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KERNEL-BASED APPROXIMATION OF THE KOOPMAN GENERATOR

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gEDMD

Elements of RKHS Theory

Generator EDMD and Kernels

Approximation of the Generator

Recall that for SDEs, the generator is the differential operator:

$$\mathcal{L}\psi(x) = b(x) \cdot \nabla\psi(x) + \frac{1}{2}a(x) : \nabla^2\psi(x).$$

Galerkin approximation to $\mathcal{L}$ on a trial space $\mathbb{W} = \mathrm{span}\{\psi_i\}_{i=1}^n$:

$$\mathbf{L} = \mathbf{G}^{-1}\mathbf{A}, \qquad \mathbf{G}_{ij} = \langle \psi_i, \psi_j \rangle_\mu, \qquad \mathbf{A}_{ij} = \langle \psi_i, \mathcal{L}\psi_j \rangle_\mu.$$

By ergodicity, data-driven approximations are (gEDMD):

$$\mathbf{G} = \frac{1}{M}\mathbf{X}\mathbf{X}^T, \quad \mathbf{A} = \frac{1}{M}\mathbf{X}\mathbf{dX}^T, \quad \mathbf{X}_{im} = \psi_i(X_{t_m}), \quad \mathbf{dX}_{im} = \mathcal{L}\psi_i(X_{t_m}).$$

Klus and **Nüske** et al, *Physica D* (2020) gEDMD

Elements of RKHS Theory

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Reproducing Kernel Hilbert Space

Let $\mathbb{H} \subset C(\mathbb{X})$ be a Hilbert space of continuous functions on a domain $\mathbb{X}$. Assume the point evaluation functional $\delta_x f = f(x)$ is continuous for some $x \in \mathbb{X}$. Then there is a function $k_x(\cdot) \in \mathbb{H}$ such that

$$f(x) = \delta_x f = \langle f,\ k_x(\cdot)\rangle_{\mathbb{H}}$$

for all $f \in \mathbb{H}$. If the above is true for all $x \in \mathbb{X}$, we can define a two-parameter function

$$k(x, y) := k_x(y)$$

which is called the *reproducing kernel* for $\mathbb{H}$.

Definition RKHS

Definition

Let $\mathbb{X}$ be a suitable domain and $\mathbb{H}$ a space of continuous functions $f: \mathbb{X} \to \mathbb{R}$. Then $\mathbb{H}$ is called a *reproducing kernel Hilbert space* (RKHS) with inner product $\langle \cdot, \cdot \rangle_{\mathbb{H}}$ if a function $k: \mathbb{X} \times \mathbb{X} \to \mathbb{R}$ exists such that

1. $\mathbb{H} = \overline{\mathrm{span}\{k(x, \cdot),\ x \in \mathbb{X}\}}$,
2. $\langle f, k(x, \cdot) \rangle_{\mathbb{H}} = f(x)$ for all $f \in \mathbb{H}$.

Basic Properties

1. Symmetry:

$$\begin{aligned} k(x,y) &= \delta_y k_x(\cdot) = \langle k(x,\cdot),\, k(y,\cdot)\rangle_{\mathbb{H}} \\ &= \langle k(y,\cdot),\, k(x,\cdot)\rangle_{\mathbb{H}} = k(y,x) \end{aligned}$$

2. Positive semi-definiteness: let $x_j \in \mathbb{X}$, $c_j \in \mathbb{R}$, $j = 1, \ldots, N$:

$$\sum_{j,k=1}^{N} c_j c_k k(x_j, x_k) = \left\langle \sum_{j=1}^{N} c_j k(x_j,\cdot),\, \sum_{j=1}^{N} c_j k(x_j,\cdot) \right\rangle_{\mathbb{H}} \geq 0.$$

The *Gramian* matrix is always positive semi-definite.

A two-argument function with these properties is called *positive semi-definite*.

Equivalence Result

Theorem (Moore-Aronszajn)

Let $k(\cdot, \cdot)$ be a positive semi-definite function. Then there is a unique RKHS $\mathbb{H}$ with k as its reproducing kernel.

Idea of the Proof.

