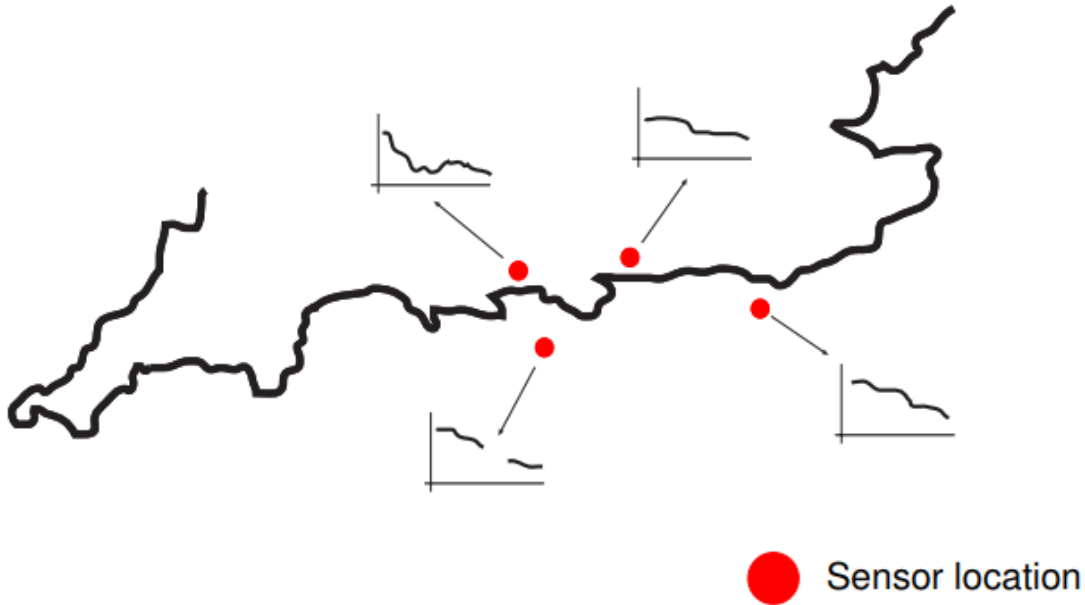


Multiple-Output Gaussian Process

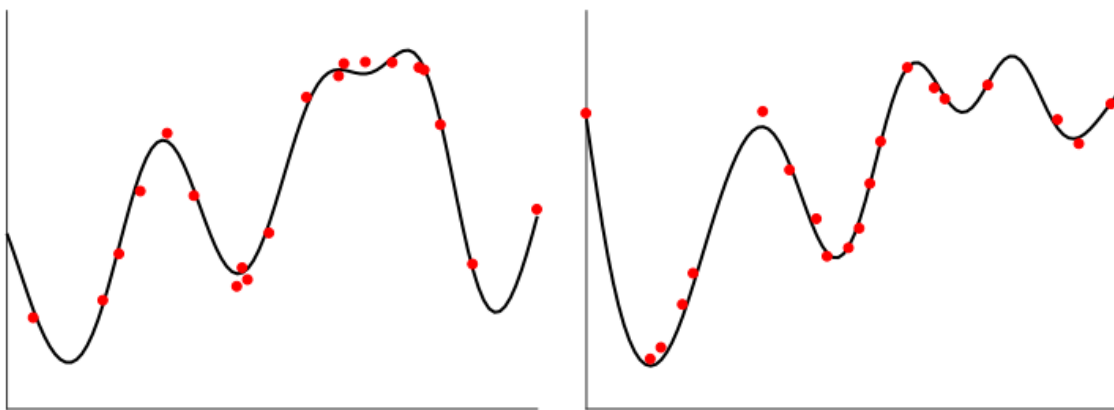
Working Situation



As the picture shows, we want to learn from the three sensors (with complete signal information) to recover the fourth one.

