A Guide to the GauPro R package

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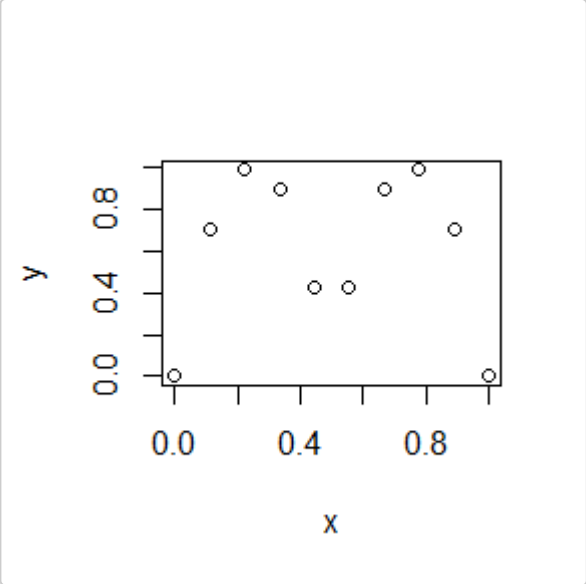
This R package provides R code for fitting Gaussian process models to data. The code is created using the `R6` class structure, which is why `$` is used to access object methods.

A Gaussian process fits a model to a dataset, which gives a function that gives a prediction for the mean at any point along with a variance of this prediction.

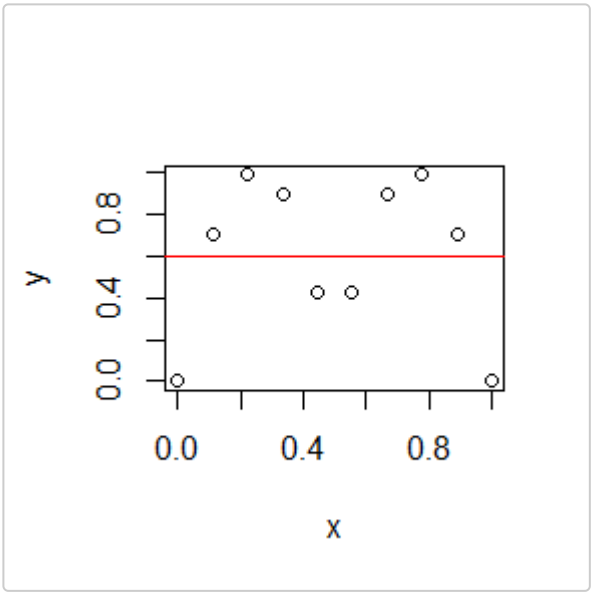
Suppose we have the data below

```
x <- seq(0,1,l=10)
y <- abs(sin(2*pi*x))^.8
plot(x, y)
```



A linear model (LM) will fit a straight line through the data and clearly does not describe the underlying function producing the data.

```
lm_mod <- lm(y ~ x)
plot(x, y)
abline(a=lm_mod$coef[1], b=lm_mod$coef[2], col='red')
```



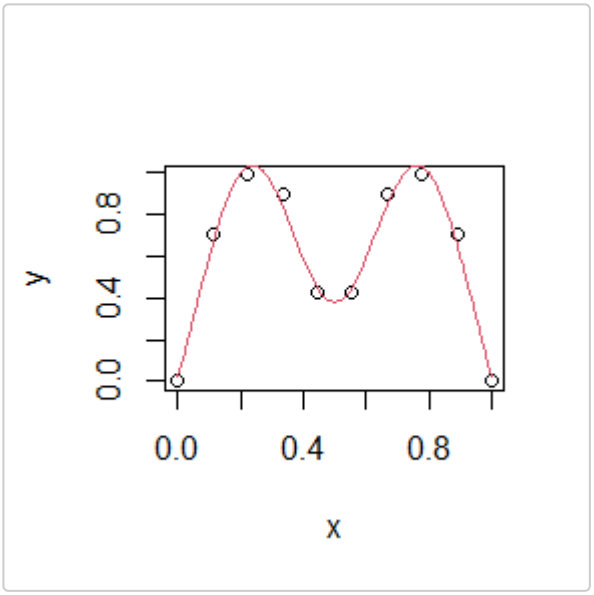
A Gaussian process is a type of model that assumes that the distribution of points follows a multivariate distribution.

