Data-Driven Design & Analyses of Structures & Materials (3dasm)

Lecture 2

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OPTION 1. Run this notebook **locally in your computer**:

1. Confirm that you have the '3dasm' mamba (or conda) environment (see Lecture 1).
2. Go to the 3dasm_course folder in your computer and pull the last updates of the **repository**:

   ```
   git pull
   ```

3. Open command window and load jupyter notebook (it will open in your internet browser):

   ```
   jupyter notebook
   ```

4. Open notebook of this Lecture and choose the '3dasm' kernel.

OPTION 2. Use **Google's Colab** (no installation required, but times out if idle):

1. go to **https://colab.research.google.com**
2. login
3. File > Open notebook
4. click on Github (no need to login or authorize anything)
5. paste the git link: **https://github.com/bessagroup/3dasm_course**
6. click search and then click on the notebook for this Lecture.

In [1]:
```python
# Basic plotting tools needed in Python.

import matplotlib.pyplot as plt # import plotting tools to create figures
import numpy as np # import numpy to handle a lot of things!

%config InlineBackend.figure_format = "retina" # render higher resolution images in the notebook
plt.rcParams["figure.figsize"] = (8,4) # rescale figure size appropriately for slides
```

Outline for today

- Handling data and handling pandas!
- Application of knowledge gained in Lecture 1
- Understanding the governing model for the car stopping distance problem

Reading material: This notebook

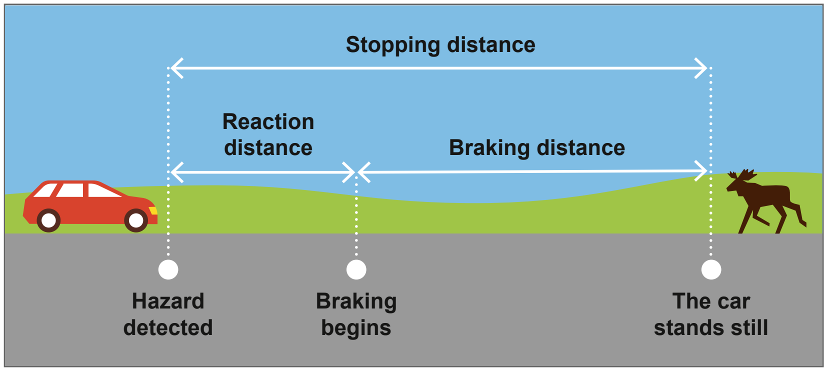
The car stopping distance problem (again!)

Imagine we want to predict y for a given x but that **we had no idea** that this problem is governed by:

$y = zx + 0.1x^2$

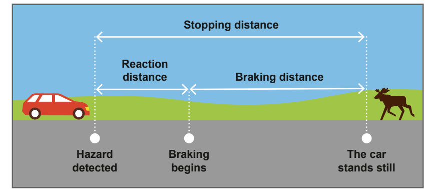
- y is the **output**: the car stopping distance
- x is the **input**: the car velocity
- z is a hidden variable: an rv z representing the driver's reactiontime (in seconds)

where $z \sim N(\mu_z = 1.5, \sigma_z^2 = 0.5^2)$



The car stopping distance problem

Instead, you are just provided with the data D that contains N measurements of different people stopping the car.
How does the data D look like?



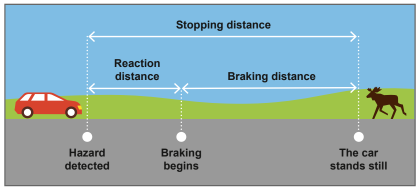
A table with N rows and 2 columns (input $\mathrm{x} = \mathrm{D_x}$ and output $\mathrm{y} = \mathrm{D_y}$).

x (m/s)	**y (m)**
15.5	21.4
5.3	11.8
78.0	701.6
...	...
10.8	22.1

Note that z is nowhere to be found! We could only measure the velocity of the car and the stopping distance, but we could not measure how quickly each driver reacts to seeing the deer!

