GP - Rasmussen & Williams - Ch. 2: Regression

Outline

1. Regression
   - Sampling from prior
   - Posterior
   - Python toolboxes
   - Haskell code

GP prior

$$k(x,y) = \exp(-\tfrac{1}{2}|x-y|^2) \tag{1}$$

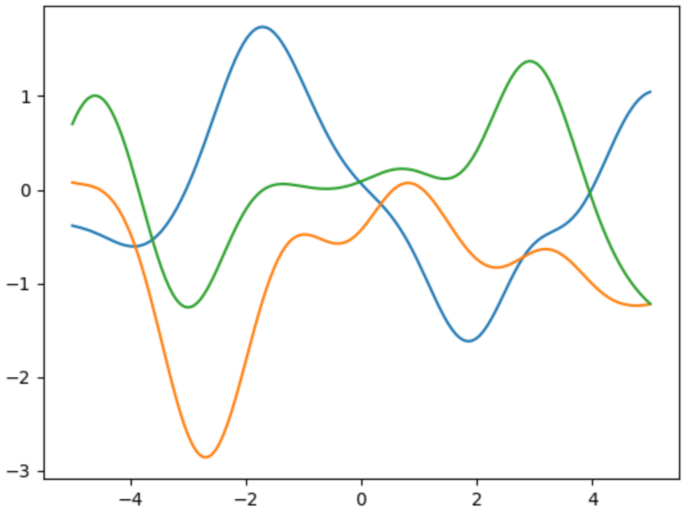
$$\mathbf{f} \sim \mathcal{N}(\mathbf{0}, K(\mathbf{x},\mathbf{x})) \tag{2}$$

Sampling from prior: Python code

```
from numpy import sum, eye, exp #, zeros
from numpy.linalg import cholesky
from numpy.random import normal #, multivariate_normal

def rbf(length_scale):
    def k(x,y):
        if len(x.shape)==1:
            d = 1
        else:
            d  = x.shape[1]
        lx = x.shape[0]
        ly = y.shape[0]
        dists =  sum(((x.T.reshape([d,lx,1]) -  y.T.reshape([d,1,ly]))/length_scale)**2,0)
        return exp(-.5 * dists)
    return k

def genSamplesSimple(x, k):
    n = x.shape[0]
    L = cholesky(k(x,x)+eye(n)*1e-8)
    return L.dot(normal(size=n))
# Same as:
#    return multivariate_normal(zeros(n), k(x,x) + eye(n)*1e-8)
```

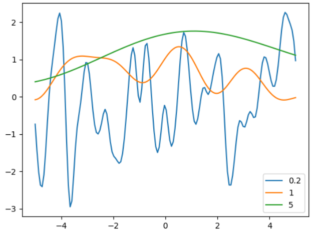
```
from matplotlib.pyplot import figure, plot, savefig, close, legend
from numpy import linspace

figure()
x = linspace(-5,5,150)
k = rbf(1)
for i in range(3): plot(x, genSamplesSimple(x,k));
```

Random functions in 1D



Different length scales

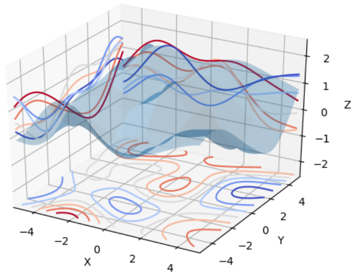
```
scales = [0.2, 1, 5]
for i in scales:
  plot(x, genSamplesSimple(x,rbf(i)))
legend(scales)
```



Two dimensions

```
from numpy import meshgrid, concatenate

x = linspace(5, -5, 50)
xx, yy = meshgrid(x, x)
xy = concatenate([xx.reshape([1, -1]),
                  yy.reshape([1, -1])]).T
z = genSamplesSimple(xy, rbf(2)).reshape([50, 50]
```

```
fig = figure()
ax = fig.gca(projection='3d')
ax.plot_surface(xx, yy, z, rstride=8,
                cstride=8, alpha=0.3)
cset = ax.contour(xx, yy, z, zdir='z',
                  offset=-2.5, cmap=cm.coolwarm)
cset = ax.contour(xx, yy, z, zdir='x',
                  offset=-5, cmap=cm.coolwarm)
cset = ax.contour(xx, yy, z, zdir='y',
                  offset=5, cmap=cm.coolwarm)

ax.set_xlabel('X')
ax.set_xlim(-5, 5)
ax.set_ylabel('Y')
ax.set_ylim(-5, 5)
ax.set_zlabel('Z')
ax.set_zlim(-2.5, 2.5)
```



