Regularization in Reproducing Kernel Banach Spaces

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Outline

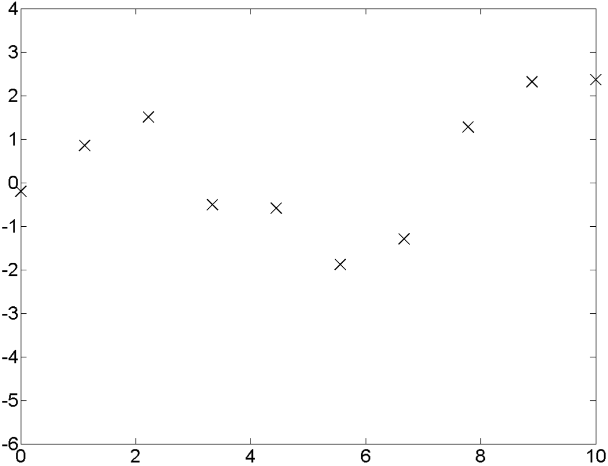
1. Scattered Data Approximation
2. Reproducing Kernel Hilbert Spaces
3. Reproducing Kernel Banach Spaces

Setting:

- Given data $\{(\boldsymbol{x}_j, y_j) : j = 1, 2, \ldots, n\}$ in $\mathbb{R}^d \times \mathbb{R}$.
- Find a function Pf which is a “good fit” to the given data.

Question 1

What is a “good fit”?



scattered data points

A Regularization Approach

- We want to control
  - the closeness to the given data
  - the complexity of the function
- A regularization approach:
  - Target function: $L(f, \mathbf{y}, \mathcal{H}) := \sum_{j=1}^{n} (f(\mathbf{x}_j) - y_j)^2 + \lambda \|f\|_{\mathcal{H}}^2$
  - $Pf := \arg\min_{f \in \mathcal{H}} L(f, \mathbf{y}, \mathcal{H})$.
  - Some fancy names: penalized least square, ridge regression, smoothing spline

Question 2

What is the hypothesis space $\mathcal{H}$?

Reproducing Kernel Hilbert Spaces (RKHS)

- We need
  - $\mathcal{H}$ is a Hilbert space
  - $\|f_n - f\|_{\mathcal{H}} \to 0 \Longrightarrow f_n(x) - f(x) \to 0$ for all $x \in \mathcal{X}$
- RKHS: a Hilbert space $\mathcal{H}$ on which the point evaluation functional is continuous.
  - $|f(x)| \leq M_x \|f\|_{\mathcal{H}}$ for all $x \in \mathcal{X}$

Question 3

Where is the "kernel"?

Kernel

- Suppose $\mathcal{X}$ is a subset of $\mathbb{R}^d$.
- K is a real-valued function on $\mathcal{X} \times \mathcal{X}$:

$$K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$$

- K is a kernel if for any positive integer m and $X := \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m\} \subset \mathcal{X}$, the kernel gram matrix

$$\mathsf{K}_m := [K(\boldsymbol{x}_j, \boldsymbol{x}_l) : 1 \leq j, l \leq m]$$

is symmetric and positive semi-definite.

Connections Between RKHS and Kernels

- [Aronszajn, 1950] There is a bijective mapping from the RKHS to the set of kernels such that
  - ▷ $K(\cdot, \boldsymbol{x}) \in \mathcal{H}$ for any $\boldsymbol{x} \in \mathcal{X}$,
  - ▷ $f(\boldsymbol{x}) = (f(\cdot), K(\cdot, \boldsymbol{x}))_{\mathcal{H}}$ for any $f \in \mathcal{H}$.

- Some properties of RKHS $\mathcal{H}_K$ and the kernel K
  - ▷ $\mathcal{H}_0 := \text{span}\{K(\cdot, \boldsymbol{x}) : \boldsymbol{x} \in \mathcal{X}\}$ is dense in $\mathcal{H}_K$.
  - ▷ For any $f = \sum_{j=1}^{m} c_j K(\cdot, \boldsymbol{x}_j) \in \mathcal{H}_0$,

$$\|f\|_{\mathcal{H}_K} = \|\mathsf{K}_m^{1/2} \boldsymbol{c}\|_2.$$

Some Examples of RKHS and Kernels

- Sobolev space $H^2(\mathbb{R})$: $K(s,t) = \frac{\sqrt{3}}{3} e^{-\frac{\sqrt{3}}{2}|s-t|} \sin\left(\frac{|s-t|}{2} + \frac{\pi}{6}\right)$.
- C^0 Matérn kernel: $K(s,t) = \mathrm{e}^{-|s-t|}$
- Gaussian kernel: $K(s,t) = \mathrm{e}^{-w(s-t)^2},\ w > 0$.
- Sinc kernel: $K(s,t) = \operatorname{sinc}(s-t)$.
- Polynomial kernels: $K(s,t) = (st)^d,\ d = 1, 2, \ldots$.
- $L^2(\mathbb{R})$ is NOT a RKHS.

