A tutorial introduction to the design and analysis of computer experiments

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Computer models

Computer experiments

- Due to the expense of running complex codes, it is necessary to carefully *design experiments* for computer models, somewhat analogous to physical designed experiments
- Just as we perform real experiments to reduce our uncertainty about the behaviour of physical systems, we can perform experiments on computer models to reduce our uncertainty about their (pre-determined, but unknown) behaviour
- Computer models often have various *input parameters*, which we denote by $\mathbf{x}$, which alter the behaviour of the computer model
- Models will often generate lots of output. For this session, we will consider a *single output* of primary interest, y, which is a *deterministic* function of the inputs (even if there is some *stochasticity* internal to the computer model)

Emulating a computer model

- An **emulator** is a *cheap* (fast) surrogate for the computer model, which has many potential uses
- Principally, it can be used instead of the real model in algorithms that require many evaluations of the simulator at many different input configurations
- Some emulators are good and some are bad — to be useful, they should have a measure of *uncertainty* associated with them
- *Stochastic process* emulators define a probability distribution on the space of functions consistent with any known evaluations of the *simulator* (expensive computer model)
- *Gaussian processes* (GPs) are one of the simplest and most tractable stochastic processes on function space

Gaussian processes (GPs)

Gaussian processes

- A GP is a probability distribution on functions defined so that the marginal distribution of any finite number of points always has a multivariate normal (MVN) distribution
- Points close together in input space are typically more highly correlated than points far away
- Stationary GPs are defined by a *covariance function* - many different possible choices - here I've used a Gaussian kernel

$$\mathrm{Cov}[f(\mathbf{x}), f(\mathbf{x}')] = K(\mathbf{x}, \mathbf{x}') = \sigma^2 \exp\left\{ -\left(\frac{\|\mathbf{x} - \mathbf{x}'\|_2}{r} \right)^2 \right\},$$

containing two parameters: an asymptotic variance, σ^2, and a correlation length scale, r.

- A GP *conditioned* on observations is also a GP (*Kriging*)

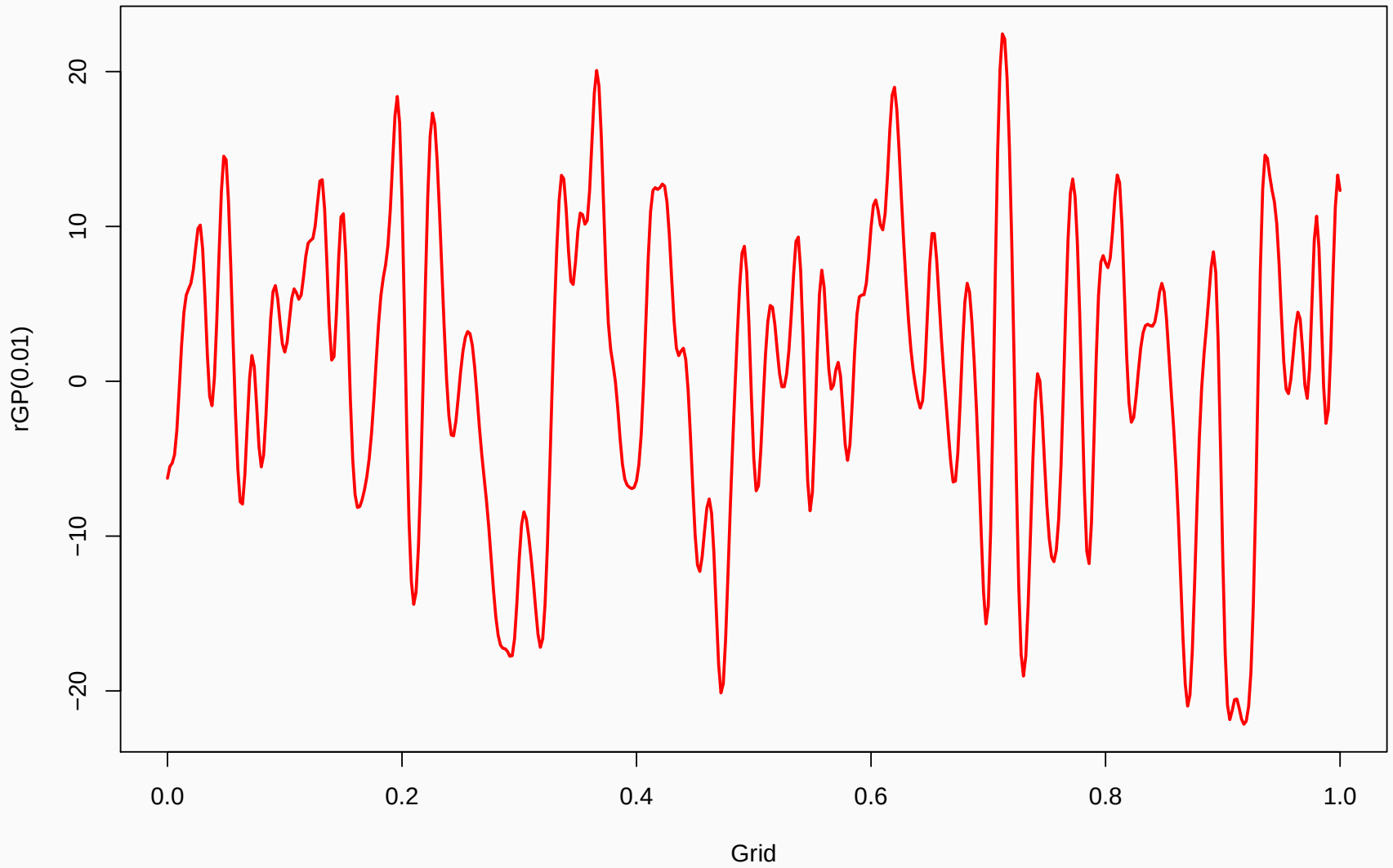
1d GP

- 1d GPs are simplest to visualise and understand

```
Grid = seq(0,1,0.002)
Dist = as.matrix(dist(Grid))
K = function(d, lengthScale=0.4, scale=10)
  (scale^2)*exp(-(d/lengthScale)^2)
rGP = function(r=0.4, s=10) {
  Var = K(Dist,r,s) + (1e-5)*diag(length(Grid))
  t(chol(Var)) %*% rnorm(length(Grid))
  }
set.seed(1)
```

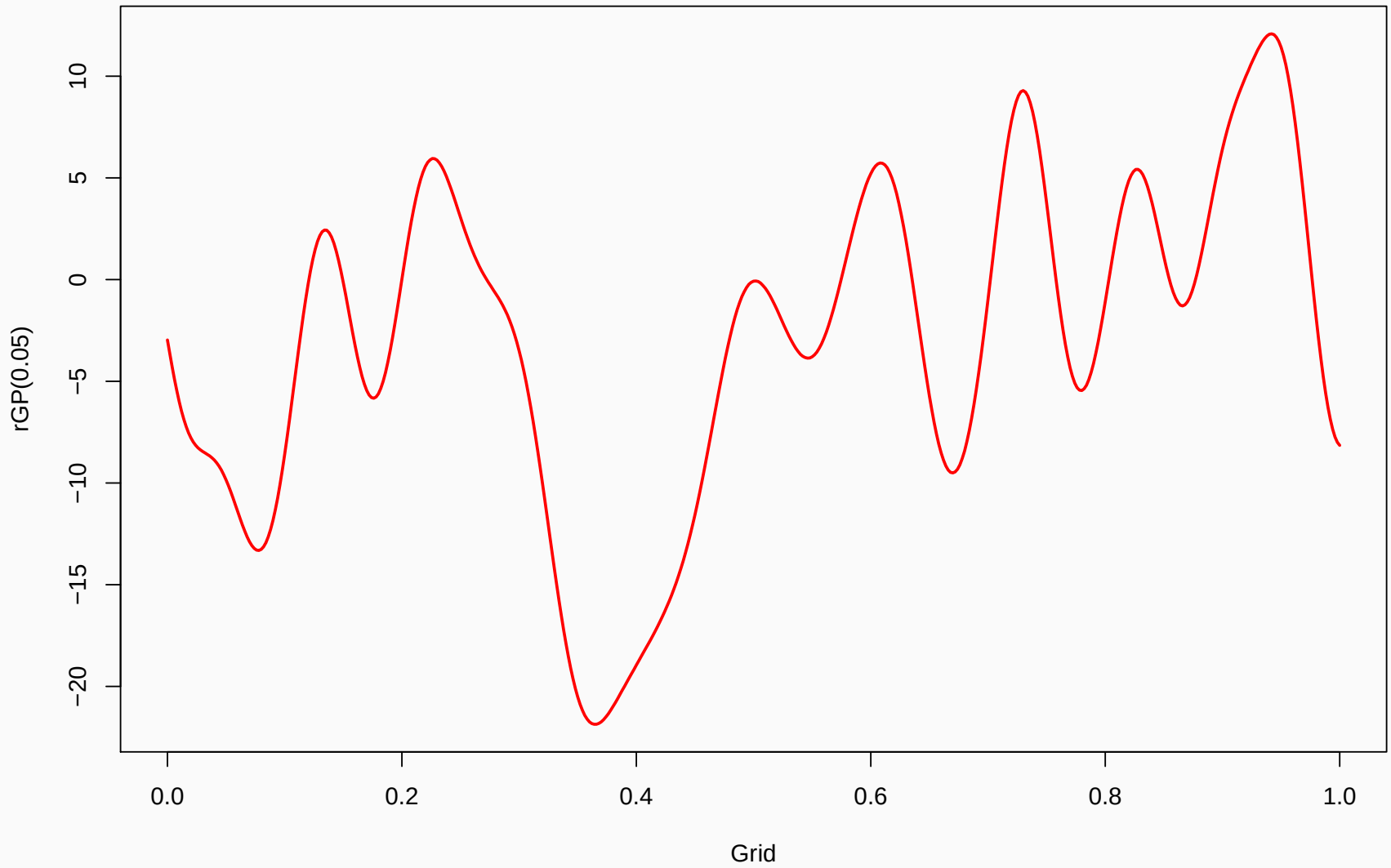
$r = 0.01$

```
plot(Grid,rGP(0.01),type="l",lwd=2,col="red")
```



