STA4502 MiniProject

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We are applying MCMC algorithm to Bayesian linear regression in the context of polynomial fitting problem. In particular, we are interested in the predictive distribution. In this mini-project, we first define an arbitrary nonlinear function

$$f(x) = \frac{1}{6}(3\sin(2(x/3+1)^2) + 6\cos(2(x/3+1)^2) + 8)$$

Then we generate 301 data points from $f(x)$ with noise as our training data. Our goal is to use Bayesian linear regression to predict $\hat{f}(x^*)$ and then we can compare it to $f(x^*)$ to see how well our algorithm did.
In this project we assume $p(t|x, w, \beta) \sim N(t|\sum_{j=0}^{D} w_j x^j, \beta^{-1})$, which means we want to fit a polynomial to the training data set. Also, we give a normal prior to the weights $p(w) \sim N(w|0, aI)$. Then we can write down the predictive distribution, let D denote the training data set, x^* denote the given input, and t^* is our prediction,

$$p(t^*|x^*, D) = \int\int\int p(t^*|x^*, w, \beta)p(w|D, a, \beta)p(a, \beta|D)dwdad\beta$$

We can consider $p(t^*|x^*, w, \beta)$ as the likelihood function and $p(w|D, a, \beta)$ as the posterior distribution.
In general, let M be the number of iterations in MCMC algorithm. To simplify the model, we assume positive $f(x)$, then we only have to consider positive t^*. Also, we generate an alphalist and a betalist with normal distribution with mean 0 and corresponding training data variance. So within one MCMC iteration, we treat a, β as constants, so $p(a, \beta|D)$ is removed, which implies,

$$p(t^*|x^*, D) = \int p(t^*|x^*, w, \beta)p(w|D, a, \beta)dw$$

.
Next we are interested in the mean of predictive distribution. So we want to compute

$$\begin{aligned} E(t^*) &= \int t^* p(t^*|x^*, D)dt^* && (1)\\ &= \int\int t^* p(t^*|x^*, w, \beta)p(w|D, a, \beta)dwdt^* && (2)\\ &= \int\int e^{t^*} t^* p(t^*|x^*, w, \beta)p(w|D, a, \beta)e^{-t^*}dwdt^* && (3)\end{aligned}$$

In this model, we fit a 5-degree polynomial and try to predict values for 20 new inputs, so we have the following likelihood function

$$p(t|x, w, \beta) \sim N(t|\sum_{j=0}^{5} w_j x^j, \beta^{-1})$$

Also we let $\pi = p(w|D, a, \beta)$, which it is the posterior distribution of w. i.e.

$$\pi(w) \propto p(w|a, \beta) * p(target|input, w, a, \beta)$$

To be consistent to the notation in class, we set $h(t^*, w) = e^{t^*} t^* p(t^*|x^*, w, \beta)$, where $p(t^*|x^*, w, \beta)$ is the likelihood function for new input.
In the MCMC algorithm, we first initialize w according to the prior, which it is a 6-dimensional vector. Next