Computing posterior

$$\begin{aligned}
\begin{bmatrix} \mathbf{y} \\ \mathbf{f}_* \end{bmatrix} &\sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} K(X,X)+\sigma^2 I & K(X,X_*) \\ K(X_*,X) & K(X_*,X_*) \end{bmatrix}\right) \\
\mathbf{f}_*|X,\mathbf{y},X_* &\sim \mathcal{N}(\bar{\mathbf{f}}_*, \mathrm{cov}(\mathbf{f}_*)) \\
\bar{\mathbf{f}}_* &= K(X_*,X)[K(X,X)+\sigma^2 I]^{-1}\mathbf{y} \\
&= K(X_*,X)\alpha \\
\mathrm{cov}(\mathbf{f}_*) &= K(X_*,X_*) - K(X_*,X)[K(X,X)+\sigma^2 I]^{-1}K(X,X_*) \\
&= K(X_*,K_*) - V^T V
\end{aligned}$$

Where

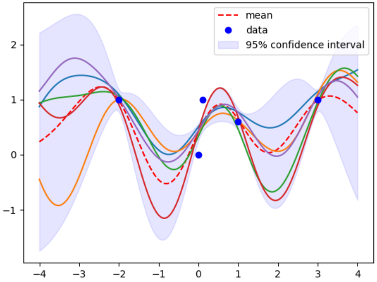
$$\begin{aligned}
L &= \mathrm{chol}(K(X,X)+\sigma^2 I) \rightarrow LL^T = K(X,X)+\sigma^2 I \\
\alpha &= [K(X,X)+\sigma^2 I]^{-1}\mathbf{y} = L^{-T}L^{-1}\mathbf{y} \\
V &= L^{-1}K(X,X_*)
\end{aligned}$$

Python code

```python
from numpy import pi, eye, log, diag
from numpy.random import normal
from numpy.linalg import cholesky, solve #, inv
# solve(A,b) equals inv(A)*v, but it is more robust

def compPosterior(y, x, k, X, snoise):
    n = x.shape[0]
    K = k(x,X)
    L = cholesky(k(x, x) + eye(n)*(snoise + 1e-8))
    alpha = solve(L.T,solve(L,y))
    f_mean = K.T.dot(alpha)
    v = solve(L,K)
    V = k(X,X) - v.T.dot(v)
    log_p = -.5*y.T.dot(alpha) - sum(log(diag(L))) - .5*n*log(2*pi)
    return f_mean, V, log_p

def genSamples(x, m, K):
    n = x.shape[0]
    L = cholesky(K+eye(n)*1e-8)
    return m + L.dot(normal(size=n))
```

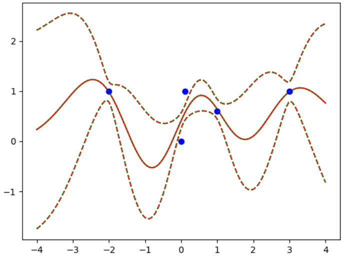
Fitting some data

```
from numpy import array, sqrt

x = array([-2, 0, 0.1,   1, 3])
y = array([ 1, 0,   1, 0.6, 1])
X = linspace(-4, 4, 150)

k = rbf(1)
f_m, V, _ = compPosterior(y, x, k, X, 0.01)

s = sqrt(diag(V))

plot(X, f_m, '--r', label='mean')
fill_between(X, f_m - 2*s, f_m + 2*s, color = 
       alpha = 0.1, label='95% confidence inte
for i in range(5):
  plot(X, genSamples(X, f_m, V))
plot(x, y, 'ob', label='data')
legend()
```



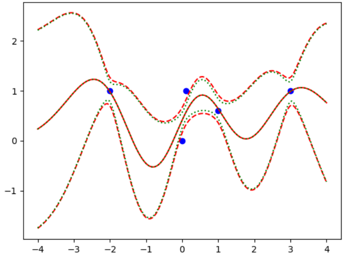
scikit-learn

```
from sklearn.gaussian_process import GaussianProcessRegressor as GPR
from sklearn.gaussian_process.kernels import RBF
      # other kernels: Matern, WhiteKernel, ConstantKernel

k = RBF(1) # exactly the same behaviour as before
# but many kernels can be combined more easily:
# ConstantKernel() + Matern(length_scale=2, nu=3/2)
#      + WhiteKernel(noise_level=1)

x = x.reshape([-1,1])  # but now x must be a 2D array
X = X.reshape([-1,1])

gp = GPR(alpha = 0.01, kernel=k, optimizer = None)
# it has many more options, in particular, optimizer
# must be set to None to prevent ML kernel estimation

gp.fit(x, y)

y_pred, sigma = gp.predict(X, return_std=True)

plot(x,y,'ob')
plot(X, y_pred, 'r')
plot(X, y_pred + 2*sigma, 'r--'); plot(X, y_pred - 2*sigma, 'r--')

# same results as raw python code
plot(X, f_m, 'g:')
plot(X, f_m + 2*s, 'g:'); plot(X, f_m - 2*s, 'g:')
```



