### February 12, 2021

### 0.1 Q1: 1D Gaussians

### Can the probability density function (pdf) of X ever take values greater than 1?

yes, it can. In fact the only important thing is the sum of the area under the pdf curve. Also, pdf can not be negative as it is the derivative of the CDF function which is a non-decreasing function.

Write the expression for the pdf of a univariate gaussian:

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2}$$

Write the code for the function that computes the pdf at x.

```
[1]: import numpy as np from math import pi
```

Test your implementation against a standard implementation:

```
[5]: from scipy.stats import norm
```

```
[8]: def test(x, mean, variance):
    assert gaussian_pdf(x, mean, variance) == norm.pdf(x, loc=mean, u
    ⇒scale=variance)
```

What is the value of the pdf at x = 0? What is probability that x = 0? value of pdf at 0 is  $\frac{1}{\sqrt{2\pi}\sigma}$  but the probability of drawing x=0 is zero.

Write the transformation that takes  $x \sim \mathcal{N}(0., 1.)$  to  $z \sim \mathcal{N}(\mu, \sigma^2)$ 

```
[6]: def transform(x, mu, sigma):
    return sigma * x + mu
```

Write a code to sample from  $\mathcal{N}(\mu, \sigma^2)$ :

```
[7]: def sample_gaussian(n, mean=0, variance=0.01):
    return [transform(np.random.normal(), mean, variance ** 0.5) for _ in_
    →range(n)]
```

Test your implementation by computing statistics on the samples:

```
[9]: import statistics

mean = 10.
variance = 1.28

sample = sample_gaussian(100000, mean=mean, variance=variance)

assert abs(statistics.mean(sample) - mean) < 1e-2
assert abs(statistics.variance(sample) - variance) < 1e-2

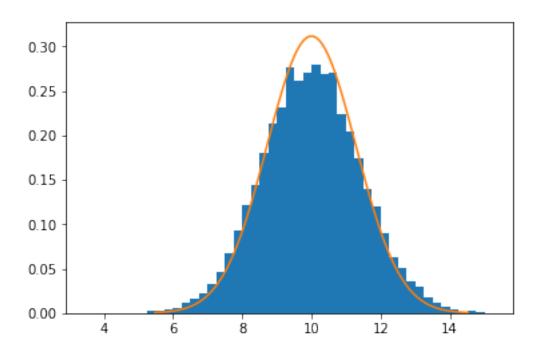
print('Yaaay!')</pre>
```

Yaaay!

Plot pdf and normalized histogram of samples:

```
[12]: import matplotlib.pyplot as plt
from scipy import stats

sample = sample_gaussian(10000, mean=10., variance=2.)
plt.hist(sample, density=True, bins=np.arange(3.5, 15.5, 0.25))
sigma = variance ** 0.5
x = np.linspace(mean - 4 * sigma, mean + 4 * sigma, 100)
plt.plot(x, stats.norm.pdf(x, mean, variance))
plt.show()
```



[]:

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# 1 Q2: High Dimensional Gaussians

### 1.1 Distance of Gaussian samples from origin

if we have  $x = [x_1, x_2, ..., x_d]^T$  then:

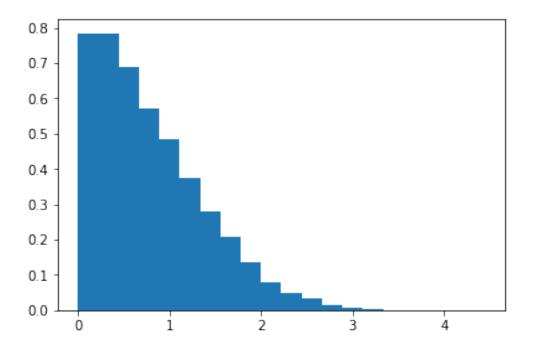
Euclidean dist. = Euclidean distance = 
$$\sqrt{\sum_{i=1}^{d} (x_i - 0)^2} = \sqrt{\sum_{i=1}^{d} x_i^2} = x^T x$$

```
[6]: import numpy as np
import matplotlib.pyplot as plt
from scipy.stats import chi
import scipy.stats as stats
```

# 1.2 Distribution of distances of Gaussian samples from origin

```
[3]: def norm(x): return x.dot(x) ** 0.5
```

```
[183]: V = np.random.randn(10000, 1)
dists = [norm(x) for x in V]
plt.hist(dists, density=True, bins=20)
plt.show()
```

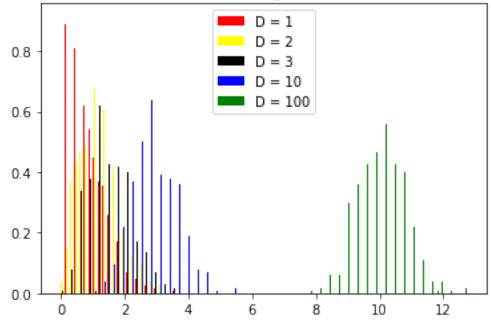


# Does this confirm your intuition that the samples will be near the origin?

As seen above, The first bin is higher than the others which is completely congruent with my intuition that most of the samples should be close to 0 (as the pdf is larger for them, they are more probable to be drawn).

### 1.3 Plot samples from distribution of distances





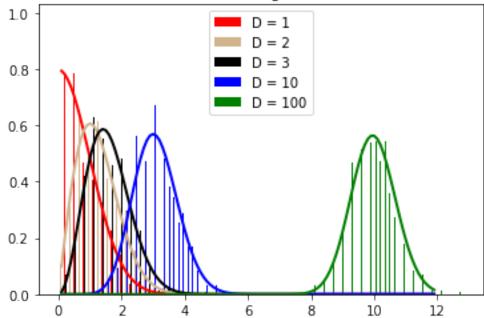
As the dimensionality of the Gaussian increases, what can you say about the expected distance of the samples from the Gaussian's mean (in this case, origin)?

The expected distance from origin increases as d increseas.

### 1.4 Plot samples from distribution of distances

```
plt.plot(x, stats.chi.pdf(x, df=3), color='black', lw=2)
plt.plot(x, stats.chi.pdf(x, df=10), color='blue', lw=2)
plt.plot(x, stats.chi.pdf(x, df=100), color='green', lw=2)
plt.show()
```

# Distrution of distances from the origin for different dimensionalities



### 1.5 Distribution of distance between samples

Taking two samples from the *D*-dimensional unit Gaussian,  $x_a, x_b \sim \mathcal{N}(0_D, I_D)$  how is  $x_a - x_b$  distributed?

One can easily prove that if X1 and X2 are two independent Gaussian RVs, with means  $\mu_1$  and  $\mu_2$  and variances  $\sigma_1^2$  and  $\sigma_2^2$ , then X + Y is another Gaussian random variable with mean  $\mu_1 + \mu_2$  and variance  $\sigma^2 = \sigma_1^2 + \sigma_2^2$  (This is a well known theorem and we can prove it using various methods, such as the characteristic or the moment generating function. For a more complete list of proofs you can visit this wikipedia page).

We can write  $x_a - x_b$  as  $x_a + (-x_b)$  where  $x_a$  and  $-x_b$  are distributed according to  $\mathcal{N}(0_D, I_D)$ . Therefore, sum of them would be a Gaussian random variable with the distribution  $\mathcal{N}(0_D, \sqrt{2}I_D)$ .

Using the above result about  $\chi$ -distribution, derive how  $||x_a - x_b||_2$  is distributed.

