Defn:

A random matrix-valued function $X: \mathbb{R}^k \to \mathbb{R}^{d \times n}$ is a <u>multivariate GP</u> on $\mathbb{R}^k$,

$$X \sim \mathrm{MatGP}(\mu, \kappa, \Omega)$$

with <u>mean function</u> $\mu: \mathbb{R}^k \to \mathbb{R}^{d\times n}$

<u>kernel function</u> $\kappa: \mathbb{R}^k \times \mathbb{R}^k \to \mathbb{R}$ &

positive semi-definite <u>parameter covariance matrix</u>

$\Omega \in \mathbb{R}^{dn \times dn}$ if the vectorization of any finite collection of evaluations of X at given locations have a joint multivariate

Gaussian distribution. I.e., if $\forall N \in \mathbb{N}$ & any $\{\underline{s}_i\}_{i=1}^N \subset \mathbb{R}^k$ we have:

$$\mathrm{vec}(X_s) \sim N_{dnN}(\mathrm{vec}(M), K \otimes \Omega)$$

where $X_s := [X(\underline{s}_1), \ldots, X(\underline{s}_N)] \in \mathbb{R}^{d \times nN}$,

$$M = [\mu(\underline{s}_1), \ldots, \mu(\underline{s}_N)] \in \mathbb{R}^{d \times nN}$$

$K \in \mathbb{R}^{N \times N}$ has ijth entry $K_{ij} = \kappa(\underline{s}_i, \underline{s}_j)$

Notes:

- $$\mathrm{vec}(X_s) = \begin{pmatrix} \mathrm{vec}(X(\underline{s}_1)) \\ \vdots \\ \mathrm{vec}(X(\underline{s}_N)) \end{pmatrix}$$

$$K \otimes \Omega = \begin{pmatrix} K_{11}\Omega & \cdots & K_{1N}\Omega \\ \vdots & \ddots & \vdots \\ K_{N1}\Omega & \cdots & K_{NN}\Omega \end{pmatrix}$$

$$\Rightarrow \mathrm{cov}(\mathrm{vec}(X(\underline{s}_i))) = k(\underline{s}_i, \underline{s}_i)\,\Omega \qquad \forall i \in \{1, \ldots, N\}$$

&

$$\mathrm{cov}(\mathrm{vec}(X(\underline{s}_i)), \mathrm{vec}(X(\underline{s}_j))) = k(\underline{s}_i, \underline{s}_j)\,\Omega$$

$$\forall i \neq j \in \{1, \ldots, N\}$$

- $$\mathbb{E}(X(\underline{s}_i)) = \mu(\underline{s}_i) \qquad \forall i \in \{1, \ldots, N\}.$$

Predictions for MatGP

$$\tilde{s} = (s_{\mathcal{D}^*}, s_{\mathcal{D}})$$

$$X_{\tilde{s}} = (X_{\mathcal{D}^*}, X_{\mathcal{D}})$$

$$\mathrm{vec}(X_{\tilde{s}}) = \begin{pmatrix} \mathrm{vec}(X_{\mathcal{D}^*}) \\ \mathrm{vec}(X_{\mathcal{D}}) \end{pmatrix}$$

$$\mathrm{vec}(X_{\tilde{s}}) \sim N\left(\begin{pmatrix} \mathrm{vec}(M_{\mathcal{D}^*}) \\ \mathrm{vec}(M_{\mathcal{D}}) \end{pmatrix}, \begin{pmatrix} K_{\mathcal{D}^*\mathcal{D}^*} \otimes \Omega & K_{\mathcal{D}^*\mathcal{D}} \otimes \Omega \\ K_{\mathcal{D}\mathcal{D}^*} \otimes \Omega & K_{\mathcal{D}\mathcal{D}} \otimes \Omega \end{pmatrix} \right)$$

$$\mathrm{vec}(X_{\mathcal{D}^*}) \mid \mathrm{vec}(X_{\mathcal{D}}) \sim N(\bar{m}, \bar{\Sigma})$$

$$\bar{m} = \mathrm{vec}(M_{\mathcal{D}^*}) + (K_{\mathcal{D}^*\mathcal{D}} \otimes \Omega)(K_{\mathcal{D}\mathcal{D}} \otimes \Omega)^{-1}(\mathrm{vec}(X_{\mathcal{D}}) - \mathrm{vec}(M_{\mathcal{D}}))$$

$$\bar{\Sigma} = K_{\mathcal{D}^*\mathcal{D}^*} \otimes \Omega - (K_{\mathcal{D}^*\mathcal{D}} \otimes \Omega)(K_{\mathcal{D}\mathcal{D}} \otimes \Omega)^{-1}(K_{\mathcal{D}\mathcal{D}^*} \otimes \Omega)$$

$$\bar{M} = vec(M_{\mathcal{D}*}) + (K_{\mathcal{D}*\mathcal{D}} \otimes \Omega)(K_{\mathcal{D}\mathcal{D}} \otimes \Omega)^{-1}(vec(X_{\mathcal{D}}) - vec(M_{\mathcal{D}}))$$

Note:

$$\bar{M} = vec(M_{\mathcal{D}*}) + (\overbrace{\underbrace{K_{\mathcal{D}*\mathcal{D}}}_{N_* \times N} \underbrace{K_{\mathcal{D}\mathcal{D}}^{-1}}_{N \times N}}^{N_* \times N} \otimes I_{dn}) vec(X_{\mathcal{D}} - M_{\mathcal{D}})$$

$$= vec(M_{\mathcal{D}*}) + \underbrace{((K_{\mathcal{D}\mathcal{D}}^{-1} K_{\mathcal{D}\mathcal{D}*})^T \otimes I_{dn})}_{dn N_* \times dn N} \underbrace{vec(\underbrace{X_{\mathcal{D}} - M_{\mathcal{D}}}_{d \times n N})}_{dn N \times 1}$$

$$(B \otimes I_{dn}) vec(Y)$$

$$= \begin{pmatrix} B_{11} I & B_{12} I & \cdots & B_{1N} I \\ B_{21} I & & & \\ \vdots & & & \\ B_{N_*1} I & \cdots & \cdots & B_{N_*N} I \end{pmatrix} \begin{pmatrix} vec(Y(s_1)) \\ \vdots \\ vec(Y(s_N)) \end{pmatrix}$$