Distributed Kernel Representations for Variational Sparse Gaussian Processes

Michalis K. Titsias
Department of Informatics,
Athens University of Economics and Business, Greece

Outline

- Variational learning of inducing variables
- Distributed representations of GPs (kernel functions) that can facilitate approximations in large datasets

Gaussian process regression

Inputs $X = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$ and outputs $\mathbf{y} = (y_1, \ldots, y_n)$ such that

$$y_i = f(\mathbf{x}_i) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

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Given that we have n data our current "marginal model" is

$$p(\mathbf{y}|\mathbf{f})p(\mathbf{f}) = \mathcal{N}(\mathbf{y}|\mathbf{f}, \sigma^2 I)\mathcal{N}(\mathbf{f}|\mathbf{0}, \mathbf{K}_{ff}), \quad [\mathbf{K}_{ff}]_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$$

where $\mathbf{f} = (f_1, \ldots, f_n)$ are the parameters

Inducing variables

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The size of $\mathbf{u}$ must be user-controllable based on current computational resources

- it could grow if the computational capacity increase in future

Inducing variables

Inducing variables $\mathbf{u}$ form a vector of user-controllable size that augments the GP prior:

$$p(\mathbf{f}, \mathbf{u}) = \mathcal{N}\left(\begin{bmatrix} \mathbf{f} \\ \mathbf{u} \end{bmatrix} \middle| \mathbf{0}, \begin{bmatrix} \mathbf{K}_{ff} & \mathbf{K}_{fu} \\ \mathbf{K}_{uf} & \mathbf{K}_{uu} \end{bmatrix} \right), \; \mathbf{K}_{fu} = \mathbb{E}[\mathbf{f}\mathbf{u}^T], \; \mathbf{K}_{uu} = \mathbb{E}[\mathbf{u}\mathbf{u}^T]$$

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$\mathbf{u}$ can be:

- a subset of $\mathbf{f}$
- values of $f(\mathbf{x})$ at arbitrary "pseudo-inputs"
- arbitrary linear functionals, e.g. $u = z_i f(\mathbf{x}_i) + z_j f(\mathbf{x}_j)$

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The augmentation with $\mathbf{u}$ adds some parameters Z

- indices that specify the subset in $\mathbf{f}$, pseudo-inputs, weights etc
- $\mathbf{K}_{fu}$ and $\mathbf{K}_{uu}$ depend on those parameters

Inducing variables

The whole purpose of adding **u** is to help us obtain an approximation to our Bayesian non-parametric model (**without changing its non-parametric nature**) that will scale better computationally

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The whole purpose of adding $\mathbf{u}$ is to help us obtain an approximation to our Bayesian non-parametric model (**without changing its non-parametric nature**) that will scale better computationally

How do we "turn around" $\mathbf{u}$ in order to make it the basis of our approximation? Further, how do we learn the augmentation parameters Z?

Variational learning of inducing variables

Augmented joint

$$p(\mathbf{y}, \mathbf{f}, \mathbf{u}) = p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{u})p(\mathbf{u})$$

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Marginal likelihood is invariant to the augmentation parameters Z

$$p(\mathbf{y}) = \int p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{u})p(\mathbf{u})d\mathbf{f}d\mathbf{u}$$

and the marginal posterior $p(\mathbf{f}|\mathbf{y})$ is also invariant to Z

- **I.e. Z is not model parameter**
- **$\Rightarrow$ we can turn it into variational parameter by lower bounding**

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This choice encourages $\mathbf{u}$ to become approximate sufficient statistic

if $p(\mathbf{f}|\mathbf{u}) \approx p(\mathbf{f}|\mathbf{u}, \mathbf{y})$, then $\mathbf{u}$ summarizes well the data

Variational learning of inducing variables

Minimize KL $[q(\mathbf{f}, \mathbf{u})||p(\mathbf{f}, \mathbf{u}|\mathbf{y})]$ or equivalently maximize the bound on the log marginal likelihood

$$\log p(\mathbf{y}) = \log \int p(\mathbf{y}|\mathbf{f}) p(\mathbf{f}|\mathbf{u}) p(\mathbf{u}) d\mathbf{f} d\mathbf{u}$$

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Maximize over $q(\mathbf{u})$:

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Variational learning of inducing variables

Bound:

For arbitrary GP model:

$$p(\mathbf{y}) \geq \int G(\mathbf{y}, \mathbf{u}) p(\mathbf{u}) d\mathbf{u}, \quad G(\mathbf{y}, \mathbf{u}) = e^{\int p(\mathbf{f}|\mathbf{u}) \log p(\mathbf{y}|\mathbf{f}) d\mathbf{f}}$$

For GP regression:

$$\mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}_{ff} + \sigma^2 I) \geq \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf} + \sigma^2 I) e^{-\frac{1}{2\sigma^2}\mathrm{tr}\left(\mathbf{K}_{ff} - \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf}\right)}$$

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Monotonicity property: If we have inducing variables $\mathbf{u}$ and add an extra u_i the bound can only increase

$$\int G(\mathbf{y}, \mathbf{u}, u_i) p(\mathbf{u}, u_i) d\mathbf{u} \geq \int G(\mathbf{y}, \mathbf{u}) p(\mathbf{u}) d\mathbf{u}$$

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Computation of the bound and the approximate GP prediction scale as $O(nm^2)$ where m is the number of inducing variables

Variational learning of inducing variables

For GP regression the bound has an interesting form:

$$\mathcal{F}(Z,\theta) = \log \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf} + \sigma^2 I) - \frac{1}{2\sigma^2}\mathrm{tr}\left(\mathbf{K}_{ff} - \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf}\right)$$

Variational learning of inducing variables

The approximate posterior/predictive Gaussian process:

$$
\begin{aligned}
q(\mathbf{f}_*) &= \int p(\mathbf{f}_*|\mathbf{f},\mathbf{u})q(\mathbf{f},\mathbf{u})d\mathbf{f}d\mathbf{u} \\
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where we used the consistency $\int p(\mathbf{f}_*|\mathbf{f},\mathbf{u})p(\mathbf{f}|\mathbf{u})d\mathbf{f} = p(\mathbf{f}|\mathbf{u})$