Regularization in the RKHS $\mathcal{H}_K$

- [Kimeldorf and Wahba, 1971] Representer Theorem :
  - Target function: $L(f, \boldsymbol{y}, \mathcal{H}_K) = \sum_{j=1}^{n} (f(\boldsymbol{x}_j) - y_j)^2 + \lambda \|f\|_{\mathcal{H}_K}^2$.
  - Let $\mathcal{S}_n := \text{span}\{K(\cdot, \boldsymbol{x}_j) : j = 1, 2, \ldots, n\}$.
  - The optimization problem reduces to finite-dimensional:

$$\min_{f \in \mathcal{H}_K} L(f, \boldsymbol{y}, \mathcal{H}_K) = \min_{f \in \mathcal{S}_n} L(f, \boldsymbol{y}, \mathcal{H}_K)$$

  - The minimizer is explicitly given:

$$Pf = \sum_{j=1}^{n} \alpha_j K(\cdot, \boldsymbol{x}_j), \qquad \text{where } \boldsymbol{\alpha} = (\mathsf{K}_n + \lambda \mathsf{I}_n)^{-1} \boldsymbol{y}.$$

Reproducing Kernel Banach Spaces

- We try to construct
  - a Banach space $\mathcal{B}$
  - point evaluation functional $\delta_{\boldsymbol{x}}$ is continuous on $\mathcal{B}$
- A specific construction
  - Let $\mathcal{B}_0 := \operatorname{span}\{K(\cdot, \boldsymbol{x}) : \boldsymbol{x} \in \mathcal{X}\}$.
  - For any $f = \sum_{j=1}^m c_j K(\cdot, \boldsymbol{x}_j) \in \mathcal{B}_0$, define

$$\|f\|_{\mathcal{B}} := \|\boldsymbol{c}\|_1.$$

  - $\delta_{\boldsymbol{x}}$ is continuous on $\mathcal{B}_0$ if $K(\cdot, \cdot)$ is uniformly bounded.
  - Let $\mathcal{B}$ be the Banach completion of $\mathcal{B}_0$ with the norm $\|\cdot\|_{\mathcal{B}}$.

Some Properties of RKBS

- [Song2010+] Point evaluation functional is continuous on $\mathcal{B}$ if and only if

$$\sum_{j=1}^{\infty} \alpha_j K(\cdot, \boldsymbol{x}_j) = 0 \Longrightarrow \boldsymbol{\alpha} = 0.$$

- [Song2010+] Reproducing property still holds.
  - ▷ Define a bilinear form $< \cdot, \cdot >$ on $\mathcal{B}_0 \times \mathcal{B}_0$ such that

$$< \sum_{j=1}^{m} \alpha_j K(\cdot, \boldsymbol{x}_j), \sum_{j=1}^{m} \beta_j K(\cdot, \boldsymbol{x}_j) >= \boldsymbol{\alpha}^T \mathsf{K}_m \boldsymbol{\beta}$$

  - ▷ The bilinear form $< \cdot, \cdot >$ can be extended to $\mathcal{B} \times \mathcal{B}$ such that

$$< f, K(\cdot, \boldsymbol{x}) >= f(\boldsymbol{x}), \qquad \boldsymbol{x} \in \mathcal{X}, f \in \mathcal{B}.$$

Regularization in RKBS

- Target function: $L(f, \boldsymbol{y}, \mathcal{B}) = \sum_{j=1}^{n} \left(f(\boldsymbol{x}_j) - y_j\right)^2 + \lambda \|f\|_{\mathcal{B}}$.
- Recall $\mathcal{S}_n = \operatorname{span}\{K(\cdot, \boldsymbol{x}_j) : j = 1, 2, \ldots, n\}$.
- Does the optimization problem reduce to finite-dimensional?

$$\min_{f \in \mathcal{B}} L(f, \boldsymbol{y}, \mathcal{B}) \overset{??}{=} \min_{f \in \mathcal{S}_n} L(f, \boldsymbol{y}, \mathcal{B})$$

- If it can reduce to finite-dimensional, how to find the minimizer $Pf = \sum_{j=1}^{n} \alpha_j K(\cdot, \boldsymbol{x}_j)$?