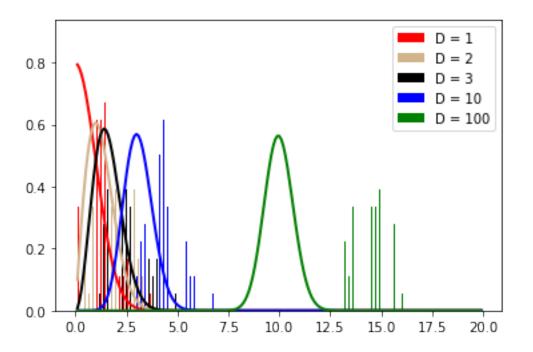
We know that  $Y=x_a-x_b$  is a Gaussian RV where its different dimensions are iid. Therefore,

based on what we know from previous parts, the following RV would be a Chi RV:

$$Z = \sqrt{\sum_{i=1}^{D} (\frac{Y_i - 0}{\sqrt{2}})^2} = \sqrt{\sum_{i=1}^{D} \frac{{Y_i}^2}{2}} = \frac{1}{\sqrt{2}} \sqrt{\sum_{i=1}^{D} Y_i^2}$$

Also,  $T = ||Y||_2 = \sqrt{\sum_{i=1}^D Y_i^2} = \sqrt{2}Z$ . We can compute the pdf of T using change of variables formula easily:

$$f(T=t) = f(\sqrt{2}Z=t) = f(Z=\frac{t}{\sqrt{2}};D) = \frac{1}{2^{k/2-1}\Gamma(k/2)}(\frac{t}{\sqrt{2}})^{D-1}\exp(-t^2/4)$$



# 1.6 Linear and Polar Interpolation Between Samples

[5]: from math import pi

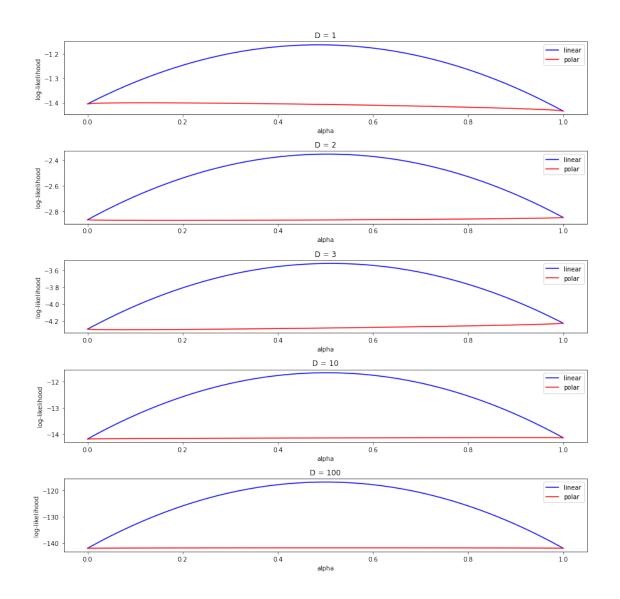
```
[6]: lin_interp = lambda alpha, x_a, x_b: alpha * x_a + (1 - alpha) * x_b
polar_interp = lambda alpha, x_a, x_b: alpha**0.5 * x_a + (1 - alpha)**0.5 * x_b

def ll_norm_stable(x):
    """
    stable log likelihood implementation of Normal distribution...
    """
    d = x.shape[0]
    return d * (-0.5 * np.log(2 * pi)) - 1/2 * np.sum(x ** 2)

[8]: D = [1, 2, 3, 10, 100]

fig, axs = plt.subplots(5, figsize=(15,15))
plt.subplots_adjust(hspace=0.5)

for i, d in enumerate(D):
    sample_1 = np.random.randn(1000, d)
    sample_2 = np.random.randn(1000, d)
```



Is a higher log-likelihood for the interpolated points necessarily better? Given this, is it a good idea to linearly interpolate between samples from a high dimensional Gaussian?

I do not think that higher likelihood implies betterness. Higher likelihood just shows that interpolated points on average are closer than the original sample points to the origin. In fact, the interpolated points are coming from another Gaussian distribution with the variance less than one  $(a^2 + (1-a)^2 < (a+1-a)^2 = 1)$ . Therefore they tend to be closer to the origin and have higher probabilities of begin drawn from the unit Gaussian distribution. In fact, one could sample arbitrary points from a Gaussian distribution with a variance close to zero and get much larger likelihood values from them. But again, this does not imply that these points are better than the original and interpolated points. They are just closer to the origin.

But I think for comparison we need a context. If, as mentioned in the forum of the course, we are going to use these interpolated points as inputs to a generative model, interpolated points would

better come from the original distribution on which the model is trained.

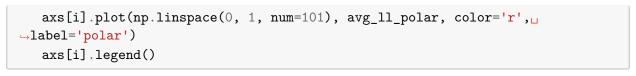
As the number of dimensions increases, the difference between likelihoods of original sample points and interpolated points gets bigger, which might result in a more dramatic change in the geometry of interplated points comparing to that of the original points. Again in particular, if we are going to feed these points to a generative model, it might be better to stick to the same distribution rather than change it.

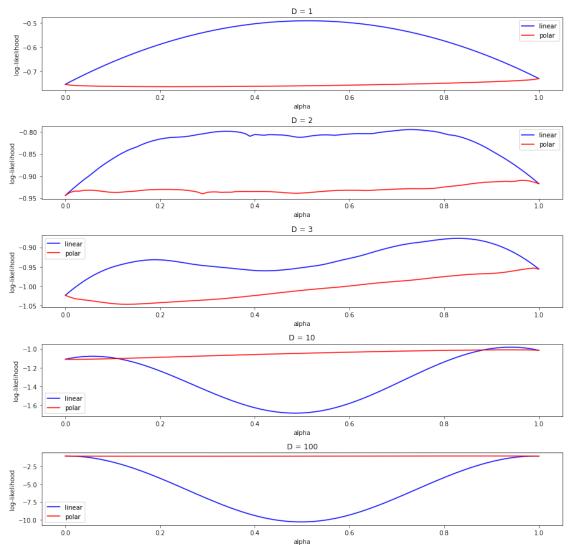
Comment on the log-likelihood under the unit Gaussian of points along the polar interpolation. Give an intuitive explanation for why polar interpolation is more suitable than linear interpolation for high dimensional Gaussians.

As seen in the plots, the log-likelihood of the interpolated points is approximately equal to the log-likelihood of original sample points across different  $\alpha$ 's. This is due to the fact that the polar interpolated points come from the same distribution which is unit Gaussian (Their mean is zero and the variance is  $\sqrt{a^2} + \sqrt{1-a^2} = 1$ ). This is also true for high dimensions whereas in the linear case, the difference gets bigger.

# 1.7 Norm along interpolation

```
[15]: from scipy.stats import chi
[16]: D = [1, 2, 3, 10, 100]
      fig, axs = plt.subplots(5, figsize=(15,15))
      plt.subplots_adjust(hspace=0.5)
      for i, d in enumerate(D):
          sample_1 = np.random.randn(1000, d)
          sample_2 = np.random.randn(1000, d)
          avg_ll_norm = np.zeros(101, dtype=np.float64)
          for j, alpha in enumerate(np.linspace(0, 1, num=101)):
              norm_linear = [norm(lin_interp(alpha, x1, x2))
                             for x1, x2 in zip(sample_1, sample_2)]
              norm_polar = [norm(polar_interp(alpha, x1, x2))
                            for x1, x2 in zip(sample_1, sample_2)]
              avg_ll_linear[j] = np.mean([chi.logpdf(x, df=d) for x in norm_linear])
              avg ll polar[j] = np.mean([chi.logpdf(x, df=d) for x in norm polar])
          axs[i].set_title(f'D = {d}')
          axs[i].set_xlabel('alpha')
          axs[i].set_ylabel('log-likelihood')
          axs[i].plot(np.linspace(0, 1, num=101), avg_ll_linear, color='b',__
       →label='linear')
```





# How does the log-likelihood along the linear interpolation compare to the log-likelihood of the true samples (endpoints)?

