{2}\|\bar{\omega}_{x_r(t)}(t)\|_S^2 - \frac{1}{2}\|D(\hat{x}(t), t)\|_M^2,
\end{aligned}$$

by the HJB equation. Suppose for the moment that there is no model noise $\omega_r(\cdot) \equiv 0$, no measurement noise $\chi \equiv 0$ and that B is linear. In this case, the error dynamics is stable, since the total derivative of $\tilde{V}(\tilde{x}(\cdot), \cdot)$ is:

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{V}(\tilde{x}(t), t) = -\frac{1}{2}\|\partial_\xi V(x_r(t), t)\|_{B^T S^{-1} B} - \frac{1}{2}\|D(\hat{x}(t), t)\|_M^2 \leq 0,$$

by abuse of notation, since $B^T S^{-1} B$ is not necessarily a norm.

	Control	Filtering	
$[t, T]$	time window	time window	$[0, t]$
s	time	time	$t - s$
$x(t) = \zeta$	initial condition	final condition	$x(t) = \zeta$
$u(\cdot)$	control	model noise	$\omega(\cdot)$
$L(\cdot, \cdot)$	trajectory error	innovation	$D(\cdot, \cdot)$
$x_r(\cdot)$	reference trajectory	real system	$x_r(\cdot)$

Table 1: Duality of control and estimation

3 The optimal reduced filtering problem

The approach of reduced filtering is to reduce the uncertainty to the so-called reduced state (in our case consisting of parameters[8]), and consider that the rest of the uncertainty (state) is taken care of. E.g. in our case, joint state-parameter filtering is applied that is a Luenberger type filter is applied to the state of the system, and the optimal reduced filter is applied to determine the unknown parameters of the system. In this way, one is able to implement computationally demanding filters for parameters that require more accurate estimates by applying the filter only to a small part of the state, and applying another type of filter (Luenberger) to the large remaining state. In the simulations conducted for this work, the parameters to be determined are the stiffness and mass parameters of the different regions of a bar clamped at one end, and the rest of the state is constituted by the displacements and the velocities of the bar's particles.

3.1 Reduced filtering

The reduced estimation case is formally presented in this short introduction, then exact definitions follow. The idea of reduced estimation is as follows: the full state is decomposed into two parts, the state, and the reduced state. The *reduced* term refers to the fact that the uncertainty is only present in x_ϑ, a part of the full state. E.g. one could consider a system, with a set of unknown parameters ϑ that are to be estimated. The state space, extended by these parameters also defines a dynamic system, with the extended dynamics (0 dynamics on parameters in most of the cases). For the sake of generality, we do not pose restrictions on this so-called *reduced state* and its dynamics.

Methods for conducting reduced filtering have already been investigated in the MACS team, see [32], [33]. These methods rely on the Extended and Unscented Kalman Filtering (EKF, UKF). These reduced filtering methods, as their full counterparts, often possess good stability properties, this however depends on the nonlinearity of the system. However, from the nature of the problem it is unevitable, to apply a joint state estimation method to obtain convergence, since even with 'good' parameter estimates, if the state doesn't converge, it is hopeless to expect convergence of the parameter. However the stability of such a joint state-parameter filter must be examined, for details, see [33].

The goal of this section, is to present the reduced formulation of the filter proposed by Mortensen [36], presented in the previous section.

[8]The distinction of state/parameter is purely conceptual; as we shall see in this chapter, the parameters can be added to the state space, thus they can also be considered as part of the state. However we emphasize the fundamental difference with the reduced state, which is characterized by containing the uncertainty. Also note that in most applications the reduced state coincides with the parameters, but the purpose of this footnote is to state that this is not imperative.

3.2 Problem formulation

In this section the previously introduced optimal filtering approach is adapted for the *reduced* state estimation case. $x_\xi(\cdot)$ is referred to as state trajectory, and $x_\vartheta(\cdot)$ is referred to as reduced state trajectory.

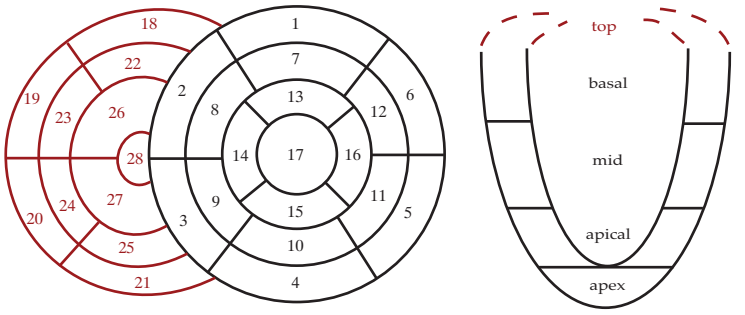
Thus the system to be considered is:

$$\begin{aligned} \dot{x}_\xi(t) &= A^\xi(x_\xi(t), x_\vartheta(t), t) && (3.1)\\ \dot{x}_\vartheta(t) &= A^\vartheta(x_\xi(t), x_\vartheta(t), t) && (3.2)\\ x_\xi(0) &= \xi_0 && (3.3)\\ x_\vartheta(0) &= \vartheta_0 + \eta_\vartheta && (3.4) \end{aligned}$$

with the notations of the previous section, with additionally $x_\vartheta : [0, T] \to \Theta$ a parameter vector with an unkown reference parameter $x^r_\vartheta : [0, T] \to \Theta$ to be estimated.

Remark In real applications, the assumption of a known initial condition is justified, since state estimation (see section B) can be jointly conducted with the parameter estimation to find ξ_0. Of course, the stability of the joint filter must be examined. With some prior knowledge on the system, a ϑ_0 *a priori* estimate of the unknown parameter is given, and the uncertainty on this parameter is noted η_ϑ ($x^r_\vartheta(0) = \vartheta_0 + \eta_\vartheta$).

Remark In the case of the the bar clamped at one end, x_ξ represents the displacements and velocities of the vibrating bar, and x_ϑ represents the unknown stiffness parameters in the different regions of the bar. In the case of the heart, the different parameters are the contractility parameters of the different regions, see Figure 1.



1. basal anterior
2. basal anteroseptal
3. basal inferoseptal
4. basal inferior
5. basal inferolateral
6. basal anterolateral
7. mid anterior
8. mid anteroseptal
9. mid inferoseptal
10. mid inferior
11. mid inferolateral
12. mid anterolateral
1.3 apical anterior
14. apical septal
15. apical inferior
16. apical lateral
17. apex
18. basal anterior
19. basal anterolateral
20. basal inferolateral
21. basal inferior
22. mid anterior
23. mid anterolateral
24. mid inferolateral
25. mid inferior
26. basal anterior
27. basal inferior
28. apex

Figure 1: Official (AHA - American Heart Association) ventricular regions

By extending the state space with the parameter, the system can be reformulated as follows:

$$\dot{x}(t) = A(x(t), t) \tag{3.5}$$
$$x(0) = x_0 + \eta, \tag{3.6}$$

with $x(\cdot) := (x_\xi(\cdot), x_\vartheta(\cdot))^T$, $x_0 := (\xi_0, \vartheta_0)^T$, $\eta := (0, \eta_\vartheta)^T$ and

$$A(x, t) = \begin{pmatrix} A^\xi(x_\xi, x_\vartheta, t) \\ A^\vartheta(x_\xi, x_\vartheta, t) \end{pmatrix},$$

thus transforming the parameter uncertainty to an initial condition uncertainty that has been studied in the previous chapter. However the fact that there is no uncertainty on $x(0)$ requires certain modifications, and thus the *reduced filter* is obtained. The extended reference variable is noted by $x_r(\cdot)$. In the following discussion, since there is no uncertainty on the state, we drop the subscript of η_ϑ.

Similarly to the previous problem, an observation $H : \mathcal{X}\times\Theta\times[0,T] \to \mathcal{Z}$ and an innovation $\tilde{D} : \mathcal{X} \times \Theta \times [0,T] \to \mathcal{Z}$ are given:

$$D(x_\xi, x_\vartheta, t) := z(t) - H(x_\xi, x_\vartheta, t)$$

The parameter estimation problem writes as:

$$J\left((\xi,\eta)^T, t\right) := \begin{cases} \frac{1}{2}\|\eta\|^2_{U_0} + \frac{1}{2}\int_0^t \|D(x_\xi(s), x_\vartheta(s), s)\|^2_M \,\mathrm{d}s & \xi = \xi_0 \\ \infty & \xi \neq \xi_0. \end{cases}$$

with $x_\xi(\cdot)$, $x_\vartheta(\cdot)$ satisfying (3.1), (3.2) with initial conditions $x_\xi(0) = \xi$ and $x_\vartheta(0) = \vartheta_0 + \eta$.

Remark Since we have an absolute knowledge of the initial value of the state, the norm $\|\cdot\|_{U_0}$ considered in the previous section degenerates to the case $\|(\xi,\eta)^T\|_{U_0} = \infty$ iff $\xi \neq \xi_0$; thus it is no longer a norm.

Remark The cost function in shows how 'good' an actual estimate is, through the system dynamics and the observations on the system; in other words how 'far' we are actually from the real model.

Since the values of interest of the cost function do not depend on ξ, it can be reduced to η by adding the constraint $x_\xi(0) = \xi_0$. By adding this constraint, the *reduced cost function* is obtained:

$$J_\vartheta(\eta, t) := \frac{1}{2}\|\eta\|^2_{U_0} + \frac{1}{2}\int_0^t \|D(x_\xi(s), x_\vartheta(s), s)\|^2_M \,\mathrm{d}s,$$

with the state and parameter trajectories satisfying the initial/final conditions $x_\xi(0) = \xi_0$, $x_\vartheta(0) = \vartheta_0 + \eta$

3.3 Optimal parameter filtering law

Fix $(\eta, t) \in \Theta \times [0, T]$. To a given trajectory $x(\cdot) = \begin{pmatrix} x_\xi(\cdot) \\ x_\vartheta(\cdot) \end{pmatrix}$ on $[0, t]$, defined by the fixed η, introduce the adjoint variable

$$p(\cdot) := \begin{pmatrix} p_\xi(\cdot) \\ p_\vartheta(\cdot) \end{pmatrix} : [0, t] \to \mathcal{X} \times \Theta$$

by

$$\frac{\mathrm{d}}{\mathrm{d}t} p(s) = -\left.\frac{\partial A}{\partial x}\right|_{x(s),s}^{T} p(s) + \left.\frac{\partial D}{\partial x}\right|_{x(s),s}^{T} MD(x(s), s) \tag{3.7}$$

$$\begin{pmatrix} p_\xi(t) \\ p_\vartheta(t) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{3.8}$$

Remark The adjoint variable appears when differentiating the cost functional J that has to be minimized, and facilitates calculation of the optimal filtering law, see the following theorem for details. It is quite commonly used in variational methods.

