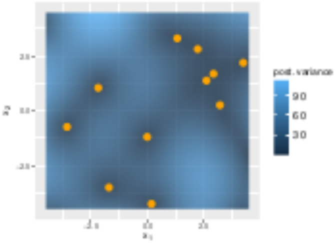
Introduction to Machine Learning

Gaussian Process Prediction



Learning goals

- Know how to derive the posterior process
- GPs are interpolating and spatial models
- Model noise via a nugget term

POSTERIOR PROCESS

- Let us now distinguish between observed training inputs, also denote by a design matrix $\mathbf{X}$, and the corresponding observed values

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

  and one single **unobserved test point** $\mathbf{x}_*$ with $f_* = f\left(\mathbf{x}_*\right)$.

- We now want to infer the distribution of $f_* | \mathbf{x}_*, \boldsymbol{X}, \boldsymbol{f}$.

$$f_* = f\left(\mathbf{x}_*\right)$$

- Assuming a zero-mean GP prior $\mathcal{GP}\left(\mathbf{0}, k(\mathbf{x}, \mathbf{x}')\right)$ we know

$$\begin{bmatrix} \boldsymbol{f} \\ f_* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \mathbf{K} & \boldsymbol{k}_* \\ \boldsymbol{k}_*^T & \boldsymbol{k}_{**} \end{bmatrix}\right).$$

  Here, $\mathbf{K} = \left(k\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right)\right)_{i,j}$, $\boldsymbol{k}_* = \left[k\left(\mathbf{x}_*, \mathbf{x}^{(1)}\right), \dots, k\left(\mathbf{x}_*, \mathbf{x}^{(n)}\right)\right]$ and $\boldsymbol{k}_{**} = k(\mathbf{x}_*, \mathbf{x}_*)$.

POSTERIOR PROCESS / 2

- Given that $\boldsymbol{f}$ is observed, we can apply the general rule for condition $^{(*)}$ of Gaussian random variables and obtain the following formula:

$$f_* \mid \mathbf{x}_*, \mathbf{X}, \boldsymbol{f} \sim \mathcal{N}(\boldsymbol{k}_*^T \mathbf{K}^{-1} \boldsymbol{f}, \boldsymbol{k}_{**} - \boldsymbol{k}_*^T \mathbf{K}^{-1} \boldsymbol{k}_*).$$

- As the posterior is a Gaussian, the maximum a-posteriori estimate, i.e. the mode of the posterior distribution, is $\boldsymbol{k}_*^T \mathbf{K}^{-1} \boldsymbol{f}$.

POSTERIOR PROCESS / 3

[*] General rule for condition of Gaussian random variables:

If the m-dimensional Gaussian vector $\boldsymbol{z} \sim \mathcal{N}(\mu, \Sigma)$ can be partitioned with $\boldsymbol{z} = (\boldsymbol{z}_1, \boldsymbol{z}_2)$ where $\boldsymbol{z}_1$ is m_1-dimensional and $\boldsymbol{z}_2$ is m_2-dimensional, and:

$$(\mu_1, \mu_2)\,, \quad \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix},$$

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$$\mathcal{N}\left(\mu_2 + \Sigma_{21}\Sigma_{11}^{-1}(\boldsymbol{a} - \mu_1), \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}\right)$$

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GP PREDICTION: TWO POINTS

Let us visualize this by a simple example:

- Assume we observed a single training point $\mathbf{x} = -0.5$, and want to make a prediction at a test point $\mathbf{x}_* = 0.5$.
- Under a zero-mean GP with $k(\mathbf{x}, \mathbf{x}') = \exp(-\frac{1}{2}\|\mathbf{x} - \mathbf{x}'\|^2)$, we compute the cov-matrix:

$$\begin{bmatrix} f \\ f_* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} 1 & 0.61 \\ 0.61 & 1 \end{bmatrix}\right).$$

- Assume that we observe the point $f(\mathbf{x}) = 1$.
- We compute the posterior distribution:

$$\begin{aligned} f_* \mid \mathbf{x}_*, \mathbf{x}, f &\sim \mathcal{N}(\boldsymbol{k}_*^T \mathbf{K}^{-1} f, k_{**} - \boldsymbol{k}_*^T \mathbf{K}^{-1} \boldsymbol{k}_*) \\ &\sim \mathcal{N}(0.61 \cdot 1 \cdot 1, 1 - 0.61 \cdot 1 \cdot 0.61) \\ &\sim \mathcal{N}(0.61, 0.6279) \end{aligned}$$

- The MAP-estimate for $\mathbf{x}_*$ is $f(\mathbf{x}_*) = 0.61$, and the uncertainty estimate is 0.6279.