GPFlow

```
import gpflow

Y = y.reshape(-1,1)

k = gpflow.kernels.RBF(1)

m = gpflow.models.gpr(x, Y, kern=k)

m.likelihood.variance = 0.01

f, sgpf =  m.predict_y(X)


plot(x,y,'ob')
plot(X, f, 'r')
plot(X, f + 2*sqrt(sgpf), 'r--'); plot(X, f - 2*sqrt(s

# similar (not identical) to previous results
plot(X, f_m, 'g:')
plot(X, f_m + 2*s, 'g:'); plot(X, f_m - 2*s, 'g:')
```



PyMC3

Edward

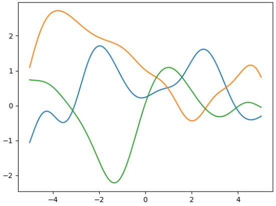
PyStan

```
data {
  int<lower=1> N;
  real x[N];
  real<lower=0> alpha;
  real<lower=0> rho;
  real<lower=0> sigma;
}
transformed data {
  matrix[N, N] K = cov_exp_quad(x, alpha, rho);
  matrix[N, N] L;
  vector[N] mu = rep_vector(0, N);
  for (n in 1:N)
    K[n, n] = K[n, n] + sigma^2;
  L = cholesky_decompose(K);
}
// this should not be necessary when fixed_param option is set,
// but "The fixed_param sampler doesn't work in PyStan v2.9.0."
parameters {  real<lower=0, upper=1> theta; }
generated quantities {
  vector[N] y;
  vector[N] eta;
  for (n in 1:N)
    eta[n] = normal_rng(0, 1);
  y = mu + L*eta;
}
```

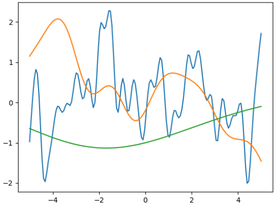
Naive code

```
data {
  int<lower=1> N;
  real x[N];
  real<lower=0> alpha;
  real<lower=0> rho;
  real<lower=0> sigma;
}
transformed data {
  matrix[N, N] K = cov_exp_quad(x, alpha, rho);
  vector[N] mu = rep_vector(0, N);
  for (n in 1:N)
    K[n, n] = K[n, n] + sigma^2;
}
/*
  transformed data {
  matrix[N, N] K;
  vector[N] mu = rep_vector(0, N);
  for (i in 1:(N - 1)) {
  K[i, i] = alpha^2 + sigma^2;
  for (j in (i + 1):N) {
  K[i, j] = alpha^2 * exp(-0.5/rho^2 * square(x[i] - x[j]));
  K[j, i] = K[i, j];
  }
  }
  K[N, N] = alpha^2 + sigma^2;
  }
*/
generated quantities {
  vector[N] y;
  y = multi_normal_rng(mu, K);
}
```

```
# Random functions in 1D

from pystan import stan

N = 150
x = linspace(-5,5,N)
data = {'N': N, 'x': x, 'alpha': 1, 'rho': 1, 'sigma': 1e-4}

model_filename = "stan-models/Gp00.c"
nchains = 1; nthin=1; niter = 1;
fit_GP = stan(file=model_filename, data=data, iter=niter,
                                   thin=nthin, chains=nchains)

figure();
for i in range(3):
  fit_GP = stan(fit=fit_GP, data=data, iter=niter,
                            thin=nthin, chains=nchains)
  plot(x,fit_GP['y'][0]);
```



```
# Different length scales

figure()
for i in range(3):
  data['rho'] = scales[i]
  fit_GP = stan(fit=fit_GP, data=data, iter=niter,
                            thin=nthin, chains=nchains)
  plot(x,fit_GP['y'][0]);
```



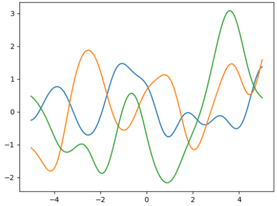
Sampling from prior: Haskell code

```haskell
module Gp00 where
import Numeric.LinearAlgebra

type DVector = Vector Double
type DMatrix = Matrix Double
type CovarianceMatrix = Matrix Double
type Kernel = DMatrix -> DMatrix -> CovarianceMatrix

sumElems :: DVector -> Double
sumElems = sumElements

rbf :: Double -> Kernel
rbf l xm ym = exp $ - (len xm >< len ym) [d x y | x <- toRows xm, y <- toRows ym ]
  where d a b = sumElems $ (( a - b ) / scalar l)^2
        len   = fst . size
-- forDVectors: rbf l x y = exp $ -((asColumn x - asRow y) / scalar l )^2
```

