Simulation of Chen

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2023-04-14

In this section, we are going to reproduce the same result as Chen did in the deep Kriging paper. For 1d case, they simulated the z in this way:

$$z(s) = \mu + \nu(s) + \epsilon(s)$$

with $\mu = 1$, and $\nu(s)$ being a zero mean GP with an exponential covariance function:

$$C(s, s') = \sigma^2 exp\{-|s - s'|/\rho\}$$

with variance $\sigma^2 = 1$ and the range parameter $\rho = 0.1$, and the ϵ is a Gaussian white noise with the nugget variance $\tau^2 = 0.01$.

Step 1

They generated 100 replicates for $z(s_1), z(s_2), ..., z(s_N)$ with $N = 1000$, and equally spaced locations over $[0, 1]$, with 800 locations randomly selected as training data and the rest are testing data. Here we have no observed covariates except for the intercept.

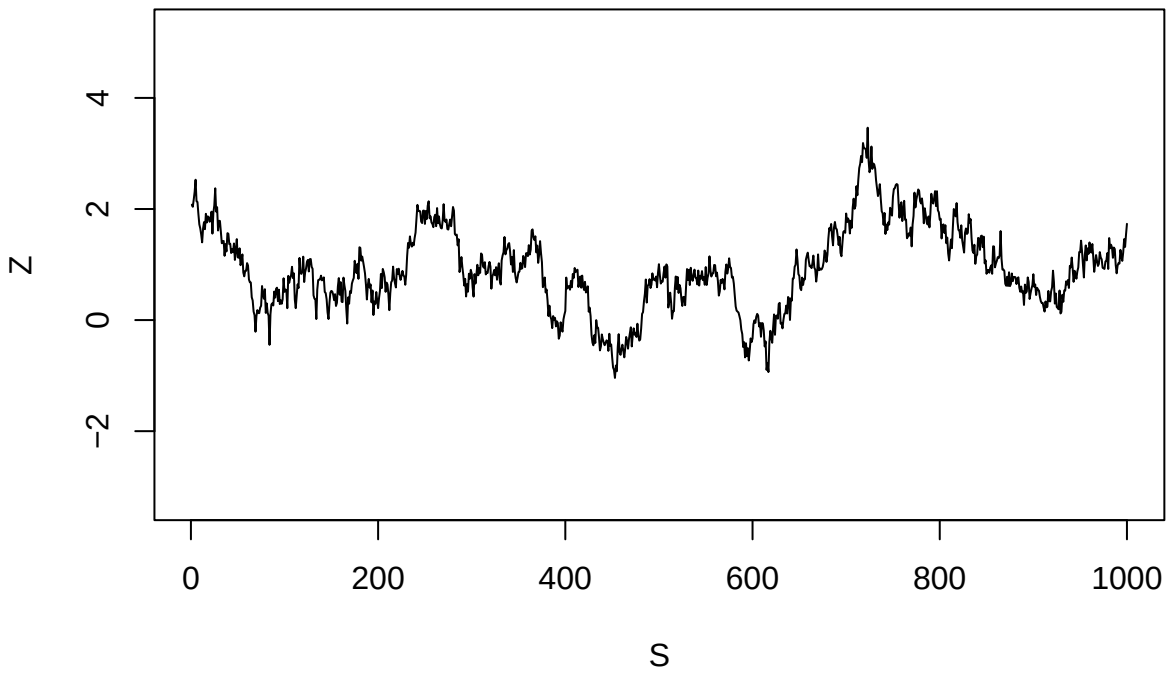
```
# Generate the GP

sim_all <- matrix(NA, nrow = 100, ncol = 1000)
s <- seq(from = 0, to = 1, length.out = 1000)

exp_cor <- function(d){
  return(exp(-abs(d)/0.1))
}
#
dis <- spDists(cbind(s, 1))
cov_mat <- exp_cor(dis)
# for (i in 1:100) {
#   sim_all[i,] <- mvtnorm::rmvnorm(1, mean = rep(1,1000), sigma = cov_mat) + rnorm(1000, mean = 0, sd =
#   print(i)
# }
# write.csv(sim_all, here::here("pm_small/sim_dat.csv"))

sim_dat <- read.csv(here::here("pm_small/sim_dat.csv"))[,-1]

plot(x = 1:1000, sim_dat[1,], type = 'l', ylim = c(min(sim_dat)-0.3, max(sim_dat)+0.3), ylab = "Z", xlab
```




```
# Create basis function for DK
  basis_1 <- seq(from = 0, to = 1, length.out = 10)
  basis_2 <- seq(from = 0, to = 1, length.out = 19)
  basis_3 <- seq(from = 0, to = 1, length.out = 37)
  basis_4 <- seq(from = 0, to = 1, length.out = 73)

  basis_dist_1 <- spDists(cbind(1,s), cbind(1, basis_1))
  basis_dist_2 <- spDists(cbind(1,s), cbind(1, basis_2))
  basis_dist_3 <- spDists(cbind(1,s), cbind(1, basis_3))
  basis_dist_4 <- spDists(cbind(1,s), cbind(1, basis_4))

  theta_1 <- 2.5* diff(seq(from = 0, to = 1, length.out = 10))[1]
  theta_2 <- 2.5* diff(seq(from = 0, to = 1, length.out = 19))[1]
  theta_3 <- 2.5* diff(seq(from = 0, to = 1, length.out = 37))[1]
  theta_4 <- 2.5* diff(seq(from = 0, to = 1, length.out = 73))[1]

  basis_fun_1 <- matrix(nychka_fun(basis_dist_1, theta_1), nrow = length(s))