POSTERIOR PROCESS

- We can generalize the formula for the posterior process for multiple unobserved test points:

$$\boldsymbol{f}_* = \left[f\left(\mathbf{x}_*^{(1)}\right), ..., f\left(\mathbf{x}_*^{(m)}\right)\right].$$

- Under a zero-mean Gaussian process, we have

$$\begin{bmatrix}\boldsymbol{f}\\ \boldsymbol{f}_*\end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix}\mathbf{K} & \mathbf{K}_*\\ \mathbf{K}_*^T & \mathbf{K}_{**}\end{bmatrix}\right),$$

with $\mathbf{K}_* = \left(k\left(\mathbf{x}^{(i)}, \mathbf{x}_*^{(j)}\right)\right)_{i,j}$, $\mathbf{K}_{**} = \left(k\left(\mathbf{x}_*^{(i)}, \mathbf{x}_*^{(j)}\right)\right)_{i,j}$.

POSTERIOR PROCESS / 2

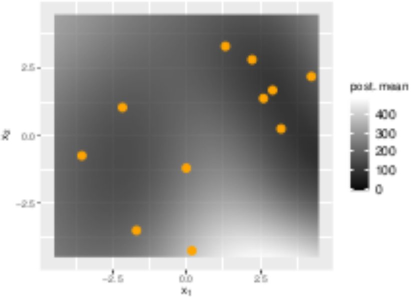
- Similar to the single test point situation, to get the posterior distribution, we exploit the general rule of conditioning for Gaussians:

$$\boldsymbol{f}_* \mid \mathbf{X}_*, \mathbf{X}, \boldsymbol{f} \sim \mathcal{N}(\mathbf{K}_*^T \mathbf{K}^{-1} \boldsymbol{f}, \mathbf{K}_{**} - \mathbf{K}_*^T \mathbf{K}^{-1} \mathbf{K}_*).$$

- This formula enables us to talk about correlations among different test points and sample functions from the posterior process.

GP AS A SPATIAL MODEL

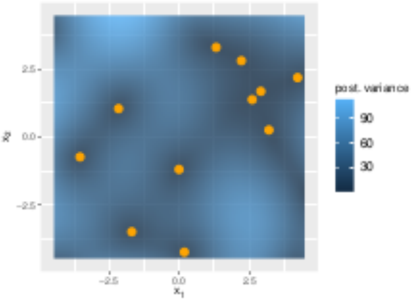
- The correlation among two outputs depends on distance of the corresponding input points $\mathbf{x}$ and $\mathbf{x}'$ (e.g. Gaussian covariance kernel $k(\mathbf{x}, \mathbf{x}') = \exp\left(\frac{-\|\mathbf{x}-\mathbf{x}'\|^2}{2l^2}\right)$)
- Hence, close data points with high spatial similarity $k(\mathbf{x}, \mathbf{x}')$ enter into more strongly correlated predictions: $\mathbf{k}_*^\top \mathbf{K}^{-1}\mathbf{f}$ ($\mathbf{k}_* := \left(k(\mathbf{x}, \mathbf{x}^{(1)}), \ldots, k(\mathbf{x}, \mathbf{x}^{(n)})\right)$).



Example: Posterior mean of a GP that was fitted with the Gaussian covariance kernel with $l = 1$.

GP AS A SPATIAL MODEL / 2

- Posterior uncertainty increases if the new data points are far from the design points.
- The uncertainty is minimal at the design points, since the posterior variance is zero at these points.



Example (continued): Posterior variance.

NOISY GAUSSIAN PROCESS / 2

- In reality, however, this is often not the case.
- We often only have access to a noisy version of the true function value

$$y = f(\mathbf{x}) + \epsilon, \epsilon \sim \mathcal{N}\left(0, \sigma^2\right).$$

- Let us still assume that $f(\mathbf{x})$ is a Gaussian process.
- Then,

$$\begin{aligned} \text{Cov}(y^{(i)}, y^{(j)}) &= \text{Cov}\left(f\left(\mathbf{x}^{(i)}\right) + \epsilon^{(i)}, f\left(\mathbf{x}^{(j)}\right) + \epsilon^{(j)}\right) \\ &= \text{Cov}\left(f\left(\mathbf{x}^{(i)}\right), f\left(\mathbf{x}^{(j)}\right)\right) + 2 \cdot \text{Cov}\left(f\left(\mathbf{x}^{(i)}\right), \epsilon^{(j)}\right) + \text{Cov}\left(\epsilon^{(i)}, \epsilon^{(j)}\right) \\ &= k\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) + \sigma^2 \delta_{ij}. \end{aligned}$$

- σ^2 is called **nugget**.

