Probabilistic Graphical Models
Lecture 20: Gaussian Processes

Andrew Gordon Wilson

www.cs.cmu.edu/~andrewgw
Carnegie Mellon University

March 30, 2015
What is Machine Learning?

- Machine learning algorithms adapt with data versus having fixed decision rules.
- Machine learning aims not only to equip people with tools to analyse data, but to create algorithms which can learn and make decisions without human intervention.¹,²
- In order for a model to automatically learn and make decisions, it must be able to discover patterns and extrapolate those patterns to new situations.

¹E.g., N.D. Lawrence (2010), “What is Machine Learning?”
Function Learning Example
Function Learning Example
Function Learning Example

Airline Passengers (Thousands)

Year

Train
Alien?
Function Learning Example

![Airline Passengers (Thousands) vs. Year]

- **Train** (Blue Line)
- **Human?** (Black Line)

- **Y-axis**: Airline Passengers (Thousands)
- **X-axis**: Year

Data points from 1949 to 1961:
- 1949: 100
- 1951: 200
- 1953: 300
- 1955: 400
- 1957: 500
- 1959: 600
- 1961: 700

The graph illustrates the trend in airline passengers over the years, with fluctuations that appear to be influenced by human factors (e.g., holidays, events, etc.).
Function Learning Example
Function Learning Example

Airline Passengers (Thousands)

Year

Train
Alien?
Test
Human?

The ability for a model to learn from data depends on its:

1. Support: what solutions we think are a priori possible.
2. Inductive biases: what solutions we think are a priori likely.

- Examples: Function Learning, Character Recognition
- Human ability to make remarkable generalisations from data could derive from an expressive prior combined with Bayesian inference.
Basic Regression Problem

- Training set of $N$ targets (observations) $\mathbf{y} = (y(x_1), \ldots, y(x_N))^T$.
- Observations evaluated at inputs $\mathbf{X} = (x_1, \ldots, x_N)^T$.
- Want to predict the value of $y(x_*)$ at a test input $x_*$. 

For example: Given CO$_2$ concentrations $\mathbf{y}$ measured at times $\mathbf{X}$, what will the CO$_2$ concentration be for $x_* = 2024$, 10 years from now?

Just knowing high school math, what might you try?
Guess the parametric form of a function that could fit the data

- $f(x, w) = w^T x$ [Linear function of $w$ and $x$]
- $f(x, w) = w^T \phi(x)$ [Linear function of $w$] (Linear Basis Function Model)
- $f(x, w) = g(w^T \phi(x))$ [Non-linear in $x$ and $w$] (E.g., Neural Network)

$\phi(x)$ is a vector of basis functions. For example, if $\phi(x) = (1, x, x^2)$ and $x \in \mathbb{R}^1$ then $f(x, w) = w_0 + w_1 x + w_2 x^2$ is a quadratic function.

Choose an error measure $E(w)$, minimize with respect to $w$

- $E(w) = \sum_{i=1}^{N} [f(x_i, w) - y(x_i)]^2$
A probabilistic approach

We could explicitly account for noise in our model.

\[ y(x) = f(x, w) + \epsilon(x) \], where \( \epsilon(x) \) is a noise function.

One commonly takes \( \epsilon(x) = \mathcal{N}(0, \sigma^2) \) for i.i.d. additive Gaussian noise, in which case

\[
p(y(x)|x, w, \sigma^2) = \mathcal{N}(y(x); f(x, w), \sigma^2) \quad \text{Observation Model} \quad (1)
\]

\[
p(y|x, w, \sigma^2) = \prod_{i=1}^{N} \mathcal{N}(y(x_i); f(x_i, w), \sigma^2) \quad \text{Likelihood} \quad (2)
\]

- Maximize the likelihood of the data \( p(y|x, w, \sigma^2) \) with respect to \( \sigma^2, w \).

For a Gaussian noise model, this approach will make the same predictions as using a squared loss error function:

\[
\log p(y|X, w, \sigma^2) \propto -\frac{1}{2\sigma^2} \sum_{i=1}^{N} [f(x_i, w) - y(x_i)]^2 \quad (3)
\]
The probabilistic approach helps us interpret the error measure in a deterministic approach, and gives us a sense of the noise level $\sigma^2$.

