Vector-valued Gaussian Processes

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I. Overview of Gaussian Processes

Gaussian processes generalize the multivariate Gaussian dist. and can describe probability distributions over functions. [1]

i. Multivariate Gaussian Distribution

$$\begin{aligned} \boldsymbol{z} \in \mathbb{R}^N &\sim \mathcal{N}_N(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \; z_i \sim \mathcal{N}(\mu_i, \boldsymbol{\Sigma}_{ii}) \\ \boldsymbol{\mu} \in \mathbb{R}^N &= (\mu_1, \mu_2, ..., \mu_N)^\top = (\mathbb{E}(z_1), \mathbb{E}(z_2), ..., \mathbb{E}(z_N))^\top \\ \boldsymbol{\Sigma} \in \mathbb{R}^{N\times N} &= \mathbb{E}\Big((\boldsymbol{z}-\mu)(\boldsymbol{z}-\mu)^\top\Big) = \big[\mathrm{cov}(z_i, z_j)\big]_{i,j=1}^{N} \end{aligned} \tag{1}$$

ii. Gaussian Processes (GPs)

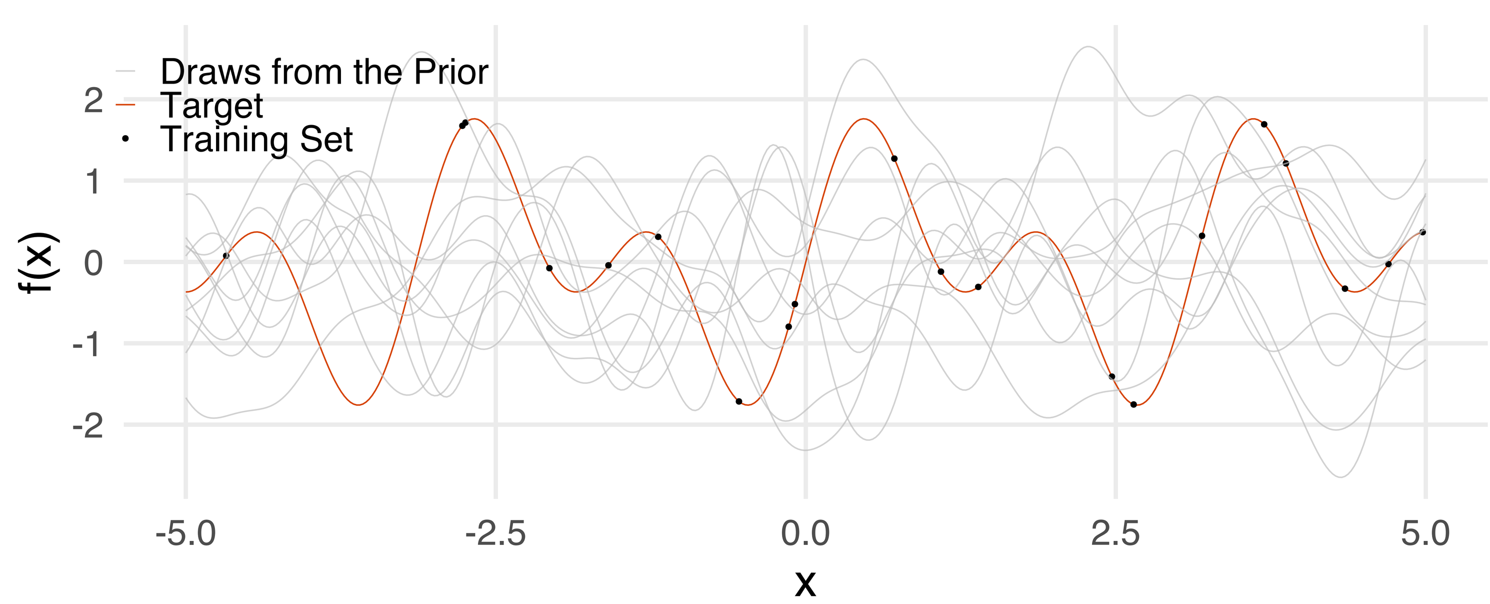
- GP: an uncountably infinite collection of random variables; any finite sample is a draw from a MV Gaussian distribution.
- GPs fully specified by *mean* and *covariance (kernel)* functions.
- The covariance function k must produce a positive semi-definite matrix.
- Squared exponential kernel, $k : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$:

$$k(x, x') = \alpha^2 \exp\left(-\frac{1}{2\rho^2}\|x - x'\|^2\right). \tag{2}$$

- α and ρ are *hyperparameters* (chosen, or estimated from data)

