Gaussian Processes for Jigsaw Puzzles

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Abstract

Background: Gaussian Processes (GP) are an important tool in non-parametric statistics. They can also be aesthetically pleasing .

Methods: I used the Free/Libre Open Source Software (FLOSS) Python PyMC GP package to generate cute, random puzzle nubs for making jigsaw puzzles. This also serves as demonstration and exploration of the 3 parameters of the Matérn covariance function, which is an important, and sometimes confusing mathematical object popular in GP modeling.

Results: The Matérn parameters have a complex interdependence, and setting any one incorrectly can lead to non-nubby puzzle pieces. Furthermore, the non-nubbyness can be similarly accomplished by setting any one of the three parameters incorrectly.

Conclusions: FLOSS math and stats tools are good for recreational math projects, which can also serve as educational tools. The Matérn covariance function is very expressive, but its parameters are highly interdependent in a way that can be surprising.

Background

Wikipedia provides a fine background:

> In probability theory and statistics] a *Gaussian process* is a stochastic process whose realizations consist of random variable associated with every point in a range of times (or of space) such that each such random variable has a normal distribution. Moreover, every finite collection of those random variables has a multivariate normal distribution.
>
> Gaussian processes are important in statistical modeling because of properties inherited from the normal distribution. For example, if a random process is modeled as a Gaussian process, the distributions of various derived quantities can be obtained explicitly. Such quantities include: the average value of the process over a range of times; the error in estimating the average using sample values at a small set of times.
>
> A Gaussian process is a stochastic process $\{X_t : t \in T\}$ for which any finite linear combination of samples will be normally distributed (or, more generally, any linear functional applied to the sample function X_t will give a normally distributed result).
>
> Alternatively, a process is Gaussian if and only if for every finite set of indices $t_{1,\ldots,k}$ in the index set T,
>
> $$\vec{\mathbf{X}}_{t_1,\ldots,t_k} = (\mathbf{X}_{t_1}, \ldots, \mathbf{X}_{t_k})$$
>
> is a vector-valued Gaussian random variable. Using characteristic functions of random variables, the Gaussian property can be formulated as follows: $\{X_t : t \in T\}$ is Gaussian if and only if, for every finite set of indices $t_1, \ldots, t_k$, there are reals σ_{lj} with $\sigma_{ii} > 0$ and reals μ_j such that
>
> $$\mathrm{E}\left(\exp\left(i\ \sum_{\ell=1}^{k} t_\ell\ \mathbf{X}_{t_\ell}\right)\right) = \exp\left(-\frac{1}{2}\sum_{\ell,j}\sigma_{\ell j} t_\ell t_j + i\sum_{\ell}\mu_\ell t_\ell\right).$$
>
> The numbers σ_{lj} and μ_j can be shown to be the covariances and means of the variables in the process [1].
>
> The "Matérn covariance" (named after the Swedish forestry statistician Bertil Matérn) is a covariance function used in spatial statistics, geostatistics, machine learning, image analysis, and other applications of multivariate statistical analysis on metric spaces. It is commonly used to define the statistical covariance between measurements made at two points that are d units

distant from each other. Since the covariance only depends on distances between points, it is stationary process. If the distance is Euclidean distance, the Matérn covariance is also isotropic.

The Matérn covariance between two points separated by d distance units is given by

$$C(d) = \sigma^2 \frac{1}{\Gamma(\nu)2^{\nu-1}} \left(2\sqrt{\nu}\frac{d}{\rho}\right)^{\nu} K_\nu\left(2\sqrt{\nu}\frac{d}{\rho}\right),$$

where Γ is the gamma function, K_ν is the modified Bessel function of the second kind, and ρ and ν are non-negative parameters of the covariance.

A Gaussian process with Matérn covariance has sample paths that are $\lceil \nu - 1 \rceil$ times differentiable. As $\nu \to \infty$, the Matérn covariance converges to the squared exponential covariance function

$$C(d) = \sigma^2 \exp(-d^2/\rho^2).$$

When $\nu = 0.5$, the Matérn covariance is identical to the exponential covariance function [2].

