Data-driven Design and Analyses of Structures and Materials (3dasm)

Lecture 3

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

1. Confirm that you have the 3dasm 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):

```
conda activate 3dasm
jupyter notebook
```

4. Open notebook of this Lecture.

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

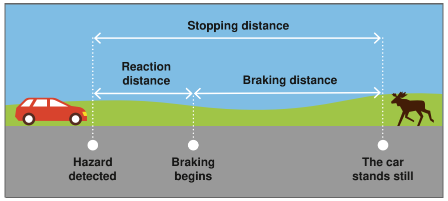
1. go to **https://colab.research.google.com**
2. login
3. File > Open notebook
4. click on Github (no need to login or authorize anything)
5. paste the git link: **https://github.com/bessagroup/3dasm_course**
6. click search and then click on the notebook for this Lecture.

Outline for today

- Probability: multivariate models
    - Covariance
    - Introduction to joint pdfs: the multivariate Gaussian
    - Marginal pdfs
    - Conditional pdfs

Reading material: This notebook + Chapter 3 (until Section 3.3)

Consider an even simpler car distance problem



For now, let's focus on the case where every driver is going at the same velocity $x = 75$ m/s.
Then, the governing model is even simpler:
$y = z \cdot 75 + 0.1 \cdot 75^2 = 75z + 562.5$

- y is the **output**: the car stopping distance (in meters)
- z is a hidden variable: an rv representing the driver's reaction time (in seconds)

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

In [3]:

```
# Let's make different observations
from scipy.stats import norm # import the normal dist, as we learned before!
# Define our car stopping distance function
def y_for_fixed_x(N_samples):
    x = 75
    samples_z = norm.rvs(1.5, 0.5, size=N_samples) # randomly draw samples from the normal dist.
    samples_y = samples_z*x + 0.1*x**2 # compute the stopping distance for samples of z
    return samples_y # return samples of y

print("Stopping distance for x=75 m/s is:",y_for_fixed_x(N_samples=1)) # drawing random samples of y
```

```
Stopping distance for x=75 m/s is: [670.53290312]
```

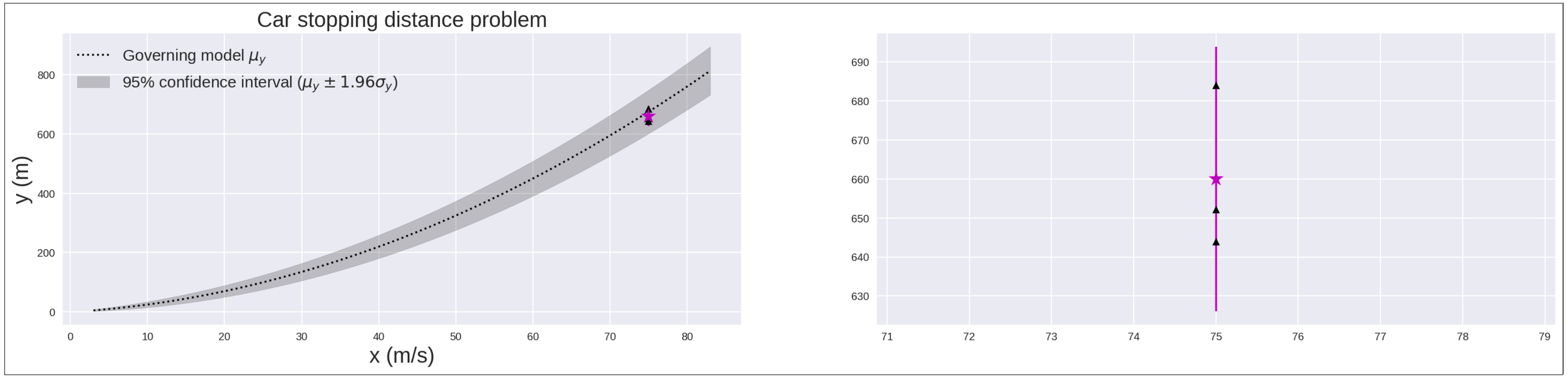
Let's estimate the confidence interval for $x = 75$ m/s

