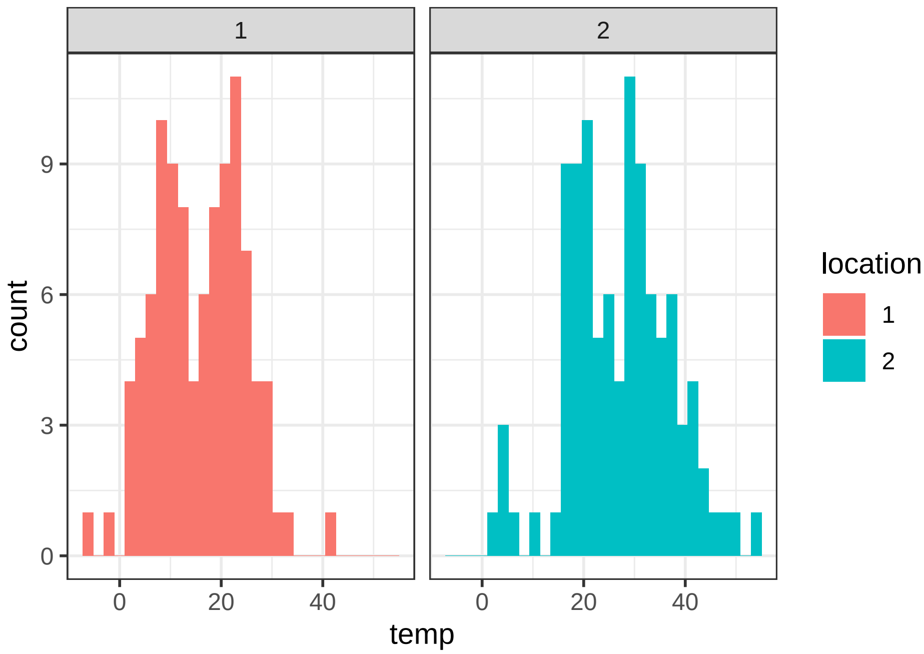
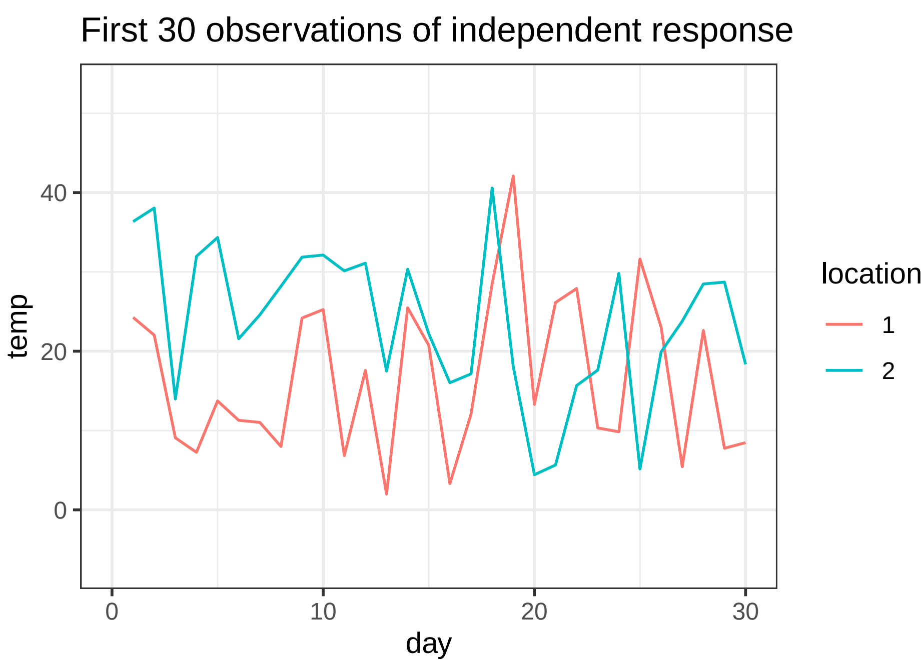
GP demo

Multivariate Normal Distribution First we will start with the a bivariate normal distribution:

```
library(mnormt)
n <- 100
theta <- c(15,25)
sigma <- diag(2) * 100
fake_temperatures <- rmnorm(n, theta , sigma)
```