Dependencies between processes

Multiple-independent Output GP



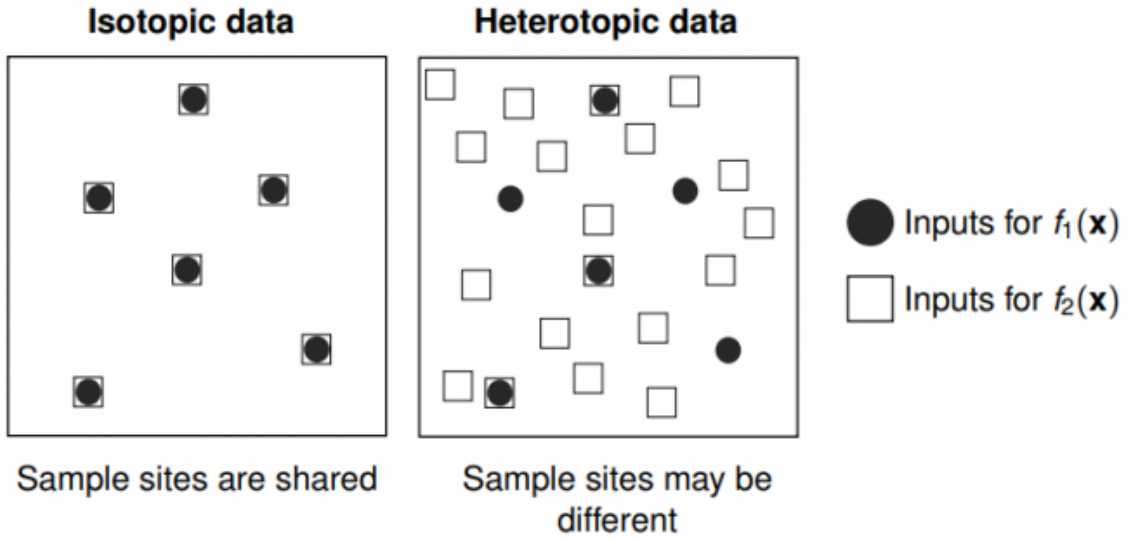
$$\begin{aligned} f_1(\mathbf{x}) &\sim \mathcal{GP}(0, k_1(\mathbf{x}, \mathbf{x}')) \\ D_1 &= \{(\mathbf{x}_{i,1}, y_1(\mathbf{x}_{i,1})) \mid i = 1, \dots, N_1\} \\ \mathbf{y}_1 &\sim \mathcal{N}(\mathbf{0}, \mathbf{K}_1 + \sigma_1^2 \mathbf{1}) \\ f_2(\mathbf{x}) &\sim \mathcal{GP}(0, k_2(\mathbf{x}, \mathbf{x}')) \\ D_2 &= \{(\mathbf{x}_{i,2}, y_2(\mathbf{x}_{i,2})) \mid i = 1, \dots, N_2\} \\ \mathbf{y}_2 &\sim \mathcal{N}(\mathbf{0}, \mathbf{K}_2 + \sigma_2^2 \mathbf{1}) \\ \begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix} &\sim \mathcal{N}\left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{K}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{K}_2 \end{bmatrix} + \begin{bmatrix} \sigma_1^2 \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \sigma_2^2 \mathbf{1} \end{bmatrix}\right) \end{aligned} \quad (1)$$

How to find the independences for kernel design

$$\mathbf{K}_{f,f} = \begin{bmatrix} \mathbf{K}_1 & ? \\ ? & \mathbf{K}_2 \end{bmatrix} \quad (2)$$

Build a cross-covariance function $\text{cov}[f_1(x), f_2(x')]$ such that $\mathbf{K}_{f,f}$ is positive semi-definite.

Different input configurations of data



$$\begin{aligned} \mathcal{D}_1 &= \{(\mathbf{x}_i, f_1(\mathbf{x}_i))_{i=1}^N\} & \mathcal{D}_1 &= \{(\mathbf{x}_{i,1}, f_1(\mathbf{x}_{i,1}))_{i=1}^{N_1}\} \\ \mathcal{D}_2 &= \{(\mathbf{x}_i, f_2(\mathbf{x}_i))_{i=1}^N\} & \mathcal{D}_2 &= \{(\mathbf{x}_{i,2}, f_2(\mathbf{x}_{i,2}))_{i=1}^{N_2}\} \end{aligned} \quad (3)$$

Intrinsic Coregionalization Model

Two outputs

Sample Once

Consider two outputs $f_1(x)f_2(x)$ with $x \in \mathcal{R}^p$.

1. Sample from a GP $u(\mathbf{x}) \sim \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}'))$ to obtain $u^1(\mathbf{x})$
2. Obtain $f_1(x)$ and $f_2(x)$ by linearly transforming:

$$\begin{aligned} f_1(\mathbf{x}) &= a_1^1 u^1(\mathbf{x}) \\ f_2(\mathbf{x}) &= a_2^1 u^1(\mathbf{x}) \end{aligned}$$

For a fixed value x . we can group $f_1(x)$ and $f_2(x)$ in a vector:

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \end{bmatrix} \quad (4)$$

and this vector will be refer as a **vector — valued function**.

The covariance for $f(x)$ is computed as:

$$\text{cov}(\mathbf{f}(\mathbf{x}), \mathbf{f}(\mathbf{x}')) = \mathbb{E} \left\{ \mathbf{f}(\mathbf{x}) [\mathbf{f}(\mathbf{x}')]^\top \right\} - \mathbb{E} \{ \mathbf{f}(\mathbf{x}) \} [\mathbb{E} \{ \mathbf{f}(\mathbf{x}') \}]^\top \quad (5)$$

