Statistical Modelling and Inference: Week 2 Exercises

Questions from Bayesian Regression

1. For a Bayesian linear regression model with prior on $p(w) = N(w|\mu, D^{-1})$ and q known, show that w_{Bayes} solves $(D + q\phi^T\phi)w_{Bayes} = q\phi^T t + D\mu$

To solve for bayes we take the known posterior probability:

$-2logp(w|t, X) = -2qt^T\phi w + qw^T\phi^T\phi w + (w - \mu)^T D(w - \mu) + const$

To get the best estimate of w, we take the derivative of the posterior probability and set it equal to zero:

$\frac{d(-2logp(w|t,X))}{dw} = 0$

The derivative of the **first term:**

$\frac{d(-2qt^T\phi w)}{dw} = -2qt^T\phi$

The derivative of the **second term** uses the property $\frac{d(x^TAx)}{dx} = 2Ax$

$\frac{d(qw^T\phi^T\phi w}{dw} = 2q\phi^T\phi w$

Expanding the third term $(w - \mu)^T D(w - \mu)$ gives:

$= (w^T D - \mu^T D)(w - \mu)$

$= w^T Dw - \mu^T Dw - w^T D\mu + \mu^T D\mu$

$\partial(w^T Dw - \mu^T Dw - w^T D\mu + \mu^T D\mu)/\partial w = 2w^T D - 2\mu^T D$

So we have:

$0 = -2qt^T\phi + 2qw^T\phi^T\phi + 2w^T D - 2\mu^T D$

Move negative terms to the LHS and divide both sides by 2:

$qt^T\phi + \mu^T D = qw^T\phi^T\phi + w^T D$

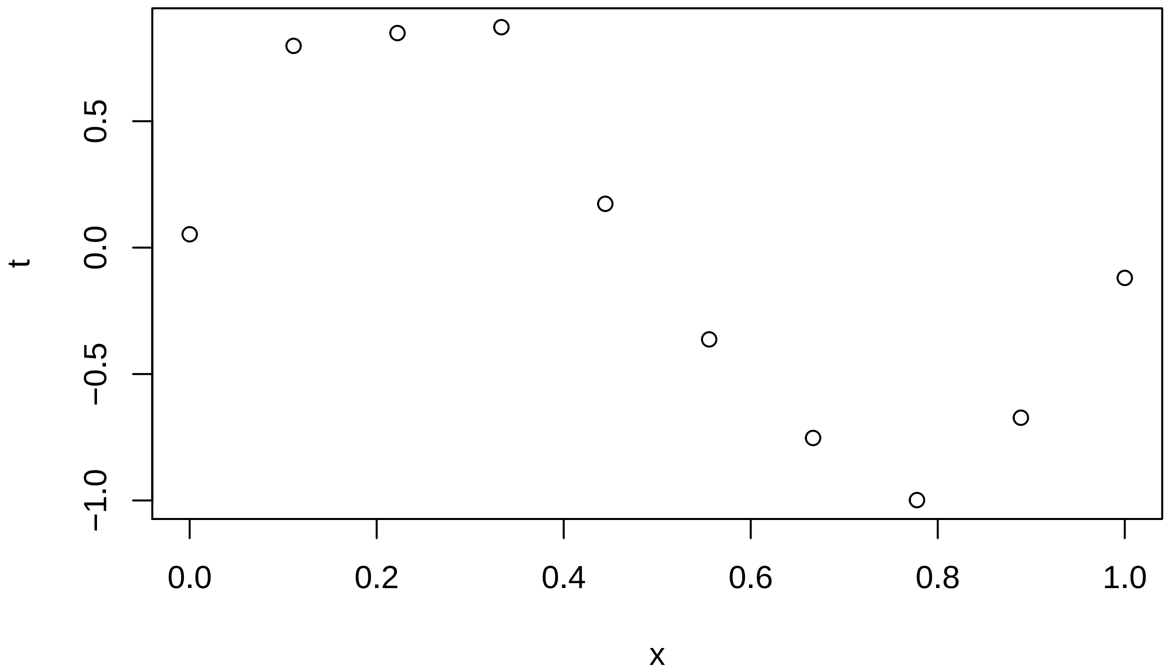
$qw^T\phi^T\phi + w^T D = qt^T\phi + \mu^T D$