Regularization and Interpolation

- Define the interpolation space
  $\mathcal{I}_n(\boldsymbol{y}) = \{f \in \mathcal{B} : f(\boldsymbol{x}_j) = y_j,\ j = 1, 2, \ldots, n\}$.

- [Song2010+] The following two statements are equivalent.
  - $\min_{f \in \mathcal{B}} L(f, \boldsymbol{y}, \mathcal{B}) = \min_{f \in \mathcal{S}_n} L(f, \boldsymbol{y}, \mathcal{B}),$ for all $\boldsymbol{y} \in \mathbb{R}^n$.
  - $\min_{f \in \mathcal{I}_n(\boldsymbol{y})} \|f\|_{\mathcal{B}} = \min_{f \in \mathcal{I}_n(\boldsymbol{y}) \cap \mathcal{S}_n} \|f\|_{\mathcal{B}},$ for all $\boldsymbol{y} \in \mathbb{R}^n$.

- Note that $\mathcal{I}_n(\boldsymbol{y}) \cap \mathcal{S}_n$ has only one element when K_n is invertible.

- We only need to show that the minimal norm interpolation problem admits a minimizer in the finite-dimensional space $\mathcal{S}_n$.

Representer Theorem in RKBS

- Let $\boldsymbol{k}(\boldsymbol{x}) := (K(\boldsymbol{x}, \boldsymbol{x}_1), \ldots, K(\boldsymbol{x}, \boldsymbol{x}_n))^T$.
- [Song2010+] Minimal norm interpolation

$$\min_{f \in \mathcal{I}_n(\boldsymbol{y})} \|f\|_{\mathcal{B}} = \min_{f \in \mathcal{I}_n(\boldsymbol{y}) \cap S_n} \|f\|_{\mathcal{B}}, \qquad \text{for all } \boldsymbol{y} \in \mathbb{R}^n$$

$$\Longleftrightarrow \quad \left\|K_n^{-1}\boldsymbol{k}(\boldsymbol{x})\right\|_1 \leq 1, \qquad \text{for all } \boldsymbol{x} \in \mathcal{X}.$$

- [Song2010+] Regularization

$$\min_{f \in \mathcal{B}} L(f, \boldsymbol{y}, \mathcal{B}) = \min_{f \in \mathcal{S}_n} L(f, \boldsymbol{y}, \mathcal{B}), \qquad \text{for all } \boldsymbol{y} \in \mathbb{R}^n$$

$$\Longleftrightarrow \quad \left\|K_n^{-1}\boldsymbol{k}(\boldsymbol{x})\right\|_1 \leq 1, \qquad \text{for all } \boldsymbol{x} \in \mathcal{X}.$$

Some Examples

- The condition $\left\|K_n^{-1}\boldsymbol{k}(\boldsymbol{x})\right\|_1 \leq 1$ is not easy to check.
- We have only been able to find two kernels satisfying it so far.
  - ▷ $K(s,t) = \min\{s,t\} - st, \quad s,t \in [0,1]$
  - ▷ $K(s,t) = \mathrm{e}^{-|s-t|}, \quad s,t \in \mathbb{R}$
- Counter examples that does not satisfy this condition
  - ▷ Gaussian kernels: $K(s,t) = \mathrm{e}^{-(s-t)^2}, \quad s,t \in \mathbb{R}$
  - ▷ Sinc Kernel: $K(s,t) = \operatorname{sinc}(s-t), \quad s,t \in \mathbb{R}$

How to find the minimizer?

- $\min_{f \in \mathcal{S}_n} L(f, \boldsymbol{y}, \mathcal{B}) = \min \left\{ \sum_{j=1}^{n} (f(\boldsymbol{x}_j) - y_j)^2 + \lambda \|\boldsymbol{c}\|_1 : f = \sum_{j=1}^{n} c_j K(\cdot, \boldsymbol{x}_j) \right\}$
- We do not have a closed form of the minimizer.
- Standard optimization methods may do, but we still need efficient methods especially for large size of data.

Thank you !