$$\begin{aligned}
\mathbb{E} \left\{ \begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \end{bmatrix} \begin{bmatrix} f_1(\mathbf{x}') & f_2(\mathbf{x}') \end{bmatrix} \right\} &= \begin{bmatrix} \mathbb{E} \{f_1(\mathbf{x})f_1(\mathbf{x}')\} & \mathbb{E} \{f_1(\mathbf{x})f_2(\mathbf{x}')\} \\ \mathbb{E} \{f_2(\mathbf{x})f_1(\mathbf{x}')\} & \mathbb{E} \{f_2(\mathbf{x})f_2(\mathbf{x}')\} \end{bmatrix} \\
\mathbb{E} \{f_1(\mathbf{x})f_1(\mathbf{x}')\} &= \mathbb{E} \{a_1^1 u^1(\mathbf{x})a_1^1 u^1(\mathbf{x}')\} = (a_1^1)^2 \mathbb{E} \{u^1(\mathbf{x})u^1(\mathbf{x}')\} \\
\mathbb{E} \{f_1(\mathbf{x})f_2(\mathbf{x}')\} &= \mathbb{E} \{a_1^1 u^1(\mathbf{x})a_2^1 u^1(\mathbf{x}')\} = a_1^1 a_2^1 \mathbb{E} \{u^1(\mathbf{x})u^1(\mathbf{x}')\} \\
\mathbb{E} \{f_2(\mathbf{x})f_2(\mathbf{x}')\} &= \mathbb{E} \{a_2^1 u^1(\mathbf{x})a_2^1 u^1(\mathbf{x}')\} = (a_2^1)^2 \mathbb{E} \{u^1(\mathbf{x})u^1(\mathbf{x}')\}
\end{aligned}$$

So that term could be written as:

$$\begin{aligned}
\mathbb{E} \left\{ \mathbf{f}(\mathbf{x})[\mathbf{f}(\mathbf{x}')]^\top \right\} &= \begin{bmatrix} (a_1^1)^2 \mathbb{E} \{u^1(\mathbf{x})u^1(\mathbf{x}')\} & a_1^1 a_2^1 \mathbb{E} \{u^1(\mathbf{x})u^1(\mathbf{x}')\} \\ a_1^1 a_2^1 \mathbb{E} \{u^1(\mathbf{x})u^1(\mathbf{x}')\} & (a_2^1)^2 \mathbb{E} \{u^1(\mathbf{x})u^1(\mathbf{x}')\} \end{bmatrix} \\
&= \begin{bmatrix} (a_1^1)^2 & a_1^1 a_2^1 \\ a_1^1 a_2^1 & (a_2^1)^2 \end{bmatrix} \mathbb{E} \{u^1(\mathbf{x})u^1(\mathbf{x}')\}
\end{aligned} \tag{6}$$

The term $\mathbb{E}\{\mathbf{f}(\mathbf{x})\}$ is computed as:

$$\mathbb{E} \left\{ \begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \end{bmatrix} \right\} = \begin{bmatrix} \mathbb{E} \{f_1(\mathbf{x})\} \\ \mathbb{E} \{f_2(\mathbf{x})\} \end{bmatrix} = \begin{bmatrix} \mathbb{E} \{a_1^1 u^1(\mathbf{x})\} \\ \mathbb{E} \{a_2^1 u^1(\mathbf{x})\} \end{bmatrix} = \begin{bmatrix} a_1^1 \\ a_2^1 \end{bmatrix} \mathbb{E} \{u^1(\mathbf{x})\} \tag{7}$$

Putting them together, the covariance for $f(\mathbf{x}')$ follows as:

$$\begin{bmatrix} (a_1^1)^2 & a_1^1 a_2^1 \\ a_1^1 a_2^1 & (a_2^1)^2 \end{bmatrix} \mathbb{E} \{u^1(\mathbf{x})u^1(\mathbf{x}')\} - \begin{bmatrix} a_1^1 \\ a_2^1 \end{bmatrix} \begin{bmatrix} a_1^1 & a_2^1 \end{bmatrix} \mathbb{E} \{u^1(\mathbf{x})\} \mathbb{E} \{u^1(\mathbf{x}')\} \tag{8}$$

Defining $\mathbf{a} = \begin{bmatrix} a_1^1 & a_2^1 \end{bmatrix}^\top$,

$$\begin{aligned}
\text{cov}(\mathbf{f}(\mathbf{x}), \mathbf{f}(\mathbf{x}')) &= \mathbf{a}\mathbf{a}^\top \mathbb{E} \{u^1(\mathbf{x})u^1(\mathbf{x}')\} - \mathbf{a}\mathbf{a}^\top \mathbb{E} \{u^1(\mathbf{x})\} \mathbb{E} \{u^1(\mathbf{x}')\} \\
&= \mathbf{a}\mathbf{a}^\top \underbrace{\left[\mathbb{E} \{u^1(\mathbf{x})u^1(\mathbf{x}')\} - \mathbb{E} \{u^1(\mathbf{x})\} \mathbb{E} \{u^1(\mathbf{x}')\} \right]}_{k(\mathbf{x}, \mathbf{x}')} \\
&= \mathbf{a}\mathbf{a}^\top k(\mathbf{x}, \mathbf{x}')
\end{aligned}$$

We define $\mathbf{B} = \mathbf{a}\mathbf{a}^\top$, leading to

$$\text{cov}(\mathbf{f}(\mathbf{x}), \mathbf{f}(\mathbf{x}')) = \mathbf{B}k(\mathbf{x}, \mathbf{x}') = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} k(\mathbf{x}, \mathbf{x}') \tag{9}$$

