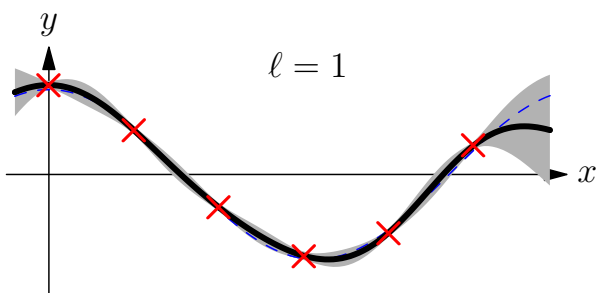


Advanced Machine Learning

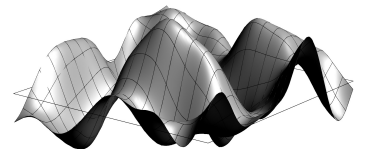
Gaussian Processes



Gaussian Processes, regression

Outline

1. **Introduction**
2. Gaussian Processes
3. Bayesian Inference
4. Hyper-parameters



Gaussian Processes

- Gaussian processes (GPs) are a mathematically defined ensemble of functions
- They can be combined with Bayesian inference to give one of the most powerful regression techniques
- Although Bayesian they can be used in a black-box fashion due to the ubiquity of the prior
- Mathematically they are a bit complicated (because Gaussians involve the inverse of matrices which are a real pain to work with)
- In practice they aren't that difficult to use

Regression

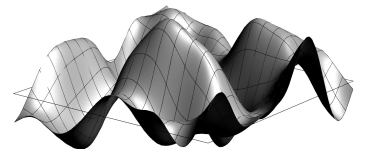
- In regression we try to fit a multi-dimensional function to our data
- (You can use Gaussian Processes for classification, e.g. by inferring the probabilities of being in a class, but we ignore this as regression is where GP excel)
- In regression we have some p dimensional feature vectors x_i and some target $y_i \in \mathbb{R}$
- Our task is to fit a function through all the data points

Priors on Functions

- We can think of a solution as a function $f(\mathbf{x})$
- We can put a prior probability distribution, $p(f)$, on a function, f , that prefers smooth functions
- We can then compute a posterior probability distribution on functions given the data, $p(f|\mathcal{D})$
- As a likelihood, $p(y_i|f(\mathbf{x}_i))$, we use the probability of observing y_i given the true function value is $f(\mathbf{x}_i)$
- In general, this would be next to impossible to compute except in the special case where everything is Gaussian (normally) distributed

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Gaussian Processes

- Gaussian Processes are probability distributions over functions
- (Functions can be viewed as vectors in an infinite dimensional vector space)
- In the Gaussian Process, $\mathcal{GP}(m, k)$, the probability of a function, f , is proportional
$$p(f|m, k) \propto e^{-\frac{1}{2} \int (f(\mathbf{x}) - m(\mathbf{x})) k^{-1}(\mathbf{x}, \mathbf{y}) (f(\mathbf{y}) - m(\mathbf{y})) d\mathbf{x} d\mathbf{y}}$$
- The function $m(\mathbf{x})$ is the mean $\mathbb{E}[f(\mathbf{x})]$ (usually taken to be zero in most inference problems)

Meaning of GP

- To understand GP's we can discretise space, \mathbf{x} , into a lattice of points $\{\mathbf{x}_i\}$
- Then (assuming $m(\mathbf{x}) = 0$)

$$p(f|m, k) \propto \prod_i e^{-\frac{f_i^2 k^{-1}(\mathbf{x}_i, \mathbf{x}_i)}{2} + f_i \sum_j k^{-1}(\mathbf{x}_i, \mathbf{x}_j) f_j}$$

where $f_i = f(\mathbf{x}_i)$

- We see that the value of the function at each point is normally distributed with a mean that depends on functions at neighbouring points

Covariance function

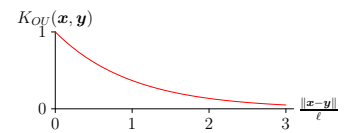
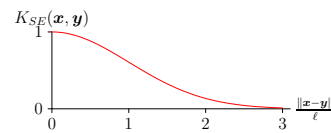
- $k(\mathbf{x}, \mathbf{y})$ is a covariance function

$$\mathbb{E}[(f(\mathbf{x}) - m(\mathbf{x}))(f(\mathbf{y}) - m(\mathbf{y}))] = k(\mathbf{x}, \mathbf{y})$$

