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

Lecture 4

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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
    - The multivariate Gaussian: joint pdf, conditional pdf and marginal pdf
    - Covariance and covariance matrix

Reading material: This notebook (+ Bishop's book Section 2.3)

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.

Diving deeper into 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 (a.k.a. MVN distribution)

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!

$$\begin{aligned}
\boldsymbol{\Sigma} = \mathrm{Cov}[\mathbf{x}] &= \mathbb{E}\left[(\mathbf{x}-\mathbb{E}[\mathbf{x}])(\mathbf{x}-\mathbb{E}[\mathbf{x}])^T\right] &(3)\\
&= \begin{bmatrix} \mathbb{V}[x_1] & \mathrm{Cov}[x_1,x_2] & \cdots & \mathrm{Cov}[x_1,x_D] \\ \mathrm{Cov}[x_2,x_1] & \mathbb{V}[x_2] & \cdots & \mathrm{Cov}[x_2,x_D] \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{Cov}[x_D,x_1] & \mathrm{Cov}[x_D,x_2] & \cdots & \mathbb{V}[x_D] \end{bmatrix} &(4)
\end{aligned}$$

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

Notes about covariance and normalized covariance (correlation coefficient)

The covariance between two rv's y and z measures the degree to which y and z are **linearly** related.
Covariances can be between negative and positive infinity.
Sometimes it is more convenient to work with a normalized measure, with a finite lower and upper bound.
The (Pearson) **correlation coefficient** between y and z is defined as

$$\rho = \mathrm{corr}[y, z] = \frac{\mathrm{Cov}[y, z]}{\sqrt{\mathbb{V}[y]\mathbb{V}[z]}}$$

Covariance and correlation coefficient measure the same relationship.

Note about normalized covariance (correlation coefficient)

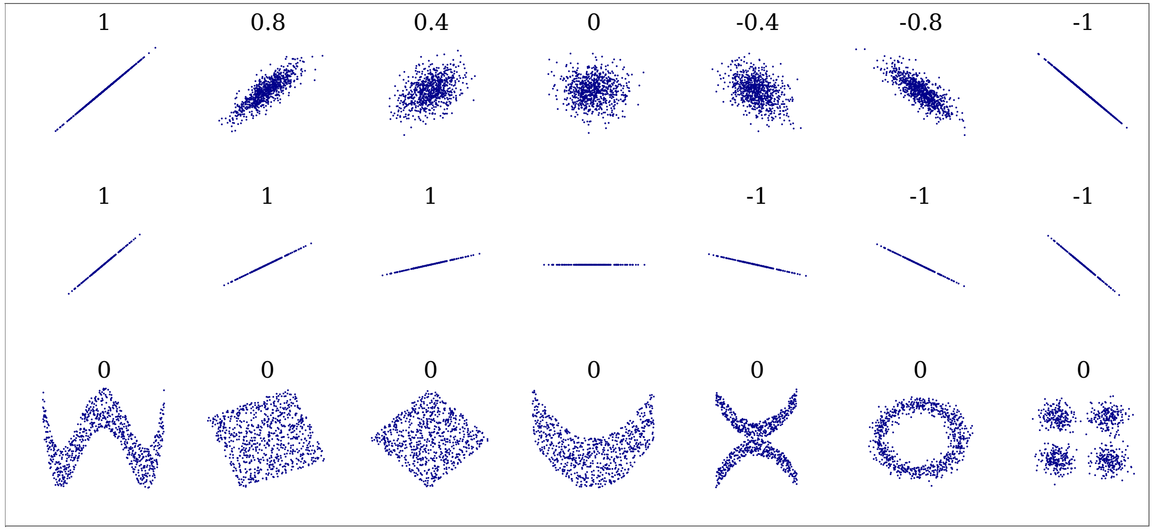
Several sets of (y_i, z_i) points, with the correlation coefficient of y and z for each set.

Top row: $\mathrm{corr}[y, z]$ reflects the noisiness and direction of a linear relationship.

Middle row: $\mathrm{corr}[y, z]$ **does not** reflect the slope of that relationship

Bottom row: $\mathrm{corr}[y, z]$ **does not** reflect many aspects of nonlinear relationships.