Theorem 3.1 *On a fix window* $[0, t]$*, for the optimal parameter trajectory* $\bar{x}_\vartheta(\cdot)$ *(satisfying* $\bar{x}_\vartheta(0) = \vartheta_0 + \bar{\eta} := \vartheta_0 + \bar{\eta}_t$*) the resulting adjoint variable* $\bar{p}_\vartheta(\cdot)$ *satisfies:*

$$\bar{p}_\vartheta(0) = U_0 \bar{\eta}.$$

Proof. Using (3.7) and (3.8), the partial derivative of J with respect to η writes as:

$$\begin{aligned}
\left.\frac{\partial J}{\partial \eta}\right|_{\eta,t} \delta\vartheta &= \eta^T U_0 \delta\vartheta + \int_0^t D(x(s), s)^T M \left.\frac{\partial D}{\partial x}\right|_{x(s),s} \left.\frac{\partial x}{\partial \eta}\right|_s \delta\vartheta \, \mathrm{d}s \\
&= \eta^T U_0 \delta\vartheta + \int_0^t \left(\dot{p}(s) + \left.\frac{\partial A}{\partial x}\right|_{x(s),s}^{T} p(s) \right)^T \left.\frac{\partial x}{\partial \eta}\right|_s \delta\vartheta \, \mathrm{d}s \\
&= \eta^T U_0 \delta\vartheta + \left[p(s)^T \left.\frac{\partial x}{\partial \eta}\right|_s \delta\vartheta \right]_0^t \\
&\qquad - \int_0^t p(s)^T \frac{\mathrm{d}}{\mathrm{d}t} \left(\left.\frac{\partial x}{\partial \eta}\right|_s \delta\vartheta \right) \mathrm{d}s + \int_0^t p(s)^T \left.\frac{\partial A}{\partial x}\right|_{x(s),s} \left.\frac{\partial x}{\partial \eta}\right|_s \delta\vartheta \, \mathrm{d}s \\
&= \eta^T U_0 - p_\vartheta(0)^T \delta\vartheta
\end{aligned}$$

by partial integration, and since the sensitivity of the state with respect to the initial condition

of the parameter η satisfies:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial x}{\partial \eta}\right)\Big|_s = \frac{\partial A}{\partial x}\Big|_{x(s),s} \frac{\partial x}{\partial \eta}\Big|_s \tag{3.9}$$

$$\frac{\partial x_\xi}{\partial \eta}\Big|_0 = 0 \tag{3.10}$$

$$\frac{\partial x_\vartheta}{\partial \eta}\Big|_0 = \mathbb{1}. \tag{3.11}$$

For the optimal $\bar{\eta}$

$$\frac{\partial J}{\partial \eta}\Big|_{\bar{\eta},t} = 0$$

must hold, which gives:

$$\bar{p}_\vartheta(0) = U_0\bar{\eta}. \qquad \square$$

Remark Note that by fixing $x_\xi(0) = x_0$ the sense of both the corresponding sensitivity equation and thus the corresponding adjoint equation has changed.

Introduce the *reduced filter Hamiltonian*:

$$\begin{aligned} \mathcal{H} : (\mathcal{X}\times\Theta)\times(\mathcal{X}\times\Theta)\times[0,T] &\to \mathbb{R} \\ (x,p,t) \mapsto \mathcal{H}(x,p,t) &:= \frac{1}{2}\|D(x,t)\|_M^2 - p^T A(x,t) \end{aligned} \tag{3.12}$$

For a given trajectory $x(\cdot)$ and the associated $p(\cdot)$ adjoint variable the following relationships hold:

$$\frac{\partial \mathcal{H}}{\partial x}\Big|_{x(s),p(s),s}^{T} = \dot{p}(s) \qquad \forall s \in [0,t],$$

$$\frac{\partial \mathcal{H}}{\partial p}\Big|_{x(s),p(s),s}^{T} = -\dot{x}(s) \qquad \forall s \in [0,t].$$

Since we consider the parameter dynamics without model noise, the dynamic programming problem degenerates to an optimization problem, with the *reduced value function* coinciding with the reduced cost function:

$$V_\vartheta(\eta,t) = J_\vartheta(\eta,t).$$

The analogue version of Theorem 2.2 results in the previous identity:

Theorem 3.2 *$V_\vartheta(\cdot,\cdot)$ satisfies the* reduced HJB equation*:*

$$\frac{\partial V_\vartheta}{\partial t}\Big|_{\eta,t} - \frac{1}{2}\|D(x_\xi(t), x_\vartheta(t), t)\|_M^2 = 0 \tag{3.13}$$

$$V_\vartheta(\eta,0) = \frac{1}{2}\|\eta\|_{U_0}^2 \tag{3.14}$$

with $x_\xi(0) = \xi_0$ and $x_\vartheta(0) = \vartheta_0 + \eta$.

Proof. Fix $t \in [0, T]$. Bellman's principle of optimality reduces to a simple additivity of the integral:

$$V_\vartheta(\eta, t) = V_\vartheta(\eta, t - \delta t) + \frac{1}{2} \int_{t-\delta t}^{t} \|D(x_\xi(s), x_\vartheta(s), s)\|_M^2 \, \mathrm{d}s, \qquad \forall\, \delta t \in [0, t]$$

where x_ϑ satisfies $x_\vartheta(0) = \vartheta_0 + \eta$ and $x_\xi(0) = \xi_0$. Using the continuity of $D(\cdot, \cdot)$ and $x_\vartheta(\cdot)$ leads to

$$\begin{aligned} 0 &= \lim_{\delta t \to 0} \left(\frac{1}{2\delta t} \left(\delta t \|D(x_\xi(t), x_\vartheta(t), t)\|_M^2 + o(\delta t) \right) - \frac{V_\vartheta(\eta, t) - V_\vartheta(\eta, t - \delta t)}{\delta t} \right) \\ &= \frac{1}{2} \|D(x_\xi(t), x_\vartheta(t), t)\|_M^2 - \left. \frac{\partial V_\vartheta}{\partial t} \right|_{\eta, t} \\ &= \frac{1}{2} \|D(x_\xi(t), x_\vartheta(t), t)\|_M^2 - \left. \frac{\partial V_\vartheta}{\partial t} \right|_{\eta, t}. \end{aligned}$$

The initial condition is satisfied by definition. □

The analogue version of Theorem 2.3 is stated as:

Theorem 3.3 *For* $\forall t \in [0, T]$*:*

$$\partial_\eta V_\vartheta(\eta, s)^T = p(s)^T \left. \frac{\partial x}{\partial \eta} \right|_s, \qquad \forall s \in [0, t] \tag{3.15}$$

with $p(\cdot)$ *the adjoint variable associated with* $x(\cdot)$ *(both determined by a choice of* η*).*

Proof. Fix arbitrarily $t \in [0, T]$ and the $(x(\cdot), p(\cdot))$ pair. The boundary conditions write as

$$\partial_\eta V_\vartheta(x_\vartheta(0), 0)^T = \eta^T U_0 \left. \frac{\partial x_\vartheta}{\partial \eta} \right|_0 = p(0)^T \left. \frac{\partial x}{\partial \eta} \right|_0$$

By differentiating the right hand side of the equation, after simplifications, one has:

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(p(s)^T \left. \frac{\partial x}{\partial \eta} \right|_s \right) = D(x_\xi(s), x_\vartheta(s), s) M \partial_\eta D(x_\xi(s), x_\vartheta(s), s)$$

using the equations of the state sensitivity with respect to the parameter (3.9) and the adjoint equations (3.7). Differentiating the reduced HJB equation by η, it follows that the two sides satisfy the same differential equation with the same initial conditions. □

The Mortensen conditions for the optimal filter are $\hat{x}(t)$ satisfying the initial condition $\hat{x}_\vartheta(0) = \vartheta_0 + \hat{\eta}(t)$. Using the previous result the following condition can be given on the value function:

$$\partial_\eta V_\vartheta(\hat{\eta}(t), t) = 0, \qquad \forall t \in [0, T].$$

Remark The following intuitive remark can be made: the Mortensen filter minimizes at each time instant t the value function $V_\vartheta(\eta, t)$, and the preceding condition is exactly the necessary condition for $\hat{x}_\vartheta(t)$ to be a minimizer of $V_\vartheta(\cdot, t)$. However by the previous proofs, further insight is gained on the relationships that hold between the value function, sensitivity and adjoint variables.

Taking the total derivative of the previous identity by t and differentiating the reduced HJB equation by η it follows that:

$$\begin{aligned} 0 &= \left.\frac{\partial^2 V_\vartheta}{\partial \eta^2}\right|_{\hat{\eta}(t),t} \dot{\hat{\eta}}(t) + \left.\frac{\partial^2 V_\vartheta}{\partial \eta \partial t}\right|_{\hat{\eta}(t),t} \\ &= \left.\frac{\partial^2 V_\vartheta}{\partial \eta^2}\right|_{\hat{\eta}(t),t} \dot{\hat{\eta}}(t) + \left.\frac{\partial \hat{x}}{\partial \eta}\right|_t^T \left.\frac{\partial D}{\partial x}\right|_{\hat{x}(t),t}^T MD(\hat{x}(t), t) \end{aligned}$$

the last term being zero by the condition on the value function, which gives the equation for the optimal filter for the reduced uncertainty η:

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\eta}(t) = -\left(\partial_\eta^2 V(\hat{\eta}(t), t)\right)^{-1} \left.\frac{\partial \hat{x}}{\partial \eta}\right|_t^T \left.\frac{\partial D}{\partial x}\right|_{\hat{x}(t),t}^T MD(\hat{x}(t), t)$$

To obtain the optimal state estimation associated with the optimal parameter estimation

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{x}(t) = \partial_t \hat{x}(t) + \partial_\eta \hat{x}(t)\dot{\eta}(t)$$

Thus the equations of the optimal joint state-parameter filter are obtained:

$$\begin{aligned} \dot{\hat{x}}(t) &= A(\hat{x}(t), t) - \left.\frac{\partial x}{\partial \eta}\right|_{\hat{\eta}(t),t} \left(\partial_\eta^2 V(\hat{\eta}(t), t)\right)^{-1} \left.\frac{\partial x}{\partial \eta}\right|_{\hat{\eta}(t),t}^T \left.\frac{\partial D}{\partial x}\right|_{\hat{x}(t),t}^T MD(\hat{x}(t), t) \\ \dot{\hat{\eta}}(t) &= -\left(\partial_\eta^2 V(\hat{\eta}(t), t)\right)^{-1} \left.\frac{\partial x}{\partial \eta}\right|_{\hat{\eta}(t),t}^T \left.\frac{\partial D}{\partial x}\right|_{\hat{x}(t),t}^T MD(\hat{x}(t), t) \\ \hat{x}(0) &= \begin{pmatrix} \xi_0 \\ \vartheta_0 \end{pmatrix} \\ \hat{\eta}(0) &= 0 \end{aligned}$$

In these equations one recognizes the sensitivity of the state w.r.t. the uncertainty on the initial condition and also, the Hessian of the value function $V(\cdot, \cdot)$. The first equation can be decomposed into two parts, the dynamics $A(\cdot, \cdot)$, responsible for our system to behave as the target system in case there is no measured difference, and the correction term. This prediction-correction type decomposition is significant in the discrete case. The equation on η shows that by gathering information, our optimal guess for the initial condition $\bar{x}_\vartheta(0)$ (determined by the uncertainty ϑ) changes in time, described by the obtained differential equation.