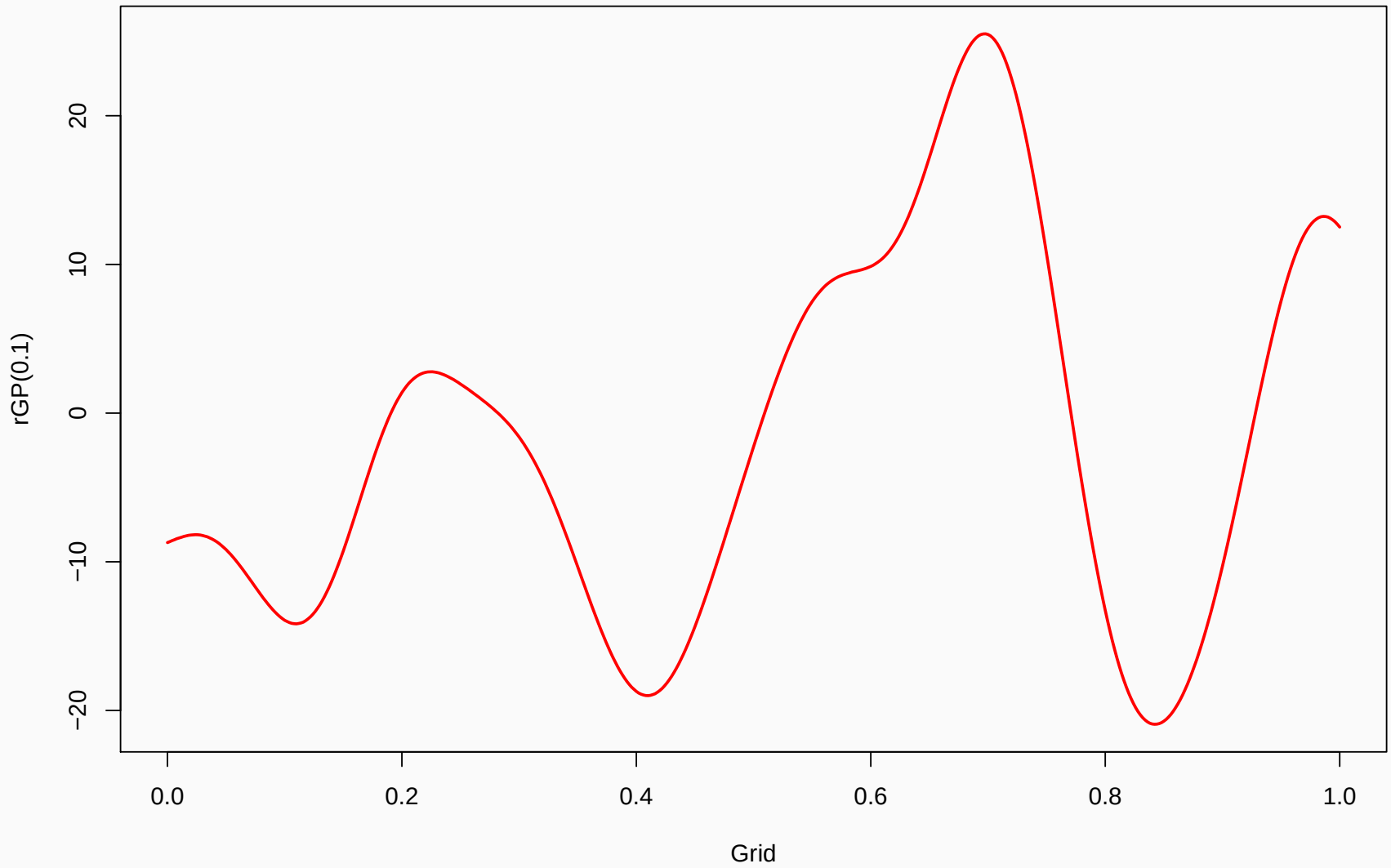
$r = 0.05$

```
plot(Grid,rGP(0.05),type="l",lwd=2,col="red")
```



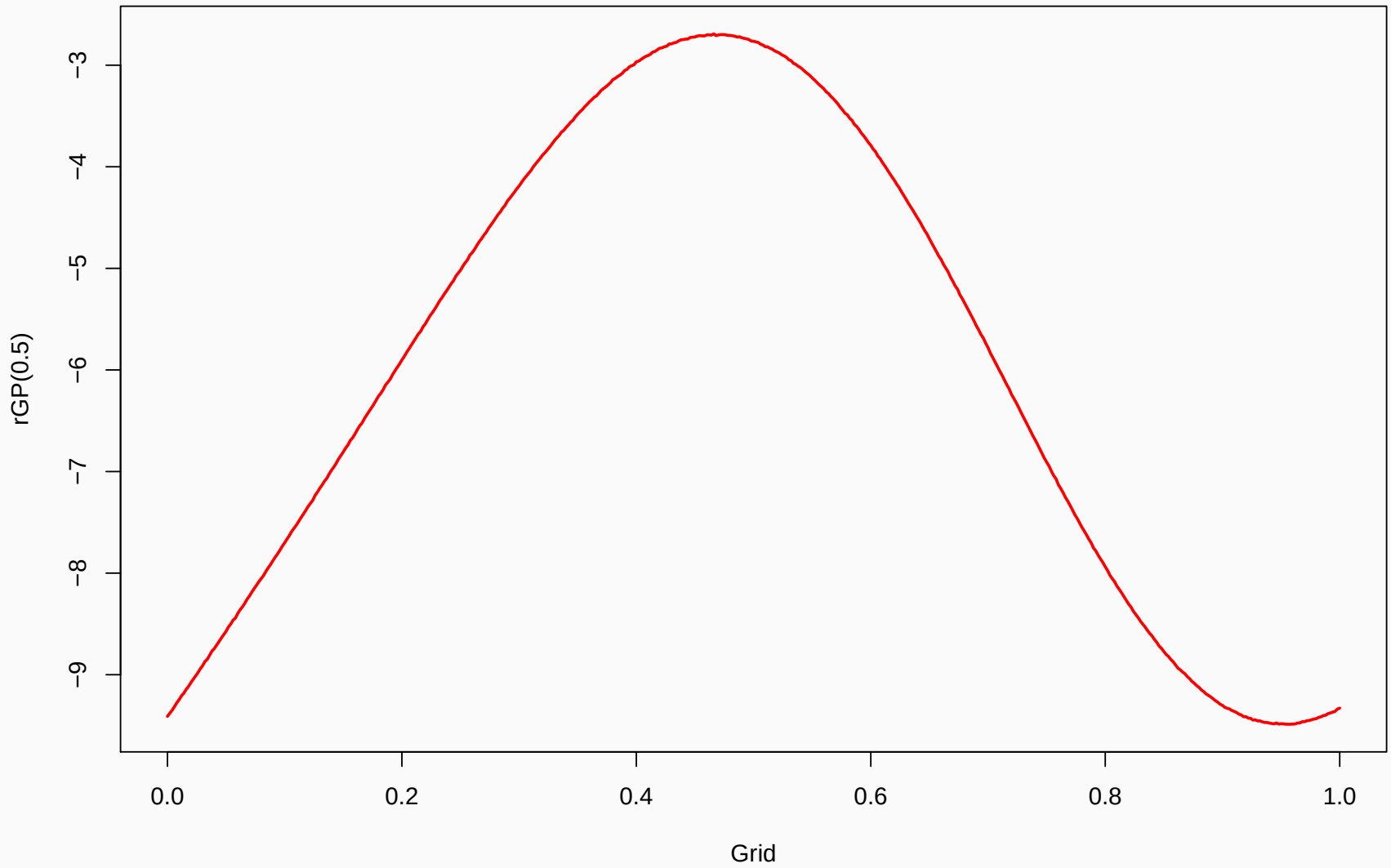
$r = 0.1$

```
plot(Grid,rGP(0.1),type="l",lwd=2,col="red")
```