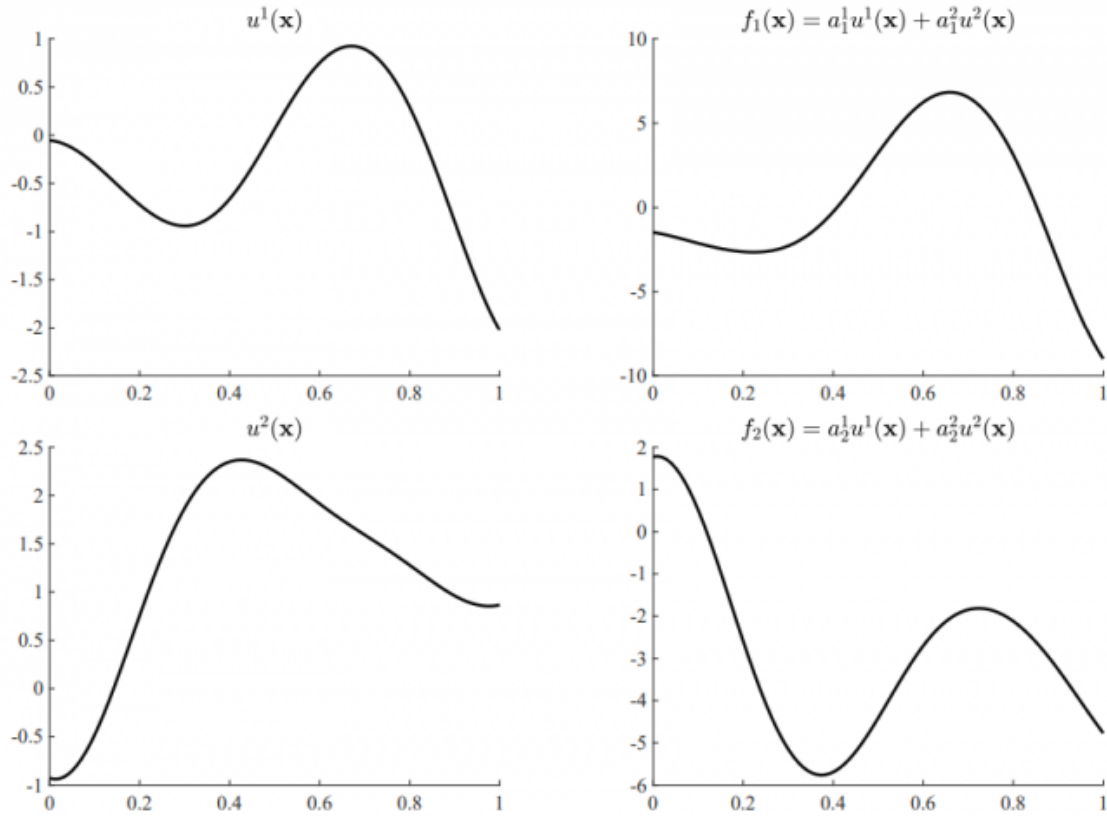
and the \mathbf{B} has rank one, since it is the result of the multiplication of two column-vector.

Sample Twice

Sample **twice** from a GP $u(\mathbf{x}) \sim \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}'))$ to obtain $u^1(\mathbf{x})$ and $u^2(\mathbf{x})$.

Adding a scaled transformation.:

$$\begin{aligned}
f_1(\mathbf{x}) &= a_1^1 u^1(\mathbf{x}) + a_1^2 u^2(\mathbf{x}) \\
f_2(\mathbf{x}) &= a_2^1 u^1(\mathbf{x}) + a_2^2 u^2(\mathbf{x})
\end{aligned} \tag{10}$$



**

Notice that the u_1 and u_2 are independent, although they share the same covariance k .

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} a_1^1 & a_1^2 \\ a_2^1 & a_2^2 \end{bmatrix} \begin{bmatrix} u^1 \\ u^2 \end{bmatrix} \quad (11)$$

The vector-valued function can be written as $f(x)$, where $\mathbf{a}^1 = [a_1^1 \ a_2^1]^\top$ and $\mathbf{a}^2 = [a_1^2 \ a_2^2]^\top$

The covariance for $f(x)$ is computed as:

$$\begin{aligned} \text{cov}(\mathbf{f}(\mathbf{x}), \mathbf{f}(\mathbf{x}')) &= \mathbf{a}^1 (\mathbf{a}^1)^\top \text{cov}(u^1(\mathbf{x}), u^1(\mathbf{x}')) + \mathbf{a}^2 (\mathbf{a}^2)^\top \text{cov}(u^2(\mathbf{x}), u^2(\mathbf{x}')) \\ &= \mathbf{a}^1 (\mathbf{a}^1)^\top k(\mathbf{x}, \mathbf{x}') + \mathbf{a}^2 (\mathbf{a}^2)^\top k(\mathbf{x}, \mathbf{x}') \\ &= [\mathbf{a}^1 (\mathbf{a}^1)^\top + \mathbf{a}^2 (\mathbf{a}^2)^\top] k(\mathbf{x}, \mathbf{x}') \end{aligned}$$

