

Gaussian Processes Part 1

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Agenda

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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 - Priors on time or spatial effects
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 - Does not change much
 - Volatile
 - Can take values from y_0 to y_1
 - Extrapolates periodically
 - And more structural assumptions
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- Is not only about Gaussian Processes
 - Dirichlet Processes
 - Bayesian Additive Regression Trees
 - Many Others



Notation

$x \in \mathbb{R}^n, y \in \mathbb{R}$

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- ① \mathcal{GP} Gaussian Process - simply, a normal distribution with special mean $m(x)$ and covariance $k(x, x')$



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- ➋ $m(x)$ - mean function, e.g.
 - Linear regression $m(x) = x^\top \beta$
 - Simply Constant or Zero $m(x) = c$
 - Other custom functions $m(x) = \sin(x)$



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- ➌ $k(x, x')$ - 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:

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

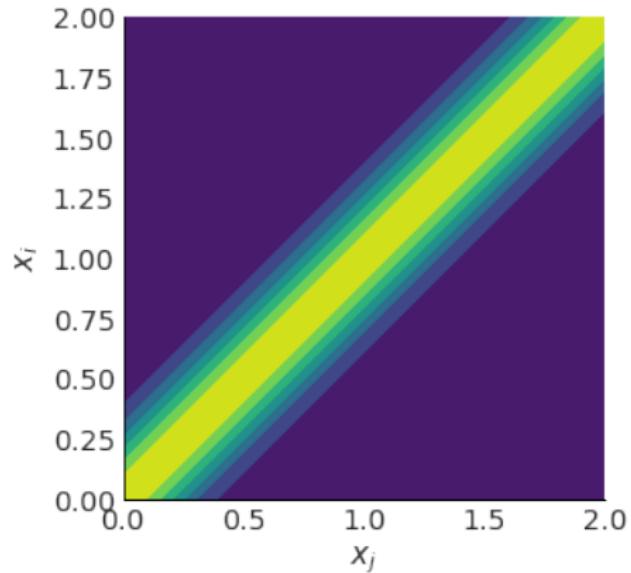


Figure: RBF kernel (data space)



