

MAXIMUM ENTROPY PROPERTY OF DISCRETE-TIME STABLE SPLINE KERNEL

Tohid Ardeshiri and Tianshi Chen

Division of Automatic Control, Department of Electrical Engineering,
Linköping University, 581 83 Linköping, Sweden,
email: {tohid,tschen}@isy.liu.se

ABSTRACT

In this paper, the maximum entropy property of the discrete-time first-order stable spline kernel is studied. The advantages of studying this property in discrete-time domain instead of continuous-time domain are outlined. One of such advantages is that the differential entropy rate is well-defined for discrete-time stochastic processes. By formulating the maximum entropy problem for discrete-time stochastic processes we provide a simple and self-contained proof to show what maximum entropy property the discrete-time first-order stable spline kernel has.

Index Terms— Machine learning, Gaussian process, impulse response estimation, maximum entropy (MaxEnt).

1. INTRODUCTION

System identification is about how to construct mathematical models based on observed data, see e.g., [1]. For linear time-invariant (LTI) and causal systems, the identification problem can be stated as follows. Consider

$$y(t_i) = f * u(t_i) + v(t_i), \quad i = 0, 1, \dots, N \quad (1)$$

where $t_i, i = 0, 1, \dots, N$ are the time instants at which the measured input $u(t)$ and output $y(t)$ are collected, $v(t)$ is the disturbance, $f(t)$ is the impulse response with $t \in \mathbb{R}^+ \triangleq [0, \infty)$ for continuous-time systems and $t = t_i, i = 0, 1, \dots$ for discrete-time systems, and $f * u(t_i)$ is the convolution of $f(\cdot)$ and $u(\cdot)$ evaluated at $t = t_i$. The goal is to estimate $f(t)$ as good as possible.

Recently, there have been increasing interests in system identification community to study system identification problems with machine learning methods, see e.g., [2], [3]. An emerging trend among others is to apply Gaussian process regression methods for LTI, stable and causal system identification problems, see [4] and its follow up papers [5], [6], [7]. Its idea is to model the impulse response $f(t)$ with a suitably defined Gaussian process which is characterized by

$$f(t) \sim \text{GP}(m(t), k(t, s)), \quad (2)$$

where $m(t)$ is the mean function and is often set to be zero, and $k(t, s)$ is the covariance function, also called the kernel function in machine learning and statistics, see e.g., [8].

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The kernel $k(t, s)$ is parametrized by a hyper-parameter β and further written as $k(t, s; \beta)$. The key issue is to design a suitable parametrization of $k(t, s; \beta)$, or in other words, the structure of $k(t, s; \beta)$, because it reflects our prior knowledge about the system to be identified. Several kernel structures have been proposed in the literature, e.g., the stable spline (SS) kernel in [4] and the diagonal and correlated (DC) kernel in [6].

Our prior knowledge is however never complete and it is thus worth to note Jaynes's maximum entropy rationale [9] to derive complete statistical prior distributions from incomplete a priori information. By maximizing the entropy rate of a stochastic process subject to constraints imposed by prior knowledge, the stochastic process which encompasses the least assumptions about the data can be obtained.

Interestingly, [10] shows based on a result in [11] that for continuous-time systems, the continuous-time first-order SS kernel (also derived by deterministic arguments in [6] and called Tuned Correlated (TC) kernel):

$$k(t, s) = \min\{e^{-\beta t}, e^{-\beta s}\}, \quad t, s \in \mathbb{R}^+ \quad (3)$$

has a certain maximum entropy property.

In Section 1.1 the maximum entropy property of the continuous-time kernel (3) is briefly presented. Then, we explain why it is worthwhile to study the maximum entropy property for the discrete-time first order SS kernel

$$k(t, s) = \min\{e^{-\beta t}, e^{-\beta s}\}, \quad t, s = t_i, i = 0, 1, \dots \quad (4)$$

and we will further elaborate our results in Section 2.