In low dimensional cases, it is bigger but in high dimensional cases it is smaller. This can imply that the linearly interpolated points have fallen in an area of the space where the probability of drawing a point is smaller. In fact, if we are going to again feed these interpolated points to a generative model, it could cause problems as the model might have not been trained well for these samples with low probabilities.

[]:

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# 1 Q3. Regression

### 1.1 Manually derived linear regression

### 1. What happens if n < m?

 $X^T$  is a  $n \times m$  matrix. if n < m, the null space of  $X^T$  is at least m - n > 0. Therefore the null space of  $XX^T$  is at least 1. Hence  $XX^T$  is not invertible. Tu put it differently,  $X^T\beta = y$  has infinitely many solutions and solving the linear regression problem in this case would be useless.

# 2. What are the expectation and covariance matrix of $\hat{\beta}$ , for a given true value of $\beta$ ?

Note that the only random variable here is y and X is a matrix of constant numbers. In fact we can write  $y = X^T \beta + \epsilon$  where  $\epsilon \sim \mathcal{N}(0, \sigma^2 I)$ . Therefore we can write:

$$\begin{split} E[(XX^T)^{-1}Xy] &= (XX^T)^{-1}E[X(X^T\beta + \epsilon)] \\ &= (XX^T)^{-1}[(XX^T)\beta + XE[\epsilon]] \\ &= (XX^T)^{-1}[(XX^T)\beta + 0] = (XX^T)^{-1}(XX^T)\beta = \beta \end{split}$$

Where we used  $E[\epsilon] = 0$ . Thus  $E[\hat{\beta}] = \beta$ .

For the variance we can write:

$$Var(\hat{\beta}) = E[((XX^T)^{-1}Xy)((XX^T)^{-1}Xy)^T]$$
$$-E[(XX^T)^{-1}Xy]E[(XX^T)^{-1}Xy]^T$$
$$= E[((XX^T)^{-1}Xy)((XX^T)^{-1}Xy)^T] - \beta\beta^T$$

We can simplify the first term:

$$E[((XX^{T})^{-1}Xy)((XX^{T})^{-1}Xy)^{T}]$$

$$= E[((XX^{T})^{-1}Xy)(y^{T}X^{T}((XX^{T})^{-1})^{T})]$$

$$= E[(XX^{T})^{-1}Xyy^{T}X^{T}((XX^{T})^{-1})^{T}]$$

$$= (XX^{T})^{-1}XE[yy^{T}]X^{T}((XX^{T})^{-1})^{T}$$

but we have  $E[yy^T] = \sigma^2 I$ . Therefore:

$$\begin{split} (XX^T)^{-1}XE[yy^T]X^T((XX^T)^{-1})^T \\ &= (XX^T)^{-1}X\sigma^2IX^T((XX^T)^{-1})^T \\ &= \sigma^2(XX^T)^{-1}(XX^T)((XX^T)^{-1})^T \\ &= \sigma^2((XX^T)^{-1})^T \end{split}$$

As  $(A^T)^{-1} = (A^{-1})^T$ , we can write:

$$Var(\hat{\beta}) = \sigma^2((XX^T)^{-1})^T = \sigma^2((XX^T)^T)^{-1} = \sigma^2(XX^T)^{-1}$$

Show that maximizing the likelihood is equivalent to minimizing the squared error  $\sum_{i=1}^{n} (y_i - x_i \beta)^2$ . [Hint: Use  $\sum_{i=1}^{n} a_i^2 = a^T a$ ]

Instead of working likelihood, we show that maximizing log-likelihood is equivalent to minimizing SELoss which derives the same result. We can write log-likelihood as:

$$\log L(\beta) = \log \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y_i - \beta x_i)^2}{2\sigma^2}\right)$$

which is equal to:

$$\sum_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp(-\frac{(y_i - \beta x_i)^2}{2\sigma^2}) = n \log \frac{1}{\sqrt{2\pi}\sigma} - \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - \beta x_i)^2$$

The first term in the above expression is independent of  $\beta$ . Therefore, only the second term remains. Thus, maximizing log-likelihood is equivalent to minimizing the second term which is  $\sum_{i=1}^{n} (y_i - x_i \beta)^2$  (if we ignore the constant  $\frac{1}{2\sigma^2}$  in the denominator)

4. Write the squared error in vector notation, (see above hint), expand the expression, and collect like terms. [Hint: Use  $\beta^T x^T y = y^T x \beta$  and  $x^T x$  is symmetric]

Squarred error loss would be:

$$(y - X^T \beta)^T (y - X^T \beta) = (y^T - \beta^T X)(y - X^T \beta) = (y^T y - y^T X^T \beta - \beta^T X y + \beta^T X X^T \beta)$$

According to the given hint we can rewrite this as:

$$y^Ty - 2\beta^TXy + \beta^TXX^T\beta$$

5. Use the likelihood expression to write the negative log-likelihood. Write the derivative of the negative log-likelihood with respect to  $\beta$ , set equal to zero, and solve to show the maximum likelihood estimate  $\hat{\beta}$  as above.

We have to minimize the value derived above in wrt beta. The derivative would be:

$$0 - 2Xy + 2XX^T\beta$$

If we set it equal to zero we have:

$$Xy = XX^T\beta$$

and by multiplying both sides, from left, in  $XX^T$  we can get  $\hat{\beta}$ :

$$\hat{\beta} = (XX^T)^{-1}Xy$$

```
[1]: import jax.numpy as jnp
      from numpy.random import randn
      from random import randint
      from jax import random, grad
      from matplotlib import pyplot as plt
 [2]: def generate_random_seed():
          return randint(0, 10000)
 [3]: def target_f1(x, sigma_true=0.3):
          key = random.PRNGKey(generate_random_seed())
          noise = random.normal(key, shape=x.shape)
          return (2 * x + sigma_true * noise).ravel()
[80]: def norm(a: float):
          return (a * a) ** 0.5
      def element_wise_norm(x):
          shape = x.shape
          return jnp.array([norm(el) for el in x.ravel()]).reshape(shape)
      def element_wise_sin(x):
          shape = x.shape
          return jnp.sin(x.ravel()).reshape(shape)
 [5]: def target_f2(x: jnp.ndarray):
          key = random.PRNGKey(generate_random_seed())
          noise = random.normal(key, shape=x.shape)
          y = 2 * x + element_wise_norm(x) * 0.3 * noise
          return y.ravel()
 [6]: def target_f3(x):
          key = random.PRNGKey(generate_random_seed())
          noise = random.normal(key, shape=x.shape)
         y = 2 * x + 5 * element_wise_sin(x * 0.5) + element_wise_norm(x) * 0.3 * noise
          return y.ravel()
```

# 1.2 Sample data from the target functions

```
[7]: def sample_batch(target_f, batch_size):
    key = random.PRNGKey(generate_random_seed())
    x = random.uniform(key, shape=(1, batch_size), minval=0., maxval=20.)
    y = target_f(x)
    return x, y
```

# 1.3 Test assumptions about your dimensions

```
[9]: n = 200
m = 1

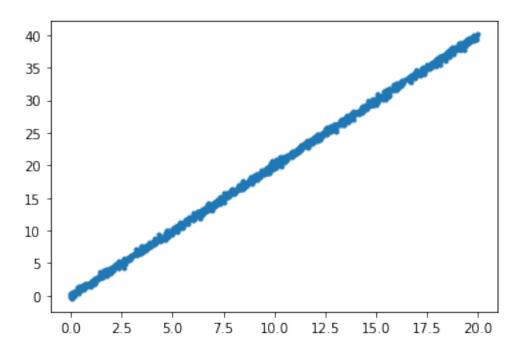
for target_f in [target_f1, target_f2, target_f3]:
    x, y = sample_batch(target_f, n)
    assert x.shape == (m, n)
    assert y.shape == (n,)
print('Yaay!')
```

Yaay!