4 Numerical strategy

To implement the above described filtering methods, the calculation of the value function is necessary. This however requires the solution of either a HJB equation, or in the case with no model noise, a time integration of the innovation; even the latter requires the simulation of the dynamical system on the given time window $[0, T]$; such a simulation for high dimensional systems is very demanding in calculation time. In this realization we considered the case without ω model noise, that is we do not solve a HJB equation. In this section we present the numerical methods used for the realization of the *reduced Mortensen filter*.

4.1 On-line and off-line approach

The *off-line* approach here refers to the fact, that we consider the measurements on $[0, T]$ to be available at $t = 0$, while the *on-line* approach implies that the measurements are considered to be arriving continuously in "real-time"[9]. For the implementation of the reduced filter, both the value function and the sensitivity must be calculated.

There are (at least) two approaches for the approximation of the sensitivity $\partial_\vartheta x_{\hat{\vartheta}(t)}(t)$:

1. Simulate the sensitivity for ϑ_0, giving $\partial_\eta x_{\hat{\vartheta}(t)}(t) \approx \partial_\eta x_{\vartheta_0}(t)$ (giving quite a rough approximation)

2. Take at each time instant t a local approximation of the sensitivity, by taking a discretization Ω_d of a pre-defined domain $\Omega \subset \Theta$ and approximating by some sort of interpolation; e.g. $\partial_\eta x_{\hat{\vartheta}(t)}(t) \approx \dfrac{\hat{x}_{\vartheta_i}(t) - \hat{x}_{\vartheta_{i-1}}(t)}{d\vartheta}$

In the Verdandi implementation the first approach is used in the off-line method, and the second is used in the on-line realisation. The reason is that the second method requires the state trajectories to be calculated for a set of i particles. However, for large systems, off-line precalculation and more importantly the *storage* of the trajectories would be impossible. This however can be avoided in the on-line version by storing at each time t only $\hat{x}_{\vartheta_i}(t), \hat{x}_{\vartheta_i}(t-1)$ for a set of the i particles.

Remark One might wonder, if the value function has been calculated off-line on the domain Ω (which supposedly contains the optimum), one has an approximation of all $V(\cdot, T)$ values; why not simply take the minimum of $V(\vartheta, T)$ with $\vartheta \in \Omega$? The answer is, that for an application-oriented version of the filter, this idea should not be automatically rejected; see Appendix C on the *reduced order variational*

[9] Real-time here shouldn't be confused with real-time engineering applications; since our goal is diagnostics, the measurement data (MRI images) can be processed off-line, separately from the real-time system (heart). In this context, real-time means simply that the measurements are processed consecutively.

method. However, the interest of a realization of such an optimal filter lies in its possibility to be compared to other, more easily implementable nonlinear filters. As a comparison take e.g.

$$\|\hat{x}_{\text{ROUKF}} - \hat{x}_{\text{ROHJB}}\|_{\mathcal{X}}$$

with $\mathcal{X} = L^p(0,T), W^p(0,T), \ldots$ (Of course instead of ROUKF any other filter can be taken.)

4.2 Discretization

Depending on the approach, both the value function and the trajectories (on-line approach), or only the value function (off-line approach) have to be calculated on Ω. Thus both a discretization and an interpolation strategy must be chosen.

First of all a domain to be discretized $\Omega \subset \Theta := \mathbb{R}^N$ must be determined; this can be done around ϑ_0, depending on the initial error variance U_0. The domains considered are of the "box" type: $\Omega := I_1 \otimes I_2 \otimes \ldots \otimes I_N$ with I_i denoting an interval of the i-th dimension.

Two discretization approaches have been implemented. The first version takes a *dense* discretization of the domain, see section 4.2.1. However, such a discretization suffers from the *curse of dimensionality*, and with increasing dimensions of the parameter vector, quickly becomes intractable. In the solution of partial differential equations and quadrature methods, this problem is treated to some extent by using the so-called *sparse grid* methods, which for the same order of precision require significantly less number of points. Thus the second approach was to apply the sparse grid method to approximate the Hessian of the value function.

For the interpolation strategy the dense grid uses a piecewise linear interpolation method, while the sparse grid uses either a polynomial, or piecewise linear interpolation method. For approximation of the derivatives finite differences are available in both cases, and for sparse grids analytic differentiation of the polynomial interpolant is also available. In the following these two approaches are presented.

4.2.1 Dense grid

A dense discretization of this domain gives

$$\Omega \supset \Omega_d := I_1^d \otimes I_2^d \otimes \ldots \otimes I_N^d$$

with I_i^d a certain discretization of I_i; $i = 1 \ldots N$. In our case only equidistant discretization is examined; this can be determined by a $h = (h_1, h_2, \ldots h_N) \in \mathbb{R}^N$ discretization vector and the lower and upper bounds of $I_i, i = 1, 2 \ldots N$.

Since the evaluation of the value function for a given $\vartheta_i \in \Theta_d$ can be done recursively, for a computationally demanding problem it is worthwhile doing an off-line precalculation of these values using parallel computation techniques. In this implementation MPI has been used.

Once the value function calculated on the domain, 3-point and a 5-point stencil finite difference methods are used for the approximation of the Hessian.

4.2.2 Sparse grid

Sparse Grids are generally attributed to Smolyak [42]. For the reference on polynomial sparse grid interpolation see [4]. A good introduction to the sparse grid techniques is [14]. On implementation aspects [22] and especially Klimke's [21] is instructive. We base this compactified introduction on these articles.

The sparse grid techniques have evolved primarily from quadrature techniques, see [42] and [15]. The main advantage of the method is that supposing certain regularity conditions on the given function, good approximation properties can be obtained using a significantly less number of points, thus to some extent reducing the effect of the 'curse of dimensionality' (a term coined by Richard Bellman). To give an idea of the number of points used for a certain discretization level of sparse grids compared with that of the dense discretization see Figure 2. This comparison is made in 2 dimensions, and for a relatively low level, for higher dimensions and higher levels the contrast is even more sharp.

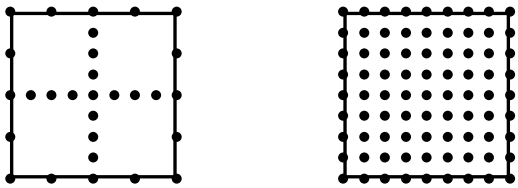


Figure 2: Sparse vs. Dense discretization (29 vs. 81 points)

The basic idea of the sparse grid methods, is to take a hierarchical discretization of the I_i intervals in each dimension i, giving $I_{i,l}$-s, $l = 0 \dots L$ with L the hierarchical level and $I_{i,l}$ the (finite) set of points, whose union gives the discretized I_i; $\bigcup_{l=1\dots L} I_{i,l} = I_i^d$. Then the tensor products of these $I_{i,l}$-s are taken in such a way, that only those with a limited number of points are added on each level $l = 1 \dots L$. The gain in the number of points originates from the fact that *not all tensor products are taken into account*. The idea of the hierarchical discretization is best illustrated on figure 3 (taken from Garcke's Sparse Grid Tutorial [14]).

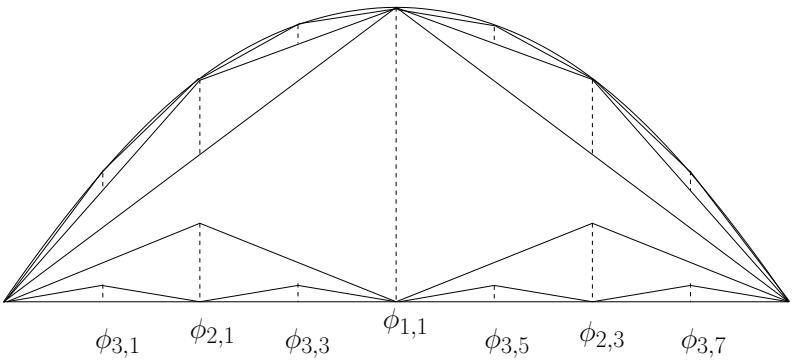


Figure 3: Hierarchical Sparse Grid interpolation of a 1-D function by piecewise linear basis functions (taken from Garcke's Sparse Grid tutorial [14])

There are several parameters to the creation of a sparse grid:

1. Where to place the nodes of the I_i^d? (Equidistant, Chebyshev, ...)
2. How, in what order to divide the I_i^d-s to $I_{i,l}$ hierarchical levels? (Clenshaw-Curtis (CC), maximum-norm (MN) based, maximum-norm based with no boundary points (MNNB), ...)
3. What kind of approximation to use? (Linear, Polynomial, ...)

The methods in parentheses and their combinations have been implemented in the library. In the following a more formal exposition is presented of the previous notions.

The Sparse Grid method This paragraph is based on Barthelmann et al. [4]. Without loss of generality, take $I_1 = I_2 = \ldots = I_N = [-1, 1]$.