- Let's estimate the confidence interval (error bar) using samples of different sizes.
- We will also overlay this with the plot for the governing model (recall **Exercise 2** from Lecture 2)

In [4]:

```
               # vvvvvvvvvvv this is just a trick so that we can run this cell multiple times vvvvvvvvvvv
fig_car_new, ax_car_new = plt.subplots(1,2); plt.close() # create figure and close it
if fig_car_new.get_axes():
    del ax_car_new; del fig_car_new # delete figure and axes if they exist
    fig_car_new, ax_car_new = plt.subplots(1,2) # create them again
# ^^^^^^^^^^^ end of the trick ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
N_samples = 3 # CHANGE THIS NUMBER AND RE-RUN THE CELL
real_x = 75; empirical_y = y_for_fixed_x(N_samples); # Empirical measurements of N_samples
empirical_mu_y = np.mean(empirical_y); empirical_sigma_y = np.std(empirical_y); # empirical mean and std
car_fig(ax_car_new[0]) # a function I created to include the background plot of the governing model
for i in range(2): # create two plots (one is zooming in on the error bar)
    ax_car_new[i].errorbar(real_x , empirical_mu_y,yerr=1.96*empirical_sigma_y, fmt='*m', markersize=15);
    ax_car_new[i].plot(75*np.ones_like(empirical_y),empirical_y,'k^')
print("Empirical mean[y] is",empirical_mu_y, "(real mean[y]=675)")
print("Empirical std[y] is",empirical_sigma_y,"(real std[y]=37.5)")
fig_car_new.set_size_inches(25, 5) # scale figure to be wider (since there are 2 subplots)
```

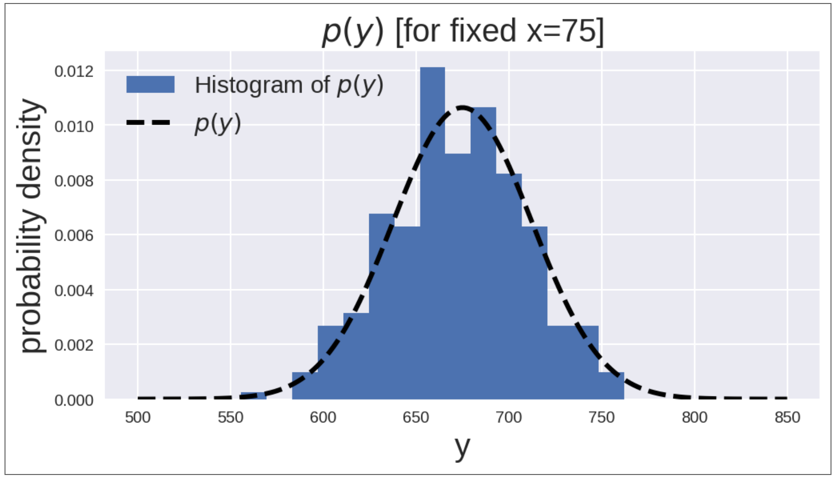
```
Empirical mean[y] is 659.9932360726916 (real mean[y]=675)
Empirical std[y] is 17.290343602599062 (real std[y]=37.5)
```



In [10]:

```
fig_hist, ax_hist_y = plt.subplots()
# Plot the histogram obtained by sampling p(y) with data
samples_y = y_for_fixed_x(N_samples=300)
ax_hist_y.hist(samples_y, bins='auto', # Change Number of samples and see histogram
               density=True, label='Histogram of $p(y)$')
ax_hist_y.set_title("$p(y)$ [for fixed x=75]", fontsize=20)

# Plot the actual p(y|z) pdf:
yrange = np.linspace(500, 850, 200) # to show the real Gaussian distribution
ax_hist_y.plot(yrange, norm.pdf(yrange, 675, 37.5), 'k--', linewidth = 3, label='$p(y)$')
ax_hist_y.set_xlabel("y", fontsize=20)
ax_hist_y.set_ylabel("probability density", fontsize=20)
ax_hist_y.legend(fontsize=15, loc='upper left');
```



