On the Connections and Equivalences between Gaussian Processes and Kernel Methods in Nonparametric Regression

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Outline

Learning with Positive Definite Kernels

- In machine learning, positive definite kernels have been widely used in modeling nonlinear relationships between variables.

- There are two major approaches:

Bayesian learning with Gaussian Processes (GP)
[Rasmussen and Williams, 2006]:

- Positive definite kernels appear as covariance kernels
- e.g., Gaussian process regression, Bayesian optimization, probabilistic numerics, etc.

Learning with Positive Definite Kernels

Kernel methods using Reproducing Kernel Hilbert Spaces (RKHS) [Schölkopf and Smola, 2002]:

- Positive definite kernels appear as reproducing kernels.
- e.g., kernel ridge regression, support vector machines, kernel mean embedding, etc.

- These two approaches have been studied extensively in the literature (also in the context of neural networks).

The Aim of the Talk

- I will discuss the connections between the GP– and RKHS–based approaches, focusing on the problem of nonparametric regression.

- There is a well-known result for the equivalence between the two approaches to regression [Kimeldorf and Wahba, 1970].

- On the other hand, it is known that a sample path of the GP prior does not belong to the corresponding RKHS with probability 1 [Driscoll, 1973].

- This apparent difference in the "hypothesis spaces" may give an impression that the connection between the two approaches is rather superficial.

— How can we explain this difference? Does it contradict the equivalence?

The Aim of the Talk

- The aim of the talk is to clarify how these two approaches are related by studying the connections in their theoretical convergence properties.

- It will be shown that the above "apparent difference" does not lead to any contradiction, and there is a clear correspondence in the convergence results.

- The key is to understand that the RKHS approach has two ways of controlling the complexity of a model; the RKHS itself and regularization.

Contents and Collaborators

- The contents of the talk is based on Section 5 of

Kanagawa et al. (2018) Gaussian Processes and Kernel Methods: A Review on Connections and Equivalences, *arXiv preprint* (under revision)

- Collaborators:

- Philipp Hennig (University of Tuebingen and Max Planck Institue)
- Dino Sejdinovic (University of Oxford)
- Bharath K. Sriperumbudur (Penn State University)

Outline

Positive Definite Kernels

- Let $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be a symmetric function on a set $\mathcal{X}$.
- The function $k(x, x')$ is called **positive definite kernel**, if

$$\sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j k(x_i, x_j) \geq 0 \quad \text{holds}$$

$$\text{for all} \quad n \in \mathbb{N}, \quad c_1, \ldots, c_n \in \mathbb{R}, \quad x_1, \ldots, x_n \in \mathcal{X}.$$

- Examples of positive definite kernels on $\mathcal{X} \subset \mathbb{R}^d$:

$$\begin{aligned}
\text{Gaussian} \quad & k(x, x') &&= \exp(-\|x - x'\|^2/\gamma^2). \\
\text{Laplace} \quad & k(x, x') &&= \exp(-\|x - x'\|/\gamma). \\
\text{Linear} \quad & k(x, x') &&= \langle x, x' \rangle. \\
\text{Polynomial} \quad & k(x, x') &&= (\langle x, x' \rangle + c)^m.
\end{aligned}$$

- In this talk, I will simply say kernels to indicate positive definite kernels.

Matérn Kernels

- In this talk, Matérn kernels will play the key role (Let $\mathcal{X} \subset \mathbb{R}^d$).

Example (Matern Kernels)

- For constants $\alpha > 0$ and $h > 0$, the Matérn kernel is defined by

$$k_{\alpha,h}(x, x') = \frac{1}{2^{\alpha-1}\Gamma(\alpha)} \left(\frac{\sqrt{2\alpha}\|x - x'\|}{h} \right)^{\alpha} K_\alpha \left(\frac{\sqrt{2\alpha}\|x - x'\|}{h} \right)$$

where Γ is the Gamma function, and K_α is the modified Bessel function of the second kind of order α.