1.1. Maximum entropy property of continuous-time SS kernel

In [10], the maximum differential entropy rate *continuous-time* stochastic process subject to constraints on smoothness and bounded-input bounded-output (BIBO) stability is sought. The definition of the differential entropy rate of a stationary *continuous-time Gaussian* process $g(t)$ with power spectrum $S(\omega)$ is adopted from [11] in [10]:

$$\overline{H}(g) = \frac{1}{4\pi} \int_{-\pi}^{+\pi} \log(S(\omega)) d\omega. \quad (5)$$

We describe how smoothness and stability constraints are expressed in [10] in separate items.

1) Smoothness: The smoothness constraint on the impulse responses is addressed by using [11, Theorem 1] which suggests that the smoothness of a signal (with some of its derivatives continuous and bounded) can be imposed by assuming that the variances of these derivatives are finite. The main result in [11, Theorem 1] is given in Proposition 1 for the sake of completeness.

Proposition 1. [11, Theorem 1] Let $g(t)$ be a zero-mean bandlimited stationary Gaussian process with power spectrum $S(\omega) = 0$ for $|\omega| > B$. Given finite λ_k^2 , $k = 0, 1, \dots, m$, assume that there exist real numbers α_j , $j = 0, 1, \dots, m$ such that $\int_{-B}^B \frac{\omega^{2k}}{\sum_{j=0}^m \alpha_j \omega^{2j}} d\omega = 2\pi \lambda_k^2$, $k = 0, 1, \dots, m$. Under this assumption, if there exists $S(\omega)$ that maximizes $\bar{H}(g)$ in (5) subject to constraints $\text{Var}[\frac{d^k g(t)}{dt^k}] = \lambda_k^2$, $k = 0, 1, \dots, m$, then the spectrum is given by $S(\omega) = \frac{1}{\sum_{j=0}^m \alpha_j \omega^{2j}}$. In particular, if there is no constraints on the first $m-1$ order derivatives, then the spectrum becomes $S(\omega) = \frac{1}{\alpha_m \omega^{2m}}$.

It is further claimed in [10] that as $B \rightarrow \infty$, the Wiener process is the maximum differential entropy rate process among all Gaussian processes whose 1st-order derivatives are stationary Gaussian processes with finite variance.

2) Stability: The BIBO stability constraint on the impulse response $f(t)$ is imposed by using a stable time transformation: $f(t) = g(e^{-\beta t})$ where $g(t)$ is the Wiener process defined on $[0, 1]$ and $\beta \in \mathbb{R}^+$. Adding this on top of [11, Theorem 1] leads to the maximum differential entropy rate result in [10, Proposition 2] regarding the SS kernel (3).

Deriving the maximum entropy process in continuous-time in [11] and [10] is quite involved, due to the infinite-dimensional nature of the problem and absence of a well-defined differential entropy rate for a generic continuous-time stochastic process.

1.2. Our contributions

In this paper, we focus on discrete-time impulse responses (stochastic processes), and provide a simple and self-contained proof to show the maximum entropy property of the discrete-time first-order SS kernel (4). The advantages of working in discrete-time domain include

1. The differential entropy rate is well-defined for discrete-time stochastic process.
2. Given a stochastic process, its finite difference process can be well-defined in discrete-time domain.
3. It is possible to show what maximum entropy property a zero-mean discrete-time Gaussian process with covariance function (4) has.

Also, we define the discrete-time Wiener process and prove its maximum entropy property.

2. THE DISCRETE-TIME STABLE SPLINE KERNEL

Before deriving the maximum entropy kernels for discrete-time processes, we give some definitions. In the rest of the paper the ordered index set \mathcal{T} is defined as $\mathcal{T} = \{t_i | t_0 =$

$0, t_i < t_{i+1}, i = 0, 1, \dots, \infty\}$ also, the points t_i in the index set \mathcal{T} do not have to be equidistant.