Take the transpose of both sides (note: $D^T = D$:

$q\phi^T\phi w + Dw = q\phi^T t + D\mu$

$(D + q\phi^T\phi)w_{Bayes} = q\phi^T t + D\mu$

2. Curve fitting (pt1) The aim is to learn a smooth function from the cloud of points stored in curve_data.txt using Bayesian linear regression models. In all that follows the prior $p(w) = N(w|0, \delta^{-1}I)$ is used and q, δ are constants specified by the user. 2.1 Plot the data



2.2 Write a function in R, called phix that takes as input a scalar x (the input in curve fitting), with values in [0, 1], M the number of bases functions, and a categorical variable that specifies the type of basis used, and returns the vector of basis functions evaluated at x. Hence a call of the function phix(0.3,4,"poly") should return c(1.0000, 0.3000, 0.0900, 0.0270, 0.0081). Code it up so that the option "poly" gives the polynomial bases and "Gauss" the Gaussian kernels with means mui equally spaced in [0, 1], with $\mu = 0$ and $mu_M = 1$.

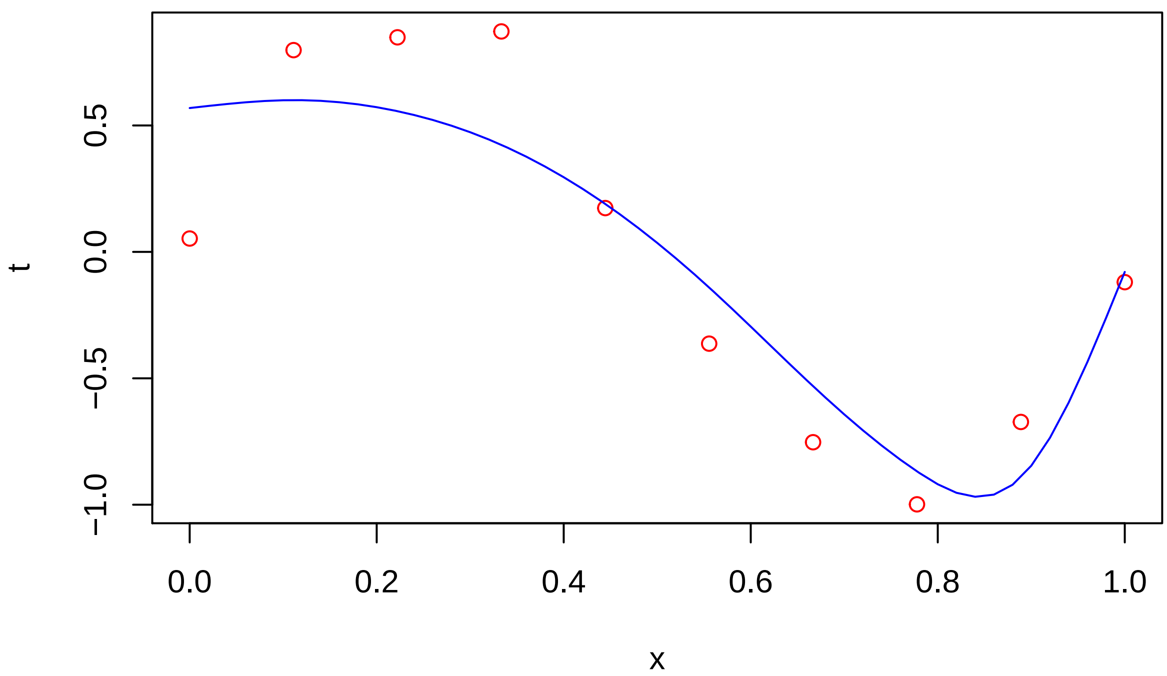
```
phix <- function(x, M, option) {
  phi <- rep(0, M)
  if (option == "poly") {
    for (i in 1:(M)) {
      phi[i] <- x**i
    }
  }
  if (option == "Gauss") {
    for (i in 1:(M)) {
      phi[i] <- exp(-((x-i/(M))**2)/0.1)
    }

  }
  phi
}
```