Matérn Kernels

- If α is a half integer, an analytic form is known: e.g.,

$$k_{1/2,h}(x,x') = \exp\left(-\frac{\|x-x'\|}{h}\right) \quad \text{(Laplace kernel)},$$

$$k_{3/2,h}(x,x') = \left(1+\frac{\sqrt{3}\|x-x'\|}{h}\right)\exp\left(-\frac{\sqrt{3}\|x-x'\|}{h}\right),$$

$$k_{5/2,h}(x,x') = \left(1+\frac{\sqrt{5}\|x-x'\|}{h}+\frac{5\|x-x'\|^2}{3h^2}\right)\exp\left(-\frac{\sqrt{5}\|x-x'\|}{h}\right).$$

- The Gaussian kernel is given by the limit $\alpha \to \infty$ of the Matérn kernel.

$$\lim_{\alpha\to\infty} k_{\alpha,h}(x,x') = \exp\left(-\frac{\|x-x'\|^2}{2h^2}\right), \quad x,x' \in \mathbb{R}^d.$$

- One of the most standard kernels in the literature (e.g., geostatistics, Bayesian optimization)

Gaussian Processes (GP)

- For a given kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ and a function $m : \mathcal{X} \to \mathbb{R}$, we can consider a corresponding Gaussian process (GP), which we denote by

$$g \sim \mathcal{GP}(m, k).$$

- The g is a random function on $\mathcal{X}$ satisfying the following:

  - Take any finite set $X := (x_1, \ldots, x_n) \subset \mathcal{X}$ of any size $n \in \mathbb{N}$,
  - Then the corresponding random vector induced by g

$$g_X := (g(x_1), \ldots, g(x_n))^\intercal \in \mathbb{R}^n$$

  follows the Gaussian distribution $\mathcal{N}(m_X, k_{XX})$ with
  — mean vector $m_X = (m(x_1), \ldots, m(x_n))^\intercal \in \mathbb{R}^n$
  — covariance matrix $k_{XX} = (k(x_i, x_j))_{i,j=1}^n \in \mathbb{R}^{n \times n}$

- $g \sim \mathcal{GP}(m, k)$ is a GP with mean function m and covariance kernel k.

Reproducing Kernel Hilbert Spaces (RKHS)

- For a given kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, there exists a uniquely associated Hilbert space $\mathcal{H}$ consisting of functions on $\mathcal{X}$ such that

$$\text{(i)} \quad k(\cdot, x) \in \mathcal{H} \quad \text{for all } x \in \mathcal{X}$$

where $k(\cdot, x)$ is the function of the first argument with x fixed:

$$x' \in \mathcal{X} \to k(x', x).$$

$$\text{(ii)} \quad f(x) = \langle f, k(\cdot, x) \rangle_{\mathcal{H}} \quad \text{for all } f \in \mathcal{H} \text{ and } x \in \mathcal{X},$$

which is called the **reproducing property**.

– $\mathcal{H}$ is called the RKHS of k.

– $\mathcal{H}$ can be written as

$$\mathcal{H} = \overline{\text{span}\,\{k(\cdot, x) \mid x \in \mathcal{X}\}}$$

Outline

Regression Problem

- Let $(x, y) \in \mathcal{X} \times \mathbb{R}$ be population random variables ($\mathcal{X} \subset \mathbb{R}^d$), such that

$$y = f_0(x) + \varepsilon,$$

where

— $f_0 : \mathcal{X} \to \mathbb{R}$ is the regression function (the "unknown true function");

— ε is an independent, zero-mean noise variable.

- Assume that n i.i.d. observations of (x, y)

$$(x_1, y_1), \ldots, (x_n, y_n)$$

are given as training data: let $D_n := (x_i, y_i)_{i=1}^n$.

- The task of regression is to estimate the unknown true function f_0 using D_n.

Gaussian Process Regression (GPR)

- For the regression problem, GPR takes the Bayesian approach.