Following the conventions of the Matérn implementation in the PyMC GP Package, I call σ the amplitude, ρ the scale, and ν the degree of differentiability.

Methods

The Free/Libre Open Source Software (FLOSS) package PyMC has an efficient set of Gaussian Process routines, including an implementation of the Matérn covariance function. In order to use this to generate the nubs for jigsaw puzzles, I designed a set of "observations" which lead a pair of GPs through the contortions expected of a jigsaw puzzle nub (Fig. 1).

Realizing this GP is straightforward with PyMC, requiring little more than the following code:

```
M, C = uninformative_prior_gp(0., diff_degree, amp, scale)
gp.observe(M, C, data.puzzle_t, data.puzzle_x, data.puzzle_V)
GPx = gp.GPSubmodel('GP', M, C, pl.arange(1))
X = GPx.value.f(pl.arange(0., 1.0001, 1. / steps))
```

By mapping the nubs from these pairs of GPs to the edges of graphs embedded in the plane, I automatically generated random puzzles (for example, Fig 2).

To explore the effects of the amplitude, scale, and degree of differentiability parameters, I varied each parameter individually through a range of values, while holding the other two fixed at good parameters for puzzle nubs.

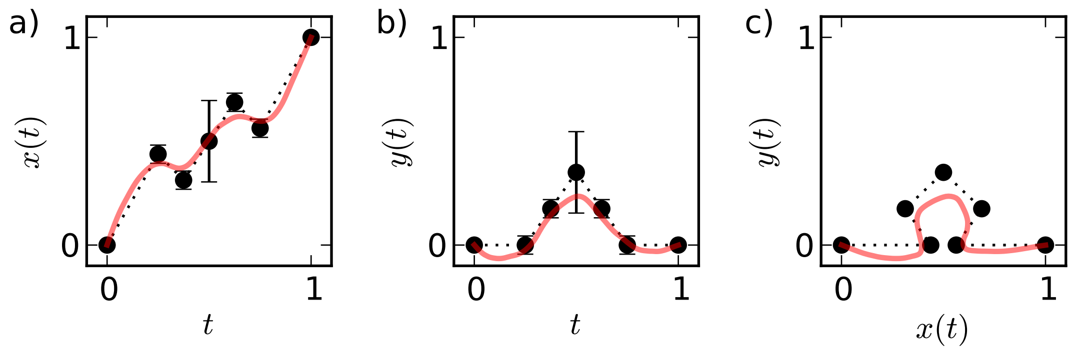

Figure 1: Two Gaussian Processes (panel a) for $x(t)$ and panel b) for $y(t)$ with Matérn covariance functions and 7 "observations" that look like a puzzle nub when plotted as a two dimensional function of time (panel c). The GP realizations (solid red lines) show the results of choosing good nub-like parameters for the Matérn covariance function of $\sigma = 1, \rho = 1.5, \nu = 2$.