$r = 0.5$

```
plot(Grid,rGP(0.5),type="l",lwd=2,col="red")
```



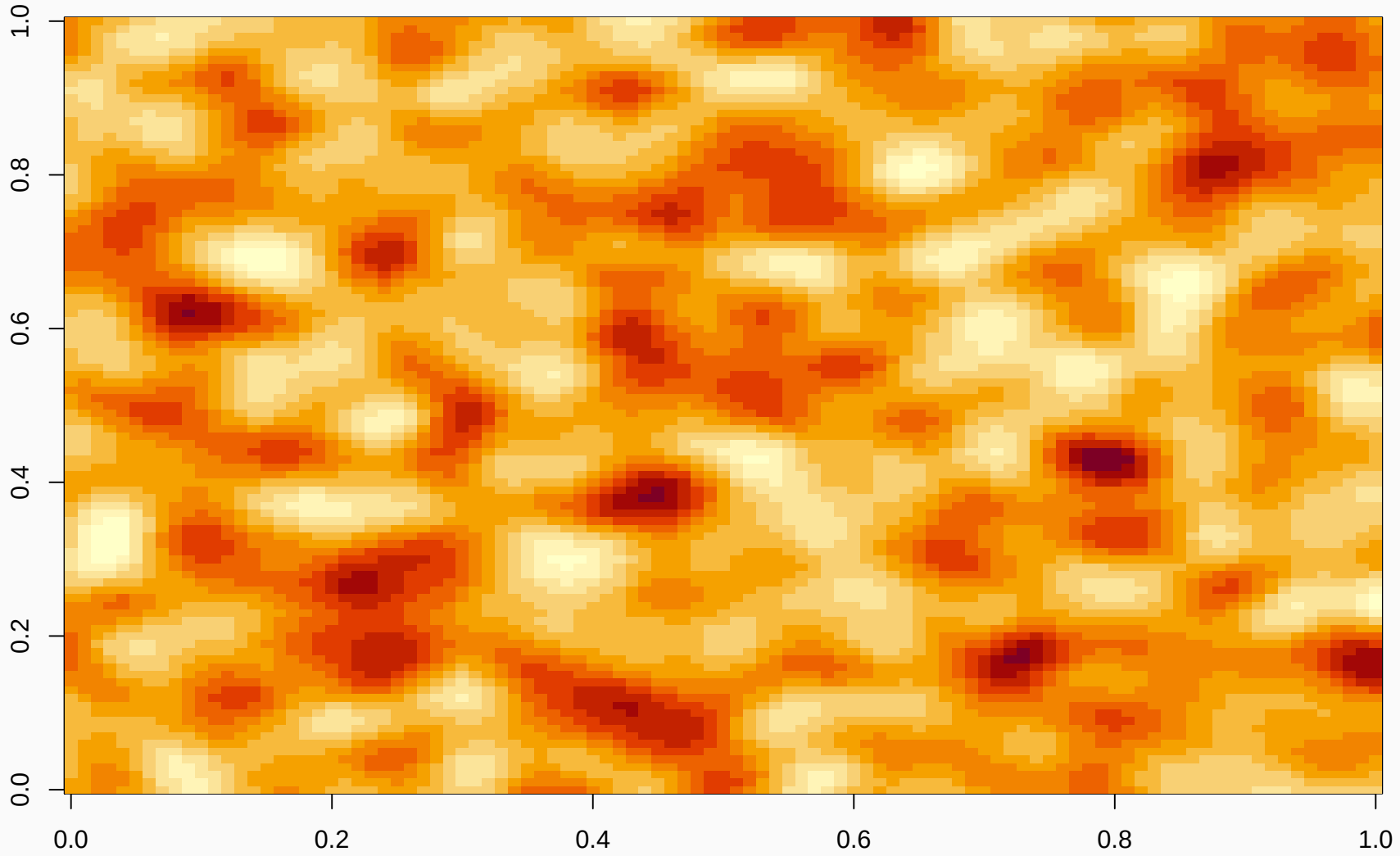
2d GP

- 2d (and 3d) GPs can be useful for modelling smooth spatial heterogeneity

```
Grid = seq(0,1,0.01)
xGrid = expand.grid(Grid,Grid)
Dist = as.matrix(dist(xGrid))
rGP2d = function(r=0.1, s=10) {
  Var = K(Dist,r,s) + (1e-5)*diag(length(Grid)^2)
  z = t(chol(Var)) %*% rnorm(length(Grid)^2)
  matrix(z,nrow=length(Grid))
  }
```

