Gaussian Process

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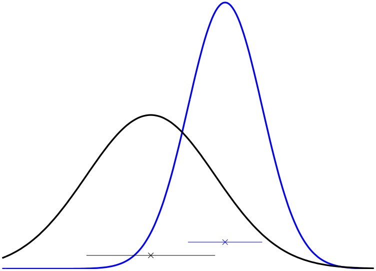
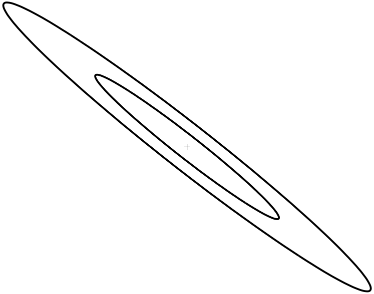
Key concepts

- generalize: scalar Gaussian, multivariate Gaussian, Gaussian process
- Key insight: functions are like infinitely long vectors
- Surprise: Gaussian processes are practical, because of
  - the marginalization property
- generating from Gaussians
  - joint generation
  - sequential generation

The Gaussian Distribution





The univariate Gaussian distribution is given by

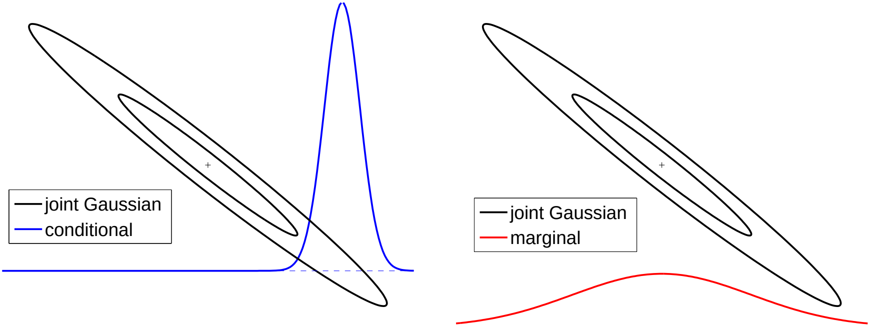
$$p(x|\mu, \sigma^2) \;=\; (2\pi\sigma^2)^{-1/2} \exp\big(-\frac{1}{2\sigma^2}(x-\mu)^2\big)$$

The multivariate Gaussian distribution for D-dimensional vectors is given by

$$p(\mathbf{x}|\mu, \Sigma) \;=\; \mathcal{N}(\mu, \Sigma) \;=\; (2\pi)^{-D/2}|\Sigma|^{-1/2} \exp\big(-\tfrac{1}{2}(\mathbf{x}-\mu)^\top \Sigma^{-1}(\mathbf{x}-\mu)\big)$$

where μ is the mean vector and Σ the covariance matrix.

Conditionals and Marginals of a Gaussian, pictorial



Both the conditionals $p(x|y)$ and the marginals $p(x)$ of a joint Gaussian $p(x, y)$ are again Gaussian.

Conditionals and Marginals of a Gaussian, algebra

If $\mathbf{x}$ and $\mathbf{y}$ are jointly Gaussian

$$p(\mathbf{x}, \mathbf{y}) \;=\; p\left(\begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix}\right) \;=\; \mathcal{N}\left(\begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} A & B \\ B^\top & C \end{bmatrix}\right),$$

we get the marginal distribution of $\mathbf{x}$, $p(\mathbf{x})$ by

$$p(\mathbf{x}, \mathbf{y}) \;=\; \mathcal{N}\left(\begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} A & B \\ B^\top & C \end{bmatrix}\right) \;\Longrightarrow\; p(\mathbf{x}) \;=\; \mathcal{N}(\mathbf{a},\; A),$$

and the conditional distribution of $\mathbf{x}$ given $\mathbf{y}$ by

$$p(\mathbf{x}, \mathbf{y}) = \mathcal{N}\left(\begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} A & B \\ B^\top & C \end{bmatrix}\right) \;\Longrightarrow\; p(\mathbf{x}|\mathbf{y}) = \mathcal{N}(\mathbf{a}+BC^{-1}(\mathbf{y}-\mathbf{b}),\; A-BC^{-1}B^\top),$$

where $\mathbf{x}$ and $\mathbf{y}$ can be scalars or vectors.

What is a Gaussian Process?

A *Gaussian process* is a generalization of a multivariate Gaussian distribution to infinitely many variables.

