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Assignment 01 Companion Notebook

This notebook contains some examples that show off various properties of linear regression. This notebook is mostly focused on linear regression from a top-down perspective. That is, we are concerned with how does the algorithm behave rather than how it is implemented. As such we will be using a built-in solver for linear regression and treating it essentially as a black box (you will be opening that black box later in the assignment).

Numpy Practice

While you will not be doing any programming in this assignment, in order to understand the provided examples it helps to have at least a little bit of knowledge of `numpy`. Additionally, we will be using `numpy` extensively in this course. Please use the code block below to play around a bit with `numpy` (assuming you aren't already well-versed in `numpy`'s use').

In order to help you learn how to use `numpy`, you may consider consulting one of these tutorials.

- Numpy for MATLAB Users
- Numpy Cheatsheet

In [1]:

```
# play around with numpy here
import numpy as np
```

A Toy Linear Regression Problem

The notion of a toy problem is very useful for validating that a machine learning algorithm is working as it is intended to. The basic structure of a toy problem is as follows.

Suppose you are given a learning algorithm designed to estimate some model parameters $\mathbf{w}$ from some training data $(\mathbf{X}, \mathbf{y})$.

1. Generate values for the model parameters $\mathbf{w}$ (e.g., set them to some known values or generate them randomly). If you were applying your algorithm to real data, you would of course not know these parameters, but instead estimate them from data. For our toy problem, we'll proceed with values that we generate so we can test our algorithms.
2. Generate some training input data, $\mathbf{X}$, (random numbers work well for this). Generate the training output data, $\mathbf{y}$, by applying the model with parameters $\mathbf{w}$. For example, for a linear regression problem if $\mathbf{w}$ represents the regression coefficients, then we can generate each training label, y_i as $y_i = \mathbf{x_i}^\top \mathbf{w}$.
3. Run your learning algorithms on the synthesized training data $(\mathbf{X}, \mathbf{y})$ to arrive at estimated values of the model parameters, $\hat{\mathbf{w}}$.
4. Compare $\mathbf{w}$ and $\hat{\mathbf{w}}$ as a way of understanding whether your learning algorithm is working.

In the next code block, you'll see an example of a toy regression problem where we set $\mathbf{w} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$, generate some training data, and then recover $\mathbf{w}$ by applying the linear regression algorithm.

In [2]:

```
import numpy as np

def linear_regression(X, y):
    w, _, _, _ = np.linalg.lstsq(X, y, rcond=-1)
    return w

n_points = 50
X = np.random.randn(n_points,2)
w_true = np.array([1, 2])
y = X.dot(w_true)
w_estimated = linear_regression(X, y)

w_estimated
```

Out[2]:

Out[2]:

```
array([1., 2.])
```

Notebook Exercise 1

(a) What should be true about the relationship between `w_true` and `w_estimated` if the algorithm is working properly?

(b) Are there values of `n_points` that would cause `w_true` to be different from `w_estimated'? (this is a bit tricky, so try some corner cases, values at the extremes, and see if you get a different result. If you do, try ot understand why.)

Solution

(a) These two vectors should be equal since the inferences of the model should match the true parameters.

(b) `n_points = 1` will give you a value for `w_estimated` that doesn't match `w_true`. This is because them problem is underconstrained (there are more unknowns than equations). Thus, the linear regression method can find multiple solutions that drive the cost to 0 and has no way of knowing which the correct one was.

Investigating Noise

One thing you might be interested in knowing is how well the algorithm will work when the data doesn't perfectly conform to the hypothesized model (i.e., $y \neq \mathbf{x}^\top \mathbf{w}$).

In the next code block we'll add some noise to the labels and see if the linear regression algorithm can still reconstruct the true parameters $\mathbf{w}$. In particular, we are going to add noise generated from a Gaussian distribution with a specified standard deviation. By modifying `noise_standard_deviation`, you can explore how the magnitude of the noise influences the quality of the results (we'll be exploring standard deviation and Gaussians in more detail later in this course). For now you can just think of `noise_standard_deviation` as controlling the magnitude of corruption applied to the training outputs.

Additionally, By modifying `n_points` you can change how many training points are available to the linear regression model for parameter estimation.