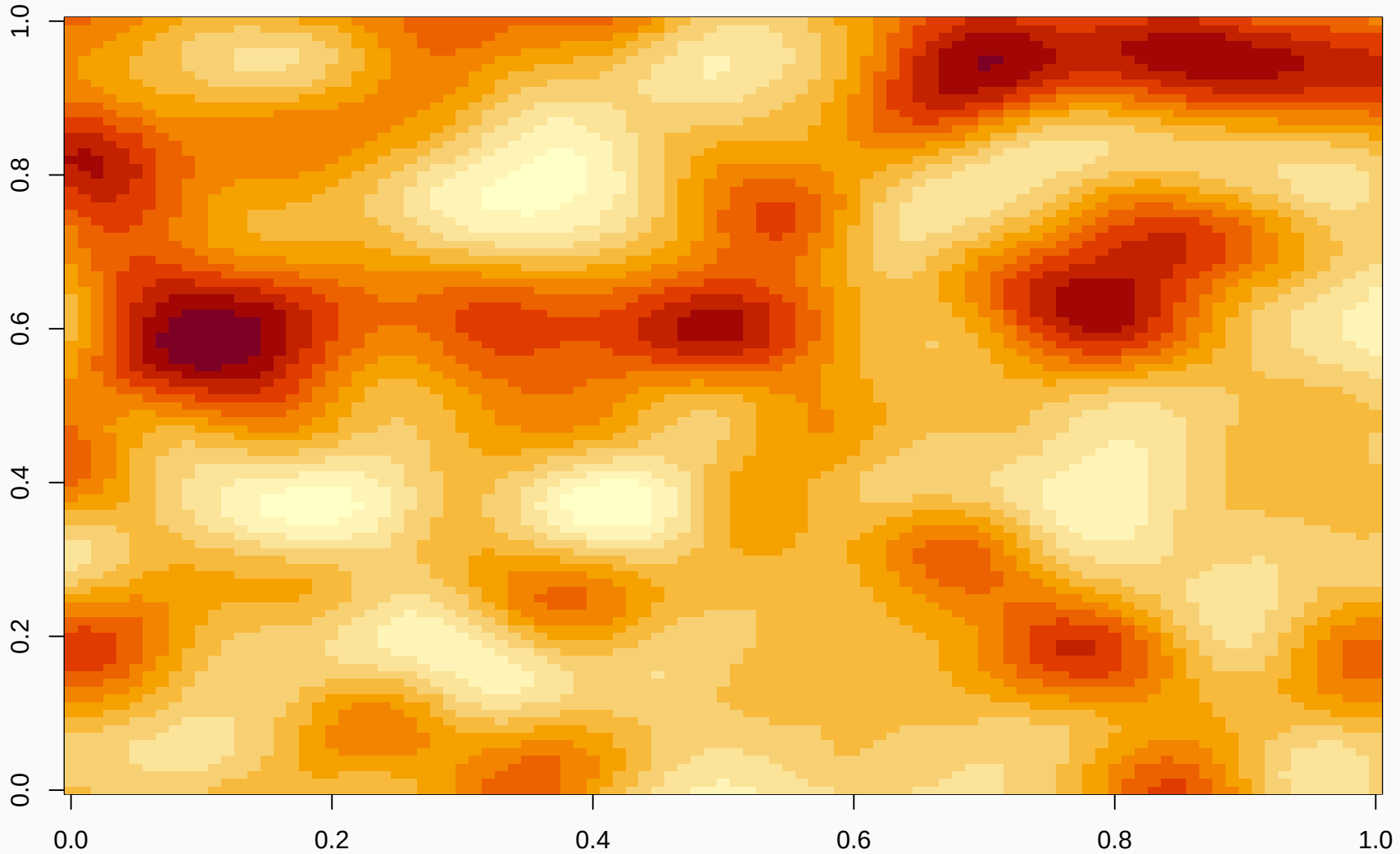
$r = 0.05$

```
image(rGP2d(0.05))
```



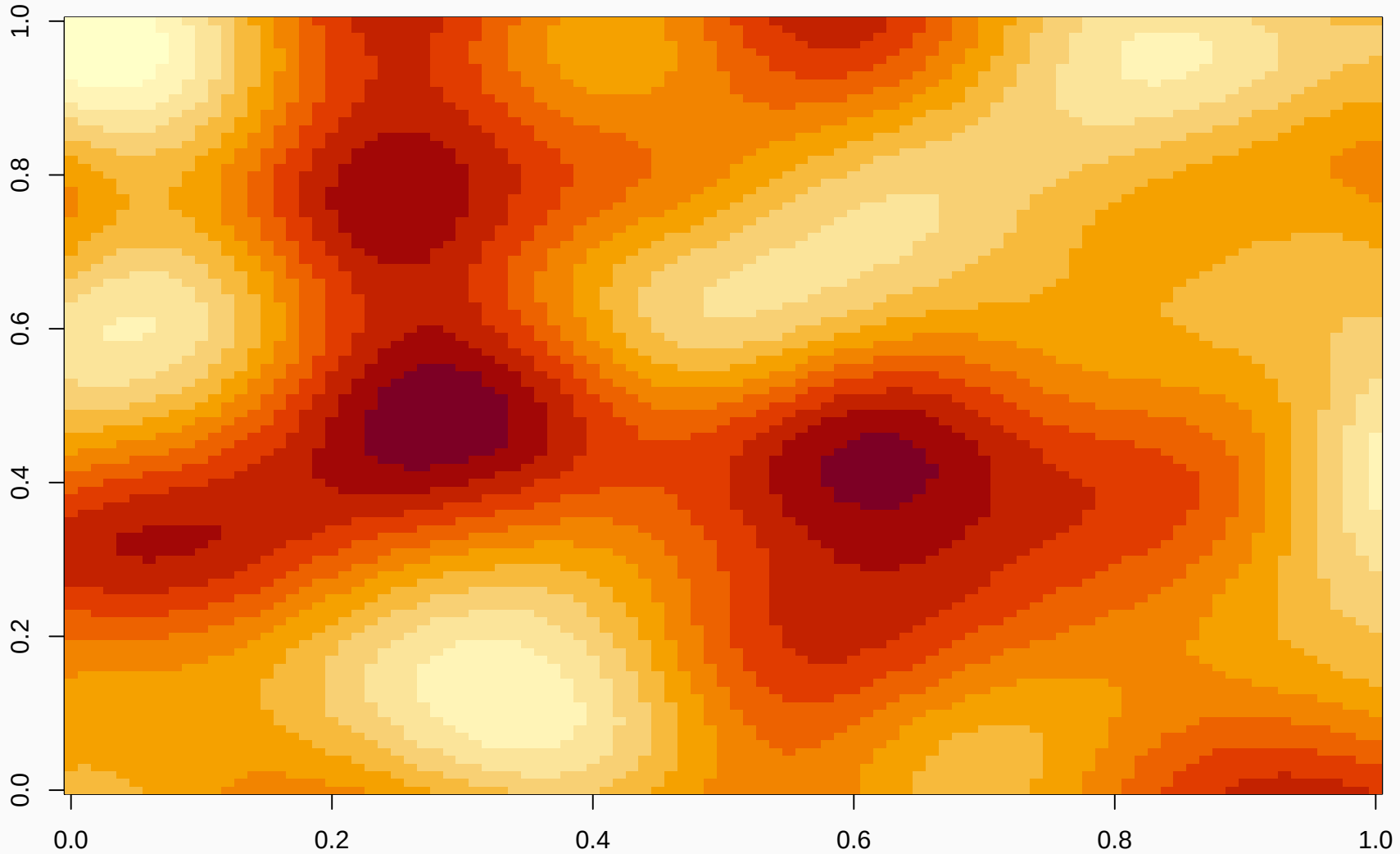
$r = 0.1$

```
image(rGP2d(0.1))
```



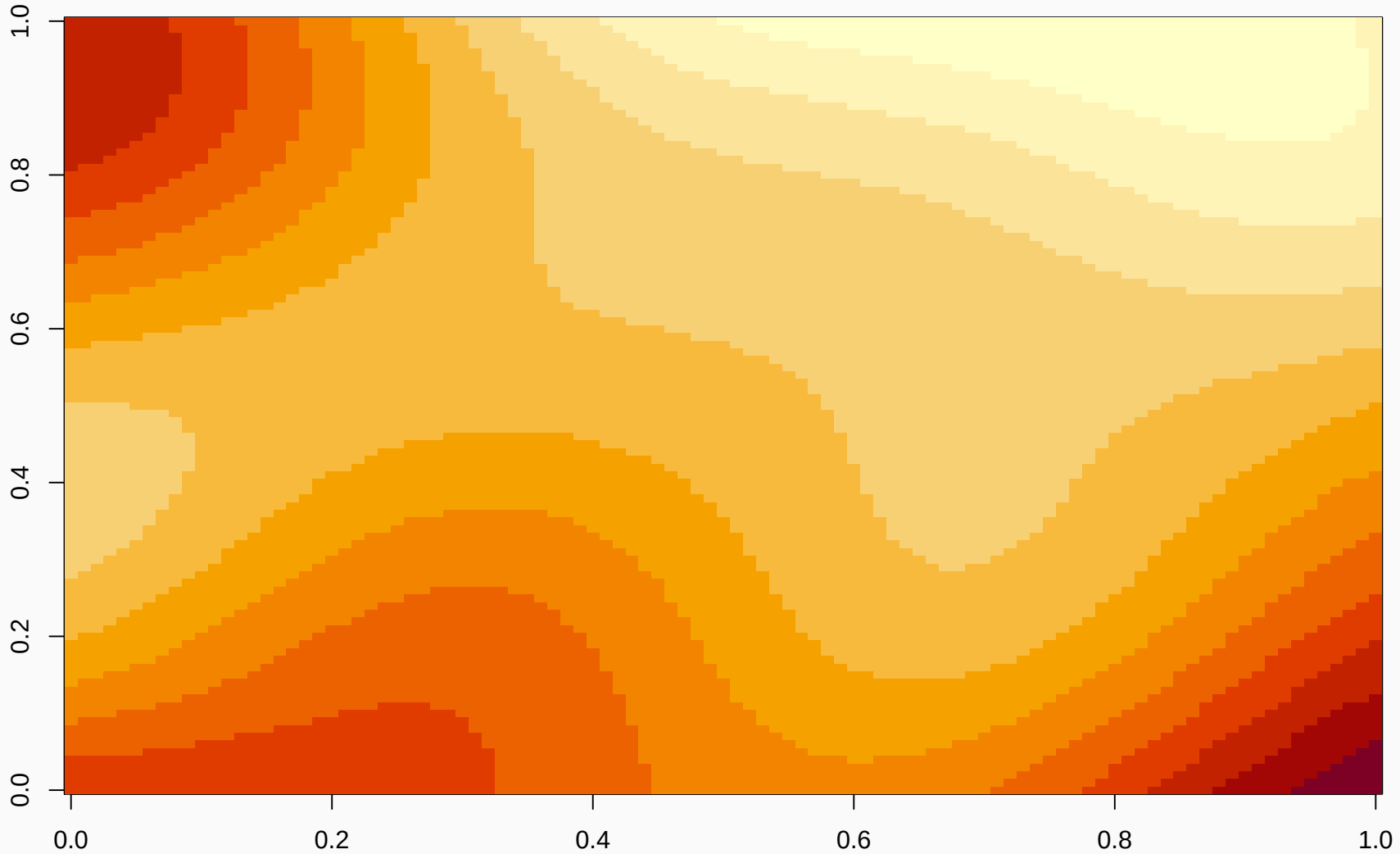
$r = 0.2$

```
image(rGP2d(0.2))
```



$r = 0.5$

```
image(rGP2d(0.5))
```



Gaussian process emulation

GP emulation of a computer code

- A GP defines a (tractable) probability distribution over (univariate) functions
- We can *condition* the GP on some observations and the conditional process is also a GP, but with a new mean and covariance function that is a function of the observations
- This new GP can represent our uncertainty about a function given some observations
- This uncertain representation of our knowledge of the function can be used to *emulate* an expensive function, such as a complex computer code
- The uncertainty associated with the GP can be used to properly quantify and propagate uncertainty associated with the fact that we don't actually know the expensive model everywhere

DiceKriging

- `DiceKriging` is a popular R package with a range of functionality

```
library(DiceKriging)
set.seed(1)
nd = 20
x = as.matrix(runif(nd,0,5))
colnames(x)=c("x")
y = sin(x)+rnorm(nd,0,0.1)
```

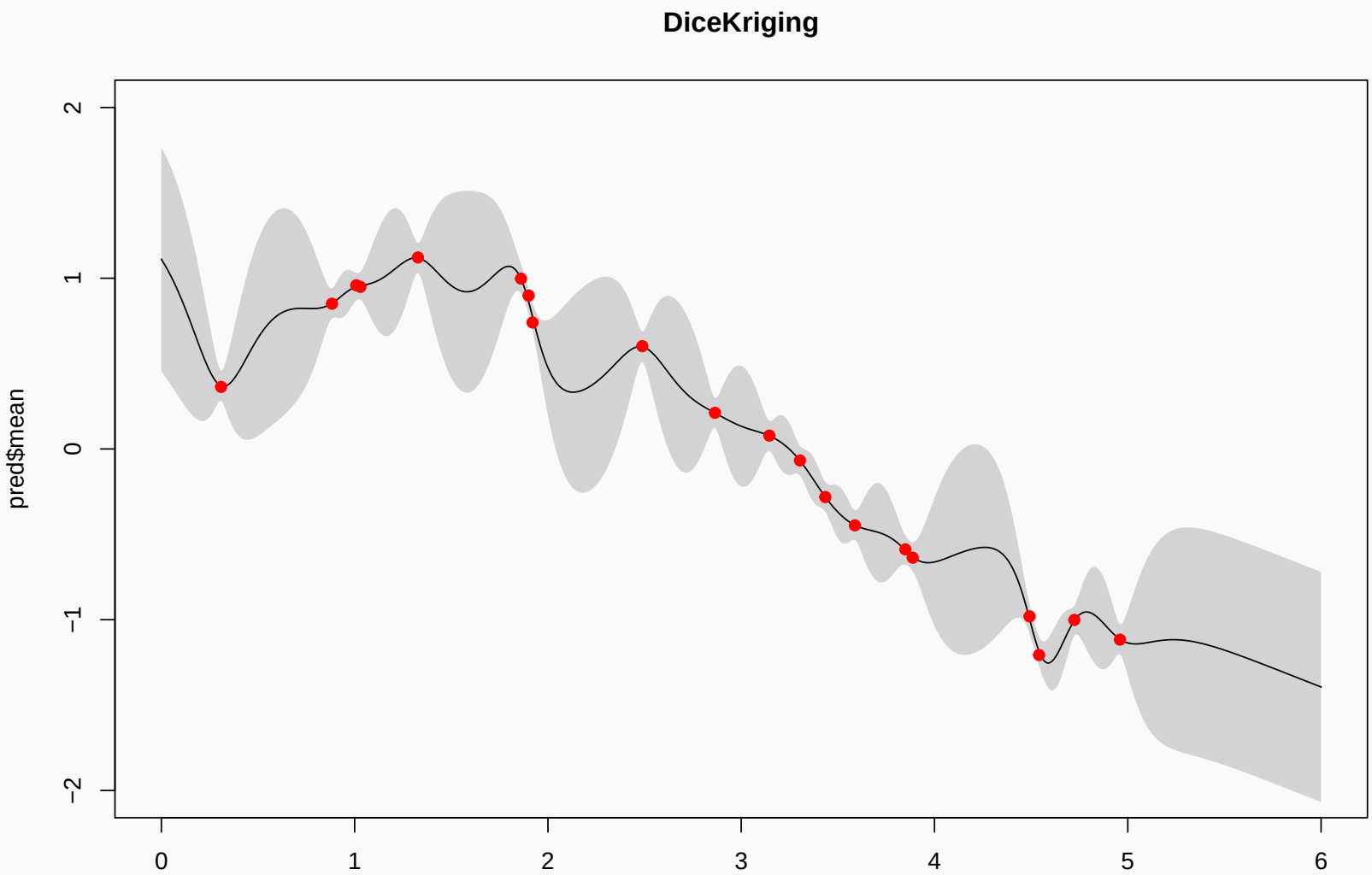
```
mod = km(~x,design=x,response=y,nugget=0.001)
```

```
##
## optimisation start
## ------------------
## * estimation method   : MLE
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~x
## * covariance model :
##   - type :  matern5_2
##   - nugget : 0.001
##   - parameters lower bounds :  1e-10
##   - parameters upper bounds :  9.301198
##   - variance bounds :  0.0101135 1.467872
##   - best initial criterion value(s) :  -10.60975
##
```

```r
px = seq(0,6,0.01)
pred = predict(mod,px,type="SK")
```

```
## Warning in checkNames(X1 = X, X2 = newdata, X1.name = "t
## = "newdata"): newdata not named: newdata's variables are
## design
```

```
plot(px,pred$mean,type="l",ylim=c(-2,2),main="DiceKriging")
polygon(c(px,rev(px)),c(pred$upper,rev(pred$lower)),col="li
lines(px,pred$mean,type="l")
points(x,y,pch=19,col=2)
```



