
On Gaussian Processes for Regression

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Abstract

1 Gaussian processes emerged in machine learning as a powerful tool for regression
2 and classification that provides interpretability through kernel choice and uncertainty
3 quantification. By leveraging properties of multivariate normal distributions
4 and Bayes's rule, we may infer a probability distribution over possible functions
5 when fitting a dataset. This Bayesian framework allows flexibility through choosing
6 a covariance function as a prior belief about the dataset, which can provide further
7 insight into the trends of the training data. We implement a multi-dimensional Gaussian
8 process regressor and evaluate its performance on the Boston Housing dataset,
9 which is comparable to those in the top 25 of the Kaggle competition. Furthermore,
10 we perform optimization on the hyperparameters through maximum likelihood
11 estimation, to remove the need for manual tuning of the hyperparameters.

12 1 Gaussian Random Variables

13 A random variable is a function that maps from an event space to a measurable space. The event
14 space represents a set of all possible outcomes that the random variable may take, and the measurable
15 space is a probability measure between 0 and 1 (inclusive). We say that a random variable X is
16 normally distributed if the event space has a probability distribution that behaves like a Gaussian,
17 fully characterized by two parameters: a mean μ and variance σ^2 :

$$X \sim \mathcal{N}(\mu, \sigma^2).$$

18 For a one-dimensional Gaussian random variable, we refer to its distribution as a univariate Gaussian
19 distribution. A set of Gaussian random variables may be characterized jointly as a multivariate
20 Gaussian distribution, with joint probability distribution fully characterized by a mean vector and a
21 covariance matrix:

$$X = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_n \end{bmatrix} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma).$$

22 where $\boldsymbol{\mu}$ is the mean vector, and Σ is the covariance matrix whose entries describe the covariance
23 between each pair of random variables.

24 2 Gaussian Process

25 A random process is essentially a collection of random variables jointly characterized as a set or
26 vector of random variables with a multivariate joint probability distribution. A Gaussian process
27 $f(\mathbf{x})$ is defined as a random process where each set of random variable in the random process is

28 has a multivariate Gaussian distribution. $f(\mathbf{x})$ is fully characterized by a mean function $m(\mathbf{x})$ and
29 covariance function, or kernel $K(\mathbf{x}, \mathbf{x}')$:

$$f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), K(\mathbf{x}, \mathbf{x}'))$$

30 **3 Regression**

31 **3.1 Kernels**

32 **References**

33 References follow the acknowledgments. Use unnumbered first-level heading for the references. Any
34 choice of citation style is acceptable as long as you are consistent. It is permissible to reduce the font
35 size to small (9 point) when listing the references. **Note that the Reference section does not count**
36 **towards the eight pages of content that are allowed.**

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