In [3]:

```
n_points = 50
noise_standard_deviation = 2
X = np.random.randn(n_points,2)
w_true = np.array([1, 2])
y = X.dot(w_true) + np.random.randn(n_points,) * noise_standard_deviation
w_estimated = linear_regression(X, y)

w_estimated
```

Out[3]:

```
array([1.21351413, 2.18360576])
```

Notebook Exercise 2

(a) Keeping `noise_standard_deviation` constant, characterize qualitatively the relationship between `n_points` and how close `w_estimated` is to `w_true`? Why do you think this is the case (you don't have the formal language to describe this yet, so try to give a conceptual argument)?

(b) Keeping `n_points` constant, characterize qualitatively the relationship between `noise_standard_deviation` and how close `w_estimated` is to `w_true`? Why do you think this is the case (you don't have the formal language to describe this yet, so try to give a conceptual argument)?

Solution

(a) as `n_points` gets higher `w_estimated` gets closer to `w_true`. This makes sense intuitively since the random noise added to the training outputs `y` gets averaged out as more training poitns are provided.

(b) as `noise_standard_deviation` gets higher `w_estimated` gets farther from `w_true`. This makes sense intuitively since the random noise added to each to training output is greater and thus has the parameter estimates from linear regression are noisier as well.

Adding a y-intercept (bias) term

The beautiful thing about linear regression is that we can make it work for non-linear functions quite easily. The easiest way to do this is by augmenting the input data with additional features. In this way, functions that are non-linear in the original input space become linear in the agumented space.

For instance, the function $\mathbf{w}^\top\mathbf{x} + b$ (where b is a scalar or bias term) is non-linear (We know it looks linear but it is actually affine. If you are not convinced, you can test it against the properties of a linear map). On the other hand if we construct the vectors $\tilde{\mathbf{x}} = \begin{bmatrix}\mathbf{x}\\1\end{bmatrix}$ and $\tilde{\mathbf{w}} = \begin{bmatrix}\mathbf{w}\\b\end{bmatrix}$, then $\mathbf{w}^\top\mathbf{x} + b = \tilde{\mathbf{w}}^\top\tilde{\mathbf{x}}$ where $\tilde{\mathbf{w}}^\top\tilde{\mathbf{x}}$ is now a linear function!

In the code block below, you'll see how this idea can be used to fit a linear regression model to model with a bias term.

In [4]:

```
b = 3
y = X.dot(w_true) + b
linear_regression(np.hstack((X, np.ones((X.shape[0],1)))), y)
```

Out[4]:

```
array([1., 2., 3.])
```

Handling Other types of Non-linear Functions

Provided you know the form of the non-linear function you are fitting, you can use linear regression to fit arbitrary non-linear functions.

In the code below we will explore an example where the $y_i = w^\top x_i + x_{i,1}^2$. We'll create modified feature vector $\tilde{\mathbf{x}} = \begin{bmatrix}x\\x^2\end{bmatrix}$, and apply linear regression to those vectors. You'll see that the linear regression with the additional feature will match much better to the training data (have a lower error) than the one where we don't allow for this new feature.

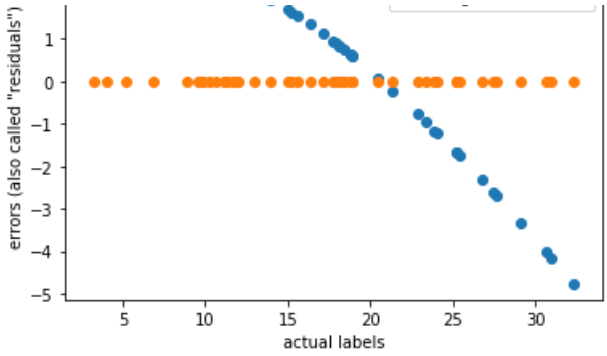
In [5]:

```
n_points = 50
X = np.random.randn(n_points,1) + 3
w_true = np.array([3])
y = X.dot(w_true) + np.square(X[:,0])
w_estimated = linear_regression(X, y)
original_model_preds = X.dot(w_estimated)
print("w_estimated", w_estimated)
print("Sum of squares for original model", np.sum(np.square(original_model_preds - y)))

X_augmented = np.column_stack((X, np.square(X[:,0])))
w_estimated_augmented = linear_regression(X_augmented, y)
print("w_estimated_augmented", w_estimated_augmented)

augmented_model_preds = X_augmented.dot(w_estimated_augmented)
print("Sum of squares for augmented model", np.sum(np.square(augmented_model_preds - y)))
%matplotlib inline
import matplotlib.pyplot as plt
plt.scatter(y, original_model_preds - y)
plt.scatter(y, augmented_model_preds - y)
plt.xlabel('actual labels')
plt.ylabel('errors (also called "residuals")')
plt.legend(['original model', 'augmented model'])
plt.show()
```

```
w_estimated [6.28834633]
Sum of squares for original model 233.8487631525443
w_estimated_augmented [3. 1.]
Sum of squares for augmented model 4.599059077438499e-28
```