Definition 1. The differential entropy of a continuous random variable X with density $p(x)$ is defined as

$$H(X) = - \int_S p(x) \log p(x) dx, \quad (6)$$

where, S is the support set of the random variable [12]. ■

Definition 2. The differential entropy rate of a real-valued discrete-time stochastic process $\{f(t_i) : f(t_i) \in \mathbb{R}, t_i \in \mathcal{T}\}$ is defined as

$$\bar{H}(f) = \lim_{n \rightarrow \infty} \frac{1}{n} H(f(t_1), f(t_2), \dots, f(t_n)) \quad (7)$$

if the limit exists [12]. ■

Definition 3. The discrete-time Gaussian white noise process is a discrete-time Gaussian process whose covariance function is $\sigma^2 \delta(t - \tau)$ [13] where $\delta(t - \tau)$ is equal to 1 for $t = \tau$ and 0 otherwise. ■

In Lemma 1 we show that Gaussian white noise process is the maximum differential entropy rate stochastic process with constant and finite variance. The proof is an adaptation of proof of Burg's maximum entropy theorem in [12].

Lemma 1. The discrete-time Gaussian white noise process is the maximum differential entropy rate stochastic process on \mathcal{T} with constant and finite variance.

Proof. First, let us formulate the maximum differential entropy rate problem.

$$\begin{aligned} & \underset{h}{\text{maximize}} && \bar{H}(h) \\ & \text{subject to} && \text{Var}[h(t)] = \lambda \quad \text{for } 0 < \lambda < \infty \end{aligned} \quad (8)$$

where, $\text{Var}[\cdot]$ is the variance operator. In the following, we show that $h(t)$ is a Gaussian white noise process with variance λ .

Let $h(t_1), h(t_2), \dots, h(t_n)$ be any stochastic process that satisfies the constraint $\text{Var}[h(t)] = \lambda$.

Also, let $q(t_1), q(t_2), \dots, q(t_n)$ be a Gaussian process with the same covariance matrix as $h(t_1), h(t_2), \dots, h(t_n)$ ¹. The multivariate Gaussian distribution maximizes the entropy over all n -dimensional vector valued random variables under a covariance constraint [12], therefore

$$H(h(t_1), h(t_2), \dots, h(t_n)) \leq H(q(t_1), q(t_2), \dots, q(t_n)).$$

using the chain rule and owing to the fact that conditioning reduces the entropy we obtain

$$\begin{aligned} & H(q(t_1), q(t_2), \dots, q(t_n)) \\ &= H(q(t_1)) + \sum_{i=2}^n H(q(t_i) | q(t_{i-1}), q(t_{i-2}), \dots, q(t_1)) \\ &\leq H(q(t_1)) + \sum_{i=2}^n H(q(t_i)) = \sum_{i=1}^n H(q(t_i)). \end{aligned} \quad (9)$$

¹Note that we are not making any assumptions regarding the off-diagonal elements of the covariance matrix

Since $q(t_1), q(t_2), \dots, q(t_n)$ obeys a multivariate Gaussian distribution and all the diagonal entries of the covariance matrix are equal to λ , all $q(t_i)$ are distributed according to a uni-variate Gaussian distribution with variance λ . Also, it is known that the entropy of a uni-variate Gaussian distribution depends only on its variance. Hence, $\sum_{i=1}^n H(q(t_i)) = nH(q(t_1))$.

Now define $q'(t_1), q'(t_2), \dots, q'(t_n)$ as a Gaussian white noise process where $q'(t_1), q'(t_2), \dots, q'(t_n)$ are identically distributed as $q(t_1)$. Since

$$H(q'(t_1), q'(t_2), \dots, q'(t_n)) = nH(q(t_1)), \quad (10)$$

we obtain

$$H(h(t_1), h(t_2), \dots, h(t_n)) \leq H(q'(t_1), q'(t_2), \dots, q'(t_n)). \quad (11)$$

Dividing by n and taking the limit, we obtain

$$\begin{aligned} & \lim_{n \rightarrow \infty} \frac{1}{n} H(h(t_1), h(t_2), \dots, h(t_n)) \\ & \leq \lim_{n \rightarrow \infty} \frac{1}{n} H(q'(t_1), q'(t_2), \dots, q'(t_n)) = \overline{H}^* \end{aligned} \quad (12)$$

where $\overline{H}^* = \frac{1}{2} \log(2\pi e \lambda)$ and is the differential entropy rate of the Gaussian white noise process. Hence, the maximum differential entropy rate stochastic process with constant and finite variance λ is the Gaussian white noise process with variance λ . \square