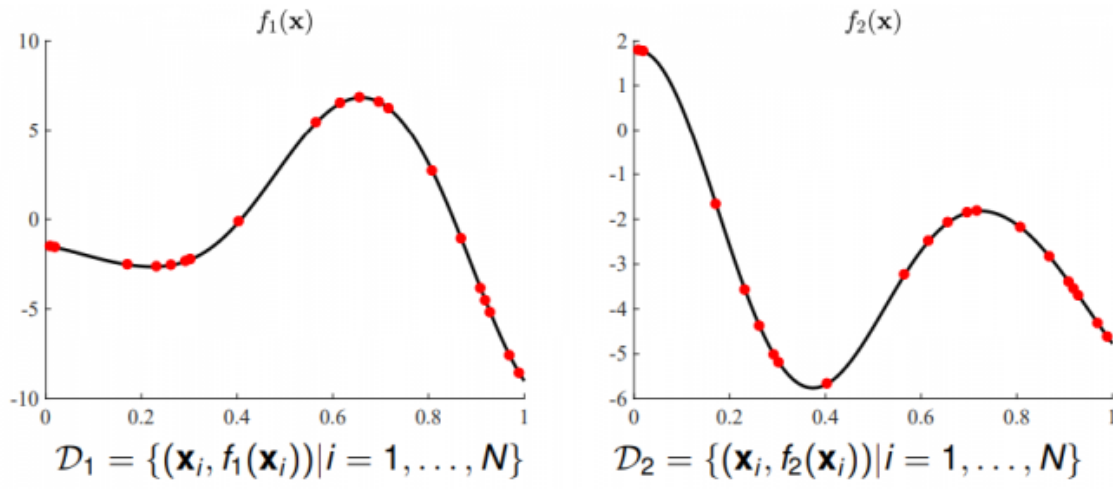
notice that u_1 and u_2 are independent, so their variance could be added directly.

we define $\mathbf{B} = \mathbf{a}^1 (\mathbf{a}^1)^\top + \mathbf{a}^2 (\mathbf{a}^2)^\top$, leading to:

$$\text{cov}(\mathbf{f}(\mathbf{x}), \mathbf{f}(\mathbf{x}')) = \mathbf{B} k(\mathbf{x}, \mathbf{x}') = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} k(\mathbf{x}, \mathbf{x}') \quad (12)$$

Notice that B has rank two.

Observed Data:



$$\begin{bmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{bmatrix} = \begin{bmatrix} f_1(\mathbf{x}_1) \\ \vdots \\ f_1(\mathbf{x}_N) \\ f_2(\mathbf{x}_1) \\ \vdots \\ f_2(\mathbf{x}_N) \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} b_{11}\mathbf{K} & b_{12}\mathbf{K} \\ b_{21}\mathbf{K} & b_{22}\mathbf{K} \end{bmatrix} \right) \quad (13)$$

The matrix $\mathbf{K} \in \mathcal{R}^{N \times N}$ has elements $k(x_i, x_j)$.

If we use **Kronecker product** we would get:

$$\begin{bmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{bmatrix} = \begin{bmatrix} f_1(\mathbf{x}_1) \\ \vdots \\ f_1(\mathbf{x}_N) \\ f_2(\mathbf{x}_1) \\ \vdots \\ f_2(\mathbf{x}_N) \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \mathbf{B} \otimes \mathbf{K} \right) \quad (14)$$

General Case

Consider a set of functions $\{f_d(\mathbf{x})\}_{d=1}^D$.

In the ICM,

$$f_d(\mathbf{x}) = \sum_{i=1}^R a_d^i u^i(\mathbf{x}) \quad (15)$$

where the functions $u_i(x)$ are GPs sampled independently, and share the same covariance function $k(x, x')$.

For $\mathbf{f}(\mathbf{x}) = [f_1(\mathbf{x}) \cdots f_D(\mathbf{x})]^\top$, the covariance is given as:

$$\text{cov}[\mathbf{f}(\mathbf{x}), \mathbf{f}(\mathbf{x}')] = \mathbf{A}\mathbf{A}^\top k(\mathbf{x}, \mathbf{x}') = \mathbf{B}k(\mathbf{x}, \mathbf{x}') \quad (16)$$

where

$$\mathbf{A} = [\mathbf{a}^1 \mathbf{a}^2 \cdots \mathbf{a}^R] \quad (17)$$

and the Rank of B is given by R .

ICM: autokrigeability

If the outputs are considered to be noise-free, prediction using the ICM under an isotopic data case is equivalent to independent prediction over each output. This circumstance is also known as autokrigeability.

