Lecture 02: Reproducing Kernel Hilbert Spaces

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Reproducing kernel Hilbert spaces (RKHS) are function spaces that play an important role in the analysis of neural networks and other machine learning models. These spaces contain "complex" non-linear functions, yet the spaces are surprisingly structured in a way that's amenable to theoretical analysis.

Most texts introduce RKHS from a functional analysis perspective. Here we will provide a simpler introduction, starting with spaces of finite-dimensional linear functions and gaining complexity. The goal is to elevate concepts from standard matrix-based linear algebra into abstract infinite-dimensional spaces of functions.

These notes are a brief introduction to RKHS, foregoing many important properties and theorems. See [Wainwright, 2019, Ch. 12] for a thorough reference.

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1) Linear Functions and Inner Products

Consider the space of $\mathbb{R} \to \mathbb{R}$ functions

$$\mathcal{H} = \left\{ f(x) = \sum_{j=1}^{d} \left[\theta_{2j-1} \cos(jx) + \theta_{2j} \sin(jx) \right] \; : \; \theta_1, \ldots, \theta_{2d} \in \mathbb{R} \right\}$$

for some $d \in \mathbb{N}$. The space considers all linear functions that can be built off of a $2d$-dimensional Fourier basis expansion of x. Note that any function $f(\cdot) \in \mathcal{H}$ can be written as:

$$f(x) = \left\langle \underbrace{\begin{bmatrix} \theta_1 \\ \vdots \\ \theta_{2d} \end{bmatrix}}_{\boldsymbol{\theta}}, \underbrace{\begin{bmatrix} \cos(x) \\ \vdots \\ \sin_{dx}(x) \end{bmatrix}}_{\boldsymbol{z}(x)} \right\rangle, \tag{1}$$

where $\boldsymbol{\theta} \in \mathbb{R}^{2d}$ are the function parameters and $\boldsymbol{z} : \mathbb{R} \to \mathbb{R}^{2d}$ is the Fourier basis expansion function. We refer to $\boldsymbol{z}(x) \in \mathbb{R}^{2d}$ as a **feature representation** of x. Assuming the basis expansion is fixed, any $f(\cdot) \in \mathbb{R}^{2d}$ is entirely specified by $\boldsymbol{\theta}$, and so we can implicitly define $f(\cdot)$ through $\boldsymbol{\theta}$. We thus refer to $\boldsymbol{\theta}$ as the **function representation** of $f(\cdot)$.

Evaluating $f(\cdot)$ on any input x requires computing an inner product between two vectors: $\boldsymbol{\theta}$ and $\boldsymbol{z}(x)$. While this fact may seem straightforward, it unearths a lot of interesting complexities:

- The inner product we use to evaluate $f(x)$ can also be used to compare two functions. I.e., given $f(x) = \langle \boldsymbol{\theta}, \boldsymbol{z}(x) \rangle$ and $\tilde{f}(x) = \langle \tilde{\boldsymbol{\theta}}, \boldsymbol{z}(x) \rangle$, we can compute $\langle \boldsymbol{\theta}, \tilde{\boldsymbol{\theta}} \rangle$.
  - We can also use the same inner product to define a norm $\|\boldsymbol{\theta}\| = \langle \boldsymbol{\theta}, \boldsymbol{\theta} \rangle^{1/2}$.
- For any $x' \in \mathbb{R}$, the vector $\boldsymbol{z}(x')$ is also a $\mathbb{R}^{2d}$ vector and thus parameterizes a function in $\mathcal{H}$. (I.e. there exists some $k_{x'}(x) = \langle \boldsymbol{z}(x'), \boldsymbol{z}(x) \rangle$.)
  - In other words, for every x, we have a *function representation* $k_x(\cdot)$ in addition to its *feature representation* $\boldsymbol{z}(x)$!

2) From Inner Products on Vectors to Inner Products on Functions

Because there is a one-to-one mapping between vectors $\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}}, \boldsymbol{z}(x') \in \mathbb{R}^{2d}$ to functions $f(\cdot), \tilde{f}(\cdot), k_{x'}(\cdot) \in \mathcal{H}$, we can define an *inner product on* $\mathcal{H}$ using our inner product over $\mathbb{R}^{2d}$:

$$\left\langle f(\cdot), \tilde{f}(\cdot) \right\rangle_{\mathcal{H}} := \left\langle \boldsymbol{\theta}, \tilde{\boldsymbol{\theta}} \right\rangle \qquad (f(\cdot) = \langle \boldsymbol{\theta}, \boldsymbol{z}(\cdot) \rangle, \quad \tilde{f}(\cdot) = \langle \tilde{\boldsymbol{\theta}}, \boldsymbol{z}(\cdot) \rangle)$$

Curiously, since $k_{x'}(\cdot) = \langle \boldsymbol{z}(x'), \boldsymbol{z}(\cdot) \rangle \in \mathcal{H}$, our inner product over $\mathcal{H}$ can be used to *evaluate* $\mathcal{H}$ functions!

$$f(x') = \langle f(\cdot), k_{x'}(\cdot) \rangle_{\mathcal{H}} = \langle \boldsymbol{\theta}, \boldsymbol{z}(\cdot) \rangle \qquad (f(\cdot) = \langle \boldsymbol{\theta}, \boldsymbol{z}(\cdot) \rangle, \quad k_{x'}(\cdot) = \langle \boldsymbol{z}(x'), \boldsymbol{z}(\cdot) \rangle)$$

We thus refer to $k_{x'}(\cdot)$ as the **evaluation function** for x'.