The Wiener process $W(t)$ is a continuous-time stochastic process which can be defined as the definite integral of continuous-time zero-mean Gaussian white noise, has many applications in applied mathematics and signal processing [14]. The Wiener process can be characterized by these properties [15]

1. The initial condition $W(0) = 0$.
2. The function $W(t)$ is almost surely continuous everywhere.
3. $W(t)$ has independent increments with $W(t) - W(\tau) \sim \mathcal{N}(0, \lambda(t - \tau))$ for $0 \leq \tau < t$, where $\mathcal{N}(\mu, \sigma^2)$ denotes the Gaussian distribution with mean μ and variance σ^2 .

In the following we will define a stochastic process, we refer to as discrete-time Wiener process and show two of its properties in Lemmas 2 and 3 and its maximum differential entropy rate property in Proposition 2.

Definition 4. The discrete-time Wiener process $\{f(t_i) : f(t_i) \in \mathbb{R}, t_i \in \mathcal{T}\}$ is characterized by these properties

1. $f(t_0) = 0$,
2. $f(t)$ has independent increments with $f(t_i) - f(t_j) \sim \mathcal{N}(0, \lambda(t_i - t_j))$ for $0 \leq t_j < t_i$. \blacksquare

Lemma 2. The discrete-time stochastic process $g(t)$ on \mathcal{T} is a discrete-time Wiener process if and only if $g(t_0) = 0$ and

$$g(t_n) = \sum_{i=1}^n h(t_i) \sqrt{t_i - t_{i-1}}, \quad n \geq 1 \quad (13)$$

where $h(t)$ is the zero-mean Gaussian white noise process.

Proof. First, we prove the necessary part. That is, we show if $g(t)$ is a discrete-time Wiener process, it can be expressed in the form of (13). Let $w(t_i) \triangleq \frac{g(t_i) - g(t_{i-1})}{\sqrt{t_i - t_{i-1}}}$ for $i \in \mathbb{N}$. Since $g(t_i) - g(t_{i-1}) \sim \mathcal{N}(0, \lambda(t_i - t_{i-1}))$ we have

$$w(t_i) \sim \mathcal{N}(0, \lambda). \quad (14)$$

Also, since $g(t)$ has independent increments it follows that $w(t)$ is a discrete-time zero-mean Gaussian white noise process. Also, from the definition of $w(t)$ we have

$$g(t_n) = w(t_n) \sqrt{t_n - t_{n-1}} + g(t_{n-1}) = \sum_{i=1}^n w(t_i) \sqrt{t_i - t_{i-1}}.$$

Now we prove the sufficient part, i.e., the stochastic process (13) is a discrete-time Wiener process. Since Gaussian processes are closed under linear operations [8], $g(t)$ is a Gaussian process. Also $\mathbb{E}[g(t_n)] = \mathbb{E}[\sum_{i=1}^n h(t_i) \sqrt{t_i - t_{i-1}}] = 0$. Furthermore, let $0 \leq t_j < t_i$,

$$\begin{aligned} \text{Var}[g(t_i) - g(t_j)] &= \mathbb{E} \left[\left(\sum_{r=j+1}^i h(t_r) \sqrt{t_r - t_{r-1}} \right)^2 \right] \\ &= \sum_{r=j+1}^i \lambda(t_r - t_{r-1}) = \lambda(t_i - t_j). \end{aligned} \quad (15)$$

Therefore, $g(t_i) - g(t_j) \sim \mathcal{N}(0, \lambda(t_i - t_j))$ for $0 \leq t_j < t_i$. Since $h(t)$ is a Gaussian white noise process, the increments of $g(t)$ are independent and the proof follows. \square

Lemma 3. The covariance of the discrete-time Wiener process is given by

$$\mathbb{V}[g(t_i), g(t_j)] = \lambda \min\{t_i, t_j\} \quad \text{for } t_i, t_j \in \mathcal{T} \quad (16)$$

where, λ is the variance of the underlying Gaussian white noise process.