2.3 Write a function in R, called post.params, that takes as input the training data, M, the type of basis, the function phix, δ and q and returns the parameters of the posterior distribution, w_{Bayes} and Q.

```
post.params <- function(data, M, option, delta, q) {
  phi = phix(data$x[1],M, option)
```

```
  for (i in 2:length(data$x)) {
    phi_ <- phix(data$x[i], M, option)
    phi = rbind(phi, phi_)
  }
  phi <- cbind(rep(1,M+1), phi)

  Q = delta * diag(ncol(phi)) + q * (t(phi) %*% phi)
  w = solve(Q)%*%(q*t(phi)%*%data$t)
  t <- phi%*%w

  return(list(Q, w, t))
}
```

2.4 Plot the estimated linear predictor, by plugging in w_{Bayes}, and superimpose the training data; use $q = (1/0.1)^2$, $\delta = 2.0$ and $M = 9$

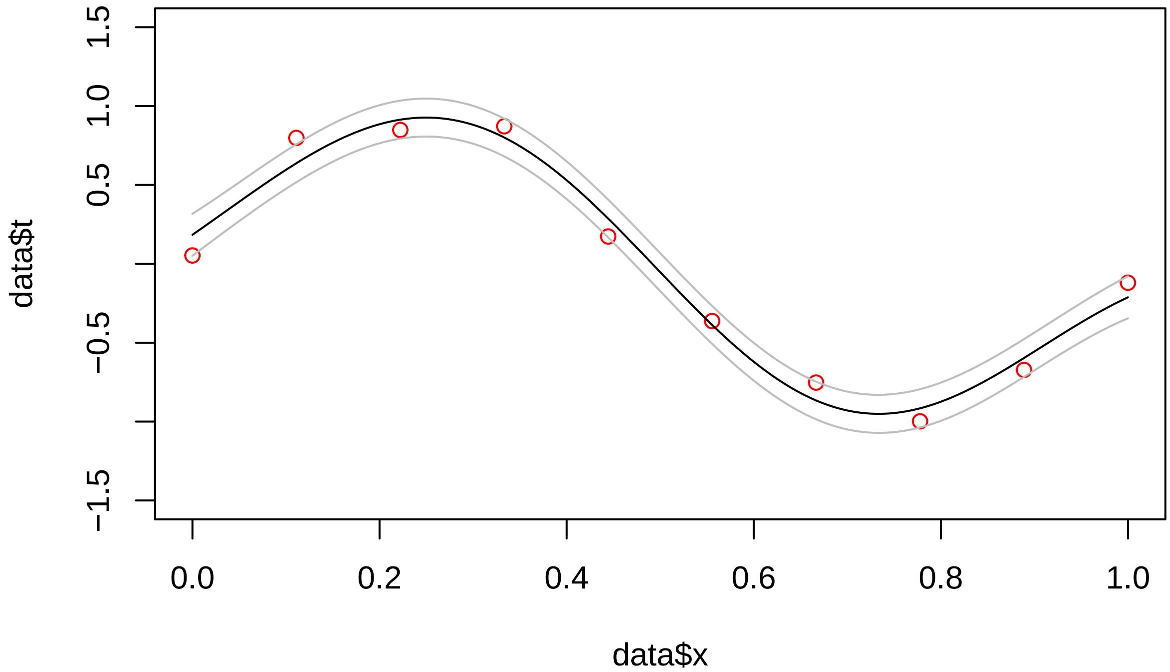


Questions from Bayesian Prediction

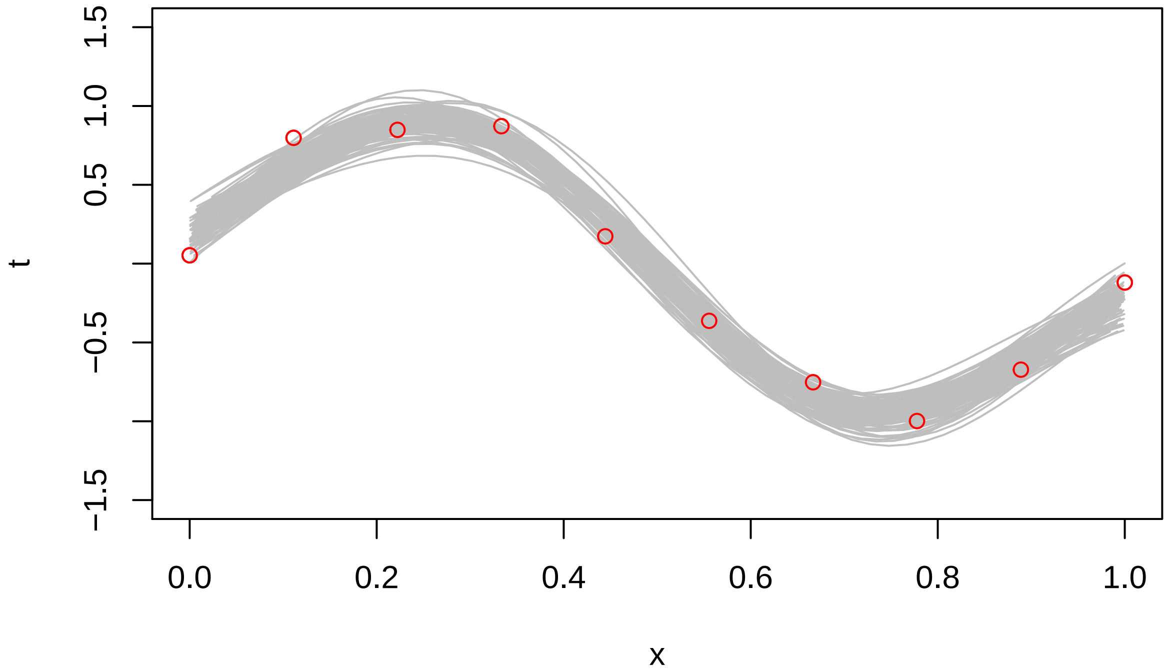
1. Continuation of your work on smooth function estimation with the data in curve_data.txt.

```
library(MASS)

M = 9
basis_type = 'Gauss'
delta = 1.0
q = (1/0.1)**2
data <- read.table("curve_data.txt")
test.x <- seq(0,1,1/1000)
```