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3) Dual (Data-Based) Representations and Kernel Functions

Given a set of $x_1, \ldots, x_{2d}$ so that $\boldsymbol{z}(x_1), \ldots, \boldsymbol{z}(x_{2d})$ spans $\mathbb{R}^{2d}$, any $\theta \in \mathbb{R}^{2d}$ can be defined as $\sum_{j=1}^{2d} \alpha_j \boldsymbol{z}(x_j)$ for some $\alpha_1, \ldots, \alpha_{2d}$, and thus any $f(\cdot) \in \mathcal{H}$ can be written as

$$f(\cdot) = \left\langle \left(\sum_{j=1}^{2d} \alpha_j \boldsymbol{z}(x_j) \right), \boldsymbol{z}(\cdot) \right\rangle = \sum_{j=1}^{2d} \alpha_j \left\langle \boldsymbol{z}(x_j), \boldsymbol{z}(\cdot) \right\rangle = \sum_{j=1}^{2d} \alpha_j \underbrace{\left\langle k_{x_j}(\cdot), k_x(\cdot) \right\rangle}_{:=k(x_j, x)}.$$

In other words, any function $f \in \mathcal{H}$ admits a **dual (data-based) representation** through the **kernel function** $k(\cdot, \cdot)$:

$$\mathcal{H} = \left\{ f(\cdot) = \sum_{j=1}^{2d} \alpha_j k(x_j, \cdot), : \ \alpha_j \in \mathbb{R}, \ x_j \in \mathbb{R} \right\}. \tag{2}$$

There is a deep connection between this dual representation and standard training of machine learning algorithms:

Theorem 1 (Representer Theorem [Kimeldorf and Wahba, 1970, Schölkopf et al., 2001])**.** *Given training data $(x_1, y_1), \ldots, (x_n, y_n)$, some loss function $\ell(f(x), y)$, and some regularization parameter $\lambda > 0$, the solution to the regularized training objective can be written as*

$$f^*(x) = \sum_{j=1}^{n} \alpha_j k(x_j, x)$$

for some $\alpha_1, \ldots, \alpha_n$.

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4) Spectrum of the Kernel Function

The kernel function $k(x, x') = \langle \boldsymbol{z}(x), \boldsymbol{z}(x') \rangle$ has some curious properties.

- For any $x_1, \ldots, x_n$, the matrix

  $$\begin{bmatrix} k(x_1, x_1) & \ldots & k(x_1, x_n) \\ \vdots & \ddots & \vdots \\ k(x_n, x_1) & \ldots & k(x_n, x_n) \end{bmatrix} = \begin{bmatrix} \boldsymbol{z}(x_1)^\top \\ \vdots \\ \boldsymbol{z}(x_n)^\top \end{bmatrix} \begin{bmatrix} \boldsymbol{z}(x_1) & \ldots & \boldsymbol{z}(x_n) \end{bmatrix}$$

  is positive definite.

- $k(x, x')$ can be defined through the eigenvalues of the matrix $\mathbb{E}[\boldsymbol{z}(x)\boldsymbol{z}(x)^\top] \in \mathbb{R}^{2d\times 2d}$. Letting $\boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^\top$ be an eigendecomposition of $\boldsymbol{\Sigma} := \mathbb{E}[\boldsymbol{z}(x)\boldsymbol{z}(x)^\top]$, define

$$\{\phi_j(\cdot) = \lambda^{-1/2}\langle \boldsymbol{v}_j, \boldsymbol{z}(\cdot)\rangle\}_{j=1}^{2d}$$

as **eigenfunctions** of $\mathcal{H}$ (where $\boldsymbol{v}_j$ and λ_j are the columns of $\boldsymbol{V}$ and diagonals of $\boldsymbol{\Lambda}$ respectively). Then:

$$\begin{aligned} k(x, x') = \langle \boldsymbol{z}(x), \boldsymbol{z}(x')\rangle &= \left(\boldsymbol{z}(x)\boldsymbol{V}\boldsymbol{\Sigma}^{-1/2}\right)\boldsymbol{\Sigma}\left(\boldsymbol{\Sigma}^{-1/2}\boldsymbol{V}\boldsymbol{z}(x')\right) \\ &= \sum_{j=1}^{2d} \lambda_j \left(\lambda_j^{-1/2}\boldsymbol{v}_j\boldsymbol{z}(x)\right)\left(\lambda_j^{-1/2}\boldsymbol{v}_j\boldsymbol{z}(x)\right) \\ &= \sum_{j=1}^{2d} \lambda_j \phi_j(x)\phi_j(x'). \end{aligned} \tag{3}$$

