Gaussian Processes Part 1

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MSU

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Agenda

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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  - Dirichlet Processes
  - Bayesian Additive Regression Trees
  - Many Others

Notation

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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:

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k(x, x') &= RBF(x, x') \\
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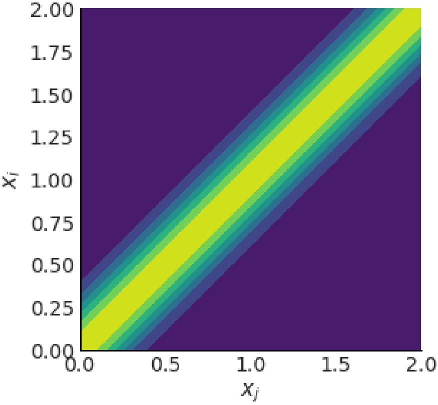

Figure: RBF kernel (data space)

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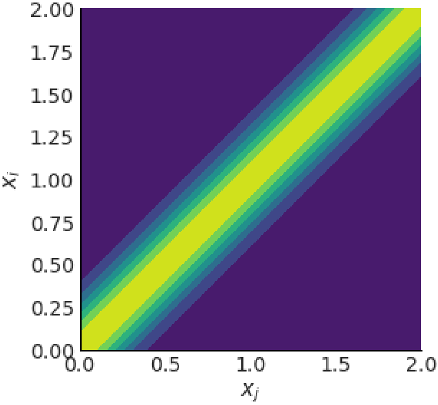

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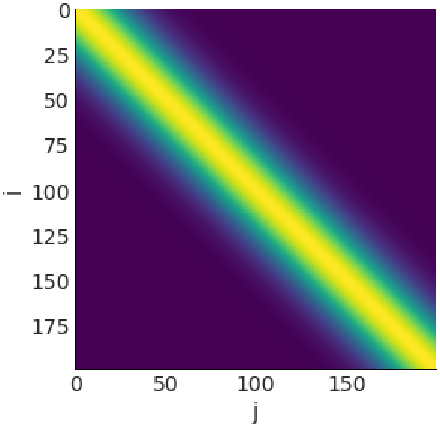

Figure: RBF kernel (covariance matrix)

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
   - $a, b > 0$
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Basic parametrisation often includes the following

- White Noise ε
- Amplitude σ
- Lengthscale L

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

Understanding the lengthscale

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

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

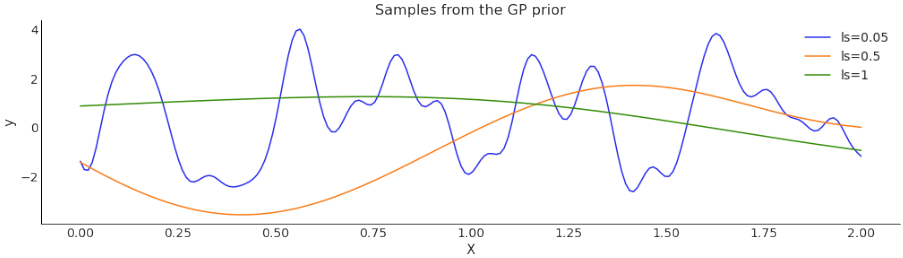

Figure: Lenthscales comparison

Educated guess on lenthscales

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

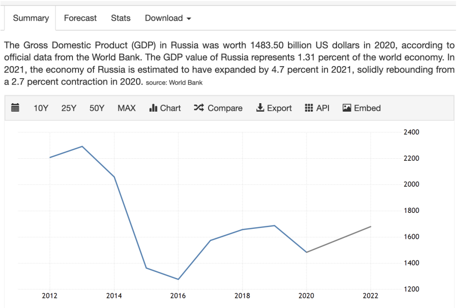

Figure: Russian GDP (tradingeconomics.com)

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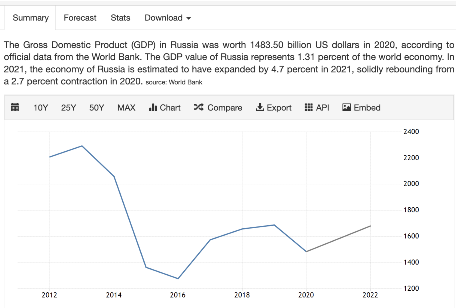
- **Other**
  - Spatial distance (km, m, cm)
  - Age
  - Education duration