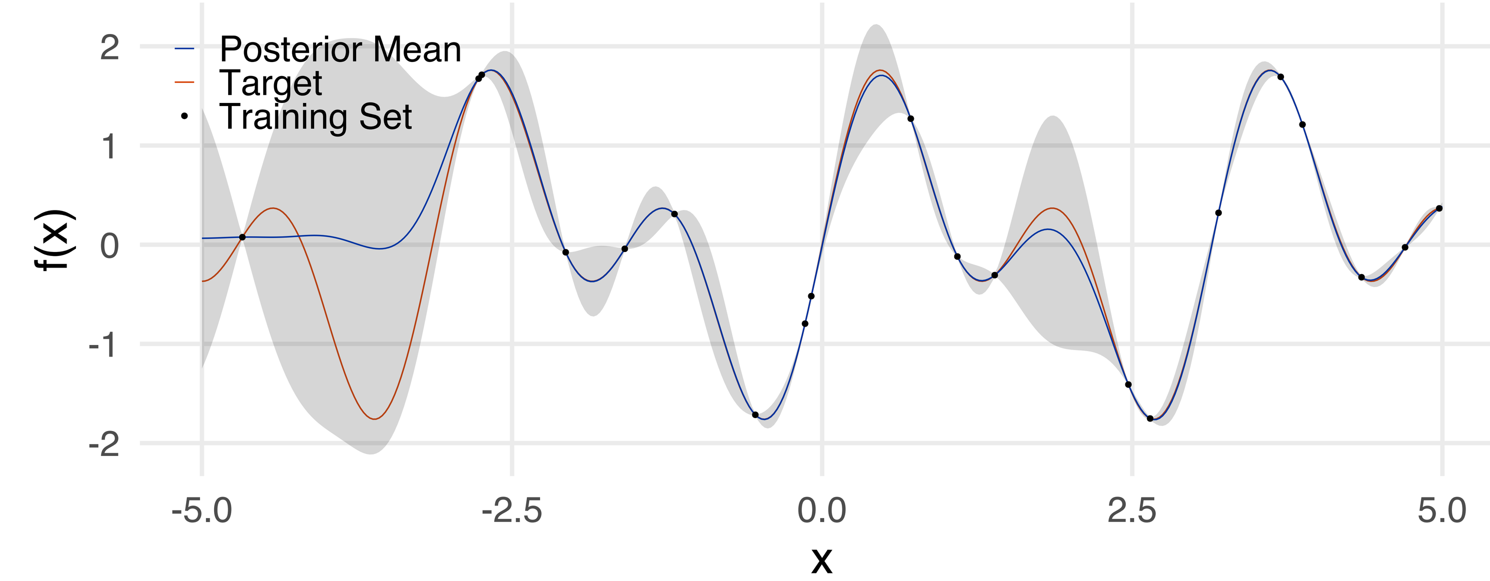
II. Gaussian Process Regression – Univariate $\mathbf{y}$

$$\begin{aligned} S &= (\boldsymbol{x}, \boldsymbol{y}) = \{(x_i, y_i) : x_i, y_i \in \mathbb{R}, i \in 1, 2, ..., N\} \\ f &\sim \mathcal{GP}(\boldsymbol{0}, k) \;\; \boldsymbol{y}_* \sim \mathcal{N}_M(\boldsymbol{0}, k(\boldsymbol{x}_*, \boldsymbol{x}_*)) \\ k(\boldsymbol{x}_*, \boldsymbol{x}_*) \in \mathbb{R}^{M\times M} &= \big[k(x_{*i}, x_{*j})\big]_{i,j=1}^{M}. \end{aligned} \tag{3}$$



$$\begin{aligned} \boldsymbol{y}_* \mid \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{x}_* &\sim \mathcal{N}_M\big(\hat{\mu}, \hat{\Sigma}\big) \\ \hat{\mu} \in \mathbb{R}^M &= k(\boldsymbol{x}_*, \boldsymbol{x})k(\boldsymbol{x}, \boldsymbol{x})^{-1}\boldsymbol{y} \\ \hat{\Sigma} \in \mathbb{R}^{M\times M} &= k(\boldsymbol{x}_*, \boldsymbol{x}_*) - k(\boldsymbol{x}_*, \boldsymbol{x})k(\boldsymbol{x}, \boldsymbol{x})^{-1}k(\boldsymbol{x}_*, \boldsymbol{x})^\top \end{aligned} \tag{4}$$

$$\begin{aligned} k(\boldsymbol{x}, \boldsymbol{x}) \in \mathbb{R}^{N\times N} &= \big[k(x_i, x_j)\big]_{i,j=1}^{N} \\ k(\boldsymbol{x}_*, \boldsymbol{x}) \in \mathbb{R}^{M\times N} &= \big[k(x_{*i}, x_j)\big]_{i,j=1}^{M,N}. \end{aligned} \tag{5}$$