mlegp

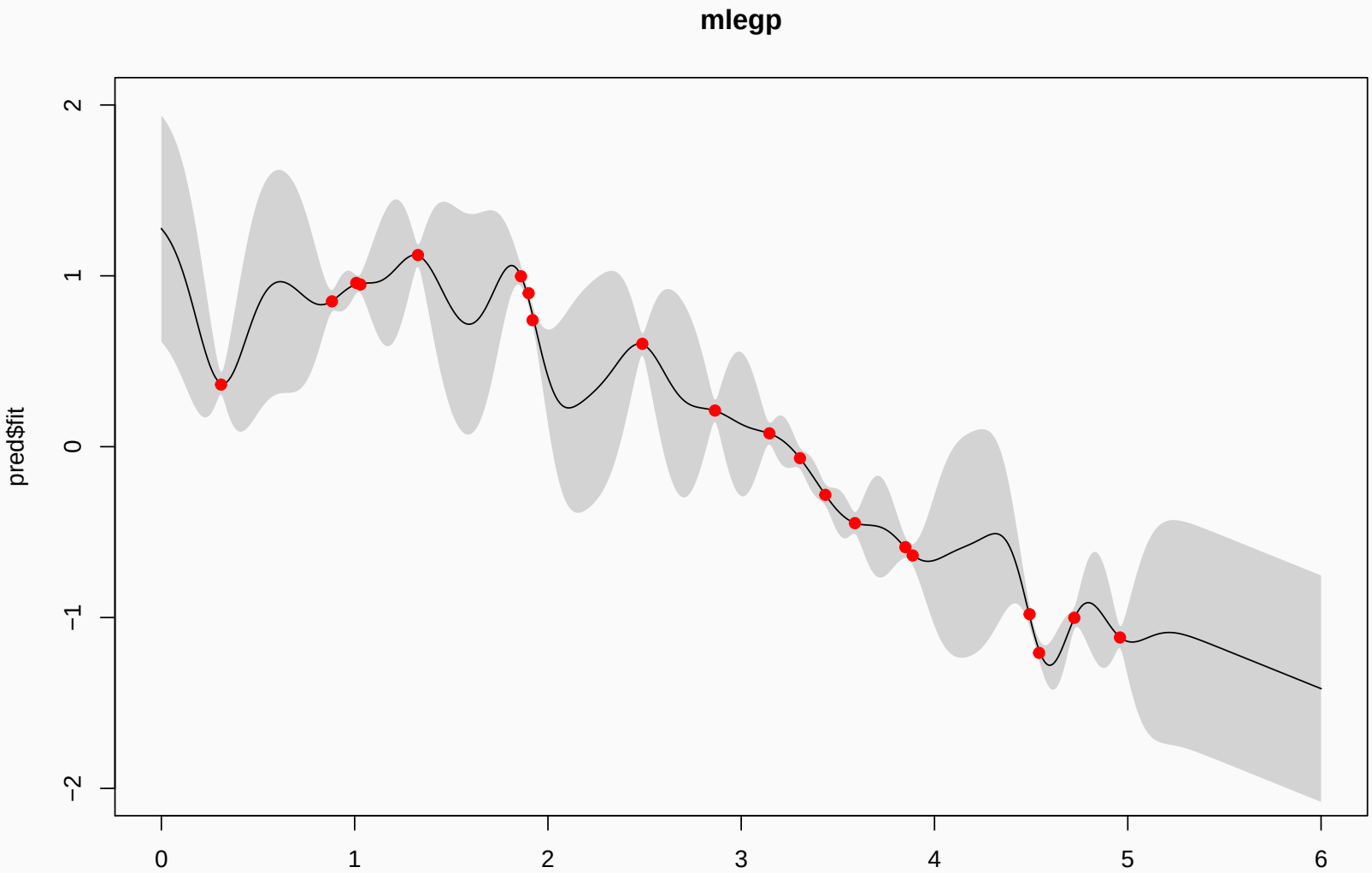
- mlegp is an alternative package, based on the book by Santner et al.

```
library(mlegp)
mod = mlegp(x,y,constantMean=0,nugget.known=1,nugget=0.001)

## no reps detected in meanPerReps, returning originals...
##
## ========== FITTING GP # 1 ============================
## running simplex # 1...
## ...done
## ...simplex #1 complete, loglike = 0.895601 (convergence)
## running simplex # 2...
## ...done
## ...simplex #2 complete, loglike = 0.895601 (convergence)
```

```
pred = predict(mod,as.matrix(px),se.fit=TRUE)
pred$upper = pred$fit + 2*pred$se.fit
pred$lower = pred$fit - 2*pred$se.fit
```

```r
plot(px,pred$fit,type="l",ylim=c(-2,2),main="mlegp")
polygon(c(px,rev(px)),c(pred$upper,rev(pred$lower)),col="li
lines(px,pred$fit,type="l")
points(x,y,pch=19,col=2)
```



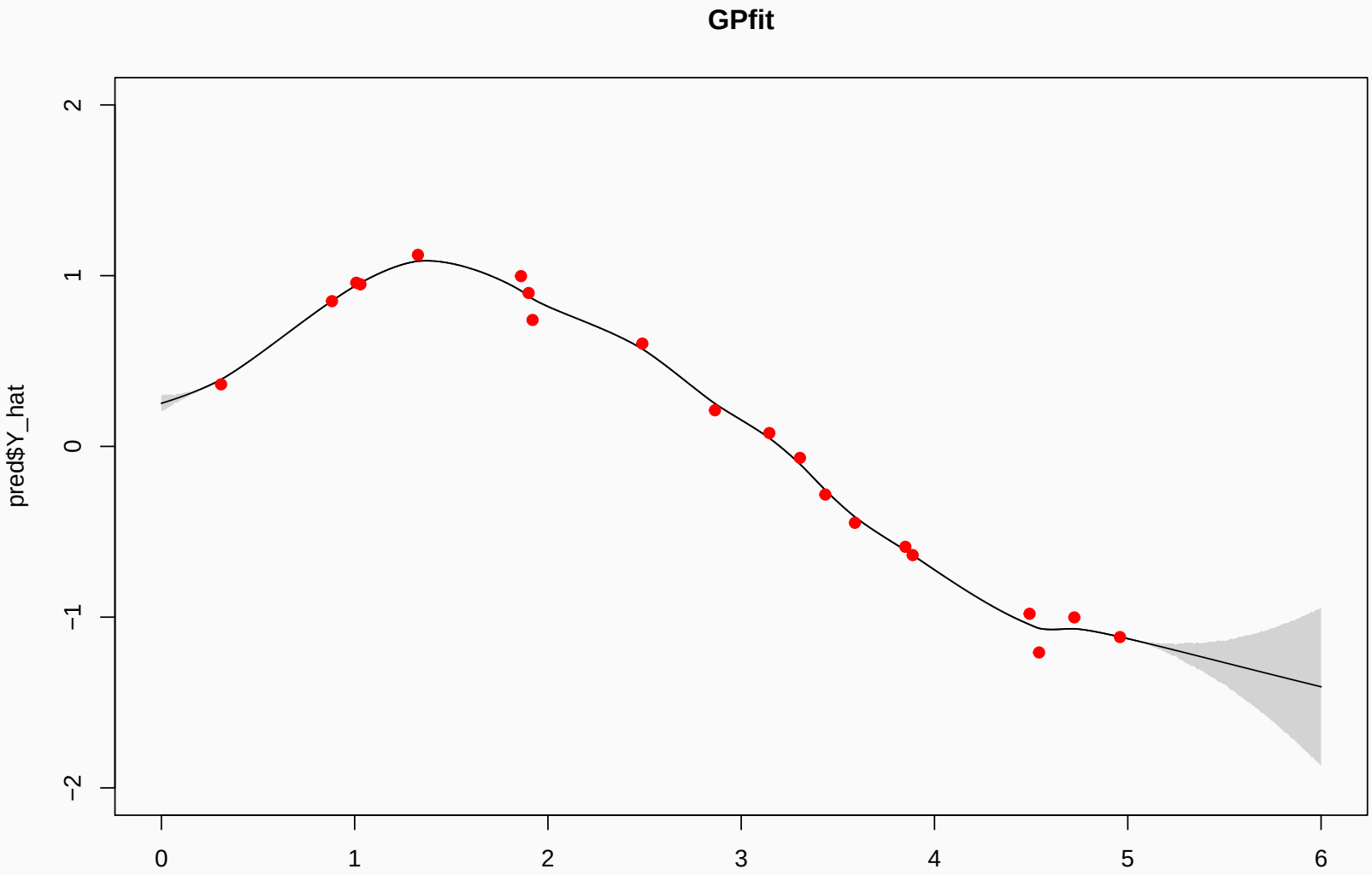
GPfit

- `GPfit` is another R package, which has more sophisticated parameter estimation procedures than some other packages

```
library(GPfit)
xScaled = x/5
mod = GP_fit(xScaled,y)
```

```r
pxScaled = px/5
pred = predict(mod,as.matrix(pxScaled))
pred$upper = pred$Y_hat + 2*pred$MSE
pred$lower = pred$Y_hat - 2*pred$MSE
```

```r
plot(px,pred$Y_hat,type="l",ylim=c(-2,2),main="GPfit")
polygon(c(px,rev(px)),c(pred$upper,rev(pred$lower)),col="li
lines(px,pred$Y_hat,type="l")
points(x,y,pch=19,col=2)
```

