

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

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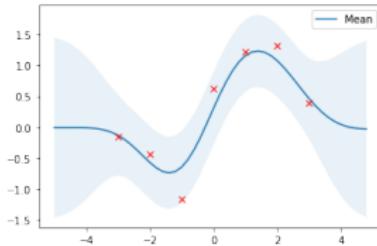
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Source: <http://krasserm.github.io/2018/03/19/gaussian-processes/>

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

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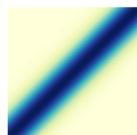
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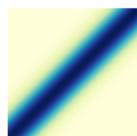
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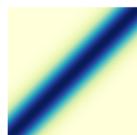


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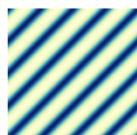
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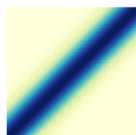
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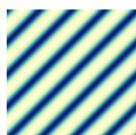
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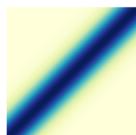


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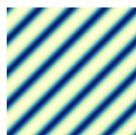
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- **Automatic relevancy determination (ARD) kernel**
- Kernels can be composed by addition, multiplication and other operations

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

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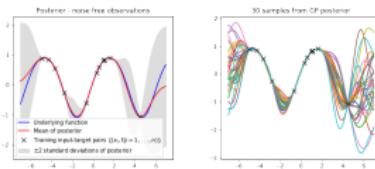
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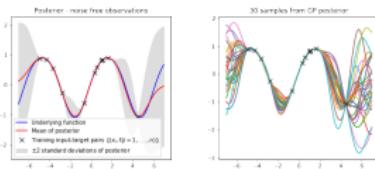
Source: <https://www.aidanscannell.com/post/gaussian-process-regression/>

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$$\mathcal{D} = \{(\mathbf{x}_n, y_n) : n = 1 : N\} \quad (12)$$

$$y_n = f(\mathbf{x}_n) \quad (\text{noise-free observation}) \quad (13)$$



Source: <https://www.aidanscannell.com/post/gaussian-process-regression/>

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

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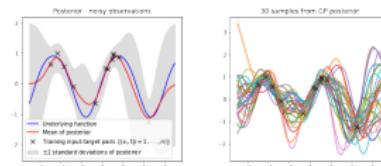
Note that this has the same form as the joint distribution in the noise-free case, except: $\mathbf{K}_{x,x}$ is replaced by $\hat{\mathbf{K}}_{x,x}$, which is the covariance of the training inputs with a constant variance σ_y^2 added to all the diagonal terms.

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

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

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>