  basis_fun_2 <- matrix(nychka_fun(basis_dist_2, theta_2), nrow = length(s))
  basis_fun_3 <- matrix(nychka_fun(basis_dist_3, theta_3), nrow = length(s))
  basis_fun_4 <- matrix(nychka_fun(basis_dist_4, theta_4), nrow = length(s))

  basis_fun_all <- cbind(basis_fun_1,basis_fun_2,basis_fun_3,basis_fun_4)
```

```
# Classical Kriging with true covariance function
pred_grid <- seq(from = 0, to = 1, length.out = 200)
krig_mse <- rep(NA, 100)
```

```
mkrig_mse <- rep(NA, 100)
dkrig_mse <- rep(NA, 100)
ckrig_mse<- rep(NA, 100)
nn_mse <- rep(NA, 100)

krig_grid_pred <- matrix(NA, ncol = 200, nrow = 100)
mkrig_grid_pred <- matrix(NA, ncol = 200, nrow = 100)
dkrig_grid_pred <- matrix(NA, ncol = 200, nrow = 100)
ckrig_grid_pred <- matrix(NA, ncol = 200, nrow = 100)
nn_grid_pred <- matrix(NA, ncol = 200, nrow = 100)
```

```
for (rep_idx in 1:100) {
print(paste("Now calculating the index ",rep_idx))

train_index <- sample(1:1000, 800, replace = FALSE)
train_x <- s[train_index]
test_x <- s[-train_index]
train_y <- sim_dat[rep_idx,train_index]
test_y <- sim_dat[rep_idx,-train_index]

exp_sig_11 <- cov_mat[train_index, train_index]
exp_sig_12 <- cov_mat[train_index, -train_index]
exp_sig_21 <- t(exp_sig_12)
exp_sig_22 <- cov_mat[-train_index, -train_index]
krig_mean_temp <- 1 + exp_sig_21 %*% solve(exp_sig_11) %*%
                              matrix( as.numeric(sim_dat[rep_idx,train_index] - 1), ncol = 1 )
krig_mse[rep_idx] <- mean((krig_mean_temp - as.numeric(test_y))^2)

dist_pred <- spDists(cbind(1, c(train_x,pred_grid)))
cov_pred <- exp_cor(dist_pred)
grid_sig_11 <- cov_pred[(1:length(train_x)),(1:length(train_x))]
grid_sig_12 <- cov_pred[(1:length(train_x)),((length(train_x)+1):nrow(cov_pred))]
grid_sig_21 <- t(grid_sig_12)
grid_sig_22 <- cov_pred[((length(train_x)+1):nrow(cov_pred)),((length(train_x)+1):nrow(cov_pred))]
krig_grid_pred[rep_idx,] <-  1 + grid_sig_21 %*% solve(grid_sig_11) %*%
                              matrix( as.numeric(train_y) - 1, ncol = 1 )
}
```

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```
neg_llh_matern <- function(params){
  mu <- params[1]
  phi <- params[2]
  sig <- params[3]
  out <- mvtnorm::dmvnorm(curr_sim_y, mean = rep(mu, length(curr_sim_y)),
                          sigma = sig* Matern( spDists(cbind(1,s)), range = phi, nu = 1.5), log = TRUE )
  return(-out)