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Parameter Interpretation

L - **lengthscale** for x such that y does not change much

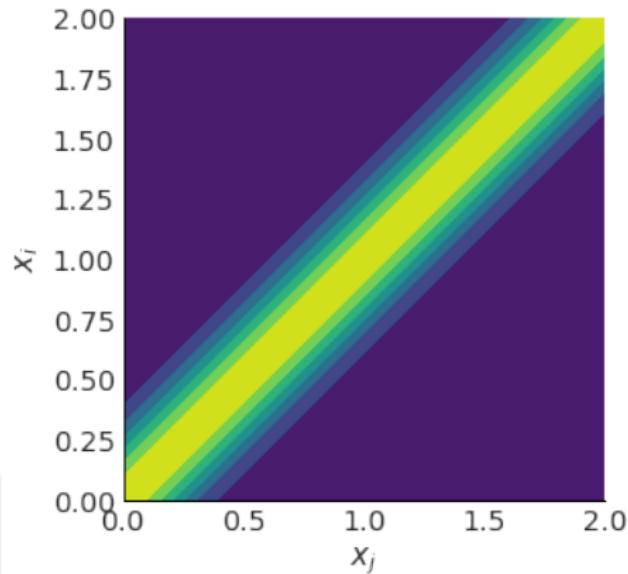


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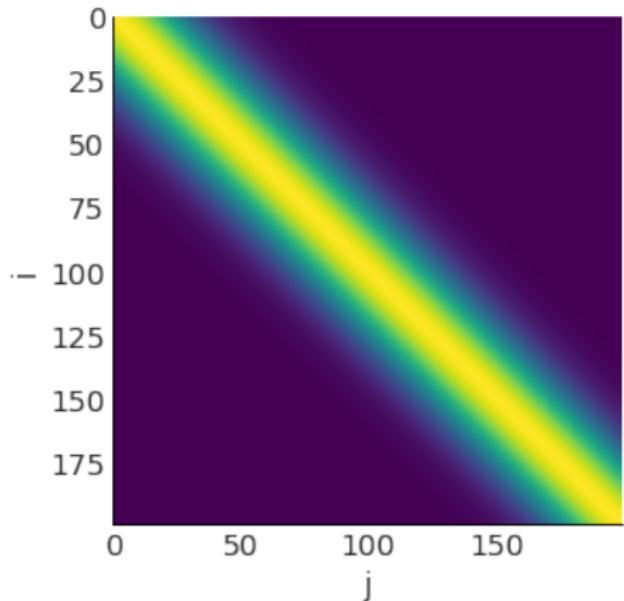


Figure: RBF kernel (covariance matrix)



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 ε
- Amplitude σ
- 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

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

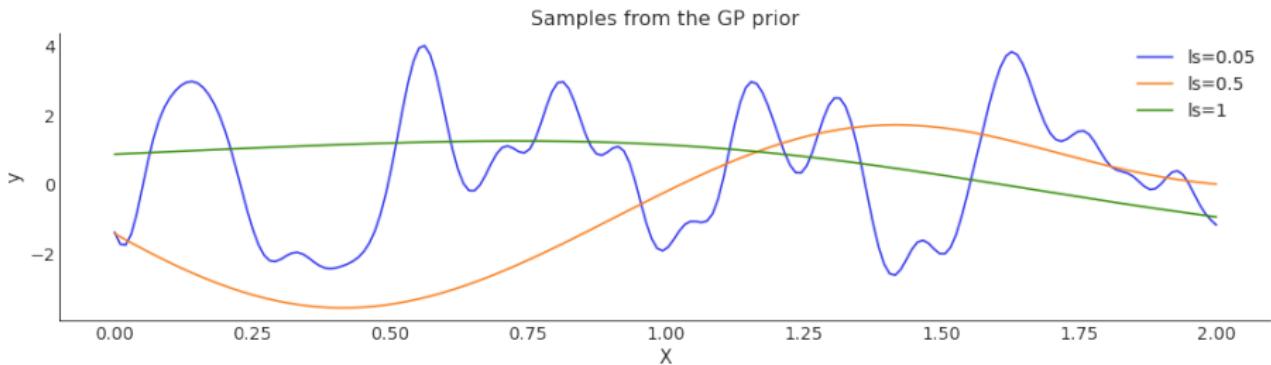


Figure: Lengthscales comparison



Educated guess on lengthscales

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

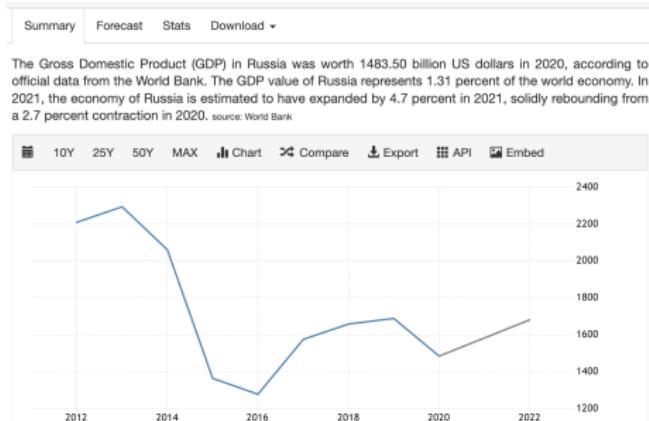


Figure: Russian GDP
(tradingeconomics.com)



Educated guess on lengthscales

- **Granularity** of time series data
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- **Other**
 - Spatial distance (km, m, cm)
 - Age
 - Education duration

