

# Gaussian Processes Part 1

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10 Nov, 2025



## ① Intro

- Preliminaries
- Kernel Math
- Basic Hyper-Parameters
- Kernel Types
- Kernel Math

## ② Example

- Spatial Hierarchy



# Non-parametrics

- Assumptions are vague
- Structure (of a function) is your prior.
- Is not only about Gaussian Processes



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  - Can take values from  $y_0$  to  $y_1$
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  - And more structural assumptions
- Is not only about Gaussian Processes
  - Dirichlet Processes
  - Bayesian Additive Regression Trees
  - Many Others



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  - Simply Constant or Zero  $m(x) = c$
  - Other custom functions  $m(x) = \sin(x)$



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- ③  $k(x, x')$  - kernel function, simply - measure of similarity for  $x$  and  $x'$ 
  - $[K]_{ij} = k(x_i, x_j)$  is an SPD matrix



# Kernel Function

Recall,  $\mathcal{GP}(M(x), K(x, x'))$  is a kind of normal distribution. This how a kernel might look like:

$$\begin{aligned}k(x, x') &= RBF(x, x') \\ &= \exp(-\|x - x'\|/2L)\end{aligned}$$

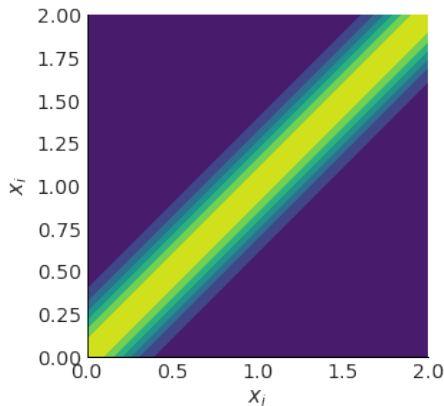


Figure: RBF kernel (data space)



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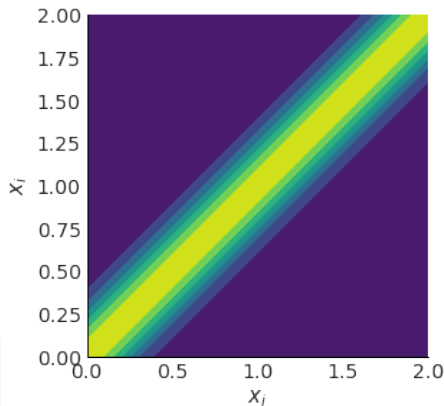


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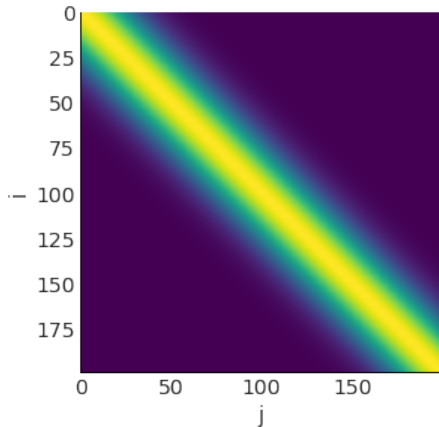


Figure: RBF kernel (covariance matrix)



# Kernel Math

Kernels can be combined (read more [2]). If  $k_1(x, x')$  and  $k_2(x, x')$  are valid kernels, then

- ①  $k_*(x, x') = a \cdot k_1(x, x') + b \cdot k_2(x, x')$  is a valid kernel
  - sum rule
  - $a, b > 0$
- ②  $k_*(x, x') = k_1(x, x')^a \cdot k_2(x, x')^b$  is a valid kernel
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Basic parametrisation often includes the following

- White Noise  $\varepsilon$
- Amplitude  $\sigma$
- Lengthscale  $L$

$$k(x, x') \cdot \sigma^2 + \varepsilon^2$$



# Understanding the lengthscale

- How **quickly**  $y$  is changed
- Not the magnitude!
- Often known up to a good value
- Hard to infer in practice

$$k(\mathbf{x}, \mathbf{x}') \cdot \sigma^2 + \epsilon^2$$

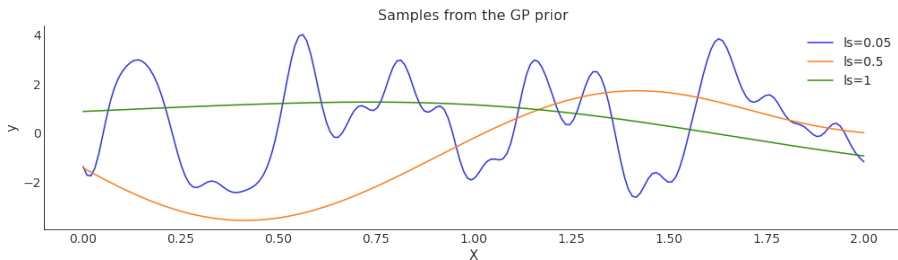


Figure: Lengthscales comparison





# Educated guess on lenthcales

- **Granularity** of time series data
  - If data is yearly, 1y lenthscale is a good fit
  - Interpolate missing observations
  - Interpolate higher granularity (months)