Conclusions about y and z

- We conclude that y is also an rv because z is an rv.
- In this case, we empirically found that $p(y)$ is also a Gaussian distribution, just like z but with different parameters. This makes sense because y is just linearly dependent on z.
- Also recall that in **Exercise 2** from Lecture 2 we calculated the expected value (mean) and variance of y.

These observations lead to the conclusion:

$$p(y) = \mathcal{N}(\mu_y = 675, \sigma_y^2 = 37.5^2)$$

with $p(z) = \mathcal{N}(\mu_z = 1.5, \sigma_z^2 = 0.5^2)$ and for $x = 75$.

Transformation of random variables

This empirical conclusion can be reached analytically from the **change of variables formula**.
This formula says that if $y = f(z)$ and if this function is invertible, i.e. $z = f^{-1}(y) = g(y)$, then:

$$p_y(y) = p_z\left(g(y)\right)\left|\frac{d}{dy}g(y)\right|$$

where $g(y) = f^{-1}(z)$.

Exercise 1

Use the change of variables formula to demonstrate that $p(y)$ is a Gaussian distribution with the expected value and variance determined in Lecture 2 (Exercise 2). In other words, that $p(y) = \mathcal{N}(y|\mu_y = x\mu_z + 0.1x^2, \sigma_y^2 = \sigma_z^2 x^2)$ when $y = xz + 0.1x^2$.

Introducing joint probability density of y and z

Just like in Lecture 1 where we talked about **joint probability** of two events, $\Pr(A \wedge B) = \Pr(A, B)$, the **joint probability density** is:

$$p(y \wedge z) = p(y, z)$$

- But how do we **calculate** $p(y, z)$?

If the two rv's were independent, then it would be: $p(y, z) = p(y)p(z)$
But... We know that y is dependent on z... So now what do we do?

What is the joint probability density of y and z?

As we saw in Lecture 1,

$$p(y, z) = p(y|z)p(z) = p(z|y)p(y) = p(z, y)$$

Here, we already know $p(y)$ and $p(z)$.

- But what is the **conditional pdf** $p(y|z)$? Tell me what you think!

What is the joint probability density of y and z?

Since y and z are dependent, the joint pdf $p(y, z)$ is

$$p(y, z) = \delta\left(y - (zx + 0.1x^2)\right) p(z)$$

where $p(y|z) = \delta\left(y - (zx + 0.1x^2)\right)$ is the Dirac delta pdf, assigning zero probability everywhere except when $y = zx + 0.1x^2$.
Recall that $p(z) = \mathcal{N}(\mu_z = 1.5, \sigma_z^2 = 0.5^2)$ (for now you can also forget about x since $x = 75$).

- Note: $p(y, z)$ and $p(y|z)$ are pdf's that depends on *both* y and z, i.e. both pdf's are multivariate (depending on more than one rv; in this case on 2 rvs).

Why do we care about joint pdfs?

In general, from a joint pdf $p(y, z)$ we can obtain $p(y)$ and $p(z)$ simply by **integrating out** wrt the other variable. This is called **marginalizing**:

$$p(y) = \int p(y, z) dz$$

$$p(z) = \int p(y, z) dy$$

Therefore, $p(y)$ and $p(z)$ are also called **marginal distributions** of $p(y, z)$.

Exercise 2

Knowing that $p(y, z) = \delta\left(y - (zx + 0.1x^2)\right) \mathcal{N}(z|\mu_z, \sigma_z^2)$, calculate $p(y)$ and $p(z)$.

In general, do we know the true conditional distribution $p(y|z)$?

Unfortunately, we usually don't know the true conditional pdf $p(y|z)$ because z is hidden!
(Remember: we are cheating with the *car stopping distance problem* because we already know that $y = zx + 0.1x^2$)
In general, we don't know the true relationship between y and z...