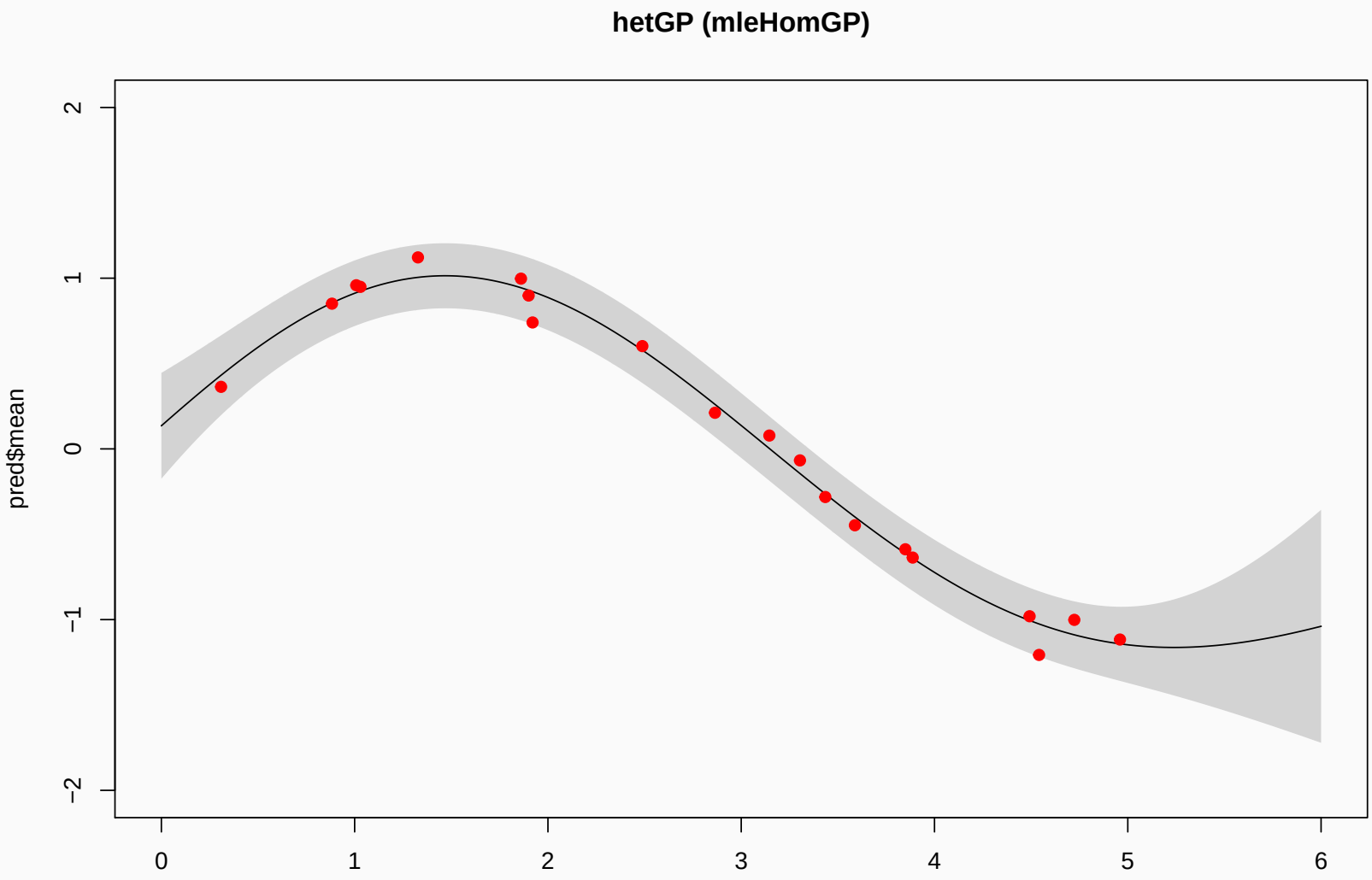


hetGP

- `hetGP` is a modern, sophisticated package for GP emulation, including good support for large datasets, stochastic kriging for noisy models with replication, and heteroskedastic GP modelling

```
library(hetGP)
mod = mleHomGP(x,y) # homoskedastic GP fit
pred = predict(mod,as.matrix(px))
pred$var = pred$sd2 + pred$nugs
pred$sd = sqrt(pred$var)
pred$upper = pred$mean + 2*pred$sd
pred$lower = pred$mean - 2*pred$sd
```

```r
plot(px,pred$mean,type="l",ylim=c(-2,2),main="hetGP (mleHo
polygon(c(px,rev(px)),c(pred$upper,rev(pred$lower)),col="l
lines(px,pred$mean,type="l")
points(x,y,pch=19,col=2)
```

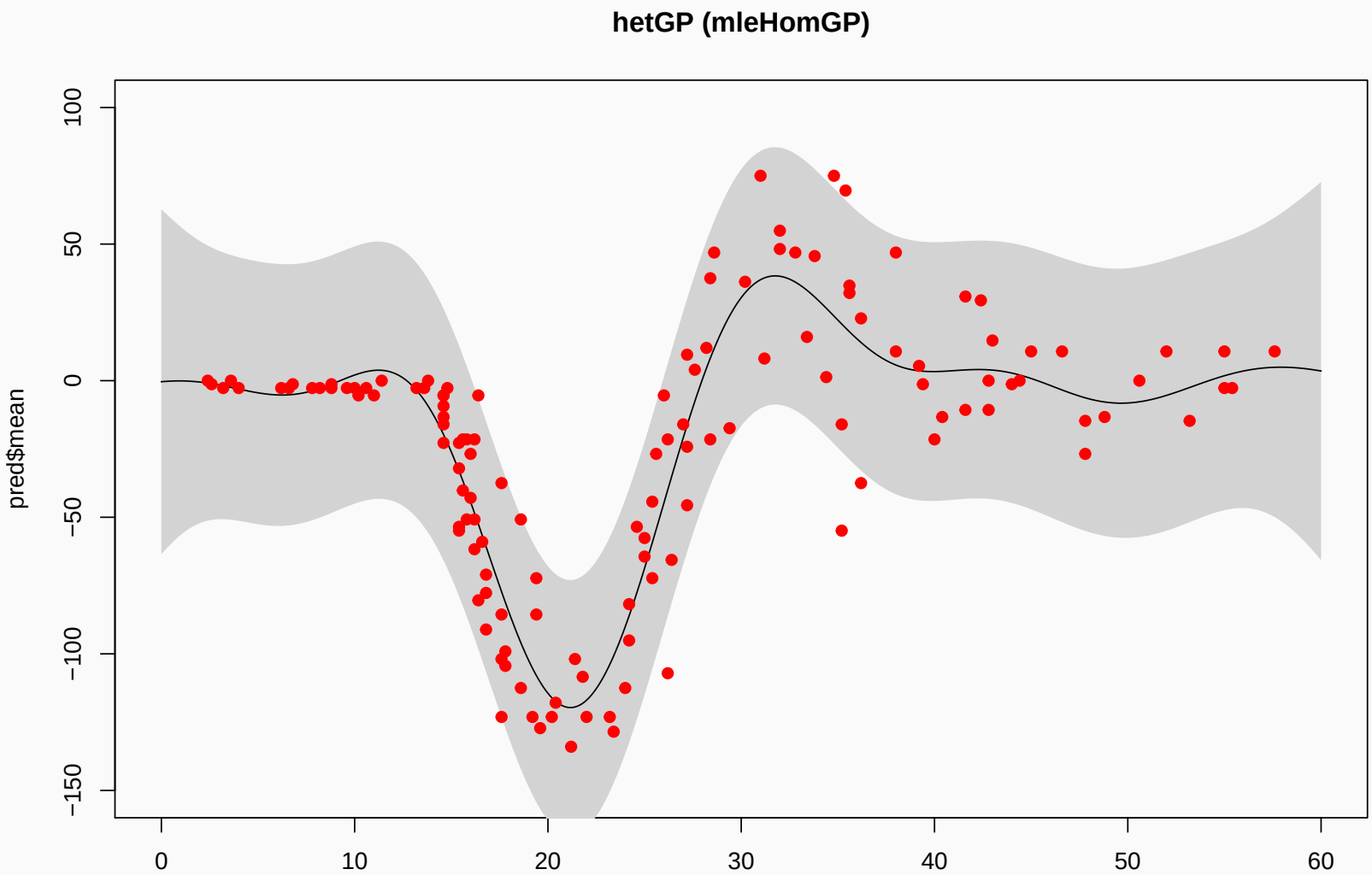


Heteroskedasticity and the Motorcycle data

- The `mcycle` dataset from the `MASS` package is output from a computer model exhibiting heteroskedasticity - non-stationary variance
- We will start with a homoskedastic fit

```
library(MASS)
mod = mleHomGP(mcycle$time,mcycle$accel) # homoskedastic
px=seq(0,60,0.1)
pred = predict(mod,as.matrix(px))
pred$var = pred$sd2 + pred$nugs
pred$sd = sqrt(pred$var)
pred$upper = pred$mean + 2*pred$sd
pred$lower = pred$mean - 2*pred$sd
```