Take a smooth $f : [-1, 1]^N \to \mathbb{R}$ function, that is to be approximated. For the moment in one dimension ($g : [-1, 1] \to \mathbb{R}$) choose an interpolation method:

$$\mathcal{M}^i(g) = \sum_{j=1}^{m_i} g(x_j^i)\varphi_j^i,$$

where $i \in \mathbb{N}$ is the order of the interpolation, $\varphi_j^i \in C([-1, 1])$ are basis functions and $x_j^i \in [-1, 1]$ are the interpolating nodes. Now using these 1-D interpolation formulas, define the tensor product:

$$\left(\mathcal{M}^{i_1} \otimes \cdots \otimes \mathcal{M}^{i_N}\right)(f) = \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_N=1}^{m_{i_N}} f(x_{j_1}^{i_1}, \ldots, x_{j_N}^{i_N})\,(\varphi_{j_1}^{i_1} \otimes \cdots \otimes \varphi_{j_N}^{i_N})$$

Take $|\mathbf{s}| := s_1 + s_2 + \ldots + s_N$ for $\mathbf{i} \in \mathbb{R}^N$. Now by defining the difference formulas as:

$$\Delta^s = \mathcal{M}^s - \mathcal{M}^{s-1},$$

the Smolyak algorithm writes as

$$\mathcal{S}(l) = \sum_{|\mathbf{s}| \leq l} \Delta^{s_1} \otimes \ldots \otimes \Delta^{s_N}.$$

In other words, we take the tensor products on the N-dimensional diagonal of the l^N sized "interpolation box" (see figure for illustration of $N = 2$ with Chebyshev points, Clenshaw-Curtis ordering and piecewise linear basis functions).

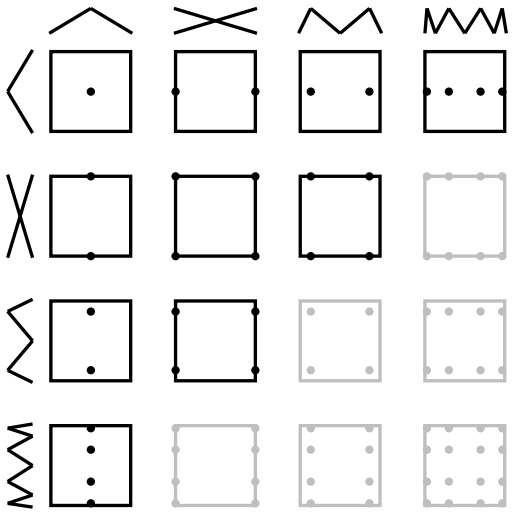


Figure 4: Hierarchical subgrid spaces with Chebyshev discretization points and basis functions in 2 dimensions (adapted from Garcke's Sparse Grid tutorial [14])

In [15] the following are chosen as the parameters of the sparse grid:

1. Chebyshev
2. Clenshaw-Curtis
3. Polynomial

For these parameters the authors obtain the following error bounds:

$$\|I_d - \mathcal{A}(l)\| \leq c_{N,k} \cdot n^{-k} (\log n)^{(k+2)(N-1)+1}$$

with $c_{N,k}$ constants depending on the order of continuity $f \in C^k$ and the dimension of the problem N; n denotes the number of nodes used by $\mathcal{A}(l)$.

4.3 Interpolation

For interpolation with basis functions that have disjoint support, it suffices to identify and evaluate only the contributing basis function, which leads to fast interpolation. For an efficient evaluation of multivariate Lagrange type interpolation, a barycentric interpolation type scheme is used.

A very clear and concise introduction to barycentric interpolation and its history can be found in [6]; the univariate case is based on this article. Klimke in his thesis [21] presents an approach to apply barycentric interpolation for sparse grids. In the following first the barycentric interpolation for the univariate case, and then an implementation of barycentric interpolation for Sparse Grids is presented.

4.3.1 Barycentric Interpolation

Univariate case The Lagrange polynomial interpolation problem is the following: Find the polynomial $p \in \Pi_n$ that interpolates a given $f : \mathbb{R} \to \mathbb{R}$ at given points $\{x_j\}_{j=0\ldots n}$:

$$p(x_j) = f_j, \qquad j = 0, \ldots, n,$$

by noting $f_j := f(x_j)$. The classical solution of this problem due to Lagrange can be written as

$$p(x) = \sum_{j=0}^{n} f_j \varphi_j(x), \qquad \varphi_j(x) = \frac{\prod_{k=0,k\neq j}^{n}(x - x_k)}{\prod_{k=0,k\neq j}^{n}(x_j - x_k)}$$

Note that the φ_j *Lagrange basis polynomials* can be characterized by

$$\varphi_j(x_k) = \delta_{j,k},$$

with $\delta_{j,k}$ denoting the Kronecker symbol.

Remark A simple calculation gives, that the evaluation of $p(x)$ in this form requires $O(n^2)$ multiplications. (n basis functions each requiring n multiplications.)

Introduce $\varphi(x) := \prod_{j=0}^{n}(x - x_j)$. Now to proceed, define the *barycentric weights* w_j by

$$w_j := \frac{1}{\prod_{k=0,k\neq j}^{n}(x_j - x_k)}, \qquad j = 0, \ldots, n$$

By using these weights, the basis functions simplify:

$$\varphi_j(x) = \varphi(x)\frac{w_j}{x - x_j},$$

and the Lagrange interpolation formula writes as:

$$p(x) = \varphi(x) \sum_{j=0}^{n} \frac{w_j}{x - x_j} f_j$$

In this form, the w_j are quantities that can be evaluated independently of x, and the evaluation of $\varphi(x)$ requires $O(n)$ multiplications. This has been called the *first form of the barycentric interpolation formula*. This can be further simplified by the following observation:

$$1 \equiv \sum_{j=0}^{n} \varphi_j(x) = \varphi(x) \sum_{j=0}^{n} \frac{w_j}{x - x_j}.$$

and dividing the first form by 1, the *second*, or *true form of the barycentric interpolation formula* is obtained:

$$p(x) = \frac{\sum_{j=0}^{n} \frac{w_j}{x - x_j} f_j}{\sum_{j=0}^{n} \frac{w_j}{x - x_j}}$$

This formula is a numerically stable one, for further details, see [6]; however special care must be taken, when interpolating at a point x_k, since certain numerators turn 0. However, knowing that p satisfies $p(x_j) = f_j$, by storing the function values f_j alongside the w_j coefficients, the problem is easily circumvented.

Barycentric interpolation for Sparse Grids Now for sparse grids, when using multivariate polynomial interpolation at a given $(x_1, \ldots, x_N) = \mathbf{x} \in \Omega$ point, polynomials of the type:

$$\sum_{|\mathbf{s}| \leq L} \sum_{\mathbf{b} \in B_\mathbf{s}} c_\mathbf{b}^\mathbf{s} \varphi_\mathbf{b}^\mathbf{s}(\mathbf{x})$$

have to be evaluated, where L is the level of refinement of the sparse grid, $\mathbf{s} \in \mathbb{N}^N$ is the subgrid index, $\mathbf{b} \in B_\mathbf{s} \subset \mathbb{N}^N$ is an indexation of the $\varphi_\mathbf{b}^\mathbf{s} : [0,1]^N \to \mathbb{R}$ basis functions, $c_\mathbf{b}^\mathbf{s}$ denotes the coefficient (also called *surplus*) of a $\varphi_\mathbf{b}^\mathbf{s}(\mathbf{x}) := \prod_{d=1}^{N} \varphi_{b_d}^{s_d}(x_d)$ basis function, and a certain $\varphi_{b_d}^{s_d} : [0,1] \to \mathbb{R}$ writes as

$$\varphi_{b_d}^{s_d}(x_d) := \frac{1}{\alpha_{b_d}^{s_d}} \prod_{\substack{0 \leq l \leq s_d, 0 \leq m \leq m_l \\ l = s_d \Rightarrow m \neq b_d}} (x_d - x_m^l),$$

where m_l denotes the number of nodes on subgrid level l, $\alpha_{b_d}^{s_d}$ being the normalizing factor:

$$\alpha_{b_d}^{s_d} := \prod_{\substack{0 \leq l \leq s_d, 0 \leq m \leq m_l \\ l = s_d \Rightarrow m \neq b_d}} (x_{b_d}^{s_d} - x_m^l),$$

such that $\varphi_{b_d}^{s_d}(x_{b_d}^{s_d}) = 1$; thus the $c_{\mathbf{b}}^{\mathbf{s}}$ coefficients can be chosen to be $f(x_{\mathbf{b}}^{\mathbf{s}}) - \mathcal{S}^{L-1}(f)(x_{\mathbf{b}}^{\mathbf{s}})$. In a complete form:

$$\mathcal{S}^L(f)(\mathbf{x}) = \sum_{|\mathbf{s}|\leq L} \sum_{\mathbf{b}\in B_{\mathbf{s}}} \left(f(x_{\mathbf{b}}^{\mathbf{s}}) - \mathcal{S}^{L-1}(f)(x_{\mathbf{b}}^{\mathbf{s}})\right) \prod_{d=1}^{N} \prod_{\substack{0\leq l\leq s_d, 0\leq m\leq m_l \\ l=s_d \Rightarrow m\neq b_d}} \frac{x_d - x_m^l}{x_{b_d}^{s_d} - x_m^l}$$

Thus to have a sparse grid representation of a function, one first has to evaluate the function values on the sparse grid nodes $\left\{ x_{\mathbf{b}}^{\mathbf{s}} \middle| |\mathbf{s}| \leq L, \mathbf{b} \in B_{\mathbf{s}} \right\}$, then to interpolate on intermediate values $\mathbf{x}$, one has to calculate products of differences of the type $x_d - x_m^l$.

Now note, that compared to the barycentric interpolation problem, the hierarchical representation of the sparse grid interpolation doesn't enable evaluating the interpolant in the same way; the roots of the hierarchical basis functions do not coincide with the Lagrangian basis functions. However, they do coincide up to the level of the basis function; thus for evaluation of each basis function barycentric interpolation can be used independently. This requires calculation of intermediate $\varphi(\cdot)$ functions, and barycentric weights.

1	0	$\psi^l(x)$
0	$x - x_0^0$	$x - x_0^0$
1	$x - x_0^1$ $x - x_1^1$	$(x - x_0^0)$ $(x - x_0^1)(x - x_1^1)$
2	$x - x_0^2$ $x - x_1^2$ $x - x_2^2$ $x - x_3^2$	 $(x - x_0^0)$ $(x - x_0^1)(x - x_1^1)$ $(x - x_0^2)(x - x_1^2)(x - x_2^2)(x - x_3^2)$
$\vdots$		
L	$x - x_0^L$ $x - x_1^L$ $\vdots$	$\prod_{\substack{0\leq l\leq L \\ 0\leq m\leq m_l}} (x - x_m^l)$

Table 2: Barycentric Interpolation scheme for polynomial sparse grid evaluation

Such a scheme (denoted by M) can be calculated efficiently by the recursive formula:

$$\psi^l(x) = \psi^{l-1}(x) \prod_{0\leq m\leq m_l} (x - x_m^l),$$

and the evaluation of a $\varphi_{b_d}^{s_d}$ basis function can be done by taking

$$\varphi_{b_d}^{s_d}(x) = \begin{cases} \dfrac{\psi^{s_d}(x)}{x - x_{b_d}^{s_d}}, & x \neq x_{b_d}^{s_d} \\ \psi^{s_d - 1}(x) \cdot \displaystyle\prod_{\substack{b=1,\ldots,m_{s_d} \\ b \neq b_d}} (x_{b_d}^{s_d} - x_b^{s_d}), & x = x_{b_d}^{s_d}. \end{cases}$$

The Chebyshev nodes in the Clenshaw-Curtis ordering are $x_0^0 = 0$, $x_0^1 = -1$, $x_1^1 = 1$ and:

$$x_b^l = \cos \frac{2(m_l - b) - 1}{2m_l} \pi, \qquad b = 1, \ldots, m_l$$

for $l > 1$ with $m_0 = 2^l$ for $l = 0, 1$ and $m_l = 2^{l-1}$. (Equidistant points on the perimeter of a semicircle projected onto the diameter.)