- So, what can we do?

We can **observe** the effect caused by the hidden z in y by taking measurements of y.
In other words, within the measurements of y (which we call data $\mathcal{D}_y$) lies the *effect* of the hidden z.

- The Bayes' rule provides a way to estimate the distribution of the hidden rv z given data $\mathcal{D}_y$.

Remember the amazing Bayes' rule

Bayes' rule: a formula for computing the probability distribution over possible values of an unknown (or hidden) quantity z given some observed data y:

$$p(z|y) = \frac{p(y|z)p(z)}{p(y)}$$

Bayes' rule follows automatically from the identity: $p(z|y)p(y) = p(y|z)p(z) = p(y,z) = p(z,y)$

Bayes' rule

The pdfs we have been discussing in this lecture are what enable us to create ML models via the Bayes' rule when we apply it on **observed data** $\mathcal{D}_y$:

$$p(z|y=\mathcal{D}_y) = \frac{p(y=\mathcal{D}_y|z)p(z)}{p(y=\mathcal{D}_y)}$$

- $p(z)$ is the **prior** distribution: this term represents what we know (or what we believe we know!) about possible values of the unknown (hidden) rv z before we see any data.

Bayes’ rule

The pdfs we have been discussing in this lecture are what enable us to create ML models via the Bayes' rule when we apply it on **observed data** $\mathcal{D}_y$:

$$p(z|y=\mathcal{D}_y) = \frac{p(y=\mathcal{D}_y|z)p(z)}{p(y=\mathcal{D}_y)}$$

- $p(y|z)$ is the **observation** distribution (not yet the likelihood!): represents the distribution over the possible outcomes y we expect to see given a particular hidden variable z.
  - When we evaluate the observation distribution $p(y|z)$ at a point corresponding to the actual observations, $y=\mathcal{D}_y$, we get the function $p(y=\mathcal{D}_y|z)$:
    - $p(y=\mathcal{D}_y|z)$ is the **likelihood** function: it is a function of z, since y is *fixed* to the observations $\mathcal{D}_y$, but **it is not a probability distribution** (it does not sum to one).

Bayes’ rule

The pdfs we have been discussing in this lecture are what enable us to create ML models via the Bayes' rule when we apply it on **observed data** $\mathcal{D}_y$:

$$p(z|y=\mathcal{D}_y) = \frac{p(y=\mathcal{D}_y|z)p(z)}{p(y=\mathcal{D}_y)}$$

- $p(y=\mathcal{D}_y)$ is the **marginal likelihood**, which is obtained by *marginalizing* over the unknown z.

Bayes' rule

The pdfs we have been discussing in this lecture are what enable us to create ML models via the Bayes' rule when we apply it on **observed data** $\mathcal{D}_y$:

$$p(z|y = \mathcal{D}_y) = \frac{p(y = \mathcal{D}_y|z)p(z)}{p(y = \mathcal{D}_y)}$$

- $p(z|y = \mathcal{D}_y)$ is the **posterior**, which represents our *belief state* about the possible values of the unknown z.

Summary of Bayes' rule

$$p(z|y=\mathcal{D}_y) = \frac{p(y=\mathcal{D}_y|z)p(z)}{p(y=\mathcal{D}_y)} = \frac{p(y=\mathcal{D}_y, z)}{p(y=\mathcal{D}_y)}$$

- $p(z)$ is the **prior** distribution
- $p(y=\mathcal{D}_y|z)$ is the **likelihood** function
- $p(y=\mathcal{D}_y, z)$ is the **joint likelihood** (product of likelihood function with prior distribution)
- $p(y=\mathcal{D}_y)$ is the **marginal likelihood**
- $p(z|y=\mathcal{D}_y)$ is the **posterior**

We can write Bayes' rule as posterior $\propto$ likelihood $\times$ prior , where we are ignoring the denominator $p(y=\mathcal{D}_y)$ because it is just a **constant** independent of the hidden variable z.