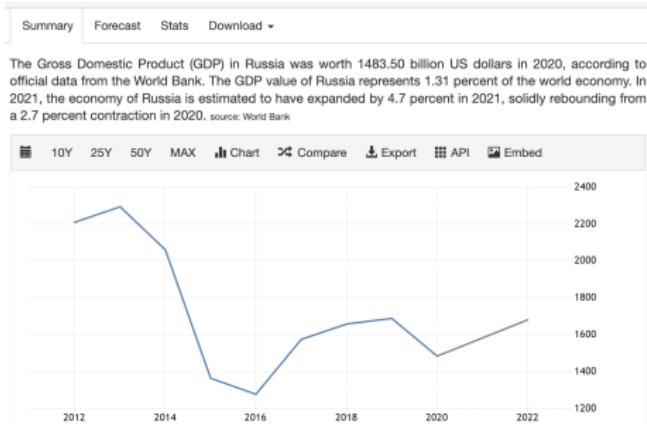


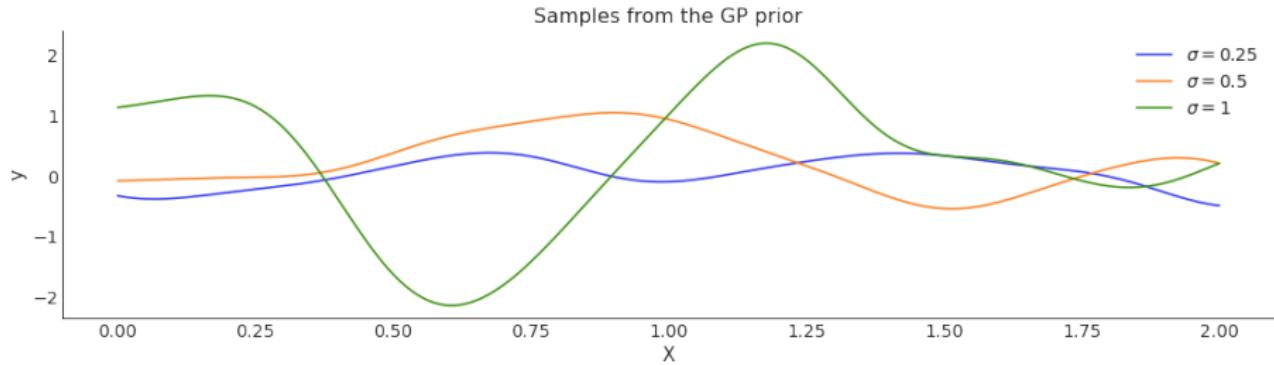
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Understanding Amplitude