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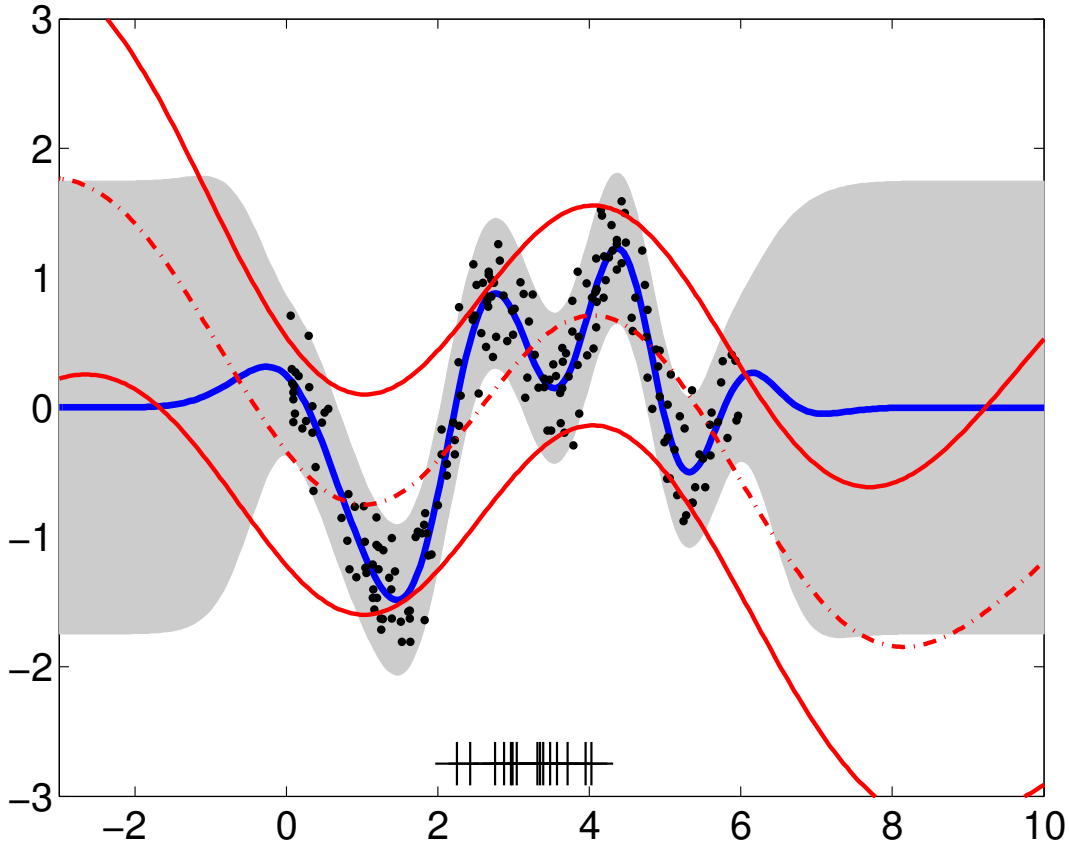
The approximation can be thought of been **restricted not to explore freely the information in the training data**. But it maintains fully the non-parametric nature of the model

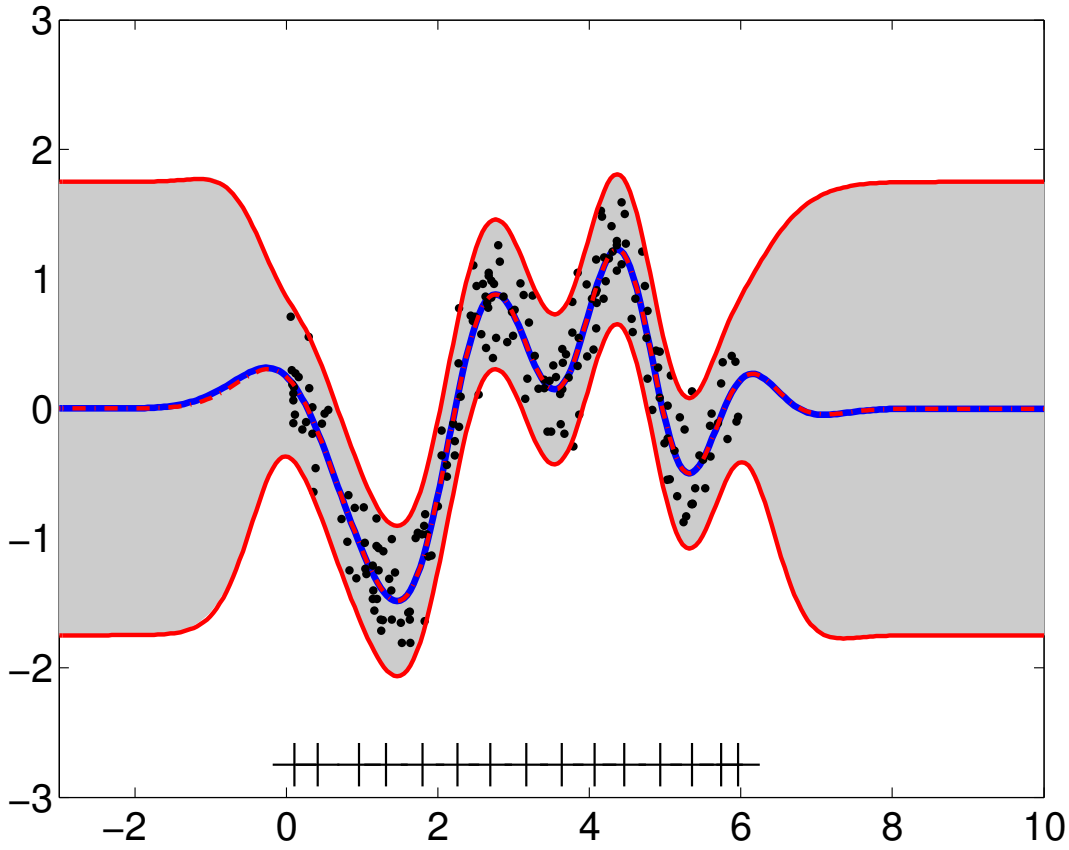
Variational learning of inducing variables



Full GP that scales as $O(n^3) = O(200^3)$
Variational approximation that scales as $O(nm^2) = O(200 \times 15^2)$ **at initialization**

- The crosses $(+)$ are the initial values of the inducing inputs Z

Variational learning of inducing variables



Full GP that scales as $O(n^3) = O(200^3)$

Variational approximation that scales as $O(nm^2) = O(200 \times 15^2)$ **after having maximized the bound**

Distributed representation of GPs

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If we could construct distributed representations of a given GP

- then our approximations (based on inducing variables or by other means) could computationally become more distributed

Distributed representation of GPs

So the precise problem we wish to address here (and the framework to approach it) is the following:

Assume a GP with pre-specified/known kernel function $k(\mathbf{x}, \mathbf{x}')$

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Construct a set of GP function $f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_J(\mathbf{x})$ so that their sum has the same probability law as $f(\mathbf{x})$:

$$f_1(\mathbf{x}) + f_2(\mathbf{x}) + \ldots + f_J(\mathbf{x}) \sim \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}'))$$

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There are many ways to consctruct these f_js $\Rightarrow$ but to facilitate approximations we need these functions to be (in some sense) local!