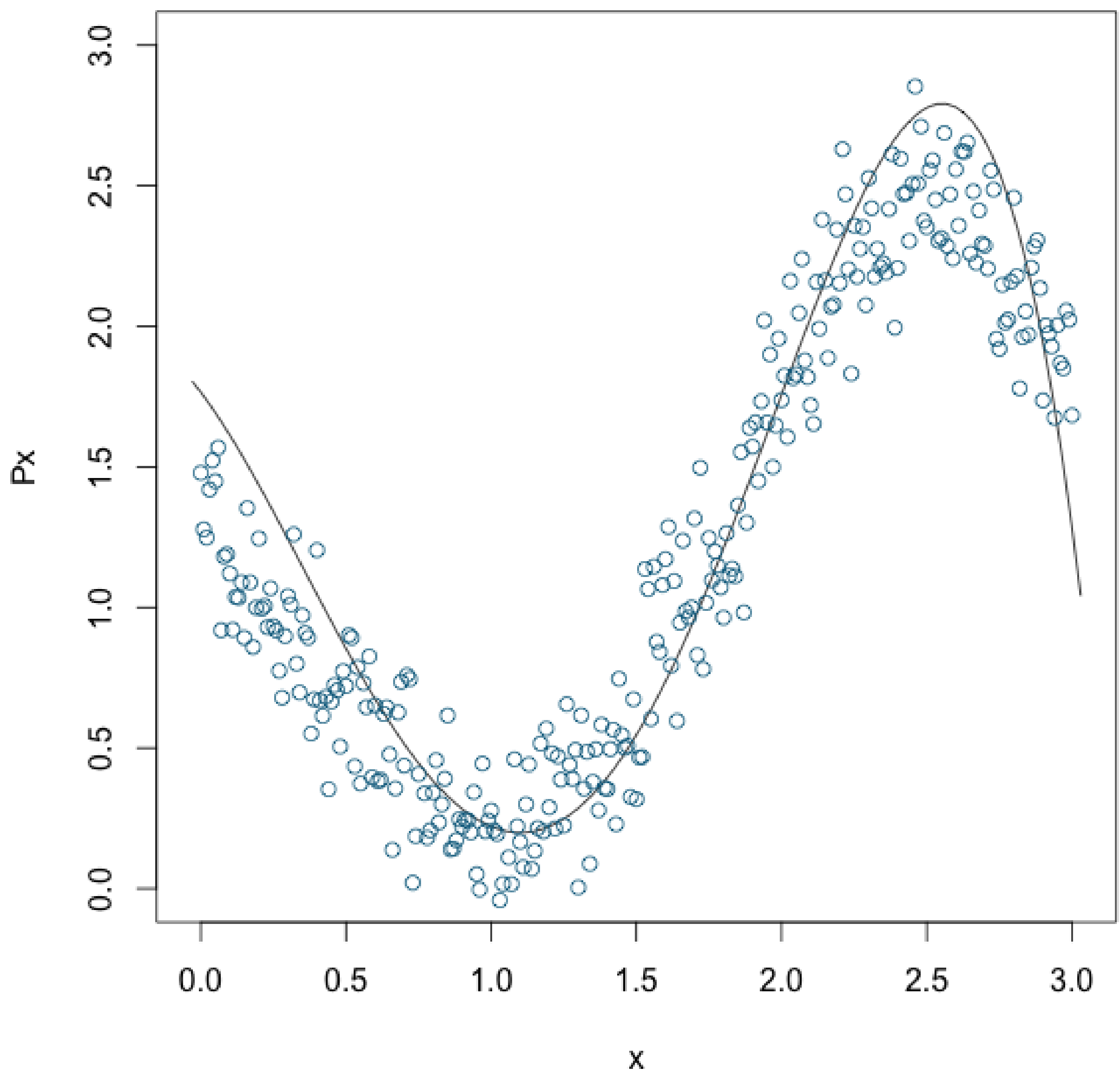
we ran something similar to Metropolis algorithm. Specifically, we propose a new vector w', and accept it with probability $\frac{\pi(w')}{\pi(w)}$. Then with this w (it's w' if we accept otherwise it is the w from last iteration), and sampling t^* from $exp(1)$, we can compute $h(t^*, w, x)$ within this iteration, where x is the new input value and we have 20 of them.
Repeat the above procedure M times, the mean of hlist after burn-in is our final prediction for 20 new inputs. Also we keep track of the value of w, so we can write down our fitted polynomial.