- For the true unknown function f_0, we first define a prior distribution as a Gaussian process:

$$f_0 \sim \mathcal{GP}(0, k). \tag{1}$$

(For simplicity, we assume the zero-mean function, $m(x) = 0$).

- Given training data $D_n = (x_i, y_i)_{i=1}^n$, we also define a likelihood function

$$p(D_n|f_0) := \prod_{i=1}^{n} p_{\text{gauss}}(y_i; f_0(x_i), \sigma^2)$$

assuming the i.i.d. Gaussian noise model

$$y_i = f_0(x_i) + \varepsilon_i, \quad \text{where} \quad \varepsilon_i \overset{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2), \quad i = 1, \ldots, n.$$

- Here, $\sigma^2 > 0$ is the noise variance.

Gaussian Process Regression (GPR)

- Then Bayes' rule is applied to obtain the posterior distribution of the true function f_0:

$$P(f_0|D_n) \propto p(D_n|f_0)P(f_0),$$

where $P(f_0)$ indicates the GP prior

$$f_0 \sim \mathcal{GP}(0, k).$$

Gaussian Process Regression (GPR)

- Importantly, the posterior $P(f_0|D_n)$ is also given as a Gaussian process:

- Let $X := (x_1, \ldots, x_n) \in \mathcal{X}^n$ and $Y := (y_1, \ldots, y_n)^\intercal \in \mathbb{R}^n$. Then

$$P(f_0|D_n) = \mathcal{GP}(\bar{m}, \bar{k}),$$

where $\bar{m} : \mathcal{X} \to \mathbb{R}$ and $\bar{k} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ are given by

$$\begin{aligned} \bar{m}(x) &= k_X(x)^\top (k_{XX} + \sigma^2 I_n)^{-1} Y, \quad x \in \mathcal{X}, \\ \bar{k}(x, x') &= k(x, x') - k_X(x)^\top (k_{XX} + \sigma^2 I_n)^{-1} k_X(x'), \quad x, x' \in \mathcal{X}, \end{aligned}$$

where $I_n \in \mathbb{R}^{n \times n}$ is the identity matrix, and

$$k_X(x) := (k(x_1, x), \ldots, k(x_n, x))^\top \in \mathbb{R}^n, \quad k_{XX} := (k(x_i, x_j))_{i,j=1}^n \in \mathbb{R}^{n \times n}.$$

— $\bar{m} : \mathcal{X} \to \mathbb{R}$ is called the posterior mean function;

— $\bar{k} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called the posterior covariance function.

Kernel Ridge Regression (KRR)

- On the other hand, KRR deals with regression by solving the following optimization problem in the RKHS $\mathcal{H}_k$:

$$\hat{f}_\lambda := \arg\min_{f \in \mathcal{H}_k} \frac{1}{n} \sum_{i=1}^{n} (f(x_i) - y_i)^2 + \lambda \|f\|^2_{\mathcal{H}_k},$$

where $\lambda > 0$ is a regularization constant.

- This is a regularized least-squares problem.

— The first term quantifies the fit to the training data $D_n = (x_i, y_i)_{i=1}^n$:

— The second term controls the complexity of the estimate $\hat{f}_\lambda$:

i.e., a larger λ makes $\hat{f}_\lambda$ smoother.

Kernel Ridge Regression (KRR)

- By the representor theorem, the solution $\hat{f}_\lambda$ is given in a closed form.

- Let $X := (x_1, \ldots, x_n) \in \mathcal{X}^n$ and $Y := (y_1, \ldots, y_n)^\intercal \in \mathbb{R}^n$. Then

$$\hat{f}_\lambda(x) = k_X(x)^\top (k_{XX} + n\lambda I_n)^{-1} Y, \quad x \in \mathcal{X},$$

where $I_n \in \mathbb{R}^{n \times n}$ is the identity matrix, and

$$k_X(x) := (k(x_1, x), \ldots, k(x_n, x))^\top \in \mathbb{R}^n, \quad k_{XX} := (k(x_i, x_j))_{i,j=1}^n \in \mathbb{R}^{n \times n}.$$