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

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





Amplitude vs White Noise

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

- White Noise is separate thing from amplitude

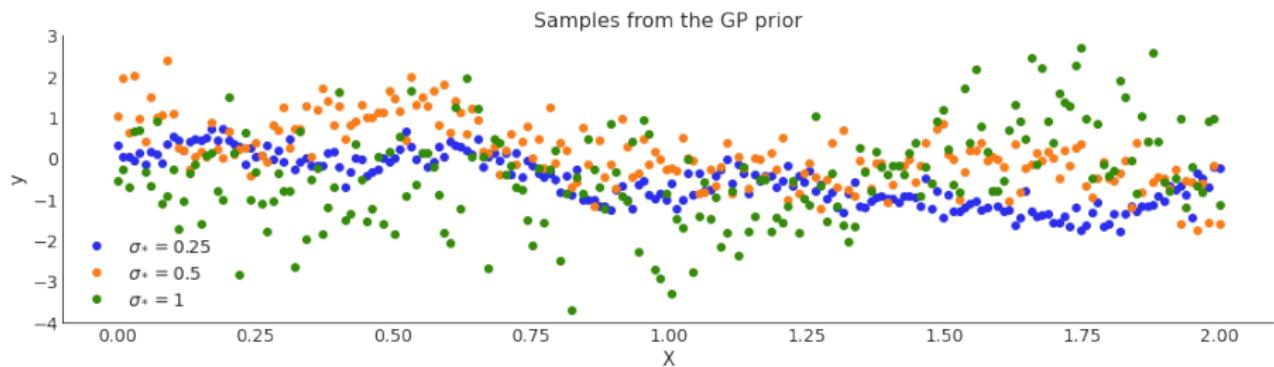


Figure: White Noise (ε) comparison



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

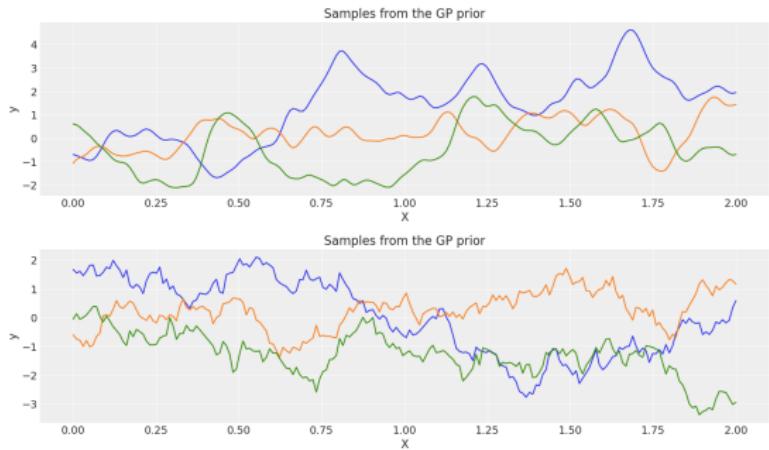
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- Periodic/Circular
- Linear/Polynomial (non stationary)



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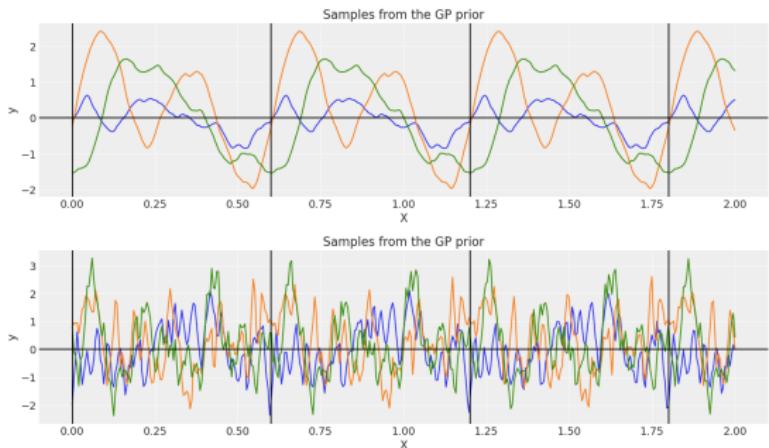




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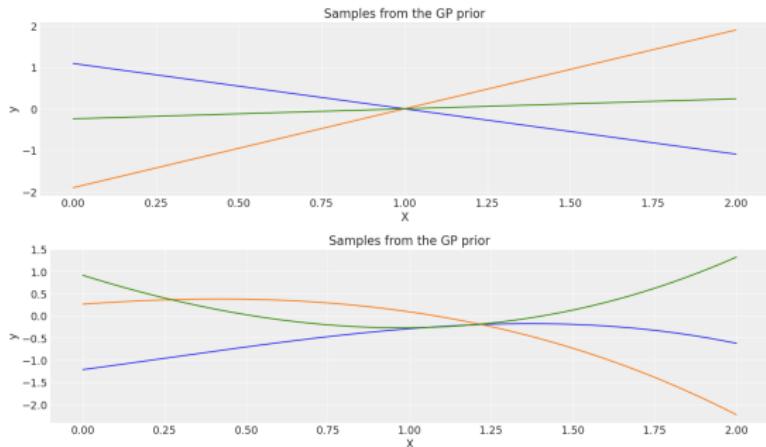