Consider the linear span $\tilde{\mathbb{H}}$ of all finite combinations $\sum_{j=1}^{N} c_j k(x_j, \cdot)$, with semi inner product $\sum_{j,k} c_j d_k k(x_j, x_k)$. It can be shown that this is actually a genuine inner product, and $\tilde{\mathbb{H}}$ is a pre-Hilbert space. Complete it and identify elements $\tilde{f}$ of the completion $\mathbb{H}$ with a function by $f(x) = \left\langle \tilde{f},\ k(x, \cdot) \right\rangle_{\mathbb{H}}$. □

Kernel Trick

In summary, a RKHS is a Hilbert space of functions where inner products can be evaluated by kernel evaluations (*the "kernel trick"*).

Example

- The most popular kernel is the Gaussian $k(x, y) = \exp(-\frac{1}{2\sigma^2}\|x - y\|^2)$.
- Many other kernels with rich properties have been developed for a broad range of applications.

Derivative Reproducing Property

The Reproducing Property can be extended to derivatives if the kernel is smooth:

Theorem

Let $k(\cdot, \cdot) \in C^{2k}(\mathbb{X} \times \mathbb{X})$ *be a positive definite function on an open set* $\mathbb{X}$*. Then all functions in* $\mathbb{H}$ *are* C^k *and we have for all* $|\alpha| \leq k$*:*

$$D^\alpha f(x) = \langle f,\, D^\alpha k(x, \cdot)\rangle_{\mathbb{H}} \,,$$

where the derivative acts on the first argument of k*.*

References

Berlinet and Thomas-Agnan, *Reproducing Kernel Hilbert Spaces in Probability and Statistics* (2004)

Wendland, *Scattered Data Approximation* (2005)

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Rank-one Operators

In order to approximate the generator on an RKHS, we introduce rank-one operators of the type:

$$\mathcal{T}_x^\alpha : \mathbb{H} \mapsto \mathbb{H}, \; x \in \mathbb{X},$$
$$\mathcal{T}_x^\alpha f := \langle f, \, D^\alpha k(x, \cdot) \rangle_{\mathbb{H}} \, k(x, \cdot).$$

We can verify for all $f, g \in \mathbb{H}$:

$$\begin{aligned} \langle \mathcal{T}_x^\alpha f, \, g \rangle_{\mathbb{H}} &= \langle f, \, D^\alpha k(x, \cdot) \rangle_{\mathbb{H}} \, \langle k(x, \cdot), \, g \rangle_{\mathbb{H}} \\ &= D^\alpha f(x) \, \langle k(x, \cdot), \, g \rangle_{\mathbb{H}} = D^\alpha f(x) g(x). \end{aligned}$$

kgEDMD

Approximating Differential Operators

Consider a formal operator

$$\mathcal{T}_{\mathbb{H}}^{\alpha} f = \int_{\mathbb{X}} w(x) \left\langle f,\; D^{\alpha} k(x,\cdot) \right\rangle_{\mathbb{H}} k(x,\cdot)\, \mathrm{d}\mu(x),$$

where w is a weight function. This is a bounded linear operator on $\mathbb{H}$ if:

$$\int_{\mathbb{X}} |w(x)| \|D^{\alpha} k(x,\cdot)\|_{\mathbb{H}} \|k(x,\cdot)\|_{\mathbb{H}} \,\mathrm{d}\mu(x) < \infty.$$

Approximating Differential Operators

We can then verify that

$$
\begin{aligned}
\langle \mathcal{T}_{\mathbb{H}}^{\alpha} f,\, g \rangle_{\mathbb{H}} &= \left\langle \int_{\mathbb{X}} w(x) \, \langle f,\, D^{\alpha} k(x,\cdot) \rangle_{\mathbb{H}} \, k(x,\cdot) \, \mathrm{d}\mu(x),\, g \right\rangle_{\mathbb{H}} \\
&= \int_{\mathbb{X}} w(x) \, \langle f,\, D^{\alpha} k(x,\cdot) \rangle_{\mathbb{H}} \, \langle k(x,\cdot),\, g \rangle_{\mathbb{H}} \, \mathrm{d}\mu(x) \\
&= \int_{\mathbb{X}} w(x) D^{\alpha} f(x) g(x) \, \mathrm{d}\mu(x).
\end{aligned}
$$

The last term is an inner product in L^2_μ between a function g and the action of a differential operator $w(\cdot)D^{\alpha} f(\cdot)$ on another function f.

