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GP2D

HAJIME KAWAHARA[1]

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ABSTRACT

GP2D: 2D input → 2D prediction

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1. GP2D

The multivariate normal distribution:

$$p(\boldsymbol{f}|\boldsymbol{d}) = \mathcal{N}(\boldsymbol{f}|\boldsymbol{\mu}, \Sigma_{\boldsymbol{f}|\boldsymbol{d}}) \tag{1}$$

$$\Sigma_{\boldsymbol{f}|\boldsymbol{d}} = (\Sigma_{\boldsymbol{d}}^{-1} + \Sigma_{\boldsymbol{f}}^{-1})^{-1} \tag{2}$$

$$\boldsymbol{\mu} = \Sigma_{\boldsymbol{f}|\boldsymbol{d}} \Sigma_{\boldsymbol{d}}^{-1} \boldsymbol{d} = \Sigma_{\boldsymbol{f}} (I + \Sigma_{\boldsymbol{d}}^{-1} \Sigma_{\boldsymbol{f}})^{-1} \Sigma_{\boldsymbol{d}}^{-1} \boldsymbol{d} \tag{3}$$

Assuming

$$\Sigma_{\boldsymbol{d}} = \sigma^2 I \tag{4}$$

$$\Sigma_{\boldsymbol{f}} = K = K_Y \otimes K_X \tag{5}$$

and an eigendecomposition of K, K_X, and K_Y as

$$K \equiv Q \Lambda Q^\top = (U_Y \otimes U_X)(\Lambda_Y \otimes \Lambda_X)(U_Y \otimes U_X)^\top \tag{6}$$

$$K_X \equiv U_X \Lambda_X U_X^\top \tag{7}$$

$$K_Y \equiv U_Y \Lambda_Y U_Y^\top, \tag{8}$$

and an identity

$$(A^\top \otimes B)\mathrm{vec}(X) = \mathrm{vec}(BXA), \tag{9}$$

we obtain (isomorphism, $\boldsymbol{d} = \mathrm{vec}(D)$, $D = \mathrm{mat}(\boldsymbol{d}) \in \mathcal{R}^{N_X \times N_Y}$)

$$\boldsymbol{\mu} = K(K + \sigma^2 I)^{-1} \boldsymbol{d} \tag{10}$$

$$= KQ(\Lambda + \sigma^2 I)^{-1} Q^\top \boldsymbol{d} \tag{11}$$

$$= KQ(\Lambda + \sigma^2 I)^{-1} (U_Y \otimes U_X)^\top \boldsymbol{d} \tag{12}$$

$$= KQ(\Lambda + \sigma^2 I)^{-1} (U_Y^\top \otimes U_X^\top) \boldsymbol{d} \tag{13}$$

$$= KQ(\mathrm{diag}(\Lambda + \sigma^2 I)^{-1} \odot \mathrm{vec}(\mathrm{U_X^\top D U_Y})) \tag{14}$$

$$= K(U_Y \otimes U_X)(\mathrm{diag}(\Lambda + \sigma^2 I)^{-1} \odot \mathrm{vec}(\mathrm{U_X^\top D U_Y})) \tag{15}$$

$$= K(U_Y \otimes U_X)\boldsymbol{p} \tag{16}$$

$$= (K_Y \otimes K_X)\mathrm{vec}(U_X P U_Y^\top) \tag{17}$$

$$= \mathrm{vec}(K_X U_X P U_Y^\top K_Y) \tag{18}$$

where $\boldsymbol{p} = (\mathrm{diag}(\Lambda + \sigma^2 I)^{-1} \odot \mathrm{vec}(U_X^\top D U_Y))$ and

$$P = \mathrm{mat}(\boldsymbol{p}) = L \odot (U_X^\top D U_Y) \tag{19}$$

$$L = \mathrm{mat}(\boldsymbol{l}) = 1 \oslash (\boldsymbol{\kappa}_S^\top \otimes \boldsymbol{\kappa}_T + \sigma^2 E) \tag{20}$$

where $\oslash$ is an element-wise devision, E is a matrix whose elemenets are unity, and $\boldsymbol{\kappa}_S^\top$ and $\boldsymbol{\kappa}_T$ are the colmun vector made of the eigenvalues of K_S and K_T.

The isomorphic expression for $M = \mathrm{mat}(\boldsymbol{\mu})$ is given by

$$M = K_X U_X P U_Y^\top K_Y. \tag{21}$$

For the prediction of $K^* = (K_Y^* \otimes K_X^*)$, we obtain

$$\boldsymbol{\mu} = K^* \mathrm{vec}(U_X P U_Y^\top) \tag{22}$$

$$= (K_Y^* \otimes K_X^*)\mathrm{vec}(U_X P U_Y^\top) \tag{23}$$

$$= \mathrm{vec}(K_X^* U_X P U_Y^\top (K_Y^*)^\top) \tag{24}$$

The isomorphic expression is

$$M^* = K_X^* U_X P U_Y^\top (K_Y^*)^\top \tag{25}$$

Corresponding author: Hajime Kawahara