Advanced Machine Learning

Gaussian Processes: From Discrete to Continuous

$$\sim \mathcal{N}\left(\mu, \boldsymbol{\Sigma}\right)$$

Learning goals

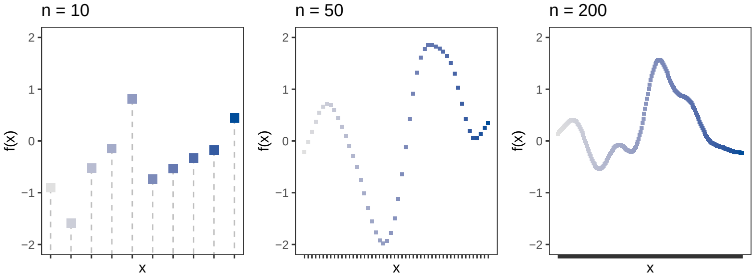
- GPs model distributions over functions
- The marginalization property makes this distribution easily tractable

FROM DISCRETE TO CONTINUOUS FUNCTIONS

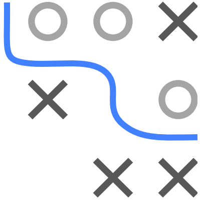
- We defined distributions on functions with finite domain by putting a finite Gaussian on it

$$\mathbf{f} = [f(\mathbf{x}^{(1)}), f(\mathbf{x}^{(2)}), \dots, f(\mathbf{x}^{(n)})] \sim \mathcal{N}(\boldsymbol{m}, \boldsymbol{K})$$

- We can do this for $n \to \infty$ (as “granular” as we want)

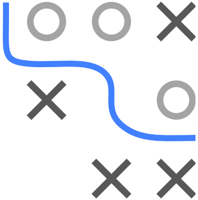


FROM DISCRETE TO CONTINUOUS FUNCTIONS



- No matter how large *n* is, we are still considering a function over a discrete domain.
- How can we extend our definition to functions with **continuous domain** $\mathcal{X} \subset \mathbb{R}$?
- Intuitively, a function *f* drawn from **Gaussian process** can be understood as an “infinite” long Gaussian random vector.
- It is unclear how to handle an “infinite” long Gaussian random vector!

GAUSSIAN PROCESSES: INTUITION

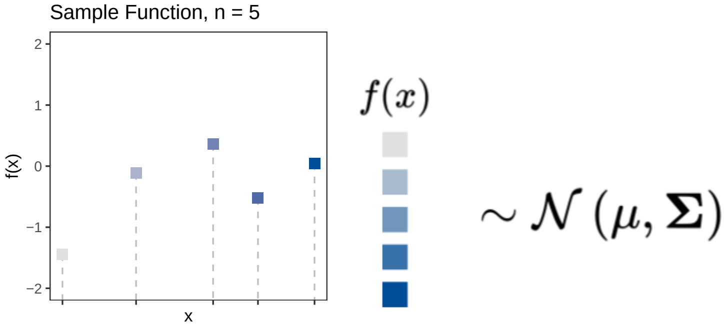


- Thus, it is required that for **any finite set** of inputs $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\} \subset \mathcal{X}$, the vector **f** has a Gaussian distribution

$$\boldsymbol{f} = \left[f\left(\mathbf{x}^{(1)}\right), \dots, f\left(\mathbf{x}^{(n)}\right)\right] \sim \mathcal{N}\left(\boldsymbol{m}, \boldsymbol{K}\right),$$

  with $\boldsymbol{m}$ and $\boldsymbol{K}$ being calculated by a mean function $m(.)$ / covariance function $k(.,.)$.

- This property is called **marginalization property**.



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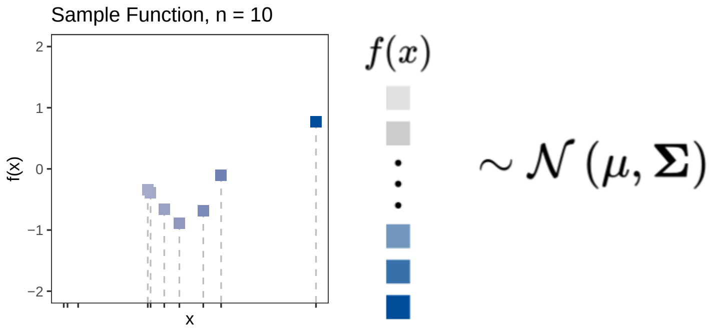