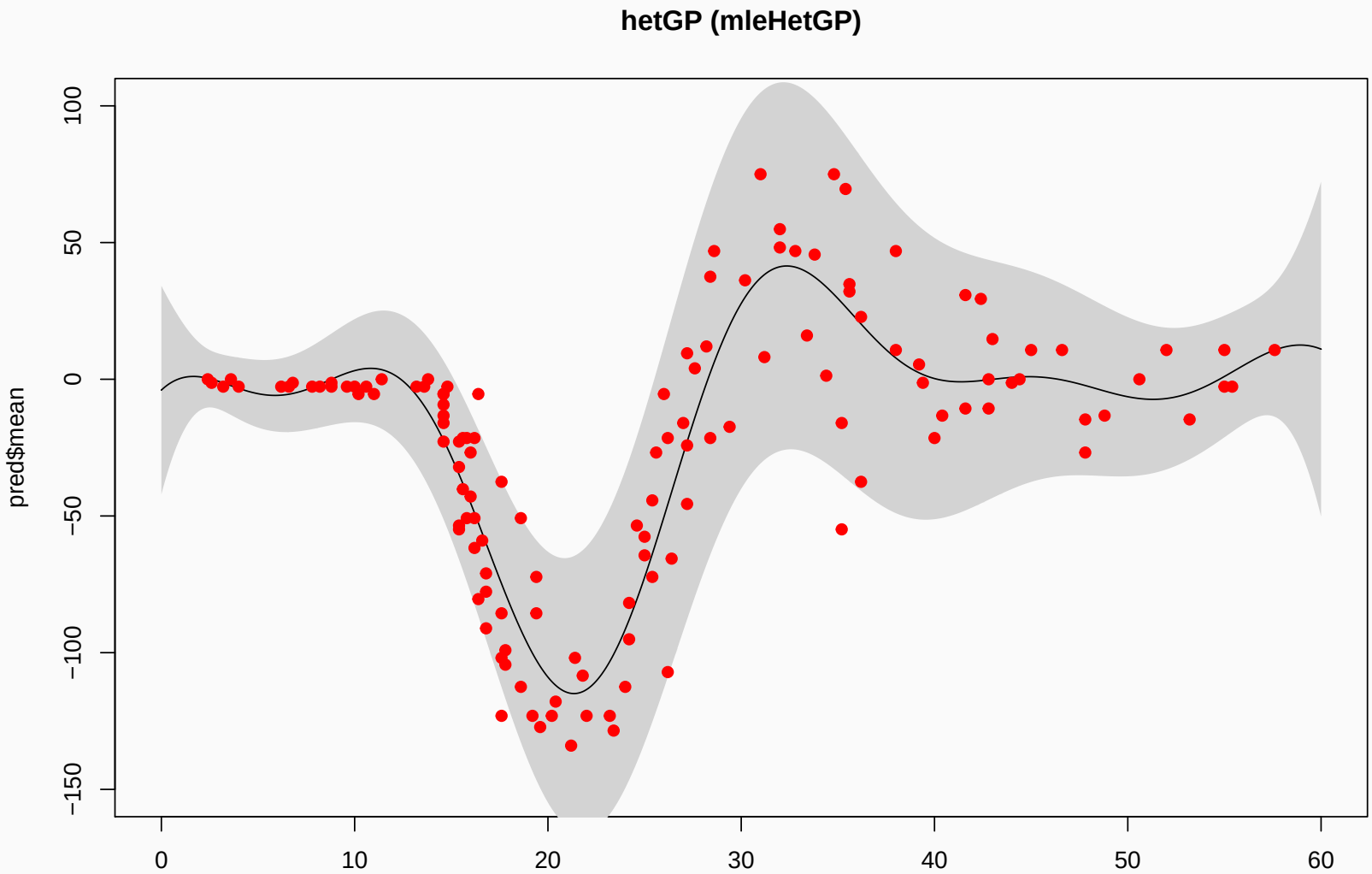
```
plot(px,pred$mean,ylim=c(-150,100),type="l",main="hetGP (ml
polygon(c(px,rev(px)),c(pred$upper,rev(pred$lower)),col="li
lines(px,pred$mean,type="l")
points(mcycle,pch=19,col=2)
```



- Next we will do a heteroskedastic fit

```
mod = mleHetGP(mcycle$time,mcycle$accel) # heteroskedastic
pred = predict(mod,as.matrix(px))
pred$var = pred$sd2 + pred$nugs
pred$sd = sqrt(pred$var)
pred$upper = pred$mean + 2*pred$sd
pred$lower = pred$mean - 2*pred$sd
```

```
plot(px,pred$mean,ylim=c(-150,100),type="l",main="hetGP (ml
polygon(c(px,rev(px)),c(pred$upper,rev(pred$lower)),col="li
lines(px,pred$mean,type="l")
points(mcycle,pch=19,col=2)
```



Bayesian versus frequentist parameter fitting

- Although the essential essence of GP emulation is fundamentally Bayesian (conditioning a joint probability distribution on observations), the estimation of parameters such as scale and length scale can be done in various ways
- All of the R packages described above used frequentist fitting procedures of some sort, typically based around the method of *maximum likelihood*
- The emulator produced is then *conditional* on a single point estimate of those parameters, which means that the uncertainties associated with them typically (significantly) underestimate the true uncertainty associated with the unknown function

Bayesian fitting, UQ, and uncertainty propagation

- Computationally intensive Bayesian methods can be used which properly account for (quantify) all uncertainties in the problem, and so then samples from the emulation distribution can be used to form Monte Carlo ensembles that can correctly propagate uncertainty through further downstream analyses
- In this context, GP emulators can be usefully embedded into large Bayesian hierarchical models
- It can be challenging to fit such large and complex Bayesian hierarchical models - often custom code is written, tailored to a specific application, but general purpose software such as Stan is adding support for GPs

Design of computer experiments

Latin hypercube sampling

- When working with expensive computer models with input parameters, the choice of which combination of inputs to run is important, and worth doing carefully
- For a single tunable parameter, a uniform grid can be sensible
- For multiple input parameters, a Cartesian product design seems intuitive, but is actually a very poor choice, and gets worse in higher dimensions
- LHS is a technique for choosing points such that the univariate margins essentially form a uniform grid
- The simplest approaches give random designs subject to the constraint of uniform margins
- More sophisticated variants try to optimise some desirable property of the design, such as maximising the minimum distance between points

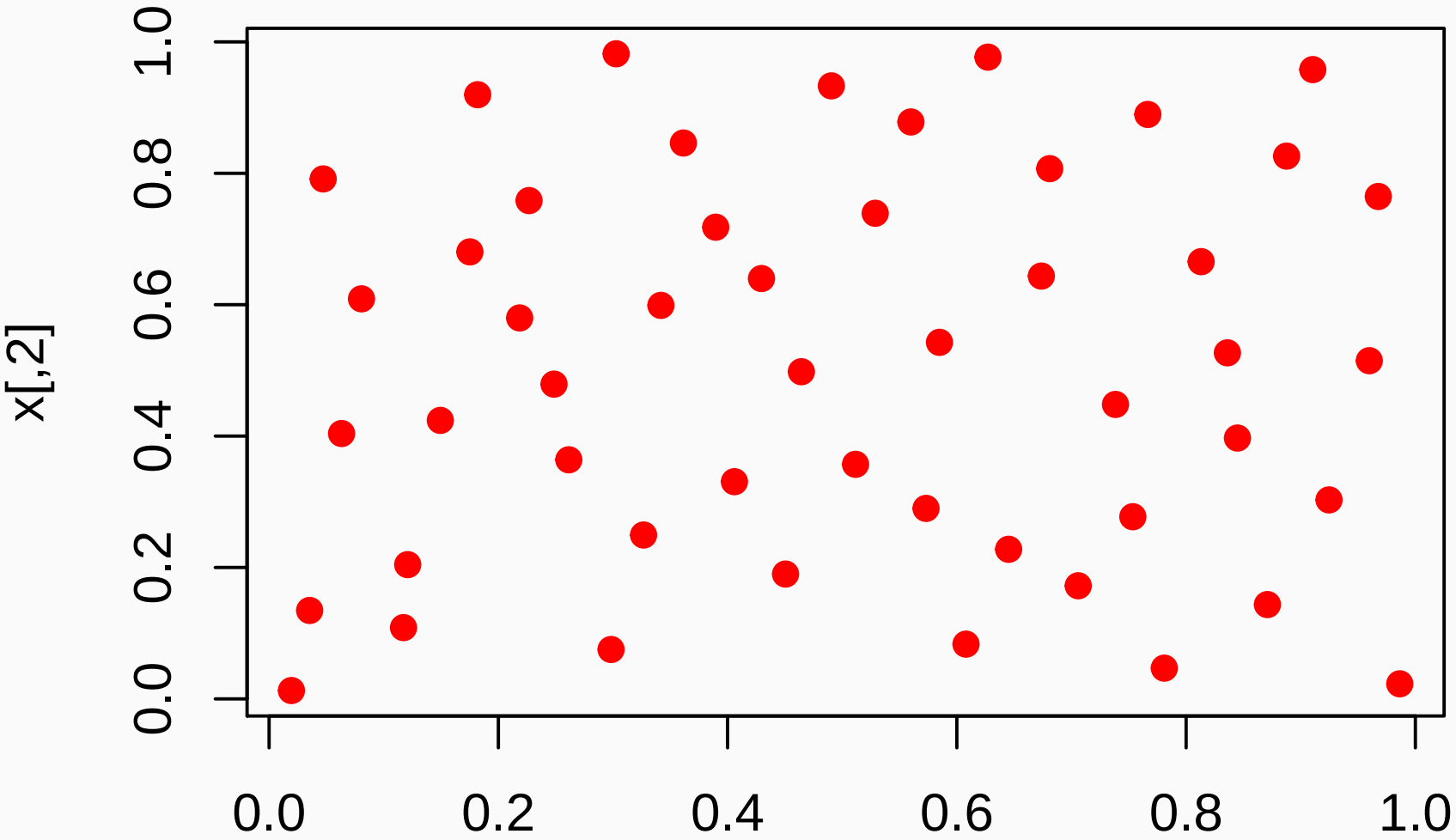
The lhs R package

```
library(lhs)
set.seed(1)

help(package="lhs")
?randomLHS
?maximinLHS
vignette(package="lhs")
vignette("lhs_basics")
```