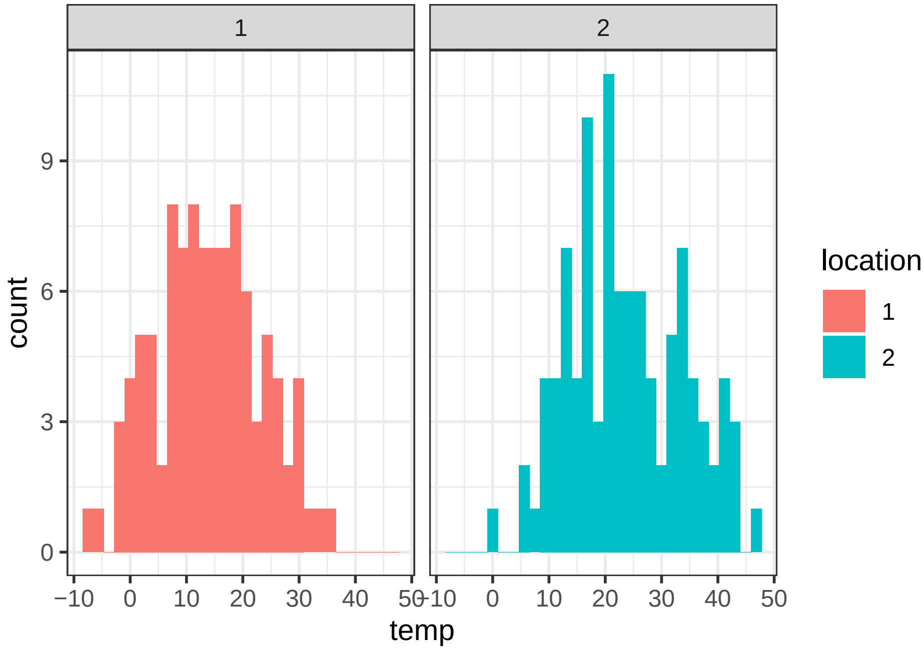
Independent bivariate normal

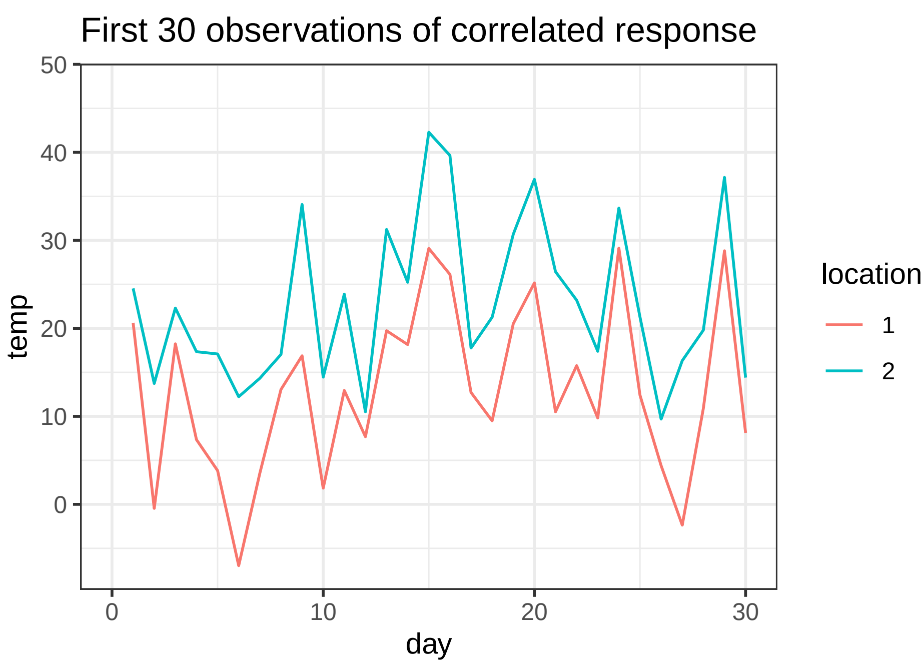




```r
sigma <- matrix(c(1, .9, .9, 1), nrow = 2, ncol = 2) * 100
fake_temperatures_corr <- rmnorm(n, theta , sigma)
```

Correlated bivariate normal





In many statistical models there is an assumption about independence. When independence is violated, uncertainty is under estimated and in incorrect inferences can be made.