Distributed representation of GPs

But let's assume we have some suitable functions f_js. How can we can distribute the approximations?

The initial GP model has joint $p(\mathbf{y}, \mathbf{f}) = p(\mathbf{y}|\mathbf{f})p(\mathbf{f})$

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$$p(\mathbf{y}, \mathbf{f}_1, \ldots, \mathbf{f}_J) = p(\mathbf{y}|\sum_{j=1}^{J} \mathbf{f}_j) \times \prod_{j=1}^{J} p(\mathbf{f}_j)$$

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Introduce a separate set of m inducing variables $\mathbf{u}_j$ to approximate the correspoding f_j

Assume a factorized $\prod_{j=0}^{J} p(\mathbf{f}_j|\mathbf{u}_j)q(\mathbf{u}_j)$ and compute the bound

$$\int \prod_{j=1}^{J} p(\mathbf{f}_j|\mathbf{u}_j)q(\mathbf{u}_j) \log p(\mathbf{y}|\sum_{j=0}^{J} \mathbf{f}_j) - \sum_{j=1}^{J} \mathrm{KL}[q(\mathbf{u}_j)||p(\mathbf{u}_j)]$$

which has complexity $O(n * J * m^2)$ (and we are using $J * m$ inducing variables!)

Distributed representation of GPs

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$$f(\mathbf{x}) \sim \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}'))$$

$$f_1(\mathbf{x}) + f_2(\mathbf{x}) + \ldots + f_J(\mathbf{x}) \sim \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}'))$$

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Essentially we need a way to divide the kernel function so that

$$k(\mathbf{x}, \mathbf{x}') = \sum_{j=1}^{J} k_j(\mathbf{x}, \mathbf{x}')$$

and each k_j is positive definite and hopefully local (variance drops to zero outside from a certain input region)

Distribute the kernel in 1-D

GP regression problem in 1-D with covariance function

$$k(x, x') = \sigma_f^2 e^{-\frac{1}{2\ell^2}(x-x')^2}$$

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Explicitly write this as a feature dot product

$$k(x, x') = \int_{-\infty}^{\infty} \phi(x, z)\phi(x', z)dz$$

where $\phi(x, z) = \frac{\sigma_f}{\left(\frac{\pi\ell^2}{2}\right)^{\frac{1}{4}}} e^{-\frac{1}{\ell^2}(x-z)^2}$

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Divide the real axis $a_1 = -\infty < a_2 < a_3 < \ldots < a_J < a_{J+1} = \infty$ and write the kernel

$$k(x, x') = \sum_{j=1}^{J} \int_{a_j}^{a_{j+1}} \phi(x, z)\phi(x', z)dz = \sum_{j=1}^{J} k_j(x, x')$$

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Each $k_j(x, x')$ is

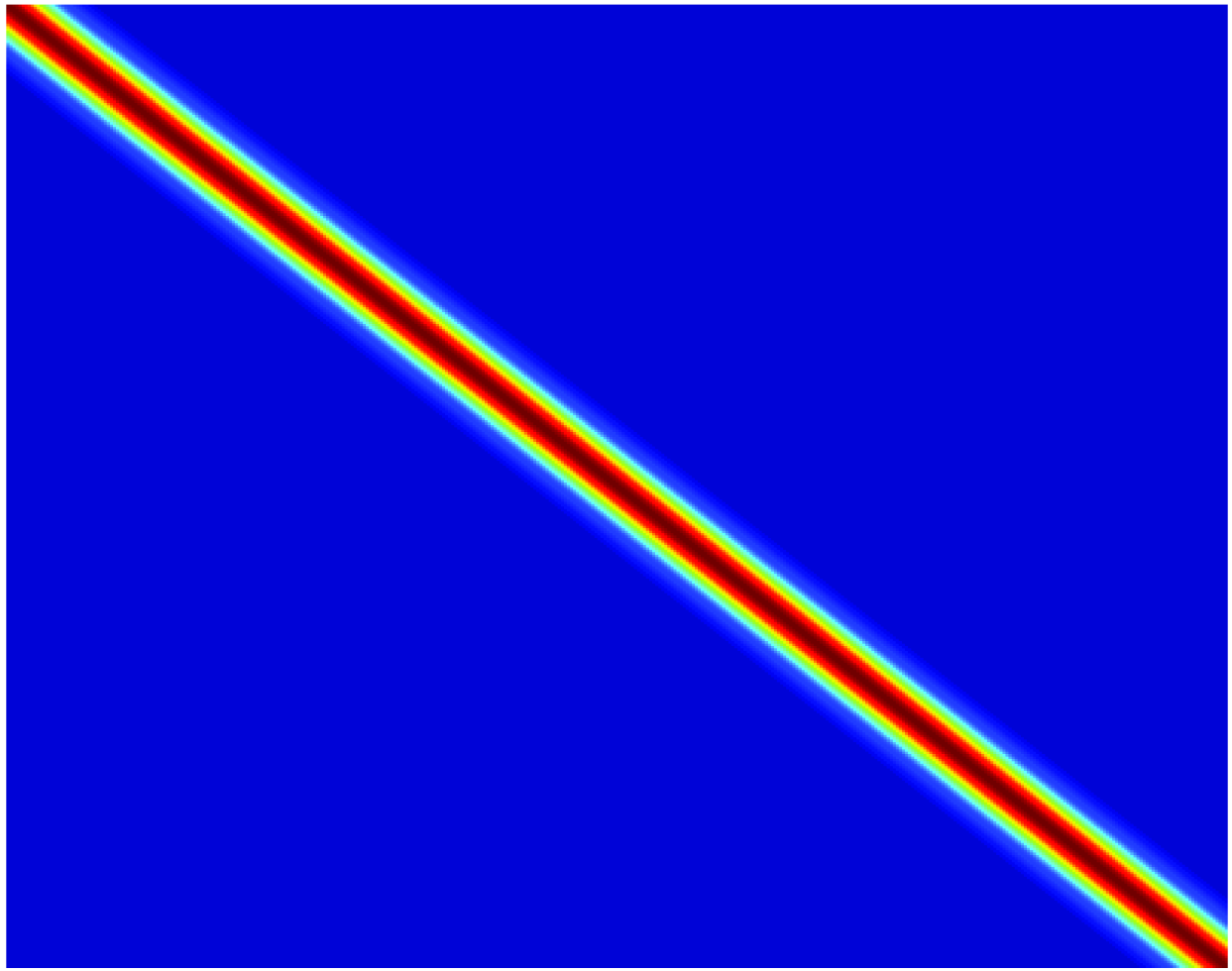
$$k_j(x, x') = k(x, x') \times \frac{\text{erfc}(s_j) - \text{erfc}(s_{j+1})}{2}$$

where the complementary error function is $\text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-s^2} ds$ and

$$s_j = \frac{a_j - \bar{x}}{\ell/\sqrt{2}}, \; s_{j+1} = \frac{a_{j+1} - \bar{x}}{\ell/\sqrt{2}}, \quad \bar{x} = \frac{x + x'}{2}$$