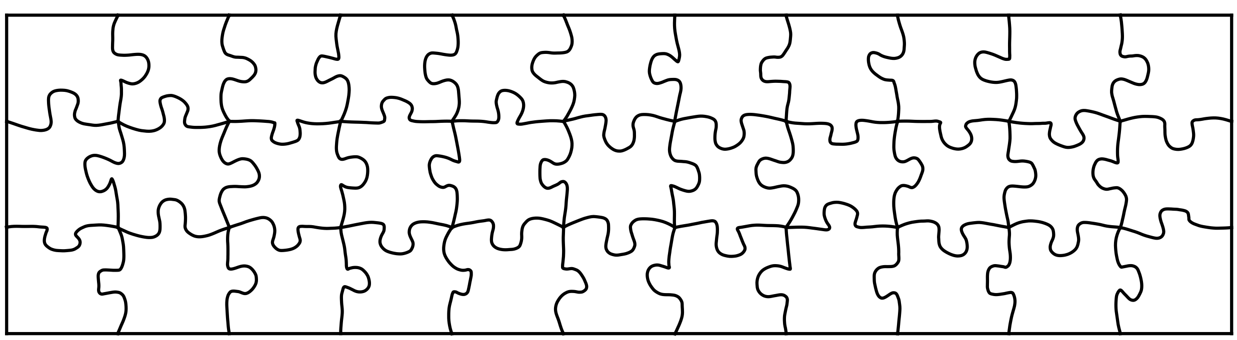

Figure 2: A small, randomly generated puzzle, using pairs of Gaussian Processes with Matérn covariance functions and 7 "observations" when good nub-like parameters for the Matérn covariance function ($\sigma = 1, \rho = 1.5, \nu = 2$) are selected.

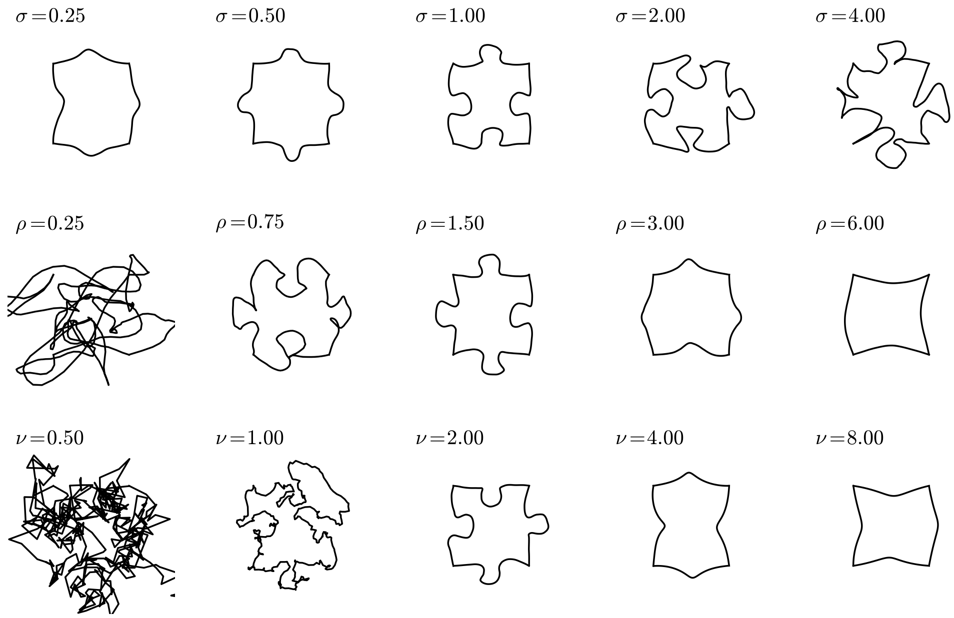

Figure 3: Realizations of GP puzzle pieces with varying Matérn parameters, using pairs of Gaussian Processes with Matérn covariance functions and 7 "observations". The parameters not listed in each row are the nub-like parameters $\sigma = 1, \rho = 1.5$, and/or $\nu = 2$.

Results and Discussion

The results are summarized by Fig 3.

As shown in Fig 3, the Matérn parameters have a complex interdependence structure, and setting any one incorrectly can lead to e non-nubby puzzle pieces. The middle column of the figure shows the nubby settings, while the entry with $\sigma = .25$ looks qualitatively very similar to that with $\rho = 3.00$ and also $\nu = 4.00$.

Conclusions

GPs are an important tool in non-parametric statistics, but be careful with the parameters, because they have complex interdependencies.

Competing interests

The author declares that he has no competing interests.

Authors contributions

AF designed the study, performed the analysis, and wrote the paper.

References

1. **Gaussian Process** [http://en.wikipedia.org/wiki/Gaussian_process].
2. **Matérn Covariance Function** [http://en.wikipedia.org/wiki/Matern_covariance_function].

Additional Files

Additional file 1 — Source Code

The source code used to generate puzzles and all plots in this paper with the Python PyMC GP Package is available under FLOSS GPL 3.0 Licence from http://github.com/aflaxman/pymc-gp-pzzle.