Regularization

tion properties as Υ . Next, we formally state the equivalence between RKHS and regularization operator view.

Theorem 4.9 (RKHS and Regularization Operators) For every RKHS \mathcal{H} with reproducing kernel k there exists a linear operator $\Upsilon : \mathcal{H} \to \mathcal{D}$ such that for all $f \in \mathcal{H}$

$$\langle \Upsilon k(x,\cdot), \Upsilon f(\cdot) \rangle_{\mathcal{D}} = f(x), \tag{4.19}$$

and in particular,

$$\langle \Upsilon k(x,\cdot), \Upsilon k(x',\cdot) \rangle_{\mathcal{D}} = k(x,x'). \tag{4.20}$$

Matching RKHS Likewise, for every positive definite linear self-adjoint operator $\tilde{\Upsilon} : \mathcal{F} \to \mathcal{F}$ for which a Green's function exists, there exists a corresponding RKHS \mathcal{H} with reproducing kernel k, a dot product space \mathcal{D} , and an operator $\Upsilon : \mathcal{F} \to \mathcal{D}$ such that (4.19) and (4.20) are satisfied.

Equation (4.20) is useful to analyze smoothness properties of kernels, in particular if we pick \mathcal{D} to be $L_2(\mathcal{X})$. Here we will obtain an explicit form of the dot product induced by the RKHS which helps us to understand why kernel methods work.

From Section 2.2.4 we can see that minimization of $\|\mathbf{w}\|^2$ is equivalent to minimization of $\Omega[f]$ (4.18), due to the feature map $\Phi(x) := k(x, \cdot)$.

Proof We prove the first part by explicitly constructing an operator that takes care of the mapping. One can see immediately that $\Upsilon = \mathbf{1}$ and $\mathcal{D} = \mathcal{H}$ will satisfy all requirements.¹

For the converse statement, we have to obtain k, \mathcal{D} and Υ from $\tilde{\Upsilon}$ and show that k is, in fact, the kernel of an RKHS (note that this does not imply that $\mathcal{F} = \mathcal{H}$ since it may be equipped with a different dot product than \mathcal{H}).

Set $\mathcal{D} = \mathcal{F}$. Since $\tilde{\Upsilon}$ is positive definite, there exists an operator Υ such that $\tilde{\Upsilon} = \Upsilon^* \Upsilon$ (e.g., set $\Upsilon = (\tilde{\Upsilon})^{\frac{1}{2}}$). Next we show that the Green's function $G_x(\cdot)$ of $\tilde{\Upsilon}$ is a kernel. Green's functions are known to satisfy

$$f(x) = \left\langle \tilde{\Upsilon}G_x(\cdot), f \right\rangle_{\mathcal{F}} = \left\langle \Upsilon G_x(\cdot), \Upsilon f \right\rangle_{\mathcal{F}}.$$
(4.21)

for all $f \in \Upsilon^* \Upsilon \mathcal{F}$ is called *Green's function* of the operator $\Upsilon^* \Upsilon$ on \mathcal{F} . For further information on Green's functions, see ?). Note that this amounts to our desired reproducing property (4.19), on the set $\Upsilon^* \Upsilon \mathcal{F}$. The second equality in (4.21) follows from the definition of the adjoint operator Υ^* .

By applying (4.21) to G_x it follows immediately that G is symmetric, for every $f \in \tilde{\Upsilon}\mathcal{F}$. The second equality follows from the factorization $\tilde{\Upsilon} = \Upsilon^* \Upsilon$. It implies that G_x satisfies the reproducing property (4.19). Furthermore $G_x(x')$ is symmetric in (x, x'), since

$$G_x(x') = \left\langle \tilde{\Upsilon} G_{x'}(\cdot), G_x(\cdot) \right\rangle_{\mathcal{F}} = \left\langle G_{x'}(\cdot), \tilde{\Upsilon} G_x(\cdot) \right\rangle_{\mathcal{F}} = \left\langle \tilde{\Upsilon} G_x(\cdot), G_{x'}(\cdot) \right\rangle_{\mathcal{F}} = G_{x'}(x).$$
(4.22)

^{1.} $\Upsilon = \mathbf{1}$ is not the most useful operator. Typically we will seek an operator Υ corresponding to a *specific* dot product space \mathcal{D} . Note that \mathcal{D} and Υ associated with $\tilde{\Upsilon}$ are not unique.