Distribute the kernel in 1-D

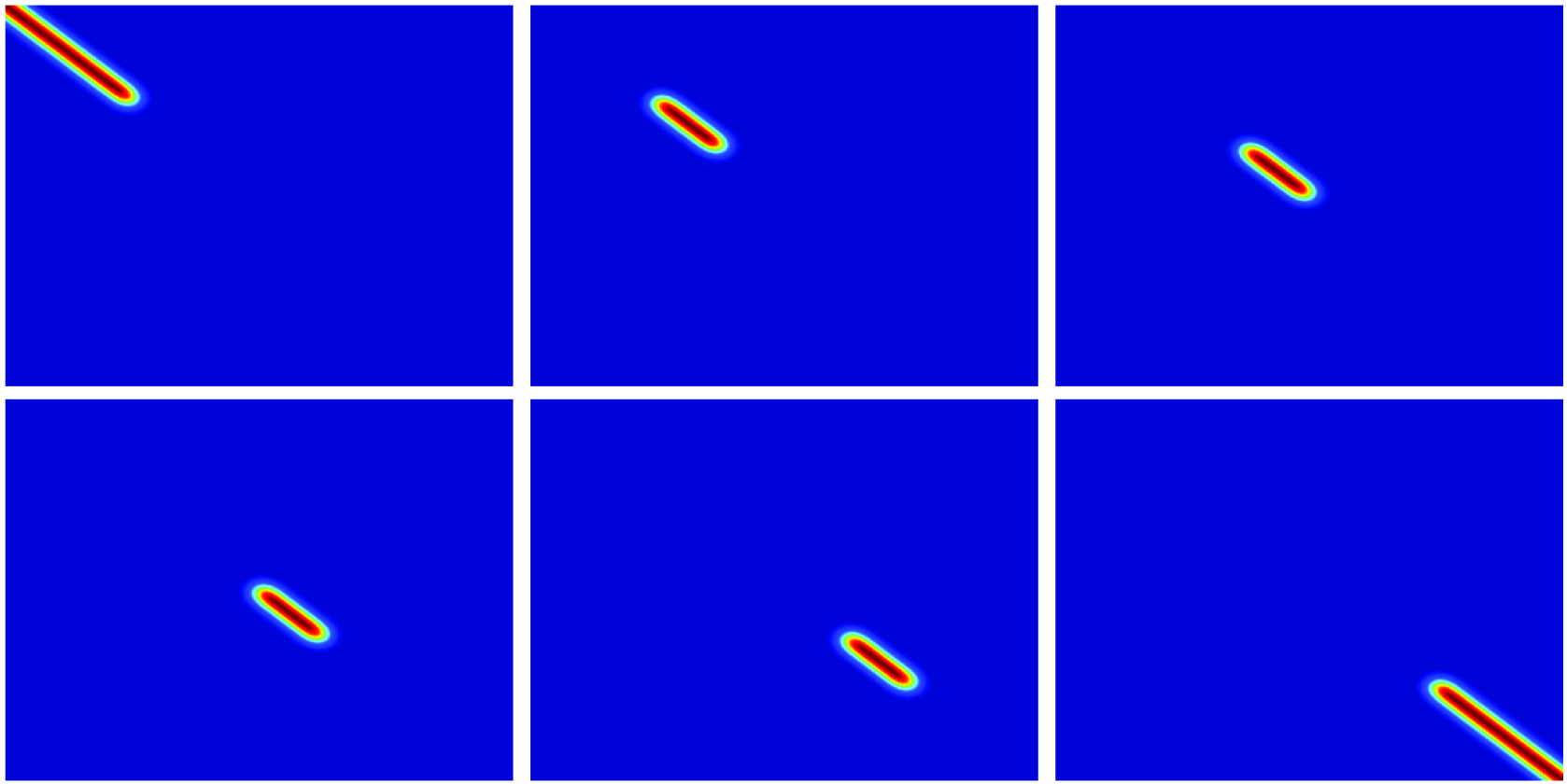
Example



Assume $k(x, x') = e^{-\frac{1}{2}(x-x')^2}$. Figure shows the corresponding kernel matrix in the range $[-20, 20]$