Notebook Exercise 3

(a) Explain the observed differences in the sum of squares error for the two models. Why is the augmented model more accurate?

(b) In the original model, the coefficient estimated for the input feature is much higher than the true value (roughly twice as large). Explain why this occurs and why the augmented model doesn't have this problem?

(c) If you were applying linear regression to a real problem, how might you determine features to add to your model to capture non-linearities? There are many right answers to this, so you should be thinking of this as an open-ended question rather than one with a specific right answer.

Solution

(a) The augmented model is much more accurate (has a lower sum of squares) because due to the additional feature it can model the non-linear behavior in the training data.

(b) The original model is forced to artificially inflate the weight placed on the input feature to compensate for not being able to model the non-linear (quadratic behavior). It winds up overestimating the outputs for low input values and underestimating them for high input values. Since the augmented model has the quadratic feature, it can properly assign weight to that feature and keep the weight on the original feature at the appropriate value.

(c) There are lots of ways to do this. Here are three (we know you'll come up with more good ideas):

- See if there are any patterns in the plot of model residuals (e.g., the plot above shows a quadratic pattern in the errors, which might point towards the need to add a quadratic feature).
- Use domain-specific knowledge. For instance, there might be a reason why you expect a particular non-linear behavior to show up (e.g., you are modeling data that is periodic, such as temperature fluctuations over the year, and you know there is some sinusoidal behavior).
- You can use brute force search to try a bunch of different non-linearities and see which ones fit the data the best (there are a lot of machine learning models that work like this).

Predicting Bikeshare Data (Your First Machine Learning Application!)

The University of California maintains a repository of machine learning datasets. These datasets have been used over the years to benchmark algoirthms in order to faciltate comparisons to previously published work. In this next section of the notebook you will be exploring the Bikeshare dataset. The Bikeshare dataset contains daily usage data over a roughly two year period. Along with each record of user counts, there are independent variables that measure various characteristics of the day in question (e.g., whether it was a weekday or a weekend, the air temperature, the wind speed).

Here is what the data looks like (Note: we're using Pandas for this example. We'll be learning some Pandas later in the course, but for now don't worry about it).

In [6]:

```
import pandas as pd
bikeshare =
pd.read_csv('https://raw.githubusercontent.com/kylecho/nd101_p1_neural_network/master/Bike-Sharing
-Dataset/day.csv')
bikeshare
```

Out[6]:

	instant	dteday	season	yr	mnth	holiday	weekday	workingday	weathersit	temp	atemp	hum	windspeed	casual