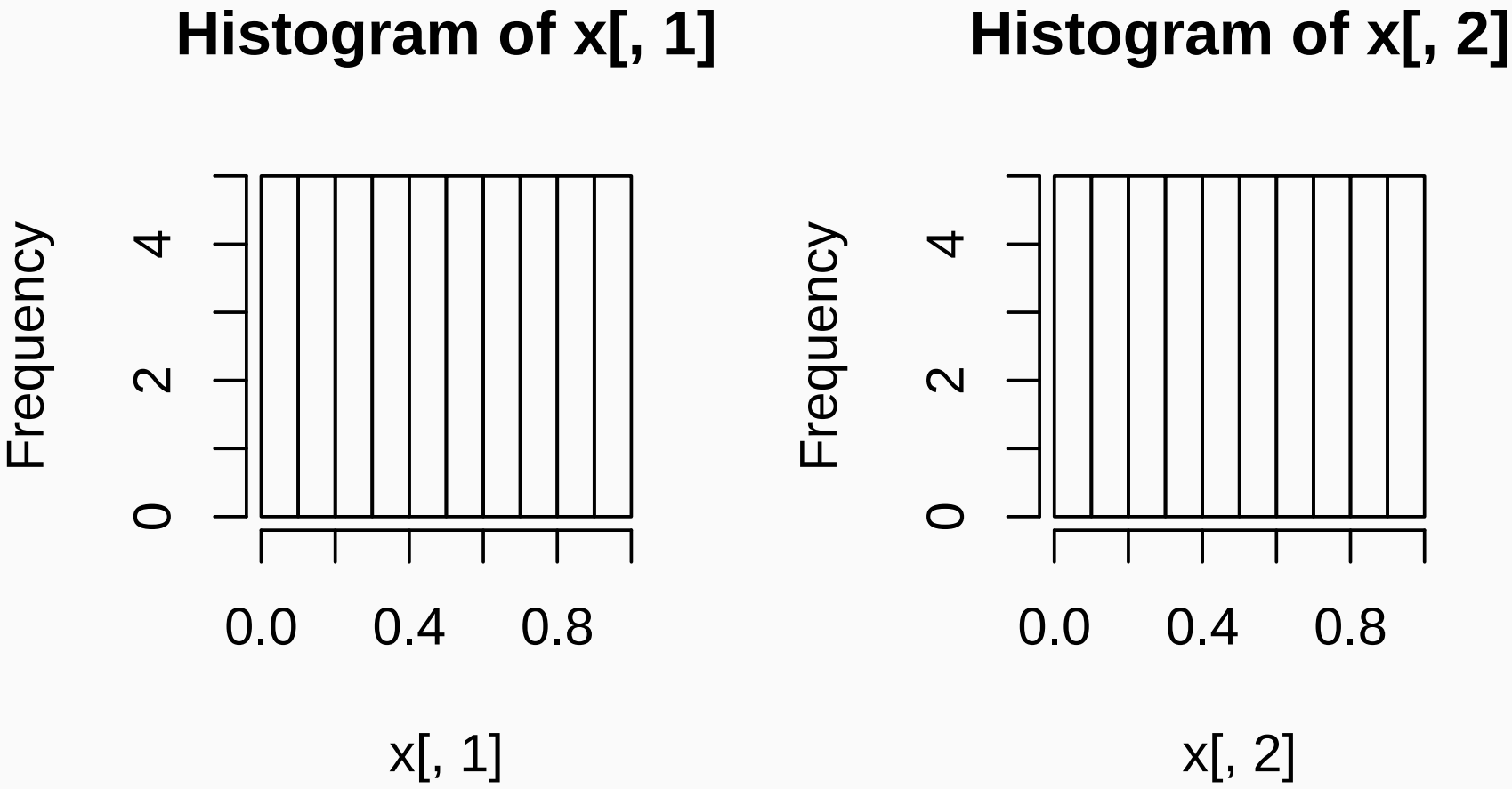
A 2d example

```
x = maximinLHS(50,2)
plot(x, pch=19, col=2)
```



Univariate margins are uniform

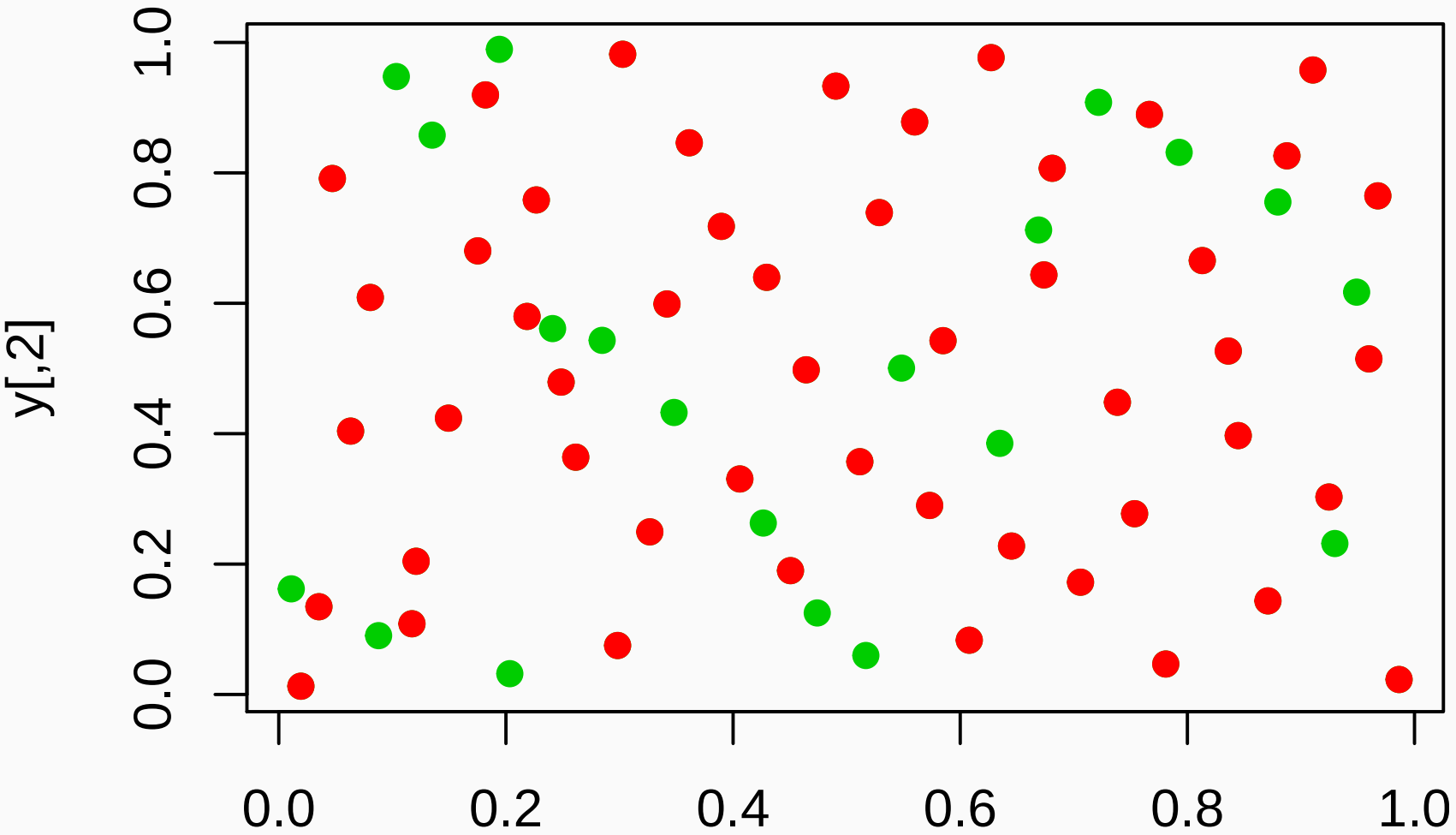
```
op = par(mfrow=c(1,2))
hist(x[,1]); hist(x[,2])
```




```
par(op)
```

Augmenting a design

```
y = augmentLHS(x,20)
plot(y,pch=19,col=3); points(x,pch=19,col=2)
```



Further reading

Software

R

- CRAN Task Views
  - Spatial
  - Spatio-Temporal
- R Packages
  - hetGP (heteroskedastic GPs)
  - DiceKriging
  - GPfit (robust fitting)
  - mlegp (multiple outputs)
  - lhs (latin hypercube sampling)

Python

- GPy

Books and on-line articles

Wikipedia

- Computer experiment
- Gaussian process
- Latin hypercube sampling
- Uncertainty quantification

Books

- The Design and Analysis of Computer Experiments (Santner et al.) - ISBN 1493988476
- Gaussian processes for machine learning (Rasmussen and Williams) - ISBN 026218253X