Probabilistic Interpretation of Least Squares - Estimating the Measurement Noise

Contents


```
import numpy as np
np.set_printoptions(precision=3)
import matplotlib.pyplot as plt
%matplotlib inline
import seaborn as sns
sns.set(rc={"figure.dpi":100, "savefig.dpi":300})
sns.set_context("notebook")
sns.set_style("ticks")
```

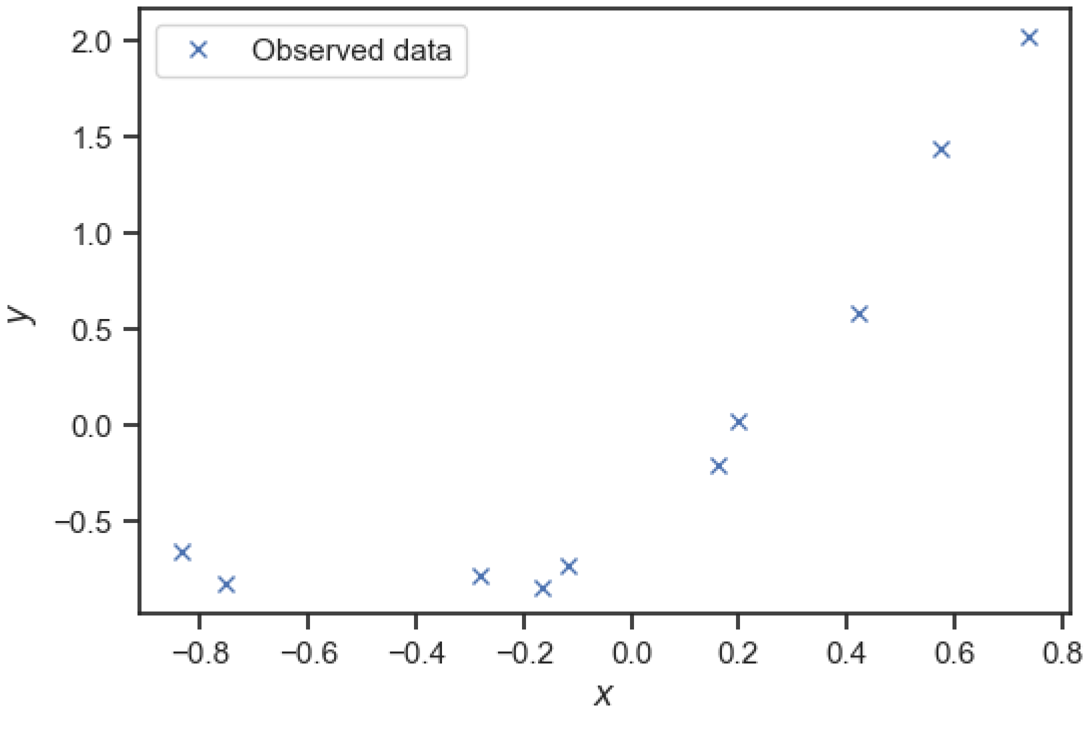
Let's reuse our synthetic dataset:

$$y_i = -0.5 + 2x_i + +2x_i^2 + 0.1\epsilon_i,$$

where $\epsilon_i \sim N(0,1)$ and where we sample $x_i \sim U([0,1])$. Here is how to generate this synthetic dataset and how it looks like:

```
num_obs = 10
x = -1.0 + 2 * np.random.rand(num_obs)
w0_true = -0.5
w1_true = 2.0
w2_true = 2.0
sigma_true = 0.1
y = (
    w0_true
    + w1_true * x
    + w2_true * x ** 2
    + sigma_true * np.random.randn(num_obs)
)

fig, ax = plt.subplots()
ax.plot(x, y, 'x', label='Observed data')
ax.set_xlabel('$x$')
ax.set_ylabel('$y$')
plt.legend(loc='best');
```



We will be fitting polynomials, so let's copy-paste the code we developed for computing the design matrix:

```
def get_polynomial_design_matrix(x, degree):
    """
    Returns the polynomial design matrix of ``degree`` evaluated at ``x``.
    """
    # Make sure this is a 2D numpy array with only one column
    assert isinstance(x, np.ndarray), 'x is not a numpy array.'
    assert x.ndim == 2, 'You must make x a 2D array.'
    assert x.shape[1] == 1, 'x must be a column.'
    # Start with an empty list where we are going to put the columns of the matrix
    cols = []
    # Loop over columns and add the polynomial
    for i in range(degree+1):
        cols.append(x ** i)
    return np.hstack(cols)
```

In the previous section, we saw that when least squares are interpreted probabilistically the weight estimate does not change. So, we can obtain it just like before:

```
# The degree of the polynomial
degree = 2
# The design matrix
Phi = get_polynomial_design_matrix(x[:, None], degree)
# Solve the least squares problem
w, sum_res, _, _ = np.linalg.lstsq(Phi, y, rcond=None)
```