Proof. Since $\mathbb{E}[g(t_i)] = \mathbb{E}[g(t_j)] = 0$, then

$$\begin{aligned} \mathbb{V}[g(t_i), g(t_j)] &= \mathbb{E}[g(t_i) \cdot g(t_j)] \\ &= \mathbb{E} \left[\left(\sum_{r=1}^i h(t_r) \sqrt{t_r - t_{r-1}} \right) \left(\sum_{s=1}^j h(t_s) \sqrt{t_s - t_{s-1}} \right) \right] \\ &= \sum_{q=1}^{\min(i,j)} \lambda(t_q - t_{q-1}) = \lambda \min\{t_i, t_j\} \end{aligned} \quad (17)$$

\square

In Proposition 2 the maximum differential entropy rate property of the discrete-time Wiener process when the index set is unbounded from above is studied. For the continuous-time case, the smoothness constraint on the stochastic process is expressed by constraining the variance of its first-order derivative to be constant and finite, see Proposition 1. Due to the absence of derivative for the Wiener process we use the variance of the finite difference of the discrete-time stochastic process defined below.

Definition 5. The finite difference of a discrete-time stochastic process $f(t)$ on \mathcal{T} , at $t_i \in \mathcal{T}$ is an expression of the form

$$\Delta[f](t_i) \triangleq f(t_{i+1}) - f(t_i). \quad (18)$$

■

Proposition 2. The discrete-time Wiener process is the maximum differential entropy rate stochastic process on \mathcal{T} with $t_\infty = \infty$ and $\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n \log \sqrt{t_i - t_{i-1}} < \infty$ such that its value at origin is zero and is zero-mean and variance of its finite difference at all $t_i \in \mathcal{T}$ is proportional to the time increment $t_{i+1} - t_i$ and $t_{i+1} - t_i$ is bounded from below by a positive number. That is, the discrete-time Wiener process is the optimal solution to the problem:

$$\begin{aligned} & \underset{g}{\text{maximize}} \quad \overline{H}(g) \\ & \text{subject to} \quad g(t_0) = 0 \\ & \mathbb{E}[g(t)] = 0 \\ & \text{Var}[\Delta[g](t_i)] = \lambda(t_{i+1} - t_i), \quad \lambda > 0, \\ & t_{i+1} - t_i \geq \delta > 0, \quad i = 0, 1, \dots, \infty \end{aligned} \quad (19)$$

Proof. Let $g(t)$ be any discrete-time stochastic process on \mathcal{T} . Now we define the stochastic process $w(t)$ as

$$w(t_{i+1}) \triangleq \frac{\Delta[g](t_i)}{\sqrt{t_{i+1} - t_i}}. \quad (20)$$

Therefore, $\mathbb{E}[w(t)] = 0$ and the variance of the finite difference of $g(t)$ obeys, $\text{Var}[\Delta[g](t_i)] = \mathbb{E}[w(t_{i+1})^2] (t_{i+1} - t_i)$. So the third constraint in the maximization problem (19) can be written as $\text{Var}[w(t_{i+1})] = \lambda$. Also, from (20) we have

$$g(t_{n+1}) = g(t_n) + w(t_{n+1})\sqrt{t_{n+1} - t_n} \quad (21)$$

$$= \sum_{i=1}^{n+1} w(t_i)\sqrt{t_i - t_{i-1}}. \quad (22)$$

Let $\mathcal{G} \triangleq [g(t_1), \dots, g(t_n)]^T$ and $\mathcal{W} \triangleq [w(t_1), \dots, w(t_n)]^T$. We have $\mathcal{G} = A\mathcal{W}$ where A is a lower triangular non-singular matrix independent of \mathcal{W} and \mathcal{G} . Using (7) and [12, Corollary to Theorem 8.6.4] we obtain

$$H(\mathcal{G}) = H(\mathcal{W}) + \log |A| \quad (23)$$

Therefore, it is sufficient to maximize the differential entropy rate of the underlying stochastic process $w(t)$ such that the variance of $w(t)$ is constant and $\mathbb{E}[w(t)] = 0$. Using Lemma 1 $w(t)$ turns out to be a zero-mean Gaussian white noise process. Consequently, using Lemma 2 the maximum differential entropy rate stochastic process $g(t)$ turns out to be the discrete-time Wiener process. □