Data generation

However, it's more instructive if we *create* the data from the governing equation.
This is more interesting than just being provided with the data!



- Usually, in ML literature people don't create the data...
  - Data is collected from somewhere (Internet?) and we don't have a clue about the hidden variables involved in the data generation process (unknown causes that explain the data!).
- **But**... In engineering practice this can be different! Sometimes you *can create data* (e.g. from computer simulations, from conducting your own experiments, etc.)
  - Although, models/measurements are never perfect (errors) and can be stochastic (noise)!

Anyway, let's create the dataset for our problem...

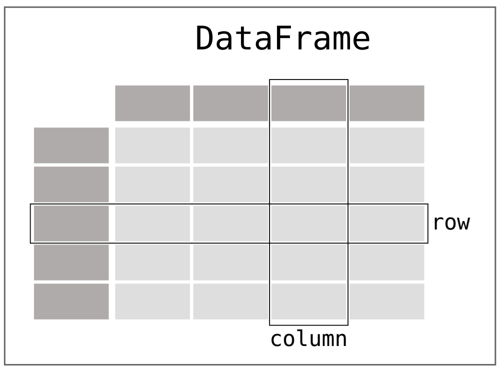
```python
In [2]: from scipy.stats import norm # import the normal dist, as we learned before!
        # Define our car stopping distance function
def y(x):
    z = norm.rvs(1.5, 0.5, size=1) # randomly draw 1 sample from the normal dist.
    y = z*x + 0.1*x**2 # compute the stopping distance
    return y

N = 33 # number of points to generate data
Data_x = np.linspace(3, 83, N) # generate a dataset with N points for velocities x between 3 and 83 m/s
print("Let's see the Data_x vector:\n", Data_x)

Data_y = np.zeros_like(Data_x) # create an empty vector for Data_y with same size as Data_x
i = 0 # initialize the counter
for x_i in Data_x:
    Data_y[i] = y(x_i)
    i += 1

print("\nLet's see the Data_y vector:\n", Data_y)
# IMPORTANT NOTE: Every time you run this cell you generate a new Data_y vector because of the z rv!!!
```

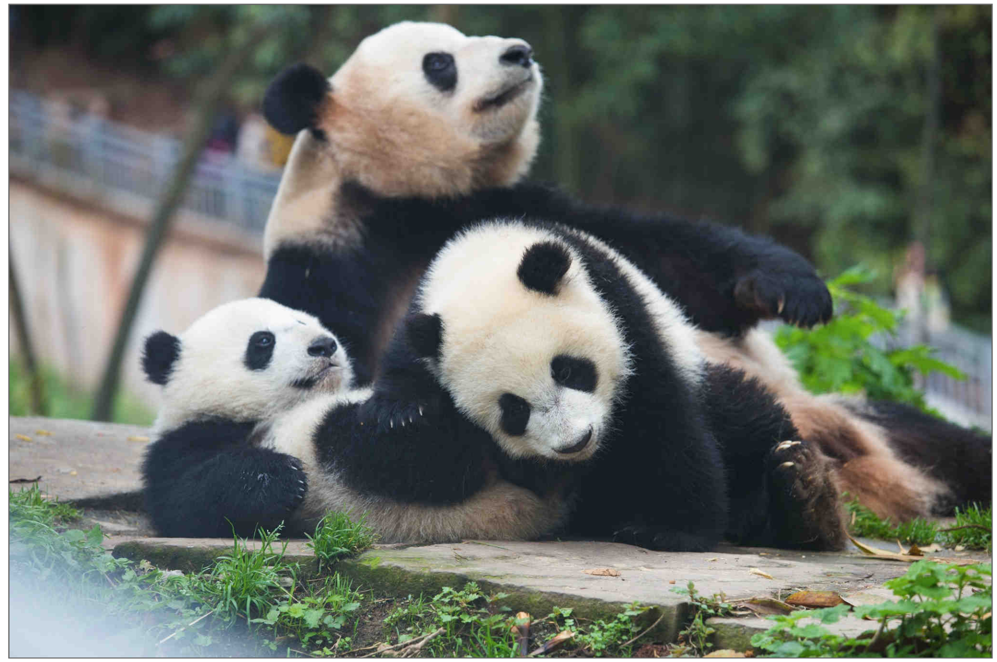
```
Let's see the Data_x vector:
 [ 3.   5.5  8.  10.5 13.  15.5 18.  20.5 23.  25.5 28.  30.5 33.  35.5
 38.  40.5 43.  45.5 48.  50.5 53.  55.5 58.  60.5 63.  65.5 68.  70.5
 73.  75.5 78.  80.5 83. ]

Let's see the Data_y vector:
 [  5.57525631  13.24258085  15.47257693  25.94986652  35.30847489
  38.69409239  58.09915111  80.33654285  72.44303492 109.23455188
 125.11703437 134.21363273 142.90099508 147.4460397  188.81252583
 225.43736634 204.11157173 297.64525874 281.30739377 306.53582559
 343.56209994 405.70124713 381.3237814  469.88060802 457.63831804
 563.89772439 564.05703623 602.80886772 629.78299347 652.9564992
 732.53869976 803.05686486 788.0898396 ]
```