Probabilistic methods thus provide an intuitive framework for representing uncertainty, and model development.

Both approaches are prone to over-fitting for flexible $f(x, w)$: low error on the training data, high error on the test set.

Regularization

Use a penalized log likelihood (or error function), such as

$$\log p(y|X, w) \propto -\frac{1}{2\sigma^2} \sum_{i=1}^{n} (f(x_i, w) - y(x_i))^2 - \lambda w^T w.$$  

But how should we define complexity, and how much should we penalize complexity?

Can set $\lambda$ using cross-validation.
Bayesian Inference

Bayes’ Rule

\[ p(a|b) = \frac{p(b|a)p(a)}{p(b)}, \quad p(a|b) \propto p(b|a)p(a). \quad (5) \]

\[ \text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{marginal likelihood}}, \quad p(w|y, X, \sigma^2) = \frac{p(y|X, w, \sigma^2)p(w)}{p(y|X, \sigma^2)}. \quad (6) \]

Predictive Distribution

\[ p(y|x_*, y, X) = \int p(y|x_*, w)p(w|y, X)dw. \quad (7) \]

- Average of infinitely many models weighted by their posterior probabilities.
- No over-fitting, automatically calibrated complexity.
- Typically more interested in distribution over functions than in parameters \( w \).
Different types of uncertainty:

- Uncertainty through lack of knowledge
- Intrinsic uncertainty; e.g., radioactive decay.

Uncertainty through lack of knowledge can seem like intrinsic uncertainty (e.g., rolling dice).

Regardless of whether or not the universe is deterministic – whether there is some underlying true answer – we will always have uncertainty. We can represent this belief using probability distributions (Bayesian methods, probabilistic modelling).
Parametric Regression Review

Deterministic

\[ E(w) = \sum_{i=1}^{N} (f(x_i, w) - y_i)^2. \]  \hspace{1cm} (8)

Maximum Likelihood

\[ p(y(x)|x, w) = \mathcal{N}(y(x); f(x, w), \sigma^2_n), \]  \hspace{1cm} (9)

\[ p(y|X, w) = \prod_{i=1}^{N} \mathcal{N}(y(x_i); f(x_i, w), \sigma^2_n). \]  \hspace{1cm} (10)

Bayesian

\[ \text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{marginal likelihood}}, \quad p(w|y, X) = \frac{p(y|X, w)p(w)}{p(y|X)}. \]  \hspace{1cm} (11)
Model Selection and Marginal Likelihood

\[ p(y|\mathcal{M}_1, X) = \int p(y|f_1(x, w))p(w)dw \]  

18 / 53
Blackboard: Examples of Occam’s Razor in Everyday Inferences

For further reading, see MacKay (2003) textbook, Information Theory, Inference, and Learning Algorithms.
Occam’s Razor Example

-1, 3, 7, 11, ??, ??

- H₁: the sequence is an arithmetic progression, add $n$, where $n$ is an integer.
- H₂: the sequence is generated by a cubic function of the form $cx^3 + dx^2 + e$, where $c$, $d$, and $e$ are fractions. \((-\frac{1}{11}x^3 + \frac{9}{11}x^2 + \frac{23}{11}\)
Observations $y(x)$. Assume $p(y(x)|f(x)) \sim \mathcal{N}(y(x); f(x), \sigma^2)$. Consider polynomials of different orders. As always, observations are out of the chosen model class! Which model should we choose?

$$f_0(x) = a_0,$$  \hspace{1cm} (14)

$$f_1(x) = a_0 + a_1 x,$$  \hspace{1cm} (15)

$$f_2(x) = a_0 + a_1 x + a_2 x^2,$$  \hspace{1cm} (16)

$$\vdots$$  \hspace{1cm} (17)

$$f_J(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_J x^J.$$  \hspace{1cm} (18)
Marginal likelihood (evidence) as a function of model order, using an isotropic prior $p(a) = \mathcal{N}(0, \sigma^2 I)$.
Marginal likelihood (evidence) as a function of model order, using an anisotropic prior $p(a_i) = \mathcal{N}(0, \gamma^{-i})$, with $\gamma$ learned from the data.
Occam’s Razor

For further reading, see Rasmussen and Ghahramani (2001) (*Occam’s Razor*) and Kass and Raftery (1995) (*Bayes Factors*)
Consider the simple linear model,

\[ f(x) = a_0 + a_1 x, \]  
(19)

\[ a_0, a_1 \sim \mathcal{N}(0, 1). \]  
(20)
We are interested in the induced distribution over functions, not the parameters...
Let’s characterise the properties of these functions directly:

\[
\begin{align*}
 f(x|a_0, a_1) &= a_0 + a_1 x, \quad a_0, a_1 \sim \mathcal{N}(0, 1). \\
 \mathbb{E}[f(x)] &= \mathbb{E}[a_0] + \mathbb{E}[a_1] x = 0. \\
 \text{cov}[f(x_b), f(x_c)] &= \mathbb{E}[f(x_b)f(x_c)] - \mathbb{E}[f(x_b)]\mathbb{E}[f(x_c)] \\
 &= \mathbb{E}[a_0^2 + a_0 a_1(x_b + x_c) + a_1^2 x_b x_c] - 0 \\
 &= \mathbb{E}[a_0^2] + \mathbb{E}[a_1^2 x_b x_c] + \mathbb{E}[a_0 a_1(x_b + x_c)] \\
 &= 1 + x_b x_c + 0 \\
 &= 1 + x_b x_c.
\end{align*}
\]
Therefore any collection of values has a joint Gaussian distribution

\[ [f(x_1), \ldots, f(x_N)] \sim \mathcal{N}(0, K), \quad (28) \]

\[ K_{ij} = \text{cov}(f(x_i), f(x_j)) = k(x_i, x_j) = 1 + x_b x_c. \quad (29) \]

By definition, \( f(x) \) is a Gaussian process.

**Definition**

A Gaussian process (GP) is a collection of random variables, any finite number of which have a joint Gaussian distribution. We write \( f(x) \sim \mathcal{GP}(m, k) \) to mean

\[ [f(x_1), \ldots, f(x_N)] \sim \mathcal{N}((\mu, K) \quad (30) \]

\[ \mu_i = m(x_i) \quad (31) \]

\[ K_{ij} = k(x_i, x_j), \quad (32) \]

for any collection of input values \( x_1, \ldots, x_N \). In other words, \( f \) is a GP with mean function \( m(x) \) and covariance kernel \( k(x_i, x_j) \).
Model Specification

\[ f(x, w) = w^T \phi(x) \quad (33) \]
\[ p(w) = \mathcal{N}(0, \Sigma_w) \quad (34) \]

Moments of Induced Distribution over Functions

\[ \mathbb{E}[f(x, w)] = m(x) = \mathbb{E}[w^T] \phi(x) = 0 \quad (35) \]
\[ \text{cov}(f(x_i), f(x_j)) = k(x_i, x_j) = \mathbb{E}[f(x_i)f(x_j)] - \mathbb{E}[f(x_i)]\mathbb{E}[f(x_j)] \quad (36) \]
\[ = \phi(x_i)^T \mathbb{E}[ww^T] \phi(x_j) - 0 \quad (37) \]
\[ = \phi(x_i)^T \Sigma_w \phi(x_j) \quad (38) \]

- \( f(x, w) \) is a Gaussian process, \( f(x) \sim \mathcal{N}(m, k) \) with mean function \( m(x) = 0 \) and covariance kernel \( k(x_i, x_j) = \phi(x_i)^T \Sigma_w \phi(x_j) \).
- The entire basis function model of Eqs. (33) and (34) is encapsulated as a distribution over functions with kernel \( k(x, x') \).
We are ultimately more interested in – and have stronger intuitions about – the *functions* that model our data than weights $w$ in a parametric model, and we can express those intuitions using a covariance kernel.

The kernel controls the support and inductive biases of our model, and thus its ability to generalise.
Example: RBF Kernel

\[ k_{RBF}(x, x') = \text{cov}(f(x), f(x')) = a^2 \exp\left(-\frac{||x - x'||^2}{2\ell^2}\right) \] (39)

- Far and above the most popular kernel.
- Expresses the intuition that function values at nearby inputs are more correlated than function values at far away inputs.
- The kernel hyperparameters \( a \) and \( \ell \) control amplitudes and wiggliness of these functions.
- GPs with an RBF kernel have large support and are universal approximators.
Sampling from a GP with an RBF Kernel

```matlab
x = [-10:0.2:10]'; % inputs (where we query the GP)
N = numel(x); % number of inputs
K = zeros(N,N); % covariance matrix

% very inefficient way of creating K in Matlab
for i=1:N
    for j=1:N
        K(i,j) = k_rbf(x(i),x(j));
    end
end

K = K + 1e-6*eye(N); % add jitter for conditioning
CK = chol(K);
f = CK'*randn(N,1); % draws from N(0,K)

plot(x,f);
```
Samples from a GP with an RBF Kernel

Gaussian process sample prior functions

output, f(x)

input, x
1D RBF Kernel with Different Length-scales

\[ k_{\text{RBF}}(x, x') = \text{cov}(f(x), f(x')) = a^2 \exp\left(-\frac{||x - x'||^2}{2\ell^2}\right) \]  

(40)

**Figure:** SE kernels with different length-scales, as a function of \( \tau = x - x' \).
The covariance matrix $K$ for ordered inputs on a 1D grid. $K_{ij} = k_{\text{RBF}}(x_i, x_j)$. 

\[ k_{\text{RBF}}(x, x') = \text{cov}(f(x), f(x')) = a^2 \exp\left(-\frac{||x - x'||^2}{2\ell^2}\right) \] 

(41)
Gaussian Process Inference

- Observed noisy data $y = (y(x_1), \ldots, y(x_N))^T$ at input locations $X$.
- Start with the standard regression assumption: $\mathcal{N}(y(x); f(x), \sigma^2)$.
- Place a Gaussian process distribution over noise free functions $f(x) \sim \mathcal{GP}(0, k_\theta)$. The kernel $k$ is parametrized by $\theta$.
- Infer $p(f^*|y, X, X^*)$ for the noise free function $f$ evaluated at test points $X^*$.

**Joint distribution**

$$
\begin{bmatrix}
y \\
f^*_x
\end{bmatrix} \sim \mathcal{N}\left(0, \begin{bmatrix} K_\theta(X, X) + \sigma^2 I & K_\theta(X, X^*) \\ K_\theta(X^*, X) & K_\theta(X^*, X^*) \end{bmatrix}\right).$$

(42)

**Conditional predictive distribution**

$$f^*_x|X^*, X, y, \theta \sim \mathcal{N}(\bar{f}^*_x, \text{cov}(f^*)),$$

(43)

$$\bar{f}^*_x = K_\theta(X^*, X)[K_\theta(X, X) + \sigma^2 I]^{-1}y,$$

(44)

$$\text{cov}(f^*) = K_\theta(X^*, X^*) - K_\theta(X^*, X)[K_\theta(X, X) + \sigma^2 I]^{-1}K_\theta(X, X^*).$$

(45)
Inference using an RBF kernel

- Specify \( f(x) \sim \mathcal{GP}(0, k) \).
- Choose \( k_{\text{RBF}}(x, x') = a_0^2 \exp\left(-\frac{|x-x'|^2}{2\ell_0^2}\right) \). Choose values for \( a_0 \) and \( \ell_0 \).
- Observe data, look at the prior and posterior over functions.

Does something look strange about these functions?
Increase the length-scale $\ell$. 

Samples from GP Prior

Samples from GP Posterior

(a)

(b)
Learning and Model Selection

\[
p(M_i | y) = \frac{p(y | M_i) p(M_i)}{p(y)}
\]  
\[\text{(46)}\]

We can write the evidence of the model as

\[
p(y | M_i) = \int p(y | f, M_i) p(f) df,
\]  
\[\text{(47)}\]
Learning and Model Selection

- We can integrate away the entire Gaussian process \( f(x) \) to obtain the marginal likelihood, as a function of kernel hyperparameters \( \theta \) alone.

\[
p(y|\theta, X) = \int p(y|f, X)p(f|\theta, X)df .
\]  
\[ \text{model fit} \quad - \quad \text{complexity penalty} \]

\[
\log p(y|\theta, X) = -\frac{1}{2}y^T(K_{\theta} + \sigma^2 I)^{-1}y - \frac{1}{2} \log |K_{\theta} + \sigma^2 I| - \frac{N}{2} \log(2\pi) .
\]

- An extremely powerful mechanism for kernel learning.
A fully Bayesian treatment would integrate away kernel hyperparameters $\theta$.

$$p(f_*|X_*, X, y) = \int p(f_*|X_*, X, y, \theta)p(\theta|y)d\theta$$  \hspace{1cm} (50)

For example, we could specify a prior $p(\theta)$, use MCMC to take $J$ samples from $p(\theta|y) \propto p(y|\theta)p(\theta)$, and then find

$$p(f_*|X_*, X, y) \approx \frac{1}{J} \sum_{i=1}^{J} p(f_*|X_*, X, y, \theta^{(i)}) , \quad \theta^{(i)} \sim p(\theta|y) .$$ \hspace{1cm} (51)

If we have a non-Gaussian noise model, and thus cannot integrate away $f$, the strong dependencies between Gaussian process $f$ and hyperparameters $\theta$ make sampling extremely difficult. In my experience, the most effective solution is to use a deterministic approximation for the posterior $p(f|y)$ which enables one to work with an approximate marginal likelihood.
Gaussian Process Covariance Kernels

Let \( \tau = x - x' \):

\[
\begin{align*}
    k_{SE}(\tau) &= \exp(-0.5\tau^2/\ell^2) \\
    k_{MA}(\tau) &= a(1 + \frac{\sqrt{3}\tau}{\ell}) \exp(-\frac{\sqrt{3}\tau}{\ell}) \\
    k_{RQ}(\tau) &= (1 + \frac{\tau^2}{2\alpha \ell^2})^{-\alpha} \\
    k_{PE}(\tau) &= \exp(-2 \sin^2(\pi \tau \omega)/\ell^2)
\end{align*}
\]
1. **Learning:** Optimize marginal likelihood,

\[
\log p(y|\theta, X) = \underbrace{-\frac{1}{2}y^T(K_\theta + \sigma^2 I)^{-1}y}_{\text{model fit}} - \frac{1}{2} \log |K_\theta + \sigma^2 I| - \frac{N}{2} \log(2\pi) ,
\]

with respect to kernel hyperparameters \( \theta \).

2. **Inference:** Conditioned on kernel hyperparameters \( \theta \), form the predictive distribution for test inputs \( X_* \):

\[
f_*|X_*, X, y, \theta \sim \mathcal{N}(\bar{f}_*, \text{cov}(f_*)) ,
\]

\[
\bar{f}_* = K_\theta(X_*, X)[K_\theta(X, X) + \sigma^2 I]^{-1}y ,
\]

\[
\text{cov}(f_*) = K_\theta(X_*, X_*) - K_\theta(X_*, X)[K_\theta(X, X) + \sigma^2 I]^{-1}K_\theta(X, X_*) .
\]
- Squared are observed, circles are latent, the thick bar is a set of fully connected nodes.
- Each $y_i$ is conditionally independent given $f_i$.
- Because of the marginalization property of a GP, addition of further inputs $x_*$ and unobserved targets $y_*$ does not change the distribution of any other variables.

Figure from GPML, Rasmussen and Williams (2006)
Worked Example: Combining Kernels, CO$_2$ Data

Example from Rasmussen and Williams (2006), *Gaussian Processes for Machine Learning*. 
Worked Example: Combining Kernels, CO$_2$ Data
Worked Example: Combining Kernels, CO₂ Data

- **Long rising trend:** \( k_1(x_p, x_q) = \theta_1^2 \exp \left( -\frac{(x_p-x_q)^2}{2\theta_2^2} \right) \)
- **Quasi-periodic seasonal changes:** \( k_2(x_p, x_q) = k_{\text{RBF}}(x_p, x_q)k_{\text{PER}}(x_p, x_q) = \theta_3^2 \exp \left( -\frac{(x_p-x_q)^2}{2\theta_4^2} - \frac{2 \sin^2(\pi (x_p-x_q))}{\theta_5^2} \right) \)
- **Multi-scale medium term irregularities:**
  \( k_3(x_p, x_q) = \theta_6^2 \left( 1 + \frac{(x_p-x_q)^2}{2\theta_8\theta_7^2} \right)^{-\theta_8} \)
- **Correlated and i.i.d. noise:** \( k_4(x_p, x_q) = \theta_9^2 \exp \left( -\frac{(x_p-x_q)^2}{2\theta_10^2} \right) + \theta_{11}^2 \delta_{pq} \)
- **Total kernel:** \( k_{\text{total}}(x_p, x_q) = k_1(x_p, x_q) + k_2(x_p, x_q) + k_3(x_p, x_q) + k_4(x_p, x_q) \)
Hand crafted a kernel combination to perform extrapolation
Confidence in the extrapolation is high (suggests that model is well specified).
Can interpret the learned kernel hyperparameters $\theta$ to learn information about our dataset.
A lot of the interesting pattern recognition has been done by a human in this example. We would like to completely automate this modelling procedure.
Non-Gaussian Likelihoods

We can no longer analytically integrate away the Gaussian process. But we can use a simple Monte carlo sum:

\[
p(f_* | y, X, x_*) = \int p(f_* | f, x_*) p(f | y) df \\
\approx \frac{1}{J} \sum_{j=1}^{J} p(f_* | f^{(j)}, x_*) , \quad f^{(j)} \sim p(f | y)
\]

But how do we sample from \( p(f | y) \)?
We can no longer analytically integrate away the Gaussian process. But we can use a simple Monte carlo sum:

\[
p(f_* | y, X, x_*) = \int p(f_* | f, x_*) p(f | y) df
\]
\[
\approx \frac{1}{J} \sum_{j=1}^{J} p(f_* | f^{(j)}, x_*) , \quad f^{(j)} \sim p(f | y)
\]

But how do we sample from \( p(f | y) \)?

*Elliptical slice sampling*. Murray et. al. AISTATS 2010.
But what about hyperparameters? It’s easy to implement Gibbs sampling:

\[ p(f|y, \theta) \propto p(y|f)p(f|\theta) \]  \hspace{1cm} (56)
\[ p(\theta|f,y) \propto p(f|\theta)p(\theta) . \]  \hspace{1cm} (57)

But this won’t work because of strong correlations between \( f \) and \( \theta \).
Non-Gaussian Likelihoods

But what about hyperparameters? It’s easy to implement Gibbs sampling:

\[
p(f|y, \theta) \propto p(y|f)p(f|\theta) \tag{58}
\]

\[
p(\theta|f, y) \propto p(f|\theta)p(\theta) \tag{59}
\]

But this won’t work because of strong correlations between \( f \) and \( \theta \).

- Transform into a whitened space, \( f = L\nu \), and sample from \( \nu \) and \( \theta \), which decouples correlations.
Non-Gaussian Likelihoods

But what about hyperparameters? It’s easy to implement Gibbs sampling:

\[
p(f|y, \theta) \propto p(y|f)p(f|\theta) \tag{60}
\]

\[
p(\theta|f, y) \propto p(f|\theta)p(\theta) . \tag{61}
\]

But this won’t work because of strong correlations between \(f\) and \(\theta\).

- Transform into a whitened space, \(f = L \nu\), and sample from \(\nu\) and \(\theta\), which decouples correlations.
- Use a deterministic approach to approximately integrate away \(f\) to access a marginal likelihood, conditioned only on kernel hyperparameters \(\theta\):

\[
p(y|\theta) = \int p(y|f)p(f|\theta) df \tag{62}
\]

- The Laplace approximation, for example, approximates \(p(f|y)\) as a Gaussian.
Readings for Next Time

- C. Rasmussen and C. Williams, GPML, Ch. 4, 5