(Additional note: the figure in the center has a slope of 0 but in that case the correlation coefficient is undefined because the variance of z is zero.)



Understanding the MVN pdf (a common joint pdf)

$$
\begin{aligned}
p(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) &= \frac{e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(x-\mu)}}{\sqrt{(2\pi)^D|\boldsymbol{\Sigma}|}} && (5) \\
&= \frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right] && (6)
\end{aligned}
$$

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**.

- Multivariate Gaussian pdf's are very important in ML and Statistics.
- Let's discover their properties by working out some examples.

Exercise 1: MVN from independent Gaussian rv's

Consider two **independent** rv's x_1 and x_2 where each of them is a univariate Gaussian pdf:

$$x_1 = \mathcal{N}(x_1|\mu_{x_1}, \sigma^2_{x_1})$$

$$x_2 = \mathcal{N}(x_2|\mu_{x_2}, \sigma^2_{x_2})$$

where $\mu_{x_1} = 10$, $\sigma^2_{x_1} = 5^2$, $\mu_{x_2} = 0.5$ and $\sigma^2_{x_2} = 2^2$.
Answer the following questions:

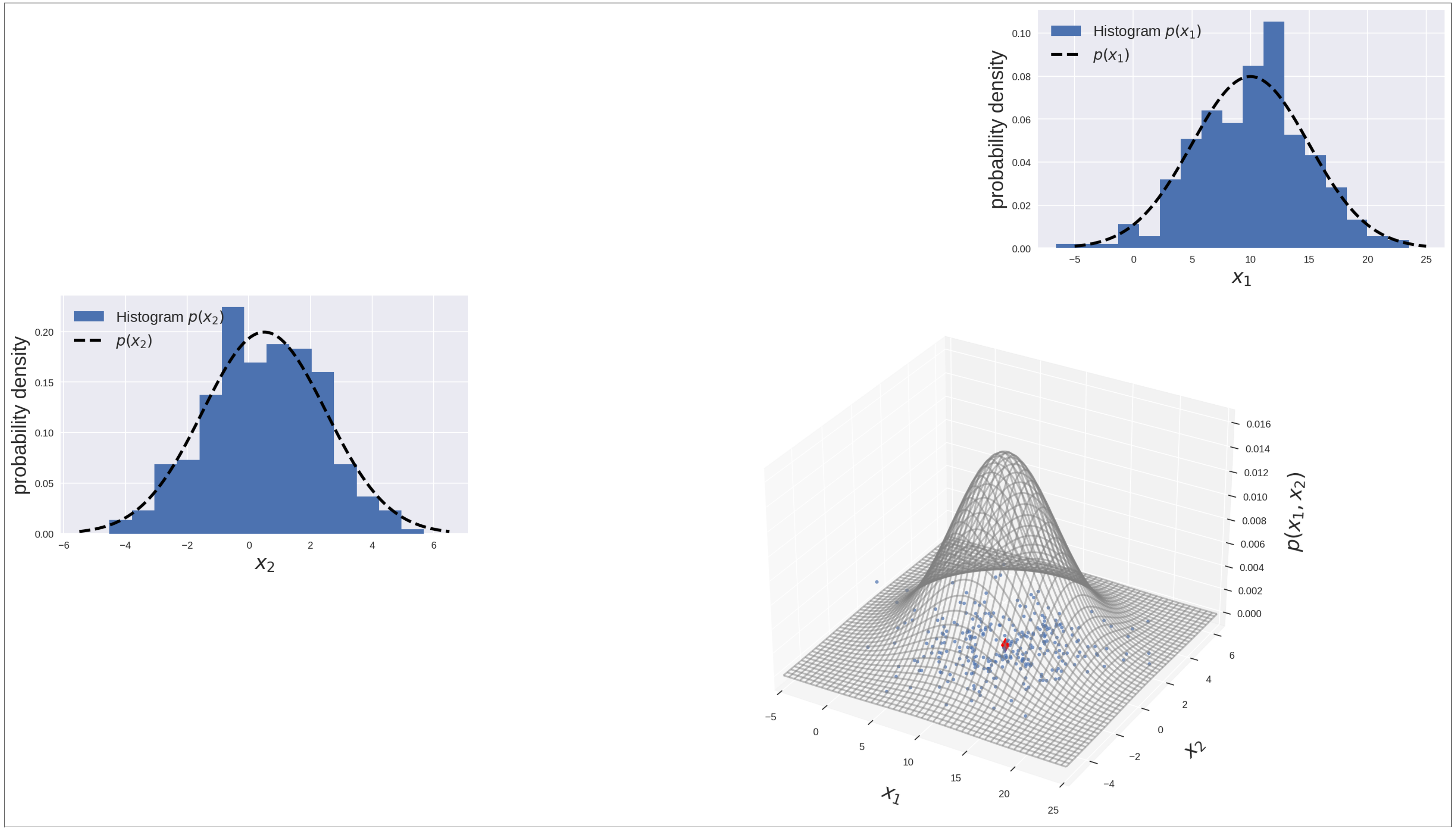
1. What is the joint pdf $p(x_1, x_2)$?
2. Calculate the covariance matrix for $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$.