Listing 1: Random Walk Metropolis R code

```
#Target polynomial:

f = function(x) {(3*sin(2*(x/3+1)^2) + 6*cos(2*(x/3+1)^2) + 8 )/6}
input = seq(from=0, to=3, by=0.01)
y = f(input)
target = y + rnorm(301,0,0.2)
plot(input,target,col='deepskyblue4',xlab='x',main='Observed data')

# Define function for varfact
varfact <- function(series) { 2 * sum(acf(series, plot=FALSE)$acf) - 1 }

D = 6

noise = sd(target)

# points want to extimates
xstarlist = runif(20)

# exact values
ylist = f(xstarlist)

# return polynomial with coefficients in w
poly = function(w,x,D){
  s = 0
  for (i in 1:D){
    s = s + w[i]*x^(i-1)
  }
  return(s)
}

h = function(t,w,beta,x){
  return(exp(t)*t*dnorm(t, mean = poly(w,x,D), sd = 1/beta))
}

logmultinorm = function(w,alpha,D){
  log((2*pi)^(-0.5*D)*(1/alpha)^(-0.5*D)*exp(-0.5*alpha*sum(w^2)))
}

logg = function(w,input,target,alpha,beta,D){
  s = 0
  for (i in 1:length(target)){
    s = s + dnorm(target[i],poly(w,input[i],D),1/beta,log = TRUE)
  }
  return(s + logmultinorm(w,alpha,D))
}
```

```
M = 110000   # run length
B = 10000   # amount of burn-in
alphalist = abs(rnorm(M,0,noise))
betalist = abs(1/rnorm(M,0,noise))
tlist = rexp(M)
# for keeping track of values
wmatrix = matrix(rep(0,M*D),nrow = D,ncol = M)
hmatrix = matrix(rep(0,M*20),nrow = 20,ncol = M)
numaccept = 0
# overdispersed starting distribution (dim=D)
W = rnorm(D,0,1/alphalist[1])
sigma = 0.5   # proposal scaling


for (i in 1:M) {
  Y = W + sigma * rnorm(D)   # proposal value (dim=D)
  U = runif(1)   # for accept/reject
  a = logg(Y,input,target,alphalist[i],betalist[i],D) -
  logg(W,input,target,alphalist[i],betalist[i],D)   # for accept/reject
  if (log(U) < a) {
    W = Y   # accept proposal
    numaccept = numaccept + 1
  }
  for (j in 1:D){
    wmatrix[j,i] = W[j]
  }
  for (k in 1:20){
    hmatrix[k,i] = h(tlist[i],W,betalist[i],xstarlist[k]);
  }
}

for (k in 1:20){
  estimate = mean(hmatrix[k,(B+1):M])
  iidse =  sd(hmatrix[k,(B+1):M]) / sqrt(M-B)
  se = iidse*sqrt(varfact(hmatrix[k,(B+1):M]) )
  cat("Estimate for x = ", xstarlist[k], "=" , estimate, ",
  True value (f(x))= ", ylist[k], "\n")
  cat("approximate 95% confidence interval is (", estimate - 1.96 * se, ",",
      estimate + 1.96 * se, ")\n\n")
}

w = wmatrix[,M]
predictpoly = polynomial(coef = w)


plot(predictpoly,xlim = c(0,3),ylim = c(0,3))
points(input,target,type = "p", col='deepskyblue4',xlab='x',main='Observed data')
```

And we get the output



Listing 2: R output

```
Estimate for x =  0.160577 is 1.419294 , True value (f(x))=  1.127248
approximate 95% confidence interval is ( 1.391167 , 1.44742 )

Estimate for x =  0.9899601 is 0.4158945 , True value (f(x))=  0.2178462
approximate 95% confidence interval is ( 0.4081417 , 0.4236472 )

Estimate for x =  0.453312 is 0.9170817 , True value (f(x))=  0.6876926
approximate 95% confidence interval is ( 0.9031105 , 0.9310528 )
```

```
Estimate for x =  0.5914694 is 0.7158354 , True value (f(x))=  0.5068513
approximate 95% confidence interval is ( 0.7059315 , 0.7257393 )

Estimate for x =  0.7428511 is 0.5504592 , True value (f(x))=  0.3479855
approximate 95% confidence interval is ( 0.5426297 , 0.5582888 )

Estimate for x =  0.464768 is 0.9075627 , True value (f(x))=  0.671718
approximate 95% confidence interval is ( 0.8920921 , 0.9230332 )

Estimate for x =  0.07897275 is 1.522164 , True value (f(x))=  1.252638
approximate 95% confidence interval is ( 1.49407 , 1.550257 )

Estimate for x =  0.6387615 is 0.6542706 , True value (f(x))=  0.4520785
approximate 95% confidence interval is ( 0.645401 , 0.6631402 )

Estimate for x =  0.5817941 is 0.7331457 , True value (f(x))=  0.5185618
approximate 95% confidence interval is ( 0.7220487 , 0.7442426 )

Estimate for x =  0.7518658 is 0.5440949 , True value (f(x))=  0.3401651
approximate 95% confidence interval is ( 0.5359097 , 0.5522802 )

Estimate for x =  0.08717507 is 1.513882 , True value (f(x))=  1.24011
approximate 95% confidence interval is ( 1.482046 , 1.545719 )

Estimate for x =  0.9182943 is 0.4404978 , True value (f(x))=  0.2361555
approximate 95% confidence interval is ( 0.4326342 , 0.4483613 )

Estimate for x =  0.3694 is 1.046509 , True value (f(x))=  0.8087238
approximate 95% confidence interval is ( 1.030208 , 1.06281 )

Estimate for x =  0.5742994 is 0.7416084 , True value (f(x))=  0.5277443
approximate 95% confidence interval is ( 0.7308318 , 0.752385 )

Estimate for x =  0.6752285 is 0.6152825 , True value (f(x))=  0.4128695
approximate 95% confidence interval is ( 0.6068049 , 0.6237601 )

Estimate for x =  0.8706393 is 0.4635071 , True value (f(x))=  0.2575953
approximate 95% confidence interval is ( 0.4556642 , 0.4713501 )

Estimate for x =  0.2876286 is 1.197784 , True value (f(x))=  0.9316992
approximate 95% confidence interval is ( 1.177637 , 1.21793 )

Estimate for x =  0.674066 is 0.6179598 , True value (f(x))=  0.4140761
approximate 95% confidence interval is ( 0.6088086 , 0.6271109 )

Estimate for x =  0.7465105 is 0.5465784 , True value (f(x))=  0.3447863
approximate 95% confidence interval is ( 0.5390394 , 0.5541173 )

Estimate for x =  0.1921243 is 1.367434 , True value (f(x))=  1.078529
approximate 95% confidence interval is ( 1.341655 , 1.393213 )

estimate polynomial :
1.76558 - 1.370776*x - 1.774254*x^2 + 1.83905*x^3 - 0.1733876*x^4 -
0.06588073*x^5
```