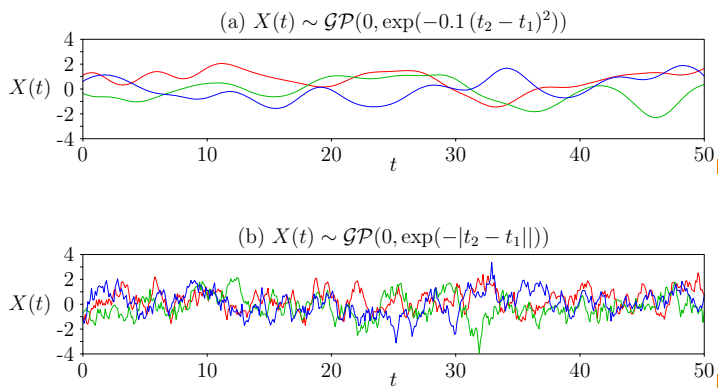
- This is sometimes known as a **kernel**—it must be positive semi-definite (just like in SVMs)
- It is a free “parameter” that the user gets to choose (although we can learn its parameters too)
- If $k(\mathbf{x}, \mathbf{y})$ is a function of $\mathbf{x} - \mathbf{y}$ it is “**stationary**”
- If $k(\mathbf{x}, \mathbf{y})$ is a function of $\|\mathbf{x} - \mathbf{y}\|$ it is also “**isometric**”

Popular Choices of GP Kernel Function

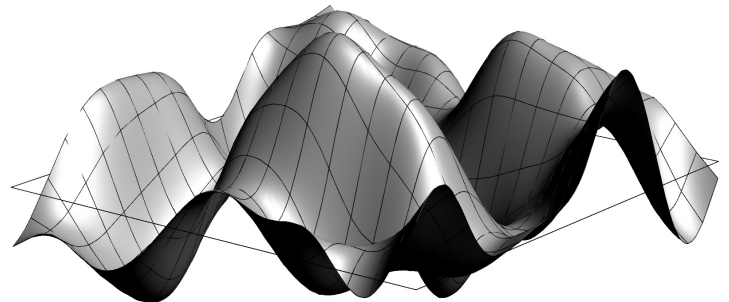
- Constant: $k_C(\mathbf{x}, \mathbf{y}) = C$
- Gaussian noise: $k_{GN}(\mathbf{x}, \mathbf{y}) = \sigma^2 \delta_{\mathbf{x}, \mathbf{y}}$
- Squared exponential: $k_{SE}(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{\|\mathbf{x} - \mathbf{y}\|^2}{2\ell^2}\right)$
- Ornstein–Uhlenbeck: $k_{OU}(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{\|\mathbf{x} - \mathbf{y}\|}{\ell}\right)$



Gaussian Process Worlds

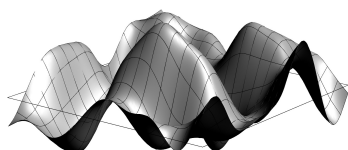


2-D Gaussian Processes



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Alternative Derivation

- Denoting the target values as a vector \mathbf{y} with elements y_i
- Denoting the matrices of covariances between data points as \mathbf{K} with elements $k(\mathbf{x}_i, \mathbf{x}_j)$
- Denoting the covariance between the data points and a particular position, \mathbf{x}_* as \mathbf{k}_* with elements $k(\mathbf{x}_i, \mathbf{x}_*)$
- Denoting the variance at a point \mathbf{x}_* as $k_* = k(\mathbf{x}_*, \mathbf{x}_*)$
- Then the distribution of function values at points at \mathbf{x}_i and \mathbf{x}_* is

$$p(\mathbf{y}, f_*) = \mathcal{N}\left(\begin{pmatrix} \mathbf{y} \\ f_* \end{pmatrix} \middle| \mathbf{0}, \begin{pmatrix} \mathbf{K} + \sigma^2 \mathbf{I} & \mathbf{k}_* \\ \mathbf{k}_*^\top & k_* \end{pmatrix}\right)$$

Observed Gaussian Processes

- Given some data points $\mathcal{D} = ((\mathbf{x}_i, y_i) | i = 1, \dots, m)$ the likelihood (assuming Gaussian error and independence of the data point) is given by

$$p(\mathcal{D} | f) = \prod_{i=1}^m \mathcal{N}(y_i | f(\mathbf{x}_i), \sigma^2)$$

- Using a Gaussian Process prior we can compute a posterior using Bayes's rule
- The posterior is a Gaussian Process with a shifted mean and variance depending on the data-points
- This direct Bayesian derivation gives the answer involving the inverse matrix of the correlation function, $k^{-1}(\mathbf{x}, \mathbf{y})$ —this is a pain to work with

Conditional Probability

- To compute the posterior $p(f_* | \mathbf{y})$ we use

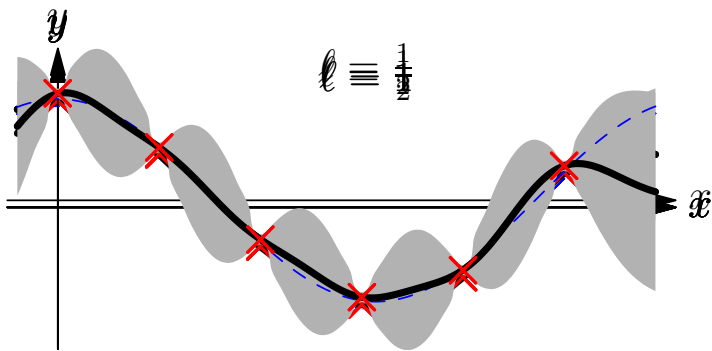
$$p(f_* | \mathbf{y}) = \frac{p(f_*, \mathbf{y})}{p(\mathbf{y})}$$

