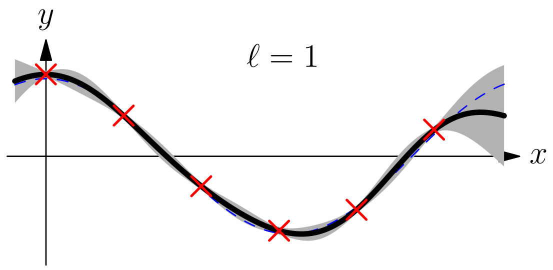
Advanced Machine Learning

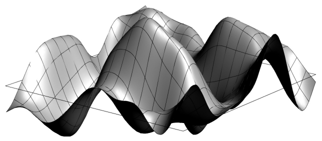
Gaussian Processes



Gaussian Processes, regression

Outline

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



Gaussian Proccesses

- 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 $\boldsymbol{x}_i$ 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 $f(\boldsymbol{x})$
- 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, $p(y_i|f(\boldsymbol{x}_i))$, we use the probability of observing y_i given the true function value is $f(\boldsymbol{x}_i)$
- 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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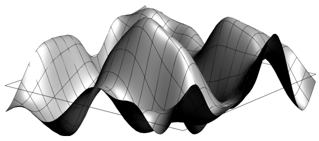


Gaussian Processes

- 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

$$p(f|m,k) \propto \mathrm{e}^{-\frac{1}{2}\int (f(\boldsymbol{x}) - m(\boldsymbol{x}))k^{-1}(\boldsymbol{x},\boldsymbol{y})(f(\boldsymbol{y}) - m(\boldsymbol{y}))\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y}}$$

- The function $m(\boldsymbol{x})$ is the mean $\mathbb{E}[f(\boldsymbol{x})]$ (usually taken to be zero in most inference problems)

Meaning of GP

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

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

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

- 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

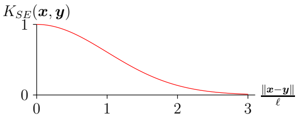
- $k(\boldsymbol{x},\boldsymbol{y})$ is a covariance function

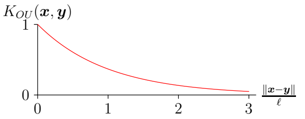
$$\mathbb{E}\big[\big(f(\boldsymbol{x})-m(\boldsymbol{x})\big)\big(f(\boldsymbol{y})-m(\boldsymbol{y})\big)\big]=k(\boldsymbol{x},\boldsymbol{y})$$

- This is sometimes know 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 $k(\boldsymbol{x},\boldsymbol{y})$ is a function of $\boldsymbol{x}-\boldsymbol{y}$ it is **"stationary"**
- If $k(\boldsymbol{x},\boldsymbol{y})$ is a function of $\|\boldsymbol{x}-\boldsymbol{y}\|$ it is also **"isometric"**

Popular Choices of GP Kernel Function

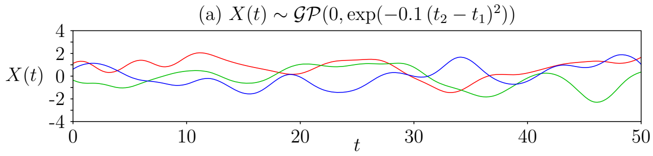
- Constant: $k_{\mathrm{C}}(\boldsymbol{x},\boldsymbol{y})=C$
- Gaussian noise: $k_{\mathrm{GN}}(\boldsymbol{x},\boldsymbol{y})=\sigma^2\delta_{\boldsymbol{x},\boldsymbol{y}}$
- Squared exponential: $k_{\mathrm{SE}}(\boldsymbol{x},\boldsymbol{y})=\exp\left(-\frac{\|\boldsymbol{x}-\boldsymbol{y}\|^2}{2\ell^2}\right)$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