}

for (rep_idx in 1:100) {
print(paste("Now calculating the index ",rep_idx))

train_index <- sample(1:1000, 800, replace = FALSE)
train_x <- s[train_index]
test_x <- s[-train_index]
train_y <- sim_dat[rep_idx,train_index]
test_y <- sim_dat[rep_idx,-train_index]

curr_sim_y <- as.numeric(sim_dat[rep_idx,])
curr_params <- optim(c(1,0.1,1), neg_llh_matern)$par
curr_mu <- curr_params[1]
```

```
curr_phi <- curr_params[2]
curr_sig <- curr_params[3]
curr_cov_mat <- curr_sig * Matern( spDists(cbind(1,s)), range = curr_phi, nu = 1.5)


mat_sig_11 <- curr_cov_mat[train_index, train_index]
mat_sig_12 <- curr_cov_mat[train_index, -train_index]
mat_sig_21 <- t(mat_sig_12)
mat_sig_22 <- curr_cov_mat[-train_index, -train_index]
mkrig_mean_temp <- curr_mu + mat_sig_21 %*% solve(mat_sig_11) %*%
                             matrix( as.numeric(sim_dat[rep_idx,train_index] - curr_mu), ncol = 1 )

mkrig_mse[rep_idx] <- mean((mkrig_mean_temp - as.numeric(test_y))^2)

dist_pred <- spDists(cbind(1, c(train_x,pred_grid)))
cov_pred <- Matern(dist_pred, range = curr_phi, nu = 1.5)

grid_sig_11 <- cov_pred[(1:length(train_x)),(1:length(train_x))]
grid_sig_12 <- cov_pred[(1:length(train_x)),((length(train_x)+1):nrow(cov_pred))]
grid_sig_21 <- t(grid_sig_12)
grid_sig_22 <- cov_pred[((length(train_x)+1):nrow(cov_pred)),((length(train_x)+1):nrow(cov_pred))]
mkrig_grid_pred[rep_idx,] <-  curr_mu + grid_sig_21 %*% solve(grid_sig_11) %*%
                             matrix( as.numeric(train_y) - curr_mu, ncol = 1 )



}
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```

```
for (rep_idx in 1:100) {
print(paste("Now calculating the index ",rep_idx))

train_index <- sample(1:1000, 800, replace = FALSE)
train_x <- s[train_index]
test_x <- s[-train_index]
train_y <- sim_dat[rep_idx,train_index]
test_y <- sim_dat[rep_idx,-train_index]


x_tr <- cbind(1, matrix(as.numeric(train_x), ncol = 1))
x_te <- cbind(1, matrix(as.numeric(test_x), ncol = 1))
x_tr <- array_reshape(x_tr, c(nrow(x_tr), 2))
x_te <- array_reshape(x_te, c(nrow(x_te), 2))

z_tr <- as.numeric(sim_dat[rep_idx,train_index])
z_te <- as.numeric(sim_dat[rep_idx,-train_index])

  model_dnn <- keras_model_sequential()

  model_dnn %>%
  layer_dense(units = 100, activation = 'relu', input_shape = c(ncol(x_tr))) %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 1, activation = 'linear')

  model_dnn %>% compile(
    loss = "mse",
```

```
    optimizer = optimizer_adam(),
    metrics = list("mse")
  )

  mod_train_dnn <- model_dnn %>%
    fit(x = x_tr, y = z_tr, epochs = 100, batch_size = 32)

  nn_mean_temp <- predict(model_dnn, x_te)

  nn_mse[rep_idx] <- mean((krig_mean_temp - as.numeric(test_y))^2)

  nn_grid_pred[rep_idx,] <- predict(model_dnn, cbind(1, pred_grid))
}
```

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for (rep_idx in 1:100) {

  print(paste("Now calculating the index ",rep_idx))

  train_index <- sample(1:1000, 800, replace = FALSE)
  train_x <- s[train_index]
  test_x <- s[-train_index]
  train_y <- sim_dat[rep_idx,train_index]
  test_y <- sim_dat[rep_idx,-train_index]

  x_tr <- cbind(1, matrix(as.numeric(train_x), ncol = 1), basis_fun_all[train_index,])
  x_te <- cbind(1, matrix(as.numeric(test_x), ncol = 1), basis_fun_all[-train_index,])

  z_tr <- as.numeric(sim_dat[rep_idx,train_index])
  z_te <- as.numeric(sim_dat[rep_idx,-train_index])

  model_dk <- keras_model_sequential()