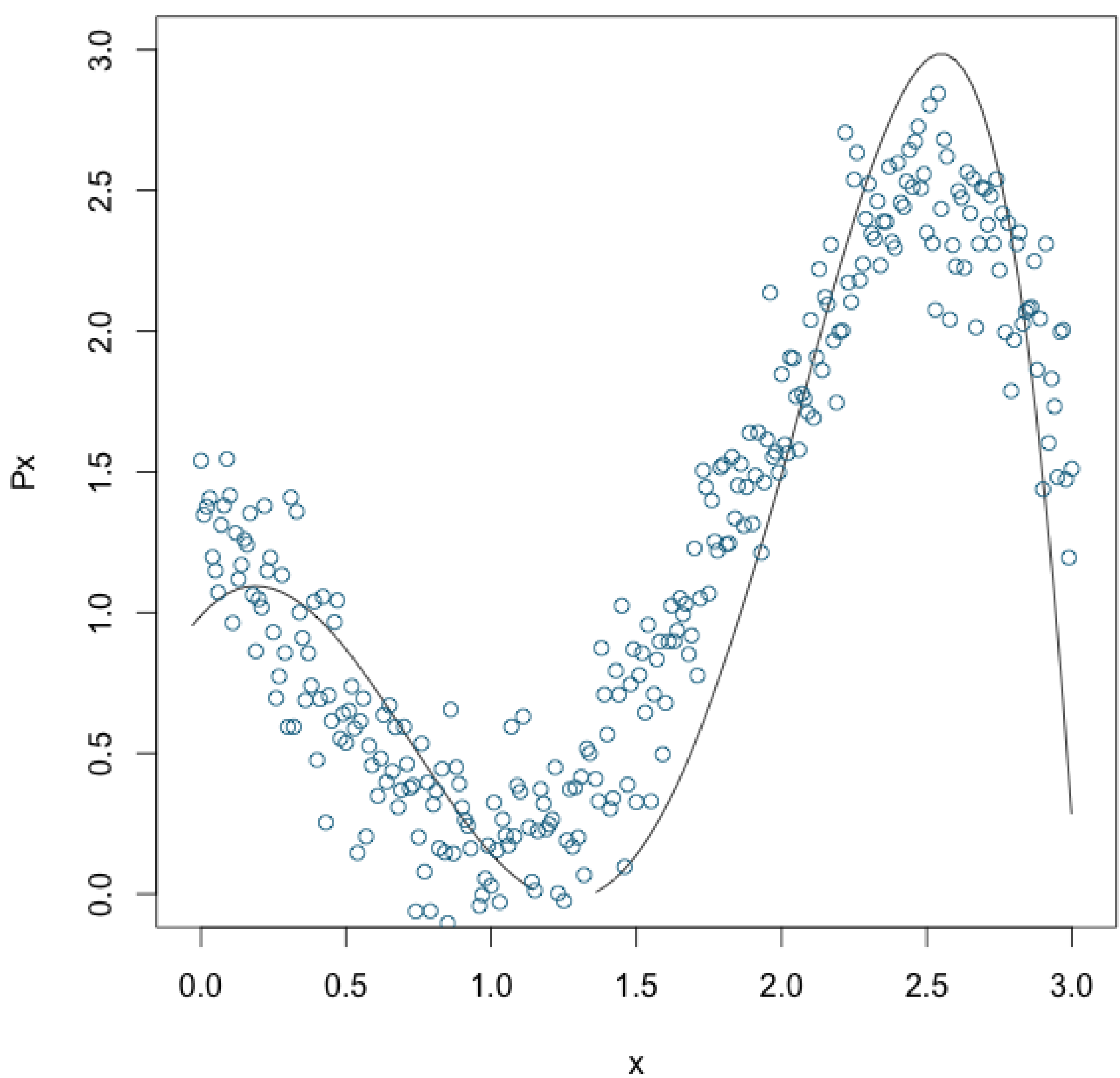
Here is the code for Variable-At-A-Time Algorithm