Say hello to the pandas!

pandas is an open source library that is very common to handle data in ML

Let's create a pandas dataframe D that includes both the input $\mathrm{D_x}$ and output $\mathrm{D_y}$ that we created.





```
In [3]: import pandas as pd # Pandas dataframe (very common in ML)
        #
# Create a dictionary with the names of the input and output variables
# and their respective values:
input_dictionary = {
            'x' : Data_x, # vector with input values of x
            'y' : Data_y, # vector with output values of y
            }
#
# Then, we create a Pandas data frame:
car_df = pd.DataFrame(input_dictionary)

print(car_df)
```

```
       x           y
0    3.0    5.575256
1    5.5   13.242581
2    8.0   15.472577
3   10.5   25.949867
4   13.0   35.308475
5   15.5   38.694092
6   18.0   58.099151
7   20.5   80.336543
8   23.0   72.443035
9   25.5  109.234552
10  28.0  125.117034
11  30.5  134.213633
12  33.0  142.900995
13  35.5  147.446040
14  38.0  188.812526
15  40.5  225.437366
16  43.0  204.111572
17  45.5  297.645259
18  48.0  281.307394
19  50.5  306.535826
20  53.0  343.562100
21  55.5  405.701247
22  58.0  381.323781
```

23	60.5	469.880608
24	63.0	457.638318
25	65.5	563.897724
26	68.0	564.057036
27	70.5	602.808868
28	73.0	629.782993
29	75.5	652.956499
30	78.0	732.538700
31	80.5	803.056865
32	83.0	788.089840

Say hello to the pandas!

The **pandas** DataFrame we created is quite simple!
Today we won't go through many of the powerful data handling features of pandas.
We will try to introduce things as we need them.

- A basic need: save your data!

```
In [4]: # Saving our "car_df" pandas dataframe to the "your_data" folder in our computer is quite simple!
        car_df.to_pickle("your_data/car_dataframe.pkl") # done!
```

Go check in the "your_data" folder if you have created the "car_dataframe.pkl" file!

Load data from someone else

As mentioned, many ML problems start in a different way:

- We are provided with a dataset in some format.
    - For example, someone else conducted the car stopping distance experiment and saved the measurements in a csv file called "**data_for_car_prob.csv**".
    - Then we receive the file and have to use it in our analysis!

We have that file in folder "../data". The "../" just means that folder "data" is one level below the current folder (currently we are on "Lecture2" folder).