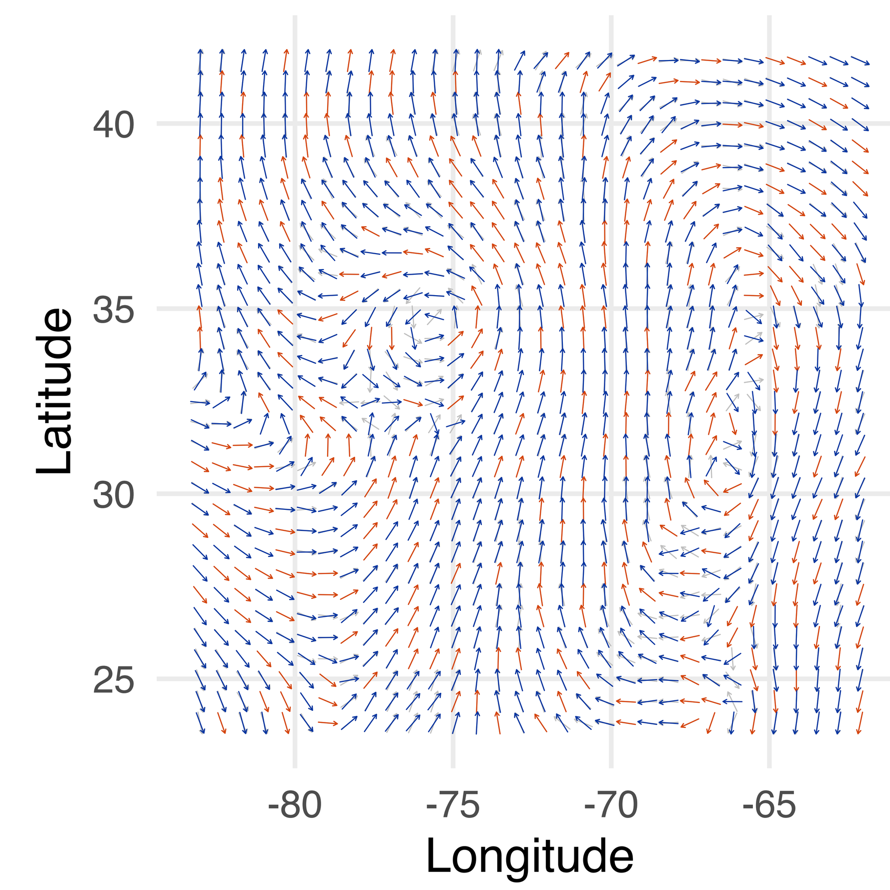


III. Multioutput GPR – Vector-valued $\mathbf{y}$

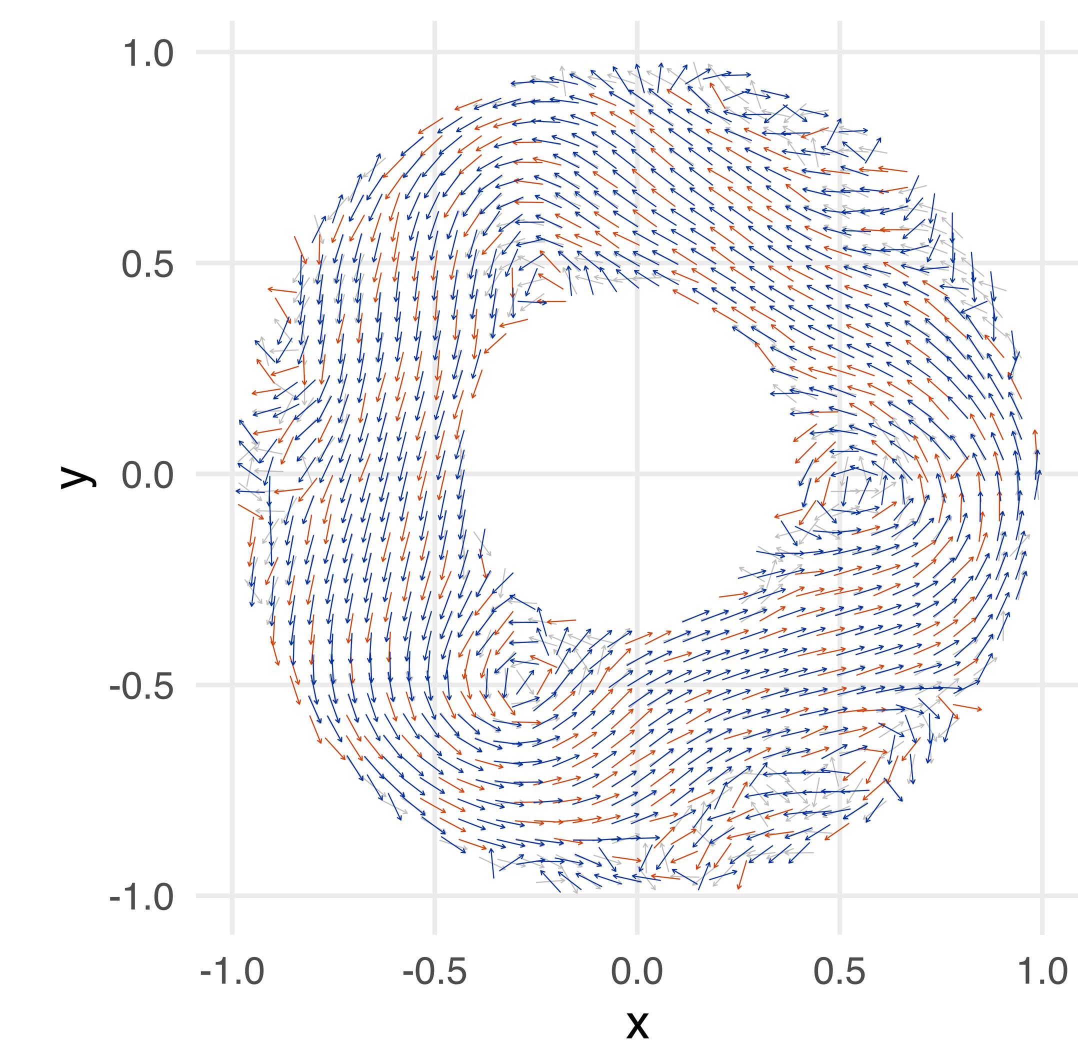
- Velocity fields: $\boldsymbol{X}, \boldsymbol{Y} \in \mathbb{R}^{N\times 2}$, $\boldsymbol{y} \in \mathbb{R}^{2N} = \mathrm{vec}(Y)$, $\boldsymbol{X}_* \in \mathbb{R}^{M\times 2}$
- Intrinsic Coregionalization Model (ICM) [2], [3]

$$\begin{aligned} \boldsymbol{y}_* \mid \boldsymbol{X}, \boldsymbol{y}, \boldsymbol{X}_* &\sim \mathcal{N}_{2M}\big(\hat{\mu}, \hat{\Sigma}\big) \\ \hat{\mu} \in \mathbb{R}^{2M} &= K_{\boldsymbol{X}_*\boldsymbol{X}}K_{\boldsymbol{X}\boldsymbol{X}}^{-1}\boldsymbol{y} \\ \hat{\Sigma} \in \mathbb{R}^{2M\times 2M} &= K_{\boldsymbol{X}_*\boldsymbol{X}_*} - K_{\boldsymbol{X}_*\boldsymbol{X}}K_{\boldsymbol{X}\boldsymbol{X}}^{-1}K_{\boldsymbol{X}_*\boldsymbol{X}}^\top \\ K_{\boldsymbol{X}\boldsymbol{X}} \in \mathbb{R}^{2N\times 2N} &= B \otimes k(\boldsymbol{X}, \boldsymbol{X}) \\ K_{\boldsymbol{X}_*\boldsymbol{X}} \in \mathbb{R}^{2M\times 2N} &= B \otimes k(\boldsymbol{X}_*, \boldsymbol{X}) \\ K_{\boldsymbol{X}_*\boldsymbol{X}_*} \in \mathbb{R}^{2M\times 2M} &= B \otimes k(\boldsymbol{X}_*, \boldsymbol{X}_*) \\ B \in \mathbb{R}^{2\times 2} = \mathrm{corr}(\boldsymbol{Y}) &= \left(\frac{\langle \boldsymbol{y}_i - \overline{\boldsymbol{y}}_i, \boldsymbol{y}_j - \overline{\boldsymbol{y}}_j\rangle}{\|\boldsymbol{y}_i - \overline{\boldsymbol{y}}_i\| \; \|\boldsymbol{y}_j - \overline{\boldsymbol{y}}_j\|}\right)_{i,j=1}^{2} \end{aligned} \tag{6}$$

Case study: Hurricane Isabel Simulation [4]



Case study: Particle Image Velocimetry [5]



Note: colors reflect sample data, posterior mean, and test points.

Bibliography

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