Once you finish, let's plot the joint pdf.

In [3]:

```
            # HIGHLIGHT DIFFERENCE IN MAXIMUM PROBABILITY DENSITIES!!
fig_joint_pdf_ex1 # The joint pdf results from the multiplication...
```

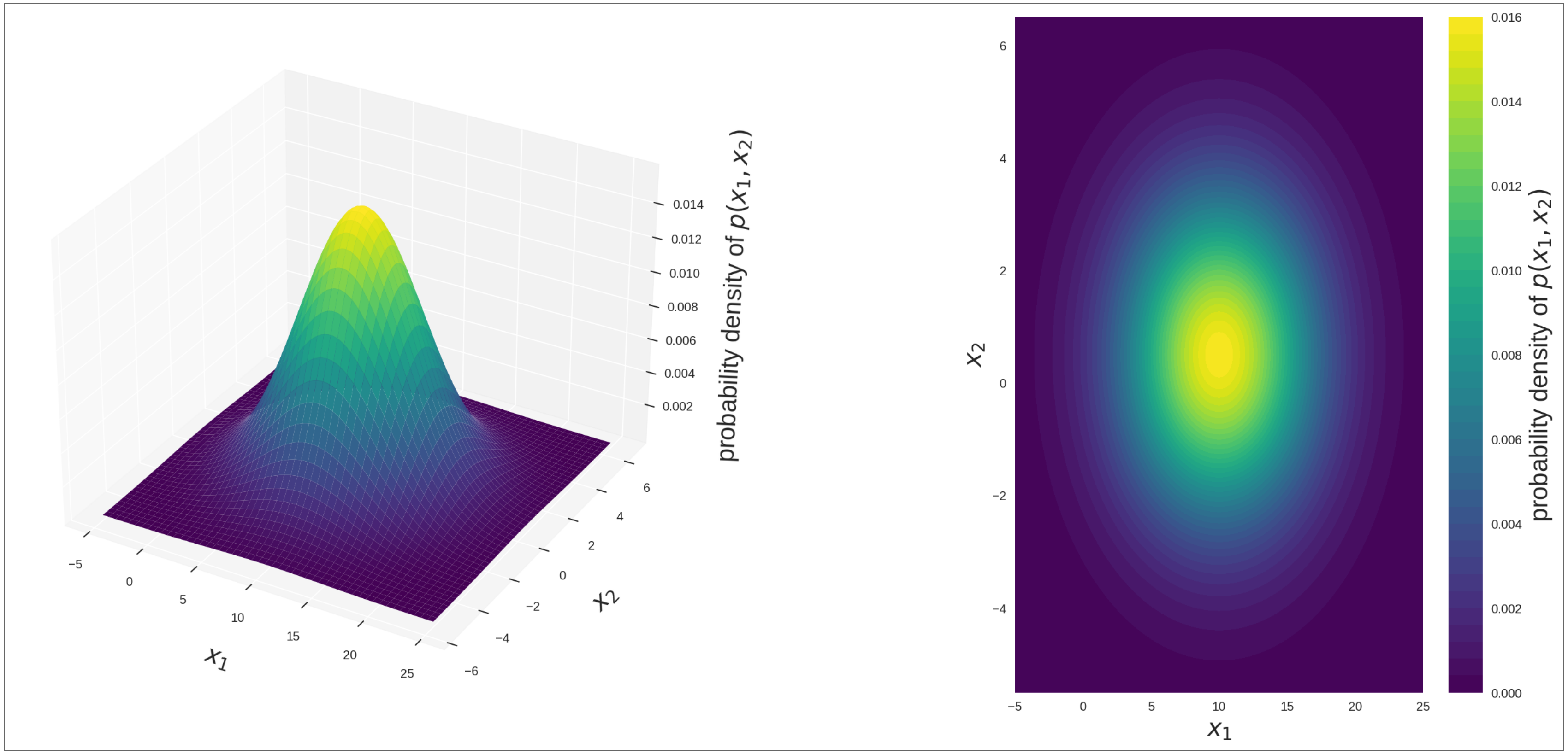
Out[3]:



In [5]:

```
# Same pdf but now as a surface plot and as a contour plot.
fig_joint_pdf_ex1_color
```

Out[5]:



Car stopping distance problem (I know how much you missed it!)

Back to our simple car stopping distance problem with constant velocity $x = 75$ m/s.
We have two rv's for this problem,

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

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

$$\begin{aligned} \mathbf{\Sigma} = \mathrm{Cov}[\mathbf{x}] &= \mathbb{E}\left[(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{x} - \mathbb{E}[\mathbf{x}])^T\right] && (7) \\ &= \begin{bmatrix} \mathbb{V}[y] & \mathrm{Cov}[y, z] \\ \mathrm{Cov}[z, y] & \mathbb{V}[z] \end{bmatrix} && (8) \end{aligned}$$

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

Exercise 2: Covariance matrix for the car problem when $x = 75$ m/s

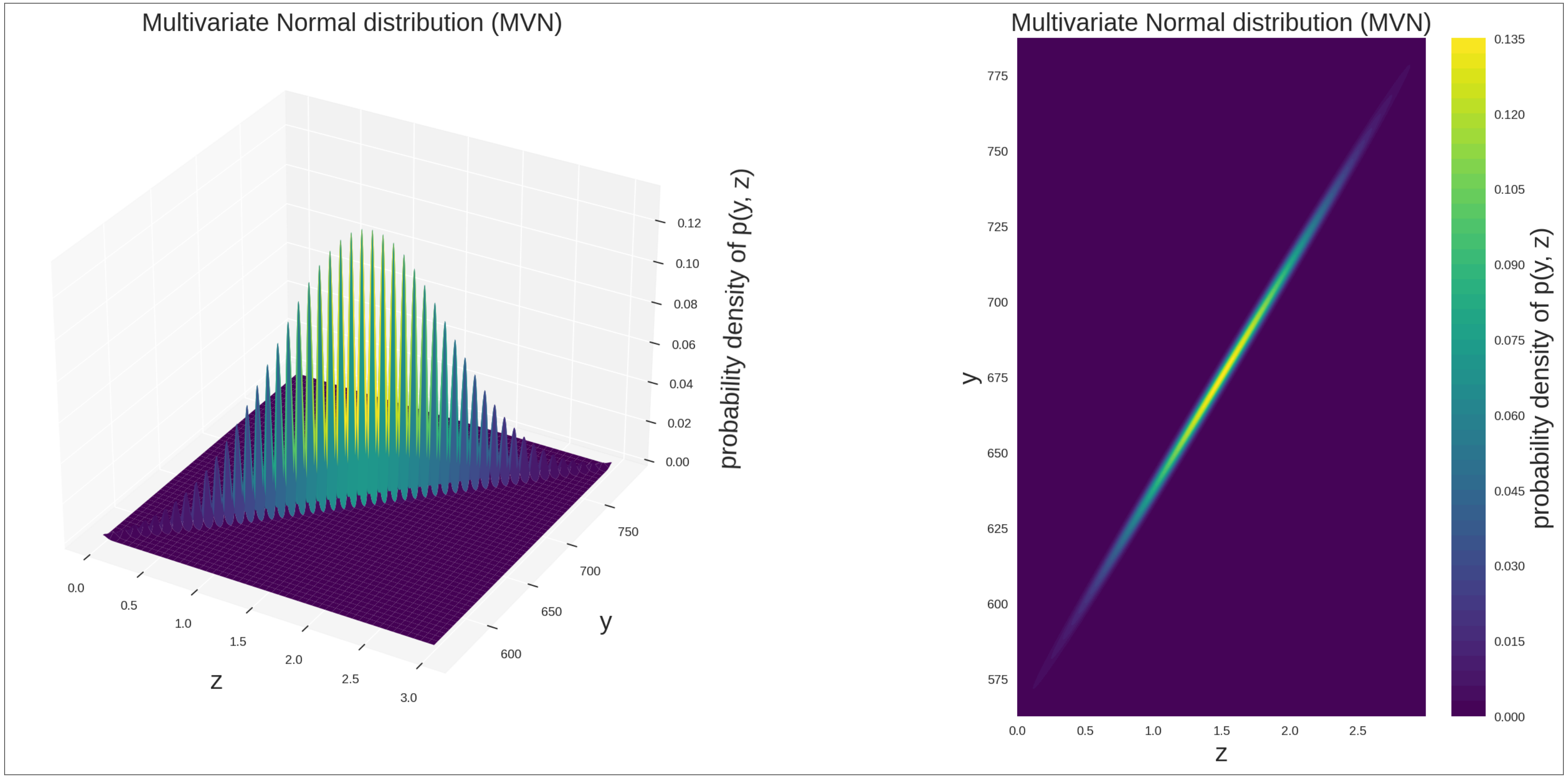
1. Calculate the mean vector and covariance matrix values for our problem (with $x = 75$ m/s). **Be careful** that y is dependent on z!
2. Calculate the determinant of the covariance matrix.

