A Probabilistic Taylor Expansion with Applications in Filtering and Differential Equations

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Abstract

We study a class of Gaussian processes for which the posterior mean, for a particular choice of data, replicates a truncated Taylor expansion of any order. The data consists of derivative evaluations at the expansion point and the prior covariance kernel belongs to the class of *Taylor kernels*, which can be written in a certain power series form. This permits statistical modelling of the uncertainty in a variety of algorithms that exploit first and second order Taylor expansions. To demonstrate the utility of this Gaussian process model we introduce new probabilistic versions of the classical extended Kalman filter for non-linear state estimation and the Euler method for solving ordinary differential equations.

1 Introduction

In one dimension, Taylor's theorem states that any function $f: \mathbb{R} \to \mathbb{R}$ that is sufficiently smooth at a point $a \in \mathbb{R}$ can be written as

$$f(x) = T_{n,a}(x) + P_{n,a}(x). (1.1)$$

Here $T_{n,a}(x) = \sum_{p=0}^n \frac{1}{p!} f^{(p)}(a) (x-a)^p$ is the nth order Taylor polynomial and $P_{n,a}(x)$ is a remainder term which satisfies $P_{n,a}(x) = \mathcal{O}(|x-a|^{n+1})$ as $|x-a| \to 0$. Multidimensional generalisations are readily available and will be introduced in Sec. 2.

Approximations derived from (1.1), in particular the first and second order Taylor approximations $f(x) \approx f(a) + f'(a)(x-a)$ and $f(x) \approx f(a) + f'(a)(x-a) + \frac{1}{2}f''(a)(x-a)^2$ for x close to a, play important roles in a wide variety of standard algorithms for optimisation (Conn et al., 2000; Moré, 1978), state estimation (Särkkä, 2013, Ch. 5), ordinary differential equations (Hairer et al., 1993, Ch. II), and approximation of exponential integrals in Bayesian statistics (Raudenbush et al., 2000), to name but a few. This paper proposes a Gaussian process (GP) model (Rasmussen and Williams, 2006) whose posterior mean, given the derivative data $(f(a), f'(a), \ldots, f^{(n)}(a))$, is exactly the Taylor polynomial $T_{n,a}$, and whose posterior variance is proven to play a role analogous to the remainder term $P_{n,a}$ in (1.1). In the spirit of probabilistic numerics (Cockayne et al., 2019b; Diaconis, 1988; Hennig et al., 2015; Larkin, 1972; O'Hagan, 1992), the posterior variance can then be used for principled

probabilistic quantification of epistemic uncertainty in the Taylor approximation $f(x) \approx T_{n,a}(x)$ at $x \neq a$, which can be exploited and propagated forward in algorithms that rely on such expansions. Taylor approximation thus joins the ranks of classical numerical methods, such as algorithms for spline interpolation (Diaconis, 1988; Kimeldorf and Wahba, 1970), numerical quadrature (Diaconis, 1988; Karvonen and Särkkä, 2017; Karvonen et al., 2018), differential equations (Schober et al., 2014, 2019; Teymur et al., 2016), and linear algebra (Cockayne et al., 2019a; Hennig, 2015), that can be cast as statistical inference.

The GP priors we use to achieve this have their covariance structure determined by positive-definite and non-stationary *Taylor kernels* which, at an expansion point a, take the form $K_a(x,y) = K(x-a,y-a)$, where

$$K(x,y) = \sigma^2 \sum_{p=0}^{\infty} \frac{c_p \lambda^p}{(p!)^2} (xy)^p$$

for constants $c_p > 0$ and parameters $\sigma, \lambda > 0$. The canonical example, used in our applications, is the *exponential kernel* $K(x,y) = \sigma^2 \exp(\lambda xy)$, obtained by setting $c_p = p!$.

Taylor kernels, often under the name *power series kernels*, have been used—and their approximation properties analysed—in the numerical analysis and scattered data approximation literature; see (De Marchi and Schaback, 2010; Dick, 2006; Zwicknagl, 2009; Zwicknagl and Schaback, 2013) and (Fasshauer and McCourt, 2015, Sec. 3.3.1). Sec. 1 in (Zwicknagl and Schaback, 2013) has been of particular inspiration for our work. The *Szegő kernel* K(x,y) = 1/(1-xy) (i.e. $c_p = (p!)^2$) and related *Bergman kernel* $K(x,y) = 1/(1-xy)^2$ (i.e. $c_{2p} = (p!)^2$ and $c_p = 0$ for odd p), which are defined on the open interval (-1,1), are particularly well studied in the approximation theory literature because their reproducing kernel Hilbert spaces (RKHSs) are important in complex analysis (e.g. (Larkin, 1970; Richter-Dyn, 1971b,a) and (Oettershagen, 2017, Sec. 6.2)).

Taylor kernels occasionally appear in the machine learning and statistics literature (see (Minka, 2000, Sec. 4), (Steinwart and Christmann, 2008, Example 4.9), and (Liang and Rakhlin, 2020)) but, to the best of our knowledge, have not been used in conjunction with derivative data in the way proposed here. Nevertheless GP regression with derivative data has been explored (e.g., (Eriksson et al., 2018; Prüher and Särkkä, 2016; Solak et al., 2002; Wu et al., 2017)), though "standard" kernels such as the Gaussian kernel are usually used.

1.1 Structure of the Paper

The remainder of the paper is structured as follows. In Sec. 2 we introduce Taylor kernels in the multivariate setting in Sec. 2.1, and briefly recall GP regression with derivative data in Sec. 2.2. In Sec. 2.3 we show that the GP posterior mean is precisely the Taylor polynomial $T_{n,a}$ when the data consists of derivative evaluations at a up to order n, prior covariance is determined by a Taylor kernel K_a , and the prior mean is an arbitrary polynomial of degree at most n. Closed-form maximum likelihood expressions for the kernel parameters are given in Sec. 2.4, and in Sec. 2.5 we consider the setting when noisy function and derivative observations are used, rather than exact observations. In Sec. 2.6 we remark that derivative data consists of the coefficients in an RKHS-orthonormal expansion of a function in the RKHS of a Taylor kernel and briefly discuss related generalisations.

To demonstrate the utility of the proposed probabilistic Taylor expansion we develop GP versions of two classical algorithms. *Firstly*, in Sec. 3 we propose a probabilistic version of the classical extended Kalman filter (EKF) (Särkkä, 2013, Ch. 5) for online state estimation in non-linear, partially

¹For multidimensional input points $p \in \mathbb{N}_0$ is essentially replaced with a multi-index $\alpha \in \mathbb{N}_0^d$ and xy usually with the Euclidean inner product; see Sec. 2.1 for details.

observed systems. Unlike conventional non-linear filters, the proposed filter is capable of incorporating the error from model linearisations into filtering error covariances, and as a result is both more robust and significantly easier to tune than other recently developed GP based filters (Deisenroth et al., 2012; Prüher and Straka, 2018; Prüher et al., 2017, 2021). The filter is shown to outperform both the EKF and the popular derivative-free unscented Kalman filter (UKF) in a challenging target tracking problem where both of these alternatives tend to diverge.

Secondly, in Sec. 4 we apply probabilistic Taylor expansions iteratively to approximate solutions of ordinary differential equations of the form y'(t) = f(t, y(t)). Interpreting the approximations y_n and $f(t_n, y_n)$ at t_n as noisy observations of $y(t_n)$ and $y'(t_n)$ yields a probabilistic numerical version of the classical Euler method which is capable of uncertainty quantification for the unknown solution and implementation of which requires no optimisation or matrix inversions. This probabilistic Euler method is applied to the logistic equation and the FitzHugh–Nagumo model.

We emphasise that there are a myriad of other potential applications for probabilistic Taylor expansions beside the two discussed in detail here; see Sec. 5. Furthermore, the two example applications we present should not be viewed as final. The probabilistic framework permits various extensions and improvements that are useful when the data are computationally expensive to obtain, some of which are suggested and briefly experimented with in Secs. 3 and 4.

2 A Probabilistic Taylor Expansion

In this section we derive a probabilistic Taylor expansion using Gaussian processes. Many of the derivations and proofs are given in Supplements A and B.

2.1 Taylor Kernels

Let $\boldsymbol{a} \in \mathbb{R}^d$ and $\Omega_{\boldsymbol{a},r} = \{\boldsymbol{x} \in \mathbb{R}^d : \|\boldsymbol{x} - \boldsymbol{a}\|_2 < r\}$ for some $r \in (0,\infty]$. A multidimensional Taylor kernel defined on $\Omega_{\boldsymbol{a},r} \times \Omega_{\boldsymbol{a},r}$ is $K_{\boldsymbol{a}}(\boldsymbol{x},\boldsymbol{y}) = K(\boldsymbol{x} - \boldsymbol{a},\boldsymbol{y} - \boldsymbol{a})$ for

$$K(\boldsymbol{x}, \boldsymbol{y}) = \sigma^2 \sum_{\boldsymbol{\alpha} \in \mathbb{N}_0^d} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^2} \boldsymbol{x}^{\boldsymbol{\alpha}} \boldsymbol{y}^{\boldsymbol{\alpha}},$$
(2.1)

where $\sigma>0$ and $\pmb{\lambda}\in\mathbb{R}^d_+$ are hyperparameters and $c_{\pmb{\alpha}}$ are positive constants such that

$$\sum_{\boldsymbol{\alpha} \in \mathbb{N}_0^d} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^2} r^{2|\boldsymbol{\alpha}|} < \infty \quad \text{or} \quad \sum_{\boldsymbol{\alpha} \in \mathbb{N}_0^d} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}! \sqrt{\boldsymbol{\alpha}!}} e^{|\boldsymbol{\alpha}|} < \infty$$
 (2.2)

if $r<\infty$ or $r=\infty$, respectively. Here \mathbb{N}_0^d stands for the collection of non-negative d-dimensional multi-indices $\pmb{\alpha}=(\pmb{\alpha}(1),\dots,\pmb{\alpha}(d))$, where $\pmb{\alpha}(j)\in\mathbb{N}_0$ is the jth index of $\pmb{\alpha}$, and we define $|\pmb{\alpha}|=\pmb{\alpha}(1)+\dots+\pmb{\alpha}(d)$. The condition (2.2) ensures the series defining $K_{\pmb{\alpha}}$ via (2.1) converges for all $\pmb{x},\pmb{y}\in\Omega_{\pmb{\alpha},r}$, which, together with $c_{\pmb{\alpha}}>0$, guarantees that Taylor kernels are positive-definite (Zwicknagl and Schaback, 2013, Thm. 2.2). However, $c_{\pmb{\alpha}}>0$ is not necessary for positive-definiteness of K in (2.1) (Zwicknagl, 2009, Sec. 2).

An important subclass of Taylor kernels are inner product kernels, defined by

$$K(\boldsymbol{x}, \boldsymbol{y}) = \sigma^2 \sum_{p=0}^{\infty} \frac{c_p}{(p!)^2} \langle \boldsymbol{x}, \boldsymbol{y} \rangle_{\boldsymbol{\lambda}}^p$$
 (2.3)

where $\langle \boldsymbol{x}, \boldsymbol{y} \rangle_{\boldsymbol{\lambda}} = \sum_{i=1}^{d} \lambda_i x_i y_i$. An inner product kernel is of the form (2.1) with $c_{\boldsymbol{\alpha}} = c_{|\boldsymbol{\alpha}|} \boldsymbol{\alpha}! / |\boldsymbol{\alpha}|!$ (see Supplement A.1). In practice, uniform scaling in each dimension is used so that $\langle \boldsymbol{x}, \boldsymbol{y} \rangle_{\lambda} = \lambda \langle \boldsymbol{x}, \boldsymbol{y} \rangle_2$ for $\lambda > 0$ and the usual Euclidean inner product $\langle \cdot, \cdot \rangle_2$. The exponential inner product kernel defined by

$$K(\mathbf{x}, \mathbf{y}) = \sigma^2 \exp(\lambda \langle \mathbf{x}, \mathbf{y} \rangle_2)$$
 (2.4)

on $\Omega_{\boldsymbol{a},r} = \mathbb{R}^d$ is used for the examples in Secs. 3 and 4.

2.2 Gaussian Process Regression with Derivative Data

A Gaussian process $f_{\mathsf{GP}} \sim \mathrm{GP}(m,R)$ with mean function $m \colon \Omega_{\boldsymbol{a},r} \to \mathbb{R}$ and covariance kernel $R \colon \Omega_{\boldsymbol{a},r} \times \Omega_{\boldsymbol{a},r} \to \mathbb{R}$ is a stochastic process such that $\mathbb{E}[f_{\mathsf{GP}}(\boldsymbol{x})] = m(\boldsymbol{x})$ and $\mathrm{Cov}[f(\boldsymbol{x}),f(\boldsymbol{y})] = R(\boldsymbol{x},\boldsymbol{y})$ for all $\boldsymbol{x},\boldsymbol{y} \in \Omega_{\boldsymbol{a},r}$ (Rasmussen and Williams, 2006). Furthermore, for any distinct points $\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N \in \Omega_{\boldsymbol{a},r}$ the joint distribution of $(f_{\mathsf{GP}}(\boldsymbol{x}_1),\ldots,f_{\mathsf{GP}}(\boldsymbol{x}_N))$ is an N-dimensional Gaussian with mean vector $(m(\boldsymbol{x}_1),\ldots,m(\boldsymbol{x}_N)) \in \mathbb{R}^N$ and covariance matrix $\boldsymbol{R} = (R(\boldsymbol{x}_i,\boldsymbol{x}_j))_{i,j=1}^N \in \mathbb{R}^N$

Let $f \colon \Omega_{\boldsymbol{a},r} \to \mathbb{R}$ be an n times differentiable function on $\Omega_{\boldsymbol{a},r}$, meaning that the partial derivatives

$$D^{\alpha} f = \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha(1)} \cdots \partial x_d^{\alpha(d)}}$$

exist for all $\alpha \in \mathbb{N}_0^d$ such that $|\alpha| \le n$. Suppose also that the prior mean m is n times differentiable and that R is n times differentiable in both arguments. When conditioned on the *noiseless* derivative data

$$f_{\boldsymbol{a}} = (D^{\boldsymbol{\alpha}} f(\boldsymbol{a}))_{|\boldsymbol{\alpha}| \le n} = (D^{\boldsymbol{\alpha}_1} f(\boldsymbol{a}), \dots, D^{\boldsymbol{\alpha}_{N_n^d}} f(\boldsymbol{a})),$$

where we use an arbitrary ordering of the N_n^d -element set $\{\alpha \in \mathbb{N}_0^d : |\alpha| \leq n\}$, the posterior is a Gaussian process: $f_{\mathsf{GP}} \mid \boldsymbol{f_a} \sim \mathrm{GP}(s_{n,\boldsymbol{a}},P_{n,\boldsymbol{a}})$. Its mean and covariance have a closed form (e.g., (Särkkä, 2011) or (Oettershagen, 2017, Cor. 3.6)) given by

$$s_{n,\boldsymbol{a}}(\boldsymbol{x}) = m(\boldsymbol{x}) + \boldsymbol{r_a}(\boldsymbol{x})^\mathsf{T} \boldsymbol{R_a}^{-1} (\boldsymbol{f_a} - \boldsymbol{m_a}),$$
 (2.5a)

$$P_{n,\boldsymbol{a}}(\boldsymbol{x},\boldsymbol{y}) = R(\boldsymbol{x},\boldsymbol{y}) - \boldsymbol{r}_{\boldsymbol{a}}(\boldsymbol{x})^{\mathsf{T}} \boldsymbol{R}_{\boldsymbol{a}}^{-1} \boldsymbol{r}_{\boldsymbol{a}}(\boldsymbol{y}). \tag{2.5b}$$

Here $m{R_a} \in \mathbb{R}^{N_n^d imes N_n^d}$ and $m{r_a}(m{x}) \in \mathbb{R}^{N_n^d}$ are each given by

$$(\mathbf{R}_{\mathbf{a}})_{ij} = \mathbf{D}_{\mathbf{y}}^{\alpha_j} \mathbf{D}_{\mathbf{x}}^{\alpha_i} R(\mathbf{x}, \mathbf{y}) \Big|_{\substack{\mathbf{x} = \mathbf{a}, \\ \mathbf{y} = \mathbf{a}}}, \tag{2.6a}$$

$$(\mathbf{r}_{a}(\mathbf{x}))_{i} = D_{\mathbf{y}}^{\alpha_{i}} R(\mathbf{x}, \mathbf{y})|_{\mathbf{y} = \mathbf{a}},$$
 (2.6b)

where subscripts denote the differentiation variable, and $m_a = (D^{\alpha_1} m(a), \dots, D^{\alpha_{N_n}^d} m(a))$. If f has multidimensional range, in this paper we opt to model each component independently, though we note that this choice may be readily generalised using vector-valued Gaussian processes (Álvarez et al., 2012).