In GauPro, we can fit a GP model with Gaussian correlation function using the function ``

```
library(GauPro)
gp <- GauPro(x, y, parallel=FALSE)
```

Now we can plot the predictions given by the model. Shown below, this model looks much better than a linear model.

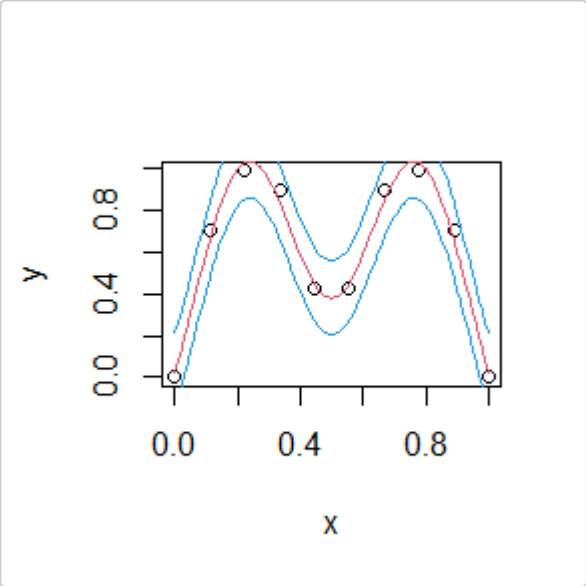
```
plot(x, y)
curve(gp$predict(x), add=T, col=2)
```



A very useful property of GP's is that they give a predicted error. The blue lines give an approximate 95% confidence interval. The width of the prediction interval is largest between points and goes to zero near data points, which is what we would hope for.

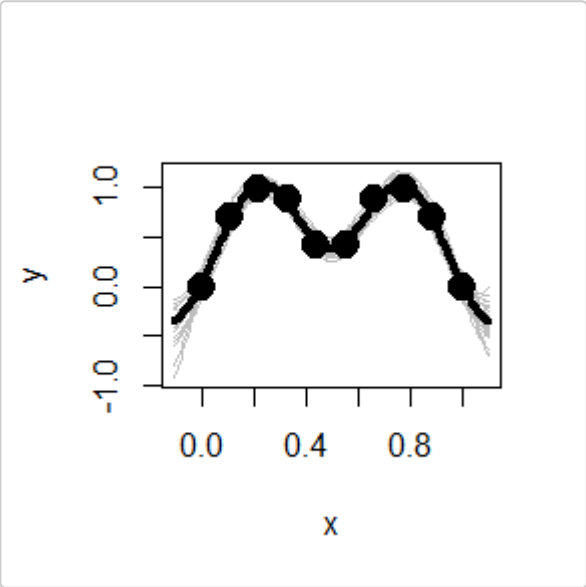
```
plot(x, y)
curve(gp$predict(x), add=T, col=2)
```

```
curve(gp$predict(x)+2*gp$predict(x, se=T)$se, add=T, col=4)
curve(gp$predict(x)-2*gp$predict(x, se=T)$se, add=T, col=4)
```



GP models give distributions for the predictions. Realizations from these distributions give an idea of what the true function may look like. Calling `plot` on the 1-D gp object shows 20 realizations. There is no visible difference between the data points, only at the ends.

```
if (requireNamespace("MASS", quietly = TRUE)) {
  plot(gp)
}
```