Outline

Formal Equivalence between GPR and KRR

- Let's compare the posterior mean function of GPR

$$\bar{m}(x) = k_X(x)^\top (k_{XX} + \sigma^2 I_n)^{-1} Y, \quad x \in \mathcal{X},$$

and the estimate of KRR

$$\hat{f}_\lambda(x) = k_X(x)^\top (k_{XX} + n\lambda I_n)^{-1} Y, \quad x \in \mathcal{X},$$

- From this, it immediately follows that the GPR and KRR estimates are equal

$$\bar{m}_n = \hat{f}_\lambda \quad \text{provided that} \quad \sigma^2 = n\lambda.$$

- This is a well known result in the literature [Kimeldorf and Wahba, 1970].

Sample Paths of a Gaussian Process

- On the other hand, it is known that a sample path $g \sim \mathcal{GP}(0, k)$ does not lie in the corresponding RKHS $\mathcal{H}_k$ (when $\mathcal{H}_k$ is infinte dimensional) [Driscoll, 1973]:

$$g \notin \mathcal{H}_k \quad \text{with probability} \quad 1.$$

- Intuitively, the sample path $g \sim \mathcal{GP}(0, k)$ becomes "rougher" than the functions in $\mathcal{H}_k$.

- For instance, assume that the kernel k is a Matern kernel of order $\alpha > 0$.

  - Then $\mathcal{H}_k$ consists of functions having smoothness $s = \alpha + d/2$ (in the sense of Sobolev; $\approx s$-times weakly differentiable), while
  - Sample path $g \sim \mathcal{GP}(0, k)$ has the smoothness α with probability 1.

— i.e., the RKHS $\mathcal{H}_k$ is $d/2$-smoother than the sample path $g \sim \mathcal{GP}(0, k)$.

Apparent Difference in Hypothesis Spaces

- Recall that GPR uses $\mathcal{GP}(0, k)$ to define a prior distribution (or as a hypothesis space) of the unknown true function f_0:

$$f_0 \sim \mathcal{GP}(0, k).$$

- Given that this prior is correct, we have

$$f_0 \notin \mathcal{H}_k \quad \text{with probability} \quad 1.$$

- Does this contradict the fact that KRR uses $\mathcal{H}_k$ as a "hypothesis space"?

$$\hat{f}_\lambda := \arg\min_{f \in \mathcal{H}_k} \frac{1}{n} \sum_{i=1}^{n} (f(x_i) - y_i)^2 + \lambda \|f\|_{\mathcal{H}_k}^2,$$

Apparent Difference in Hypothesis Spaces

- The above fact may give an impression that the formal equivalence between GPR and KRR is rather superficial.

- However, we argue below that the apparent difference between the GP and RKHS as "hypothesis spaces" does not lead to any contradiction.