Moreover, we can easily verify that:

$$\begin{aligned} \mathbb{E}[\phi_i(x)\phi_j(x)] &= \mathbb{E}[\left(\lambda_i^{-1/2}\lambda_j^{-1/2}\right)\boldsymbol{v}_i^\top \boldsymbol{z}(\boldsymbol{x})\boldsymbol{z}(\boldsymbol{x})^\top \boldsymbol{v}_j] \\ &= \left(\lambda_i^{-1/2}\lambda_j^{-1/2}\right)\boldsymbol{v}_i^\top \boldsymbol{\Sigma}\boldsymbol{v}_j \\ &= \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} \end{aligned}$$

This spectral representation of $k(\cdot, \cdot)$ contains lots of information about $\mathcal{H}$. Since $\boldsymbol{\Sigma}$ is positive definite, we know that $\lambda_1, \ldots, \lambda_d > 0$. If the eigenvalues decay quickly, then $\boldsymbol{\Sigma}$ is low-rank implying that many of the features in $\boldsymbol{z}(\cdot)$ are co-linear/redundant. This implies that $\mathcal{H}$ may be an "intrinsically low-dimensional" space (approximately few degrees of freedom) even though there are actually $2d$ parameters to fit.

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5) Reproducing Kernel Hilbert Spaces

Why did we go through the trouble of defining:

- an inner product over functions,
- a data-based representation of functions, and
- an eigendecomposition of a function?

It turns out this is the right abstraction to define powerful spaces of functions with remarkably easy-to-analyze properties. Everything we just defined holds even if we change the feature representation or even if we take $d \to \infty$.

Definition 1 (Reproducing Kernel Hilbert Spaces (RKHS))**.** *Given a positive definite kernel function $k(\cdot, \cdot) : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$; i.e. a function that can be written as:*

$$k(x, x') = \sum_{i=1}^{\infty} \lambda_i \phi_i(x)\phi_i(x'), \qquad \lambda_1 \geq \lambda_2 \geq \ldots \geq 0, \quad \mathbb{E}[\phi_i(x)\phi_i(x')] = \delta_{ij},$$

a reproducing kernel Hilbert space $\mathcal{H}$ is the space[1] *of $\mathcal{X} \to \mathbb{R}$ functions that can be written as*

$$f(\cdot) = \sum_{i=1}^{n} \alpha_i k(\boldsymbol{x}_i, \cdot), \qquad n \in \mathbb{N}, \{\boldsymbol{x}_i\}_{i=1}^{n} \in \mathcal{X}. \tag{4}$$

The inner product associated with $\mathcal{H}$ is given by

$$\left\langle f(\cdot), \tilde{f}(\cdot) \right\rangle = \sum_{i=1}^{n} \sum_{j=1}^{\tilde{n}} \alpha_i \tilde{\alpha}_j k(\boldsymbol{x}_j, \tilde{\boldsymbol{x}}_j).$$

Note that we could have alternatively defined the RKHS using the *infinite-dimensional feature expansion* implied by the eigendecomposition of $k(\cdot, \cdot)$:

$$\mathcal{H} = \left\{ f(\cdot) = \sum_{j=1}^{\infty} \theta_j \left(\lambda_j^{1/2} \phi(\cdot) \right), \quad \theta_1, \theta_2, \ldots \in \mathbb{R} \right\}.$$

(As an exercise, you should show that these two definitions yield the same space of functions.) There are many other equivalent definitions of reproducing kernel Hilbert spaces. (seee [e.g. Wainwright, 2019, Ch 12]). However, rather than dealing with infinite-dimensional vectors, we can instead deal with scalar kernel functions $k(\boldsymbol{x}, \boldsymbol{x}')$. This abstraction will yield simple closed-form expressions of neural network as well as straightforward analyses of their generalization properties.

The only portion of the feature expansion we will consider are the eigenvalues λ_1, λ_2, $\ldots$ associated with $k(\boldsymbol{x}, \boldsymbol{x}')$. As discussed above, the rate of decay of this spectrum tells us about the relative complexity of $\mathcal{H}$, which will be necessary for the analysis of generalization.

References

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B. Schölkopf, R. Herbrich, and A. J. Smola. A generalized representer theorem. In *International Conference on Computational Learning Theory*, pages 416–426, 2001.

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[1] Technically, $\mathcal{H}$ is the *completion* of the space defined by Eq. (4).