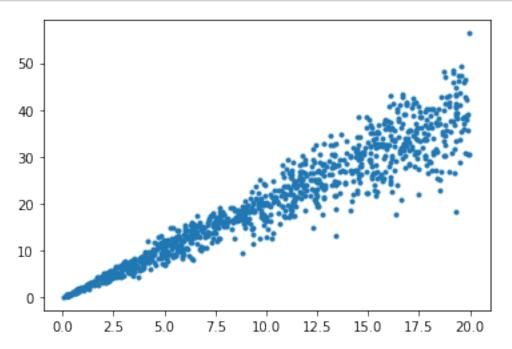
# 1.4 Plot the target functions

```
[167]: x, y = sample_batch(target_f1, 1000)

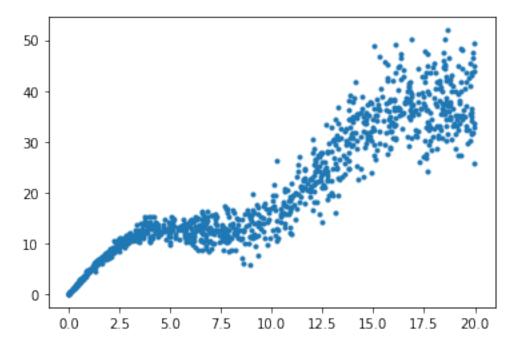
plt.plot(x[0], y, '.');
```



```
[168]: x, y = sample_batch(target_f2, 1000)
plt.plot(x[0], y, '.');
```



```
[169]: x, y = sample_batch(target_f3, 1000)
plt.plot(x[0], y, '.');
```



# 1.5 Linear regression model with $\hat{\beta}$ MLE

print(beta\_mle(\*sample\_batch(target\_f1, n)))

```
[8]: from jax.numpy.linalg import inv

def beta_mle(X, y):
    beta = inv(X.dot(X.T)) @ X @ y

    return beta
[11]: n = 1000
```

[2.0006847]

```
[172]: n = 1000
print(beta_mle(*sample_batch(target_f2, n)))
```

[1.9973272]

```
[173]: n = 1000
print(beta_mle(*sample_batch(target_f3, n)))
```

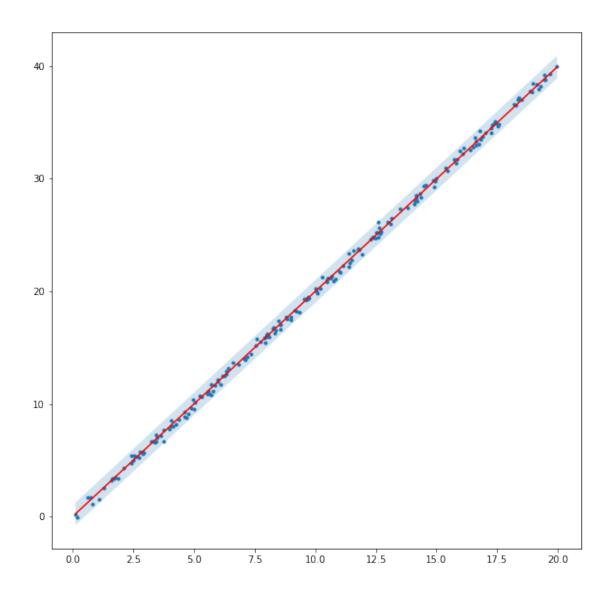
[2.0390666]

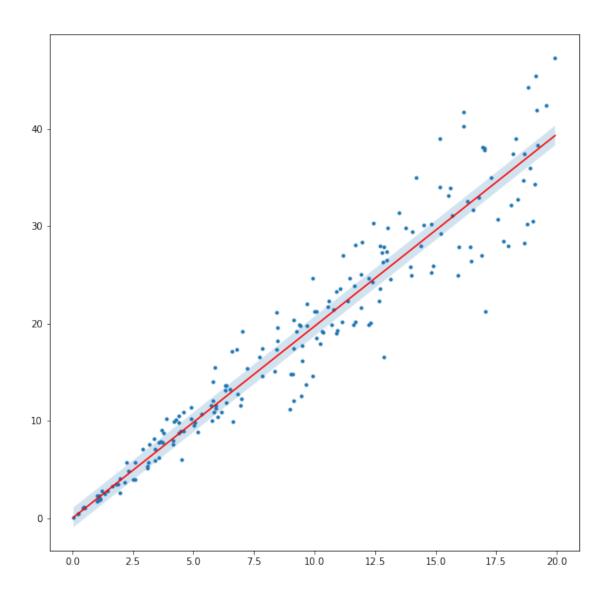
### 1.6 Plot the MLE linear regression model

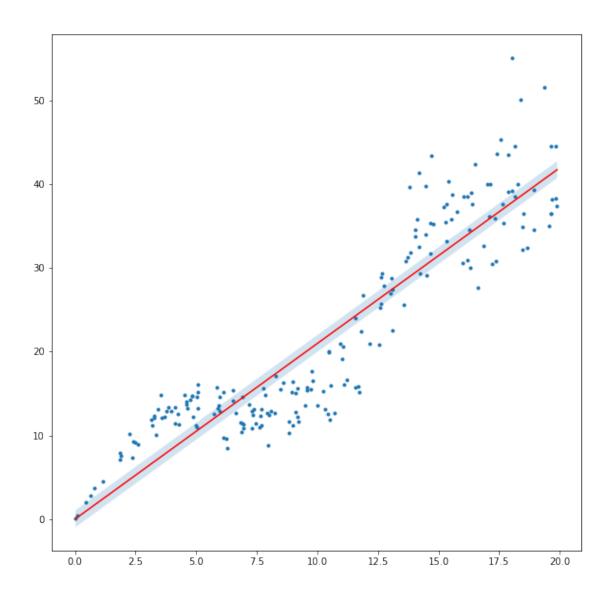
```
[180]: n = 200
X, y = sample_batch(target_f1, n)
beta_hat = beta_mle(X, y)
y_hat = (X.T @ beta_hat).ravel()
```

```
[34]: def sort_data(X, *args):
    """
    Due to the problem I had with shading in plots, I needed to sort the data
    →beforehand.
    """
    order = jnp.argsort(X)

return (X[order], *[arg[order] for arg in args])
```







# 1.7 Log-likelihood of Data under Model

```
[9]: from math import pi

def gaussian_log_likelihood(mu, sigma, x):
    return -0.5 * jnp.log(2 * pi) - jnp.log(sigma) - 0.5 * ((x - mu) / sigma) ** 2
```

### 1.8 Test Gaussian likelihood against standard implementation

```
[25]: from jax.scipy.stats import norm
      x = np.random.randn()
      mu = np.random.randn()
      sigma = np.random.rand()
      assert gaussian_log_likelihood(mu, sigma, x).shape == ()
      assert abs(gaussian_log_likelihood(mu, sigma, x) - norm.logpdf(x, mu, sigma)) <__
      →1e-2
      x = np.random.randn(100)
      mu = np.random.randn()
      sigma = np.random.rand()
      assert gaussian_log_likelihood(mu, sigma, x).shape == (100,)
      assert np.linalg.norm(gaussian_log_likelihood(mu, sigma, x) - norm.logpdf(x,__
      →mu, sigma)) < 1e-2
      x = np.random.randn(10)
      mu = np.random.randn(10)
      sigma = np.random.rand(10)
      assert gaussian_log_likelihood(mu, sigma, x).shape == (10,)
      assert np.linalg.norm(gaussian_log_likelihood(mu, sigma, x) - norm.logpdf(x,__
      →mu, sigma)) < 1e-2
      print('Yaay!')
```

Yaay!