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)
regularizer = 1e-3 # Thikhonov regularization to approximate p(y,z) for car stopping distance problem
plot_car_MVN_regularized(regularizer) # SHOW WHAT HAPPENS IF regularizer is 0, 0.1 and 1e-3
```

```
/tmp/ipykernel_100750/2672719634.py:53: MatplotlibDeprecationWarning: Auto-removal of grids by pcolor() and pcolormesh() is deprecated since 3.5 and will be removed two mi
nor releases later; please call grid(False) first.
  cbar = fig_MVN.colorbar(CS) # Make a colorbar for the ContourSet returned by the co
ntourf call.
```



Recal the joint pdf $p(y, z)$ we found for this problem in Lecture 3!

We determined in Lecture 3 that the joint pdf $p(y, z)$ for this problem is

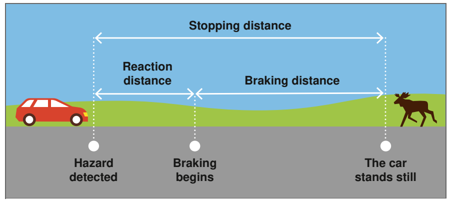
$$p(y, z) = \delta\left(y - (zx + 0.1x^2)\right) p(z)$$

where $p(z) = \mathcal{N}(\mu_z = 1.5, \sigma_z^2 = 0.5^2)$, and $p(y|z) = \delta\left(y - (zx + 0.1x^2)\right)$ is the Dirac delta pdf that assigns zero probability everywhere except when $y = zx + 0.1x^2$.

- Now we see how to approximate this pdf for plotting it:
    - We can consider that the joint pdf $p(y, z)$ is an MVN, and include a small term in the diagonal of the Covariance matrix to plot it! As this term tends to zero, we retrieve the Dirac delta effect.

A slightly more complicated car stopping distance problem

Let's focus (again) on our favorite problem, but this time we include two rv's z_1 and z_2 in the governing model:



$y = z_1 \cdot x + z_2 \cdot x^2$

- y is the **output**: the car stopping distance (in meters)