2.3 Replicating the Taylor Expansion Using Taylor Kernels

Our first theorem combines what was described in Secs. 2.1 and 2.2 to give our proposed probabilistic version of the Taylor expansion. The proof can be found in Supplement A.2.

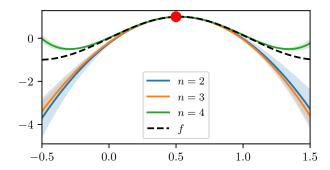


Figure 1: GP posterior means and 95% credible intervals for a prior with $m \equiv 0$ and $K(x,y) = \exp(xy)$ and data based on $f(x) = \sin(3x)$ at $a = \frac{1}{2}$.

Theorem 2.1. Let $f_{GP} \sim GP(m, K_a)$, where m is a polynomial of total degree at most n and K_a is a Taylor kernel defined as in (2.1). Let $\mathbf{f_a} = (D^{\alpha} f(\mathbf{a}))_{|\alpha| \leq n}$. Then the posterior distribution is $f_{GP} \mid \mathbf{f_a} \sim GP(s_{n,a}, P_{n,a})$, where

$$s_{n,\boldsymbol{a}}(\boldsymbol{x}) = \sum_{|\boldsymbol{\alpha}| \le n} \frac{D^{\boldsymbol{\alpha}} f(\boldsymbol{a})}{\boldsymbol{\alpha}!} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha}}, \tag{2.7a}$$

$$P_{n,\boldsymbol{a}}(\boldsymbol{x},\boldsymbol{y}) = \sigma^2 \sum_{|\boldsymbol{\alpha}| > n} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^2} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha}} (\boldsymbol{y} - \boldsymbol{a})^{\boldsymbol{\alpha}}.$$
 (2.7b)

Furthermore, $s_{n,\mathbf{a}}$ is identical to the multidimensional version of the Taylor polynomial in (1.1).

Note that the covariance is not identically zero—in fact, $P_{n,a}(x,x) \to \infty$ as $||x||_2 \to \infty$. Furthermore, while $P_{n,a}(x,y)$ takes the form of an infinite sum, provided K_a has a closed form it may be computed by subtracting the terms with $|\alpha| \le n$ in the summation form of K_a from that closed form. For intuition some posterior processes are displayed in Fig. 1.

The next theorem shows that the posterior variance has a similar interpretation to the Taylor remainder term if f is in $\mathcal{H}(K_a)$, the RKHS of K_a (see (Zwicknagl and Schaback, 2013) for characterisations of RKHSs of Taylor kernels). The proof is given in Supplement A.3.

Theorem 2.2. Let $f_{GP} \mid f_a$ be as in Theorem 2.1, and let the assumptions of that theorem hold. Further, assume that $f \in \mathcal{H}(K_a)$. Then $s_{n,a}$ and $P_{n,a}$ satisfy

$$|f(\boldsymbol{x}) - s_{n,\boldsymbol{a}}(\boldsymbol{x})| \le ||f||_{\mathcal{H}(K_{\boldsymbol{a}})} P_{n,\boldsymbol{a}}(\boldsymbol{x},\boldsymbol{x})^{1/2}$$

$$\le C_{n,r} \sigma^2 ||f||_{\mathcal{H}(K_{\boldsymbol{a}})} ||\boldsymbol{x} - \boldsymbol{a}||_2^{2(n+1)}$$

for all $\mathbf{x} \in \Omega_{\mathbf{a},r}$, where $(C_{n,r})_{n=0}^{\infty}$ is a positive sequence such that $C_{n,r} \to 0$ as $n \to \infty$.

2.4 Parameter Estimation

Observe from (2.7) that, although they do not affect the posterior mean, proper selection of the positive Taylor kernel parameters λ and σ is a prerequisite for useful and reliable uncertainty quantification

via the posterior covariance $P_{n,a}(\boldsymbol{x},\boldsymbol{x})$.² Though it may result in overconfidence in the asymptotic regime (Karvonen et al., 2020; Wang, 2020) (i.e. as $n \to \infty$), we opt to use maximum likelihood estimation to identify these parameters (Rasmussen and Williams, 2006, Sec. 5.4.1). In Supplement B we show that the maximum likelihood estimate (MLE), σ_{MI} , of σ is

$$\sigma_{\mathsf{ML}}^2 = \frac{1}{N_n^d} \sum_{|\boldsymbol{\alpha}| \le n} \frac{(D^{\boldsymbol{\alpha}}[f(\boldsymbol{a}) - m(\boldsymbol{a})])^2}{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}$$
(2.8)

for a fixed λ . As shown in Supplement B.1, the MLE of λ is available in closed form in many situations. However, this tends to cause numerical instabilities and we therefore fix λ and use (2.8) in the applications presented in Secs. 3 and 4.

2.5 Noisy Observations

Suppose now that each derivative observation is corrupted by independent Gaussian noise. That is, the data vector is $\mathbf{f}_{\mathbf{a}} = (y_{\mathbf{\alpha}})_{|\mathbf{\alpha}| \leq n}$, where $y_{\mathbf{\alpha}} = \mathrm{D}^{\mathbf{\alpha}} f(\mathbf{a}) + z_{\mathbf{\alpha}}$ with noise $z_{\mathbf{\alpha}} \sim \mathrm{N}(0, \varepsilon_{\mathbf{\alpha}}^2)$ for $\varepsilon_{\mathbf{\alpha}} > 0$. It is straightforward to compute (see Supplement A.4) that in a setting otherwise identical to that in Sec. 2.3 the posterior mean and covariance become

$$s_{n,\boldsymbol{a}}(\boldsymbol{x}) = m(\boldsymbol{x}) + \sigma^2 \sum_{|\boldsymbol{\alpha}| \le n} \frac{c_{\boldsymbol{\alpha}} \lambda^{\boldsymbol{\alpha}} [y_{\boldsymbol{\alpha}} - \mathbf{D}^{\boldsymbol{\alpha}} m(\boldsymbol{a})]}{\boldsymbol{\alpha}! (\sigma^2 c_{\boldsymbol{\alpha}} \lambda^{\boldsymbol{\alpha}} + \varepsilon_{\boldsymbol{\alpha}}^2)} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha}},$$

$$P_{n,\boldsymbol{a}}(\boldsymbol{x},\boldsymbol{y}) = \sum_{|\boldsymbol{\alpha}| \le n} \frac{\sigma^2 c_{\boldsymbol{\alpha}} \lambda^{\boldsymbol{\alpha}} \varepsilon_{\boldsymbol{\alpha}}^2}{(\boldsymbol{\alpha}!)^2 (\sigma^2 c_{\boldsymbol{\alpha}} \lambda^{\boldsymbol{\alpha}} + \varepsilon_{\boldsymbol{\alpha}}^2)} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha}} (\boldsymbol{y} - \boldsymbol{a})^{\boldsymbol{\alpha}}$$

$$+ \sigma^2 \sum_{|\boldsymbol{\alpha}| > n} \frac{c_{\boldsymbol{\alpha}} \lambda^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^2} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha}} (\boldsymbol{y} - \boldsymbol{a})^{\boldsymbol{\alpha}}.$$

Unfortunately, in this setting the MLE of σ no longer has a simple expression; see Supplement B.4 for details.

2.6 Generalisations

The results in Sec. 2.3 can be interpreted and generalised using RKHS theory (Berlinet and Thomas-Agnan, 2004). Let $R\colon X\times X\to \mathbb{R}$ be a positive-definite kernel on an arbitrary set X and suppose its RKHS $\mathcal{H}(R)$ is infinite-dimensional and separable. Let $(\phi_p)_{p=0}^\infty$ be any orthonormal basis of $\mathcal{H}(R)$. If $f\in\mathcal{H}(R)$ is to be reconstructed from data consisting of projections of f against these basis functions (i.e. $(\langle f,\phi_p\rangle_{\mathcal{H}(R)})_{p=0}^{N-1}$), then a derivation similar to that in Sec. 2.3 shows that the GP posterior mean and covariance are given by $s(x)=\sum_{p=0}^{N-1}\langle f,\phi_p\rangle_{\mathcal{H}(R)}\phi_p(x)$ and $P(x,y)=\sum_{p=N}^\infty\phi_p(x)\phi_p(y)$ for $x,y\in X$. This type of orthogonal information is known to be optimal in a certain sense (Novak and Woźniakowski, 2008, Sec. 4.2.3). See also (Wendland, 2005, Ch. 16) and (Oettershagen, 2017, Cor. 3.6) for general formulae when the data consists of applications to f of arbitrary linear functionals.

For a univariate Taylor kernel K_a the basis functions are $\phi_p(x) = \sigma \sqrt{c_p \lambda^p} (p!)^{-1} (x-a)^p$ and the RKHS inner product is $\langle f,g \rangle_{\mathcal{H}(K_a)} = \sigma^{-2} \sum_{p=0}^{\infty} \frac{1}{c_p \lambda^p} f^{(p)}(a) g^{(p)}(a)$ for any $f,g \in \mathcal{H}(K_a)$. By setting $g = \phi_p$ and observing that $\phi_p^{(p)}(a) = \sigma \sqrt{c_p \lambda^p}$ we find that the mean s defined above for

²In principle, every coefficient c_{α} in (2.1) could be considered a free parameter. However, as discussed in Supplement B.3, these parameters either cannot be selected using maximum likelihood or do not affect the posterior.

N=n+1 is $s_{n,a}$ in (2.7) for d=1. Even when an orthonormal basis of an RKHS is available, one cannot typically easily evaluate $\langle f, \phi_p \rangle_{\mathcal{H}(R)}$. However, if $(\phi_p)_{p=0}^{\infty}$ is a Fourier basis the Fourier coefficients may be accessible in some applications.

3 Application I: Non-Linear Filtering

We now outline an application of the above methodology to extended Kalman filters. We begin by recalling some basic notation. In filtering the goal is to perform Bayesian inference of an unknown state variable $\mathbf{x}_j \in \mathbb{R}^d$, $j = 0, \dots, n$, which is generally assumed to describe parameters or physical state of some underlying system that evolves over the indices j. The state evolves according to the dynamics

$$\boldsymbol{x}_{j+1} = \boldsymbol{\Phi}_j(\boldsymbol{x}_j) + \boldsymbol{\eta}_j \tag{3.1}$$

where the η_j are independent random variables on \mathbb{R}^d and $\Phi_j : \mathbb{R}^d \to \mathbb{R}^d$ a function. Inference on the parameters of the system is performed using data collected according to the observation model

$$\mathbf{y}_j = \mathbf{f}_j(\mathbf{x}_j) + \mathbf{\xi}_j \tag{3.2}$$

where $y_j \in \mathbb{R}^q$, $f_j : \mathbb{R}^d \to \mathbb{R}^q$, and the ξ_j are independent random variables on \mathbb{R}^q . To perform inference a prior is placed on the initial state x_0 which is iteratively evolved according to (3.1) and then conditioned on the information in (3.2) to obtain a belief over x_j for each j. However, unless strong assumptions are made on the prior belief and the form for Φ_j , η_j , f_j , and ξ_j this inference procedure is not tractable, in the sense that a closed-form does not exist for the belief at each j.

In the EKF the posterior belief over each \boldsymbol{x}_j is approximated with a Gaussian. Assume that the prior belief over the state at index j is Gaussian, $\boldsymbol{x}_j \sim \mathrm{N}(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$, and that $\boldsymbol{\eta}_j \sim \mathrm{N}(\mathbf{0}, \boldsymbol{\Lambda}_j)$ and $\boldsymbol{\xi}_j \sim \mathrm{N}(\mathbf{0}, \boldsymbol{\Gamma}_j)$. The dynamics $\boldsymbol{\Phi}_j$ and the observation function \boldsymbol{f}_{j+1} are each approximated using a first-order Taylor expansion (denoted $\hat{\boldsymbol{\Phi}}_j$ and $\hat{\boldsymbol{f}}_{j+1}$) centred at the current belief for the mean value of the state, $\boldsymbol{\mu}_j$, and its projection $\boldsymbol{\Phi}_j(\boldsymbol{\mu}_j)$. The result is that conjugacy properties of Gaussian distributions with linear transformations can be exploited, so that the conditional distribution $\boldsymbol{x}_{j+1} \mid \boldsymbol{y}_{j+1}$ is again Gaussian, $\boldsymbol{x}_{j+1} \mid \boldsymbol{y}_{j+1} \sim \mathrm{N}(\boldsymbol{\mu}_{j+1}, \boldsymbol{\Sigma}_{j+1})$, and the procedure can be iterated. The EKF is provided as an algorithm in Supplement D.1.

The EKF is often found to be robust to mild nonlinearities in f_j and Φ_j , but when these functions are highly nonlinear the state estimate it provides can deviate dramatically from the truth as more iterations are performed and errors accumulate. Various more complex filters have been suggested to attempt to correct this that maintain the Gaussian approximation but seek to approximate the distribution over x_j by computing the mean and covariance of the distribution using quadrature. A prototypical example of such a method is the unscented Kalman filter (UKF), in which an ensemble of particles is used to approximate the next conditional distribution without resorting to an approximation of Φ_j or f_j ; for details see (Särkkä, 2013, Sec. 5.6). The quadrature rule employed in the UKF captures the posterior mean and covariance to third order (Wan and van der Merwe, 2000), but when the target distribution is not approximately Gaussian it may nevertheless fail to provide an accurate state estimate, as will be seen in our results.