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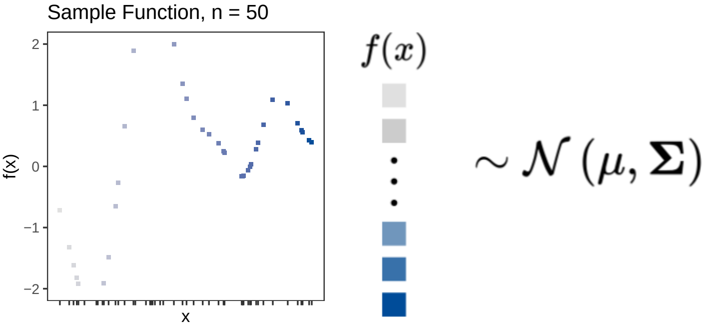


GAUSSIAN PROCESSES

This intuitive explanation is formally defined as follows:

A function $f(\mathbf{x})$ is generated by a GP $\mathcal{GP}\left(m(\mathbf{x}), k\left(\mathbf{x}, \mathbf{x}'\right)\right)$ if for **any finite** set of inputs $\left\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\right\}$, the associated vector of function values $\boldsymbol{f} = \left(f(\mathbf{x}^{(1)}), \dots, f(\mathbf{x}^{(n)})\right)$ has a Gaussian distribution

$$\boldsymbol{f} = \left[f\left(\mathbf{x}^{(1)}\right), \dots, f\left(\mathbf{x}^{(n)}\right)\right] \sim \mathcal{N}\left(\boldsymbol{m}, \boldsymbol{K}\right),$$

with

$$\mathbf{m} \; := \; \left(m\left(\mathbf{x}^{(i)}\right)\right)_i, \quad \mathbf{K} := \left(k\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right)\right)_{i,j},$$

where $m(\mathbf{x})$ is called mean function and $k(\mathbf{x}, \mathbf{x}')$ is called covariance function.

GAUSSIAN PROCESSES / 2

A GP is thus **completely specified** by its mean and covariance function

$$
\begin{aligned}
m(\mathbf{x}) &= \mathbb{E}[f(\mathbf{x})] \\
k(\mathbf{x}, \mathbf{x}') &= \mathbb{E}\Big[\big(f(\mathbf{x}) - \mathbb{E}[f(\mathbf{x})]\big)\big(f(\mathbf{x}') - \mathbb{E}[f(\mathbf{x}')]\big)\Big]
\end{aligned}
$$

Note: For now, we assume $m(\mathbf{x}) \equiv 0$. This is not necessarily a drastic limitation - thus it is common to consider GPs with a zero mean function.

SAMPLING FROM A GAUSSIAN PROCESS PRIOR

We can draw functions from a Gaussian process prior. Let us consider $f(\mathbf{x}) \sim \mathcal{GP}\left(0, k(\mathbf{x}, \mathbf{x}')\right)$ with the squared exponential covariance function $^{(*)}$

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2\ell^2}\|\mathbf{x} - \mathbf{x}'\|^2\right), \quad \ell = 1.$$

This specifies the Gaussian process completely.

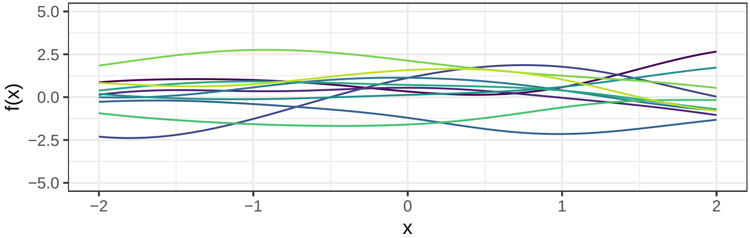
$^{(*)}$ We will talk later about different choices of covariance functions.

SAMPLING FROM A GAUSSIAN PROCESS PRIOR / 2

To visualize a sample function, we

- choose a high number n (equidistant) points $\left\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\right\}$
- compute the corresponding covariance matrix $\mathbf{K} = \left(k\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right)\right)_{i,j}$ by plugging in all pairs $\mathbf{x}^{(i)}, \mathbf{x}^{(j)}$
- sample from a Gaussian $\boldsymbol{f} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{K})$.

We draw 10 times from the Gaussian, to get 10 different samples.