- z_1 is a hidden variable: an rv representing the driver's reaction time (in seconds)
- z_2 is another hidden variable: an rv that depends on the coefficient of friction, the inclination of the road, the weather, etc. (in m^{-1}s^{-2}).
- x is the **input**: constant car velocity (in m/s).

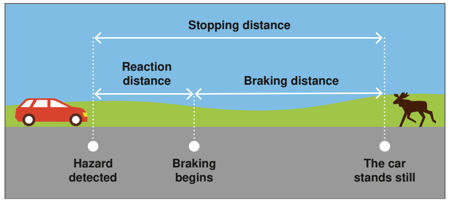
where we will assume as before that $z_1 \sim \mathcal{N}(\mu_{z_1} = 1.5, \sigma_{z_1}^2 = 0.5^2)$, but now we assume $z_2 \sim \mathcal{N}(\mu_{z_2} = 0.1, \sigma_{z_2}^2 = 0.01^2)$. Recall that in previous lectures we assumed $z_2 = 0.1$.

A slightly more complicated car stopping distance problem

For simplicity, also consider that every driver is going at the same velocity $x = 75$ m/s.

$y = z_1 \cdot 75 + z_2 \cdot 75^2 = 75z_1 + 5625z_2$

where $z_1 \sim \mathcal{N}(\mu_{z_1} = 1.5, \sigma_{z_1}^2 = 0.5^2)$, and $z_2 \sim \mathcal{N}(\mu_{z_2} = 0.1, \sigma_{z_2}^2 = 0.01^2)$
.



HOMEWORK

For the slightly more complicated car stopping distance problem, answer this:

1. Show that the conditional pdf $p(y|z_1)$ is:

$$p(y|z_1) = \mathcal{N}\left(y|\mu_{y|z_1} = 5625\mu_{z_2} + 75z_1, \sigma^2_{y|z_1} = (5625\sigma_{z_2})^2\right)$$

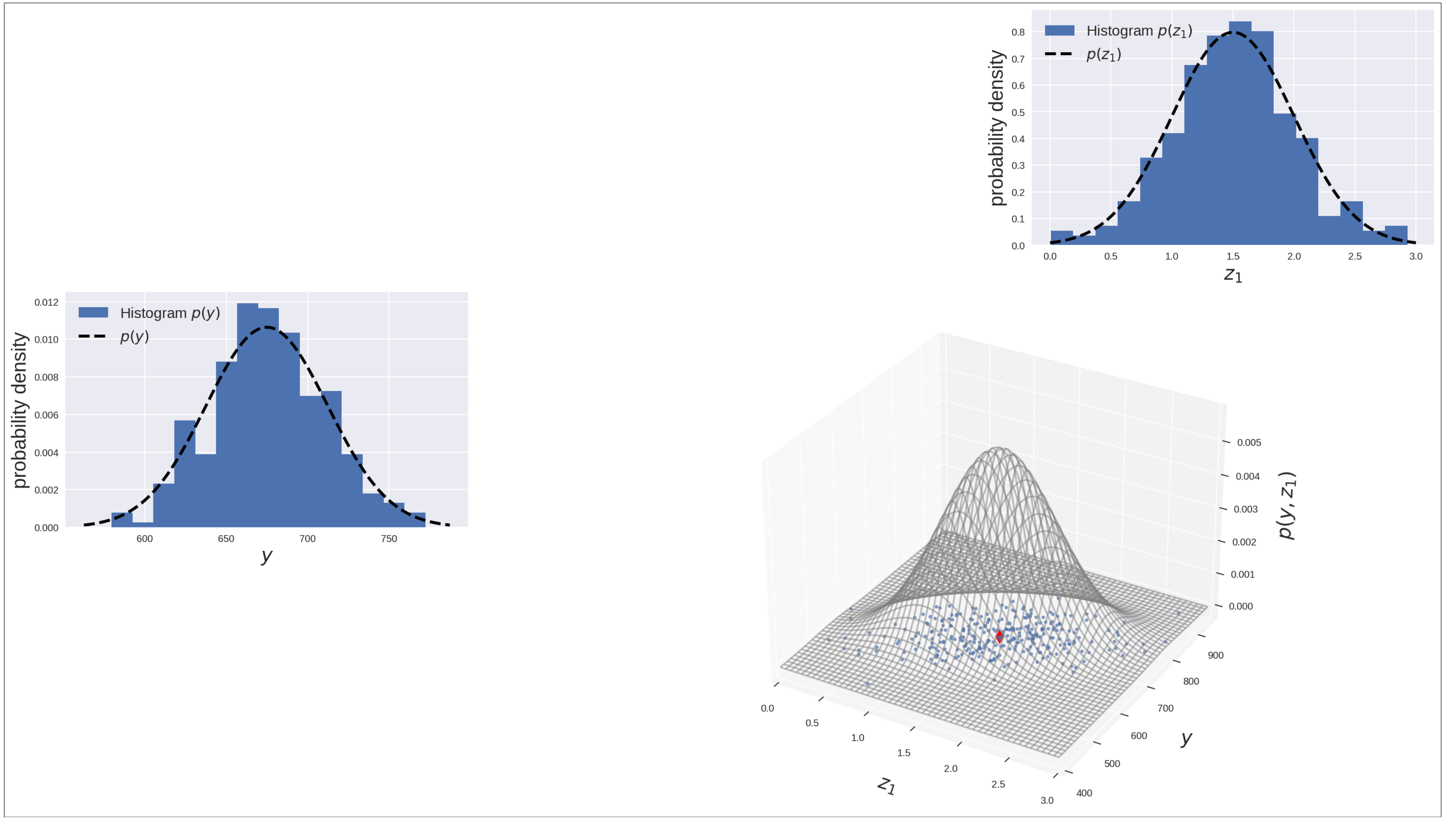
1. What is the joint pdf $p(y, z_1)$?
2. Calculate the covariance matrix for $\mathbf{x} = \begin{bmatrix} y \\ z_1 \end{bmatrix}$, i.e. $\mathrm{Cov}\left(\begin{bmatrix} y \\ z_1 \end{bmatrix}\right)$

The next cell includes the plots of $p(y|z_1)$, $p(y, z_1)$. **But do your HOMEWORK!**

In [9]:

```
             # HIGHLIGHT DIFFERENCE IN MAXIMUM PROBABILITY DENSITIES!!
fig_joint_pdf_HW # The joint pdf results from the multiplication...
```

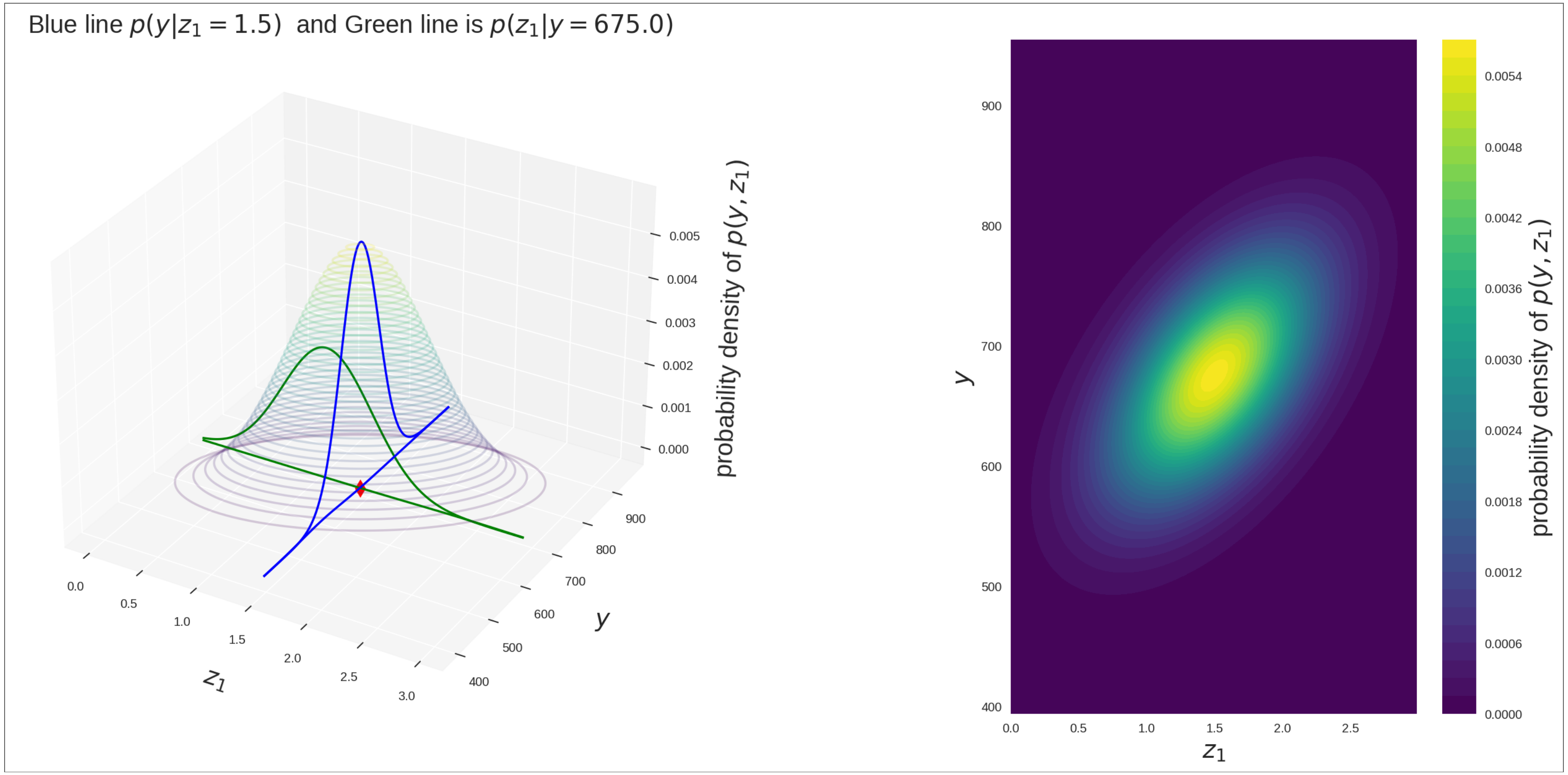
Out[9]:



In [11]:

```
                    # Code is hidden in presentation (shown as notes)
fig_joint_pdf_HW_color # plot p(y,z1), p(y|z1=mu_z1) and p(z1|y=mu_y)
```

Out[11]:



Conclusions about Gaussian distributions

Our empirical investigations in this Lecture, have led to some interesting observations! They can be generalized to:

- If two sets of variables are jointly Gaussian, i.e. if their joint pdf is an MVN, then:
    - their conditional pdfs are Gaussian, i.e. the conditional distribution of one set conditioned on the other is again Gaussian!
    - the marginal distribution of either set is also Gaussian!

This is really important because it means that Gaussians are closed under Bayesian conditioning! We will explore this later.

- Note: Bishop's book has a fantastic discussion about the univariate and multivariate Gaussian distribution (Section 2.3). **I recommend reading it.** I included it in the notes below this cell.

Summary of partitioned Gaussians

Given a joint Gaussian pdf $p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with $\boldsymbol{\Lambda} \equiv \boldsymbol{\Sigma}^{-1}$ and

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{bmatrix}, \quad \boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{bmatrix}, \quad \boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{bmatrix}, \quad \boldsymbol{\Lambda} = \begin{bmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{bmatrix}$$

We have the conditional distribution $p(\mathbf{x}_a, \mathbf{x}_b) = \mathcal{N}(\mathbf{x}_a|\boldsymbol{\mu}_{a|b}, \boldsymbol{\Lambda}_{aa}^{-1})$ with the following parameters:

$$\boldsymbol{\mu}_{a|b} = \boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ab}(\mathbf{x}_b - \boldsymbol{\mu}_b)$$

$$\boldsymbol{\Sigma}_{a|b} = \boldsymbol{\Lambda}_{aa}^{-1}$$

where $\boldsymbol{\Lambda}_{aa} = \left(\boldsymbol{\Sigma}_{aa} - \boldsymbol{\Sigma}_{ab}\boldsymbol{\Sigma}_{bb}^{-1}\boldsymbol{\Sigma}_{ba}\right)^{-1}$, and $\boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ab} = \boldsymbol{\Sigma}_{ab}\boldsymbol{\Sigma}_{bb}^{-1}$.
The marginal distribution is $p(\mathbf{x}_a) = \mathcal{N}(\mathbf{x}_a|\boldsymbol{\mu}_a, \boldsymbol{\Sigma}_{aa})$.

See you next class

Have fun!