3.1 Taylor EKF

For simplicity we assume that Φ_j is linear in \boldsymbol{x} and focus on approximation of \boldsymbol{f}_j . We further assume that $\Gamma_j = \operatorname{diag}(\gamma_{j,1},\ldots,\gamma_{j,q})$, though this may easily be generalised. The EKF is likely to perform poorly when $\Phi_j(\boldsymbol{\mu}_j)$ is far from the data generating parameter $\boldsymbol{x}_{j+1}^{\dagger}$ at iteration j. This could perhaps

be because of an outlier in the instance of the noise ξ_j , or simply because f_{j+1} is highly nonlinear. In this case, since \hat{f}_{j+1} is only a good approximation to f_{j+1} near to $\Phi_j(\mu_j)$, an unrealistic amount of bias and/or variance can be introduced.

Assume that $\boldsymbol{x}_{j-1} \sim \mathrm{N}(\boldsymbol{\mu}_{j-1}^{\mathsf{PN}}, \boldsymbol{\Sigma}_{j-1}^{\mathsf{PN}})$. The full posterior distribution over $\hat{\boldsymbol{f}}_j$ produced by the methods introduced in Sec. 2 can be incorporated into the likelihood in such a way that the strength of the likelihood diminishes far from $\boldsymbol{\Phi}_{j-1}(\boldsymbol{\mu}_{j-1}^{\mathsf{PN}})$. As mentioned in Sec. 2.2, we model the components of \boldsymbol{f}_j independently; thus, let $\boldsymbol{f}_j = (f_{j,1}, \dots, f_{j,q})$ where $f_{j,\ell} : \mathbb{R}^d \to \mathbb{R}$. Consider the likelihood at iteration j, which owing to the assumptions made factorises as

$$p(\boldsymbol{y}_j \mid \boldsymbol{x}, \boldsymbol{f}_j) = \mathrm{N}(\boldsymbol{y}_j; \boldsymbol{f}_j(\boldsymbol{x}), \Gamma_j) = \prod_{\ell=1}^q p_\ell(y_{j,\ell} \mid \boldsymbol{x}, f_{j,\ell})$$

where $p_{\ell}(y_{j,\ell} \mid \boldsymbol{x}, f_{j,\ell}) = \mathrm{N}(y_{j,\ell}; f_{j,\ell}(\boldsymbol{x}), \gamma_{j,\ell})$. Note that we have made explicit the dependence of this likelihood on $f_{j,\ell}$. The standard EKF uses the likelihood $p(\boldsymbol{y}_j \mid \boldsymbol{x}, \hat{\boldsymbol{f}}_j)$. We instead substitute the probabilistic version of the Taylor expansion from Sec. 2.1 and marginalise out the uncertainty over each $f_{j,\ell}$, that is

$$p_{\ell}^{\mathsf{PN}}(y_{j,\ell} \mid \boldsymbol{x}) = \int N(y_{j,\ell}; \tilde{f}(\boldsymbol{x}), \gamma_{j,\ell}) dN(\tilde{f}; \hat{f}_{j,\ell}, k_{\ell})$$
$$= N(y_{j,\ell}; \hat{f}_{j,\ell}(\boldsymbol{x}), \gamma_{j,\ell} + k_{\ell}(\boldsymbol{x}))$$
(3.3)

where we let $k_{\ell}(\boldsymbol{x}) = P_{1,\Phi_{j-1}(\boldsymbol{\mu}_{j-1}^{PN})}(\boldsymbol{x},\boldsymbol{x})$. Note that because the parameters of the prior are estimated using maximum likelihood as described in Sec. 2.4, the posterior covariance k_{ℓ} for each component may differ. Thus, the uncertainty is widened by an amount that depends on how accurate the Taylor series is at the point \boldsymbol{x} , according to the posterior covariance. Since $k_{\ell}(\boldsymbol{x})$ diverges as \boldsymbol{x} moves away from $\Phi_{j-1}(\boldsymbol{\mu}_{j-1}^{PN})$, using this likelihood has the effect of reverting to an uninformative likelihood far from this point.

The consequence of using the likelihood in (3.3) is that conjugate inference is no longer possible, owing to the dependence of the likelihood variance on x. This means that the posterior density

$$p^{\mathsf{PN}}(\boldsymbol{x} \mid \boldsymbol{y}_j) \propto p(\boldsymbol{x}) \prod_{\ell=1}^q p_{\ell}^{\mathsf{PN}}(y_{j,\ell} \mid \boldsymbol{x}),$$
 (3.4)

where p(x) is the Gaussian density of $x_j \mid x_{j-1}$, is not Gaussian. Here we opt to approximate it with a Gaussian using a Laplace approximation. This entails first finding a MAP point

$$\boldsymbol{\mu}_{j}^{\mathsf{PN}} = \operatorname*{arg\,max}_{\boldsymbol{x} \in \mathbb{R}^{d}} p^{\mathsf{PN}}(\boldsymbol{x} \mid \boldsymbol{y}_{j}). \tag{3.5}$$

The posterior precision matrix is then approximated by the Hessian of the negative log likelihood at μ_i^{PN} , that is,

$$(\boldsymbol{\Sigma}_j^{\mathsf{PN}})^{-1} = -\frac{\mathrm{d}^2}{\mathrm{d}\boldsymbol{x}^2} \log p^{\mathsf{PN}}(\boldsymbol{x} \mid \boldsymbol{y}_j) \Big|_{\boldsymbol{x} = \boldsymbol{\mu}_j^{\mathsf{PN}}},$$

To our knowledge (3.5) cannot be solved in closed-form, and so a numerical solution must be obtained. However as the gradients and Hessian of (3.4) with respect to \boldsymbol{x} may readily be obtained using automatic differentiation techniques, the resulting optimisation problem is relatively straightforward. A full algorithmic description is given in Supplement D.2.

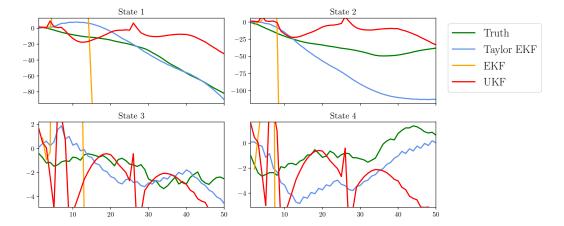


Figure 2: Results for application of the probabilistic Taylor expansion to the EKF, for the problem described in Sec. 3. Plotted are the true value of the state compared with the mean of both the standard EKF and the modification that exploits our probabilistic Taylor expansion (Taylor EKF). The unscented Kalman filter (UKF) is also displayed for comparison. The Taylor EKF is far more robust to aberrant behaviour displayed by the standard EKF.

3.2 Example: Tracking Problem

We now consider an example from (Särkkä, 2013, p93), a problem arising from passive sensor tracking. Here d=4, with $\boldsymbol{x}_j=(x_{1,j},x_{2,j},x_{3,j},x_{4,j})$ where $x_{1,j},x_{2,j}$ represent the location of the tracked object in \mathbb{R}^2 at time t_j , while $x_{3,j},x_{4,j}$ represent its velocity. Let $\delta t=t_{j+1}-t_j$. The evolution function $\Phi_j\equiv\Phi$ and variance $\Lambda_j\equiv\Lambda$ are each given by a discretised Wiener velocity model, that is,

$$oldsymbol{\Phi}(oldsymbol{x}) = egin{bmatrix} oldsymbol{I}_2 & \delta t oldsymbol{I}_2 \ oldsymbol{0}_2 & oldsymbol{I}_2, \end{bmatrix} oldsymbol{x}$$

where I_2 and $\mathbf{0}_2$ are 2×2 identity and zero matrices, and

$$\mathbf{\Lambda} = \begin{bmatrix} q_1^c(\delta t)^3/3 & 0 & q_1^c(\delta t)^2/2 & 0\\ 0 & q_2^c(\delta t)^3/3 & 0 & q_2^c(\delta t)^2/2\\ q_1^c(\delta t)^2/2 & 0 & q_1^c\delta t & 0\\ 0 & q_2^c(\delta t)^2/2 & 0 & q_2^c\delta t \end{bmatrix}.$$

We take $q_1^c=q_2^c=0.1$. The observation function ${m f}_j\equiv {m f}$ and variance ${m \Gamma}_j\equiv {m \Gamma}$ are

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} \tan^{-1} \left(\frac{x_{2,j} - s_{2,1}}{x_{1,j} - s_{1,1}} \right) \\ \tan^{-1} \left(\frac{x_{2,j} - s_{2,2}}{x_{1,j} - s_{1,2}} \right) \end{bmatrix} \quad \text{and} \quad \mathbf{\Gamma} = 0.05^{2} \mathbf{I}_{2}$$
(3.6)

where $s_1 = (s_{1,1}, s_{2,1})$ and $s_2 = (s_{1,2}, s_{2,2})$ are the location of the first and second tracking sensors in \mathbb{R}^2 , respectively. We take $s_1 = (0, 5)$ and $s_2 = (0, -5)$. Thus, while Φ is linear, f is nonlinear.

Observations were generated by simulating from the above dynamics starting from $\mathbf{x}_0 = (0,0,0.1,0.1)$ and proceeding for n=50 steps of length $\delta t=1$. Both the classic and Taylor versions of the EKF, as well as the UKF, were then applied to the problem. The UKF is included to

illustrate the performance of the Taylor EKF when compared to a more robust filter. The exponential prior (2.4) with $\lambda=1$ was used, with the MLE σ_{ML} in (2.8) used for the amplitude. For the Taylor EKF implementation the MAP point was found using the BFGS algorithm (Nocedal and Wright, 1999, Sec. 6.1) as provided in <code>scipy.optimize.minimize</code> (Virtanen et al., 2020), while gradients and Hessians were evaluated using automatic differentiation using the <code>jax</code> package (Bradbury et al., 2018).

Results are displayed in Fig. 2. The standard EKF shows a rapid divergence from the truth. The behaviour of the UKF is improved but divergence can still be seen in $x_{4,j}$. The Taylor EKF estimates the state far more accurately in general, apart from in $x_{2,j}$ where the UKF is more accurate. Note however that there is still some disagreement with the truth in the Taylor EKF. Fundamentally this version of the EKF still exploits a linearisation, it is simply adjusted to be more sceptical of observations that would indicate likely values of \boldsymbol{x} that lie far from the current mean.

4 Application II: Euler's Method

Let $y: [0,T] \to \mathbb{R}^d$ be the solution to the ODE

$$\boldsymbol{y}'(t) = \boldsymbol{f}(t, \boldsymbol{y}(t)), \tag{4.1}$$

on a non-empty interval [0,T] with the initial condition $\mathbf{y}(0) = \mathbf{y}_0$. Let $N \in \mathbb{N}$ and h = T/N. The classical Euler method computes approximations $\mathbf{y}_n \approx \mathbf{y}(t_n)$ at points $t_n = nh$ via the recursion

$$\boldsymbol{y}_{n+1} = \boldsymbol{y}_n + h\boldsymbol{f}(t_n, \boldsymbol{y}_n) \tag{4.2}$$

for $n=0,\ldots,N-1$. Each step (4.2) simply consists of assuming that $\boldsymbol{y}(t_n)=\boldsymbol{y}_n$ and evaluating the first-order Taylor expansions of the components of \boldsymbol{y} around t_n at t_{n+1} . We now use a first-order Taylor kernel to develop a probabilistic Euler method which is capable of uncertainty quantification for the unknown solution. A number of Gaussian process based (Schober et al., 2014, 2019; Teymur et al., 2016; Tronarp et al., 2019; Wang et al., 2020) and other probabilistic (Conrad et al., 2016) differential equation solvers have been proposed previously.

4.1 Probabilistic Euler's Method

Let d=1. Suppose that $y(t_n)$ has been approximated with a Gaussian approximation $\mathrm{N}(y_n,\varepsilon_n^2)$. Using (4.1) and a linearisation of f(t,y) with respect to y, we can approximate $y'(t_n)$ with $\mathrm{N}(f(t_k,y_k),f_y'(t_k,y_k)^2\varepsilon_k^2)$, where $f_y'=\frac{\partial}{\partial y}f(t,y)$. By modelling y as a GP with a Taylor covariance kernel K_{t_n} and $m\equiv 0$, interpreting y_n and $f(t_k,y_k)$ as observations of $y(t_n)$ and $y'(t_n)$ corrupted by Gaussian noise $\mathrm{N}(0,\varepsilon_n^2)$ and $\mathrm{N}(0,f_y'(t_k,y_k)^2\varepsilon_n^2)$, respectively, and thereafter using results in Sec. 2.5 we obtain a Gaussian approximation $\mathrm{N}(y_{n+1},\varepsilon_{n+1}^2)$ to $y(t_{n+1})$, where

$$y_{n+1} = a_n y_n + b_n h f(t_n, y_n), (4.3a)$$

$$\varepsilon_{n+1}^2 = \sigma^2 \left[c_0 (1 - a_n) + c_1 \lambda (1 - b_n) h^2 + r_h \right]$$
 (4.3b)

 $^{^3}$ If $y(t_n)$ is Gaussian, $y'(t_n)$ is Gaussian if and only if f(t,y) is affine in y. In the non-affine case any other Gaussian approximation to $y'(t_n)$ could be used instead of linearisation. For example, one could use numerical integration to compute approximations to the first two moments of $y'(t_n)$ and construct a moment-matched Gaussian approximation. This would be analogous to the Gaussian filtering method in Sec. 2.3 of Tronarp et al. (2019) (Sec. 2.4 contains a first-order approximation that is similar to the one we use).

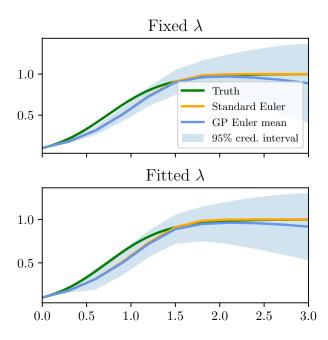


Figure 3: Approximations to the solution of the logistic equation (4.5) using the classical Euler method and our probabilistic version with N=10 steps. In the upper panel a fixed value $\lambda=1$ was used while in the lower one λ was fitted with maximum likelihood based on all available y_n .

and
$$r_h = \sum_{p=2}^{\infty} \frac{c_p \lambda^p}{(p!)^2} h^{2p}$$
,
$$a_n = \frac{\sigma^2 c_0}{\sigma^2 c_0 + \varepsilon_n^2}, \quad b_n = \frac{\sigma^2 c_1 \lambda}{\sigma^2 c_1 \lambda + f_n'(t_n, y_n)^2 \varepsilon_n^2}. \tag{4.4}$$

The recursion in (4.3) defines a *probabilistic Euler method* in which y_n functions as a point estimate of $y(t_n)$ and the variance ε_n^2 provides uncertainty quantification for the unknown solution. If $y_0 = y(0)$, the method is initialised with $\varepsilon_0 = 0$. Observe from (4.4) that as $\varepsilon_n \to 0$, the *n*th mean update step (4.3a) tends to the classical Euler step in (4.2).