NOISY GAUSSIAN PROCESS / 3

- Let us now derive the predictive distribution for the case of noisy observations.
- The prior distribution of y, assuming that f is modeled by a Gaussian process is then

$$\boldsymbol{y} = \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{pmatrix} \sim \mathcal{N}\left(\boldsymbol{m}, \boldsymbol{K} + \sigma^2 \boldsymbol{I}_n\right),$$

with

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

NOISY GAUSSIAN PROCESS / 4

- We distinguish again between
  - observed training points $\mathbf{X}$, $\mathbf{y}$, and
  - unobserved test inputs $\mathbf{X}_*$ with unobserved values $\boldsymbol{f}_*$

  and get

$$\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{f}_* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \mathbf{K} + \sigma^2 \boldsymbol{I}_n & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**} \end{bmatrix}\right).$$

NOISY GAUSSIAN PROCESS / 5

- Similarly to the noise-free case, we condition according to the rule of conditioning for Gaussians to get the posterior distribution for the test outputs $\boldsymbol{f}_*$ at $\mathbf{X}_*$:

$$\boldsymbol{f}_* \mid \mathbf{X}_*, \mathbf{X}, \boldsymbol{y} \sim \mathcal{N}(\boldsymbol{m}_{\text{post}}, \boldsymbol{K}_{\text{post}}).$$

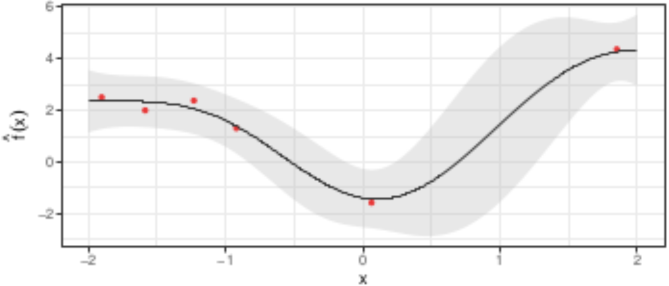
with

$$\begin{aligned} \boldsymbol{m}_{\text{post}} &= \mathbf{K}_*^T \left(\mathbf{K} + \sigma^2 \cdot \boldsymbol{I}\right)^{-1} \boldsymbol{y} \\ \boldsymbol{K}_{\text{post}} &= \mathbf{K}_{**} - \mathbf{K}_*^T \left(\mathbf{K}^{-1} + \sigma^2 \cdot \boldsymbol{I}\right) \mathbf{K}_*, \end{aligned}$$

- This converts back to the noise-free formula if $\sigma^2 = 0$.

NOISY GAUSSIAN PROCESS / 6

- The noisy Gaussian process is not an interpolator any more.
- A larger nugget term leads to a wider "band" around the observed training points.
- The nugget term is estimated during training.



After observing the training points (red), we have a nugget-band around the oberved points. (k(x,x') is the squared exponential)

RISK MINIMIZATION FOR GAUSSIAN PROCESSES

In machine learning, we learned about risk minimization. We usually choose a loss function and minimize the empirical risk

$$\mathcal{R}_{\text{emp}}(f) := \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right)$$

as an approximation to the theoretical risk

$$\mathcal{R}(f) := \mathbb{E}_{xy}[L\left(y, f(\mathbf{x})\right)] = \int L\left(y, f(\mathbf{x})\right) \mathrm{d}\mathbb{P}_{xy}.$$

- How does the theory of Gaussian processes fit into this theory?
- What if we want to make a prediction which is optimal w.r.t. a certain loss function?

RISK MINIMIZATION FOR GAUSSIAN PROCESSES / 2

- The theory of Gaussian process gives us a posterior distribution

$$p(y \mid \mathcal{D})$$

- If we now want to make a prediction at a test point $\mathbf{x}_*$, we approximate the theoretical risk in a different way, by using the posterior distribution:

$$\mathcal{R}(y_* \mid \mathbf{x}_*) \approx \int L(\tilde{y}_*, y_*) p(\tilde{y}_* \mid \mathbf{x}_*, \mathcal{D}) d\tilde{y}_*.$$

- The optimal prediciton w.r.t the loss function is then:

$$\hat{y}_* \mid \mathbf{x}_* = \arg\min_{y_*} \mathcal{R}(y_* \mid \mathbf{x}_*).$$