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Understanding Amplitude

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

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

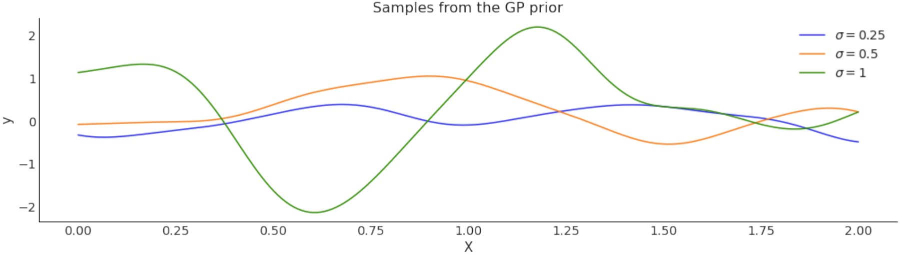

Figure: Amplitude (σ) comparison

Amplitude vs White Noise

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

- White Noise is separate thing from amplitude

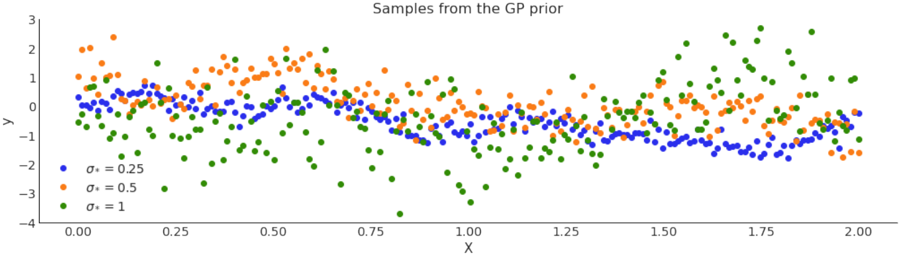

Figure: White Noise (ε) comparison

Putting All Together

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

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Note

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

$$\exp(||x - x'||/2L) = \exp(||x/L - x'/L||/2)$$

Kernel Types

Every kernel is a structural assumption

- Stationary
- Periodic/Circular
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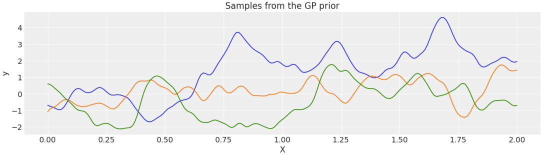

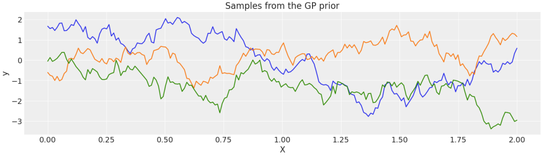

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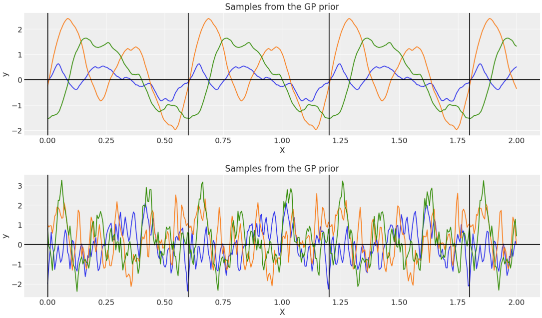

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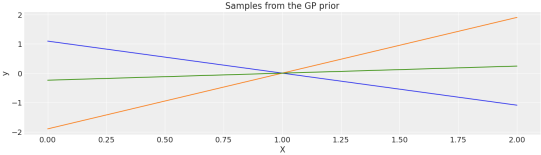

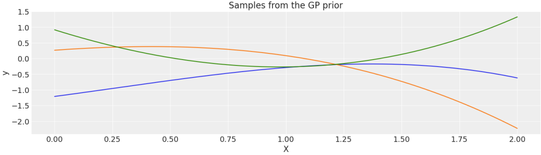

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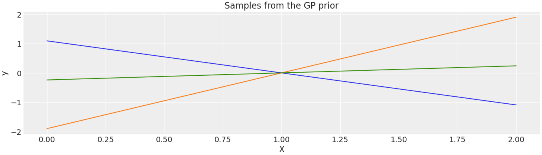

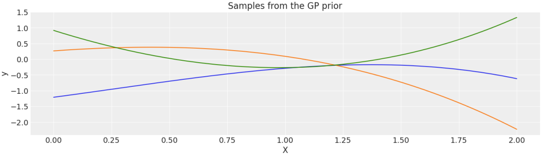

Kernel math power

You can combine basic properties of the kernels together. Examples here. Combining kernels is art. Art is for the seminar.

Combining Kernels

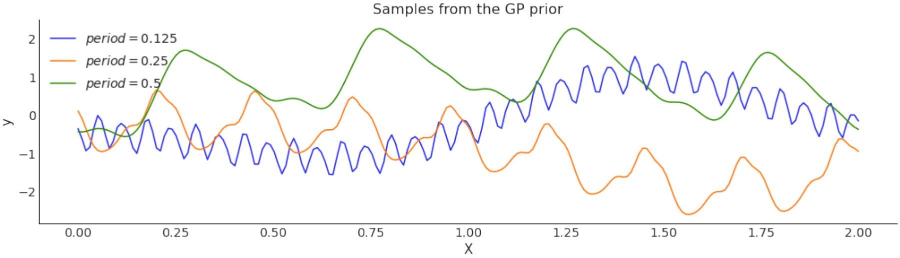

Figure: Exponential and Periodic kernel

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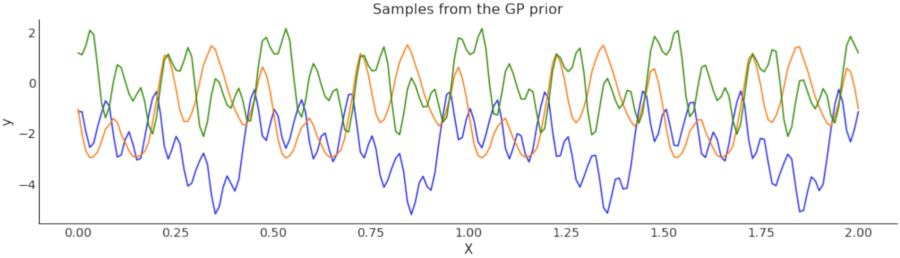