We set the parameter σ^2 independently on each time-step using maximum likelihood. As described in Supplement C.1, the MLE at the nth step, σ_n^2 , is a positive solution to a cubic equation and thus easy to solve. If $\varepsilon_n=0$ the solution is $\sigma_{n,0}^2:=\frac{1}{2}[y_n^2/c_0+f(t_n,y_n)^2/(c_1\lambda)]$, and because polynomial roots are continuous functions of the coefficients, we have $\sigma_n^2\to\sigma_{n,0}^2$ as $\varepsilon_n\to0$. Because it may happen that all these roots are non-positive, we select $\sigma_{\min}>0$ and set $\sigma_n=\sigma_{\min}$ if the roots are non-positive. The probabilistic Euler method thus consists of the iteration (4.3) with $\sigma^2=\sigma_n^2$. In Supplement C.2 we prove the following convergence result which is largely analogous to that for the standard Euler method (e.g., Atkinson, 1989, Thm. 6.3)

Theorem 4.1. Consider the probabilistic Euler method described above with $y_0 = y(0)$ and $\varepsilon_0 = 0$. If standard assumptions are satisfied (see Assumption C.1) and h is sufficiently small, then there are constants $C_1, C_2 \ge 0$ such that $|y(t_n) - y_n| \le C_1 h$ and $\varepsilon_n \le C_2 h^2$ for all $n = 0, \ldots, N$.

To solve a multivariate ODE we apply the procedure described above to each of the d coordinate functions $f_i(t, \mathbf{y}(t))$ independently at each step. That is, $y_{n+1,i}$, the ith element of \mathbf{y}_{n+1} , is obtained

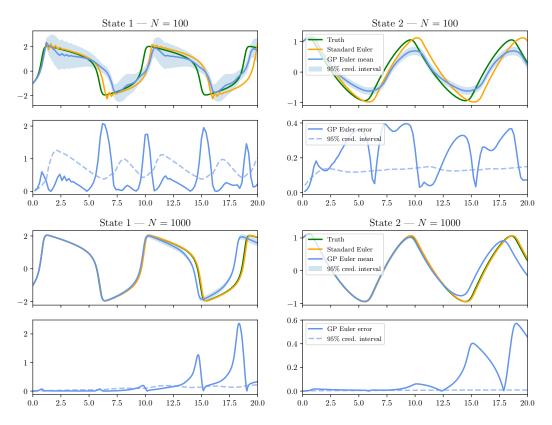


Figure 4: Approximations to the solution of the FitzHugh–Nagumo model (4.6) using the classical Euler method and our probabilistic version with N=100 and N=1000 steps.

from the one-dimensional recursion via the substitutions $y_n = y_{n,i}$, $\varepsilon_n = \varepsilon_{n,i}$, $f(t_n,y_n) = \boldsymbol{f}(t_n,\boldsymbol{y}_n)$, and $f'_y(t_n,y_n) = \frac{\partial}{\partial y_i} f_i(t,\boldsymbol{y}_n)$. See Supplement D.4 for the full algorithm.

4.2 Example: The Logistic Equation

Our first example is the logistic equation

$$y'(t) = ry(t)(1 - y(t)) \tag{4.5}$$

on [0,3] and with y(0)=0.1 and r=3. We use the exponential kernel in (2.4) with $\lambda=1$. The results are displayed in Fig. 3 with N=10 equispaced points. The probabilistic method works well and produces reasonable uncertainty quantification in that the true solution is (almost) contained within 95% credible intervals.

To illustrate potential extensions, we also display results for a version which, on the nth step, selects λ by maximum likelihood based on the noisy data (y_0, y_1, \ldots, y_n) (see, e.g., (Rasmussen and Williams, 2006, Sec. 5.4.1) for details). This results in slightly inflated uncertainty for the first few steps. For a larger number of data points this approach would likely be computationally too expensive as each evaluation of the objective function for λ requires matrix inversion and determinant computation.

4.3 Example: The FitzHugh-Nagumo Model

Our second example is the FitzHugh-Nagumo model

$$\begin{bmatrix} y_1'(t) \\ y_2'(t) \end{bmatrix} = \begin{bmatrix} c(y_1(t) - y_1(t)^3/3 + y_2(t)) \\ -(y_1(t) - a + by_2(t))/c \end{bmatrix}$$
(4.6)

on [0,20] and with $\mathbf{y}(0)=(-1,1)$ and $(a,b,c)=(\frac{1}{5},\frac{1}{5},3)$. Results are displayed in Fig. 4 for the exponential kernel in (2.4) with $\lambda=1$ and N=100 and N=1000 equispaced points. Uncertainty quantification provided by the probabilistic Euler method is reasonable for the first state component, except at points where $y_1'(t)$ is large (i.e. when t is approximately 6, 10, 15, and 19). For the second state component the probabilistic Euler method is generally overconfident, which may be caused by our independent modelling of each state component.

5 Conclusion

In this paper we have proposed a GP model based on Taylor kernels which gives rise to a probabilistic version of the classical Taylor expansion when the data consists of exact derivative evaluations up to a given order. These models have been demonstrated in non-linear filtering and ODE applications. In both cases the developed methods could be extended to various directions, often at an additional computational cost (e.g., the method to choose λ in Sec. 4.2). An interesting and potentially computationally tractable approach would be to develop a probabilistic step-size selection method for the probabilistic Euler method.

There are many other problems besides those considered here that Taylor kernel based GP regression could be applied to. Trust-region methods for optimisation (Conn et al., 2000; Schulman et al., 2015) and Bayesian optimisation (Snoek et al., 2012) are two interesting candidates. Trust-region methods typically consist of a sequence of local quadratic approximations, each of which is assumed to be valid within a small trust-region around the current minimiser; a form of this trust-region could be derived using probabilistic reasoning. Bayesian optimisation methods based on standard stationary kernels have a tendency to be over-exploitative (Bull, 2011). Because their uncertainty explodes away from the expansion point, Taylor kernels might prove a useful non-exploitative alternative in Bayesian optimisation.

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A Basic Derivations and Proofs for Sec. 2

This section contains some derivations and proofs for results in Sec. 2

A.1 Inner Product Kernels

Using the multinomial theorem an inner product kernel in (2.3) can be expanded as

$$K(\boldsymbol{x},\boldsymbol{y}) = \sigma^2 \sum_{p=0}^{\infty} \frac{c_p}{(p!)^2} \langle \boldsymbol{x}, \boldsymbol{y} \rangle_{\boldsymbol{\lambda}}^p = \sigma^2 \sum_{p=0}^{\infty} \frac{c_p}{(p!)^2} \left(\sum_{i=1}^d \lambda_i x_i y_i \right)^p = \sigma^2 \sum_{p=0}^{\infty} \frac{c_p}{(p!)^2} \sum_{|\boldsymbol{\alpha}|=p} \frac{p!}{\boldsymbol{\alpha}!} \boldsymbol{\lambda}^{\boldsymbol{\alpha}} \boldsymbol{x}^{\boldsymbol{\alpha}} \boldsymbol{y}^{\boldsymbol{\alpha}}$$
$$= \sigma^2 \sum_{\boldsymbol{\alpha} \in \mathbb{N}_d^d} \frac{c_{|\boldsymbol{\alpha}|}}{\boldsymbol{\alpha}! |\boldsymbol{\alpha}|!} \boldsymbol{\lambda}^{\boldsymbol{\alpha}} \boldsymbol{x}^{\boldsymbol{\alpha}} \boldsymbol{y}^{\boldsymbol{\alpha}}.$$

That is, an inner product kernel is of the form (2.1) with

$$c_{\alpha} = c_{|\alpha|} \frac{\alpha!}{|\alpha|!}. \tag{A.1}$$

A.2 Proof of Theorem 2.1

Proof of Theorem 2.1. It is straightforward to compute that, for any $\beta, \gamma \in \mathbb{N}_0^d$,

$$D_{\boldsymbol{y}}^{\boldsymbol{\beta}} D_{\boldsymbol{x}}^{\boldsymbol{\gamma}} K_{\boldsymbol{a}}(\boldsymbol{x}, \boldsymbol{y}) = \sigma^{2} \sum_{\boldsymbol{\alpha} \geq \boldsymbol{\beta} \wedge \boldsymbol{\gamma}} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha} - \boldsymbol{\beta}} (\boldsymbol{y} - \boldsymbol{a})^{\boldsymbol{\alpha} - \boldsymbol{\gamma}}}{(\boldsymbol{\alpha} - \boldsymbol{\beta})! (\boldsymbol{\alpha} - \boldsymbol{\gamma})!}, \tag{A.2}$$

where $\beta \wedge \gamma = (\max\{\beta(1), \gamma(1)\}, \dots, \max\{\beta(d), \gamma(d)\})$. If x = a or y = a, all terms with $\alpha - \beta \neq 0$ or $\alpha - \gamma \neq 0$, respectively, in (A.2) vanish. Therefore in the context of (2.6) we have

$$(\mathbf{R}_{\mathbf{a}})_{ij} = \sigma^2 c_{\alpha_i} \lambda^{\alpha_i} \delta_{ij}$$
 and $(\mathbf{r}_{\mathbf{a}}(\mathbf{x}))_i = \sigma^2 \frac{c_{\alpha_i} \lambda^{\alpha_i}}{\alpha_i!} (\mathbf{x} - \mathbf{a})^{\alpha_i}$.

The matrix R_a is thus diagonal and the *i*th element of the row vector $r_a(x)^T R_a^{-1}$ in (2.5) is $(\alpha_i!)^{-1}(x-a)^{\alpha_i}$. It follows that the posterior mean and covariance are

$$s_{n,\boldsymbol{a}}(\boldsymbol{x}) = m(\boldsymbol{x}) + \sum_{|\boldsymbol{\alpha}| \le n} \frac{\mathrm{D}^{\boldsymbol{\alpha}}[f(\boldsymbol{a}) - m(\boldsymbol{a})]}{\boldsymbol{\alpha}!} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha}},$$
$$P_{n,\boldsymbol{a}}(\boldsymbol{x},\boldsymbol{y}) = K_{\boldsymbol{a}}(\boldsymbol{x},\boldsymbol{y}) - \sigma^2 \sum_{|\boldsymbol{\alpha}| \le n} \frac{c_{\boldsymbol{\alpha}} \lambda^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^2} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha}} (\boldsymbol{y} - \boldsymbol{a})^{\boldsymbol{\alpha}}.$$

Because m is a polynomial of degree at most n, it holds that $m(\mathbf{x}) = \sum_{|\mathbf{\alpha}| \leq n} (\mathbf{\alpha}!)^{-1} \mathrm{D}^{\mathbf{\alpha}} m(\mathbf{a}) (\mathbf{x} - \mathbf{a})^{\mathbf{\alpha}}$. From (2.1) we recognise the covariance $P_{n,\mathbf{a}}$ as the remainder in the kernel expansion. This yields the required given final expressions given in (2.7), that is

$$s_{n,\boldsymbol{a}}(\boldsymbol{x}) = \sum_{|\boldsymbol{\alpha}| \leq n} \frac{D^{\boldsymbol{\alpha}} f(\boldsymbol{a})}{\boldsymbol{\alpha}!} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha}} \quad \text{and} \quad P_{n,\boldsymbol{a}}(\boldsymbol{x},\boldsymbol{y}) = \sigma^2 \sum_{|\boldsymbol{\alpha}| > n} \frac{c_{\boldsymbol{\alpha}} \lambda^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^2} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha}} (\boldsymbol{y} - \boldsymbol{a})^{\boldsymbol{\alpha}}.$$

By inspection it is clear that $s_{n,a}$ is identical to the Taylor expansion given in (1.1) (and its multivariate version), which completes the proof.

A.3 Proof of Theorem 2.2

Proof of Theorem 2.2. By the standard equivalence between Gaussian process regression in the noiseless setting and worst-case optimal approximation (e.g., Kanagawa et al., 2018; Scheuerer et al., 2013) the posterior mean $s_{n,a} \in \mathcal{H}(K_a)$ is the minimum-norm approximant of f such that

$$D^{\alpha} s_{n,\boldsymbol{a}}(\boldsymbol{a}) = D^{\alpha} f(\boldsymbol{a})$$
 for every $|\boldsymbol{\alpha}| \leq n$

and the posterior standard deviation at \boldsymbol{x} , $P_{n,\boldsymbol{a}}(\boldsymbol{x},\boldsymbol{x})^{1/2}$, equals the worst-case approximation error at \boldsymbol{x} in the RKHS. Consequently,

$$|f(\mathbf{x}) - s_{n,\mathbf{a}}(\mathbf{x})| \le ||f - s_{\mathbf{a}}||_{\mathcal{H}(K_{\mathbf{a}})} P_{n,\mathbf{a}}(\mathbf{x},\mathbf{x})^{1/2} \le ||f||_{\mathcal{H}(K_{\mathbf{a}})} P_{n,\mathbf{a}}(\mathbf{x},\mathbf{x})^{1/2}$$

for all $\boldsymbol{x} \in \Omega_{\boldsymbol{a},r}$ if $f \in \mathcal{H}(K_{\boldsymbol{a}})$ (Wendland, 2005, Thm. 16.3). To prove the upper bound for the posterior variance observe that from the general inequality $|\boldsymbol{x}^{\boldsymbol{\alpha}}| \leq \|\boldsymbol{x}\|_{\infty}^{|\boldsymbol{\alpha}|} \leq \|\boldsymbol{x}\|_{2}^{|\boldsymbol{\alpha}|}$ for $\boldsymbol{x} \in \mathbb{R}^{d}$ and $\boldsymbol{\alpha} \in \mathbb{N}_{0}^{d}$ it follows that, for any $\boldsymbol{x} \in \Omega_{\boldsymbol{a},r} = \{\boldsymbol{x} \in \mathbb{R}^{d} : \|\boldsymbol{x} - \boldsymbol{a}\|_{2} < r\}$,

$$P_{n,\boldsymbol{a}}(\boldsymbol{x},\boldsymbol{x}) = \sigma^{2} \sum_{|\boldsymbol{\alpha}| > n} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^{2}} (\boldsymbol{x} - \boldsymbol{a})^{2\boldsymbol{\alpha}}$$

$$= \sigma^{2} \left(\sum_{|\boldsymbol{\alpha}| = n+1} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^{2}} (\boldsymbol{x} - \boldsymbol{a})^{2\boldsymbol{\alpha}} + \sum_{|\boldsymbol{\alpha}| > n+1} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^{2}} (\boldsymbol{x} - \boldsymbol{a})^{2\boldsymbol{\alpha}} \right)$$

$$\leq \sigma^{2} \left(\sum_{|\boldsymbol{\alpha}| = n+1} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^{2}} \|\boldsymbol{x} - \boldsymbol{a}\|_{2}^{2(n+1)} + \sum_{|\boldsymbol{\alpha}| > n+1} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^{2}} \|\boldsymbol{x} - \boldsymbol{a}\|_{2}^{2|\boldsymbol{\alpha}|} \right)$$

$$= \sigma^{2} \|\boldsymbol{x} - \boldsymbol{a}\|_{2}^{2(n+1)} \left(\sum_{|\boldsymbol{\alpha}| = n+1} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^{2}} + \sum_{|\boldsymbol{\alpha}| > n+1} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^{2}} \|\boldsymbol{x} - \boldsymbol{a}\|_{2}^{2|\boldsymbol{\alpha}| - 2(n+1)} \right)$$

$$\leq \sigma^{2} \|\boldsymbol{x} - \boldsymbol{a}\|_{2}^{2(n+1)} \underbrace{\left(\sum_{|\boldsymbol{\alpha}| = n+1} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^{2}} + r^{-2(n+1)} \sum_{|\boldsymbol{\alpha}| > n+1} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^{2}} r^{2|\boldsymbol{\alpha}|} \right)}_{|\boldsymbol{\alpha}| > n+1} .$$

The summability assumption (2.2) ensures that $C_{n,r}$ is finite and that $C_{n,r} \to 0$ as $n \to \infty$.