Conditional Normal distribution In general,

$$\underline{y_1}|\underline{y_2} \sim N\left(X_1\beta + \Sigma_{12}\Sigma_{22}^{-1}\left(\underline{y_2} - X_2\beta\right), \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}\right)$$

Conditional on the values from Bridger Bowl and Big Sky, we can construct the distribution for the Rendezvous temperature.

```
fake_temperatures1 <- c(30,30)
mu_given <- mu[3] + Sigma[3,1:2] %*% solve(Sigma[1:2,1:2]) %*% (fake_temperatures1 - mu[1:2])
sigma_given <- Sigma[3,3] - Sigma[3,1:2] %*% solve(Sigma[1:2,1:2]) %*% Sigma[1:2, 3]

x_seq <- seq(-15, 55, by = 1)

tibble(x = rep(x_seq,2),
       dens = c(dnorm(x_seq, mu[3], sqrt(Sigma[3,3])),
                dnorm(x_seq, mu_given, sqrt(sigma_given))),
      type = rep(c('marginal','conditional'), each = length(x_seq) )) %>%
  ggplot(aes(x = x, y = dens, group = type, color = type)) +
  geom_line() + theme_bw() +
  geom_vline(xintercept = fake_temperatures1)
```

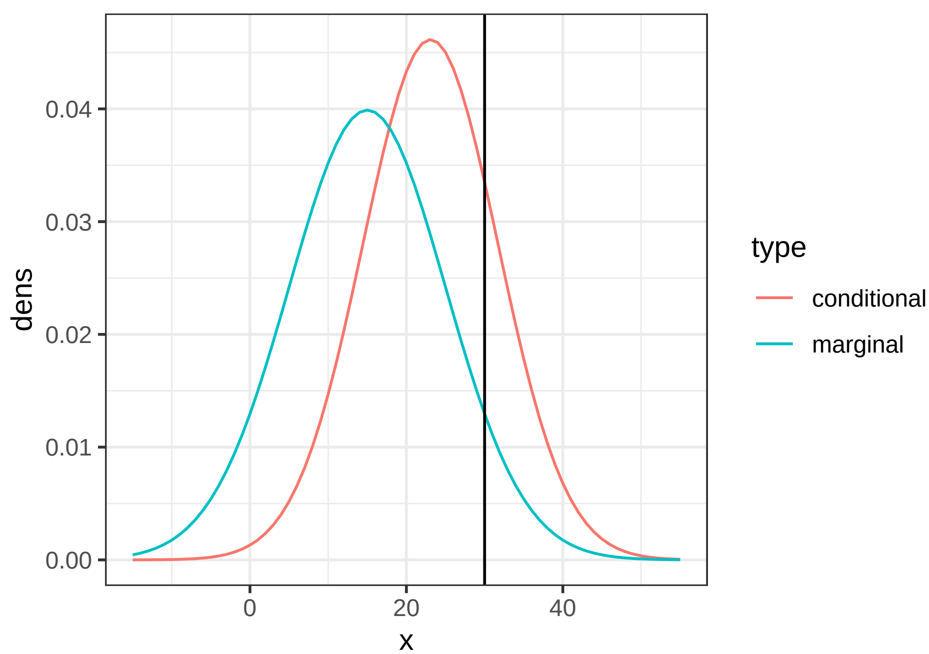


Figure 1: Black bars represent observed temperature at Big Sky and Bridger

GP regression We will simulate a Gaussian process regression, where

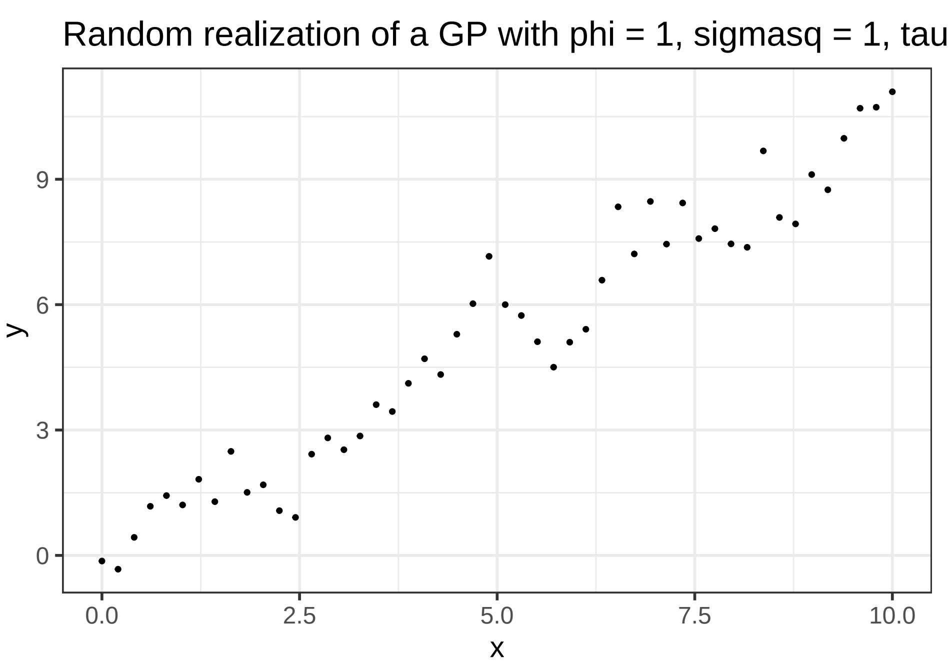
1. Set up the model parameters

```
phi <- 1
sigmasq <- 1
tausq <- .2
n <- 50
x <- seq(0, 10, length.out = n)
beta <- 1
d <- sqrt(plgp::distance(x))
eps <- sqrt(.Machine$double.eps)
H <- exp(-d/phi) + diag(eps, n)
```

2. Simulate a finite realization from the process

```
y <- rmnorm(1, x * beta,sigmasq * H + tausq * diag(n))
```

```
reg_fig <- tibble(y = y, x = x) %>% ggplot(aes(y=y, x=x)) +
  theme_bw() + ggtitle('Random realization of a GP with phi = 1, sigmasq = 1, tausq = .2') +
  geom_point(size = .5)
reg_fig
```




```
n_preds <- 50
x_preds <- seq(-1, 11, length.out = n_preds)
d_12 <- sqrt(plgp::distance(x, x_preds))
d_preds <- sqrt(plgp::distance(x_preds))
```