The prove:

Assume that we only have two outputs: f_1, f_2

the predicated mean could be written as:

$$\begin{aligned}\mu &= K_{f_*,f} (K_{f,f})^{-1} f \\ K_{f,f} &= B \otimes K \\ \mu &= B \otimes K_* (B \otimes K)^{-1} f \\ &= B \otimes K_* (B^{-1} \otimes K^{-1}) f \\ &= BB^{-1} \otimes K_* K^{-1} f \\ &= I \otimes K_* K^{-1} f \\ &= \begin{bmatrix} K_* K^{-1} & 0 \\ 0 & K_* K^{-1} \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}\end{aligned}\tag{18}$$

it means, the prediction of f_1 only depends on the data set for f_1

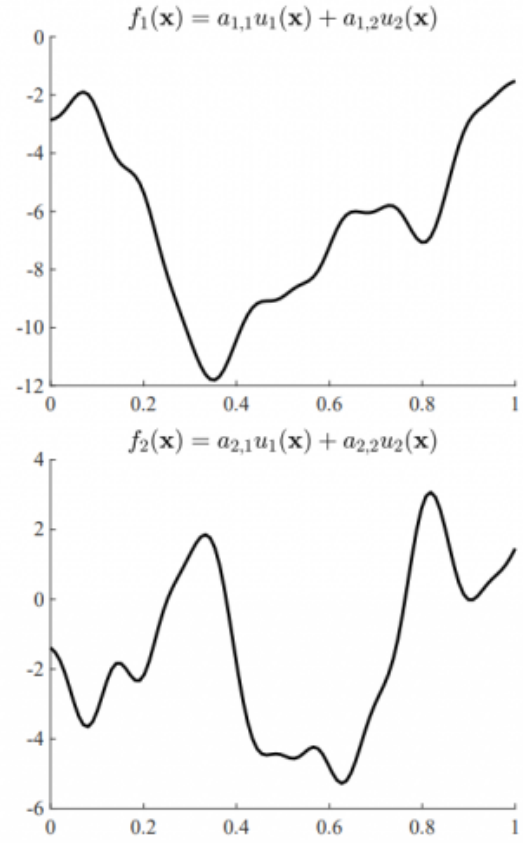
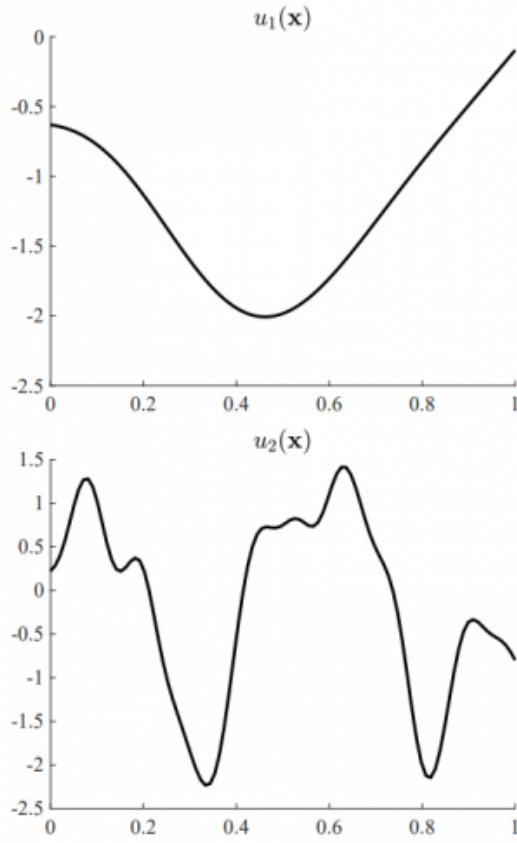
Semiparametric Latent Factor Model (SLFM)

ICM uses R samples $u^i(x)$ from $u(x)$ with the same covariance function. SLFM uses Q samples from u_q processes with different covariance functions.

Two Outputs

1. Sample from a GP $\mathcal{GP}(0, k_1(\mathbf{x}, \mathbf{x}'))$ to obtain $u_1(x)$.
2. Sample from a GP $\mathcal{GP}(0, k_2(\mathbf{x}, \mathbf{x}'))$ to obtain $u_2(x)$.
3. Adding a scaled versions:

$$\begin{aligned}f_1(\mathbf{x}) &= a_{1,1} u_1(\mathbf{x}) + a_{1,2} u_2(\mathbf{x}) \\ f_2(\mathbf{x}) &= a_{2,1} u_1(\mathbf{x}) + a_{2,2} u_2(\mathbf{x})\end{aligned}\tag{19}$$



Similar, it can be written as:

$$\mathbf{f}(\mathbf{x}) = \mathbf{a}_1 u_1(\mathbf{x}) + \mathbf{a}_2 u_2(\mathbf{x}) \quad (20)$$

with $\mathbf{a}_1 = [a_{1,1} \ a_{2,1}]^\top$ and $\mathbf{a}_2 = [a_{1,2} \ a_{2,2}]^\top$