Additional considerations about the joint pdf

Later we will dedicate a lot of effort to using Bayes' rule to update a distribution over unknown values of some quantity of interest, given relevant observed data $\mathcal{D}_y$.
This is what is called *Bayesian inference* (a.k.a. *posterior inference*).

- But before we do that, we need to understand very well multivariate pdfs.
    - In particular, let's focus on the most important one: the **multivariate Gaussian**

Multivariate Gaussian pdf

The multivariate Gaussian pdf of a D-dimensional vector $\mathbf{x}$ is given by,

$$p(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{e^{\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(x-\mu)}}{\sqrt{(2\pi)^D|\boldsymbol{\Sigma}|}} \tag{1}$$

$$= \frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}|^{1/2}}\exp\left[\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right] \tag{2}$$

where $\boldsymbol{\mu} = \mathbb{E}[\mathbf{x}] \in \mathbb{R}^D$ is the mean vector, and $\boldsymbol{\Sigma} = \mathrm{Cov}[\mathbf{x}]$ is the $D \times D$ **covariance matrix**.

Covariance matrix

The covariance matrix is a natural generalization of the variance (Lecture 1) for the multivariate case!

$$\mathbf{\Sigma} = \mathrm{Cov}[\mathbf{x}] = \mathbb{E}\left[(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{x} - \mathbb{E}[\mathbf{x}])^T\right] \tag{3}$$

$$= \begin{bmatrix} \mathbb{V}[x_1] & \mathrm{Cov}[x_1, x_2] & \cdots & \mathrm{Cov}[x_1, x_D] \\ \mathrm{Cov}[x_2, x_1] & \mathbb{V}[x_2] & \cdots & \mathrm{Cov}[x_2, x_D] \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{Cov}[x_D, x_1] & \mathrm{Cov}[x_D, x_2] & \cdots & \mathbb{V}[x_D] \end{bmatrix} \tag{4}$$

where $\mathrm{Cov}[x_i, x_j] = \mathbb{E}\left[(x_i - \mathbb{E}[x_i])(x_j - \mathbb{E}[x_j])\right] = \mathbb{E}[x_i x_j] - \mathbb{E}[x_i][x_j]$
Also note that $\mathbb{V}[x_i] = \mathrm{Cov}[x_i, x_i]$.

Let’s calculate the covariance matrix for the car problem when $x = 75$ m/s

Our simple car stopping distance problem has two rv's,

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} y \\ z \end{bmatrix}$$

- Note: this $\mathbf{x}$ has NOTHING to do with our velocity variable x. Be careful!

$$\mathbf{\Sigma} = \mathrm{Cov}[\mathbf{x}] = \mathbb{E}\left[(y - \mathbb{E}[y])(z - \mathbb{E}[z])^T\right] \tag{5}$$
$$= \begin{bmatrix} \mathbb{V}[y] & \mathrm{Cov}[y,z] \\ \mathrm{Cov}[z,y] & \mathbb{V}[z] \end{bmatrix} \tag{6}$$

where $\mathrm{Cov}[y,z] = \mathbb{E}\left[(y - \mathbb{E}[y])(z - \mathbb{E}[z])\right] = \mathbb{E}[yz] - \mathbb{E}[y][z]$