Listing 3: Variable-At-A-Time R code

```
#Target polynomial:

f = function(x) {(3*sin(2*(x/3+1)^2) + 6*cos(2*(x/3+1)^2) + 8 )/6}
input = seq(from=0, to=3, by=0.01)
y = f(input)
target = y + rnorm(301,0,0.2)
plot(input,target,col='deepskyblue4',xlab='x',main='Observed data')

# Define function for varfact
varfact <- function(series) { 2 * sum(acf(series, plot=FALSE)$acf) - 1 }

D = 6

noise = sd(target)

# points want to extimates
xstarlist = runif(20,0,3)

# exact values
ylist = f(xstarlist)

# return polynomial with coefficients in w
poly = function(w,x,D){
  s = 0
  for (i in 1:D){
    s = s + w[i]*x^(i-1)
  }
  return(s)
}

h = function(t,w,beta,x){
  return(exp(t)*t*dnorm(t, mean = poly(w,x,D), sd = 1/beta))
}

logmultinorm = function(w,alpha,D){
  log((2*pi)^(-0.5*D)*(1/alpha)^(-0.5*D)*exp(-0.5*alpha*sum(w^2)))
}

logg = function(w,input,target,alpha,beta,D){
  s = 0
  for (i in 1:length(target)){
    s = s + dnorm(target[i],poly(w,input[i],D),1/beta,log = TRUE)
  }
  return(s + logmultinorm(w,alpha,D))
}


M = 110000  # run length
B = 10000  # amount of burn-in
alphalist = abs(rnorm(M,0,noise))
betalist = abs(1/rnorm(M,0,noise))
```

```
tlist = rexp(M)
# for keeping track of values
wmatrix = matrix(rep(0,M*D),nrow = D,ncol = M)
hmatrix = matrix(rep(0,M*20),nrow = 20,ncol = M)
numaccept = 0
# overdispersed starting distribution (dim=D)
W = rnorm(D,0,1/alphalist[1])
sigma = 0.1   # proposal scaling


for (i in 1:M) {
  coord = floor( runif(1,1,D+1) )  # uniform on {1,2,...,D}
  Y = W
  Y[coord] = W[coord] + sigma * rnorm(1)  # proposal
  U = runif(1)  # for accept/reject
  a = logg(Y,input,target,alphalist[i],betalist[i],D) -
  logg(W,input,target,alphalist[i],betalist[i],D)  # for accept/reject
  if (log(U) < a) {
    W = Y  # accept proposal
    numaccept = numaccept + 1
  }
  for (j in 1:D){
    wmatrix[j,i] = W[j]
  }
  for (k in 1:20){
    hmatrix[k,i] = h(tlist[i],W,betalist[i],xstarlist[k]);
  }
}

for (k in 1:20){
  estimate = mean(hmatrix[k,(B+1):M])
  iidse =  sd(hmatrix[k,(B+1):M]) / sqrt(M-B)
  se = iidse*sqrt(varfact(hmatrix[k,(B+1):M]) )
  cat("Estimate for x = ", xstarlist[k], "is" , estimate, ",
  True value (f(x)) is ", ylist[k], "\n")
  cat("approximate 95% confidence interval is (", estimate - 1.96 * se, ",",
     estimate + 1.96 * se, ")\n\n")
}
cat("acceptance rate = ", numaccept/M )

w = wmatrix[,M]
predictpoly = polynomial(coef = w)


plot(predictpoly,xlim = c(0,3),ylim = c(0,3))
points(input,target,type = "p", col='deepskyblue4',xlab='x',main='Observed data')
```