A.4 Noisy Observations

Suppose that the data vector $\mathbf{f}_a = (y_{\alpha})_{|\alpha| < n}$ consists of noisy derivative observations at $\mathbf{a} \in \Omega$:

$$y_{\alpha} = D^{\alpha} f(\alpha) + z_{\alpha}$$
 where $z_{\alpha} \sim N(0, \varepsilon_{\alpha}^{2})$ and $\varepsilon_{\alpha} > 0$.

In this setting the GP posterior mean and covariance for a general sufficiently differentiable prior mean m and covariance kernel R are

$$s_{n,\boldsymbol{a}}(\boldsymbol{x}) = m(\boldsymbol{x}) + \boldsymbol{r_a}(\boldsymbol{x})^{\mathsf{T}} (\boldsymbol{R_a} + \boldsymbol{E})^{-1} (\boldsymbol{f_a} - \boldsymbol{m_a}), \tag{A.3a}$$

$$P_{n,\boldsymbol{a}}(\boldsymbol{x},\boldsymbol{y}) = R(\boldsymbol{x},\boldsymbol{y}) - \boldsymbol{r_a}(\boldsymbol{x})^{\mathsf{T}}(\boldsymbol{R_a} + \boldsymbol{E})^{-1}\boldsymbol{r_a}(\boldsymbol{y}), \tag{A.3b}$$

where $E = \operatorname{diag}(\varepsilon_{\boldsymbol{\alpha}_1}^2, \dots, \varepsilon_{\boldsymbol{\alpha}_{N_n^d}}^2)$ and $\boldsymbol{r_a}(\boldsymbol{x})$, $\boldsymbol{R_a}$, and $\boldsymbol{m_a}$ are defined in Sec. 2.2. Recall then from Sec. 2.3 that for R a Taylor kernel K_a we have

$$(\pmb{R_a})_{ij} = \sigma^2 c_{\pmb{lpha}_i} \pmb{\lambda}^{\pmb{lpha}_i} \delta_{ij} \quad ext{ and } \quad (\pmb{r_a}(\pmb{x}))_i = \sigma^2 rac{c_{\pmb{lpha}_i} \pmb{\lambda}^{\pmb{lpha}_i}}{\pmb{lpha}_i!} (\pmb{x} - \pmb{a})^{\pmb{lpha}_i}.$$

Therefore

$$(\mathbf{R}_{\boldsymbol{a}} + \mathbf{E})^{-1} = \frac{1}{\sigma^2 c_{\boldsymbol{\alpha}_i} \lambda^{\boldsymbol{\alpha}_i} + \varepsilon_{\boldsymbol{\alpha}_i}^2} \delta_{ij},$$

and plugging this into (A.3) yields

$$s_{n,\boldsymbol{a}}(\boldsymbol{x}) = m(\boldsymbol{x}) + \sigma^2 \sum_{|\boldsymbol{\alpha}| \leq n} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}} [y_{\boldsymbol{\alpha}} - D^{\boldsymbol{\alpha}} m(\boldsymbol{a})]}{\boldsymbol{\alpha}! (\sigma^2 c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}} + \varepsilon_{\boldsymbol{\alpha}}^2)} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha}},$$

and

$$P_{n,\boldsymbol{a}}(\boldsymbol{x},\boldsymbol{y}) = K_{\boldsymbol{a}}(\boldsymbol{x},\boldsymbol{y}) - \sigma^{2} \sum_{|\boldsymbol{\alpha}| \leq n} \frac{\sigma^{2} c_{\boldsymbol{\alpha}}^{2} \boldsymbol{\lambda}^{2\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^{2} (\sigma^{2} c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}} + \varepsilon_{\boldsymbol{\alpha}}^{2})} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha}} (\boldsymbol{y} - \boldsymbol{a})^{\boldsymbol{\alpha}}$$

$$= \sigma^{2} \left[\sum_{\boldsymbol{\alpha} \in \mathbb{N}_{0}^{d}} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^{2}} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha}} (\boldsymbol{y} - \boldsymbol{a})^{\boldsymbol{\alpha}} - \sum_{|\boldsymbol{\alpha}| \leq n} \frac{\sigma^{2} c_{\boldsymbol{\alpha}}^{2} \boldsymbol{\lambda}^{2\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^{2} (\sigma^{2} c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}} + \varepsilon_{\boldsymbol{\alpha}}^{2})} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha}} (\boldsymbol{y} - \boldsymbol{a})^{\boldsymbol{\alpha}} \right]$$

$$= \sigma^{2} \left[\sum_{|\boldsymbol{\alpha}| \leq n} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}} \varepsilon_{\boldsymbol{\alpha}}^{2}}{(\boldsymbol{\alpha}!)^{2} (\sigma^{2} c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}} + \varepsilon_{\boldsymbol{\alpha}}^{2})} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha}} (\boldsymbol{y} - \boldsymbol{a})^{\boldsymbol{\alpha}} + \sum_{|\boldsymbol{\alpha}| > n} \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\boldsymbol{\alpha}!)^{2}} (\boldsymbol{x} - \boldsymbol{a})^{\boldsymbol{\alpha}} (\boldsymbol{y} - \boldsymbol{a})^{\boldsymbol{\alpha}} \right].$$

Note that by setting $\varepsilon_{\alpha} = 0$ for every $\alpha \in \mathbb{N}_0^d$ such that $|\alpha| \le n$ we recover the noiseless posterior moments in (2.7).

B Maximum Likelihood Estimation

In this section we compute the maximum likelihood estimates, σ_{ML} and λ_{ML} , of the hyperparameters $\sigma > 0$ and $\lambda \in \mathbb{R}^d_+$ of a Taylor kernel in (2.1). First, recall that, for the Gaussian process model in Sec. 2.2, the negative log-likelihood function that is to be minimised with respect to a generic kernel hyperparameter θ is

$$\ell(\theta) = \frac{1}{2} (\boldsymbol{f_a} - \boldsymbol{m_a})^\mathsf{T} \boldsymbol{R_a^{-1}} (\boldsymbol{f_a} - \boldsymbol{m_a}) + \frac{1}{2} \log \det \boldsymbol{R_a} + \frac{N}{2} \log(2\pi).$$

Its derivative is

$$\frac{\partial}{\partial \theta} \ell(\theta) = \frac{1}{2} (\boldsymbol{f_a} - \boldsymbol{m_a})^\mathsf{T} \boldsymbol{R_a}^{-1} \frac{\partial \boldsymbol{R_a}}{\partial \theta} \boldsymbol{R_a}^{-1} (\boldsymbol{f_a} - \boldsymbol{m_a}) - \frac{1}{2} \operatorname{tr} \left(\boldsymbol{R_a}^{-1} \frac{\partial \boldsymbol{R_a}}{\partial \theta} \right). \tag{B.1}$$

In the following we denote $f_m=f-m$. Recall that N_n^d denotes the cardinality of the data set $(D^{\alpha}f(a))_{|\alpha|\leq n}$. When a Taylor kernel is used, the expressions in (A.2) yield

$$\frac{\partial}{\partial \sigma^2} \ell(\sigma^2, \lambda) = \frac{1}{2} \left(\frac{1}{\sigma^4} \sum_{|\boldsymbol{\alpha}| \leq n} \frac{(D^{\boldsymbol{\alpha}} f_m(\boldsymbol{a}))^2}{c_{\boldsymbol{\alpha}} \lambda^{\boldsymbol{\alpha}}} - \frac{N_n^d}{\sigma^2} \right)$$
(B.2)

and

$$\frac{\partial}{\partial \lambda_i} \ell(\sigma^2, \boldsymbol{\lambda}) = \frac{1}{2\lambda_i} \left(\frac{1}{\sigma^2} \sum_{|\boldsymbol{\alpha}| \leq n} \frac{\boldsymbol{\alpha}(i) (D^{\boldsymbol{\alpha}} f_m(\boldsymbol{a}))^2}{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}} - \sum_{|\boldsymbol{\alpha}| \leq n} \boldsymbol{\alpha}(i) \right)$$
(B.3)

for each $i=1,\ldots,d$. From (B.2) it is easy to solve σ_{ML} for any $\pmb{\lambda} \in \mathbb{R}^d_+$ and $n \in \mathbb{N}_0$ by setting the derivative to zero. This gives

$$\sigma_{\mathsf{ML}}^2 = \frac{1}{N_n^d} \sum_{|\boldsymbol{\alpha}| \le n} \frac{(\mathbf{D}^{\boldsymbol{\alpha}} f_m(\boldsymbol{a}))^2}{c_{\boldsymbol{\alpha}} \lambda^{\boldsymbol{\alpha}}}.$$
 (B.4)

Inserting this into (B.3) and setting the derivative shows that the maximum likelihood estimate of λ_i has to solve

$$\left(\sum_{|\boldsymbol{\alpha}| \le n} \frac{(\mathbf{D}^{\boldsymbol{\alpha}} f_m(\boldsymbol{a}))^2}{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}\right)^{-1} \sum_{|\boldsymbol{\alpha}| \le n} \frac{\boldsymbol{\alpha}(i)(\mathbf{D}^{\boldsymbol{\alpha}} f_m(\boldsymbol{a}))^2}{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}} = \frac{1}{N_n^d} \sum_{|\boldsymbol{\alpha}| \le n} \boldsymbol{\alpha}(i).$$
(B.5)

Solving (B.5) appears to be fairly complicated. This is however possible in certain important special cases. For notational simplicity we focus on inner product kernels of the form (2.3) whose general coeffcients c_{α} are given in (A.1).

B.1 Explicit Maximum Likelihood Estimates for Inner Product Kernels

Let $\partial_i^p f(x)$ denote the pth order partial derivative of f at x with respect to the ith coordinate.

B.1.1 n = 1

Note from (A.1) that $c_{\alpha} = c_0$ for $\alpha = 0$ and $c_{\alpha} = c_1$ when $|\alpha| = 1$. By (B.3), to obtain λ_{ML} we need to solve

$$\frac{1}{\sigma^2} \sum_{|\boldsymbol{\alpha}| \le 1} \frac{\boldsymbol{\alpha}(i) (\mathrm{D}^{\boldsymbol{\alpha}} f_m(\boldsymbol{a}))^2}{c_{\boldsymbol{\alpha}} \lambda^{\boldsymbol{\alpha}}} - \sum_{|\boldsymbol{\alpha}| \le 1} \boldsymbol{\alpha}(i) = \frac{(\partial_i f_m(\boldsymbol{a}))^2}{\sigma^2 c_1 \lambda_i} - 1 = 0$$
 (B.6)

for each $i = 1, \dots, d$. Eq. (B.6) readily gives the maximum likelihood estimates

$$(\lambda_{\mathsf{ML}})_i = \frac{(\partial_i f_m(\boldsymbol{a}))^2}{\sigma^2 c_1} \tag{B.7}$$

for a fixed $\sigma > 0$. If σ_{ML}^2 in (B.4) is used we get

$$\sigma_{\mathsf{ML}}^2 = \frac{1}{d+1} \left(\frac{f_m(\boldsymbol{a})^2}{c_0} + \sum_{i=1}^d \frac{(\partial_i f_m(\boldsymbol{a}))^2}{c_1(\lambda_{\mathsf{ML}})_i} \right) = \frac{1}{d+1} \left(\frac{f_m(\boldsymbol{a})^2}{c_0} + d\sigma_{\mathsf{ML}}^2 \right),$$

which is solved by $\sigma_{\rm ML}^2 = f_m(\boldsymbol{a})^2/c_0$. Plugging this in (B.7) yields

$$\sigma_{\mathsf{ML}}^2 = \frac{f_m(\boldsymbol{a})^2}{c_0}$$
 and $(\boldsymbol{\lambda}_{\mathsf{ML}})_i = \frac{c_0}{c_1} \left(\frac{\partial_i f_m(\boldsymbol{a})}{f_m(\boldsymbol{a})}\right)^2$. (B.8)

If $|f_m(a)|$ is small, the estimate for λ becomes very large and may cause numerical instabilities.

B.1.2 n=2

Note from (A.1) that (i) $c_{\alpha} = 0$ for $\alpha = 0$, (ii) $c_{\alpha} = c_1$ when $|\alpha| = 1$, (iii) $c_{\alpha} = c_2/2$ when $|\alpha| = 2$ and $\alpha(i) = \alpha(j) = 1$ for some $i \neq j$ and (iv) $c_{\alpha} = c_2$ when $|\alpha| = 2$ and $\alpha(i) = 2$ for some i.