- Find the "data" folder and open the "data_for_car_prob.csv" file inside that folder using a text editor!

- Let's learn how to import the data of this csv file into a pandas dataframe.

```
In [5]: car_csv_data = pd.read_csv("../data/data_for_car_prob.csv") # read csv data provided by someone els
        print(car_csv_data)
```

```
    Unnamed: 0          x           y
0            0   9.516939   29.749036
1            1  72.398757  642.132203
2            2  17.950326   36.648484
3            3   9.440853   18.604106
4            4  78.791008  769.656168
5            5  16.961121   57.971010
6            6  65.410368  559.093313
7            7  58.671099  463.686613
8            8  21.550603   92.242676
9            9  36.866913  197.688573
10          10  15.728748   56.885233
11          11  58.511494  388.753795
12          12  57.419190  399.807488
13          13  38.459157  213.181519
14          14   8.841742   20.387384
15          15  60.733051  516.341724
16          16  49.256663  307.931956
17          17  35.895121  181.123049
18          18  79.195652  750.178284
19          19  69.156669  553.153541
20          20  77.634896  746.031880
21          21   9.254011   20.810698
22          22  15.451468   39.872527
23          23  14.438247   42.118771
24          24  13.410999   44.775122
25          25  53.747057  375.013937
26          26  10.283719   19.438868
27          27  82.005477  742.336845
28          28  81.805562  706.620282
29          29  51.837742  345.212876
30          30  20.283785   65.303165
31          31  28.359647  155.185137
32          32  74.993715  676.628982
33          33  21.827564   81.150935
```

34	34	70.519111	700.520033
35	35	74.208532	622.453560
36	36	14.518958	40.927570
37	37	13.357644	39.770922
38	38	75.346253	707.973754
39	39	44.923956	251.300805
40	40	26.801159	124.098654
41	41	29.906265	118.100900
42	42	40.226356	215.082100
43	43	66.282662	537.845048
44	44	47.342777	308.558833
45	45	3.087674	5.947997
46	46	21.254611	101.295276
47	47	46.939484	345.778352
48	48	38.875692	219.095582
49	49	76.705452	742.720134

We see that one of the columns is redundant!

Let's delete that one

```
In [6]: car_prob_df = car_csv_data[['x','y']] # pandas has a fast way to select the
                                               # columns of interest (in this case 'x' and 'y')
        print(car_prob_df)
```

```
            x           y
0    9.516939   29.749036
1   72.398757  642.132203
2   17.950326   36.648484
3    9.440853   18.604106
4   78.791008  769.656168
5   16.961121   57.971010
6   65.410368  559.093313
7   58.671099  463.686613
8   21.550603   92.242676
9   36.866913  197.688573
10  15.728748   56.885233
11  58.511494  388.753795
12  57.419190  399.807488
13  38.459157  213.181519
14   8.841742   20.387384
15  60.733051  516.341724
16  49.256663  307.931956
17  35.895121  181.123049
18  79.195652  750.178284
19  69.156669  553.153541
20  77.634896  746.031880
21   9.254011   20.810698
22  15.451468   39.872527
23  14.438247   42.118771
24  13.410999   44.775122
25  53.747057  375.013937
26  10.283719   19.438868
27  82.005477  742.336845
28  81.805562  706.620282
29  51.837742  345.212876
30  20.283785   65.303165
31  28.359647  155.185137
32  74.993715  676.628982
```