STAN CODE

```
data {
  int<lower=0> N; // number of data points
  vector[N] y; // response
  matrix[N,N] dist; // distance matrix
  vector[N] x; // covariate
  int<lower=0> N_preds;
  matrix[N_preds, N_preds] dist_preds;
  matrix[N, N_preds] dist_12;
  vector[N_preds] x_preds; // covariate
}

parameters {
  real<lower = 0.25, upper = 9> phi;
  real<lower = 0> sigmasq;
  real<lower = 0> tausq;
  real beta;
}

transformed parameters{
  vector[N] mu_vec;
  vector[N] tausq_vec;
  corr_matrix[N] Sigma;

  for(i in 1:N) mu_vec[i] = x[i] * beta;
  for(i in 1:N) tausq_vec[i] = tausq;

  for(i in 1:(N-1)){
   for(j in (i+1):N){
     Sigma[i,j] = exp((-1)*dist[i,j]/ phi);
     Sigma[j,i] = Sigma[i,j];
    }
 }
 for(i in 1:N) Sigma[i,i] = 1;

}

model {
  y ~ multi_normal(mu_vec ,sigmasq * Sigma + diag_matrix(tausq_vec));
  phi ~ inv_gamma(10, 10);
  sigmasq ~ inv_gamma(10, 10);
  tausq ~ inv_gamma(10, 2);
  beta ~ normal(0, 10);
}


generated quantities {
  vector[N_preds] y_preds;
  vector[N] y_diff;
  vector[N_preds] mu_preds;
  corr_matrix[N_preds] Sigma_preds;
  vector[N_preds] tausq_preds;
  matrix[N, N_preds] Sigma_12;
```

```
  for(i in 1:N_preds) tausq_preds[i] = tausq;
  for(i in 1:N_preds) mu_preds[i] = x_preds[i] * beta;
  for(i in 1:N) y_diff[i] = y[i] - x[i] * beta;


  for(i in 1:(N_preds-1)){
   for(j in (i+1):N_preds){
     Sigma_preds[i,j] = exp((-1)*dist_preds[i,j]/ phi);
     Sigma_preds[j,i] = Sigma_preds[i,j];
   }
 }
 for(i in 1:N_preds) Sigma_preds[i,i] = 1;

   for(i in 1:(N)){
   for(j in (1):N_preds){
     Sigma_12[i,j] = exp((-1)*dist_12[i,j]/ phi);
   }
 }

 y_preds = multi_normal_rng(mu_preds + (sigmasq * Sigma_12)' * inverse(sigmasq * Sigma) * (y_diff),