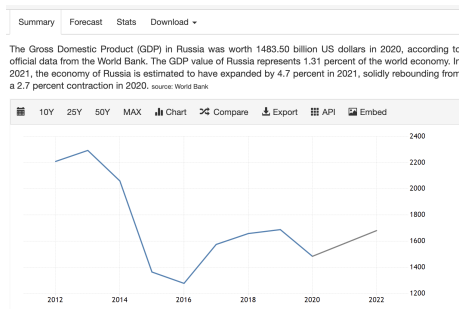


Figure: Russian GDP  
(tradingeconomics.com)



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- **Other**
  - Spatial distance (km, m, cm)
  - Age
  - Education duration

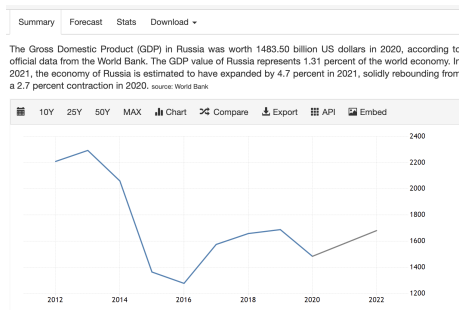


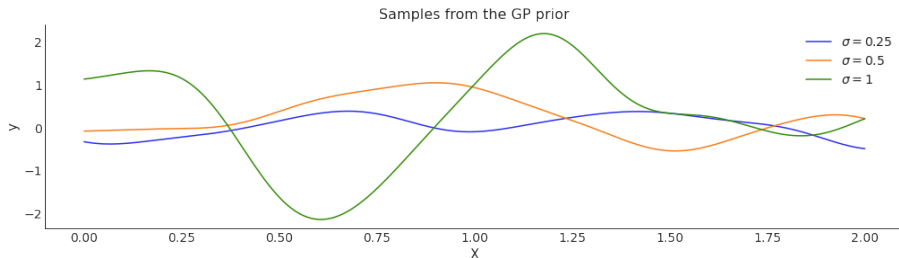
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# Understanding Amplitude

$$k(x, x') \cdot \sigma^2 + \epsilon^2$$

- How variable are the outcomes
- Not the standard deviation (aka white noise)
- Prior can be set with prior predictive checks





# Amplitude vs White Noise

$$k(x, x') \cdot \sigma^2 + \epsilon^2$$

- White Noise is separate thing from amplitude

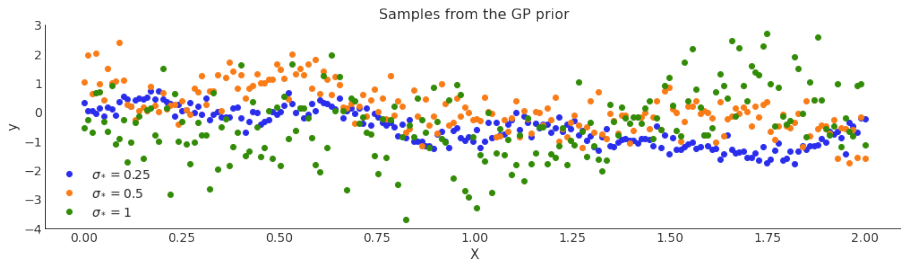


Figure: White Noise ( $\epsilon$ ) comparison



# Putting All Together

$$\begin{aligned}k(x, x') &= RBF(x, x') \cdot \sigma^2 + \varepsilon^2 \\&= \exp(-||x - x'||/2L) \cdot \sigma^2 + \varepsilon^2\end{aligned}$$



# Putting All Together

- $L$  lengthscale is input measurement unit

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## Note

Lengthscales can be put out of the kernel and are not their intrinsic property (for most of them)

$$\exp(-\|x - x'\|/2L) = \exp(-\|x/\textcolor{red}{L} - x'/\textcolor{red}{L}\|/2)$$