Remark The parallelization has been done by distributing the nodes of a subgrid; since in our case it is the evaluation of the function f (which for the filter is the value function) that is computationally demanding. (The evaluation requires simulating a PDE on the time window $[0, T]$.) Such a parallelization can be improved, by distributing the subgrids also, since subgrids on a same level do not have conflicting coefficients; however parallelization between levels is impossible, since the coefficients of the sparse grid depend on the sparse grid coefficients of the previous level, even though the function evaluations could be done.

4.4 Differentiation

Two types of differentiations must be implemented; a calculation of the $\nabla_\vartheta x_\vartheta$ sensitivity, and the Hessian $\nabla_\vartheta^2 V(\vartheta, t)$.

The following gradient methods are available in the sparse grid library:

1. Forward, Central and Backward finite differences
2. Analytic differentiation of the polynomial interpolant for the sparse grid method

For the calculation of the Hessian, a 5-point stencil and a 3-point stencil finite difference scheme has been implemented. The obvious advantage of the analytic differentiation is its precision. However the implementation is circumstantial; care must be taken to efficiently differentiate the root form of a multi-dimensional polynomial. In the following this is presented.

4.4.1 Analytic differentiation

In our implementation the divided difference type scheme presented in the previous section has been used. Two cases must be distinguished:

- $\varphi_{\mathbf{b}}^{\mathbf{s}}(\mathbf{x}) = 0$

- $\varphi^{\mathbf{s}}_{\mathbf{b}}(\mathbf{x}) \neq 0$

When $\varphi^{\mathbf{s}}_{\mathbf{b}}(\mathbf{x}) \neq 0$, the product rule must be applied to each dimension

$$\nabla_{x_d}\varphi^{s_d}_{b_d}(x) = \frac{1}{\alpha^{s_d}_{b_d}} \sum_{\substack{0\leq s\leq s_d, 0\leq j\leq m_s \\ s=s_d \Rightarrow j\neq b_d}} \prod_{\substack{0\leq l\leq s_d, 0\leq m\leq m_l \\ l=s_d \Rightarrow m\neq b_d}} \frac{x - x^l_m}{x - x^s_j} = \sum_{\substack{s\leq s_d \\ s=s_d \Rightarrow j\neq b_d}} \frac{M_{s_d,2}}{(x - x^{s_d}_{b_d})(x - x^s_j)}$$

and then

$$\nabla_{x_d}\varphi(\mathbf{x})^{\mathbf{s}}_{\mathbf{b}} = \nabla_{x_d}\varphi^{s_d}_{b_d}(x_d) \prod_{d'=1, d\neq d'}^{N} \varphi^{s_{d'}}_{b_{d'}}(x_{d'}).$$

Note that the polynomials $\varphi^{s_d}_{b_d}$ only have single roots, thus if $\varphi^{\mathbf{s}}_{\mathbf{b}}(\mathbf{x}) = 0$, then the only way for the gradient not to be 0, is for $\varphi^{s_d}_{b_d}(x_d) = 0$ to hold only for one d dimension. In this case, the gradient is non-zero only in dimension d.

5 Numerical results

The simulations (model + filter) have been implemented in C++, as part of the Verdandi [1] framework. In Verdandi the Reduced Mortensen Filter is called Reduced Order Hamilton-Jacobi-Bellman (ROHJB) filter, to imply that there is an underlying Hamilton-Jacobi-Bellman to be solved (that is for the case with model noise).

5.1 Model

The model considered is a finite element discretization of a bar clamped at one end. The bar is divided into n regions, and in each region there is a different constant parameter (stiffness, mass, force) throughout a given region. Then there is some excitation applied to the model, say at one end a certain force $F(\cdot)$ is exerted, and one observes the vibrations of the bar (displacements, as is the case for medical imaging for the heart). The goal is to determine an unknown subset of the parameters from this information.

The general partial differential equation describing such a system is:

$$\dot{x}(t) = \mathcal{A}x + \mathcal{R} \tag{5.1}$$
$$x(0) = x_0 + \eta \tag{5.2}$$

with the notations of the previous sections; additionally $x = (y, \dot{y})$ and $\mathcal{R}$ denotes a source term. In the variational form it becomes:

$$\begin{aligned}
\int_\Omega \rho \frac{\mathrm{d}y}{\mathrm{d}t} \cdot \delta y \, \mathrm{d}\Omega &= \int_\Omega \rho \, \dot{y} \cdot \delta y \, \mathrm{d}\Omega, \qquad \forall \delta y \\
\int_\Omega \rho \frac{\mathrm{d}\dot{y}}{\mathrm{d}t} \cdot \delta y \, \mathrm{d}\Omega &= -\int_\Omega \Sigma(y, \dot{y}) : \delta e \, \mathrm{d}\Omega + \int_\Omega f \cdot \delta y \, \mathrm{d}\Omega, \qquad \forall \delta y
\end{aligned}$$

Here Ω represents the domain of the equation, ρ is the mass density, Σ the second Piola-Kirchhoff stress tensor, $\delta y, \delta e$ denote the test functions (displacement, strain tensor) and f is the applied force. Assuming small displacements leads to a linear operator $\mathcal{A}$.

Now take the classical finite element approximation of the variational form described above:

$$\begin{aligned}
M_{\vartheta_m} \ddot{X} + C_{\vartheta_c} \dot{X} + K_{\vartheta_k} X &= F_{\vartheta_f} \\
X(0) &= X_0,
\end{aligned}$$

where X is a finite element discretization of y and $\vartheta_{m,c,k,f}$ denote respectively the mass, damping, stiffness and force parameters, and the matrices that they index are the corresponding

finite element matrices. This model is simulated numerically using a middle point Newmark scheme that is unconditionally stable (for details, see [5]):

$$\begin{aligned}\ddot{X}_{h+\frac{1}{2}} &= \frac{\ddot{X}_{h+1}+\ddot{X}_h}{2} = \frac{\dot{X}_{h+1}-\dot{X}_h}{\Delta t}\\ \dot{X}_{h+\frac{1}{2}} &= \frac{\dot{X}_{h+1}+\dot{X}_h}{2} = \frac{X_{h+1}-X_h}{\Delta t}\end{aligned}$$

This provides a triangular structure for the solution of the scheme:

$$\begin{pmatrix}\frac{1}{2}K_{\vartheta_k}+\frac{1}{\Delta t}C_{\vartheta_c}+\frac{2}{\Delta t^2}M_{\vartheta_m} & 0\\ \frac{2}{\Delta t}\mathbb{I} & -\mathbb{I}\end{pmatrix}\begin{pmatrix}X_{h+1}\\ \dot{X}_{h+1}\end{pmatrix} = \begin{pmatrix}\frac{2}{\Delta t}\mathbb{I} & \mathbb{I}\\ -\frac{1}{2}K_{\vartheta_k}+\frac{1}{\Delta t}C_{\vartheta_c}+\frac{2}{\Delta t^2}M_{\vartheta_m} & \frac{2}{\Delta t}M_{\vartheta_m}\end{pmatrix}\begin{pmatrix}X_h\\ \dot{X}_h\end{pmatrix}+\begin{pmatrix}0\\ F_{h+\frac{1}{2}}(\vartheta_f)\end{pmatrix},$$

$\mathbb{I}$ denoting the identity matrix. The triangular structure can be exploited by solving the equation in two passes; first for X_{h+1}, then for $\dot{X}_{h+1}$. This no longer holds for the Luenberger filtered model.

The observations are the displacements of the bar. For the solution of the finite element equations both direct and indirect methods are available; LU, GMRes in particular.

5.2 Reduced Order Mortensen filter

In fact, in order to implement the Mortensen filter, a time discretization must be chosen. The most common question is to decide whether to discretize the continuous filter, or to derive the discrete time filter from the discretized cost function. This last approach is preferable, since by supposing stability and consistency of the discretized dynamical system, the derived filter's stability and consistency properties can be derived more directly. However, as a first approach the discretization of the continuous filter as a prediction-correction model has been implemented; as the results show, this implementation is also acceptable.

1. Prediction:

$$\begin{aligned}\hat{x}^-_{n+1} &:= A_n(\hat{x}^+_n)\\ \hat{\eta}^-_{n+1} &:= \hat{\eta}^+_n\end{aligned}$$

2. Correction:

$$\begin{aligned}\hat{x}^+_{n+1} &:= \hat{x}^-_{n+1} - \left.\frac{\partial x_{n+1}}{\partial \eta}\right|_{\hat{\eta}^-_{n+1}} \left(\partial^2_\eta V_{n+1}(\hat{\eta}^-_{n+1})\right)^{-1} \left.\frac{\partial x_{n+1}}{\partial \eta}\right|^T_{\hat{\eta}^-_{n+1}} \left.\frac{\partial D_{n+1}}{\partial x}\right|^T_{\hat{x}^-_{n+1}} MD_{n+1}(\hat{x}^-_{n+1})\\ \hat{\eta}^+_{n+1} &:= \hat{\eta}^-_{n+1} - \left(\partial^2_\eta V_{n+1}(\hat{\eta}^-_{n+1})\right)^{-1} \left.\frac{\partial x_{n+1}}{\partial \eta}\right|^T_{\hat{\eta}^-_{n+1}} \left.\frac{\partial D_{n+1}}{\partial x}\right|^T_{\hat{x}^-_{n+1}} MD_{n+1}(\hat{x}^-_{n+1})\end{aligned}$$

Preliminary examinations show that the solution of the problem determined by the *discrete* cost function involves the use of Newton's method. In other words, at each step n a certain number of iterations of Newton's method must be calculated to obtain the optimal estimate for the discrete cost function.