Distribute the kernel in 1-D

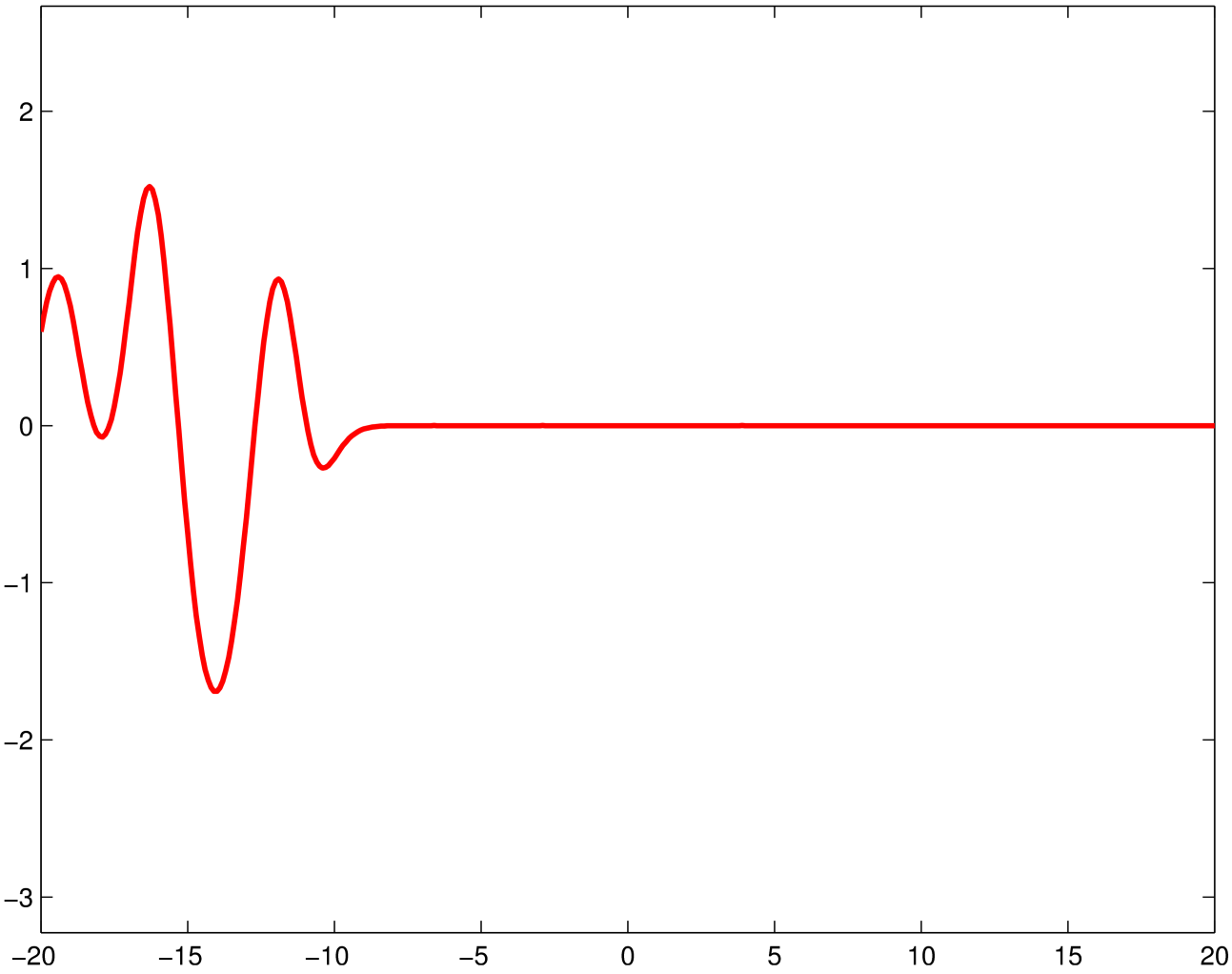
Example



Do the kernel splitting based on $-\infty < -10 < -5 < 0 < 5 < 10 < \infty$.
Figure shows all 6 local kernel matrices