Eq. (B.5) is now

$$\left(\frac{f_m(\boldsymbol{a})^2}{c_0} + \sum_{j=1}^d \left(\frac{(\partial_j f_m(\boldsymbol{a}))^2}{c_1 \lambda_j} + \frac{(\partial_j^2 f_m(\boldsymbol{a}))^2}{c_2 \lambda_j^2}\right) + \frac{2}{c_2} \sum_{j=1}^d \sum_{k>j} \frac{(\partial_k \partial_j f_m(\boldsymbol{a}))^2}{\lambda_k \lambda_j}\right)^{-1} \times \left(\frac{(\partial_i f_m(\boldsymbol{a}))^2}{c_1 \lambda_i} + \frac{2}{c_2} \left(\frac{(\partial_i^2 f_m(\boldsymbol{a}))^2}{\lambda_i^2} + \frac{1}{\lambda_i} \sum_{j \neq i} \frac{(\partial_i \partial_j f_m(\boldsymbol{a}))^2}{\lambda_j}\right)\right) = \frac{1}{N_n^d} \sum_{|\boldsymbol{a}| < n} \boldsymbol{\alpha}(i).$$

This is equivalent to the quadratic equation

$$a\lambda_i^{-2} + b\lambda_i^{-1} + c = 0,$$

where

$$\begin{split} a &= (2-M_2^d) \frac{(\partial_i^2 f_m(\boldsymbol{a}))^2}{c_2}, \\ b &= (1-M_2^d) \bigg(\frac{(\partial_i f_m(\boldsymbol{a}))^2}{c_1} + \frac{2}{c_2} \sum_{j \neq i} \frac{(\partial_i \partial_j f_m(\boldsymbol{a}))^2}{\lambda_j} \bigg), \\ c &= -M_2^d \bigg(\frac{f_m(\boldsymbol{a})^2}{c_0} + \sum_{j \neq i} \bigg(\frac{(\partial_j f_m(\boldsymbol{a}))^2}{c_1 \lambda_j} + \frac{(\partial_j^2 f_m(\boldsymbol{a}))^2}{c_2 \lambda_j^2} \bigg) + \frac{2}{c_2} \sum_{j \neq i} \sum_{k > j, \, k \neq i} \frac{(\partial_k \partial_j f_m(\boldsymbol{a}))^2}{\lambda_k \lambda_j} \bigg) \\ &= -M_2^d \bigg(\frac{f_m(\boldsymbol{a})^2}{c_0} + \sum_{j \neq i} \frac{(\partial_j f_m(\boldsymbol{a}))^2}{c_1 \lambda_j} + \frac{1}{c_2} \sum_{j \neq i} \sum_{k \neq i} \frac{(\partial_k \partial_j f_m(\boldsymbol{a}))^2}{\lambda_k \lambda_j} \bigg), \\ M_2^d &= \frac{1}{N_2^d} \sum_{|\boldsymbol{\alpha}| \leq n} \boldsymbol{\alpha}(i) \\ &= \frac{2(d+1)}{d^2 + 3d + 2}. \end{split}$$

Because c < 0 and a, b > 0 by $M_2^d < 1$, we thus get

$$(\lambda_{\mathsf{ML}})_i = \left(\frac{-b + \sqrt{b^2 - 4ac}}{2a}\right)^{-1},\tag{B.9}$$

but simplifying this does not appear easy. We therefore include an additional constraint that $\lambda = (\lambda, \dots, \lambda) \in \mathbb{R}^d$ for some $\lambda > 0$.

B.1.3
$$n=2$$
 and $\lambda=(\lambda,\ldots,\lambda)\in\mathbb{R}^d$

If $\lambda = (\lambda, \dots, \lambda) \in \mathbb{R}^d$ for some $\lambda > 0$, the log-likelihood derivative is

$$\frac{\partial}{\partial \lambda} \ell(\sigma^2, \lambda) = \frac{1}{2\lambda} \left(\frac{1}{\sigma^2} \sum_{m=1}^n m \sum_{|\boldsymbol{\alpha}| = m} \frac{(D^{\boldsymbol{\alpha}} f_m(\boldsymbol{a}))^2}{c_{\boldsymbol{\alpha}} \lambda^{|\boldsymbol{\alpha}|}} - \sum_{m=1}^n m \sum_{|\boldsymbol{\alpha}| = m} 1 \right)$$

for an arbitrary Taylor kernel and $n \in \mathbb{N}$. Specialising this to inner product kernels and n = 2 gives

$$\frac{\partial}{\partial \lambda} \ell(\sigma^2, \lambda) = \frac{1}{2\lambda} \left(\frac{1}{\sigma^2} \left[\sum_{i=1}^d \frac{(\partial_i f_m(\boldsymbol{a}))^2}{c_1 \lambda} + \frac{2}{c_2 \lambda^2} \sum_{i,j=1}^d (\partial_i \partial_j f_m(\boldsymbol{a}))^2 \right] - (d^2 + 2d) \right).$$

By using the gradient $\nabla f_m(\mathbf{a}) \in \mathbb{R}^d$ and Hessian $\mathbf{H} f_m(\mathbf{a}) \in \mathbb{R}^{d \times d}$ of f_m at \mathbf{a} we can write the derivative in the more compact form

$$\frac{\partial}{\partial \lambda} \ell(\sigma^2, \lambda) = \frac{1}{2\lambda} \left(\frac{1}{\sigma^2} \left[\frac{\left\| \nabla f_m(\boldsymbol{a}) \right\|_2^2}{c_1 \lambda} + \frac{2 \left\| \boldsymbol{H} f_m(\boldsymbol{a}) \right\|_{2,1}^2}{c_2 \lambda^2} \right] - (d^2 + 2d) \right),$$

where $\|\cdot\|_{2,1}$ denotes the entrywise 2-norm, $\|\boldsymbol{A}\|_{2,1} = (\sum_{i,j=1}^d A_{ij}^2)^{1/2}$ for any matrix $\boldsymbol{A} \in \mathbb{R}^{d \times d}$. Plugging (B.4) in and setting the derivative to zero gives the equation

$$\left(\frac{f_m(\boldsymbol{a})^2}{c_0} + \frac{\|\nabla f_m(\boldsymbol{a})\|_2^2}{c_1\lambda} + \frac{\|\boldsymbol{H}f_m(\boldsymbol{a})\|_{2,1}^2}{c_2\lambda^2}\right)^{-1} \left(\frac{\|\nabla f_m(\boldsymbol{a})\|_2^2}{c_1\lambda} + \frac{2\|\boldsymbol{H}f_m(\boldsymbol{a})\|_{2,1}^2}{c_2\lambda^2}\right) = \frac{2d(d+2)}{d^2 + 3d + 2},$$

which is equivalent to

$$a\lambda^{-2} + b\lambda^{-1} + c = 0$$

for

$$a = \frac{\|\boldsymbol{H}f_m(\boldsymbol{a})\|_{2,1}^2}{c_2} \left(2 - \frac{2d(d+2)}{d^2 + 3d + 2}\right),$$
 (B.10)

$$b = \frac{\|\nabla f_m(\mathbf{a})\|_2^2}{c_1} \left(1 - \frac{2d(d+2)}{d^2 + 3d + 2}\right),\tag{B.11}$$

$$c = -\frac{2d(d+2)}{d^2 + 3d + 2} \frac{f_m(\mathbf{a})^2}{c_0}.$$
(B.12)

It is easy to see that

$$1 \le \frac{2d(d+2)}{d^2 + 3d + 2} < 2$$
 for all $d \in \mathbb{N}$, (B.13)

which means that a > 0, $b \ge 0$ and c < 0. Therefore the maximum likelihood estimate is

$$\lambda_{\mathsf{ML}} = \left(\frac{-b + \sqrt{b^2 - 4ac}}{2a}\right)^{-1}.\tag{B.14}$$

We have not been able to simplify this further except when d=1. To summarise, in this setting the maximum likelihood estimates are given by (B.14), where the constants are defined in (B.10)–(B.12), and

$$\sigma_{\mathsf{ML}}^{2} = \frac{f_{m}(\boldsymbol{a})^{2}}{c_{0}} + \frac{\|\nabla f_{m}(\boldsymbol{a})\|_{2}^{2}}{c_{1}\lambda_{\mathsf{ML}}} + \frac{\|\boldsymbol{H}f_{m}(\boldsymbol{a})\|_{2,1}^{2}}{c_{2}\lambda_{\mathsf{MI}}^{2}}.$$
 (B.15)

B.2 Maximum Likelihood Estimates for d = 1

When d=1 the estimates derived in Supplement B.1 simplify. If λ is fixed, Eq. (B.4) yields

$$\sigma_{\mathsf{ML}}^2 = \frac{1}{n+1} \sum_{p=0}^n \frac{f_m^{(p)}(a)^2}{c_p \lambda^p} \quad \text{ for any } \quad n \in \mathbb{N}.$$

If both parameters are fitted, we get from (B.8) that

$$\sigma_{\mathsf{ML}}^2 = rac{f_m'(a)^2}{c_0}$$
 and $\lambda_{\mathsf{ML}} = rac{c_0}{c_1} \left(rac{f_m'(a)}{f_m(a)}
ight)^2$.

for n = 1 and from (B.14) and (B.15) that

$$\sigma_{\mathsf{ML}}^2 = \frac{1}{3} \left(\frac{2f_m(a)^2}{c_0} + \frac{f_m'(a)^2}{c_1} \sqrt{\frac{c_2}{c_0}} \left| \frac{f_m(a)}{f_m''(a)} \right| \right) \quad \text{ and } \quad \lambda_{\mathsf{ML}} = \sqrt{\frac{c_0}{c_2}} \left| \frac{f_m''(a)}{f_m(a)} \right|.$$

for n=2 (this simplification is due to the fraction in (B.13) being one). As remarked earlier in Supplement B.1.1, these estimates of λ may cause numerical instabilities, and some care should be exercised if they are to be used.

B.3 On Estimation of c_{α}

The approach that might strike one as the most principled one is to disregard σ and λ and instead directly estimate individual coefficients c_{α} of a Taylor kernel (2.1). Unfortunately, this is not possible because the likelihood either contains no information about them (if $|\alpha| > n$) or they do not affect the posterior (if $|\alpha| \le n$):

- Since the kernel matrix is $(\mathbf{R}_{\mathbf{a}})_{ij} = \sigma^2 c_{\alpha_i} \lambda^{\alpha_i} \delta_{ij}$, the log-likelihood derivative (B.1) is identically zero if $\theta = c_{\alpha}$ for $|\alpha| > n$.
- If $\theta = c_{\alpha}$ for $|\alpha| \le n$, then the derivative of the kernel matrix has only one non-zero diagonal element and (B.1) becomes

$$\frac{\partial}{\partial c_{\alpha}} \ell(c_{\alpha}, \sigma^2, \lambda) = \frac{1}{2c_{\alpha}} \left(\frac{(D^{\alpha} f_m(a))^2}{\sigma^2 c_{\alpha} \lambda^{\alpha}} - 1 \right),$$

which vanishes if

$$c_{\alpha} = \frac{\sigma^2 \lambda^{\alpha}}{(D^{\alpha} f_m(\boldsymbol{a}))^2}.$$

However, as seen from (2.7), the posterior mean and covariance do not depend on c_{α} for $|\alpha| \le n$ and so estimation of these coefficients confers no benefits for inference or uncertainty quantification.

B.4 Noisy Observations

Let us then briefly consider maximum likelihood estimation in the noisy setting described in Supplement A.4. In this setting the negative log-likelihood function becomes

$$\ell(\theta) = \frac{1}{2} (\boldsymbol{f_a} - \boldsymbol{m_a})^{\mathsf{T}} (\boldsymbol{R_a} + \boldsymbol{E})^{-1} (\boldsymbol{f_a} - \boldsymbol{m_a}) + \frac{1}{2} \log \det(\boldsymbol{R_a} + \boldsymbol{E})$$
(B.16)

and its derivative is

$$\frac{\partial}{\partial \theta} \ell(\theta) = \frac{1}{2} (\boldsymbol{f_a} - \boldsymbol{m_a})^\mathsf{T} (\boldsymbol{R_a} + \boldsymbol{E})^{-1} \frac{\partial \boldsymbol{R_a}}{\partial \theta} (\boldsymbol{R_a} + \boldsymbol{E})^{-1} (\boldsymbol{f_a} - \boldsymbol{m_a}) - \frac{1}{2} \operatorname{tr} \left((\boldsymbol{R_a} + \boldsymbol{E})^{-1} \frac{\partial \boldsymbol{R_a}}{\partial \theta} \right).$$

Consider then the scale parameter. Since

$$(\mathbf{R}_{\boldsymbol{a}} + \mathbf{E})^{-1} = \frac{1}{\sigma^2 c_{\boldsymbol{\alpha}_i} \boldsymbol{\lambda}^{\boldsymbol{\alpha}_i} + \varepsilon_{\boldsymbol{\alpha}_i}^2} \delta_{ij} \quad \text{ and } \quad \left(\frac{\partial \mathbf{R}_{\boldsymbol{a}}}{\partial \sigma^2}\right)_{ij} = c_{\boldsymbol{\alpha}_i} \boldsymbol{\lambda}^{\boldsymbol{\alpha}_i} \delta_{ij},$$

we get, for a fixed λ ,

$$\frac{\partial}{\partial \sigma^2} \ell(\sigma^2, \boldsymbol{\lambda}) = \frac{1}{2} \sum_{|\boldsymbol{\alpha}| \leq n} \left[\frac{(D^{\boldsymbol{\alpha}} f_m(\boldsymbol{a}))^2 c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\sigma^2 c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}} + \varepsilon_{\boldsymbol{\alpha}}^2)^2} - \frac{c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{\sigma^2 c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}} + \varepsilon_{\boldsymbol{\alpha}}^2} \right]
= \frac{1}{2} \sum_{|\boldsymbol{\alpha}| \leq n} \frac{[(D^{\boldsymbol{\alpha}} f_m(\boldsymbol{a}))^2 - \sigma^2 c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}} - \varepsilon_{\boldsymbol{\alpha}}^2] c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}}{(\sigma^2 c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}} + \varepsilon_{\boldsymbol{\alpha}}^2)^2}.$$

The zeros of this derivative, one of which is σ_{ML}^2 , are, in general, the roots of

$$\sum_{|\boldsymbol{\alpha}| \leq n} \bigg([(\mathrm{D}^{\boldsymbol{\alpha}} f_m(\boldsymbol{a}))^2 - \sigma^2 c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}} - \varepsilon_{\boldsymbol{\alpha}}^2] c_{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}} \prod_{\substack{|\boldsymbol{\beta}| \leq n \\ \boldsymbol{\beta} \neq \boldsymbol{\alpha}}} (\sigma^2 c_{\boldsymbol{\beta}} \boldsymbol{\lambda}^{\boldsymbol{\beta}} + \varepsilon_{\boldsymbol{\beta}}^2)^2 \bigg),$$

which is a polynomial of degree $2(N_n^d-1)+1$ in σ^2 . We now focus on the case d=1 which is relevant to the probabilistic Euler method in Sec. 4. The derivative of the negative-log likelihood becomes

$$\frac{\partial}{\partial \sigma^2} \ell(\sigma^2, \lambda) = \frac{1}{2} \sum_{n=0}^n \left(\frac{f_m^{(p)}(a)^2 c_p \lambda^p}{(\sigma^2 c_p \lambda^p + \varepsilon_p^2)^2} - \frac{c_p \lambda^p}{\sigma^2 c_p \lambda^p + \varepsilon_p^2} \right).$$