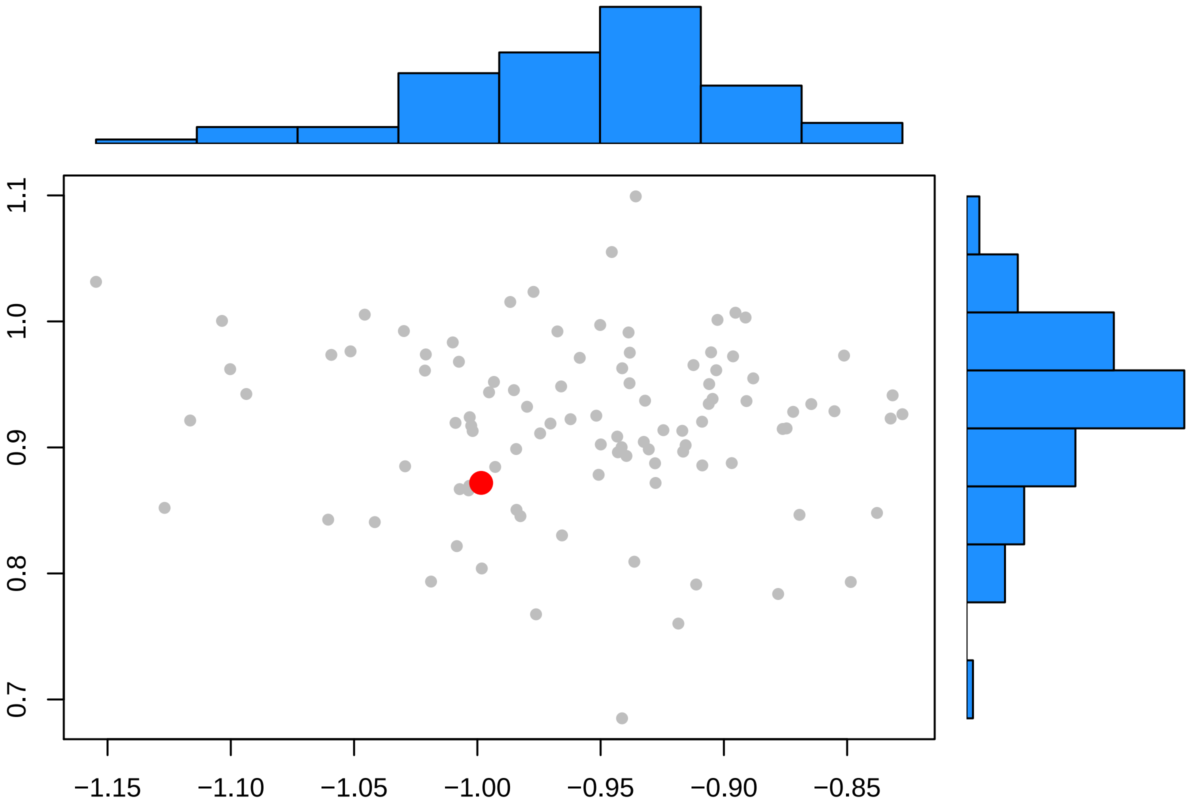
```r
pediction.bayes <- function(data, x, M, basis_type, delta, q) {
  input_data_params <- post.params(data, M, basis_type, delta, q)
  Qbayes <- input_data_params[[1]]
  wbayes <- input_data_params[[2]]

  # create phi(testx) by sending all the test x to phix
  phi.test.x <- matrix(nrow = length(test.x), ncol = M+1)
  for (n in 1:length(test.x)) {
    phi.test.x[n,] <- c(1, phix(test.x[n], M, basis_type))
  }

  test.y <- matrix(nrow = length(test.x), ncol = 2)
  dimnames(test.y)[[2]] <- list("test.x", "test.y")
  for (n in 1:nrow(phi.test.x)) {
    test.y[n,"test.x"] <- test.x[n]
    test.y[n,"test.y"] <- t(phi.test.x[n,]) %*% wbayes
  }

  Qbayesinv <- solve(Qbayes)
  covmatrix <- phi.test.x %*% Qbayesinv %*% t(phi.test.x) + 1/q

  return(list(test.y, covmatrix, Qbayes, wbayes, covmatrix))
}

result <- pediction.bayes(data, x, M, basis_type, delta, q)
test.ys <- result[1][[1]]
sds <- sqrt(diag(result[2][[1]]))
Qbayes <- result[3][[1]]
wbayes <- result[4][[1]]

plot(data$x, data$t, ylim = range(-1.5:1.5), col = 'red')
lines(x = test.ys[,"test.x"], y = test.ys[,"test.y"])
lines(x = test.ys[,"test.x"], y = (test.ys[,"test.y"] + sds), col = 'grey')
lines(x = test.ys[,"test.x"], y = (test.ys[,"test.y"] - sds), col = 'grey')
```




```
plot(data, col = 'red', ylim = range(-1.5:1.5))
nsims <- 100
mins <- rep(0, nsims)
maxs <- rep(0, nsims)
for (sim in 1:nsims) {