Distribute the kernel in 1-D

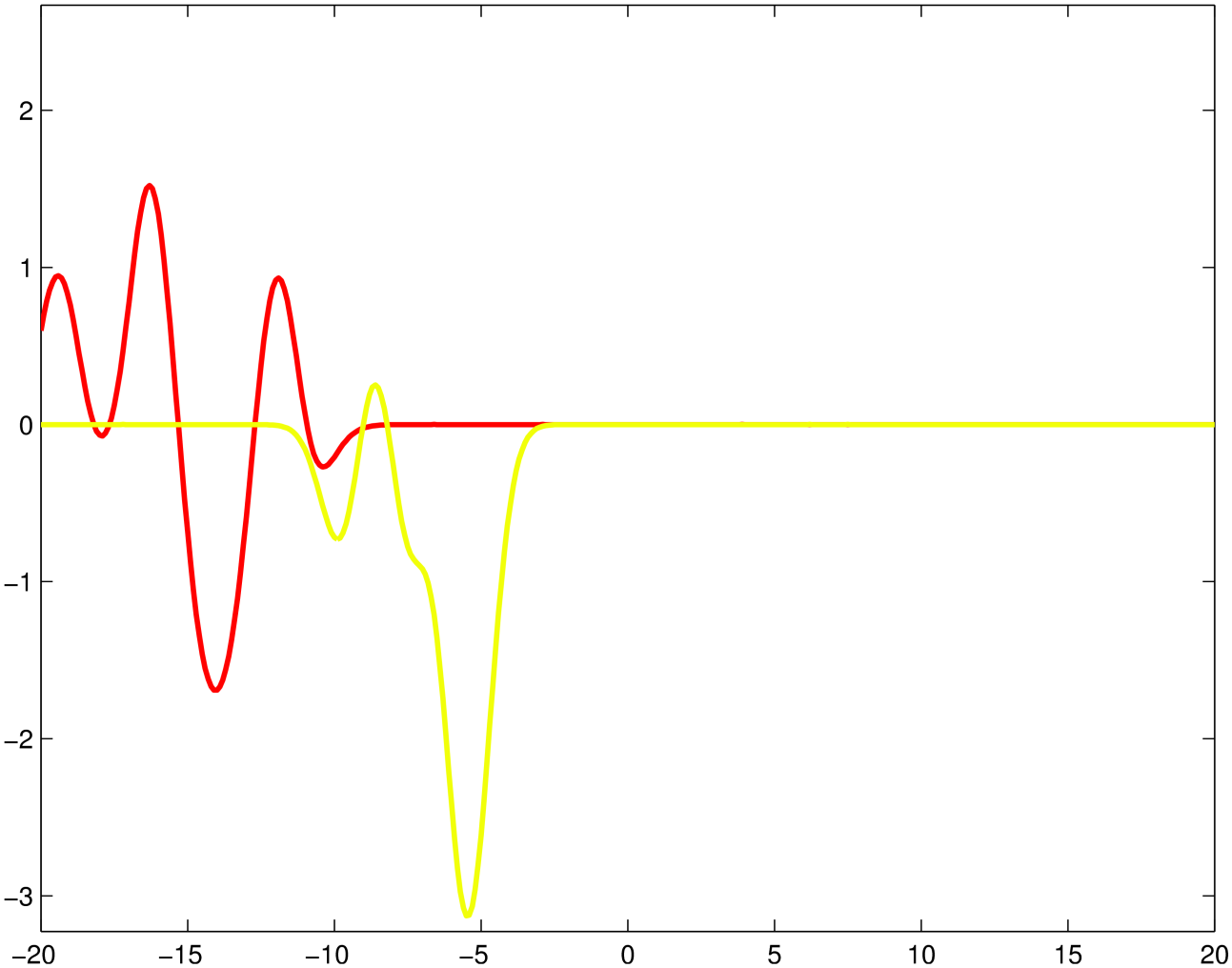
Example



Sample from the local GP associated with the segment $(-\infty, -10]$

Distribute the kernel in 1-D

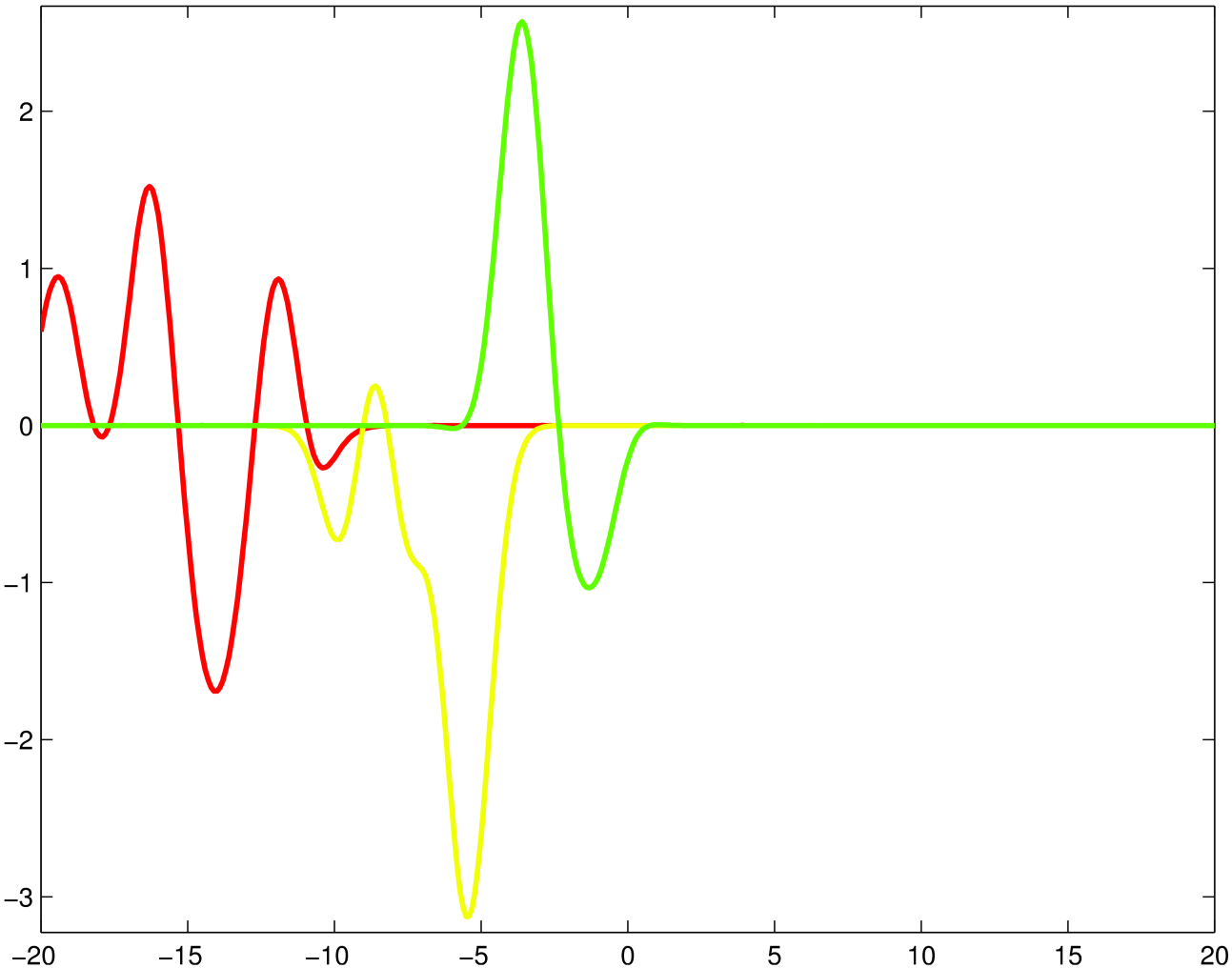
Example



A sample from the next local GP

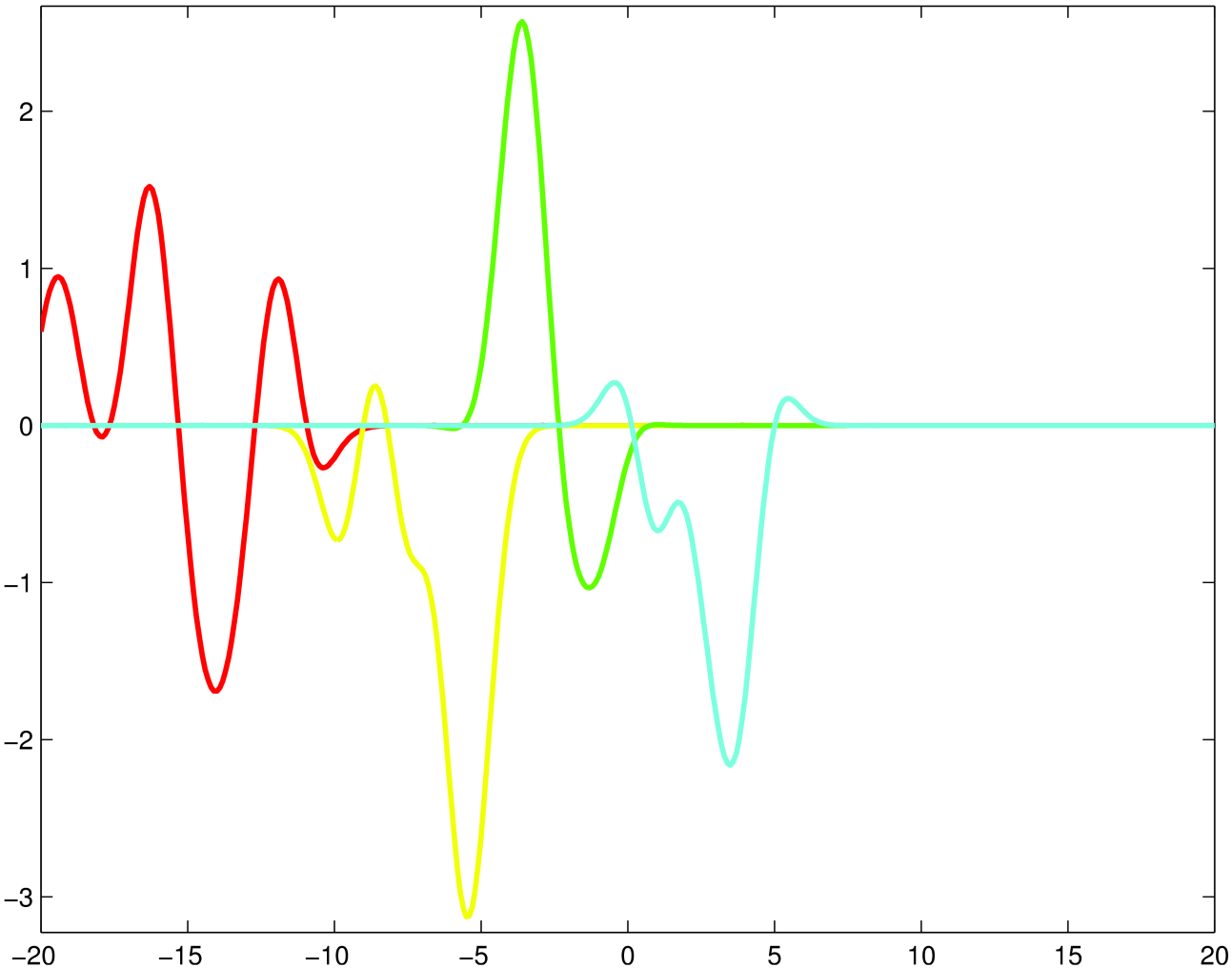
Distribute the kernel in 1-D

Example



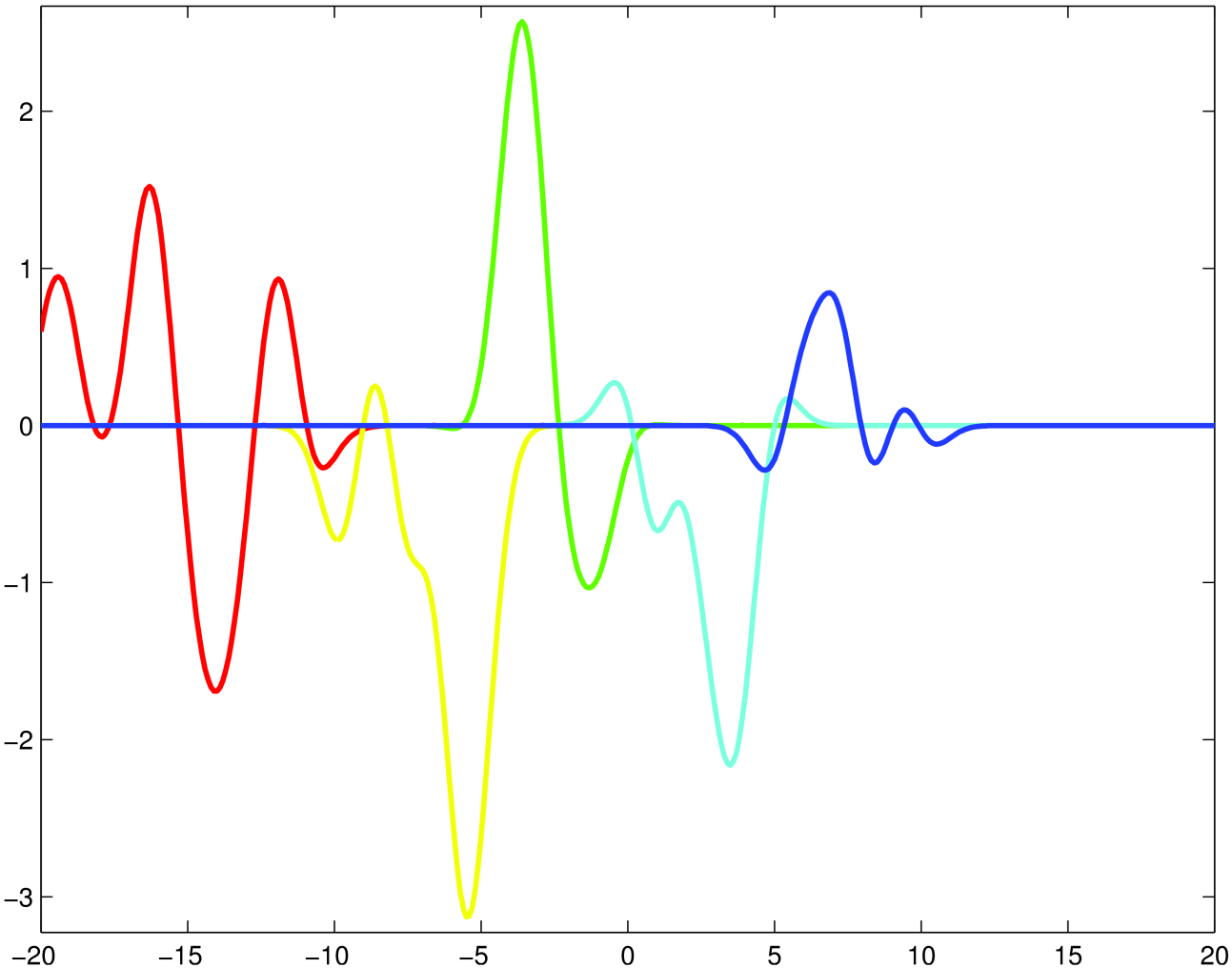
Distribute the kernel in 1-D

Example



Distribute the kernel in 1-D

Example



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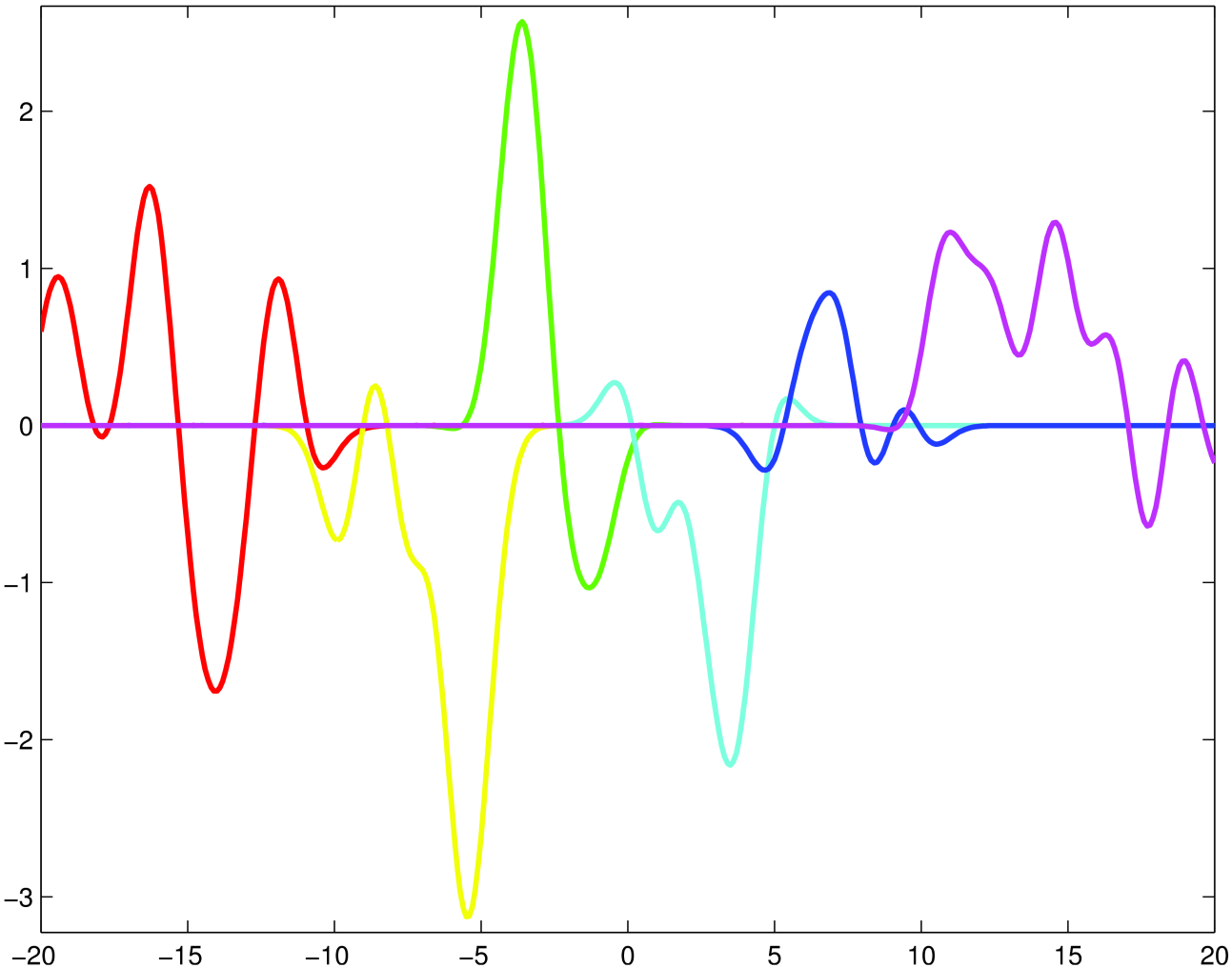
Example



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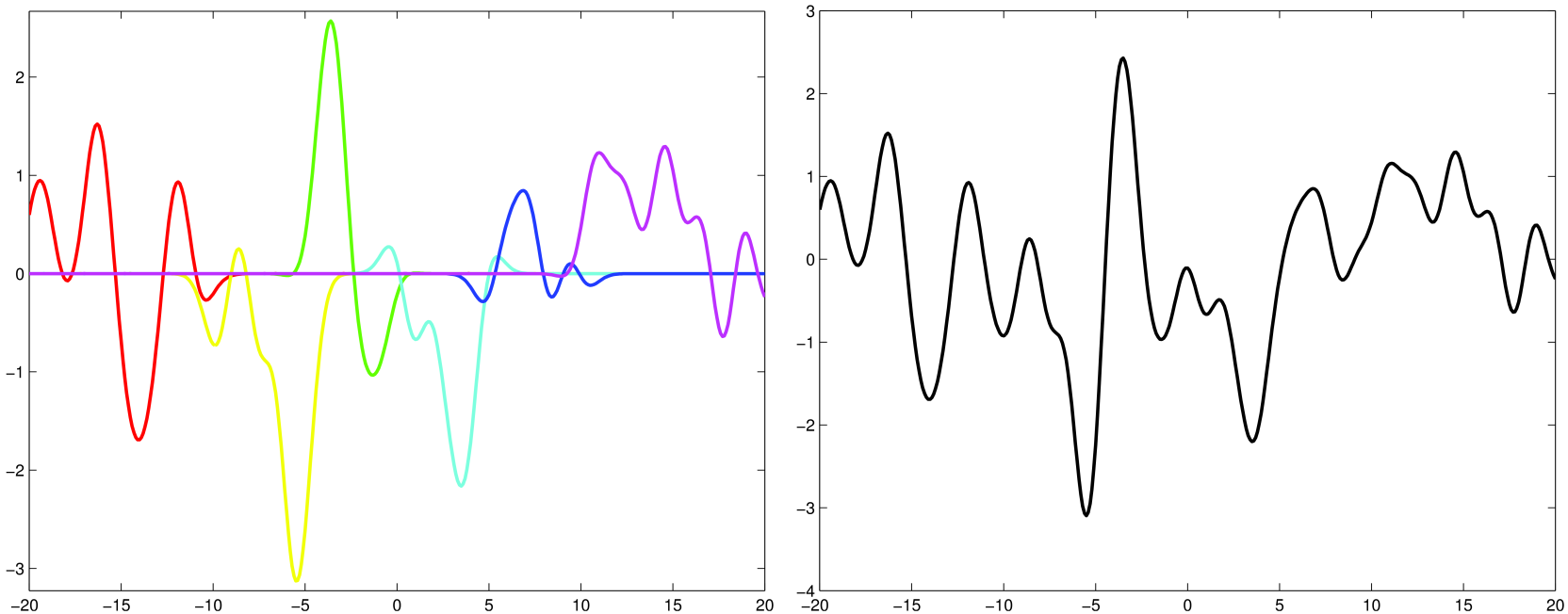

