Vector-valued Gaussian Processes

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I. Overview of Gaussian Processes

Gaussian processes are generalizations of the multivariate Gaussian distribution. Rather than characterizing a probability distributions of vectors, Gaussian processes can be used to describe a probability distribution over families of functions.

i. Multivariate Gaussian (Multivariate Normal) Distribution

The multivariate normal distribution is used to model *random vectors* (vectors whose elements are jointly distributed random variables). This distribution is parameterized by a *mean vector* $\boldsymbol{\mu}$ and *covariance matrix* $\boldsymbol{\Sigma}$. Suppose $\boldsymbol{x} \in \mathbb{R}^N$ is drawn from a multivariate Gaussian distribution. Then, we can write the following:

$$\begin{aligned} \boldsymbol{x} \in \mathbb{R}^N &\sim \mathcal{N}_N(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \\ \boldsymbol{\mu} \in \mathbb{R}^N &= (\mu_1, \mu_2, ..., \mu_N)^\top = (\mathbb{E}(x_1), \mathbb{E}(x_2), ..., \mathbb{E}(x_N))^\top \\ \boldsymbol{\Sigma} \in \mathbb{R}^{N \times N} &= \mathbb{E}\big((\boldsymbol{x}-\mu)(\boldsymbol{x}-\mu)^\top\big) = \left[\operatorname{cov}(x_i, x_j)\right]_{ij}^{N} \\ x_i &\sim \mathcal{N}(\mu_i, \boldsymbol{\Sigma}_{ii}) \end{aligned} \tag{1}$$

ii. Gaussian Processes (GPs)

Formally, a *Gaussian process* (GP) is an uncountably infinite collection of random variables, with any finite sample from the process sharing a joint multivariate Gaussian distribution. GPs are fully specified by a *mean function* m and *covariance (kernel) function* k. For notational convenience, it's often assumed that the mean function is $\mathbf{0}$, but this is not required. The kernel function must produce a positive semi-definite matrix when evaluated on a set of input points (or vectors).

Positive semi-definite matrix.
Let $M \in \mathbb{R}^{N\times N}$ be a symmetric matrix. We say that M is positive semi-definite if, for all vectors $x \in \mathbb{R}^N$ not equal to $\mathbf{0}$, the following holds: $\boldsymbol{x}^\top M \boldsymbol{x} \geq 0$.

We will focus primarily on the *squared exponential kernel* $k : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$, defined as:

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

where $\|\cdot\|$ is the Euclidean norm. The squared exponential kernel has two *hyperparameters*, α and ρ, which control the variance scale and length scale of functions drawn from the GP. Typically, α is set to 1, and ρ is specified based on domain knowledge or is estimated from observed data. This choice of kernel function reflects the assumption that the covariance between two points (or vectors) x and x' decays exponentially based on the distance between them.

iii. Gaussian Process Regression

In practice, Gaussian Processes are often brought to bear on *regression problems*, in which an analyst has collected a dataset $S = (\boldsymbol{x}, \boldsymbol{y}) = \{(x_i, y_i) : x_i \in \mathbb{R}^p, y_i \in \mathbb{R}^d, i \in 1, 2, ..., N\}$ with the goal of learning the relationship f between $\boldsymbol{x}$ and $\boldsymbol{y}$:

$$\begin{aligned} \boldsymbol{y} &= f(\boldsymbol{x}) \quad \text{or} \\ \boldsymbol{y} &= f(\boldsymbol{x}) + \varepsilon \quad \text{(with additive noise).} \end{aligned} \tag{3}$$

Once f has been estimated, it can then be used to predict the values of future or test points, which we'll refer to as $\boldsymbol{x}_* \in \mathbb{R}^M$. Gaussian Process Regression can be considered a Bayesian method for learning f. As an overview, we'll consider an example using simulated data where $x_i, y_i \in \mathbb{R}$. Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magnam aliquam quaerat voluptatem. Ut enim aeque doleamus animo, cum corpore dolemus, fieri.