- where $p(\mathbf{y}) = \int p(f_*, \mathbf{y}) df_*$
- Because all integrals are Gaussian we can compute the integral to obtain

$$p(f_* | \mathbf{y}) = \mathcal{N}\left(f_* \middle| \mathbf{k}_*^\top (\mathbf{K} + \sigma^2 \mathbf{I})^{-1} \mathbf{y}, k_* - \mathbf{k}_*^\top (\mathbf{K} + \sigma^2 \mathbf{I})^{-1} \mathbf{k}_*\right)$$

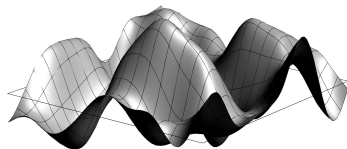
- Looks complicated, but numerically easy to evaluate

$$K(x, x') = \exp(-(x - x')^2 / (2\ell^2))$$



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Multi-dimensional Regression

- I've shown a 1-D regression example because it is easy to visualise
- This might be used with a time series
- The much more typical situation in machine learning is for x to have many features so we are doing multi-dimensional regression
- Gaussian process inference were first used in spatial problems where it was known as **kriging**
- It was re-invented by the machine learning community who call it Gaussian Processes (GP)

Choosing the Correct Covariance Function

- Choosing the correct covariance function is critical
- Most covariance functions include a continuous **hyper-parameter** (e.g. the correlation length ℓ) that we have to choose correctly
- This is typical of many Bayesian problems where we have some set of hyper-parameters, ϕ , describing the model
- These are different to the normal parameters we learn (e.g. weights w or in GP the functions $f(x)$)
- In Bayesian inference we learn the posterior for these normal parameters

$$p(f|\mathcal{D}, \phi) = \frac{p(\mathcal{D}|f, \phi)p(f|\phi)}{p(\mathcal{D}|\phi)}$$

Evidence Framework

- The normalisation factor, $p(\mathcal{D}|\phi)$ is known as the **marginal likelihood** or **evidence**

$$p(\mathcal{D}|\phi) = \int p(\mathcal{D}|f, \phi) p(f|\phi) df$$

- We can perform a Bayesian calculation at a second level by putting a prior on ϕ

$$p(\phi|\mathcal{D}) = \frac{p(\mathcal{D}|\phi)p(\phi)}{p(\mathcal{D})}$$

- From this we can now marginalise out the hyper-parameters

$$p(f|\mathcal{D}) = \int p(f|\mathcal{D}, \phi) p(\phi|\mathcal{D}) d\phi$$

Evidence for GP

- For GP the (log)-evidence can be computed in closed form

$$\log(p(\mathcal{D}|\phi)) = -\frac{1}{2} \mathbf{y}^T (\mathbf{K} + \sigma^2 \mathbf{I}) \mathbf{y} - \frac{1}{2} \log(|\mathbf{K} + \sigma^2 \mathbf{I}|) - \frac{m}{2} \log(2\pi)$$

- ★ First term measures goodness of fit
- ★ Second term measure complexity of model
- ★ Last term is a common normalisation constant

- Can efficiently compute derivatives and find best parameters
- Could overfit!

Maximum-Likelihood-II

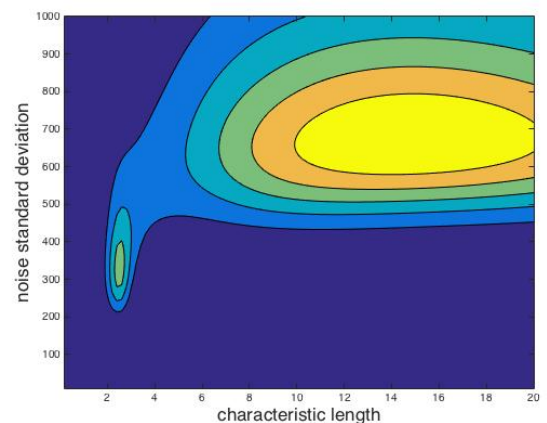
- The integral

$$p(f|\mathcal{D}) = \int p(f|\mathcal{D}, \phi) p(\phi|\mathcal{D}) d\phi$$

usually can't be computed analytically and we have to use Monte Carlo methods (see later lecture)

- An alternative is to use the most likely hyper-parameter
- We can find this by using gradient search of $p(\mathcal{D}|\phi)$
- This is sometimes referred to as ML-II
- Normally even this can be difficult, but for GP its not too difficult

Example (slightly pathological)



Conclusions

- Gaussian processes are very powerful for regression (and classification?)
- Because all calculations involve Gaussian integrals we can compute everything in closed form
- (Actually its a pain to do the mathematics because you end up working with inverse of matrices)
- Fairly generic (black-box) technique because the prior captures many continuity constraints
- We can use the evidence framework (probability of data) to do model selection and hyper-parameter optimisations