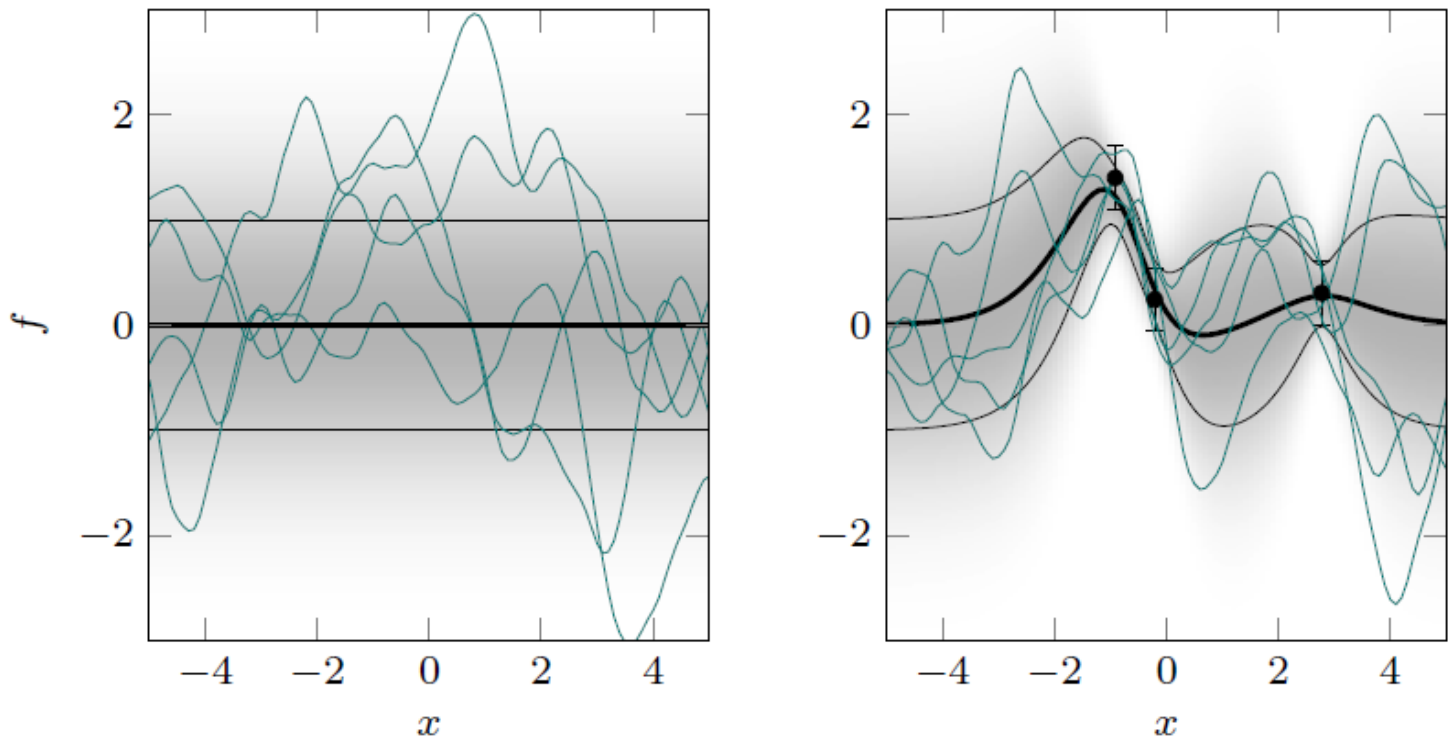
- We do this by studying the correspondence between the convergence properties of GPR and KRR.

- The key point is that KRR does not require $f_0 \in \mathcal{H}_k$ to achieve minimax optimal rates.

Illustration of GPR with a Matérn kernel order $\alpha = 5/2$

- Left: sample paths from the prior $\mathcal{GP}(0, k)$; the thick line is the prior mean function $= 0$.

- Right: sample paths from the posterior $\mathcal{GP}(\bar{m}_n, \bar{k}_n)$; the thick curve is the posterior mean function $\bar{m}_n \in \mathcal{H}_k$. The three points are training data.



Outline

Common Setting

- We assume that the true unknown function f_0 has smoothness $\beta > 0$ (in the sense of Sobolev; $\approx \beta$-times weakly differentiable).

- For simplicity we consider $\mathcal{X} := [0,1]^d \subset \mathbb{R}^d$ as an input space.

- The quality of the estimate $\hat{f}$ (either $\bar{m}_n$ in GPR or $\hat{f}_\lambda$ in KRR) is measured with the L_2 distance with respect an input distribution $P_{\mathcal{X}}$:

$$\|\hat{f} - f_0\|^2_{L_2(P_{\mathcal{X}})} = \int \left(\hat{f}(x) - f(x)\right)^2 dP_{\mathcal{X}}(x)$$

Convergence Rates for Gaussian Process Regression

- We first present a convergence result for GPR that follows from [van der Vaart and van Zanten, 2011].

