

CEE 616: Probabilistic Machine Learning

M4 Nonparametric Methods:

L4b: Gaussian Processes

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Thu, Nov 12, 2025

Outline

- ① Introduction
- ② Mercer kernels
- ③ Joint MVNs
- ④ Noise-free
- ⑤ Noisy
- ⑥ Kernel learning
- ⑦ Outlook

Gaussian processes

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$$\mathbf{f}(\mathbf{x}) = \mathcal{GP}(\boldsymbol{\mu}, \boldsymbol{\Sigma}_{ij}) \quad (1)$$

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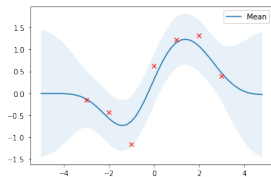
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Source: <http://krasserm.github.io/2018/03/19/gaussian-processes/>

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- Thus, a Mercer kernel is also known as a positive definite kernel

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- Kernels can be composed by addition, multiplication and other operations

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- SE is also referred to as Gaussian, RBF or exponentiated quadratic

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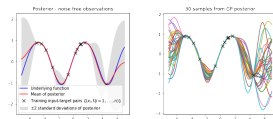
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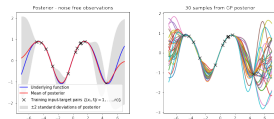
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To predict function outputs for new inputs \mathbf{x}^* , we estimate the *posterior conditional distribution*

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where:

- \mathbf{f}_X : function outputs over training set (interpolator): $[f(\mathbf{x}_1), \dots, f(\mathbf{x}_N)]$

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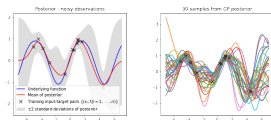
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GPR example with noisy inputs. Source: <https://www.aidancannell.com/post/gaussian-process-regression/>

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- Hyperparameters can be learned via **maximum marginal likelihood**

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To find the optimal kernel parameters $\boldsymbol{\theta}$, we maximize the **log marginal likelihood**:

Maximum marginal likelihood

Assuming the mean function is zero, the prior is given by:

$$p(\mathbf{f}|\mathbf{X}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{f}|\mathbf{0}, \mathbf{K}) \quad (25)$$

and the likelihood of each observation (conditioned on the latent function \mathbf{f}) can be written as:

$$p(\mathbf{y}|\mathbf{f}, \mathbf{X}) = \prod_{n=1}^N \mathcal{N}(y_n|f_n, \sigma_y^2) \quad (26)$$

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To find the optimal kernel parameters $\boldsymbol{\theta}$, we maximize the **log marginal likelihood**:

$$\log p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}) = \log \mathcal{N}(\mathbf{y}|\mathbf{0}, \hat{\mathbf{K}}_{\mathbf{X}, \mathbf{X}})$$

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To find the optimal kernel parameters $\boldsymbol{\theta}$, we maximize the **log marginal likelihood**:

$$\log p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}) = \log \mathcal{N}(\mathbf{y}|\mathbf{0}, \hat{\mathbf{K}}_{\mathbf{X}, \mathbf{X}}) = -\frac{1}{2} \mathbf{y}^\top \hat{\mathbf{K}}_{\mathbf{X}, \mathbf{X}}^{-1} \mathbf{y} - \frac{1}{2} \log |\hat{\mathbf{K}}_{\mathbf{X}, \mathbf{X}}| - \frac{N}{2} \log(2\pi) \quad (28)$$

Reading

- **PMLI 17.1-2**

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- https://colab.research.google.com/github/krasserm/bayesian-machine-learning/blob/dev/gaussian-processes/gaussian_processes.ipynb

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- <https://peterroelants.github.io/posts/gaussian-process-kernels/>

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- <https://peterroelants.github.io/posts/gaussian-process-kernels/>
- <https://github.com/aidanscannell/probabilistic-modelling/blob/master/notebooks/gaussian-process-regression.ipynb>