In the practically relevant case n=1 the MLE $\sigma_{\rm ML}^2$ is therefore a positive solution to the equation

$$\frac{c_0}{\sigma^2 c_0 + \varepsilon_0^2} + \frac{c_1 \lambda}{\sigma^2 c_1 \lambda + \varepsilon_1^2} - \frac{f_m(a)^2 c_0}{(\sigma^2 c_0 + \varepsilon_0^2)^2} - \frac{f_m'(a)^2 c_1 \lambda}{(\sigma^2 c_1 \lambda + \varepsilon_1^2)^2} = 0$$
 (B.17)

which has the equivalent cubic (in σ^2) form

$$a\sigma^6 + b\sigma^4 + c\sigma^2 + d = 0 \tag{B.18}$$

with constants

$$a = 2c_0^2 c_1^2 \lambda^2,$$
 (B.19a)

$$b = -f_m(a)^2 c_0 c_1^2 \lambda^2 - f_m'(a)^2 c_0^2 c_1 \lambda + 3c_0 c_1^2 \lambda^2 \varepsilon_0^2 + c_0^2 c_1 \lambda \varepsilon_1^2 + 2c_0^2 c_1 \lambda \varepsilon_1^2,$$
(B.19b)

$$c = -2f_m(a)^2 c_0 c_1 \lambda \varepsilon_1^2 - 2f_m'(a)^2 c_0 c_1 \lambda \varepsilon_0^2 + 4c_0 c_1 \lambda \varepsilon_0^2 \varepsilon_1^2 + c_0^2 \varepsilon_1^4 + c_1^2 \lambda^2 \varepsilon_0^4,$$
(B.19c)

$$d = -f_m(a)^2 c_0 \varepsilon_1^4 - f_m'(a)^2 c_1 \lambda \varepsilon_0^4 + c_0 \varepsilon_0^2 \varepsilon_1^4 + c_1 \lambda \varepsilon_0^4 \varepsilon_1^2.$$
(B.19d)

Because the first term in (B.16) is of order σ^{-2} and the second of $\log \sigma$ as $\sigma \to \infty$, we conclude that $\ell(\sigma^2, \lambda)$ is increasing to the right of the largest solution of (B.18). Therefore σ_{MI}^2 , if well defined (i.e., positive), equals either the largest or the smallest positive solution of (B.18). If all three solutions of (B.18) are non-positive, σ cannot be selected using maximum likelihood. Note that the largest solution is positive (at least) for sufficiently small ε_0 and ε_1 because for $\varepsilon_0 = \varepsilon_1 = 0$ the equation (B.18) is

$$2c_0^2c_1^2\lambda^2\sigma^6 - (f_m(a)^2c_0c_1^2\lambda^2 + f_m'(a)^2c_0^2c_1\lambda)\sigma^4 = 0,$$

whose unique solution (this is of course precisely the MLE in (B.4))

$$\sigma^2 = \frac{f_m(a)^2 c_1 \lambda + f'_m(a)^2 c_0}{2c_0 c_1 \lambda} = \frac{1}{2} \left(\frac{f_m(a)^2}{c_0} + \frac{f'_m(a)^2}{c_1 \lambda} \right)$$

is positive if either f(a) or f'(a) is non-zero.

We conclude this supplement with a discussion on why it may be a bad idea to try use maximum likelihood to select λ in the noisy setting. When d=1 and n=1 we have

$$\frac{\partial}{\partial \lambda} \ell(\sigma^2, \lambda) = \frac{\sigma^2 c_1}{2} \left(\frac{f_m'(a)^2}{(\sigma^2 c_1 \lambda + \varepsilon_1^2)^2} - \frac{1}{\sigma^2 c_1 \lambda + \varepsilon_1^2} \right),$$

which has its unique root at

$$\lambda = \frac{f_m'(a)^2 - \varepsilon_1^2}{\sigma^2 c_1}.\tag{B.20}$$

Using this value of λ in (B.17) yields the equation

$$\frac{c_0}{\sigma^2 c_0 + \varepsilon_0^2} \left(1 - \frac{f_m(a)^2}{\sigma^2 c_0 + \varepsilon_0^2} \right) = 0$$

for σ^2 , the unique solution of which is

$$\sigma^2 = \frac{f_m(a)^2 - \varepsilon_0^2}{c_0}.$$

Inserting this in (B.20) yields the maximum likelihood estimates

$$\sigma_{\mathsf{ML}}^2 = \frac{f_m(a)^2 - \varepsilon_0^2}{c_0} \quad \text{ and } \quad \lambda_{\mathsf{ML}} = \frac{c_0(f_m'(a)^2 - \varepsilon_1^2)}{c_1(f_m(a)^2 - \varepsilon_0^2)}.$$

If observation noise level is sufficiently high in comparison to $f_m(a)^2$ or $f_m'(a)^2$, these parameter estimates are negative and cannot be used. We therefore recommend fixing λ and selecting σ^2 as a solution of (B.18).

C The Probabilistic Euler Method

This supplement describes how σ_n^2 , the maximum likelihood estimate of the scaling parameter σ^2 is computed on each step and contains a proof Thm. 4.1. For ease of reference, the complete method is defined by the recursion

$$y_{n+1} = a_n y_n + b_n h f(t_n, y_n),$$

$$\varepsilon_{n+1}^2 = \sigma_n^2 \left[c_0 (1 - a_n) + c_1 \lambda (1 - b_n) h^2 + \sum_{p=2}^{\infty} \frac{c_p \lambda^p}{(p!)^2} h^{2p} \right],$$

where

$$a_n = \frac{\sigma_n^2 c_0}{\sigma_n^2 c_0 + \varepsilon_n^2}, \quad b_n = \frac{\sigma_n^2 c_1 \lambda}{\sigma_n^2 c_1 \lambda + f_y'(t_n, y_n)^2 \varepsilon_n^2},$$
 (C.1)

and σ_n^2 is a positive solution of the cubic equation (B.18) with

$$f_m(a) = y_n, \quad f'_m(a) = f(t_n, y_n), \quad \varepsilon_0 = \varepsilon_n, \quad \text{and} \quad \varepsilon_1 = f'_y(t_n, y_n)\varepsilon_n.$$
 (C.2)

If the cubic equation has not positive solutions, we set $\sigma_n^2 = \sigma_{\min}^2$ for some user-specified $\sigma_{\min} > 0$. The recursion is initialised with $y_0 = y(0)$ and $\varepsilon_0 = 0$.

C.1 Maximum Likelihood Estimation of σ^2

Using values in (C.2) in the cubic equation (B.18) means that σ_n^2 is a positive solution of

$$a\sigma^6 + b\sigma^4 + c\sigma^2 + d = 0, (C.3)$$

where

$$a = 2c_0^2 c_1^2 \lambda^2$$
, (C.4a)

$$b = -y_n^2 c_0 c_1^2 \lambda^2 - f(t_n, y_n)^2 c_0^2 c_1 \lambda + 3c_0 c_1^2 \lambda^2 \varepsilon_n^2 + c_0^2 c_1 \lambda f_y'(t_n, y_n)^2 \varepsilon_n^2 + 2c_0^2 c_1 \lambda f_y'(t_n, y_n)^2 \varepsilon_n^2,$$
(C.4b)

$$c = -2y_n^2 c_0 c_1 \lambda f_y'(t_n, y_n)^2 \varepsilon_n^2 - 2f(t_n, y_n)^2 c_0 c_1 \lambda \varepsilon_n^2 + 4c_0 c_1 \lambda f_y'(t_n, y_n)^2 \varepsilon_n^4 + c_0^2 f_y'(t_n, y_n)^4 \varepsilon_n^4$$
(C.4c)

$$+c_1^2\lambda^2\varepsilon_n^4$$
, (C.4d)

$$d = -y_n^2 c_0 f_y'(t_n, y_n)^4 \varepsilon_n^4 - f(t_n, y_n)^2 c_1 \lambda \varepsilon_n^4 + c_0 f_y'(t_n, y_n)^4 \varepsilon_n^6 + c_1 \lambda f_y'(t_n, y_n)^2 \varepsilon_n^6.$$
 (C.4e)

Since polynomial roots are continuous functions of the coefficients,

$$\lim_{\varepsilon_n \to 0} \sigma_n^2 = \sigma_{n,0}^2 = \frac{1}{2} \left(\frac{y_n^2}{c_0} + \frac{f(t_n, y_n)^2}{c_1 \lambda} \right),$$

where $\sigma_{n,0}^2$ is the unique solution to our cubic equation for $\varepsilon_n = 0$.

C.2 Convergence of the Probabilistic Euler Method

This supplement contains the proof of Thm. 4.1. The statement of this theorem is contained in Thms. C.4 and C.5.

Assumption C.1. Assume that (a) f is continuous in t and y and uniformly Lipschitz in y:

$$|f(t, y_1) - f(t, y_2)| \le L_f |y_1 - y_2|$$

for some $L \ge 0$ and all $t \in [0, T]$ and $y_1, y_2 \in \mathbb{R}$, (b) the solution y has a bounded second derivative, and (c) the Taylor kernel K is such that $\Omega_{a,r} = \mathbb{R}$.

Under part (a) of this assumption the Picard–Lindelöf theorem guarantees that there exists a unique solution $y\colon [0,T]\to \mathbb{R}$ to the ODE y'(t)=f(t,y(t)). Denote $\|y''\|_\infty\coloneqq \sup_{t\in [0,T]}|y''(t)|$ and note that the Lipschitz assumption implies the existence of a constant $C_f\geq 0$ such that

$$|f(t,y)| \le L_f |y| + C_f$$
 for all $t \in [0,T]$.

We begin by proving that $\varepsilon_n^2 = \mathcal{O}(h^2)$.

Lemma C.2. Suppose that Assumption C.1 holds Then it holds for every n = 0, ..., N that

$$|y_n| \le \left(|y(0)| + \frac{C_f}{L_f}\right) \exp(L_f T).$$

Proof. For each $n \leq N-1$ we have

$$|y_{n+1}| \le \frac{\sigma_n^2 c_0}{\sigma_n^2 c_0 + \varepsilon_n^2} |y_n| + \frac{\sigma_n^2 c_1 \lambda}{\sigma_n^2 c_1 \lambda + f_y'(t_n, y_n)^2 \varepsilon_n^2} h |f(t_n, y_n)| \le |y_n| + h |f(t_n, y_n)|$$

$$\le (1 + L_f h) |y_n| + C_f h.$$

Iterating this inequality and using the geometric sum formula and the limit definition of the exponential function yields

$$|y_n| \le (1 + L_f h)^n |y(0)| + \frac{C_f}{L_f} ((1 + L_f h)^n - 1)$$

$$= \left(1 + \frac{L_f T}{N}\right)^n |y(0)| + \frac{C_f}{L_f} \left(\left(1 + \frac{L_f T}{N}\right)^n - 1\right)$$

$$\le \left(1 + \frac{L_f T}{N}\right)^N |y(0)| + \frac{C_f}{L_f} \left(1 + \frac{L_f T}{N}\right)^N$$

$$\le \exp(L_f T) |y(0)| + \frac{C_f}{L_f} \exp(L_f T)$$

for any $n \leq N$.

Lemma C.3. Suppose that Assumption C.1 holds. Then there is a constant $C_{\sigma} \geq 0$ such that

$$\sigma_n^2 \le C_\sigma (1 + \varepsilon_n^2 + \varepsilon_n^4 + \varepsilon_n^6)$$

for every $n = 0, \dots, N - 1$.

Proof. Cauchy's upper bound for polynomial roots states that any root x_0 of a polynomial $a_p x^p + a_{p-1} x^{p-1} + \cdots + a_1 x + a_0$ satisfies

$$|x_0| \le 1 + \max\left\{\left|\frac{a_{p-1}}{a_p}\right|, \cdots, \left|\frac{a_0}{a_p}\right|\right\}.$$

Because σ_n^2 is a solution of the cubic equation (C.3),

$$\sigma_n^2 \le 1 + \max\left\{ \left| \frac{b}{a} \right|, \left| \frac{c}{a} \right|, \left| \frac{d}{a} \right| \right\},$$

where a,b,c, and d are given by (C.4). Because $a=2c_0^2c_1^2\lambda^2$ and b,c, and d consist of linear combinations of y_n^2 , $f_y'(t_n,y_n)^2$, ε_n^2 , $y_n^2f_y'(t_n,y_n)^2\varepsilon_n^2$, $f_y'(t_n,y_n)^2\varepsilon_n^4$, $f_y'(t_n,y_n)^4\varepsilon_n^4$, ε_n^4 , ε_n^4 , $v_n^2f_y'(t_n,y_n)^4\varepsilon_n^4$, $f_y'(t_n,y_n)^2\varepsilon_n^6$, $f_y'(t_n,y_n)^4\varepsilon_n^6$, and $f_y'(t_n,y_n)^2\varepsilon_n^6$, we conclude that there exists a constant $C_1 \geq 1$ such that

$$\sigma_n^2 \le 1 + C_1 (y_n^2 + f_y'(t_n, y_n)^2 + \varepsilon_n^2 + y_n^2 f_y'(t_n, y_n)^2 \varepsilon_n^2 + f_y'(t_n, y_n)^2 \varepsilon_n^4 + f_y'(t_n, y_n)^4 \varepsilon_n^4 + \varepsilon_n^4 + y_n^2 f_y'(t_n, y_n)^4 \varepsilon_n^4 + f_y'(t_n, y_n)^2 \varepsilon_n^6 + f_y'(t_n, y_n)^4 \varepsilon_n^6 + f_y'(t_n, y_n)^2 \varepsilon_n^6)$$

Lemma C.2 and f being Lipschitz in y imply that there is a constant $C_2 \ge 1$ such that $f'_y(t_n, y_n)^2 \le C_2$ and $y_n^2 \le C_2$. These bounds yield

$$\sigma_{n}^{2} \leq 1 + C_{1} \left(2C_{2} + \varepsilon_{n}^{2} + C_{2}^{2} \varepsilon_{n}^{2} + C_{2} \varepsilon_{n}^{4} + C_{2}^{2} \varepsilon_{n}^{4} + \varepsilon_{n}^{4} + C_{2}^{3} \varepsilon_{n}^{4} + C_{2} \varepsilon_{n}^{6} + C_{2}^{2} \varepsilon_{n}^{6} + C_{2} \varepsilon_{n}^{6} \right)$$

$$\leq 1 + C_{1} C_{2}^{3} \left(2 + 2 \varepsilon_{n}^{2} + 3 \varepsilon_{n}^{4} + 3 \varepsilon_{n}^{6} \right)$$

$$\leq 4C_{1} C_{2}^{3} \left(1 + \varepsilon_{n}^{2} + \varepsilon_{n}^{4} + \varepsilon_{n}^{6} \right)$$

for n < N - 1s.

Theorem C.4. Suppose that Assumption C.1 holds. If h is sufficiently small, then there is a constant $C_{\varepsilon} \geq 0$ such that

$$\varepsilon_n^2 < C_{\varepsilon} h^2$$

for every $n = 0, \dots, N$.