- Assume that (x, y) are population random variables generated as

  - $x \sim P_{\mathcal{X}}$ for an input distribution $P_{\mathcal{X}}$ on $\mathcal{X} = [0,1]^d$.
  - $y = f_0(x) + \varepsilon$, where $\varepsilon \sim \mathcal{N}(0, \sigma^2)$ is independent.

- Note that f_0 is the true unknown function.

- Assume that the data $D_n := (x_i, y_i)_{i=1}^n$ are i.i.d. with (x, y).

(Note: the Gaussian noise assumption may be relaxed [Kleijn and van der Vaart, 2006])

Convergence Rates for Gaussian Process Regression

- Assume that we perform GPR with a Matérn kernel $k_{\alpha,h}$ of order $\alpha > 0$.

— This means that a sample path from the GP prior has smoothness α.

- Assume that the true function f_0 has smoothness $\beta > 0$ and that $\min(\alpha, \beta) > d/2$.

- Then, the posterior mean $\bar{m}_n$ of GPR with data $D_n = (x_i, y_i)_{i=1}^n$ satisfies

$$\|\bar{m}_n - f_0\|_{L_2(P_X)}^2 = O_p(n^{-2\min(\alpha,\beta)/(2\alpha+d)}) \quad (n \to \infty)$$

under additional minor technical contidions.

Convergence Rates for Gaussian Process Regression

- Let's study the exponent of the rate $n^{-2\min(\alpha,\beta)/(2\alpha+d)}$:

$$\frac{2\min(\alpha,\beta)}{2\alpha+d}$$

- This becomes the largest when

$$\alpha = \beta$$

i.e., when the smoothness α of the GP prior $\mathcal{GP}(0, k_{\alpha,h})$ is equal to the smoothness β of the true function f_0.

- In this case, the rate becomes minimax optimal [Stone, 1980]:

$$\|\bar{m}_n - f_0\|^2_{L_2(P_{\mathcal{X}})} = O_p(n^{-2\beta/(2\beta+d)}) \quad (n \to \infty).$$

- This result indicates that, for GPR to perform well, the GP prior should have the same smoothness as the target function f_0

Convergence Rates for Kernel Ridge Regression

- Next, let's look at a convergence result for KRR that follows from [Steinwart et al., 2009].

- Assume that input-output variables (x, y) are given as

  - $x \sim P_{\mathcal{X}}$ for a probability distribution $P_{\mathcal{X}}$ on $\mathcal{X} = [0, 1]^d$.
  - $y = f_0(x) + \varepsilon$, where ε is an independent noise such that $\varepsilon \in [-M, M]$ for some constant $M > 0$ almost surely.

(Note: the latter boundedness assumption can be relaxed [Fischer and Steinwart, 2020])

Convergence Rates for Kernel Ridge Regression

- Assume that we perform KRR using a Matérn kernel $k_{\alpha,h}$ of order $\alpha > 0$.

— This means that the RKHS $\mathcal{H}_{k_{\alpha,h}}$ has the smoothness $s = \alpha + d/2$.

- Set the regularization constant $\lambda := \lambda_n$ as

$$\lambda_n = cn^{-2s/(2\beta+d)}$$

where $c > 0$ is an arbitrary constant independent of n.

- Assume that the true function f_0 has smoothness β and that $s \geq \beta$.

- Then for (a truncated version) of the KRR estimator $\hat{f}_{\lambda_n}$, we have

$$\|\hat{f}_{\lambda_n} - f_0\|^2_{L_2(P_{\mathcal{X}})} = O_p(n^{-2\beta/(2\beta+d)}) \quad (n \to \infty).$$

under additional minor technical conditions.

Remarks on the Rates for Kernel Ridge Regression

- The rate $n^{-2\beta/(2\beta+d)}$ is minimax optimal in nonparametric regression of a function f_0 on $\mathcal{X} \subset \mathbb{R}^d$ with smoothness β [Stone, 1980].