Exercise 3

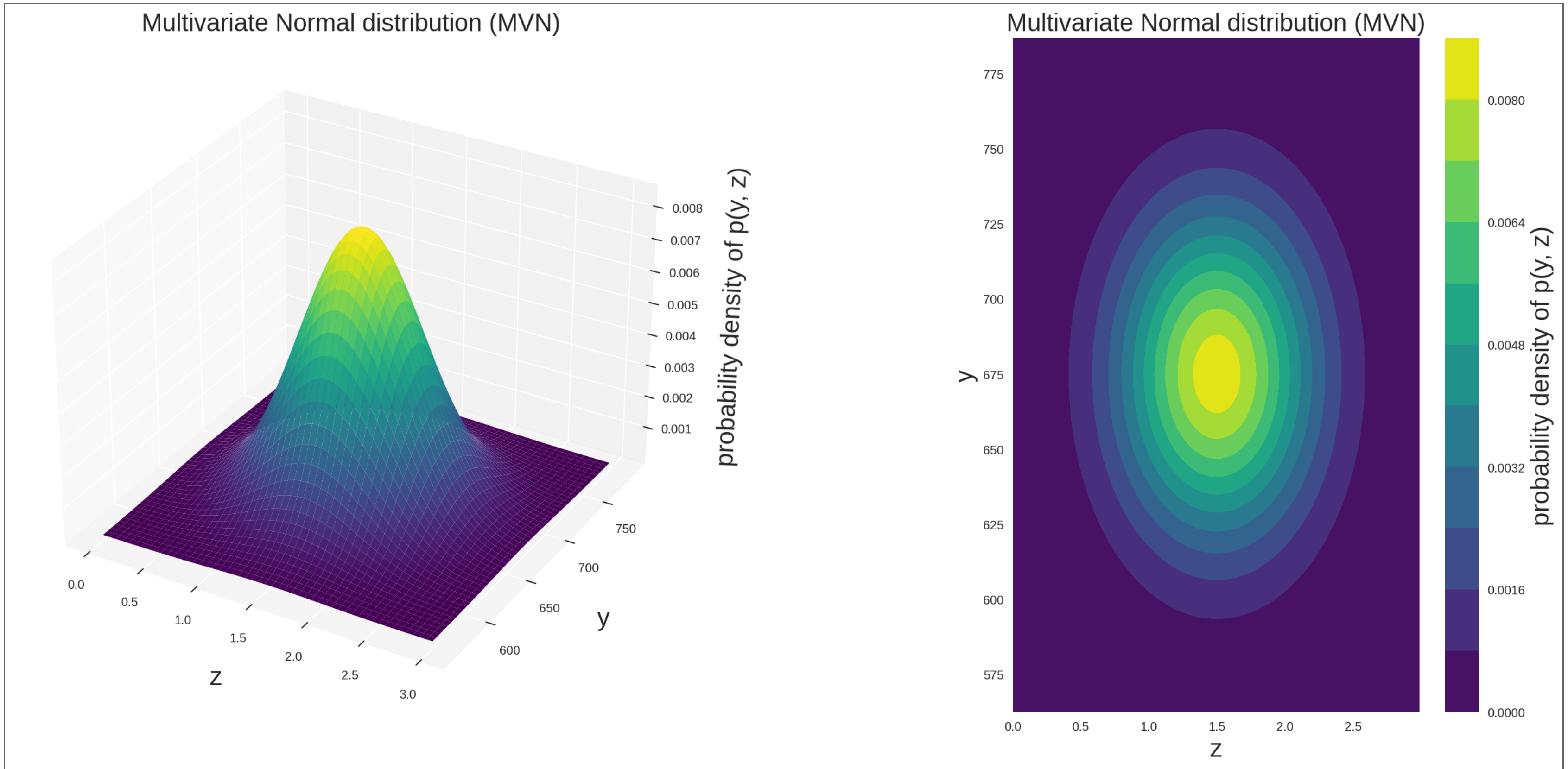
Calculate the mean vector and covariance matrix values for our problem (with $x = 75$ m/s). **Be careful** that y is dependent on z!

- Once you are done, let's plot the multivariate Gaussian $p(y, z)$ obtained from the mean vector and covariance matrix you calculated.