	instant	dteday	season	yr	mnth	holiday	weekday	workingday	weathersit	temp	atemp	hum	windspeed	casual
0	1	2011-01-01	1	0	1	0	6	0	2	0.344167	0.363625	0.805833	0.160446	331
1	2	2011-01-02	1	0	1	0	0	0	2	0.363478	0.353739	0.696087	0.248539	131
2	3	2011-01-03	1	0	1	0	1	1	1	0.196364	0.189405	0.437273	0.248309	120
3	4	2011-01-04	1	0	1	0	2	1	1	0.200000	0.212122	0.590435	0.160296	108
4	5	2011-01-05	1	0	1	0	3	1	1	0.226957	0.229270	0.436957	0.186900	82
5	6	2011-01-06	1	0	1	0	4	1	1	0.204348	0.233209	0.518261	0.089565	88
6	7	2011-01-07	1	0	1	0	5	1	2	0.196522	0.208839	0.498696	0.168726	148
7	8	2011-01-08	1	0	1	0	6	0	2	0.165000	0.162254	0.535833	0.266804	68
8	9	2011-01-09	1	0	1	0	0	0	1	0.138333	0.116175	0.434167	0.361950	54
9	10	2011-01-10	1	0	1	0	1	1	1	0.150833	0.150888	0.482917	0.223267	41
10	11	2011-01-11	1	0	1	0	2	1	2	0.169091	0.191464	0.686364	0.122132	43
11	12	2011-01-12	1	0	1	0	3	1	1	0.172727	0.160473	0.599545	0.304627	25
12	13	2011-01-13	1	0	1	0	4	1	1	0.165000	0.150883	0.470417	0.301000	38
13	14	2011-01-14	1	0	1	0	5	1	1	0.160870	0.188413	0.537826	0.126548	54
14	15	2011-01-15	1	0	1	0	6	0	2	0.233333	0.248112	0.498750	0.157963	222
15	16	2011-01-16	1	0	1	0	0	0	1	0.231667	0.234217	0.483750	0.188433	251
16	17	2011-01-17	1	0	1	1	1	0	2	0.175833	0.176771	0.537500	0.194017	117
17	18	2011-01-18	1	0	1	0	2	1	2	0.216667	0.232333	0.861667	0.146775	9
18	19	2011-01-19	1	0	1	0	3	1	2	0.292174	0.298422	0.741739	0.208317	78
19	20	2011-01-20	1	0	1	0	4	1	2	0.261667	0.255050	0.538333	0.195904	83
20	21	2011-01-21	1	0	1	0	5	1	1	0.177500	0.157833	0.457083	0.353242	75
21	22	2011-01-22	1	0	1	0	6	0	1	0.059130	0.079070	0.400000	0.171970	93
22	23	2011-01-23	1	0	1	0	0	0	1	0.096522	0.098839	0.436522	0.246600	150
23	24	2011-01-24	1	0	1	0	1	1	1	0.097391	0.117930	0.491739	0.158330	86
24	25	2011-01-25	1	0	1	0	2	1	2	0.223478	0.234526	0.616957	0.129796	186
25	26	2011-01-26	1	0	1	0	3	1	3	0.217500	0.203600	0.862500	0.293850	34
26	27	2011-01-27	1	0	1	0	4	1	1	0.195000	0.219700	0.687500	0.113837	15
27	28	2011-01-28	1	0	1	0	5	1	2	0.203478	0.223317	0.793043	0.123300	38
28	29	2011-01-29	1	0	1	0	6	0	1	0.196522	0.212126	0.651739	0.145365	123
29	30	2011-01-30	1	0	1	0	0	0	1	0.216522	0.250322	0.722174	0.073983	140
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
701	702	2012-12-02	4	1	12	0	0	0	2	0.347500	0.359208	0.823333	0.124379	892
702	703	2012-12-03	4	1	12	0	1	1	1	0.452500	0.455796	0.767500	0.082721	555