  # generate random draws of N(w,cov) and plot random xs evaluated for each
  # Procedure:
  #  1) generate a random draw of N(w, cov) -> this becomes a new (random) w (from the same distributio
  wbayesrand <- mvrnorm(n = 1, wbayes, Sigma = solve(Qbayes))
  #  2) generate 100 random xs to calculate phix(x...)
  xs <- runif(100)
  #  3) generate their y's as t(phix(xs)) %*% wbayesrand
  ys <- rep(0, length(xs))
  for (n in 1:length(xs)) {
    testphi <- c(1, phix(xs[n], M, basis_type))
    ys[n] <- t(testphi) %*% wbayesrand
  }
  mins[sim] <- min(ys)
  maxs[sim] <- max(ys)
  lines(predict(splines::interpSpline(xs, ys)), col ='grey')
}
points(data, col ='red')
```




```
observed_min <- min(data$t)
observed_max <- max(data$t)

scatterhist <- function(x, y, x1, y1, xlab="", ylab=""){
  zones=matrix(c(2,0,1,3), ncol=2, byrow=TRUE)
  layout(zones, widths=c(4/5,1/5), heights=c(1/5,4/5))
  xhist = hist(x, plot=FALSE)
  yhist = hist(y, plot=FALSE)
  top = max(c(xhist$counts, yhist$counts))
  par(mar=c(3,3,1,1))
  plot(x,y, col = 'gray', pch = 16)
  points(x1, y1, col = 'red', pch = 16, cex = 2)
  par(mar=c(0,3,1,1))
  barplot(xhist$counts, axes=FALSE, ylim=c(0, top), space=0, col = 'dodgerblue')
  par(mar=c(3,0,1,1))
  barplot(yhist$counts, axes=FALSE, xlim=c(0, top), space=0, horiz=TRUE, col = 'dodgerblue')
  par(oma=c(3,3,0,0))
  mtext(xlab, side=1, line=1, outer=TRUE, adj=0,
    at=.8 * (mean(x) - min(x))/(max(x)-min(x)))
  mtext(ylab, side=2, line=1, outer=TRUE, adj=0,
    at=(.8 * (mean(y) - min(y))/(max(y) - min(y))))
}

scatterhist(mins, maxs, observed_min, observed_max)
```