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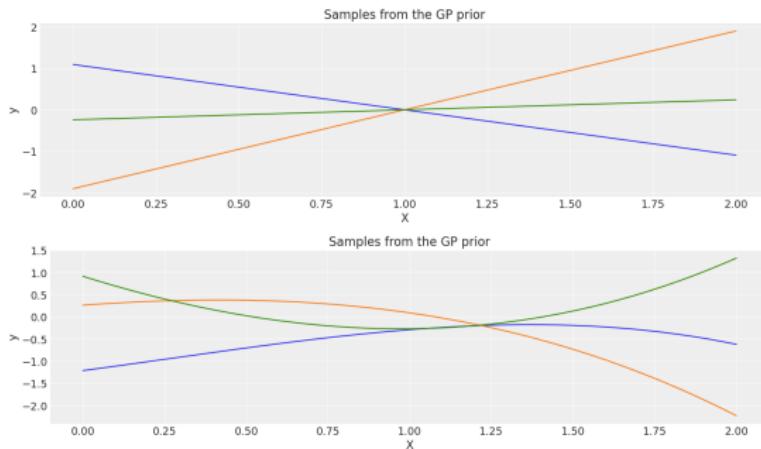




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Kernel math power

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



Combining Kernels

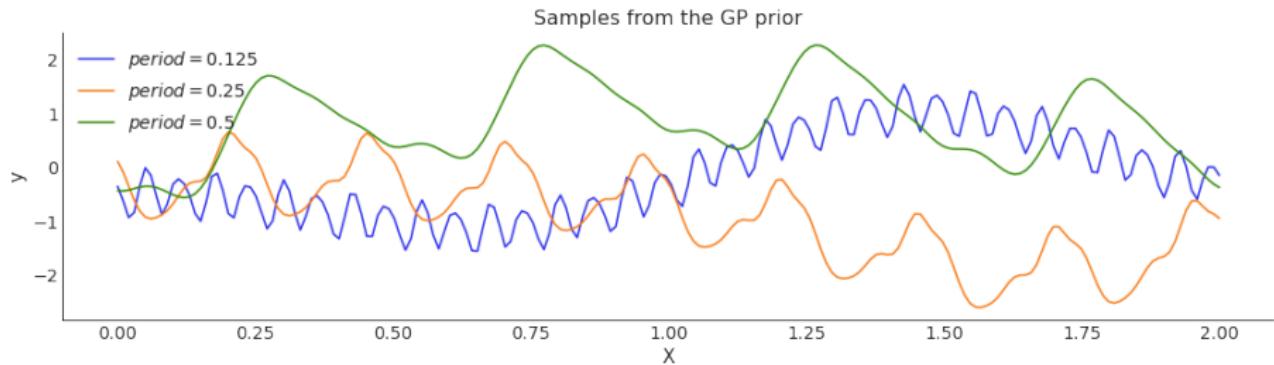


Figure: Exponential and Periodic kernel



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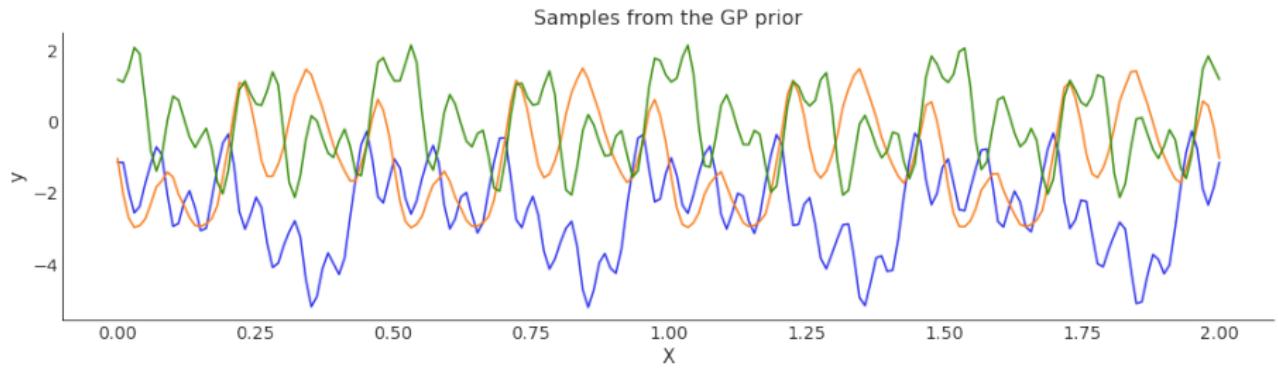