	instant	dteday	season	yr	mnth	holiday	weekday	workingday	weathersit	temp	atemp	hum	windspeed	casual
703	704	2012-12-04	4	1	12	0	2	1	1	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
704	705	2012-12-05	4	1	12	0	3	1	1	0.438333	0.428012	0.485000	0.324021	331
705	706	2012-12-06	4	1	12	0	4	1	1	0.255833	0.258204	0.508750	0.174754	340
706	707	2012-12-07	4	1	12	0	5	1	2	0.320833	0.321958	0.764167	0.130600	349
707	708	2012-12-08	4	1	12	0	6	0	2	0.381667	0.389508	0.911250	0.101379	1153
708	709	2012-12-09	4	1	12	0	0	0	2	0.384167	0.390146	0.905417	0.157975	441
709	710	2012-12-10	4	1	12	0	1	1	2	0.435833	0.435575	0.925000	0.190308	329
710	711	2012-12-11	4	1	12	0	2	1	2	0.353333	0.338363	0.596667	0.296037	282
711	712	2012-12-12	4	1	12	0	3	1	2	0.297500	0.297338	0.538333	0.162937	310
712	713	2012-12-13	4	1	12	0	4	1	1	0.295833	0.294188	0.485833	0.174129	425
713	714	2012-12-14	4	1	12	0	5	1	1	0.281667	0.294192	0.642917	0.131229	429
714	715	2012-12-15	4	1	12	0	6	0	1	0.324167	0.338383	0.650417	0.106350	767
715	716	2012-12-16	4	1	12	0	0	0	2	0.362500	0.369938	0.838750	0.100742	538
716	717	2012-12-17	4	1	12	0	1	1	2	0.393333	0.401500	0.907083	0.098258	212
717	718	2012-12-18	4	1	12	0	2	1	1	0.410833	0.409708	0.666250	0.221404	433
718	719	2012-12-19	4	1	12	0	3	1	1	0.332500	0.342162	0.625417	0.184092	333
719	720	2012-12-20	4	1	12	0	4	1	2	0.330000	0.335217	0.667917	0.132463	314
720	721	2012-12-21	1	1	12	0	5	1	2	0.326667	0.301767	0.556667	0.374383	221
721	722	2012-12-22	1	1	12	0	6	0	1	0.265833	0.236113	0.441250	0.407346	205
722	723	2012-12-23	1	1	12	0	0	0	1	0.245833	0.259471	0.515417	0.133083	408
723	724	2012-12-24	1	1	12	0	1	1	2	0.231304	0.258900	0.791304	0.077230	174
724	725	2012-12-25	1	1	12	1	2	0	2	0.291304	0.294465	0.734783	0.168726	440
725	726	2012-12-26	1	1	12	0	3	1	3	0.243333	0.220333	0.823333	0.316546	9
726	727	2012-12-27	1	1	12	0	4	1	2	0.254167	0.226642	0.652917	0.350133	247
727	728	2012-12-28	1	1	12	0	5	1	2	0.253333	0.255046	0.590000	0.155471	644
728	729	2012-12-29	1	1	12	0	6	0	2	0.253333	0.242400	0.752917	0.124383	159
729	730	2012-12-30	1	1	12	0	0	0	1	0.255833	0.231700	0.483333	0.350754	364
730	731	2012-12-31	1	1	12	0	1	1	2	0.215833	0.223487	0.577500	0.154846	439

731 rows × 16 columns

Next, we'll perform regression with the column `cnt` (number of daily riders) as the output variable and `season`, `yr`, `mnth`, `holiday`, `weekday`, `workingday`, `weathersit`, `temp`, `atemp`, `hum`, `windspeed`, and a constant (bias) term as independent (explanatory variables). Why might we do this you ask? One potential reason would be to predict when to purchase or move bikes to meet anticipated demand.

Before actually performing the regression, examine the hex plots below that show pairwise plots between each independent

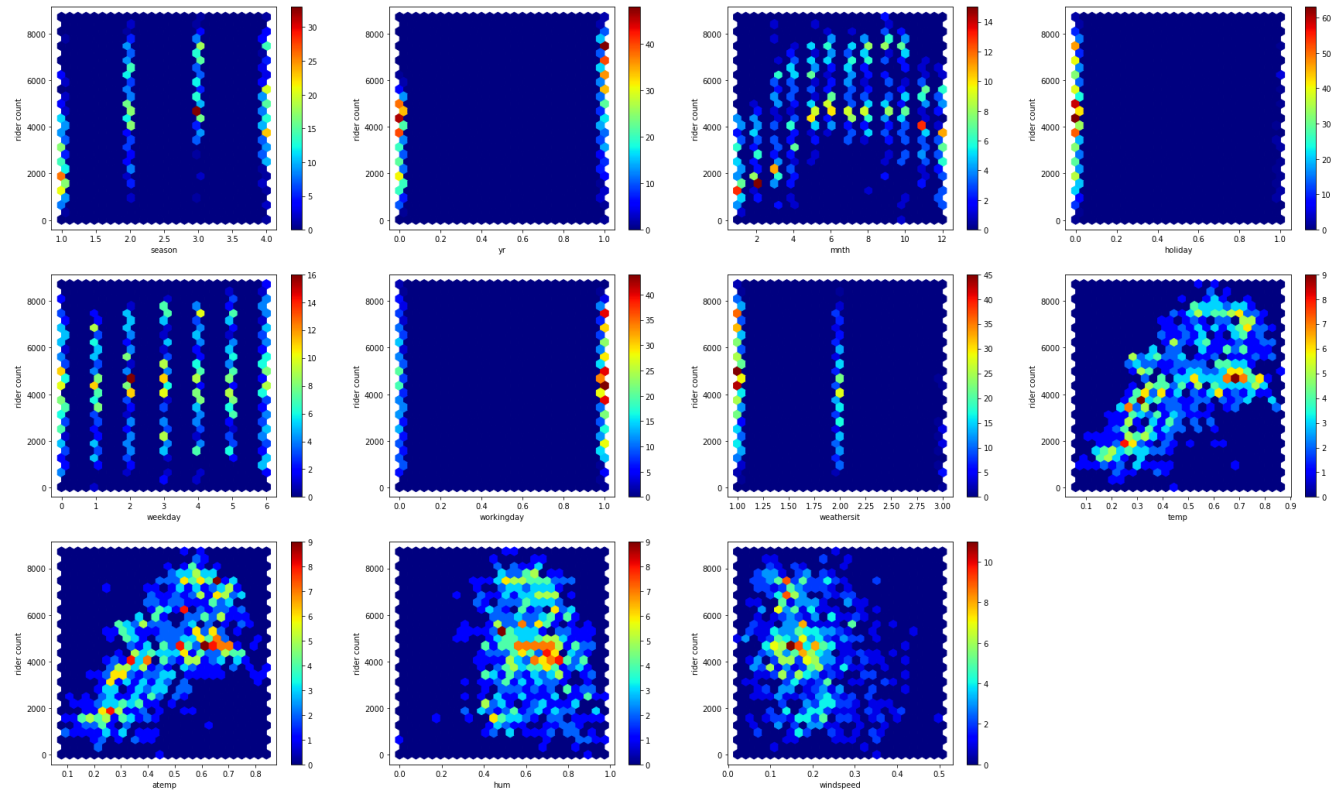
variable and the dependent variable (we avoided using scatter plots as those don't give a good sense of the density of the data when there are lots of overlapping points).