  model_dk %>%
  layer_dense(units = 100, activation = 'relu', input_shape = c(ncol(x_tr))) %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 1, activation = 'linear')


  model_dk %>% compile(
    loss = "mse",
    optimizer = optimizer_adam(),
    metrics = list("mse")
  )

  mod_train_dk <- model_dk %>%
    fit(x = x_tr, y = z_tr, epochs = 100, batch_size = 32)

  dkrig_mean_temp <- predict(model_dk, x_te)
  dkrig_mse[rep_idx] <- mean((dkrig_mean_temp - as.numeric(test_y))^2)

  pred_dist_1 <- spDists(cbind(1, pred_grid), cbind(1, basis_1))
  pred_dist_2 <- spDists(cbind(1, pred_grid), cbind(1, basis_2))
  pred_dist_3 <- spDists(cbind(1, pred_grid), cbind(1, basis_3))
  pred_dist_4 <- spDists(cbind(1, pred_grid), cbind(1, basis_4))
```

```
  pred_basis_1 <- matrix(nychka_fun(pred_dist_1, theta_1), nrow = length(pred_grid))
  pred_basis_2 <- matrix(nychka_fun(pred_dist_2, theta_2), nrow = length(pred_grid))
  pred_basis_3 <- matrix(nychka_fun(pred_dist_3, theta_3), nrow = length(pred_grid))
  pred_basis_4 <- matrix(nychka_fun(pred_dist_4, theta_4), nrow = length(pred_grid))

  pred_basis_all <- cbind(pred_basis_1,pred_basis_2,pred_basis_3,pred_basis_4)

  x_pre <- cbind(1, pred_grid, pred_basis_all)

  dkrig_grid_pred[rep_idx,] <- predict(model_dk, x_pre)
}
```

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```

```
for (rep_idx in 1:100) {

  print(paste("Now calculating the index ",rep_idx))

  train_index <- sample(1:1000, 800, replace = FALSE)
  train_x <- s[train_index]
  test_x <- s[-train_index]
  train_y <- sim_dat[rep_idx,train_index]
  test_y <- sim_dat[rep_idx,-train_index]

  x_tr <- cbind(1, matrix(as.numeric(train_x), ncol = 1), basis_fun_4[train_index,])
  x_te <- cbind(1, matrix(as.numeric(test_x), ncol = 1), basis_fun_4[-train_index,])
  x_tr <- array_reshape(x_tr, c(length(train_y), 75, 1))
  x_te <- array_reshape(x_te, c(length(test_y), 75, 1))

  input_shape <- c(75, 1)

  z_tr <- as.numeric(sim_dat[rep_idx,train_index])
  z_te <- as.numeric(sim_dat[rep_idx,-train_index])

  model_ck <- keras_model_sequential() %>%
  layer_conv_1d(filters = 64, kernel_size = 3, activation = 'relu', input_shape = input_shape) %>%
  layer_flatten() %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 1, activation = 'linear')


model_ck %>% compile(
  loss = "mse",
  optimizer = optimizer_adam(),
  metrics = list("mse")
)


mod_train_ck <- model_ck %>%
  fit(x = x_tr, y = z_tr, epochs = 100, batch_size = 32)

  ckrig_mean_temp <- predict(model_ck, x_te)
  ckrig_mse[rep_idx] <- mean((ckrig_mean_temp - as.numeric(test_y))^2)

  pred_dist_4 <- spDists(cbind(1, pred_grid), cbind(1, basis_4))
```

```
  pred_basis_4 <- matrix(nychka_fun(pred_dist_4, theta_4), nrow = length(pred_grid))

  x_pre <- cbind(1, pred_grid, pred_basis_4)

  x_pre <- array_reshape(x_pre, c(length(pred_grid), 75, 1))

  ckrig_grid_pred[rep_idx,] <- predict(model_ck, x_pre)