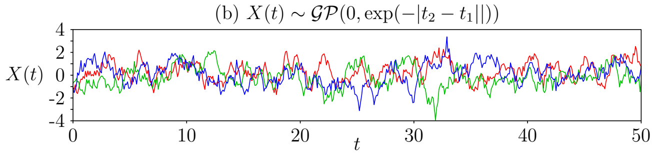


Gaussian Process Worlds

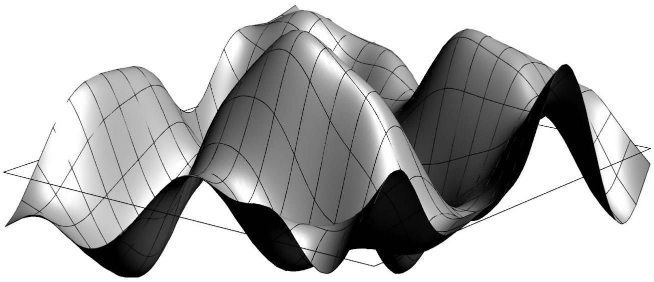
(a) $X(t)\sim\mathcal{GP}(0,\exp(-0.1\,(t_2-t_1)^2))$



(b) $X(t)\sim\mathcal{GP}(0,\exp(-|t_2-t_1||))$



2-D Gaussian Processes



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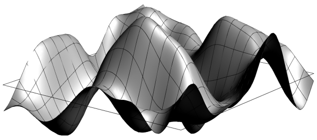


Observed Gaussian Processes

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

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

- Using a Gausssian 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, $k^{-1}(\boldsymbol{x},\boldsymbol{y})$—this is a pain to work with

Alternative Derivation

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

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

Conditional Probability

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

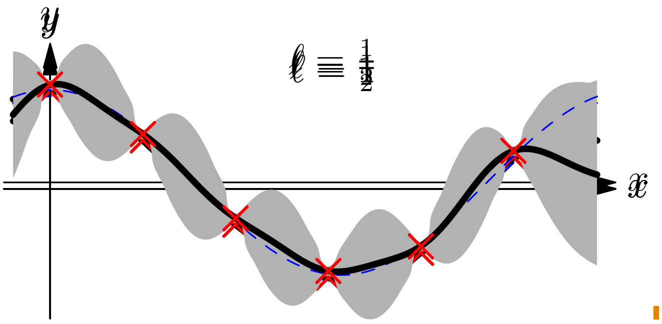
$$p(f_*|\boldsymbol{y})=\frac{p(f_*,\boldsymbol{y})}{p(\boldsymbol{y})}$$

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

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

- Looks complicated, but numerically easy to evaluate

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



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 $\boldsymbol{x}$ 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)

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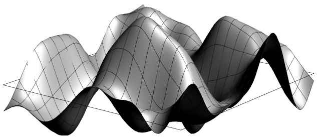


Choosing the Correct Covariance Function

- 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 were we have some set of hyper-parameters, $\boldsymbol{\phi}$, describing the model
- These are different to the normal parameters we learn (e.g. weights $\boldsymbol{w}$ or in GP the functions $f(\boldsymbol{x})$)
- In Bayesian inference we learn the posterior for these normal parameters

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

Evidence Framework

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

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

- We can perform a Bayesian calculation at a second level by putting a prior on $\boldsymbol{\phi}$

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

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

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

Maximum-Likelihood-II

- The integral

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

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 $p(\mathcal{D}|\boldsymbol{\phi})$
- This is sometimes referred to as ML-II
- Normally even this can be difficult, but for GP its not too difficult

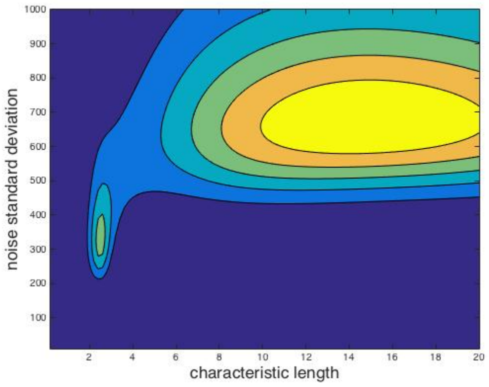
Evidence for GP

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

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

  - ⋆ 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!

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