Approximating the Generator

For the generator of an SDE, we can make the definitions:

$$\mathcal{L}_{\mathbb{H}} f = \int_{\mathbb{X}} \left[\sum_i b_i(x) \left\langle D^{e_i} k(x,\cdot),\ f \right\rangle_{\mathbb{H}} + \frac{1}{2} \sum_{i,j} a_{ij}(x) \left\langle D^{e_i + e_j} k(x,\cdot),\ f \right\rangle_{\mathbb{H}} \right] k(x,\cdot)\, \mathrm{d}\mu(x),$$

$$\mathcal{C}_{00} f = \int_{\mathbb{X}} \langle k(x,\cdot),\ f \rangle_{\mathbb{H}}\, k(x,\cdot)\, \mathrm{d}\mu(x).$$

Galerkin Approximation

Theorem

Assume that $\mathbb{H} \subset \mathcal{D}(\mathcal{L})$*, and that*

$$\int |a_{ij}(x)| \| D^{e_i + e_j} k(x, \cdot) \|_{\mathbb{H}} \| k(x, \cdot) \|_{\mathbb{H}} \, \mathrm{d}\mu(x) < \infty,$$

$$\int |b_i(x)| \| D^{e_i} k(x, \cdot) \|_{\mathbb{H}} \| k(x, \cdot) \|_{\mathbb{H}} \, \mathrm{d}\mu(x) < \infty,$$

$$\int \| k(x, \cdot) \|_{\mathbb{H}}^2 \, \mathrm{d}\mu(x) < \infty.$$

Then, for all $f, g \in \mathbb{H}$*,*

$$\langle \mathcal{L} f, g \rangle_\mu = \langle \mathcal{L}_{\mathbb{H}} f, g \rangle_{\mathbb{H}}, \qquad \langle f, g \rangle_\mu = \langle \mathcal{C}_{00} f, g \rangle_{\mathbb{H}}.$$

Klus, Nüske, and Hamzi, *Entropy* (2020)

Numerical Algorithm

Data-driven approximations of the RKHS operators:

$$\mathrm{d}k(x_m) = \frac{1}{2}\sum_{i,j} a_{ij}(x_m) D^{e_i+e_j} k(x_m, \cdot) + \sum_i b_i(x_m) D^{e_i} k(x_m, \cdot),$$

$$\widehat{\mathcal{C}}_{00} = \frac{1}{M}\sum_{m=1}^{M} \langle k(x_m, \cdot), \cdot\rangle_{\mathbb{H}}\, k(x_m, \cdot),$$

$$\widehat{\mathcal{L}}_{\mathbb{H}} = \frac{1}{M}\sum_{m=1}^{M} \langle \mathrm{d}k(x_m), \cdot\rangle_{\mathbb{H}}\, k(x_m, \cdot).$$

Convergence: $\|\mathcal{L}_{\mathbb{H}} - \widehat{\mathcal{L}}_{\mathbb{H}}\|_{\mathrm{HS}} \to 0$, $\|\mathcal{C}_{00} - \widehat{\mathcal{C}}_{00}\|_{\mathrm{HS}} \to 0$ with $m \to \infty$.

Klus, Nüske, and Hamzi, *Entropy* (2020)

Comments

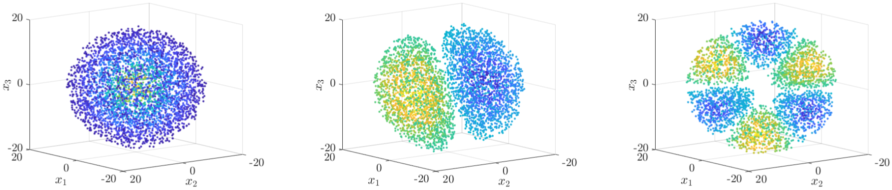
- Finite-dimensional matrix representations of these operators can be obtained. These matrices require evaluations of drift / diffusion, and of derivatives of the kernel function, at the data sites.
- The same formalism can be applied to derive kernel approximations for other differential operators, e.g. Schrödinger operators.

Klus, Nüske, and Hamzi, *Entropy* (2020)

Example

Schrödinger operator for the hydrogen atom in $\mathbb{R}^3$:

$$\mathcal{T} = -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{4\pi\epsilon_0 \|x\|}$$



Discussion

- \+ Large approximation spaces can be used implicitly to approximate the Koopman generator.
- \+ Approximation quality of RKHS has been studied for a long time.
- +- Requires solution of matrix eigenvalue problems of the same size as the data.
- \- These problems may be poorly conditioned.
- \- Hyper-parameters of the kernel function need to be tuned.