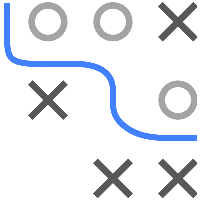


SAMPLING FROM A GAUSSIAN PROCESS PRIOR / 3

Since we specified the mean function to be zero $m(\mathbf{x}) \equiv 0$, the drawn functions have zero mean.

Gaussian Processes as Indexed Family

GAUSSIAN PROCESSES AS AN INDEXED FAMILY



A Gaussian process is a special case of a **stochastic process** which is defined as a collection of random variables indexed by some index set (also called an **indexed family**). What does it mean?

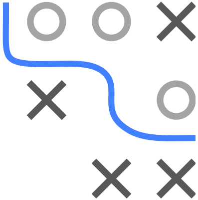
An **indexed family** is a mathematical function (or “rule”) to map indices $t \in T$ to objects in $\mathcal{S}$.

Definition

A **family of elements in $\mathcal{S}$ indexed by T** (indexed family) is a surjective function

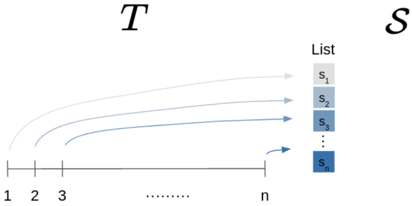
$$\begin{aligned} s : T &\rightarrow \mathcal{S} \\ t &\mapsto s_t = s(t) \end{aligned}$$

INDEXED FAMILY

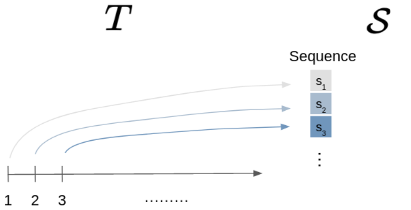


Some simple examples for indexed families are:

- finite sequences (lists): $T = \{1, 2, \ldots, n\}$ and $(s_t)_{t \in T} \in \mathbb{R}$



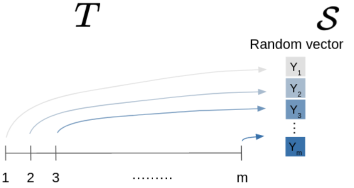
- infinite sequences: $T = \mathbb{N}$ and $(s_t)_{t \in T} \in \mathbb{R}$

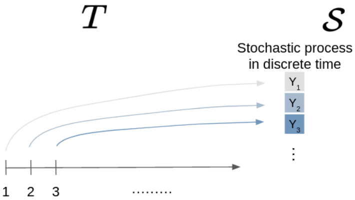


INDEXED FAMILY / 2

But the indexed set $\mathcal{S}$ can be something more complicated, for example functions or **random variables** (RV):

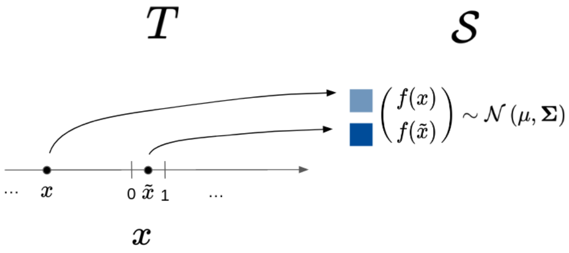
- $T = \{1, \ldots, m\}$, Y_t's are RVs: Indexed family is a random vector.
- $T = \{1, \ldots, m\}$, Y_t's are RVs: Indexed family is a stochastic process in discrete time
- $T = \mathbb{Z}^2$, Y_t's are RVs: Indexed family is a 2D-random walk.





INDEXED FAMILY

- A Gaussian process is also an indexed family, where the random variables $f(\mathbf{x})$ are indexed by the input values $\mathbf{x} \in \mathcal{X}$.
- Their special feature: Any indexed (finite) random vector has a multivariate Gaussian distribution (which comes with all the nice properties of Gaussianity!).



Visualization for a one-dimensional $\mathcal{X}$.

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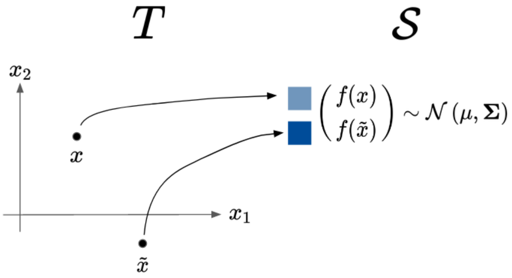

Visualization for a two-dimensional $\mathcal{X}$.