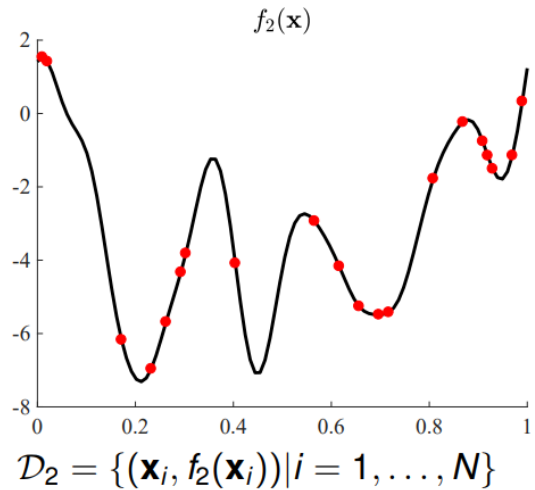
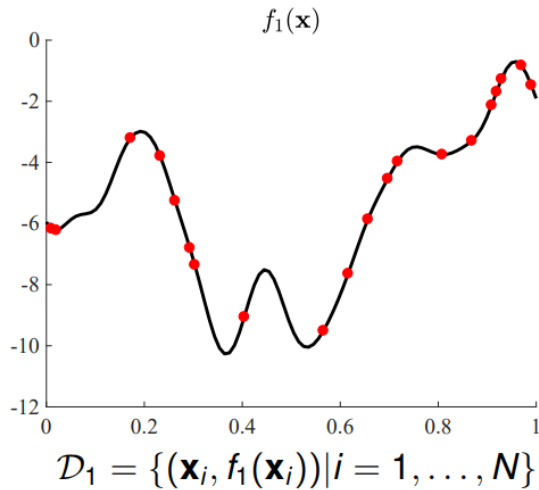
The covariance for $f(x)$ is computed as:

$$\begin{aligned} \text{cov}(\mathbf{f}(\mathbf{x}), \mathbf{f}(\mathbf{x}')) &= \mathbf{a}_1 (\mathbf{a}_1)^\top \text{cov}(u_1(\mathbf{x}), u_1(\mathbf{x}')) + \mathbf{a}_2 (\mathbf{a}_2)^\top \text{cov}(u_2(\mathbf{x}), u_2(\mathbf{x}')) \\ &= \mathbf{a}_1 (\mathbf{a}_1)^\top k_1(\mathbf{x}, \mathbf{x}') + \mathbf{a}_2 (\mathbf{a}_2)^\top k_2(\mathbf{x}, \mathbf{x}') \end{aligned}$$

We define $\mathbf{B}_1 = \mathbf{a}_1 (\mathbf{a}_1)^\top$ and $\mathbf{B}_2 = \mathbf{a}_2 (\mathbf{a}_2)^\top$, leading to:

$$\text{cov}(\mathbf{f}(\mathbf{x}), \mathbf{f}(\mathbf{x}')) = \mathbf{B}_1 k_1(\mathbf{x}, \mathbf{x}') + \mathbf{B}_2 k_2(\mathbf{x}, \mathbf{x}') \quad (21)$$

Notice that B_1 and B_2 have rank one.



$$\begin{bmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{bmatrix} = \begin{bmatrix} f_1(\mathbf{x}_1) \\ \vdots \\ f_1(\mathbf{x}_N) \\ f_2(\mathbf{x}_1) \\ \vdots \\ f_2(\mathbf{x}_N) \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \mathbf{B}_1 \otimes \mathbf{K}_1 + \mathbf{B}_2 \otimes \mathbf{K}_2 \right) \quad (22)$$

General Case:

Consider a set of functions $\{f_d(\mathbf{x})\}_{d=1}^D$

In the SLFM,

$$f_d(\mathbf{x}) = \sum_{q=1}^Q a_{d,q} u_q(\mathbf{x}) \quad (23)$$

where the functions $u_q(x)$ are GPs with covariance functions $k_q(x, x')$.

For $\mathbf{f}(\mathbf{x}) = [f_1(\mathbf{x}) \cdots f_D(\mathbf{x})]^\top$, the covariance is given as:

$$\text{cov}[\mathbf{f}(\mathbf{x}), \mathbf{f}(\mathbf{x}')] = \sum_{q=1}^Q \mathbf{A}_q \mathbf{A}_q^\top k_q(\mathbf{x}, \mathbf{x}') = \sum_{q=1}^Q \mathbf{B}_q k_q(\mathbf{x}, \mathbf{x}') \quad (24)$$

where $A_q = a_q$.

The rank of each B_q is one.

Linear model of coregionalization (LMC)

The LMC generalizes the ICM and the SLFM allowing several independent samples from GPs with different covariances.

Consider a set of functions $\{f_d(\mathbf{x})\}_{d=1}^D$

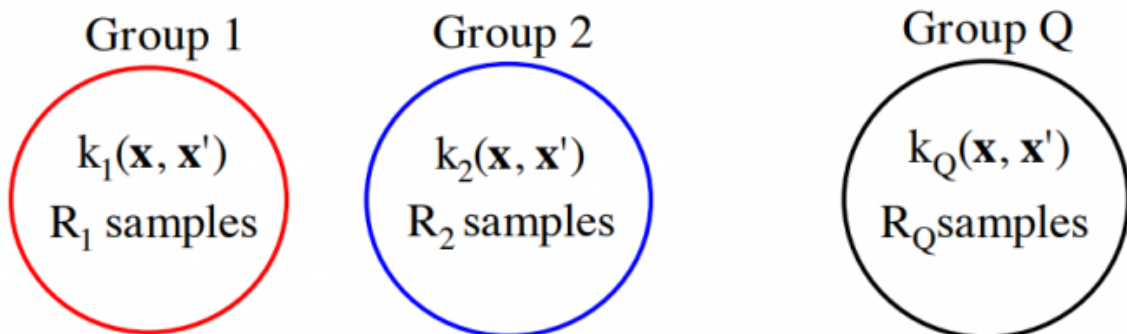
$$f_d(\mathbf{x}) = \sum_{q=1}^Q \sum_{i=1}^{R_q} a_{d,q}^i u_q^i(\mathbf{x}) \quad (25)$$