}
```

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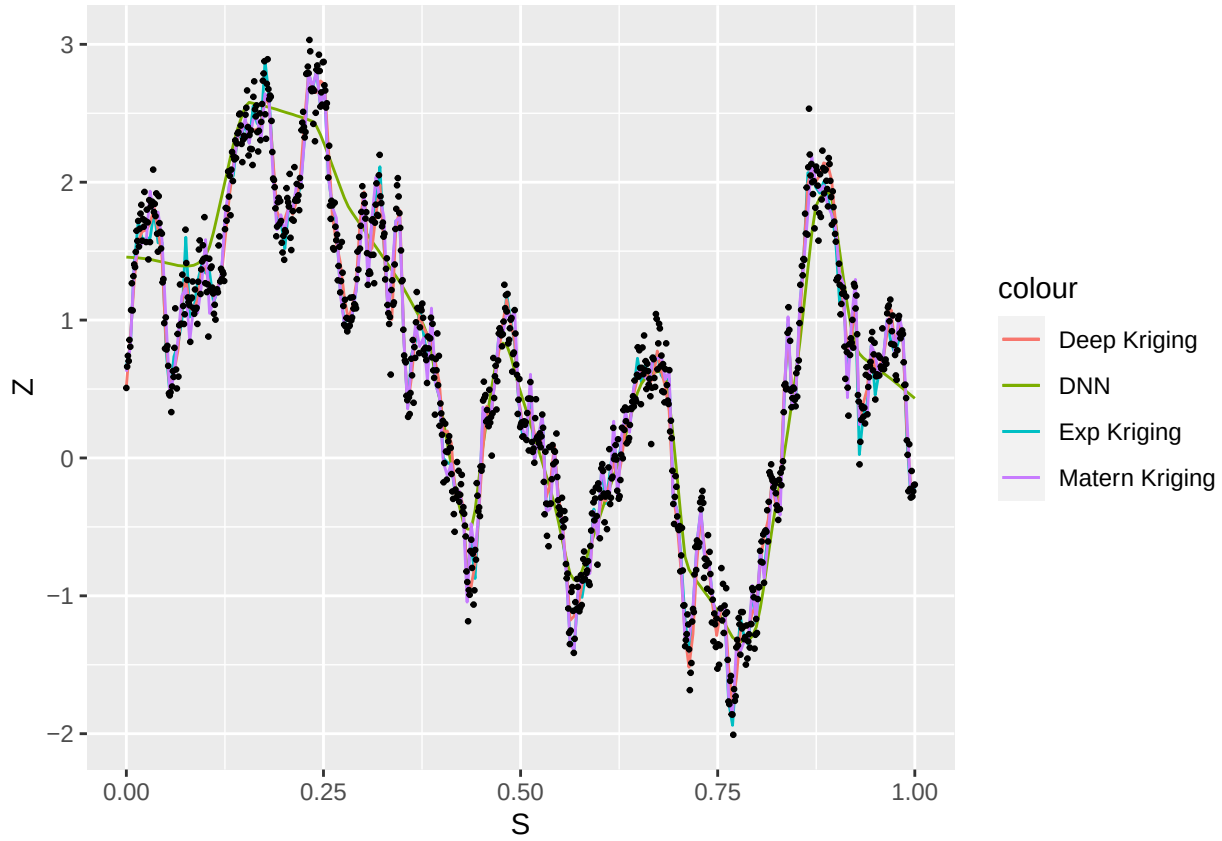
```
show_idx <- 77
ggplot() +
  geom_path(aes(x = seq(from = 0, to = 1, length.out = 200), y = krig_grid_pred[show_idx,], color = "Exp
  geom_path(aes(x = seq(from = 0, to = 1, length.out = 200), y = nn_grid_pred[show_idx,], color = "DNN"
  geom_path(aes(x = seq(from = 0, to = 1, length.out = 200), y = dkrig_grid_pred[show_idx,], color = "De
  geom_path(aes(x = seq(from = 0, to = 1, length.out = 200), y = mkrig_grid_pred[show_idx,], color = "Ma
  geom_point( aes(x = seq(from = 0, to = 1, length.out = 1000), y = as.numeric(sim_dat[show_idx,])), siz
  labs(x = "S", y = "Z")
```




```
mse.all <- cbind(krig_mse, mkrig_mse, dkrig_mse, ckrig_mse, nn_mse)
write.csv(mse.all, here::here("chen_simulation/mse_all.csv"), row.names = FALSE)
write.csv(krig_grid_pred, here::here("chen_simulation/krig_grid_pred.csv"), row.names = FALSE)
write.csv(ckrig_grid_pred, here::here("chen_simulation/ckrig_grid_pred.csv"), row.names = FALSE)
write.csv(mkrig_grid_pred, here::here("chen_simulation/mkrig_grid_pred.csv"), row.names = FALSE)
write.csv(dkrig_grid_pred, here::here("chen_simulation/dkrig_grid_pred.csv"), row.names = FALSE)
write.csv(nn_grid_pred, here::here("chen_simulation/nn_grid_pred.csv"), row.names = FALSE)
```