Vector-valued Gaussian Processes

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I. Overview of Gaussian Processes

Gaussian processes are …

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 $x \in \mathbb{R}^N$ is drawn from a multivariate Gaussian distribution. Then, we can write the following:

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

ii. Gaussian Processes

A *Gaussian Process* (GP) describes a probability distribution over a (possibly infinite) collection of random variables, such that any finite collection of those random variables is distributed by the multivariate Gaussian distribution. GPs are characterized by a *mean function* m and *covariance (kernel) function* k. By convention, it's assumed that the mean function is 0.
We will focus on the *squared exponential kernel*:

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

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

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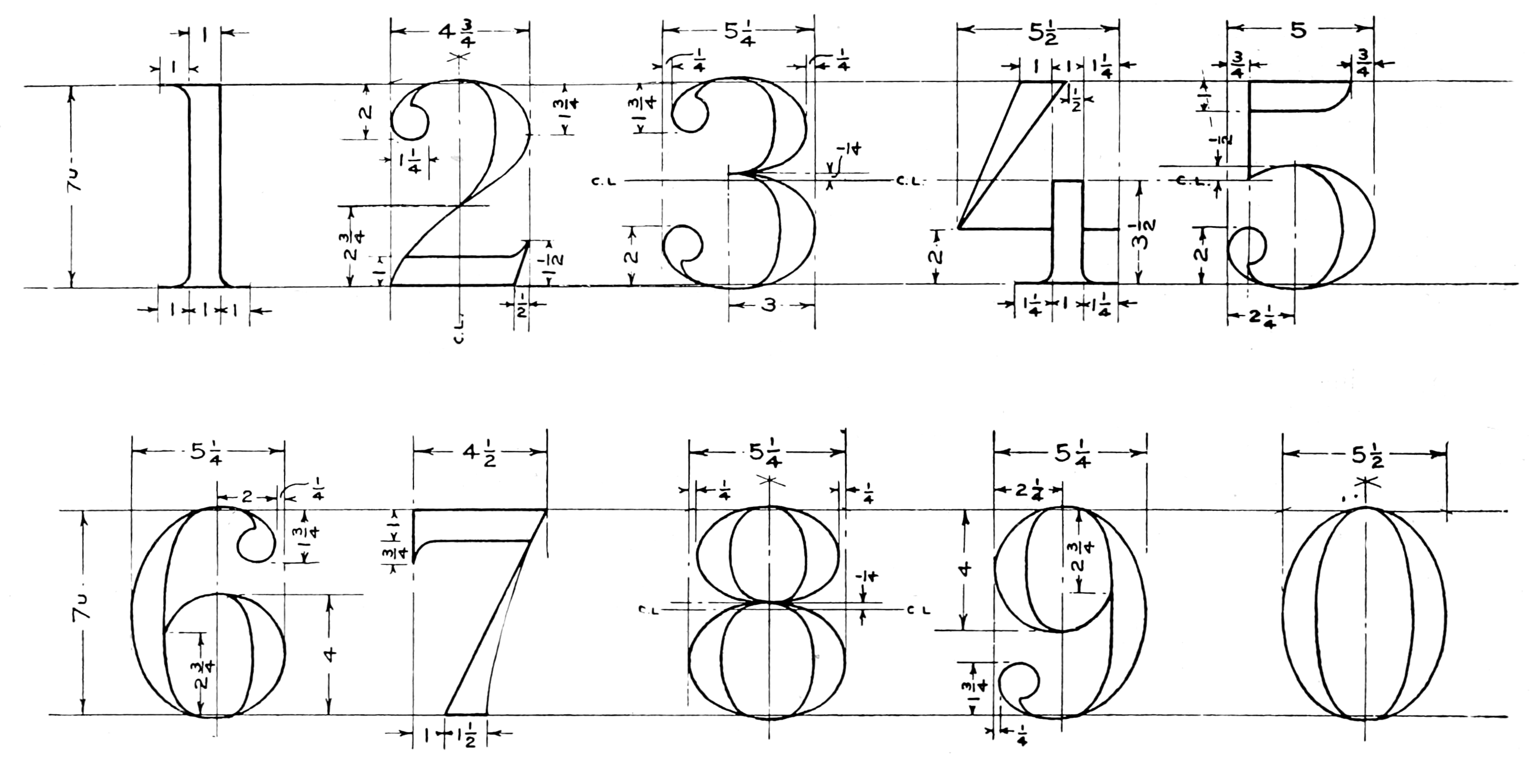

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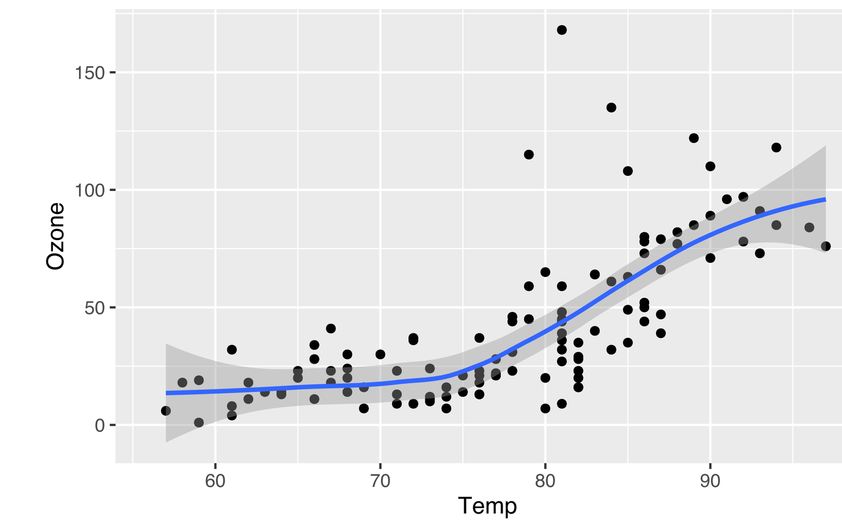

Figure 2: Temperature and ozone level

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$$\sum_{(k=1)}^{n} k = \frac{n(n+1)}{2} = \frac{n^2+n}{2} \tag{3}$$