

Linear in the parameters models and GP

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Key concepts

- Linear in the parameters model correspond to Gaussian processes
- explicitly calculate the GP from the linear model
 - mean function
 - covariance function
- going from covariance function to linear model
 - done using Mercer's theorem
 - may not always result in a **finite** linear model
- computational consideration: which is best?

From random functions to covariance functions

Consider the class of linear functions:

$$f(x) = ax + b, \text{ where } a \sim \mathcal{N}(0, \alpha), \text{ and } b \sim \mathcal{N}(0, \beta).$$

We can compute the mean function:

$$\mu(x) = \mathbb{E}[f(x)] = \iint f(x)p(a)p(b)dad b = \int axp(a)da + \int bp(b)db = 0,$$

and covariance function:

$$\begin{aligned} k(x, x') &= \mathbb{E}[(f(x) - 0)(f(x') - 0)] = \iint (ax + b)(ax' + b)p(a)p(b)dad b \\ &= \int a^2xx'p(a)da + \int b^2p(b)db + (x + x') \int ap(a)p(b)dad b = \alpha xx' + \beta. \end{aligned}$$

Therefore: a linear model with Gaussian random parameters corresponds to a GP with covariance function $k(x, x') = \alpha xx' + \beta$.

From finite linear models to Gaussian processes (1)

Finite linear model with Gaussian priors on the weights:

$$f(x) = \sum_{m=1}^M w_m \phi_m(x) \qquad p(\mathbf{w}) = \mathcal{N}(\mathbf{w}; 0, A)$$

The joint distribution of any $\mathbf{f} = [f(x_1), \dots, f(x_N)]^\top$ is a multivariate Gaussian – this looks like a Gaussian Process!

The prior $p(\mathbf{f})$ is fully characterized by the *mean* and *covariance* functions.

$$\begin{aligned} m(x) = \mathbb{E}_{\mathbf{w}(f(x))} &= \int \left(\sum_{m=1}^M w_m \phi_m(x) \right) p(\mathbf{w}) d\mathbf{w} = \sum_{m=1}^M \phi_m(x) \int w_m p(\mathbf{w}) d\mathbf{w} \\ &= \sum_{m=1}^M \phi_m(x) \int w_m p(w_m) dw_m = 0 \end{aligned}$$

The *mean function* is zero.

From finite linear models to Gaussian processes (2)

Covariance function of a finite linear model

$$\begin{aligned} f(\mathbf{x}) &= \sum_{m=1}^M \mathbf{w}_m \phi_m(\mathbf{x}) = \mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x}) \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}; 0, \mathbf{A}) \end{aligned} \quad \boldsymbol{\phi}(\mathbf{x}) = [\phi_1(\mathbf{x}), \dots, \phi_M(\mathbf{x})]^\top_{(M \times 1)}$$

$$\begin{aligned} k(\mathbf{x}_i, \mathbf{x}_j) &= \text{Cov}_{\mathbf{w}(f(\mathbf{x}_i), f(\mathbf{x}_j))} = \mathbb{E}_{\mathbf{w}(f(\mathbf{x}_i) f(\mathbf{x}_j))} - \underbrace{\mathbb{E}_{\mathbf{w}(f(\mathbf{x}_i))} \mathbb{E}_{\mathbf{w}(f(\mathbf{x}_j))}}_0 \\ &= \int \dots \int \left(\sum_{k=1}^M \sum_{l=1}^M \mathbf{w}_k \mathbf{w}_l \phi_k(\mathbf{x}_i) \phi_l(\mathbf{x}_j) \right) p(\mathbf{w}) d\mathbf{w} \\ &= \sum_{k=1}^M \sum_{l=1}^M \phi_k(\mathbf{x}_i) \phi_l(\mathbf{x}_j) \underbrace{\iint \mathbf{w}_k \mathbf{w}_l p(\mathbf{w}_k, \mathbf{w}_l) d\mathbf{w}_k d\mathbf{w}_l}_{A_{kl}} = \sum_{k=1}^M \sum_{l=1}^M A_{kl} \phi_k(\mathbf{x}_i) \phi_l(\mathbf{x}_j) \end{aligned}$$

$$\boxed{k(\mathbf{x}_i, \mathbf{x}_j) = \boldsymbol{\phi}(\mathbf{x}_i)^\top \mathbf{A} \boldsymbol{\phi}(\mathbf{x}_j)}$$

Note: If $\mathbf{A} = \sigma_{\mathbf{w}}^2 \mathbf{I}$ then $k(\mathbf{x}_i, \mathbf{x}_j) = \sigma_{\mathbf{w}}^2 \sum_{k=1}^M \phi_k(\mathbf{x}_i) \phi_k(\mathbf{x}_j) = \sigma_{\mathbf{w}}^2 \boldsymbol{\phi}(\mathbf{x}_i)^\top \boldsymbol{\phi}(\mathbf{x}_j)$

GPs and Linear in the parameters models are equivalent

We've seen that a Linear in the parameters model, with a Gaussian prior on the weights is also a GP.

Might it also be the case that every GP corresponds to a Linear in the parameters model?

The answer is **yes, but not necessarily a finite one.** (Mercer's theorem.)

Note the different computational complexity: GP: $\mathcal{O}(N^3)$, linear model $\mathcal{O}(NM^2)$ where M is the number of basis functions and N the number of training cases.

So, which representation is most efficient?