# 1.9 Model Negative Log-likelihood

```
[10]: def lr_model_nll(beta, X, y, sigma):
    """
    This function takes the average nll loss not the sum!
    """
    return -jnp.mean(gaussian_log_likelihood(X.T.dot(beta), sigma, y))
```

### 1.10 Compute Negative-Log-Likelihood on data

```
[15]: for n in [10, 100, 1000]:
    print("-----", n, "-----")
    for i, target_f in enumerate([target_f1, target_f2, target_f3], 1):
        print(f"target_f{i}:")
        for sigma_model in [0.1, 0.3, 1., 2.]:
```

```
X, y = sample_batch(target_f, n)
            beta = beta_mle(X, y)
            nll = lr_model_nll(beta, X, y, sigma_model)
            print(f'Negative Log-likelihood (sigma={sigma_model}):', nll)
        print()
----- 10 -----
target_f1:
Negative Log-likelihood (sigma=0.1): 3.0840688
Negative Log-likelihood (sigma=0.3): 0.058412135
Negative Log-likelihood (sigma=1.0): 0.9527103
Negative Log-likelihood (sigma=2.0): 1.6253029
target_f2:
Negative Log-likelihood (sigma=0.1): 18.992615
Negative Log-likelihood (sigma=0.3): 87.8604
Negative Log-likelihood (sigma=1.0): 4.381679
Negative Log-likelihood (sigma=2.0): 2.0206194
target_f3:
Negative Log-likelihood (sigma=0.1): 1068.7898
Negative Log-likelihood (sigma=0.3): 68.174416
Negative Log-likelihood (sigma=1.0): 5.471425
Negative Log-likelihood (sigma=2.0): 5.4330153
----- 100 -----
target_f1:
Negative Log-likelihood (sigma=0.1): 4.108435
Negative Log-likelihood (sigma=0.3): 0.17373458
Negative Log-likelihood (sigma=1.0): 0.971069
Negative Log-likelihood (sigma=2.0): 1.6253384
target_f2:
Negative Log-likelihood (sigma=0.1): 582.2185
Negative Log-likelihood (sigma=0.3): 45.583046
Negative Log-likelihood (sigma=1.0): 7.913444
Negative Log-likelihood (sigma=2.0): 2.577579
target_f3:
Negative Log-likelihood (sigma=0.1): 914.03516
Negative Log-likelihood (sigma=0.3): 124.541725
Negative Log-likelihood (sigma=1.0): 17.326544
Negative Log-likelihood (sigma=2.0): 4.5580425
----- 1000 -----
target f1:
Negative Log-likelihood (sigma=0.1): 3.3210075
```

```
Negative Log-likelihood (sigma=0.3): 0.23444797
Negative Log-likelihood (sigma=1.0): 0.9643055
Negative Log-likelihood (sigma=2.0): 1.6237512

target_f2:
Negative Log-likelihood (sigma=0.1): 599.31506
Negative Log-likelihood (sigma=0.3): 66.63726
Negative Log-likelihood (sigma=1.0): 6.4717426
Negative Log-likelihood (sigma=2.0): 3.0156565

target_f3:
Negative Log-likelihood (sigma=0.1): 1074.2886
Negative Log-likelihood (sigma=0.3): 129.02122
Negative Log-likelihood (sigma=1.0): 13.237523
Negative Log-likelihood (sigma=2.0): 4.361741
```

#### 1.11 Effect of model variance

### For each target function what is the best choice of sigma?

Larger sigmas works better for target\_f2 and target\_f3 which is intuitive as the there is a huge variance for larger values of y. For target\_f1  $\sigma = 0.3$  works better (very large  $\sigma$  in this case would be bad as the points are close enough to the regression line. very small  $\sigma$  would also be bad as many of the points fall out of the shaded region).

#### 1.12 Automatic differentiation and maximum likelihood

#### 1.13 Compute gradients with AD, Test against hand-derived

```
[49]: key = random.PRNGKey(generate_random_seed())
    key, subkey = random.split(key)

    beta_test = random.normal(subkey, shape=(1,))

    key, subkey = random.split(key)
    sigma_test = random.normal(subkey)

    n = 100

    X, y = sample_batch(target_f1, n)
    grad_fn = grad(lr_model_nll, argnums=0)

    ad_grad = grad_fn(beta_test, X, y, sigma_test)
    hand_derivative = 1/n * 1/(sigma_test ** 2) * (X @ X.T @ beta_test - X @ y)
```

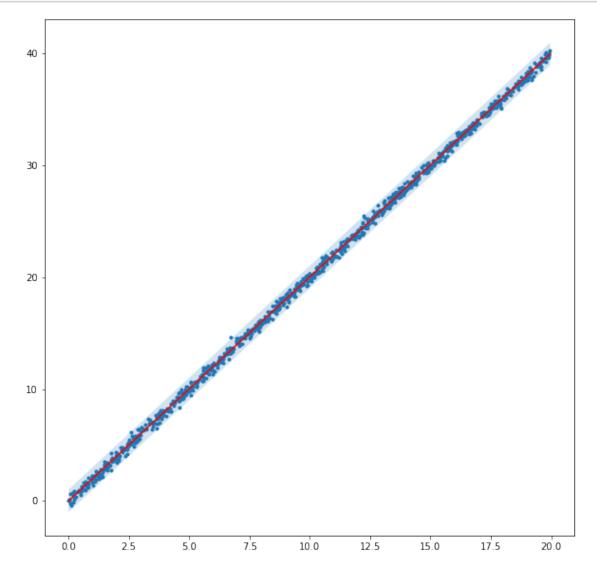
```
assert (ad_grad - hand_derivative).item() < 1e-2
print('Yaay!')</pre>
```

Yaay!

### 1.14 Train linear regression model with gradient descent

#### 1.15 Plot learned models

```
[85]: beta_init = -100.
      beta_learned_f1 = train_lin_reg(target_f1, lr=1e-3, iters= 100,__
       →beta_init=beta_init, print_every=10)
     iteration 0, loss: 695530.25, beta: -100.0
     iteration 10, loss: 31514.501953125, beta: -21.960355758666992
     iteration 20, loss: 2392.293701171875, beta: -4.108242988586426
     iteration 30, loss: 141.00570678710938, beta: 0.5659010410308838
     iteration 40, loss: 11.90237808227539, beta: 1.617439866065979
     iteration 50, loss: 1.3650925159454346, beta: 1.9091993570327759
     iteration 60, loss: 0.9935522675514221, beta: 1.977428913116455
     iteration 70, loss: 0.9624385237693787, beta: 1.9948526620864868
     iteration 80, loss: 0.9665780067443848, beta: 1.999314785003662
     iteration 90, loss: 0.9669924378395081, beta: 1.9996494054794312
     iteration 99, loss: 0.968819260597229, beta: 2.0007200241088867
[86]: X, y = sample_batch(target_f1, 1000)
      y_hat = (X.T @ jnp.array([beta_learned_f1])).ravel()
      X_sorted, y_sorted, y_hat_sorted = sort_data(X[0], y, y_hat)
```