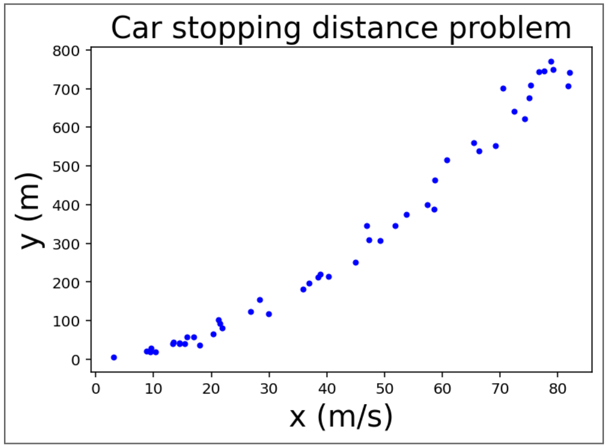
```
33  21.827564   81.150935
34  70.519111  700.520033
35  74.208532  622.453560
36  14.518958   40.927570
37  13.357644   39.770922
38  75.346253  707.973754
39  44.923956  251.300805
40  26.801159  124.098654
41  29.906265  118.100900
42  40.226356  215.082100
43  66.282662  537.845048
44  47.342777  308.558833
45   3.087674    5.947997
46  21.254611  101.295276
47  46.939484  345.778352
48  38.875692  219.095582
49  76.705452  742.720134
```

This looks better.

```
In [7]: Data_x = car_prob_df['x'].values # select the input VALUES from your dataframe into Data_x
        Data_y = car_prob_df['y'].values # select the output VALUES from your dataframe inta Data_y
print("Data_x is:\n",Data_x)
print("\nData_y is:\n",Data_y)
```

```
Data_x is:
 [ 9.51693942 72.39875748 17.95032583  9.44085299 78.79100778 16.96112056
 65.4103675  58.67109927 21.55060313 36.86691294 15.72874781 58.51149357
 57.41918959 38.45915667  8.84174221 60.73305107 49.25666345 35.89512052
 79.19565172 69.15666925 77.63489641  9.25401128 15.45146824 14.43824684
 13.41099874 53.74705712 10.28371886 82.00547705 81.80556249 51.8377421
 20.28378484 28.35964692 74.99371524 21.82756352 70.51911096 74.20853195
 14.51895792 13.35764354 75.34625316 44.92395642 26.80115926 29.90626522
 40.22635624 66.28266205 47.34277718  3.08767411 21.25461134 46.93948443
 38.87569199 76.70545196]

Data_y is:
 [ 29.74903647 642.13220315  36.64848446  18.60410602 769.65616843
  57.97101034 559.09331318 463.68661322  92.24267632 197.68857288
  56.88523327 388.75379474 399.80748803 213.18151905  20.38738432
 516.34172363 307.93195589 181.12304936 750.17828361 553.15354059
 746.03187971  20.81069833  39.87252654  42.11877078  44.77512244
 375.01393668  19.43886782 742.33684483 706.62028237 345.21287569
  65.30316533 155.18513747 676.62898211  81.15093549 700.52003305
 622.45356019  40.92757044  39.77092163 707.97375405 251.30080489
 124.09865438 118.10089977 215.08209978 537.84504756 308.55883254
   5.94799685 101.29527607 345.77835213 219.09558165 742.72013356]
```

```
In [8]: fig_car_data, ax_car_data = plt.subplots() # create a plot
        ax_car_data.plot(Data_x, Data_y, 'b.')
ax_car_data.set_xlabel("x (m/s)", fontsize=20) # create x-axis label with font size 20
ax_car_data.set_ylabel("y (m)", fontsize=20) # create y-axis label with font size 20
ax_car_data.set_title("Car stopping distance problem", fontsize=20); # create title with font size 20
```



In Homework 2...