Proof. By definition,

$$\varepsilon_{n+1}^2 = \sigma_n^2 \left[c_0 \left(1 - \frac{\sigma_n^2 c_0}{\sigma_n^2 c_0 + \varepsilon_n^2} \right) + c_1 \lambda \left(1 - \frac{\sigma_n^2 c_1 \lambda}{\sigma_n^2 c_1 \lambda + f_y'(t_n, y_n)^2 \varepsilon_n^2} \right) h^2 + \sum_{p=2}^{\infty} \frac{c_p \lambda^p}{(p!)^2} h^{2p} \right],$$

When $h \leq 1$ there exists a constant $C_K \geq 0$ such that $\sum_{p=2}^{\infty} \frac{c_p \lambda^p}{(p!)^2} h^{2p} \leq C_K h^4$. Therefore

$$\varepsilon_{n+1}^{2} \leq \sigma_{n}^{2} \left[c_{0} \left(1 - \frac{\sigma_{n}^{2} c_{0}}{\sigma_{n}^{2} c_{0} + \varepsilon_{n}^{2}} \right) + c_{1} \lambda \left(1 - \frac{\sigma_{n}^{2} c_{1} \lambda}{\sigma_{n}^{2} c_{1} \lambda + f'_{y}(t_{n}, y_{n})^{2} \varepsilon_{n}^{2}} \right) h^{2} + C_{K} h^{4} \right] \\
= \sigma_{n}^{2} \left[\frac{c_{0} \varepsilon_{n}^{2}}{\sigma_{n}^{2} c_{0} + \varepsilon_{n}^{2}} + \frac{c_{1} \lambda f'_{y}(t_{n}, y_{n})^{2} \varepsilon_{n}^{2}}{\sigma_{n}^{2} c_{1} \lambda + f'_{y}(t_{n}, y_{n})^{2} \varepsilon_{n}^{2}} h^{2} + C_{K} h^{4} \right] \\
\leq \sigma_{n}^{2} \left[\frac{\varepsilon_{n}^{2}}{\sigma_{n}^{2}} + \frac{f'_{y}(t_{n}, y_{n})^{2} \varepsilon_{n}^{2}}{\sigma_{n}^{2}} h^{2} + C_{K} h^{4} \right] \\
\leq \left(1 + f'_{y}(t_{n}, y_{n})^{2} h^{2} \right) \varepsilon_{n}^{2} + C_{K} \sigma_{n}^{2} h^{4}.$$

Because f is Lipschitz in y with Lipschitz constant L_f , we have $f'_y(t_n, y_n)^2 \leq L_f^2$. Hence

$$\varepsilon_{n+1}^2 \le \left(1 + L_f^2 h^2\right) \varepsilon_n^2 + C_K \sigma_n^2 h^4.$$

By Lemma C.3,

$$\varepsilon_{n+1}^2 \leq \left(1 + L_f^2 h^2\right) \varepsilon_n^2 + C_K C_\sigma \left(1 + \varepsilon_n^2 + \varepsilon_n^4 + \varepsilon_n^6\right) h^4.$$

Suppose that $\varepsilon_n^2 \le 1$ for all $n \le N_0$ and some $0 \le N_0 \le N-1$. In this case the above inequality and the assumption $h \le 1$ yield

$$\varepsilon_{n+1}^2 \le (1 + L_f^2 h^2) \varepsilon_n^2 + C_K C_\sigma (1 + 3\varepsilon_n^2) h^4 \le (1 + C_1 h^2) \varepsilon_n^2 + C_2 h^4$$

for constants $C_1, C_2 \ge 0$. Iterating this inequality and recalling that $\varepsilon_0 = 0$ yields

$$\varepsilon_{N_0+1}^2 \le (1 + C_1 h^2)^{N_0+1} \varepsilon_0^2 + C_2 h^4 \sum_{p=0}^{N_0} (1 + C_1 h^2)^p = \frac{C_2}{C_1} h^2 \left((1 + C_1 h^2)^{N_0+1} - 1 \right)$$

$$= \frac{C_2}{C_1} h^2 \left(\left(1 + \frac{C_1 h}{N} \right)^{N_0+1} - 1 \right)$$

$$\le \frac{C_2}{C_1} h^2 \left(\left(1 + \frac{C_1 h}{N} \right)^N - 1 \right)$$

$$\le \frac{C_2}{C_1} h^2 \left(\exp(C_1 h) - 1 \right).$$

From this we conclude that

$$\varepsilon_{N_0+1}^2 \le \frac{C_2}{C_1} h^2 \left(\exp(C_1 h) - 1 \right)$$

if h is small enough that

$$\frac{C_2}{C_1}h^2\left(\exp(C_1h) - 1\right) \le 1.$$

Because $\varepsilon_0 = 0 \le 1$ and the constants C_1 and C_2 do not depend on n, it follows by induction that

$$\varepsilon_n^2 \le \frac{C_2}{C_1} h^2 \left(\exp(C_1 h) - 1 \right)$$

for every $n = 0, \dots, N$ as claimed.

We can then proceed as in a standard proof of convergence for Euler's method (e.g., Atkinson, 1989, Sec. 6.2).

Theorem C.5. Suppose that Assumption C.1 holds. If h is sufficiently small, then there is a constant $C \ge 0$ such that

$$|y(t_n) - y_n| \le \frac{C}{L_f} \exp(L_f T) h$$

for every $n = 0, \dots, N$.

Proof. Define $e_n = |y(t_n) - y_n|$. Because the solution y is twice differentiable, Taylor's theorem implies that for each n there is $\xi_n \in [t_n, t_n + h]$ such that

$$y(t_{n+1}) = y(t_n) + hy'(t_n) + \frac{h^2}{2}y''(\xi_n).$$

Therefore

$$\begin{aligned} e_{n+1} &= \left| y(t_n) + hy'(t_n) + \frac{h^2}{2}y''(\xi_n) - a_n y_n - b_n h f(t_n, y_n) \right| \\ &\leq \left| y(t_n) - a_n y_n \right| + h \left| f(t_n, y(t_n)) - b_n f(t_n, y_n) \right| + \frac{h^2}{2} \left\| y'' \right\|_{\infty} \\ &\leq e_n + h \left| f(t_n, y(t_n)) - f(t_n, y_n) \right| + (1 - a_n) \left| y_n \right| + (1 - b_n) \left| f(t_n, y_n) \right| + \frac{h^2}{2} \left\| y'' \right\|_{\infty}. \end{aligned}$$

By Thm. C.4,

$$1 - a_n = \frac{\varepsilon_n^2}{\sigma_n^2 c_0 + \varepsilon_n^2} \le \frac{C_\varepsilon h^2}{\sigma_{\min}^2 c_0} =: C_1 h^2$$

and

$$1 - b_n = \frac{f_y'(t_n, y_n)^2 \varepsilon_n^2}{\sigma_n^2 c_1 \lambda + f_y'(t_n, y_n)^2 \varepsilon_n^2} \le \frac{L_f C_\varepsilon h^2}{\sigma_{\min}^2 c_1 \lambda} =: C_2 h^2.$$

Lemma C.2 and the fact that f is Lipschitz in y imply that, for sufficiently small h and a certain constant $C \ge 0$,

$$e_{n+1} \le e_n + h |f(t_n, y(t_n)) - f(t_n, y_n)| + C_1 h^2 |y_n| + C_2 h^2 |f(t_n, y_n)| + \frac{h^2}{2} ||y''||_{\infty}$$

$$\le e_n + h |f(t_n, y(t_n)) - f(t_n, y_n)| + Ch^2$$

$$\le (1 + L_f h)e_n + Ch^2.$$

Iteration of this inequality and the fact that $e_0 = 0$ yield

$$e_n \le Ch^2 \sum_{p=0}^{n-1} (1 + L_f h)^p = \frac{C}{L_f} h \left((1 + L_f h)^n - 1 \right) \le \frac{C}{L_f} h \left(1 + \frac{L_f T}{N} \right)^N \le \frac{C}{L_f} \exp(L_f T) h.$$

D Algorithms

This supplement collects the most important algorithms used and proposed in the paper.

D.1 Extended Kalman Filter

Consider a discrete-time system

$$\mathbf{x}_{j} = \mathbf{\Phi}_{j-1}(\mathbf{x}_{j-1}) + \mathbf{\eta}_{j-1}$$
 (D.1a)

$$\boldsymbol{y}_j = \boldsymbol{f}_j(\boldsymbol{x}_j) + \boldsymbol{\xi}_j \tag{D.1b}$$

where $\boldsymbol{x}_j \in \mathbb{R}^d$ represents a latent state and $\boldsymbol{y}_j \in \mathbb{R}^q$ are observations, $\boldsymbol{\Phi}_j \colon \mathbb{R}^d \to \mathbb{R}^d$ and $\boldsymbol{f}_j \mapsto \mathbb{R}^d$ be the Jacobian matrices of the functions $\boldsymbol{\Phi}_j$ and \boldsymbol{f}_j .

Algorithm D.1 Algorithmic description of the extended Kalman filter.

```
Input: \mu_0, \Sigma_0 for all j=1,\dots,n do 

// Compute Predictive Distribution \mu_j^- = \Phi_{j-1}(\mu_{j-1}) \Sigma_j^- = P_{j-1}(\mu_{j-1})\Sigma_{j-1}P_{j-1}^\mathsf{T}(\mu_{j-1}) + \Lambda_{j-1} // Condition on Data \delta_j = y_j - f(\mu_j^-) S_j = F_j(\mu_j^-)\Sigma_j^- F_j(\mu_j^-) + \Gamma_j K_j = \Sigma_j^- F_j(\mu_j^-)S_j^{-1} \mu_j = \mu_j^- + K_j\delta_j \Sigma_j = \Sigma_j^- - K_jS_jK_j^\mathsf{T} and for
```

D.2 Taylor Extended Kalman Filter

The Taylor extended Kalman filter computes Gaussian approximations $N(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$ to $\boldsymbol{x}_j \mid \boldsymbol{y}_1, \dots, \boldsymbol{y}_j$ for $j = 1, \dots, n$ and \boldsymbol{x}_j and \boldsymbol{y}_j defined in (D.1). It is assumed that the functions $\boldsymbol{\Phi}_j$ are linear and given by $\boldsymbol{\Phi}_j(\boldsymbol{x}) = \boldsymbol{A}_j \boldsymbol{x}$ with some matrices $\boldsymbol{A}_j \in \mathbb{R}^{d \times d}$ and that $\Gamma_j = \operatorname{diag}(\gamma_{j,1}, \dots, \gamma_{j,q})$.

Algorithm D.2 Algorithmic description of the Taylor extended Kalman filter.

```
Input: \mu_0, \Sigma_0 for all j=1,\dots,n do  // \text{ Compute Predictive Distribution}  \mu_j^- = A_{j-1}\mu_{j-1} \Sigma_j^- = A_{j-1}\Sigma_{j-1}A_{j-1}^{\mathsf{T}} + \Lambda_{j-1} p_j(\boldsymbol{x}) = \mathrm{N}(\boldsymbol{x}; \boldsymbol{\mu}_j^-, \Sigma_j^-) // \text{ Condition on Data}  for all \ell=1,\dots,q do  k_{j,\ell}(\boldsymbol{x}) = P_{1,\boldsymbol{\mu}_j^-}(\boldsymbol{x},\boldsymbol{x}) \text{ for the GP posterior covariance in (2.7b) with } \sigma^2 \text{ set as in (B.4) with } N_n^d = n = 1,   f_m = f_{j,\ell}, \text{ and } \boldsymbol{a} = \boldsymbol{\mu}_j^-  p_{j,\ell}^{\mathsf{PN}}(y_{j,\ell} \mid \boldsymbol{x}) = \mathrm{N}(y_{j,\ell}; \boldsymbol{\mu}_{j,\ell}^- + (\boldsymbol{x} - \boldsymbol{\mu}_j^-)^\mathsf{T} \nabla f_{j,\ell}(\boldsymbol{\mu}_j^-), \gamma_{j,\ell} + k_{j,\ell}(\boldsymbol{x}))  end for  // \text{ Build target } T(\boldsymbol{x}) \propto p^{\mathsf{PN}}(\boldsymbol{x} \mid \boldsymbol{y}_j)  T(\boldsymbol{x}) = p_j(\boldsymbol{x}) \prod_{\ell=1}^q p_{j,\ell}^{\mathsf{PN}}(y_{j,\ell} \mid \boldsymbol{x})  \boldsymbol{\mu}_j = \arg\max_{\boldsymbol{x} \in \mathbb{R}^d} T(\boldsymbol{x})   \Sigma_j^{-1} = -\frac{\mathrm{d}^2}{\mathrm{d}\boldsymbol{x}^2} \log T(\boldsymbol{x})|_{\boldsymbol{x} = \boldsymbol{\mu}_j}  end for
```

D.3 Euler Method

Let $f: [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$. The Euler method computes approximations $\mathbf{y}_n \approx \mathbf{y}(t_n)$ at points $t_n = nT/N, n = 1, \dots, N$, to the solution \mathbf{y} of the differential equation

$$\boldsymbol{y}'(t) = \boldsymbol{f}(t, \boldsymbol{y}(t)) \tag{D.2}$$

on the interval [0, T].

Algorithm D.3 Algorithmic description of the classical Euler method.

```
Input: m{y}_0, N
for all n=0,\ldots,N-1 do
t_n=nT/N
h=1/N
m{y}_{n+1}=m{y}_n+hm{f}(t_n,m{y}_n)
end for
```

D.4 Probabilistic Euler Method

The probabilistic Euler method computes approximations $y_n \approx y(t_n)$ at points $t_n = nT/N$, n = 1, ..., N to the solution y of the differential equation (D.2).

Algorithm D.4 Algorithmic description of the probabilistic Euler method.

```
Input: \mathbf{y}_0, \sigma_{\min}, N
\varepsilon_0 = \mathbf{0}
t_n = nT/N
h = 1/N
r_h = \sum_{p=2}^{\infty} \frac{c_p \lambda^p}{(p!)^2} h^{2p}
for all n = 0, \dots, N-1 do
\sigma^2 = \text{pos. solution of (B.17) with substitutions } f_m(a) = y_{n,i}, f'_m(a) = f_i(t_n, y_{n,i}), \varepsilon_0 = \varepsilon_{n,i},
\text{and } \varepsilon_1 = \frac{\partial}{\partial y_i} f_i(t_n, \mathbf{y}_n) \varepsilon_{n,i}
\sigma_{n,i}^2 = \max\{\sigma^2, \sigma_{\min}^2\}
Set a_{n,i} = a_n and b_{n,i} = b_n according to (C.1) and with substitutions \varepsilon_n = \varepsilon_{n,i}, \sigma_n = \sigma_{n,i},
\text{and } f'_y(t_n, y_n) = \frac{\partial}{\partial y_i} f_i(t_n, \mathbf{y}_n)
y_{n+1,i} = a_{n,i} y_{n,i} + b_{n,i} h f_i(t_n, \mathbf{y}_n)
\varepsilon_{n+1,i} = \sigma_{n,i}^2 [c_0(1 - a_{n,i}) + c_1 \lambda (1 - b_{n,i}) h^2 + r(h)]
end for
end for
```

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