- The condition $s = \alpha + d/2 \geq \beta$ means that smoothness β of the true function f_0 can be **smaller** than the smoothness s of the RKHS $\mathcal{H}_{k_{\alpha,h}}$.

— i.e., f_0 can be "rougher" than the functions in $\mathcal{H}_{k_{\alpha,h}}$.

— thus, the misspecified setting $f_0 \notin \mathcal{H}_k$ is permitted.

Remarks on the Rates for Kernel Ridge Regression

- Even in the misspecified setting $f_0 \notin \mathcal{H}_k$, KRR can achieve the optimal convergence rate $n^{-2\beta/(2\beta+d)}$.

- This is enabled by an appropriately chosen regularization constant:

$$\lambda_n = cn^{-2s/(2\beta+d)}$$

which should be smaller if β is much smaller than $s = \alpha + d/2$.

i.e., if the true function f_0 is rougher than the RKHS $\mathcal{H}_{k_{\alpha,h}}$, regularization should be weaker.

Correspondence between the Rates for GPR and KRR

- Let's study how the results for GPR and KRR are related.

- Recall that the optimal rate in GPR is achieved by setting $\alpha = \beta$, where

  - β is the smoothness of the true function f_0.
  - α is the smoothness of the GP prior $\mathcal{GP}(0, k_{\alpha,h})$.

- For KRR, this corresponds to setting the smoothness $s = \alpha + d/2$ of the RKHS as

$$s = \beta + d/2 \quad \text{since} \quad \alpha = \beta$$

and the regularization constant λ_n as

$$\lambda_n = cn^{-2(\beta+d/2)/(2\beta+d)} = cn^{-1}$$

which results in the optimal rate $n^{-2\beta/(2\beta+d)}$.

Correspondence between the Rates for GPR and KRR

- In particular, by setting $c := \sigma^2$ (= the noise variance in GPR), the regularization schedule becomes

$$\lambda_n = \sigma^2 n^{-1}.$$

- Recall that this is exactly the condition

$$\sigma^2 = n\lambda_n$$

for the equivalence between GPR and KRR:

$$\bar{m}_n = \hat{f}_{\lambda_n}.$$

Summary of the Discussion

- We started the discussion from the fact that

if the GP prior $f_0 \sim \mathcal{GP}(0, k)$ is correct, we have $f_0 \notin \mathcal{H}_k$ with probability 1.

- This should not be regarded as a contradiction, since KRR allows for the misspecified setting $f_0 \notin \mathcal{H}_k$.

— This is because KRR controls the complexity of the regressor $\hat{f}_{\lambda_n}$ by regularization;

— and the optimal regularization constant λ_n when the GP prior $f_0 \sim \mathcal{GP}(0, k)$ is correct can be given by

$$\lambda_n = \sigma^2 / n$$

which implies the equivalence of GPR and KRR.

Practical Implication of the Correspondence

- Suppose that the kernel $k_{\alpha,h}$ is well-specified (in the sense that the GP sample path has the correct smoothness, $\alpha = \beta$).

- Then, the interpretation of KRR as GPR suggests the following:

- If we set the regularization constant $\lambda_n = \sigma^2/n$ very small, this implies either that

  - we know/believe that the noise variance σ^2 is very small, or that
  - the sample size n is very large.

- If neither of the above points is correct, then we shouldn't set the regularization constant λ_n too small.

Outline

Conclusions

- In this talk, I discussed the correspondence between the GPR and KRR.

- The aim was to resolve the apparent contradiction in their way of defining hypothesis spaces.

- The contradiction is shown to be superficial: the formal equivalence between GPR and KRR is essential, carrying over into their optimal convergence results.

Further Topics

- There are several other connections between the GP and RKHS approaches:

  - RKHS interpretation of GP posterior variance.
  - Powers of an RKHS as GP sample spaces
  - GP interpretations of kernel mean embeddings (e.g., MMD, HSIC)

If you are interested, please look at [Kanagawa et al., 2018].

Contents and Collaborators

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