5.3 Simulation results

Assimilation has been conducted[10] for the stiffness parameters of the bar, with the same covariances for each method. Note that the stiffness parameter appears in a bilinear fashion in the estimation, thus the problem is nonlinear to some extent.

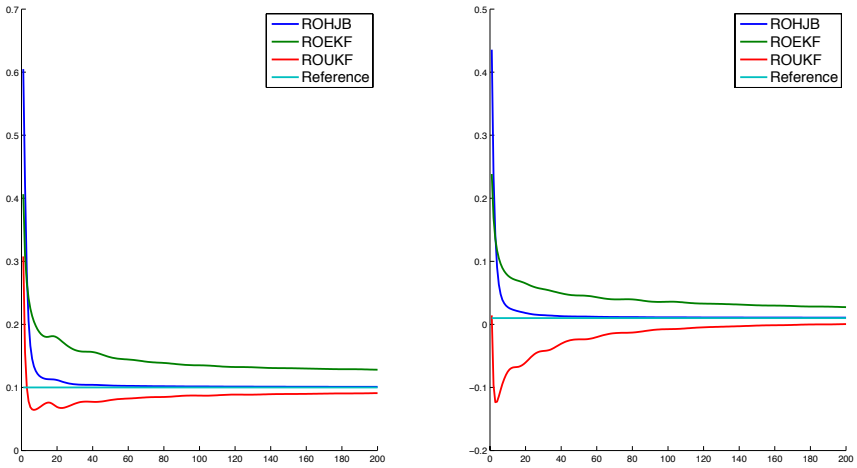


Figure 5: Estimation of the stiffness parameters of the bar with different methods

It can be seen that in this case, all three filters converge to the real value (reference), however, there is a great difference in the convergence rate. The reduced Mortensen (ROHJB) filter converges considerably faster than the suboptimal counterparts ROEKF and ROUKF. It would be interesting to see how the reduced Mortensen filter behaves for more complex cases, when the ROEKF and ROUKF don't even converge to the real value, see e.g. [31]. Nevertheless it must be noted that since the Mortensen filter requires parallel simulations of the model for a certain number of particles, the computation time of the Mortensen filter is considerably larger than as is for the ROEKF and ROUKF. However, this difference can be diminished by augmenting the number of processors involved in the parallel computations; by Moore's law, it is not completely unrealistic to expect a considerable growth (if not exponential) in the

[10]Note that several simulations have been conducted, all with similar results, this simulation is a representative sample of those simulations.

number of cores to be found in a processor, thus reducing the computation time of the reduced Mortensen filter to a comparable level to the ROEKF and ROUKF filters[11].

The value function for the specific problem examined has the following form:

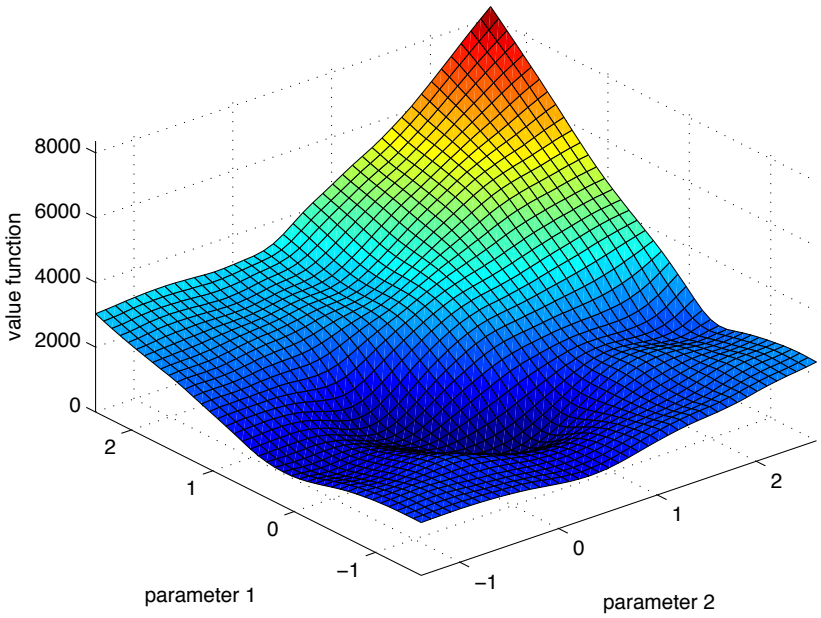


Figure 6: Value function for the stiffness parameter

Remark Note that the form of the value function contains information about the *region of attraction*. If one takes as an initial condition a point too far from the (global) optimum of the value function (which always exists and under not too harsh conditions is unique), for non-convex problems one might get stuck in a local optimum.

[11]It should be noted that since separate particles are generated that can be simulated independently, speed-up proportional with the number of cores can, and has been achieved. The limit of parallelization for the reduced Mortensen filter was far from being reached, contrary to the ROEKF and ROUKF. Further advances in this sense depend on the technological improvements to follow.

6 Conclusion and future perspectives

Conclusion In this work a reduced version of the filter first proposed by Mortensen has been implemented and examined. The filter has been implemented in the framework of the generic Data Assimilation Library, Verdandi. The filter is optimal in a certain maximum-likelihood sense and simulation results show, that it exhibits good behavior compared to other commonly used (suboptimal) nonlinear filters. A serious drawback of the method is its computational complexity, that is due to the fact that the filter requires a HJB value function to be calculated. Thus the dynamical system must be simulated for a set of particles, each of which is computationally demanding. The number of particles has been relaxed to some extent by the use of sparse grid methods for the approximation of the value function.

The usefulness of such a precise filter appears in determining unknown parameters of the heart, that could be used in clinical applications for diagnostics and prognostics. The need for an efficient filter proves to be necessary, there are cases [31] where the more common counterparts (ROEKF and ROUKF) prove to be insufficient.

Future perspectives Still, there rest some aspects of the method that are yet to be examined. Notably:

1. Derivation of the filter for the discrete cost function. Preliminary examinations show that this shall require a Newton method in the correction phase of the filter.
2. Other approximation methods, such as Kriging could be examined instead of, or in combination with, the Sparse Grid methods.
3. The interest of implementing an adaptive Sparse Grid method should also be considered.
4. The dimensional limits of the method should be examined (i.e. what dimensions are still calculable)
5. It would be interesting to see the method's performance on real applications (determining parameters of the heart model comes to mind)
6. Applying the method to state estimation through model reduction (e.g. POD, Moment matching methods . . .)

Sparse Grid aspects Also, since the sparse grid library has been implemented independently of Verdandi, for generic functions, it could be interesting to distribute the Sparse Grid Library under a public licence, since at the moment aside from Klimke's Sparse Grid Interpolation MATLAB Toolbox, and the SPARSE_GRID Python package, we have not found other

publicly available Sparse Grid Libraries (none in C++ whatsoever).

To aid development we also include a list of features that are to be added to the library in the future.

1. Determine and implement an efficient way to calculate finite difference stepsize for a certain sparse grid level L
2. Calculate domain from variance
3. Hierarchical error estimation
4. Implement all combinations of node-placement/order/approximation type
5. Possible improvement of distributing subgrids if processors are inactive (circumstantial).

A The optimal control problem

It is interesting to see the duality between the above examined optimal filtering problem and the widely known optimal control problem. The goal of the optimal control problem is to steer a system described by differential equations near a given trajectory, by minimizing one of the following: fuel, energy, peak value, time. The quantity that is to be minimized is described by a cost functional $J(\cdot)$ that associates costs with a given $u(\cdot)$ control function.

A.1 Problem formulation

Consider the following system:

$$\dot{x}(t) = A(x(t), t) + B(u(t)), \tag{A.1}$$
$$x(0) = x_0, \tag{A.2}$$

where $x \in \mathcal{X}$ represents the model state, $A(\cdot, \cdot) : \mathcal{X} \times [0, T] \to \mathcal{X}$ is the dynamical operator, $u(\cdot) : [0, T] \to \mathcal{U}$ represents the control and $x_0 \in \mathcal{X}$ is the given initial condition.

Remark Note that a solution of (A.1), (A.2) is completely determined by the choice of x_0 and $u(\cdot)$. For a fix t we note a specific solution $x_{\zeta,u(\cdot)}(\cdot)$ defined on $[t, T]$ emphasizing that we mean a solution of (A.1) with initial condition:

$$x_{\zeta,u(\cdot)}(t) = \zeta. \tag{A.3}$$

Arbitrary states shall be noted by ξ.

Consider an $x_r(\cdot) : [0, T] \to \mathcal{X}$ *reference trajectory* of the system given. Define the *trajectory error* $L(\cdot, \cdot) : \mathcal{X} \times [0, T] \to \mathcal{Z}(= \mathcal{X})$ as:

$$L(\xi, t) := x_r(t) - \xi,$$

which measures the difference between the reference trajectory at a given instant $x_r(t)$ and a given state ξ, but any other $L(\cdot, \cdot)$ can be considered.

Consider the following, general class of feedback laws:

$$\dot{x}(t) = A(x(t), t) + B(K(x(t), t)L(x(t), t)), \tag{A.4}$$
$$x(0) = x_0, \tag{A.5}$$

where $K : \mathcal{X} \times [0, T] \to \mathcal{F}(\mathcal{Z}, \mathcal{X})$ is a feedback gain of the state. The aim is to find a feedback gain $K(\cdot, \cdot)$ that is in some sense an optimal solution to this problem. To this end, introduce the following *cost functional*:

$$J(\zeta, u(\cdot), t) := \frac{1}{2}\|x_{\zeta,u(\cdot)}(T) - x_r(T)\|^2_{U_0} + \frac{1}{2}\int_t^T \|L(x_{\zeta,u(\cdot)}(s), s)\|^2_M + \|u(s)\|^2_S \, \mathrm{d}s, \tag{A.6}$$

The problem in the variational sense can be written as

$$\min_{u(\cdot)} J(x_0, u(\cdot), 0). \tag{A.7}$$

Using the *dynamic programming* approach, the problem is embedded in a larger class of problems, notably for $\forall(\zeta, t) \in \mathcal{X} \times [0, T]$ find $\bar{u}_{\zeta,t}(\cdot)$ satisfying:

$$J(\zeta, \bar{u}_{\zeta,t}(\cdot), t) = \min_{u(\cdot)} J(\zeta, u(\cdot), t), \tag{A.8}$$

for the moment supposing existence and uniqueness.