Figure: Multiple Periodic kernels

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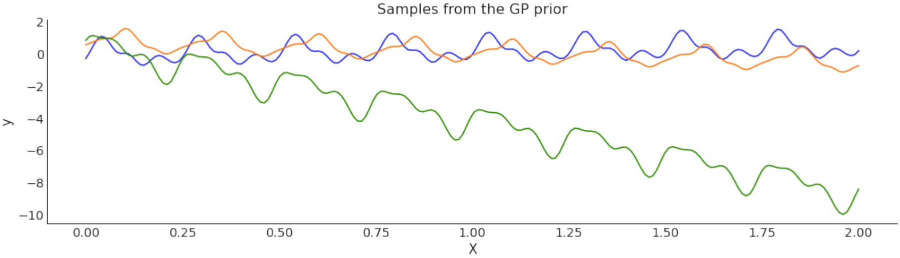

Figure: Linear and Periodic kernels

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

$$\begin{aligned} \mu &\sim \text{Normal}(0, 5) \\ \tau &\sim \text{HalfCauchy}(5) \\ \theta_i &\sim \text{Normal}(\mu, \tau) \\ y_i &\sim \text{Normal}(\theta_i, \sigma_i) \end{aligned}$$

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

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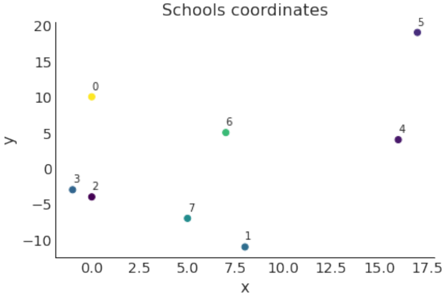
But:

- What if we have additional information?
- Coordinates of schools?



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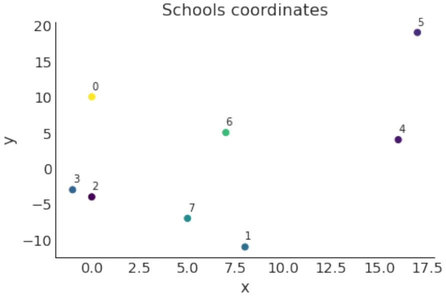
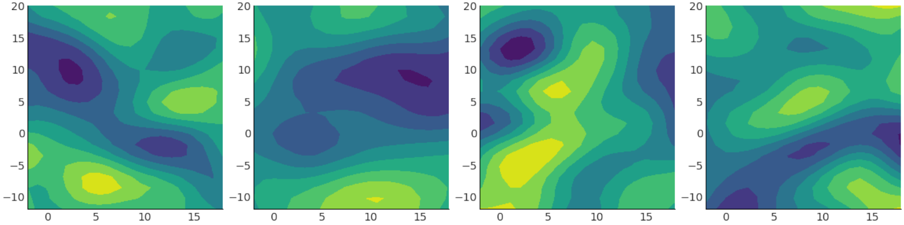


Assumption

Neighboring schools are similar

Spatial Gaussian Process

- A smooth function over 2d space
- Lengthscale is important but can be inferred



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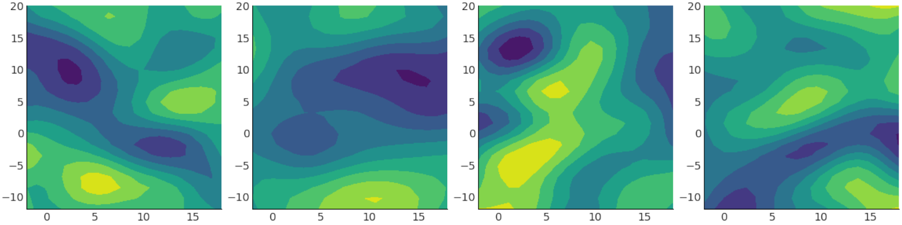

Idea

Instead of independent hierarchy, use GP hierarchy!

The GP Hierarchy

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(centered)

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

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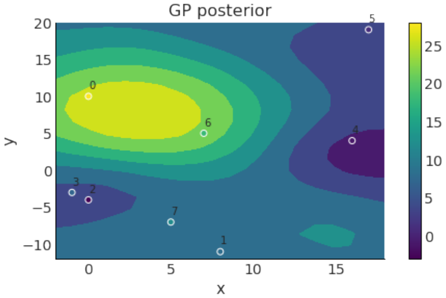
Comments

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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