2.1 Show that the mean of the predictive distribution at an input location x, $\phi(x)^T w_{Bayes}$ can be represented as

$$\sum_{n=1}^{N} q\phi(x)^T Q^{-1}\phi(x_n)t_n$$

therefore, as a linear combination of the training outputs t_n.

We know that the predictive distribution is given by (slide 3):

$t_{N+1}|t, X, x_{N+1}\tilde{}N(\phi(x_{N+1})^T w_{Bayes}, \phi(x_{N+1})^T Q^{-1}\phi(x_{N+1}) + q^{-1})$

From this we know the mean of the predictive distribution at $\mathbf{x}$ is: $\phi(\mathbf{x})^T w_{Bayes}$

and the equation is given by $w_{Bayes} = qQ^{-1}\phi^T t$

At $\mathbf{x}$, $\phi^T t$ is

$$\sum_{n=1}^{N} \phi(x_n)t_n$$

So we get the final result that the mean of the predictive distribution at $\mathbf{x}$ is:

$$\sum_{n=1}^{N} q\phi(x)^T Q^{-1}\phi(x_n)t_n$$

2.2 The weights above is a quantification of the similarity (in feature space) of the test input x and the training inputs xn. In particular, let $k(x, y) := q\phi(x)^T Q^{-1}\phi(y)$ Then, show that the weight of t_n is $k(x, x_n)$

We know from 2.1 that the mean of the predictive distribution at some input location $\mathbf{x}$ (which is denoted below as $y(\bar{\mathbf{x}})$) is given by:

$$y(\bar{\mathbf{x}}) = \sum_{n=1}^{N} q\phi(\mathbf{x})^T Q^{-1} \phi(x_n) t_n$$

We use this to solve for t_n and get

$$\frac{y(\bar{\mathbf{x}})}{\sum_{n=1}^{N} q\phi(x)^T Q^{-1} \phi(x_n) t} = t_n$$

We see $k(x, x_n)$ (the summation in the denominator) is the weight that x_n gives in calculating the predictive mean of $\mathbf{x}$, which we can take to be like an x_{n+1}, the x-value for which we want to predict.

3. Let K be the matrix with (n,k) element $k(x_n, x_k)$. Show that $K = q\phi Q^{-1} \phi^T$

We know that:

$k(x, y) := q\phi(x)^T Q^{-1} \phi(y)$

$k(x_n, x_k)$ is the value of K at the (n, k) location.

So we can exchange x and y for x_n and x_k

$k(x_n, x_k) := q\phi(x_n)^T Q^{-1} \phi(x_k)$

The interpretation of $k(x_n, x_k)$ is the impact of x_k in predicting the t_n at x_n.

The matrix produced for all n and all k, e.g. The impact of every $\mathbf{x}$ in predicting the t at any other is $\mathbf{x}$, is exactly the matrix K:

$q\phi(x_n)^T Q^{-1} \phi(x_k) = q\phi Q^{-1} \phi^T = K$

4. Notice that, by expanding Q,

$K = q\phi(\delta I + q\phi^T \phi)^{-1} \phi^T = \phi(\lambda I + \phi^T \phi)^{-1} \phi^T$.

Show that when $\lambda = 0$, and provided $\phi^T \phi$ is invertible, K is precisely the "hat" matrix of linear regression. Therefore, the matrix of kernel weights provides a Bayesian version of such matrix. We will revisit this later in the course.

The "Hat" matrix from linear regression is given by:

$H = \phi(\phi^T \phi)^{-1} \phi^T$

When $\lambda = 0$, the first term in paranthesis:

$K = \phi(\lambda I + \phi^T \phi)^{-1} \phi^T$

is a matrix of zeroes and thus when multiplied by ϕ is still a matrix of zeros so we remove it from the equation and the equation reduces to:

$K = H = \phi(\phi^T \phi)^{-1} \phi^T$