where the functions u_q^i are GPs with zero means and covariance functions:

$$\text{cov}[u_q^i(\mathbf{x}), u_{q'}^{i'}(\mathbf{x}')] = k_q(\mathbf{x}, \mathbf{x}') \quad (26)$$

if $i = i'$ and $q = q'$

There are Q groups of samples. For each group, there are R_q samples obtained independently from the same GP with covariance $k_q(x, x')$.



The LMC corresponds to the sum of Q ICMs.

Suppose we have $D = 2$, $Q = 2$, and $R_q=2$. According to LMC:

$$\begin{aligned} f_1(\mathbf{x}) &= a_{1,1}^1 u_1^1(\mathbf{x}) + a_{1,1}^2 u_1^2(\mathbf{x}) + a_{1,2}^1 u_2^1(\mathbf{x}) + a_{1,2}^2 u_2^2(\mathbf{x}) \\ f_2(\mathbf{x}) &= a_{2,1}^1 u_1^1(\mathbf{x}) + a_{2,1}^2 u_1^2(\mathbf{x}) + a_{2,2}^1 u_2^1(\mathbf{x}) + a_{2,2}^2 u_2^2(\mathbf{x}) \end{aligned} \quad (27)$$

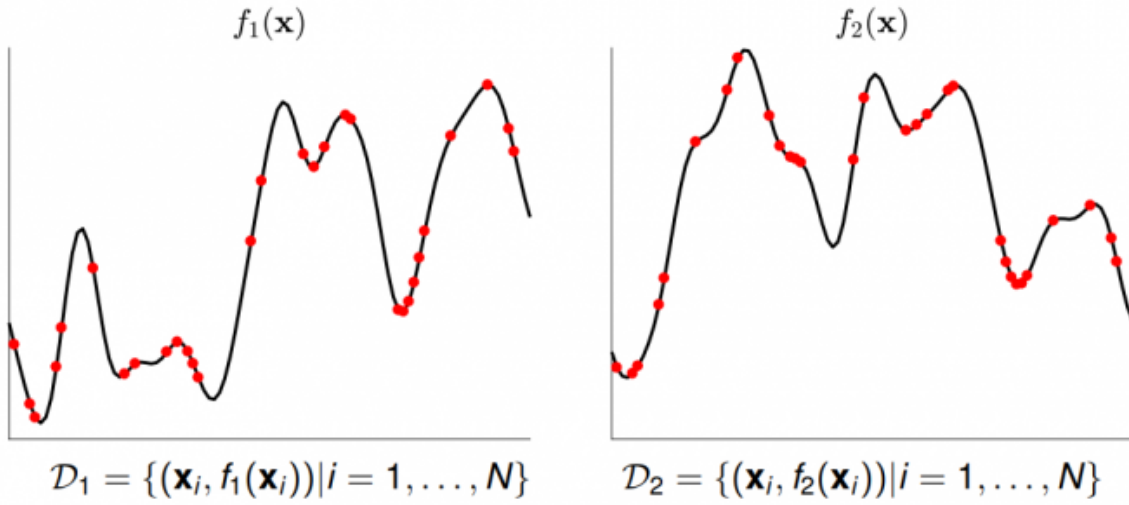
For $\mathbf{f}(\mathbf{x}) = [f_1(\mathbf{x}) \cdots f_D(\mathbf{x})]^\top$, the covariance $\text{cov}[\mathbf{f}(\mathbf{x}), \mathbf{f}(\mathbf{x}')] is given as:$

$$\text{cov}[\mathbf{f}(\mathbf{x}), \mathbf{f}(\mathbf{x}')] = \sum_{q=1}^Q \mathbf{A}_q \mathbf{A}_q^\top k_q(\mathbf{x}, \mathbf{x}') = \sum_{q=1}^Q \mathbf{B}_q k_q(\mathbf{x}, \mathbf{x}') \quad (28)$$

where $\mathbf{A}_q = [\mathbf{a}_q^1 \mathbf{a}_q^2 \cdots \mathbf{a}_q^{R_q}]$.

The rank of each B_q is R_q .

The matrices B_q are known as the coregionalization matrices.



$$\begin{bmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{bmatrix} = \begin{bmatrix} f_1(\mathbf{x}_1) \\ \vdots \\ f_1(\mathbf{x}_N) \\ f_2(\mathbf{x}_1) \\ \vdots \\ f_2(\mathbf{x}_N) \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \sum_{q=1}^Q \mathbf{B}_q \otimes \mathbf{K}_q \right) \quad (29)$$