In [7]:

```
X_bikeshare = bikeshare.drop(columns=['instant', 'dteday', 'cnt', 'registered', 'casual'])
y_bikeshare = bikeshare['cnt']

plt.figure(figsize=(30, 18))
for idx, col in enumerate(X_bikeshare):
    plt.subplot(3, 4, idx+1)
    plt.hexbin(X_bikeshare[col], y_bikeshare, gridsize=25, cmap='jet')
    plt.colorbar()
    plt.xlabel(col)
    plt.ylabel('rider count')

plt.subplots_adjust(wspace=.2)
plt.show()
```



Notebook Exercise 4

(a) Before running the regression, make a prediction as to the sign of each of the coefficients for each of the explanatory variables. That is will the corresponding weight for each of these 11 variables be positive, negative, or close to 0?

Solution

(a) Based on what we estimate to be the linear trend in each scatter plot, we make the following predictions.

- season: positive
- yr: positive
- month: weakly positive (there is some downward movement at the end)
- weekday: close to 0
- workingday: positive
- holiday: negative
- weathersit: negative
- temp: positive
- atemp: positive
- hum: close to 0
- windspeed: weakly negative

Notebook Exercise 4 (part 2)

Next, run the actual regression.

(b) Do the results match your predictions? If not, hazard a guess as to why they don't match (you won't necessarily be able to determine this given the information provided).

In [8]:

```
X_bikeshare['bias'] = 1
list(zip(linear_regression(X_bikeshare, y_bikeshare), X_bikeshare.columns))
```

Out[8]:

```
[(509.775198288188, 'season'),
 (2040.703401658302, 'yr'),
 (-38.97956441091838, 'mnth'),
 (-518.9919312460555, 'holiday'),
 (69.06221629898982, 'weekday'),
 (120.35698921300694, 'workingday'),
 (-610.9870081089621, 'weathersit'),
 (2028.916103475132, 'temp'),
 (3573.2742884028607, 'atemp'),
 (-1018.8615712186565, 'hum'),
 (-2557.5691378686074, 'windspeed'),
 (1469.0030645879083, 'bias')]
```

Solution

(b) They mostly match. Here are some more observations.

- Windspeed appeared to have a bigger influence (in the negative direction) than we intitially thought.
- `holiday` was hard to estimate mostly due to the visualization of the data as a hexplot (there isn't a lot of data in the `holiday = 1` part of the graph and thus it gets washed out in the plot. Using a different plot like a box plot could be better for this.
- `mnth` was a surprise. This looks like a few outliers at the end of the graph (`mnth` = 12) caused the weight to shift down and become negative.

It's also important to keep in mind that just because a variable is positively correlated with the output, does not imply that the OLS weight is positive. There are situations that arise when the independent variables are correlated with each other when this would not be the case. We'll be diving more into this in the next assignment.