Fix $(\zeta, t) \in \mathcal{X} \times [0, T]$. Using Bellman's *Principle of Optimality*, we have that the optimal trajectory $\bar{x}(\cdot) := x_{\zeta,\bar{u}_{\zeta,t}(\cdot)}(\cdot)$ associated with the solution $\bar{u}_{\zeta,t}(\cdot)$ of (A.8) satisfies

$$J(\bar{x}(s), \bar{u}_{\zeta,t}(\cdot), s) = \min_{u(\cdot)} J(\bar{x}(s), u(\cdot), s), \qquad \forall s \in [t, T]$$

or in other words an optimal trajectory on $[t, T]$ must be optimal on every subinterval $[s, T]$.

Remark This is a simple consequence of the additivity of the cost function J:

$$J(\zeta, u(\cdot), t) = \frac{1}{2} \int_t^s \|L(x_{\zeta,u(\cdot)}(\tau), \tau)\|_M^2 + \|u(\tau)\|_S^2 \, \mathrm{d}\tau + J(x_{\zeta,u(\cdot)}(s), u(\cdot), s), \qquad \forall s \in [t, T]$$

A.2 Optimal feedback law

Throughout this section fix arbitrarily $(\zeta, t) \in \mathcal{X} \times [0, T]$. To facilitate notation, subscripts of $x_{\zeta,u(\cdot)}$, are only noted when necessary.

To derive the equations of an optimal feedback, introduce the *adjoint variable* $p(\cdot)$ associated with a given trajectory $x(\cdot)$ on $[t, T]$:

$$\dot{p}(s) + \left.\frac{\partial A}{\partial x}\right|_{x(s),s}^{T} p(s) = \left.\frac{\partial L}{\partial x}\right|_{x(s),s}^{T} ML(x(s), s), \qquad s \in [t, T] \tag{A.9}$$

$$p(T) = -U_0^T (x(T) - x_r(T)) \tag{A.10}$$

We have the following theorem:

Theorem A.1 *The optimal feedback law minimizing $J(\xi, \cdot, t)$ is given by:*

$$\bar{u}(s) = S^{-1} B^T \bar{p}(s), \qquad \forall s \in [t, T], \tag{A.11}$$

where by $\bar{p}(\cdot)$ we denote the adjoint variable defined on $[t, T]$ associated with the trajectory determined by the given ζ and the associated optimal $\bar{u}(\cdot)$.

Proof. The partial derivative of J with respect to u writes as:

$$\begin{aligned}
\left.\frac{\partial J}{\partial u}\right|_{\zeta,u(\cdot),t} \delta u(\cdot) &= x(T)^T U_0 \left.\frac{\partial \xi}{\partial u}\right|_T \delta u(\cdot) + \int_t^T L(x(s),s)^T M \left.\frac{\partial L}{\partial x}\right|_{x(s),s} \left.\frac{\partial x}{\partial u}\right|_s \delta u(\cdot) + u(s)^T S\, \delta u(\cdot)\, \mathrm{d}s \\
&= x(T)^T U_0 \left.\frac{\partial x}{\partial u}\right|_T \delta u(\cdot) + \int_t^T \left(\dot{p}(s) + \left.\frac{\partial A}{\partial \xi}\right|_{x(s),s}^T p(s)\right)^T \left.\frac{\partial x}{\partial u}\right|_s \delta u(\cdot) + u(s)^T S\, \delta u(\cdot)\, \mathrm{d}s \\
&= x(T)^T U_0 \left.\frac{\partial x}{\partial u}\right|_T \delta u(\cdot) + \left[p(s)^T \left.\frac{\partial x}{\partial u}\right|_s \delta u(\cdot)\right]_t^T - \int_t^T p(s)^T \frac{\mathrm{d}}{\mathrm{d}t}\left(\left.\frac{\partial x}{\partial u}\right|_s \delta u(\cdot)\right) \mathrm{d}s \\
&\quad + \int_t^T p(s)^T \left.\frac{\partial A}{\partial \xi}\right|_{x(s),s} \left.\frac{\partial x}{\partial u}\right|_s \delta u(\cdot)\, \mathrm{d}s + \int_t^T u(s)^T S\, \delta u(\cdot)\, \mathrm{d}s \\
&= \int_t^T \left(u(s)^T S - p(s)^T B\right) \delta u(\cdot)\, \mathrm{d}s
\end{aligned}$$

using that p satisfies (A.9) and that the sensitivity of the state with respect to the control variable satisfies:

$$\begin{aligned}
\left.\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial x}{\partial u}\right)\right|_s &= \left.\frac{\partial A}{\partial x}\right|_{x(s),s} \left.\frac{\partial x}{\partial u}\right|_s + B \\
\left.\frac{\partial x}{\partial u}\right|_t &= 0
\end{aligned}$$

To minimize J by u, for a fix ξ we must have

$$\left.\frac{\partial J}{\partial u}\right|_{\xi,\bar{u}(\cdot),t} = 0.$$

Using the DuBois-Reymond lemma leads to the optimum of u:

$$\bar{u}(s) = S^{-1} B^T \bar{p}(s), \qquad \forall s \in [t,T]. \qquad \square$$

Since ζ and t have been fixed arbitrarilty, this theorem provides amongst its solutions the $\bar{u}$ minimizing $J(x_0, u(\cdot), 0)$.

Define the *control Hamiltonian* as

$$\begin{aligned}
&\mathcal{H}(\cdot,\cdot,\cdot,\cdot) : \mathcal{X} \times \mathcal{X} \times \mathcal{U} \times [0,T] \to \mathbb{R} \\
&(\xi, p, u, t) \mapsto \mathcal{H}(\xi, p, u, t) := \frac{1}{2}\|L(\xi,t)\|_M^2 + \frac{1}{2}\|u\|_S^2 - p^T\left(A(\xi,t) + Bu\right)
\end{aligned} \tag{A.12}$$

It can be easily verified that $\mathcal{H}$ for a given control $u(\cdot) : [t,T] \to \mathcal{U}$ with the resulting trajectory $x(\cdot) : [t,T] \to \mathcal{X}$ and the associated adjoint variable $p(\cdot) : [t,T] \to \mathcal{X}$ satisfies the following relations:

$$\left.\frac{\partial \mathcal{H}}{\partial \xi}\right|_{x(s),p(s),u(s),s}^T = \dot{p}(s), \qquad \forall s \in [t,T]$$

$$\left.\frac{\partial \mathcal{H}}{\partial p}\right|_{x(s),p(s),u(s),s}^{T} = -\dot{x}(s), \qquad \forall s \in [t,T]$$

Furthermore, from (A.11) for the *optimal* control $\bar{u}(\cdot)$ and the associated optimal trajectories $\bar{p}(\cdot)$ and $\bar{x}(\cdot)$ we also have

$$\left.\frac{\partial \mathcal{H}}{\partial u}\right|_{\bar{x}(s),\bar{p}(s),\bar{u}(s),s}^{T} = S\,\bar{u}(s) - B^T\bar{p}(s) = 0, \qquad \forall s \in [t,T]$$

Remark This characterization of the optimal control is also known as *Pontryagin's Maximum Principle*.

Now let us introduce the *value function* $V(\cdot,\cdot)$:

$$V(\zeta,t) := J(\zeta,\bar{u}(\cdot),t), \tag{A.13}$$

where $\bar{u}(\cdot)$ is the optimal control determined for the given (ζ,t) pair.

Theorem A.2 *Assume that the following minimization problem has a unique solution for* $\forall t \in [0,T]$ *and* $\forall \xi \in \mathcal{X}$*:*

$$\min_{u\in\mathcal{U}} \mathcal{H}(\xi, -\partial_x V(\xi,t)^T, u, t)$$

For a given (ξ,t) *pair, we note this solution* $\bar{u}_{\xi,t}$*. Suppose furthermore that this solution varies continuously with respect to* (ξ,t)*.*

Then $V(\cdot,\cdot)$ *is a solution of the following Hamilton-Jacobi-Bellman (HJB) equation:*

$$\partial_t V(\xi,t) + \mathcal{H}(\xi, -\partial_x V(\xi,t)^T, \bar{u}_{\xi,t}, t) = 0 \tag{A.14}$$

$$V(\xi,T) = \frac{1}{2}\|\xi - x_r(T)\|_{U_0}^2 \tag{A.15}$$

For a fixed ξ *the optimal control is given by:*

$$\bar{u}_\xi(t) = \bar{u}_{\xi,t}. \tag{A.16}$$

Proof. Define $\bar{x}_\xi(\cdot) := x_{\xi,\bar{u}_\xi(\cdot)}(\cdot)$ on $[t,T]$. By Bellman's principle of optimality:

$$V(\xi,t) = \frac{1}{2}\int_t^{t+\delta t} \|L(\bar{x}_\xi(s),s)\|_M^2 + \|\bar{u}_\xi(s)\|_S^2 \,\mathrm{d}s + V(\bar{x}_\xi(t+\delta t), t+\delta t),$$

which using the continuity of $L(\cdot,\cdot)$ and $\bar{u}_\xi(\cdot)$ leads to

$$\begin{aligned}
0 &= \lim_{\delta t\to 0}\left(\frac{V(\bar{x}_\xi(t+\delta t),t+\delta t) - V(\bar{x}_\xi(t),t)}{\delta t} + \frac{1}{2\delta t}\left(\delta t\|L(\bar{x}_\xi(t),t)\|_M^2 + \delta t\|\bar{u}_\xi(t)\|_S^2 + o(\delta t)\right)\right) \\
&= \left.\frac{\mathrm{d}V}{\mathrm{d}t}\right|_{\bar{x}_\xi(t),t} + \frac{1}{2}\|L(\xi,t)\|_M^2 + \frac{1}{2}\|\bar{u}_\xi(t)\|_S^2 \\
&= \left.\frac{\partial V}{\partial t}\right|_{\xi,t} + \left.\frac{\partial V}{\partial x}\right|_{\xi,t}\left(A(\xi,t) + B\bar{u}_\xi(t)\right) + \frac{1}{2}\|L(\xi,t)\|_M^2 + \frac{1}{2}\|\bar{u}_\xi(t)\|_S^2,
\end{aligned} \tag{A.17}$$

from which $\bar{u}_\xi(t) = \bar{u}_{\xi,t}$ follows, otherwise it would be possible to decrease the value of $V(\xi, t)$ by replacing $\bar{u}_\xi(\cdot)$ with $\bar{u}_{\xi,t}$ on a sufficiently short $[t, t + \delta t]$ interval. Expressing this equation with the Hamiltonian function gives the desired result. It is easy to see that the boundary condition is satisfied. □

Theorem A.3 *The following relationship holds between the adjoint variable and the value function:*

$$\bar{p}(t) = -\partial_\xi V(\bar{x}(t), t)^T, \qquad \forall t \in [0, T]. \tag{A.18}$$