Using kernels

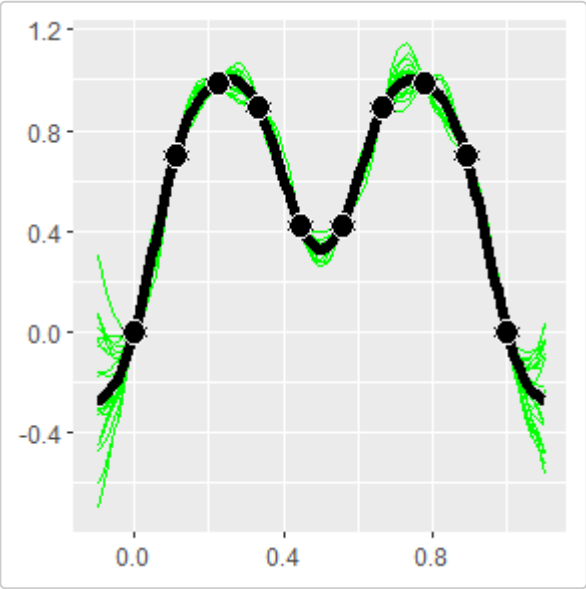
The kernel, or covariance function, has a large effect on the Gaussian process being estimated. The function `GauPro` uses the squared exponential, or Gaussian, covariance function. The newer version of GauPro has a new function that will fit a model using whichever kernel is specified.

To do this a kernel must be specified, then passed to `GauPro_kernel_model$new`. The example below shows what the Matern 5/2 kernel gives.

```
kern <- Matern52$new(0)
gpk <- GauPro_kernel_model$new(matrix(x, ncol=1), y, kernel=kern, parallel=FALSE)
```

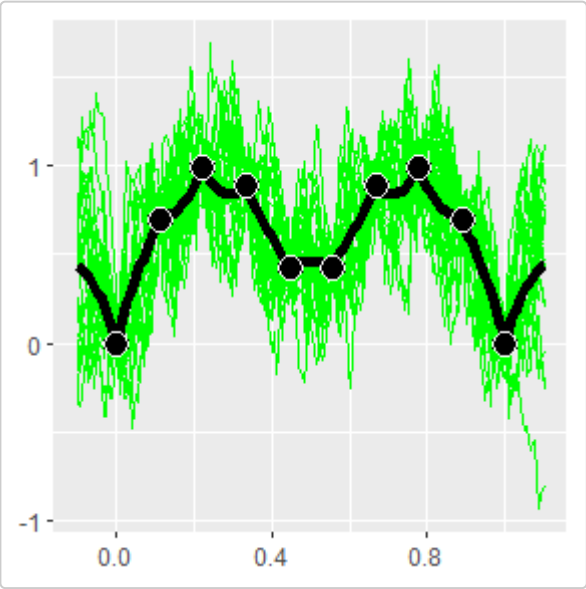
```
## nug is at minimum value after optimizing. Check the fit to see it this caused a bad fit.
Consider changing nug.min. This is probably fine for noiseless data.
```

```
if (requireNamespace("MASS", quietly = TRUE)) {
  plot(gpk)
}
```



The exponential kernel is shown below. You can see that it has a huge effect on the model fit. The exponential kernel assumes the correlation between points dies off very quickly, so there is much more uncertainty and variation in the predictions and sample paths.

```
kern.exp <- Exponential$new(0)
gpk.exp <- GauPro_kernel_model$new(matrix(x, ncol=1), y, kernel=kern.exp, parallel=FALSE)
if (requireNamespace("MASS", quietly = TRUE)) {
  plot(gpk.exp)
}
```



Trends

Along with the kernel the trend can also be set. The trend determines what the mean of a point is without any information from the other points. I call it a trend instead of mean because I refer to the posterior mean as the mean, whereas the trend is the mean of the normal distribution. Currently the three options are to have a mean 0, a constant mean (default and recommended), or a linear model.

With the exponential kernel above we see some regression to the mean. Between points the prediction reverts towards the mean of 0.2986629. Also far away from any data the prediction will near this value.

Below when we use a mean of 0 we do not see this same reversion.

```
kern.exp <- Exponential$new(0)
trend.0 <- trend_0$new()
gpk.exp <- GauPro_kernel_model$new(matrix(x, ncol=1), y, kernel=kern.exp, trend=trend.0,
          parallel=FALSE)
if (requireNamespace("MASS", quietly = TRUE)) {
  plot(gpk.exp)
}
```