# Kernel Types

Every kernel is a structural assumption

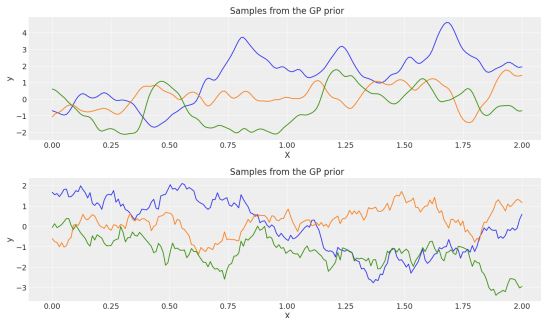
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- Periodic/Circular
- Linear/Polynomial (non stationary)



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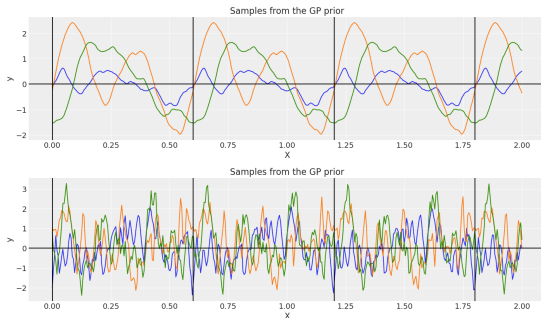




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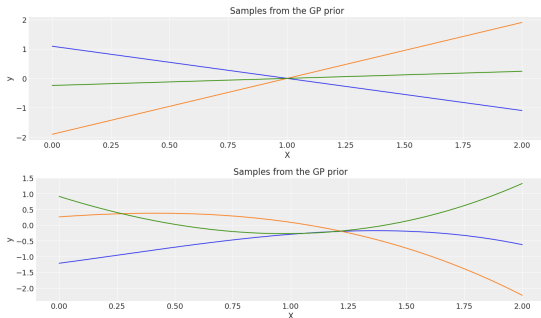




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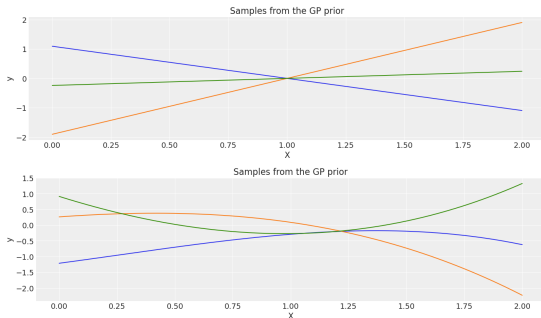




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## Kernel math power

You can combine basic properties of the kernels together. Examples [here](#).  
Combining kernels is art. Art is for the seminar.



# Combining Kernels

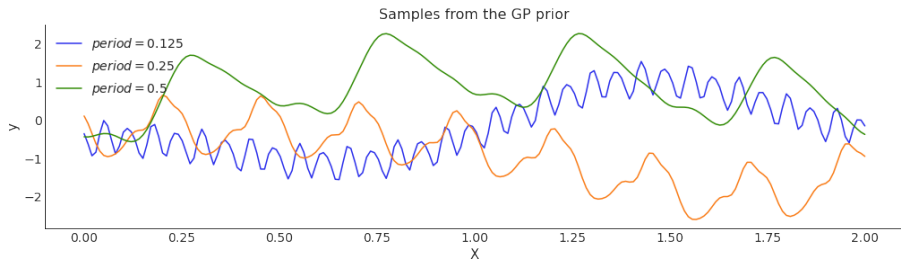


Figure: Exponential and Periodic kernel



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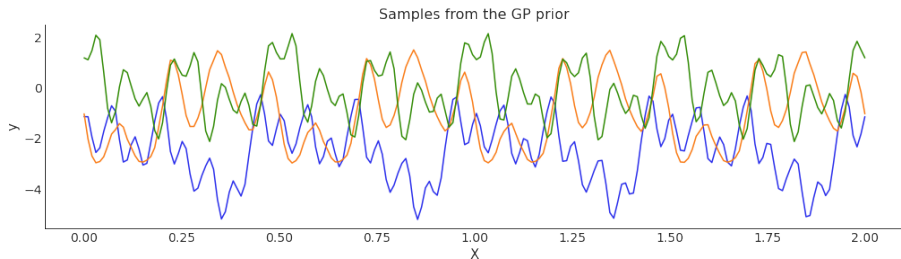


Figure: Sum of Multiple Periodic kernels





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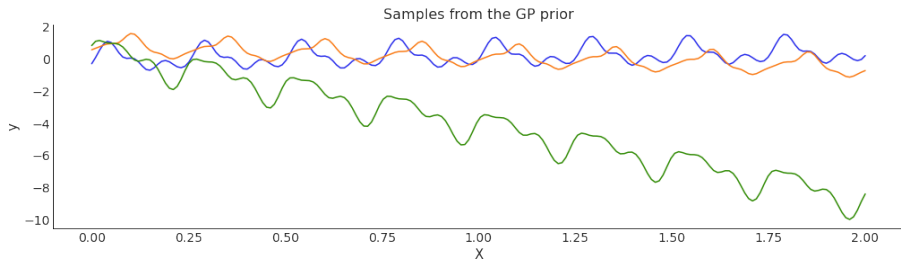