Proof. From the HJB boundary condition (A.15) we have:

$$\partial_x V(\bar{x}(T), T) = \bar{x}(T)^T U_0 = -\bar{p}(T)^T.$$

From the HJB equation (A.14), we have:

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}x}\left(\partial_t V(\xi, t) + \mathcal{H}(\xi, -\partial_x V(\xi, t)^T, \bar{u}_{\xi,t}, t)\right) \\
&\quad = \partial_\xi \partial_t V(\xi, t) + \partial_\xi \mathcal{H}(\xi, -\partial_\xi V(\xi, t)^T, \bar{u}_{\xi,t}, t) - \partial_p \mathcal{H}(\xi, -\partial_\xi V(\xi, t)^T, \bar{u}_{\xi,t}, t)\partial_\xi^2 V(\xi, t) \\
&\quad = \partial_\xi \partial_t V(\xi, t) + L(\xi, t)^T M \partial_x L(\xi, t) + \partial_\xi V(\xi, t)\partial_x A(\xi, t) + (A(\xi, t) + B\bar{u}_{\xi,t})^T \partial_\xi^2 V(\xi, t) = 0,
\end{aligned}$$

which gives on the optimal trajectory $\bar{x}(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(-\partial_\xi V(\bar{x}(t), t)^T\right) = \partial_\xi L(\bar{x}(t), t)^T M L(\bar{x}(t), t) - (-\partial_\xi A(\bar{x}(t), t)^T \partial_\xi V(\bar{x}(t), t)^T)$$

Thus $\bar{p}(t)$ associated with $\bar{x}(\cdot)$ satisfies the same dynamics as $-\partial_\xi V(\bar{x}(t), t)^T$. □

As a result of this theorem we can express the optimal feedback law as a function of V:

$$\bar{u}_\xi(t) = -S^{-1} B^T \partial_\xi V(\bar{x}(t), t)^T \tag{A.19}$$

A.3 Stability

We base this part on [39].

The stability of such a control system is a central question, it is crucial for safety issues.

Since stability of a dynamic system is defined on $\mathbb{R}^+$, the domain of the $x_r(\cdot)$ reference trajectory must be extended to $\mathbb{R}^+$ and the original cost function must be modified to:

$$\tilde{J}(\zeta, u(\cdot), t) := \frac{1}{2}\int_t^\infty \|L(x_{\zeta,u(\cdot)}(s), s)\|_M^2 + \|u(s)\|_S^2 \,\mathrm{d}s,$$

Remark The first natural question to pose is whether there exists $u(\cdot)$, for which $\tilde{J}$ is finite. For our purposes, it is supposed that such a $u(\cdot)$ exists. Note nevertheless that if there exists a control $u_r(\cdot)$, for which $J(x_r(0), u_r(\cdot), 0)$ is finite, and the system is controllable, then by composition of the control functions there exists $\bar{u}(\cdot)$ with which $\tilde{J}(x_0, \bar{u}(\cdot), 0)$ is also finite.

To examine stability, Lyapunov's *Direct Method* is applied. $\tilde{V}(\cdot,\cdot) := V(\cdot,\cdot)$ by definition is positive, thus it is a valid Lyapunov function candidate.

Theorem A.4 *$\tilde{V}(\xi, t)$ is a valid Lyapunov function, for the system* (A.1)*,* (A.2) *with feedback* (A.19)*.*

For $\tilde{V}(\cdot,\cdot)$ to be a Lyapunov function,

$$\left.\frac{\mathrm{d}\tilde{V}}{\mathrm{d}t}\right|_{\bar{x}(t),t} < 0.$$

is necessary (additionally to being a Lyapunov function candidate). From (A.17) it follows:

$$\begin{aligned}\left.\frac{\mathrm{d}\tilde{V}}{\mathrm{d}t}\right|_{\bar{x}(t),t} &= \left.\frac{\partial\tilde{V}}{\partial t}\right|_{\bar{x}(t),t} + \left.\frac{\partial\tilde{V}}{\partial x}\right|_{\bar{x}(t),t}\dot{\bar{x}}(t) \\ &= -\frac{1}{2}\left(\|L(\bar{x}(t),t)\|_M^2 + \|\bar{u}(t)\|_S^2\right),\end{aligned} \tag{A.20}$$

which is negative, hence the system is stable.

B Luenberger state estimation

Calculating the value function requires the solution of a HJB equation, which for high dimensional systems is computationally intractable. Such is the case e.g. for the systems encountered in the numerical methods of partial differential equations. In high dimensions, the computational intractability also holds for the Kalman filtering and its extensions (EKF, UKF) because of the high dimensional dense structure of the covariance matrices, that have to be propagated.

To circumvent this difficulty, it is possible [35] to use the numerically less expensive method of *Luenberger* type filters. However, the design of Luenberger type filters for high dimensional systems poses difficulties. Nevertheless, there exist operators for specific systems, that give directly in some sense an optimal feedback law.

Furthermore, in systems that are not stable, or not asymptotically (e.g. vibrating systems, as is the case of the beating heart), to obtain convergence of the parameter estimation it is desirable to enhance stability, by applying a Luenberger filter on the system, and perform the parameter estimation on the filtered system; this however entails a trade-off with observability properties.

Remark Imagine, that the state is filtered with a high gain; the innovation D thus becomes zero (or close to it) and observability is destroyed.

The following approach is based on [33] and [35]. For a detailed analysis of these filters, we refer the reader to these articles; for our purposes only a short presentation of the methods is given.

The general Luenberger filter can be formulated as follows:

$$\dot{\hat{x}}(t) = A(\hat{x}(t), t) + B(KD(\hat{x}(t), t), t), \tag{B.1}$$

$$\hat{x}(0) = x_0, \tag{B.2}$$

with the same notations introduced previously.

For the state estimation problem the finite element approximation of mechanical systems is considered:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} x_d \\ x_v \end{pmatrix} = \begin{pmatrix} 0 & \mathbb{I} \\ -M^{-1}K & -M^{-1}C \end{pmatrix}\begin{pmatrix} x_d \\ x_v \end{pmatrix} + \begin{pmatrix} 0 \\ M^{-1}F \end{pmatrix} \tag{B.3}$$

where $x_d(\cdot), x_v(\cdot) : [0, T] \to \mathcal{X}$ and M, C, K, F denote respectively the mass, damping, stiffness matrices and the force vector, or

$$\dot{X}(t) = AX(t) + R(t)$$

$$X(0) = X_0 + \eta.$$

Now the goal is to formulate a filter

$$\begin{aligned}\dot{\hat{X}}(t) &= A\hat{X}(t) + R(t) + K_X(Z(t) - H\hat{X}(t)) \\ \hat{X}(0) &= X_0,\end{aligned}$$

for which the error dynamics defined by $\tilde{X} := X - \hat{X}$, satisfying

$$\begin{aligned}\dot{\tilde{X}}(t) &= (A - K_X H)\tilde{X}(t) \\ \tilde{X}(0) &= \eta,\end{aligned}$$

is stable.

B.1 Direct Velocity Feedback

In the following the measurement $H : \mathcal{X} \to \mathcal{Z}$ is a function of the velocities:

$$z_v = H(x_v) + \chi,$$

Here $\chi \in \mathcal{Z}$ denotes the measurement error, which consists of a discretization error and the measurement noise. Now by taking as an DVF feedback as in [33]

$$K_X = \begin{pmatrix} 0 \\ \gamma M^{-1} H' \end{pmatrix},$$

the 'closed-loop' system writes as

$$M\ddot{\hat{X}} + C\dot{\hat{X}} + (K + \gamma H'H)\hat{X} = R + \gamma H'Z,$$

with K denoting the stiffness matrix.

B.2 Schur Displacement Feedback

In this section, the measurement $H : \mathcal{X} \to \mathcal{Z}$ is a function of the displacements:

$$z_d = H(x_d) + \chi,$$

This is the case e.g. in medical imaging. Now by taking as a SDF feedback as in [35]

$$K_X = \begin{pmatrix} \gamma K^{-1} H' \\ 0 \end{pmatrix},$$

such that the 'closed-loop' system writes as

$$\begin{aligned} K\dot{\hat{x}}_d &= K\hat{x}_v + \gamma H'(Z - H_d\hat{x}_d) \\ M\dot{\hat{x}}_v + C\hat{x}_v + K\hat{x}_d &= F. \end{aligned}$$

with K denoting the stiffness matrix. Note, that $\dot{\hat{x}}_d = \hat{x}_v$ no longer holds; hence the notation x_d, x_v.

By spectral analysis (of specific problems) it is possible to calculate the gain γ such, that the poles are placed in an optimal way; that is

$$\max_{\gamma} \min_{i} |\lambda_i|$$

where λ_i is the set of eigenvalues of the (discrete) operator.

C Reduced Order Variational Method

The variational approach already has all the measurements on a time window $[0, T]$, thus the problem to be solved is

$$\min_{\eta} J_{\vartheta}(\eta, T).$$

A standard approach to the solution of this minimization problem (as of all minimization problems) consists of taking an initial guess $\eta_0 = 0$ and then using the gradient (or the Hessian) of the function to be minimized - $J_{\vartheta}(\cdot, T)$. The difficulty with this strategy is that, at each iteration, to obtain the gradient of the cost function the system must be simulated for ϑ_n (n denoting the optimization iteration) on $[0, T]$, similarly for the adjoint variable, only backwards.

Another approach could be the following: Take an approximation $\tilde{J}_{\vartheta}(\cdot, T)$ of $J_{\vartheta}(\cdot, T)$, say using Sparse Grid or any other methods, and minimize the approximation of $\tilde{J}_{\vartheta}(\cdot, T)$. Note that this approach is also computationally demanding; it still requires simulation of a set of ϑ_i particles. However, a big advantage compared to the standard variational method is that the simulation for the set of particles can be done *parallelly*. On the numerical implementation of the Sparse Grid approximation of the cost (value) function, see details in section 4 on Numerical strategies.

An advantage of this method is that the simulations of the 'particles' are done parallelly as opposed to the standard variational approach (i.e. via the adjoint equation). Once the particles have been generated, the evaluation of the Sparse Grid interpolant is not demanding, the optimization problem can be solved rapidly. However the drawback of this method is the same as of the Reduced Mortensen Filter's, that is the simulation of the particles for complex systems is very demanding, and even if the 'curse of dimensionality' is treated by sparse grids to some extent, the method remains computationally demanding.

Implementation-wise, NLOPT has been used for the solution of the nonlinear optimization problem.

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