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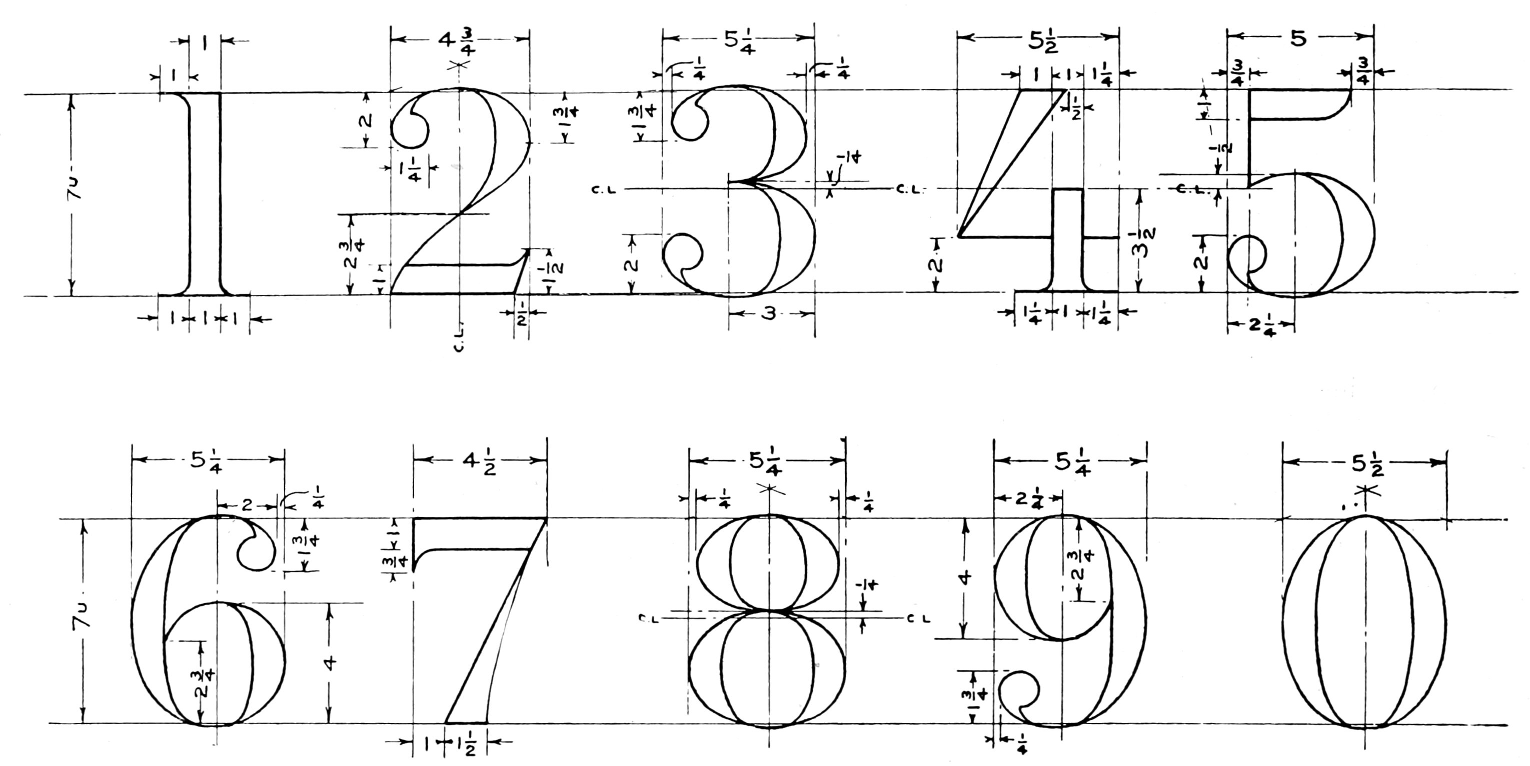

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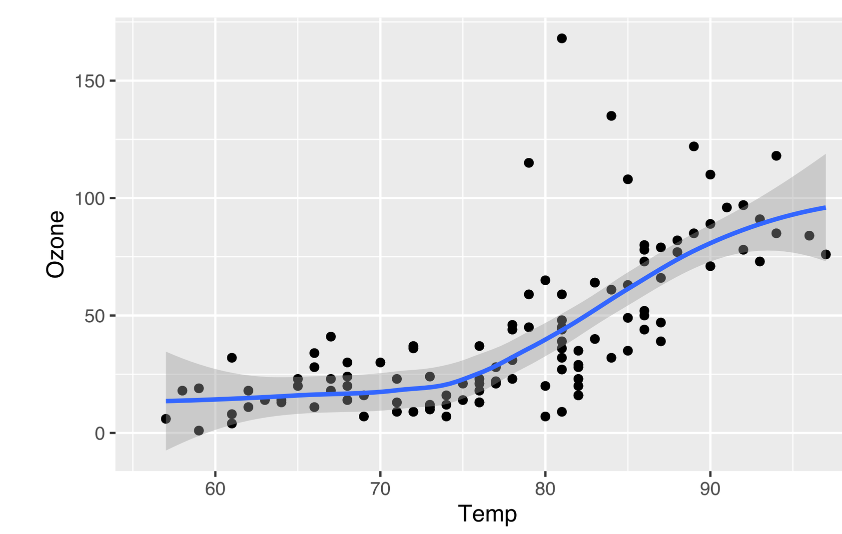

Figure 2: Temperature and ozone level

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$$\sum_{(k=1)}^{n} k = \frac{n(n+1)}{2} = \frac{n^2+n}{2} \tag{4}$$