 sigmasq * Sigma_preds + diag_matrix(tausq_preds) - (sigmasq * Sigma_12)' *
 inverse(sigmasq * Sigma + diag_matrix(tausq_vec)) *
 (sigmasq * Sigma_12) );
}
```

```r
Reg_params <- stan("GP_reg.stan",
                  data=list(N = n,
                            y = y,
                            x = x,
                            dist = d,
                            N_preds = n_preds,
                            dist_preds = d_preds,
                            dist_12 = d_12,
                            x_preds = x_preds),
                  iter = 2000)

#shinystan::launch_shinystan(Reg_params)
```

```r
print(Reg_params, pars = c('phi', 'beta','sigmasq', 'tausq',
                           'y_preds[1]', 'y_preds[50]'))
```

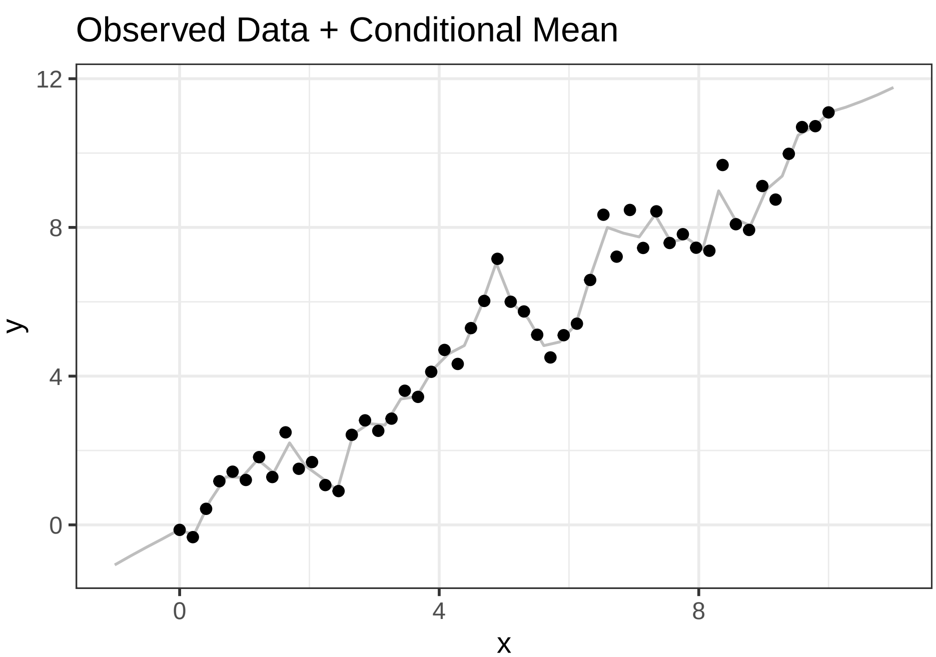
```
## Inference for Stan model: GP_reg.
## 4 chains, each with iter=2000; warmup=1000; thin=1;
## post-warmup draws per chain=1000, total post-warmup draws=4000.
##
##              mean se_mean   sd  2.5%   25%   50%   75% 97.5% n_eff Rhat
## phi          1.03    0.01 0.31  0.59  0.82  0.98  1.19  1.77  3559    1
## beta         1.05    0.00 0.07  0.93  1.01  1.05  1.09  1.19  3103    1
## sigmasq      0.92    0.00 0.24  0.55  0.76  0.89  1.06  1.49  3582    1
## tausq        0.20    0.00 0.05  0.12  0.16  0.19  0.23  0.32  3696    1
## y_preds[1]  -1.08    0.02 1.01 -3.03 -1.76 -1.10 -0.40  0.96  3840    1
## y_preds[50] 11.76    0.02 1.09  9.65 11.01 11.79 12.49 13.92  3780    1
##
## Samples were drawn using NUTS(diag_e) at Tue Mar  2 15:02:13 2021.
```

```
## For each parameter, n_eff is a crude measure of effective sample size,
## and Rhat is the potential scale reduction factor on split chains (at
## convergence, Rhat=1).
```