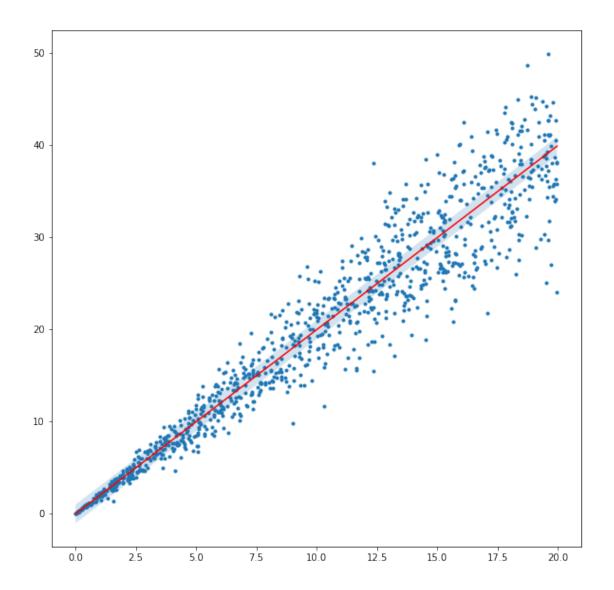


```
[87]: beta_init = -1045.43
beta_learned_f2 = train_lin_reg(target_f2, lr=1e-3, iters= 100, 

→beta_init=beta_init, print_every=10)
```

iteration 0, loss: 71597600.0, beta: -1045.4300537109375 iteration 10, loss: 3327742.75, beta: -240.8540802001953 iteration 20, loss: 246607.28125, beta: -55.82860565185547

```
iteration 30, loss: 12637.732421875, beta: -11.035815238952637
     iteration 40, loss: 741.8230590820312, beta: -1.3372020721435547
     iteration 50, loss: 51.09690475463867, beta: 1.1445693969726562
     iteration 60, loss: 3.654705286026001, beta: 1.7937183380126953
     iteration 70, loss: 1.1138404607772827, beta: 1.9534534215927124
     iteration 80, loss: 0.9887776374816895, beta: 1.9890962839126587
     iteration 90, loss: 0.9648057818412781, beta: 1.9969314336776733
     iteration 99, loss: 0.9568040370941162, beta: 1.9981322288513184
[88]: X, y = sample_batch(target_f2, 1000)
      y_hat = (X.T @ jnp.array([beta_learned_f2])).ravel()
      X_sorted, y_sorted, y_hat_sorted = sort_data(X[0], y, y_hat)
      plt.figure(figsize=(10, 10))
      plt.plot(X_sorted, y_sorted, '.');
      plt.plot(X_sorted, y_hat_sorted, 'r');
      uncertainty = [1.] * len(y_hat_sorted)
      plt.fill_between(X_sorted, y_hat_sorted.copy()-uncertainty,
                       y_hat_sorted.copy()+uncertainty, alpha=0.2);
```

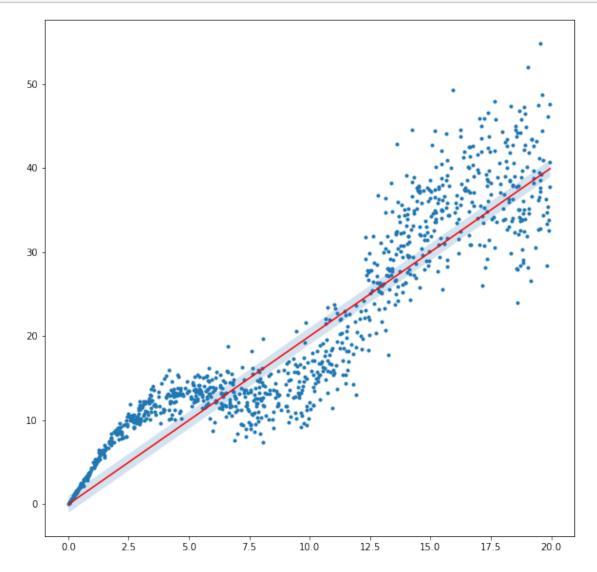


```
[89]: beta_init = -1045.43
beta_learned_f3 = train_lin_reg(target_f3, lr=1e-3, iters= 100, ____

→beta_init=beta_init, print_every=10)
```

```
iteration 0, loss: 70481304.0, beta: -1045.4300537109375 iteration 10, loss: 5197366.0, beta: -263.5350341796875 iteration 20, loss: 249470.6875, beta: -62.82470703125 iteration 30, loss: 18420.13671875, beta: -14.21027946472168 iteration 40, loss: 924.4586791992188, beta: -1.666813611984253 iteration 50, loss: 59.8269157409668, beta: 1.1058728694915771 iteration 60, loss: 4.434779167175293, beta: 1.7793068885803223 iteration 70, loss: 1.1073418855667114, beta: 1.9460408687591553 iteration 80, loss: 0.9745045304298401, beta: 1.9868106842041016 iteration 90, loss: 0.9703724384307861, beta: 1.9970945119857788
```

iteration 99, loss: 0.9639522433280945, beta: 2.001152515411377



### 1.16 Fully connected neural network

```
[91]: def neural_network(x, theta):
    w1, b1 = theta['w1'], theta['b1']
    w2, b2 = theta['w2'], theta['b2']

    out = jnp.tanh(x.T @ w1 + b1)
    out = out @ w2 + b2

    return out.ravel()
```

#### 1.17 Test model assumptions

```
[92]: theta = {'w1': randn(1, 10), 'b1': randn(10,), 'w2': randn(10, 1), 'b2': 

→randn(1,)}

n = 100

X = randn(1, n)

assert neural_network(X, theta).shape == (100,)

print('Yaay!')
```

Yaay!

### 1.18 Negative log-likelihood of NN model

```
[93]: def nn_model_nll(theta, X, y, sigma=1.):
    """
    This function takes the average nll loss not the sum!
    """
    return -jnp.mean(gaussian_log_likelihood(neural_network(X, theta), sigma, y))
```

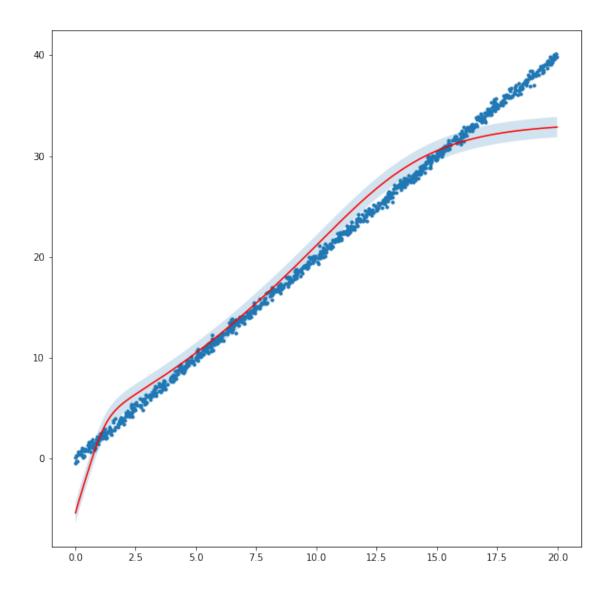
# 1.19 Training model to maximize Likelihood

```
grad_theta = grad_fn(theta_curr, X, y, sigma_model)
for par in theta_curr:
    theta_curr[par] -= lr * grad_theta[par]

return theta_curr
```