Remark 1. The assumption $\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n \log \sqrt{t_i - t_{i-1}} < \infty$ is not restrictive. For example, the assumption is trivially satisfied for uniform sampling where $t_i - t_{i-1} = T_s > 0$, $i = 1, \dots, \infty$. When the time increment $t_{i+1} - t_i$ is not bounded from below, $\lim_{n \rightarrow \infty} \frac{1}{n} \log |A|$ becomes infinite and thus the differential entropy rate is not defined. In this

case, the discrete-time Wiener process is the maximum differential entropy stochastic process on the finite segment $\{t_0, \dots, t_n\} \subset \mathcal{T}$ in the following sense: for any $n \in \mathbb{N}$, it optimizes the maximum differential entropy problem

$$\begin{aligned} & \underset{g}{\text{maximize}} \quad H(g(t_1), \dots, g(t_n)) \\ & \text{subject to} \quad g(t_0) = 0 \\ & \mathbb{E}[g(t)] = 0 \\ & \text{Var}[\Delta[g](t_i)] = \lambda(t_{i+1} - t_i), \quad \lambda > 0 \\ & i = 0, 1, \dots, n-1 \end{aligned} \quad (24)$$

Before proceeding to the maximum differential entropy property of the discrete-time stable spline kernel (4) in Proposition 3, we introduce the concept of reverse ordered index set of $\mathcal{T} = \{t_0, t_1, \dots, t_n\}$ which is defined as the ordered index set $\{t_n, \dots, t_1, t_0\}$ and denoted by $\overline{\mathcal{T}}$.

Proposition 3. Let $g(\tau)$ denote a zero-mean discrete-time stochastic process defined on an ordered index set $\{\tau_i | \tau_0 = 0, \tau_\infty = 1, 0 < \tau_i < \tau_j < 1, 0 < i < j < \infty\}$. Now consider a finite segment of g with index set $\mathcal{T}_g = \{\tau_i | \tau_0 = 0, \tau_n < 1, 0 < \tau_i < \tau_j < t_n, 0 < i < j < n\}$. Then for any $n \in \mathbb{N}$, the zero-mean Gaussian process with covariance function (4) is the solution to the maximum differential entropy problem:

$$\begin{aligned} & \underset{f}{\text{maximize}} \quad H(f(t_0), \dots, f(t_{n-1})) \\ & \text{subject to} \quad f(t) = g(e^{-\beta t}), \quad \beta > 0, t \in \overline{\mathcal{T}}_g, \\ & g(\tau_0) = 0, \\ & \mathbb{E}[g(\tau)] = 0, \\ & \text{Var}[\Delta[g](\tau_i)] = \lambda(\tau_{i+1} - \tau_i), i = 0, 1, \dots, n-1 \end{aligned} \quad (25)$$

Proof. Note that

$$\begin{aligned} H(f(t_0), \dots, f(t_{n-1})) &= H(g(e^{-\beta t_0}), \dots, g(e^{-\beta t_{n-1}})) \\ &= H(g(\tau_n), \dots, g(\tau_1)). \end{aligned} \quad (26)$$

which implies that (25) is equivalent to the maximum entropy problem (24). From Proposition 2 and Remark 1, the optimal solution to (19) is the discrete-time Wiener process $g(t)$ which is zero-mean Gaussian and has covariance function $\lambda \min\{t, s\}$, $t, s \in \{\tau_i | \tau_0 = 0, \tau_\infty = 1, 0 < \tau_i < \tau_j < 1, 0 < i < j < \infty\}$ (from Lemma 3). As a result, the optimal solution to (25) is the zero-mean Gaussian process induced by $f(t) = g(e^{-\beta t})$ which has the covariance function $\lambda \min\{e^{-\beta t}, e^{-\beta s}\}$. □

3. CONCLUSION

The maximum entropy property of the first-order discrete-time stable spline kernel for identification of LTI stable and causal systems are studied. By formulating the maximum entropy problem for discrete-time stochastic processes we provide a simple and self-contained proof to show the maximum entropy property of the discrete-time first-order stable spline kernel. Also, we define the discrete-time Wiener process and prove its maximum entropy property.

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