The sum of these local GP functions is a GP function (black line) with kernel $k(x, x') = e^{-\frac{1}{2}(x-x')^2}$

Distribute the kernel in high dimensions

GP regression with inputs $\mathbf{x} \in \mathbb{R}^D$ and covariance function

$$k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \prod_{d=1}^{D} k_d(x_d, x_d')$$

and let's assume $k(x_d, x_d') = e^{-\frac{1}{2\ell_d^2}(x_d - x_d')^2}$

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Pick a certain input dimension d (here you will need a criterion e.g. like information gain used in decision trees) to do the split:

$$\begin{aligned} k(\mathbf{x}, \mathbf{x}') &= \sigma_f^2 \left(\prod_{d' \neq d} k_d(x_d, x_d') \right) \times k_d(x_d, x_d') \\ &= \sigma_f^2 \left(\prod_{d' \neq d} k_d(x_d, x_d') \right) \times \sum_{j=1}^{J} k_{dj}(x_d, x_d') \\ &= \sum_{j=1}^{J} \sigma_f^2 \left(\prod_{d' \neq d} k_d(x_d, x_d') \right) k_{dj}(x_d, x_d') = \sum_{j=1}^{J} k_j(\mathbf{x}, \mathbf{x}') \end{aligned}$$

Discussion

The divisibility property $f_1(\mathbf{x}) + f_2(\mathbf{x}) + \ldots$ of GPs could allow to distribute approximations

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Current issues: How exactly the bound will be maximized in a computionally distributed manner