In [7]:

```
# Code to generate this figure is hidden in presentation (shown in notes)
fig_MVN
```

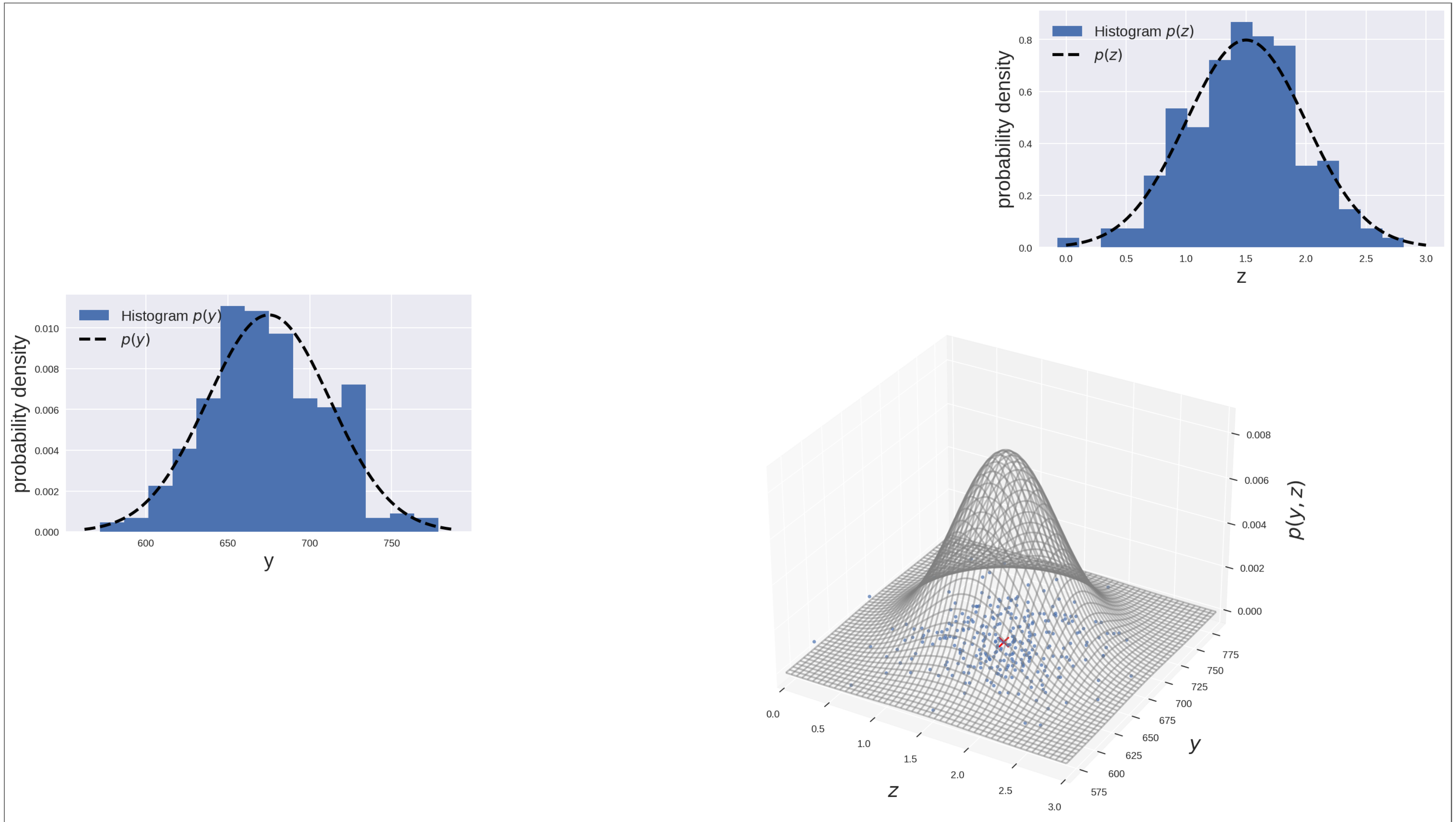
Out[7]:



In [9]:

```
            # HIGHLIGHT DIFFERENCE IN MAXIMUM PROBABILITY DENSITIES!!
fig_MVN_and_marginals #The MVN distribution and its marginal distributions
```

Out[9]:



See you next class

Have fun!