Notice that we have now also stored the second output of `numpy.linalg.lstsq`. This is the sum of the residuals, i.e., it is:

$$\sum_{i=1}^{N}\left[y_i - \sum_{j=1}^{M} w_j\phi_j(x_i)\right]^2 = \parallel \mathbf{y}_{1:N} - \mathbf{\Phi}\mathbf{w} \parallel_2^2.$$

Let's test this just to be sure…

```
print(f'sum_res = {sum_res[0]:1.4f}')
print(f'compare to = {np.linalg.norm(y-np.dot(Phi, w)) ** 2:1.4f}')
```

```
sum_res = 0.0554
compare to = 0.0554
```

It looks correct. In the video, we saw that the sum of residuals gives us the maximum likelihood estimate of the noise variance through this formula:

$$\sigma^2 = \frac{\parallel \mathbf{y}_{1:N} - \mathbf{\Phi}\mathbf{w} \parallel_2^2}{N}.$$

Let's compute it:

```
sigma2_MLE = sum_res[0] / num_obs
sigma_MLE = np.sqrt(sigma2_MLE)
print(f'True sigma = {sigma_true:1.4f}')
print(f'MLE sigma = {sigma_MLE:1.4f}')
```

```
True sigma = 0.1000
MLE sigma = 0.0744
```

Let's also visualize this noise. The prediction at each x is Gaussian with mean $\mathbf{w}^T\boldsymbol{\phi}(x)$ and variance σ^2_{MLE}. So, we can simply create a 95% credible interval by subtracting and adding (about) two σ_{MLE} to the mean.

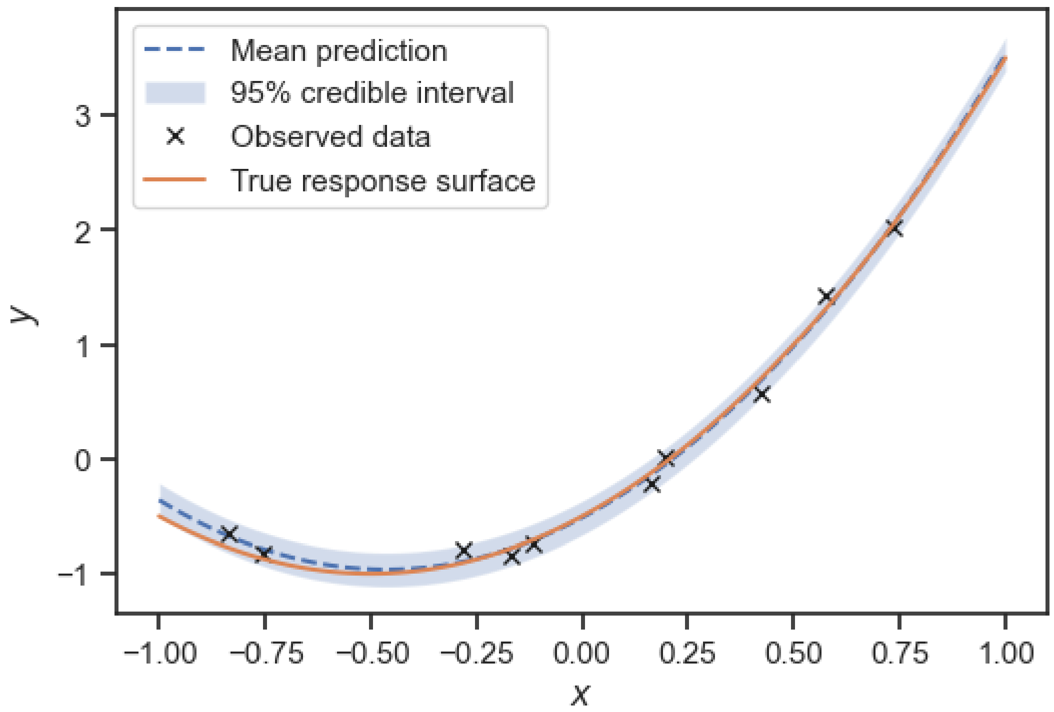
```
xx = np.linspace(-1, 1, 100)

# True response
yy_true = w0_true + w1_true * xx + w2_true * xx ** 2

# Mean predictions
Phi_xx = get_polynomial_design_matrix(
    xx[:, None],
    degree
)
yy = Phi_xx @ w

# Uncertainty (95% credible interval)
sigma_MLE = np.sqrt(sigma2_MLE)
# Lower bound
yy_l = yy - 2.0 * sigma_MLE
# Upper bound
yy_u = yy + 2.0 * sigma_MLE

# Plot
fig, ax = plt.subplots()
ax.plot(xx, yy, '--', label='Mean prediction')
ax.fill_between(
    xx,
    yy_l,
    yy_u,
    alpha=0.25,
    label='95% credible interval'
)
ax.plot(x, y, 'kx', label='Observed data')
ax.plot(xx, yy_true, label='True response surface')
ax.set_xlabel('$x$')
ax.set_ylabel('$y$')
plt.legend(loc='best');
```



Questions

- Increase the number of observations `num_obs` and notice that the likelihood noise converges to the true measurement noise.
- Change the polynomial degree to one so that you just fit a line. What does the model think about the noise now?

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