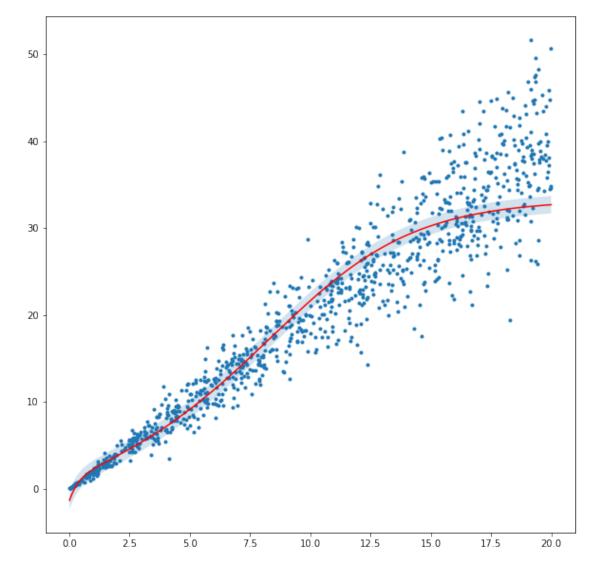
### 1.20 Learn model parameters & Plot neural network regression

```
[105]: theta_init = {'w1': randn(1, 10), 'b1': randn(10,), 'w2': randn(10, 1), 'b2':
       \rightarrowrandn(1,)}
       theta_learned = train_nn_reg(target_f1, theta_init, lr=1e-3, iters=1000,__
        →print_every=100)
      iteration 0, loss: 372.18634033203125
      iteration 100, loss: 75.48041534423828
      iteration 200, loss: 38.113563537597656
      iteration 300, loss: 22.781503677368164
      iteration 400, loss: 14.033673286437988
      iteration 500, loss: 12.48324966430664
      iteration 600, loss: 6.3160014152526855
      iteration 700, loss: 3.716982364654541
      iteration 800, loss: 5.678422451019287
      iteration 900, loss: 4.16624641418457
      iteration 999, loss: 4.429479598999023
[106]: X, y = sample_batch(target_f1, 1000)
       y_hat = neural_network(X, theta_learned)
       X_sorted, y_sorted, y_hat_sorted = sort_data(X[0], y, y_hat)
       plt.figure(figsize=(10, 10))
       plt.plot(X_sorted, y_sorted, '.');
       plt.plot(X_sorted, y_hat_sorted, 'r');
       uncertainty = [1.] * len(y_hat_sorted)
       plt.fill_between(X_sorted, y_hat_sorted.copy()-uncertainty,
                        y_hat_sorted.copy()+uncertainty, alpha=0.2);
```

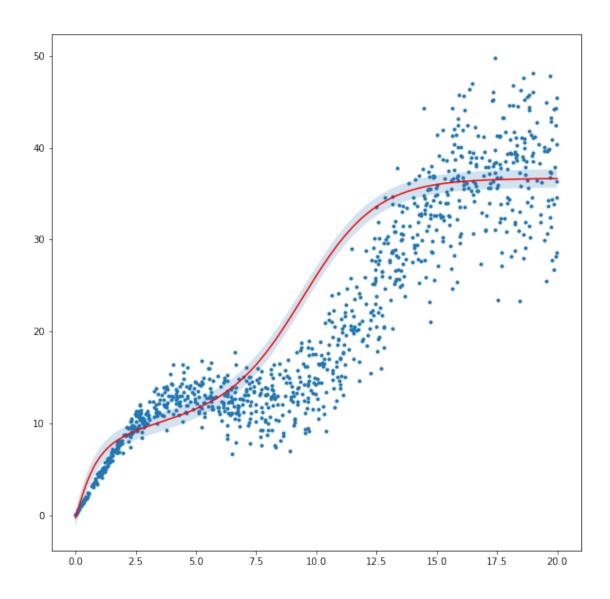


iteration 0, loss: 187.07394409179688 iteration 100, loss: 55.904972076416016 iteration 200, loss: 36.9810905456543 iteration 300, loss: 26.198501586914062 iteration 400, loss: 21.6041316986084 iteration 500, loss: 12.581140518188477 iteration 600, loss: 11.85784912109375 iteration 700, loss: 9.627582550048828 iteration 800, loss: 7.910226821899414

iteration 900, loss: 6.843225002288818 iteration 999, loss: 6.916143417358398



```
[113]: | theta init = {'w1': randn(1, 10), 'b1': randn(10,), 'w2': randn(10, 1), 'b2':
       \rightarrowrandn(1,)}
       theta_learned = train_nn_reg(target_f3, theta_init, lr=1e-3, iters=2000, __
        →print every=200)
      iteration 0, loss: 269.8338928222656
      iteration 200, loss: 46.84765625
      iteration 400, loss: 21.05194854736328
      iteration 600, loss: 27.298818588256836
      iteration 800, loss: 16.562450408935547
      iteration 1000, loss: 16.057994842529297
      iteration 1200, loss: 17.04452133178711
      iteration 1400, loss: 11.771540641784668
      iteration 1600, loss: 17.603925704956055
      iteration 1800, loss: 9.717445373535156
      iteration 1999, loss: 15.294386863708496
[114]: X, y = sample_batch(target_f3, 1000)
       y_hat = neural_network(X, theta_learned)
       X_sorted, y_sorted, y_hat_sorted = sort_data(X[0], y, y_hat)
       plt.figure(figsize=(10, 10))
       plt.plot(X_sorted, y_sorted, '.');
       plt.plot(X_sorted, y_hat_sorted, 'r');
       uncertainty = [1.] * len(y_hat_sorted)
       plt.fill_between(X_sorted, y_hat_sorted.copy()-uncertainty,
                        y_hat_sorted.copy()+uncertainty, alpha=0.2);
```



# 1.21 Input dependent variance

```
[135]: def neural_net_w_var(x, theta):
    w1, b1 = theta['w1'], theta['b1']
    w2, b2 = theta['w2'], theta['b2']

    out = jnp.tanh(x.T @ w1 + b1)
    out = out @ w2 + b2

mean = out[:, 0]
    log_sigma = out[:, 1]
```

```
return mean, log_sigma
```

### 1.22 Test model assumptions

Yaay!

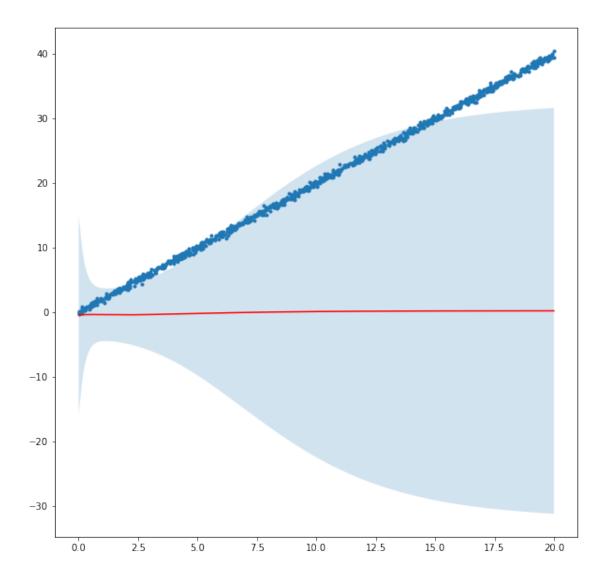
# 1.23 Negative log-likelihood with modelled variance

```
[137]: def nn_with_var_model_nll(theta, x, y):
    mean, log_sigma = neural_net_w_var(x, theta)
    return -jnp.mean(gaussian_log_likelihood(mean, jnp.exp(log_sigma), y))
```