Figure: Sum of Multiple Periodic kernels



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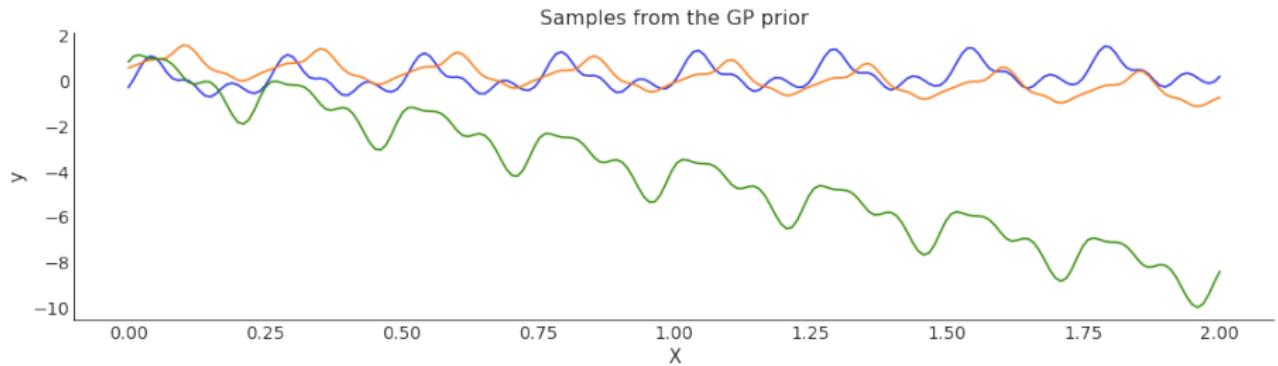


Figure: Linear and Periodic kernels



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

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

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

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

$$y_i \sim \text{Normal}(\theta_i, \sigma_i)$$

Where data are pairs $\{(y_i, \sigma_i)\}$



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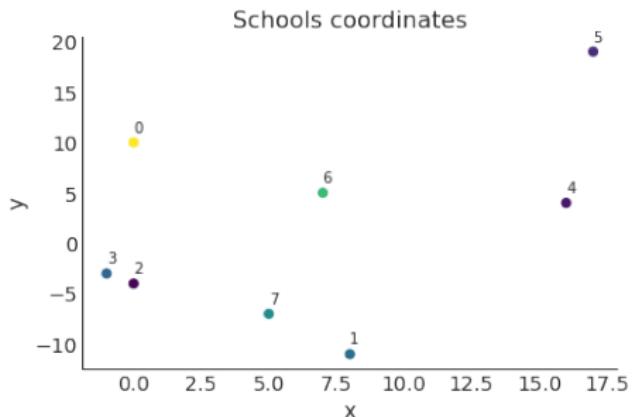
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- Coordinates of schools?





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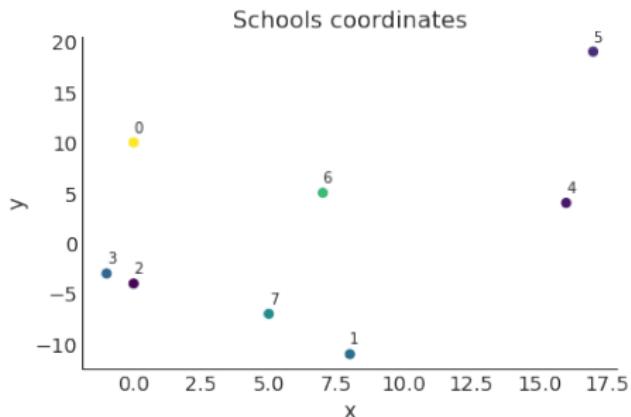
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Assumption

