Imperial College London

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PhD week 14-Weekly summary

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Since last conversation, I was looking at

- covariance matrix on the PCE

- Jacobian matrix

Multiple target regression MTR-Chain regression

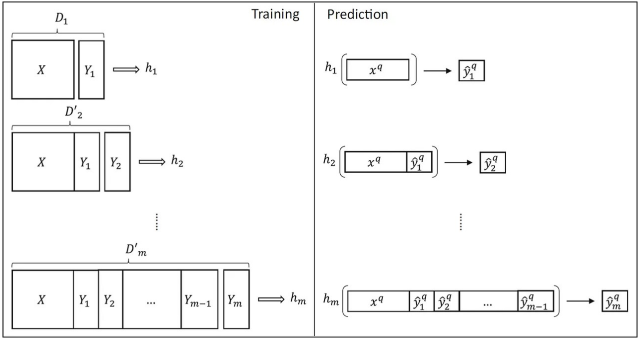

Figure 1: Regression chain model training

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Chain regression-PCE

Idea: Put 29 independent sub-PCEs into 29 dependent sub-PCEs

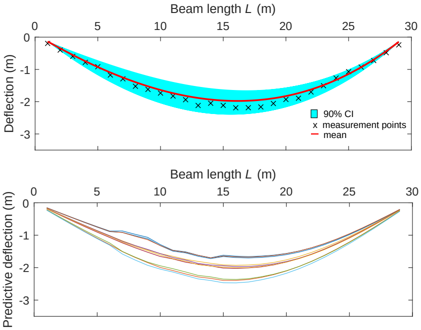

Figure 2: PCE 90% error band and predictive distribution

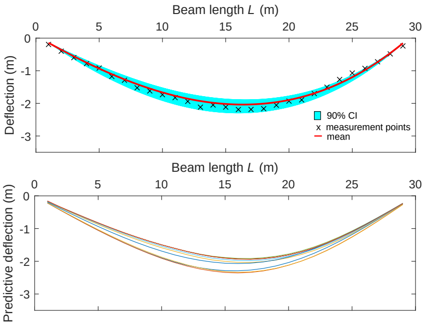

Figure 3: PCE 90% error band and predictive distribution

Jacobian matrix-scaling and rotation

Jacobian matrix is the matrix of all its first-order partial derivatives

$$\boldsymbol{J} = [\frac{\partial f}{\partial x_1} \cdots \frac{\partial f}{\partial x_n}] = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

For example, $\sigma = \mathbb{E} : \epsilon$, elastic modulus $\mathbb{E}$ is a Jacobian matrix

Multivariate Gaussian distribution

if each x_i follows Gaussian distribution $X \sim \mathcal{N}(\vec{u}, \mathbf{\Sigma})$
$\vec{u}$ is mean value; $\mathbf{\Sigma}$ is covariance matrix

Joint PDF should be:

$$p_X(x_1, \cdots, x_n) = \frac{1}{(2\pi)^{n/2}|\mathbf{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \vec{u})^{\mathsf{T}} \mathbf{\Sigma}^{-1} (\boldsymbol{x} - \vec{u})\right) \tag{1}$$

How we get the joint PDF?

Multivariate Gaussian distribution

"Any multivariate Gaussian distribution can be obtained by the linear variation of the standard Gaussian distribution"

$$\vec{Y} = A\vec{Z} + \vec{u} \tag{2}$$

in which, $\vec{Y}$ is arbitrary multivariate Gaussian distribution, $\vec{Z} = (z_1, \cdots, z_n)$ and $z_i \sim \mathcal{N}(0,1)$,$\vec{u}$ is the mean, $|A|$ is non-zero
theorem:

$$\boldsymbol{J}(Y \to Z) = A = (A^T A)^{1/2}$$
$$\boldsymbol{J}(Z \to Y) = A^{-1} = \frac{1}{A} = (A^T A)^{-1/2}$$

Multivariate Gaussian distribution

The final goal is to calculate the $p_Y(y)$:

$$\vec{Z} = A^{-1}(\vec{Y} - \vec{u}) = \Phi^{-1}(y) \tag{3}$$

$$p_Y(y) = p_Z(z)|J(Z \to Y)| = p_Z(\Phi^{-1}(y))|J(Z \to Y)| \tag{4}$$

Standard joint Gaussian distribution follows:
$p_Z(z_1, \cdots, z_n) = \frac{1}{(2\pi)^{n/2}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - 0)^{\mathsf{T}}(\boldsymbol{x} - 0)\right)$

Multivariate Gaussian distribution

Arbitrary multivariate Gaussian distribution should follow:

$$p_Y(y_1, \cdots, y_n) = p_Z(z)|J(Z \to Y)| = p_Z(\Phi^{-1}(y))|J(Z \to Y)|$$
$$= \frac{1}{(2\pi)^{n/2}} \exp\left(-\frac{1}{2}\left(A^{-1}(y-u)\right)^{\mathrm{T}}\left(A^{-1}(y-u)\right)\right) * \left(A^T A\right)^{-1/2}$$
$$= \frac{1}{(2\pi)^{n/2}} * \left(A^T A\right)^{-1/2} * \exp\left(-\frac{1}{2}(y-u)^{\mathrm{T}}(AA^T)^{-1}(y-u)\right)$$

Now, we define $A^T A = \Sigma$

$$p_Y(y_1, \cdots, y_n) = \frac{1}{(2\pi)^{n/2}} * \Sigma^{-1/2} * \exp\left(-\frac{1}{2}(y-u)^{\mathrm{T}}(\Sigma)^{-1}(y-u)\right)$$

Multivariate log-normal PDF

From above, we know the multivariate Gaussian pdf $p_Y(y)$, and $Y \sim \mathcal{N}(u, \Sigma)$

Multivariate change from Gaussian to Lognormal: $Q = \Phi(Y) = \exp(Y)$

The PDF for lognormal distribution Q is: $p_Q(q) = p_Y(\Phi^{-1}(q))|J(Y \rightarrow Q)|$

Lognormal PDF

Lognormal covariance

Something else

- PCE in UQlab explicitly mentioned that multiple output are independent. Thus, no covariance for sub-PCE
- $-\frac{1}{2}\left(\boldsymbol{x}-\vec{u}\right)^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}\left(\boldsymbol{x}-\vec{u}\right)$ is called Mahalanobis distance. So, we can get covariance between different types or magnitute of data or (height/weight or tons/gram)

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Summary

Chained PCE still has 29 sub-PCE, but related.

Jacobian matrix is an evidence for integral into 1? And Jacobian only exists when transformation exists? And I think Jacobian and covariance is the same thing

The URL mentioned Lognormal wrong? why is diagonal?