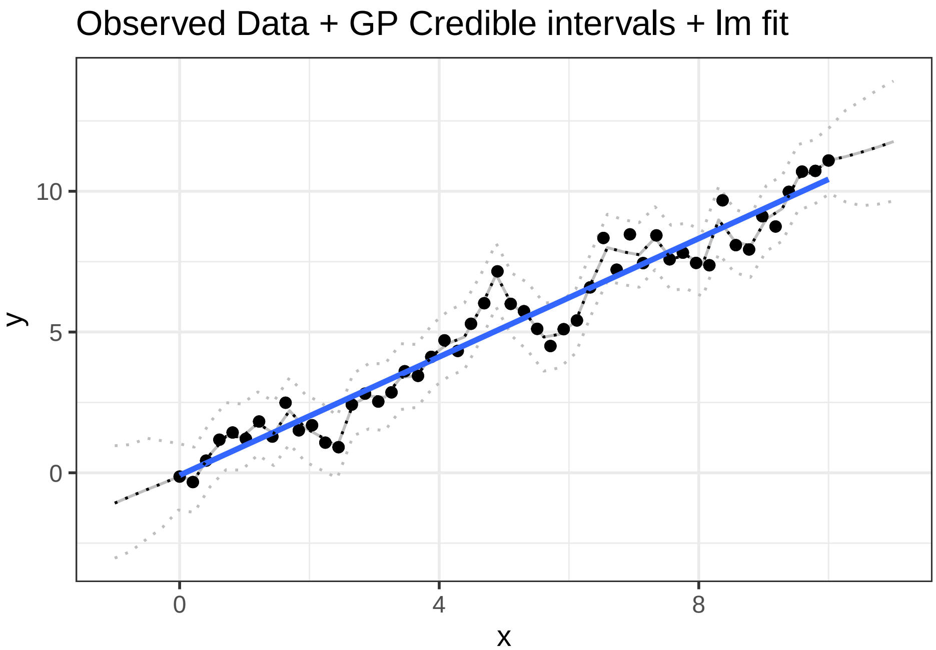
```
preds <- extract(Reg_params)['y_preds']$y_preds
mean_preds <- colMeans(preds)
lower_preds <- apply(preds, 2, quantile, probs = .025)
upper_preds <- apply(preds, 2, quantile, probs = .975)

mean_line <- tibble(y_mean = mean_preds, xnew = x_preds,
                    lower = lower_preds, upper = upper_preds)
data_and_mean <- reg_fig +
  geom_line(aes(y = y_mean, x = xnew), inherit.aes = F, data = mean_line, color = 'gray') +
  geom_point() +
  ggtitle("Observed Data + Conditional Mean")
data_and_mean
```

Making Predictions




```
data_and_mean +
  geom_line(aes(y = upper, x = xnew), inherit.aes = F,
            data = mean_line, color = 'gray', linetype = 3) +
  geom_line(aes(y = lower, x = xnew), inherit.aes = F,
            data = mean_line, color = 'gray', linetype = 3) +
  ggtitle('Observed Data + GP Credible intervals + lm fit') +
  geom_point() +
  geom_smooth(method ='lm', formula = 'y~x', se = F) +
  geom_line(aes(y = y_mean, x = xnew), inherit.aes = F,
            data = mean_line, color = 'black', linetype = 3)
```


Observed Data + GP Credible intervals + lm fit
y
10
5
0
0
4
8
x