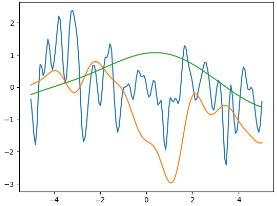
```haskell
import Numeric.LinearAlgebra
import Gp00

genSamplesSimple :: DMatrix -> Kernel -> IO DVector
genSamplesSimple x k = do
  r <- randn n 1 -- also see multivariate normal: gaussianSample
  return $ flatten (tr l <> r)
  where n = fst . size $ x
        l = chol . sym $ k x x + ident n * 1e-8
```

Random functions in 1D

```
-- 1D
import Graphics.Matplotlib

let x =  asColumn $ linspace 150 (-5, 5) :: DMatrix
let k = rbf 1

y <- sequence [genSamplesSimple x k | i <- [1..3]]

let plotCurve i z = plot (flatten x) (z!!i)

file "images/fig07.png" $ plotCurve 0 y % plotCurve 1 y % plotCurve 2 y
```



```
-- Different length scales

let scales = [0.2, 1, 5]

y' <- sequence [genSamplesSimple x (rbf (scales!!i)) | i <- [0..2]

file "images/fig08.png" $ plotCurve 0 y' % plotCurve 1 y' % plotCu
```



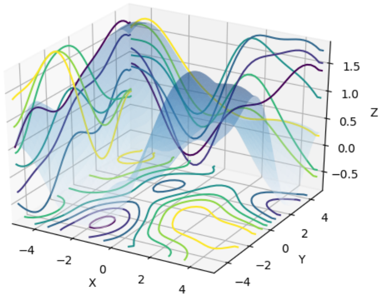
2D

```
let x =  asColumn $ linspace 50 (-5, 5) :: DMatrix
let xx = asColumn . flatten $ repmat     x   1 50
let yy = asColumn . flatten $ repmat (tr x) 50  1

let xy = xx ||| yy
```

```
z <- genSamplesSimple xy (rbf 3)
```

```
x2ind i = round $ (i + 5.1)*4.9
fz i j = reshape 50 z ! x2ind i ! x2ind j
```

```
file "images/fig09.png" $ contourF fz (-5) 5 (-5) 5 50
```

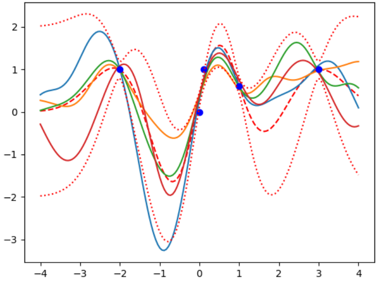


Computing posterior: Haskell code

```haskell
import Numeric.LinearAlgebra
import Gp00

compPosterior :: DVector -> DMatrix -> Kernel -> DMatrix -> Double
                     -> (DVector, DMatrix, Double)
compPosterior y x k x' snoise = (f, vf, log_p)
  where n     = fst . size $ x
        kxx'  = k x x'
        l     =  tr $ chol . sym $ k x x + ident n * scalar (snoise + 1e-8)
        alpha = triSolve Upper (tr l) $ triSolve Lower l (asColumn y)
        f     = flatten $ tr kxx' <> alpha
        v     = triSolve Lower l kxx'
        vf    = k x' x' - tr v <> v
        log_p = - 0.5* y <.> flatten alpha -  0.5*fromIntegral n * log (2*pi)
                - (sumElements . log . takeDiag ) l

genSamples :: DMatrix -> DVector -> DMatrix -> IO DVector
genSamples x m k = do
   r <- randn n 1
   return $ m + flatten (tr l <> r)
   where n = fst . size $ x
         l = chol . sym $ k + ident n * 1e-8
```

Fitting some data

```
let x  =  (5><1) [-2, 0, 0.1,   1, 3] :: DMatrix
let y  =  vector [ 1, 0,   1, 0.6, 1] :: DVector
let x' =  asColumn $ linspace 150 (-4, 4) :: DMatrix
let k = rbf 1


(f, vf, _) = compPosterior y x k x' 0.01
s = sqrt $ takeDiag vf

z <- sequence [genSamples x' f vf  | i <- [1..5]

plCurve i = plot (flatten x') (z!!i)
plCurves i = if i == 1 then plCurve 1
             else plCurve i % plCurves (i-1)

plMean = plot (flatten x') f @@ [o1 "r--"]
plCI1  = plot (flatten x') (f + 2*s) @@ [o1 "r:"
plCI2  = plot (flatten x') (f - 2*s) @@ [o1 "r:"

plData =  plot (flatten x) y @@ [o1 "bo"]


file name $ plMean % plCurves 4 % plData % plCI2 % plCI1
```


2
1
0
−1
−2
−3
−4
−3
−2
−1
0
1
2
3
4