### 1.24 Write training loop

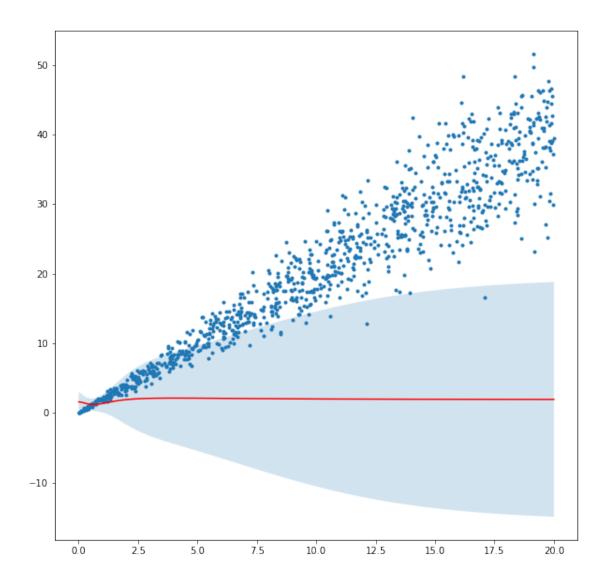
### 1.25 Learn model with input-dependent variance & Plot model

```
[155]: theta_init = \{'w1': randn(1, 10), 'b1': randn(10,), \}
                     'w2': randn(10, 2), 'b2': randn(2,)}
       theta_learned = train_nn_w_var_reg(target_f1, theta_init, iters=10000,_
       →print_every=500,
                                          lr=1e-4, bs=256)
      iteration 0, loss: 23.062238693237305
      iteration 500, loss: 4.496199607849121
      iteration 1000, loss: 4.4512224197387695
      iteration 1500, loss: 4.452008247375488
      iteration 2000, loss: 4.366448879241943
      iteration 2500, loss: 4.450658321380615
      iteration 3000, loss: 4.278117656707764
      iteration 3500, loss: 4.290834903717041
      iteration 4000, loss: 4.279414653778076
      iteration 4500, loss: 4.277789115905762
      iteration 5000, loss: 4.273720741271973
      iteration 5500, loss: 4.264880180358887
      iteration 6000, loss: 4.310825824737549
      iteration 6500, loss: 4.163493633270264
      iteration 7000, loss: 4.282164096832275
      iteration 7500, loss: 4.222474575042725
      iteration 8000, loss: 4.23431396484375
      iteration 8500, loss: 4.323176860809326
      iteration 9000, loss: 4.219166278839111
      iteration 9500, loss: 4.254668235778809
      iteration 9999, loss: 4.228629112243652
[157]: X, y = sample_batch(target_f1, 1000)
       mean, log_sigma = neural_net_w_var(X, theta_learned)
       X_sorted, y_sorted, mean_sorted, log_sigma_sorted = sort_data(X[0], y, mean,_
       →log_sigma)
       plt.figure(figsize=(10, 10))
       plt.plot(X_sorted, y_sorted, '.');
       plt.plot(X_sorted, mean_sorted, 'r');
       uncertainty = [1.] * len(mean_sorted)
       plt.fill_between(X_sorted, mean_sorted.copy()-jnp.exp(log_sigma_sorted),
                        mean_sorted.copy()+jnp.exp(log_sigma_sorted), alpha=0.2);
```



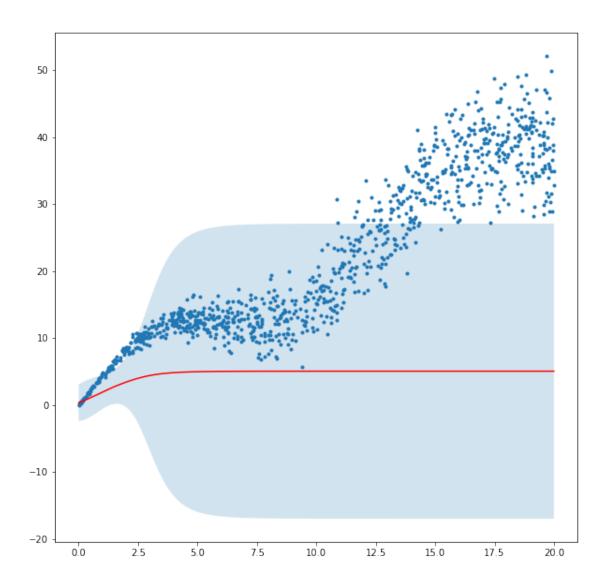
Note: It was trickier than what I thought! In fact predicting two parameters at the same time makes this process difficult... I think the problem with my model is that it is not learning mean properly and tries to compensate that by making variance bigger. In fact, this can be a local minima in which the model gets stuck. This might be overcome using better initialization. I tried different stds for the initialization of weights (0.1 and 0.01 and 0.001). However, in all of the cases the mean was not changing very much and it was mostly the variance that was being learned. I wanted to do a more exhaustive search to find better hyperparameters, however, I could not as I did not have access to any GPUs and was running on the CPU of my laptop.

```
iteration 0, loss: 32.33778381347656
      iteration 500, loss: 5.4941534996032715
      iteration 1000, loss: 4.846490383148193
      iteration 1500, loss: 4.618736267089844
      iteration 2000, loss: 4.505937576293945
      iteration 2500, loss: 4.604677200317383
      iteration 3000, loss: 4.435009956359863
      iteration 3500, loss: 4.334693908691406
      iteration 4000, loss: 4.410558700561523
      iteration 4500, loss: 4.2918500900268555
      iteration 4999, loss: 4.290377140045166
[149]: X, y = sample_batch(target_f2, 1000)
       mean, log_sigma = neural_net_w_var(X, theta_learned)
       X_sorted, y_sorted, mean_sorted, log_sigma_sorted = sort_data(X[0], y, mean,_
       →log_sigma)
       plt.figure(figsize=(10, 10))
       plt.plot(X_sorted, y_sorted, '.');
       plt.plot(X_sorted, mean_sorted, 'r');
       uncertainty = [1.] * len(mean_sorted)
       plt.fill_between(X_sorted, mean_sorted.copy()-jnp.exp(log_sigma_sorted),
                       mean_sorted.copy()+jnp.exp(log_sigma_sorted), alpha=0.2);
```



iteration 0, loss: 4.37979793548584 iteration 500, loss: 4.361379146575928 iteration 1000, loss: 4.3455047607421875 iteration 1500, loss: 4.304889678955078 iteration 2000, loss: 4.19901704788208 iteration 2500, loss: 4.258981704711914 iteration 3000, loss: 4.254028797149658 iteration 3500, loss: 4.237459182739258

```
iteration 4000, loss: 4.227425575256348
      iteration 4500, loss: 4.185097694396973
      iteration 5000, loss: 4.231231689453125
      iteration 5500, loss: 4.281516075134277
      iteration 6000, loss: 4.182871341705322
      iteration 6500, loss: 4.121823787689209
      iteration 7000, loss: 4.230964183807373
      iteration 7500, loss: 4.316128730773926
      iteration 8000, loss: 4.198155403137207
      iteration 8500, loss: 4.24950647354126
      iteration 9000, loss: 4.27836275100708
      iteration 9500, loss: 4.1965765953063965
      iteration 9999, loss: 4.181919574737549
[160]: X, y = sample_batch(target_f3, 1000)
       mean, log_sigma = neural_net_w_var(X, theta_learned)
       X_sorted, y_sorted, mean_sorted, log_sigma_sorted = sort_data(X[0], y, mean,_
       →log_sigma)
       plt.figure(figsize=(10, 10))
       plt.plot(X_sorted, y_sorted, '.');
       plt.plot(X_sorted, mean_sorted, 'r');
       uncertainty = [1.] * len(mean_sorted)
       plt.fill_between(X_sorted, mean_sorted.copy()-jnp.exp(log_sigma_sorted),
                        mean_sorted.copy()+jnp.exp(log_sigma_sorted), alpha=0.2);
```



[]: