GAUSSIAN PROCESS REGRESSION

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OVERVIEW

INTRODUCTION

GAUSSIAN PROCESSES (GPs)

REGRESSION WITH GAUSSIAN PROCESSES

APPLICATION TO MODELING LIGHTCURVES

REFERENCES
Prediction with Gaussian processes is not a new idea. It has roots that date back to Kolmogorov in the 1940s and applications to multivariate regression as early as the 1960s.
**Motivation**

Prediction with Gaussian processes is not a new idea. It has roots that date back to Kolmogorov in the 1940s and applications to multivariate regression as early as the 1960s.

- ARMA models in time series analysis
- "Kriging" in geostatistical models
- Regression splines
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Gaussian process regression is a “less” parametric tool for supervised learning.
WHAT IS A GAUSSIAN PROCESS?

A stochastic process, $Y(x)$, is a Gaussian process (GP) if it generates data such that any finite subset of the range of the process follows a multivariate Gaussian distribution.
SPECIFICATION

Because the joint distribution of $Y(x_1), Y(x_2), \ldots, Y(x_n)$ is multivariate Gaussian, we need only specify the mean and the covariance functions:

- $\mathbb{E}[Y(x)] = m(x)$
- $\mathbb{E}[\{Y(x) - m(x)\}\{Y(x') - m(x')\}^T] = k(x, x')$.

Then, we write $Y(x) \sim \mathcal{GP}(m(x), k(x, x'))$. 
Suppose that we observe $y_1, \ldots, y_n$, which are measured without error (for now).

We believe there is an underlying process $f(x)$ such that

$$y = f(x).$$

Our goal is to estimate $f(x)$. To do so, we will assume that $f(x) \sim \mathcal{GP}(0, k(x, x'))$. 
SPECIFYING A COVARIANCE FUNCTION

The covariance function, $k(x, x')$, can be any function that generates a non-negative definite covariance matrix for any finite set of points $(x_1, \ldots, x_n)$. 
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- Seems general, but these functions are tricky to find!
- Usually rely on families that are already well-studied.
**COMMON COVARIANCE FUNCTIONS**

- **Constant:**
  \[ k(x, x') = \nu_0 \]

- **Gaussian Noise:**
  \[ k(x, x') = \nu_0 \delta_{x,x'} \]

- **Squared Exponential:**
  \[ k(x, x') = \nu_0 \exp \left[ -\frac{\|x - x'\|^2}{2\ell^2} \right] \]

- **Many options:** Ornstein-Uhlenbeck, Matérn, periodic, stationary and isotropic covariance functions from spatial statistics, etc.
A MORE GENERAL COVARIANCE FUNCTION

Williams and Rasmussen (1996) propose a very general covariance function that is flexible and works well in practice.

For \( \mathbf{x} = (x_1, \ldots, x_p) \) and \( \mathbf{x}' = (x'_1, \ldots, x'_p) \),

\[
k(\mathbf{x}, \mathbf{x}') = v_0 \exp \left[ -\frac{1}{2} \sum_{\ell=1}^{p} \alpha_{\ell} (x_{\ell} - x'_{\ell})^2 \right] + \beta_0 + \beta_1 \mathbf{x}^T \mathbf{x}' + v_1 \delta_{\mathbf{x}, \mathbf{x}'}.
\]
A More General Covariance Function, Explained

\[ k(x, x') = v_0 \exp \left[ -\frac{1}{2} \sum_{\ell=1}^{p} \alpha_{\ell} (x_\ell - x'_\ell)^2 \right] + \beta_0 + \beta_1 x^T x' + v_1 \delta_{x,x'}. \]

- Nearby input values will have highly correlated outputs.
- Very similar to squared exponential, but allows a different level of smoothing for each input dimension.
- \( v_0 \) controls the overall scale of local correlations.
A More General Covariance Function, Explained

\[ k(x, x') = v_0 \exp \left[ -\frac{1}{2} \sum_{\ell=1}^{p} \alpha_\ell (x_\ell - x'_\ell)^2 \right] + \beta_0 + \beta_1 x^T x' + \nu_1 \delta_{x,x'}. \]

- \( \beta_0 \) allows for bias, i.e. correlation not explained by inputs.
- \( \beta_1 \) allows for a linear contribution to the covariance.
A More General Covariance Function, Explained

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k(x, x') = v_0 \exp \left[ -\frac{1}{2} \sum_{\ell=1}^{p} \alpha_\ell (x_\ell - x'_\ell)^2 \right] + \beta_0 + \beta_1 x^T x' + v_1 \delta_{x,x'}.
\]

- Accounts for noise or measurement error in the data.
- \(v_1\) controls the variance of the noise.
NOW WHAT?

We have specified our Gaussian process, but how do we use that to actually \textit{perform} regression?
Prediction using Gaussian Processes

For simplicity, suppose we want to predict the value at a single new point, \( y_* = f(x_*) \).

As always, first some notation:
- Let \( y = (y_1, \ldots, y_n) \) be the observed values.
- Let \( K \) be the \( n \times n \) covariance matrix where \( [K]_{ij} = k(x_i, x_j) \).
- Let \( K_* \) be the \( 1 \times n \) vector, \( K_* = [k(x_*, x_1) \ldots k(x_*, x_n)] \).
- Let \( K_{**} = k(x_*, x_*) \) be the scalar variance at the new point.
By the definition of Gaussian process, we know that the observed values and the desired predicted value have a joint multivariate normal distribution,

\[
\begin{bmatrix}
y \\
y^* 
\end{bmatrix} \sim \mathcal{N}_{n+1} \left( \begin{bmatrix}
0_n \\
0
\end{bmatrix}, \begin{bmatrix}
K & K^T \\
K^T & K_{**}
\end{bmatrix}\right).
\]
Prediction using Gaussian Processes

By the definition of Gaussian process, we know that the observed values and the desired predicted value have a joint multivariate normal distribution,

$$\begin{bmatrix} y \\ y_* \end{bmatrix} \sim \mathcal{N}_{n+1} \left( \begin{bmatrix} 0_n \\ 0 \end{bmatrix}, \begin{bmatrix} K & K^T_* \\ K_* & K_{**} \end{bmatrix} \right).$$

We know the distribution of $y_*|y$ exactly, so our best guess for $y_*$ is simply the mean of this conditional distribution

$$\hat{y}_* = K_*K^{-1}y.$$
APPLICATION TO MODELING LIGHTCURVES

The authors’ goal is to develop a new set of measures that can enhance classification of objects based on lightcurves.

To that end, they want to estimate the “true” lightcurve based on sparse-ish observations and base their measures on that estimated function.
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Because the authors estimated each lightcurve individually, we will go through this process for a single curve to demonstrate how Gaussian process regression works in this setting.
DATA

Figure: CSS111103:230309+400608, a Flare star
Regression Model

Using time, $t$, as the indexing variable for our proposed process and accounting for measurement error we posit that the process generating the observed magnitudes is of the form

$$y = f(t) + \mathcal{N}(0, \sigma_n^2),$$

where $f(t) \sim \mathcal{GP}(m(t), k(t, t'))$.

It remains to specify the functional forms of $m(t)$ and $k(t, t')$. 
SPECIFICATION

In this case, it seems that assuming $m(t) \equiv 0$ is inappropriate. Following the authors, we set $m(t) = 17.99$, the median observed magnitude in the data.

We use the squared exponential covariance kernel for $k(t, t')$. Recall that we have additional error in the observations caused by measurement error.

So, the covariance kernel for the observed magnitudes is

$$k_y(t, t') = \sigma_f^2 \exp \left[ -\frac{1}{2\ell^2} (t - t')^2 \right] + \sigma_n^2 \delta_{t,t'}.$$
PARAMETER SPECIFICATION

As the authors suggest, we set the parameter values as

- $\sigma_f^2 = 0.27$, the median observed variance in the magnitudes of non-variable objects.
- $\sigma_n^2 = 0.01$, the mean value of measurement error in the data.
- $\ell = 140$ days.
Fitted Curve

Figure: CSS111103:230309+400608, with smoothed curve in red
REFERENCES


THANK YOU!