Figure: Linear and Periodic kernels



# Summary

- Kernels represent structural patterns
- Patterns can be learned from data
- Combining kernels you combine patterns that can be learned



# Motivation

There are cases where GP is a sharp knife to solve the problem. They look like

- My parameter changes over time [3]
- I have a time series [1]
- I have spatial data
- I have spatial data and time series



# Our Example

The favorite 8 schools

$$\mu \sim \text{Normal}(0, 5)$$

$$\tau \sim \text{HalfCauchy}(5)$$

$$\theta_i \sim \text{Normal}(\mu, \tau)$$

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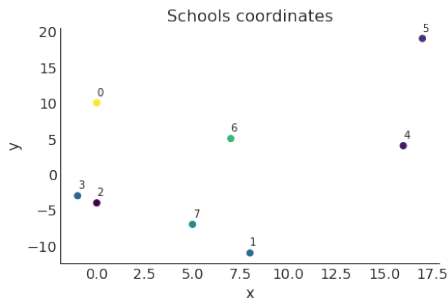
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- Coordinates of schools?





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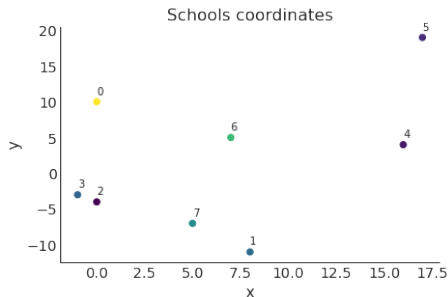
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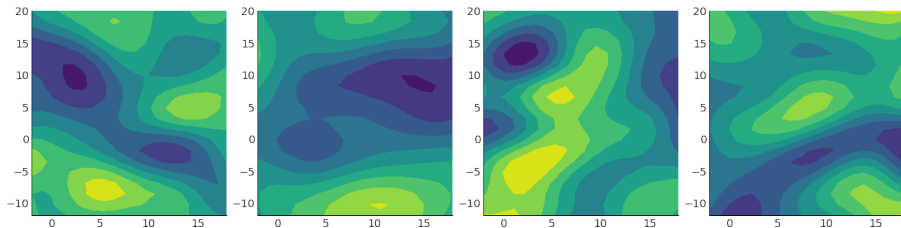
## Assumption

Neighboring schools are similar



# Spatial Gaussian Process

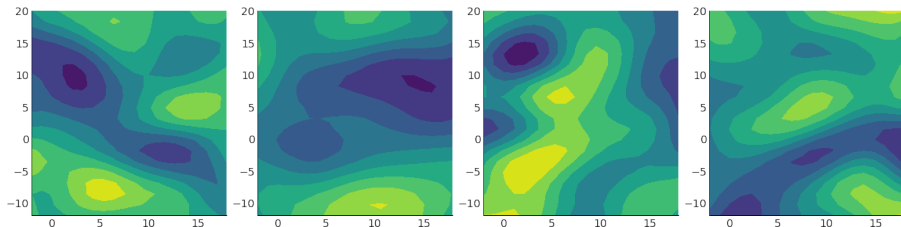
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## Idea

Instead of independent hierarchy, use GP hierarchy!





# The GP Hierarchy

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$$\theta_i = \mu + \tau \cdot \bar{\theta}_i$$

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## Comments

Centered parametrization has geometry issues (lecture 2)



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Issues can be resolved with noncentered parametrization



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## Comments

In the original model,  $\theta_i$  (or  $\bar{\theta}_i$ ) is independent per school



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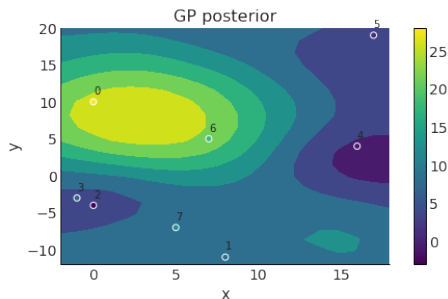
Gaussian Process adds dependencies between schools so close ones are similar.  $\sigma_{\mathcal{GP}} = 1$



# Results and Takeaways

## GP Gotchas

- 1 Flexible structure
- 2 Smart hierarchy
- 3 Predictions for new objects





# References I



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