Our famous car stopping distance problem:

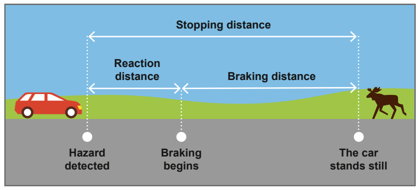
$y = zx + 0.1x^2$

where $z \sim N(\mu_z = 1.5, \sigma_z^2 = 0.5^2)$

Derive the expected value and variance for the governing model for the car stopping distance problem:

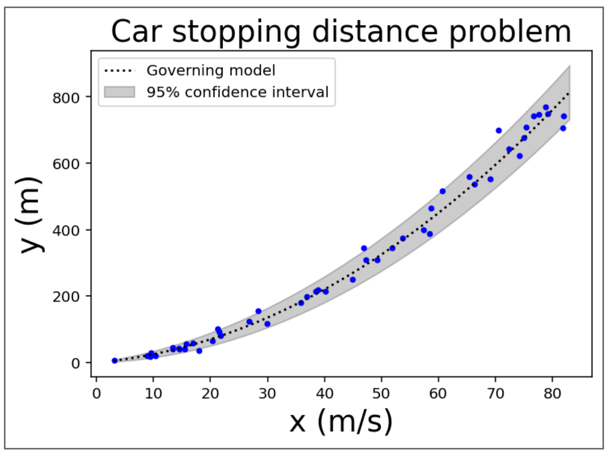
$E[y] = ?$

$V[y] = ?$



In [9]:
```
# Let's plot the model (we pretend for a moment that we know it!)
       real_x = np.linspace(3, 83, 1000)
real_mu_y = 1.5*real_x + 0.1*(real_x**2) # Recall: E[z*x+0.1*x^2] = E[z]*E[x]+0.1*E[x^2]
real_sigma_y = np.sqrt( 0.5**2*real_x**2 ) # Recall: V[z*x+x^2] = V[z*x]+V[x^2]=...=sigma_z^2*mu_x^2

ax_car_data.plot(real_x, real_mu_y, 'k:', label="Governing model")
ax_car_data.fill_between(real_x, real_mu_y - 1.9600 * real_sigma_y,
                real_mu_y + 1.9600 * real_sigma_y,
                color='k', alpha=0.2,
                label='95% confidence interval')
                # See book Sections 4.7.4 and 4.7.5 for a discussion on CI vs credible interval
ax_car_data.legend()
fig_car_data
```

Out[9]:



Question: If we didn't know the governing model, what should ML do using the data (blue dots)?

ML (supervised learning regression) goal

1. ML should find the mean response μ_y from the data $D = \{D_x, D_y\}$ (data: blue dots).

1. Of course we will always make a prediction error (we just see the data, and we don't know the model or complete reality).

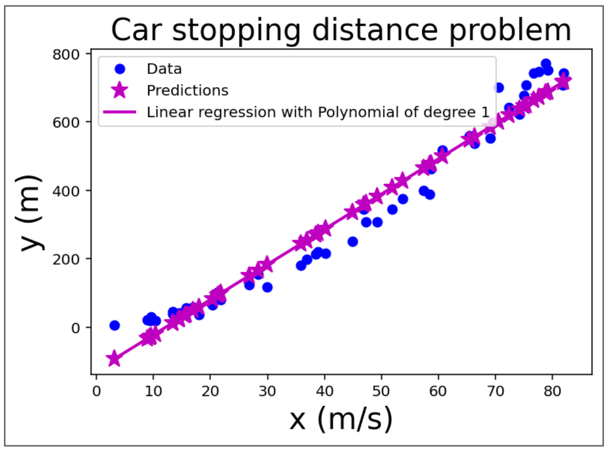
1. Ideally, ML should also tell us the confidence we have on the predictions we are making.
    - This is what probabilistic ML does!

1. **However**, even if we don't estimate our confidence (like most ML), having a probabilistic perspective over ML is advantageous because our unknowns can be modeled as rv's.
    - This helps us understand where the models come from and that the world is probabilistic.

In the next classes we will understand the simplest ML supervised learning regression models.
This will allow us to make simple predictions, so that later we make some serious predictions!
Here's a teaser for the next lectures about linear regression:

In [11]:
```
# Code to generate this figure is hidden during presentation (it's shown as notes).
# (We will learn how to do this later...)
fig_poly # show figure
```

Out[11]:



See you next class

Have fun!