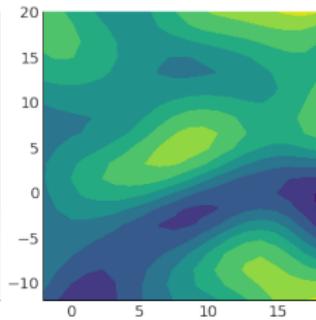
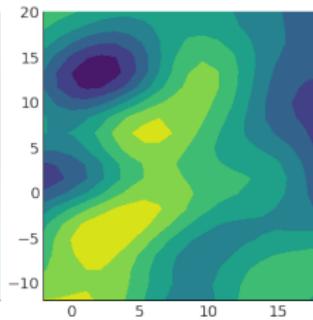
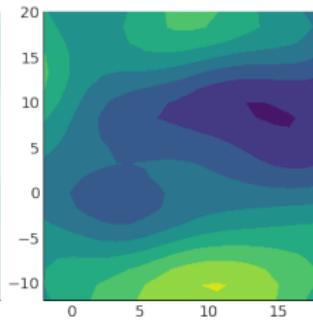
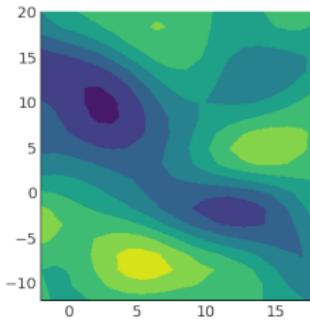
Neighboring schools are similar





Spatial Gaussian Process

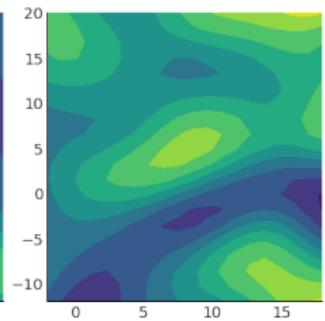
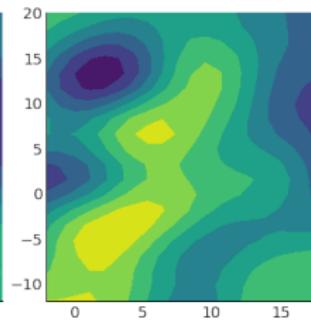
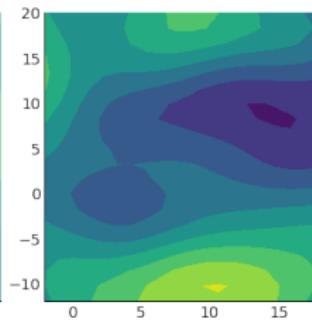
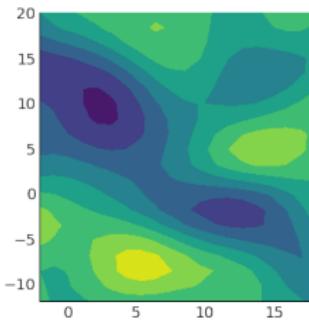
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- Lengthscale is important but can be inferred





Spatial Gaussian Process

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Idea

Instead of independent hierarchy, use GP hierarchy!



The GP Hierarchy

Before: (centered)

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

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(noncentered)

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Comments

Centered parametrization has geometry issues (lecture 2)



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Comments

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



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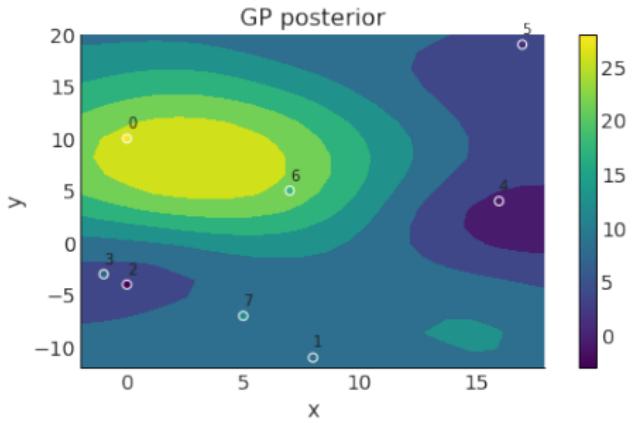
Gaussian Process adds dependencies between schools so close ones are similar. $\sigma_{\mathcal{GP}} = 1$



Results and Takeaways

GP Gotchas

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





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