Informally: infinitely long vector $\simeq$ function

> **Definition**: *a Gaussian process is a collection of random variables, any finite number of which have (consistent) Gaussian distributions.* $\square$

A Gaussian distribution is fully specified by a mean vector, μ, and covariance matrix Σ:

$$\mathbf{f} = (f_1, \ldots, f_N)^\top \sim \mathcal{N}(\mu, \Sigma), \quad \text{indexes } n = 1, \ldots, N$$

A Gaussian process is fully specified by a mean function $m(x)$ and covariance function $k(x, x')$:

$$f \sim \mathcal{N}(m, k), \quad \text{indexes: } x \in \mathcal{X}$$

here f and m are functions on $\mathcal{X}$, and k is a function on $\mathcal{X} \times \mathcal{X}$

The marginalization property

Thinking of a GP as a Gaussian distribution with an infinitely long mean vector and an infinite by infinite covariance matrix may seem impractical…

…luckily we are saved by the *marginalization property*:

Recall:

$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{y}) d\mathbf{y}.$$

For Gaussians:

$$p(\mathbf{x}, \mathbf{y}) = \mathcal{N}\left(\begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} A & B \\ B^\top & C \end{bmatrix}\right) \implies p(\mathbf{x}) = \mathcal{N}(\mathbf{a}, A),$$

which works irrespective of the size of $\mathbf{y}$.
For Gaussian processes:

$$f \sim \mathcal{N}(m, k) \implies \mathbf{f} = f(\mathbf{x}) \sim \mathcal{N}(\mu = \mathbf{m} = m(\mathbf{x}), \Sigma = K(\mathbf{x}, \mathbf{x})).$$

Key: only ever ask finite dimensional questions about functions.

Random functions from a Gaussian Process

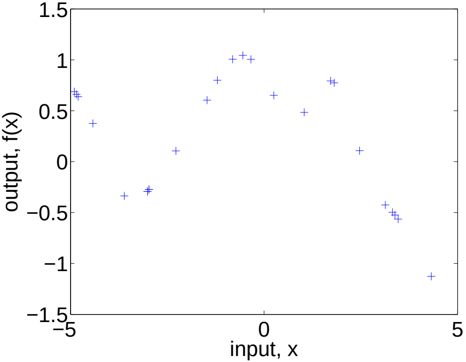
Example one dimensional Gaussian process:

$$p(f) \sim \mathcal{N}\big(m,\ k\big), \quad \text{where} \quad m(x) = 0, \quad \text{and} \quad k(x, x') = \exp(-\tfrac{1}{2}(x - x')^2).$$

To get an indication of what this distribution over functions looks like, focus on a finite subset of function values $\mathbf{f} = (f(x_1), f(x_2), \ldots, f(x_N))^\top$, for which

$$\mathbf{f} \sim \mathcal{N}(0, \Sigma), \quad \text{where} \quad \Sigma_{ij} = k(x_i, x_j).$$

Then plot the coordinates of $\mathbf{f}$ as a function of the corresponding x values.



Joint Generation

To generate a random sample from a D dimensional joint Gaussian with covariance matrix K and mean vector $\mathbf{m}$: (in octave or matlab)

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z = randn(D,1);
y = chol(K)'*z + m;
```

where `chol` is the Cholesky factor R such that $R^\top R = K$.
Thus, the covariance of $\mathbf{y}$ is:

$$\mathbb{E}[(\mathbf{y}-\mathbf{m})(\mathbf{y}-\mathbf{m})^\top] = \mathbb{E}[R^\top \boldsymbol{z}\boldsymbol{z}^\top R] = R^\top \mathbb{E}[\boldsymbol{z}\boldsymbol{z}^\top] R = R^\top I R = K.$$

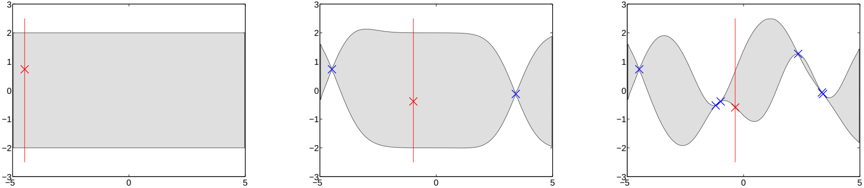
Sequential Generation

Factorize the joint distribution

$$p(f_1, \ldots, f_N | x_1, \ldots x_N) \;=\; \prod_{n=1}^{N} p(f_n | f_{n-1}, \ldots, f_1, x_n, \ldots, x_1),$$

and generate function values sequentially. For Gaussians:

$$\begin{aligned} p(f_n, \mathbf{f}_{<n}) \;&=\; \mathcal{N}\Big(\begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} A & B \\ B^\top & C \end{bmatrix}\Big) \;\Longrightarrow \\ p(f_n | \mathbf{f}_{<n}) \;&=\; \mathcal{N}(\mathbf{a} + BC^{-1}(\mathbf{f}_{<n} - \mathbf{b}),\; A - BC^{-1}B^\top). \end{aligned}$$



Function drawn at random from a Gaussian Process with Gaussian covariance