And we get the output



Listing 4: R output

```
Estimate for x =  2.157489 is 2.180967 , True value (f(x)) is  2.083078
approximate 95% confidence interval is ( 2.132901 , 2.229033 )

Estimate for x =  2.911417 is 1.408798 , True value (f(x)) is  1.919722
approximate 95% confidence interval is ( 1.383038 , 1.434559 )

Estimate for x =  1.663045 is 0.6688371 , True value (f(x)) is  0.9562295
approximate 95% confidence interval is ( 0.6610177 , 0.6766564 )
```

```
Estimate for x =  2.69406 is 2.91572 , True value (f(x)) is  2.336078
approximate 95% confidence interval is ( 2.816937 , 3.014502 )

Estimate for x =  2.895752 is 1.550337 , True value (f(x)) is  1.958341
approximate 95% confidence interval is ( 1.525694 , 1.57498 )

Estimate for x =  1.133888 is 0.3645747 , True value (f(x)) is  0.2359126
approximate 95% confidence interval is ( 0.3601866 , 0.3689627 )

Estimate for x =  0.3164865 is 1.082079 , True value (f(x)) is  0.8878831
approximate 95% confidence interval is ( 1.067628 , 1.096529 )

Estimate for x =  2.358848 is 2.861278 , True value (f(x)) is  2.377627
approximate 95% confidence interval is ( 2.77013 , 2.952425 )

Estimate for x =  2.11409 is 2.048102 , True value (f(x)) is  1.997377
approximate 95% confidence interval is ( 2.000968 , 2.095236 )

Estimate for x =  0.452603 is 1.012806 , True value (f(x)) is  0.6886861
approximate 95% confidence interval is ( 0.9994188 , 1.026194 )

Estimate for x =  0.525778 is 0.9565627 , True value (f(x)) is  0.5893972
approximate 95% confidence interval is ( 0.9426317 , 0.9704938 )

Estimate for x =  1.305032 is 0.3401239 , True value (f(x)) is  0.3593653
approximate 95% confidence interval is ( 0.3359197 , 0.344328 )

Estimate for x =  1.179608 is 0.348833 , True value (f(x)) is  0.2578536
approximate 95% confidence interval is ( 0.3445658 , 0.3531002 )

Estimate for x =  1.859953 is 1.147757 , True value (f(x)) is  1.414501
approximate 95% confidence interval is ( 1.13232 , 1.163194 )

Estimate for x =  1.335083 is 0.3455914 , True value (f(x)) is  0.392645
approximate 95% confidence interval is ( 0.3413017 , 0.349881 )

Estimate for x =  0.7642032 is 0.6878164 , True value (f(x)) is  0.3297966
approximate 95% confidence interval is ( 0.6795576 , 0.6960753 )

Estimate for x =  1.723669 is 0.7998767 , True value (f(x)) is  1.091986
approximate 95% confidence interval is ( 0.7891555 , 0.8105979 )

Estimate for x =  1.312721 is 0.3411793 , True value (f(x)) is  0.3675551
approximate 95% confidence interval is ( 0.3369647 , 0.3453939 )

Estimate for x =  1.833726 is 1.072244 , True value (f(x)) is  1.351405
approximate 95% confidence interval is ( 1.055814 , 1.088674 )

Estimate for x =  1.533271 is 0.4733783 , True value (f(x)) is  0.6935359
approximate 95% confidence interval is ( 0.4678844 , 0.4788721 )

estimate polynomial :
0.9899345 + 1.126159*x - 3.178382*x^2 + 0.4105512*x^3 + 1.108255*x^4 -
0.3141828*x^5
```