What is the meaning of the terms in the force constant matrix (FCM) ?

2D example

We have the potential energy in the quadratic form

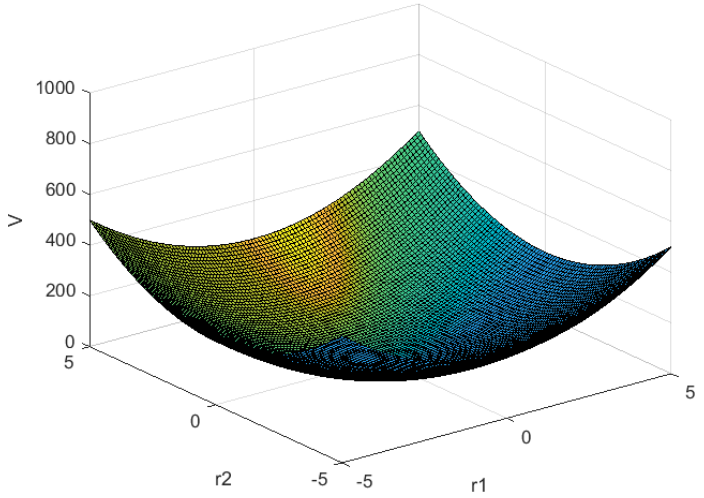
$$V = (\rho_1 \quad \rho_2) * \begin{pmatrix} f_{11} & f_{21} \\ f_{12} & f_{22} \end{pmatrix} * \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix}$$

This function is a paraboloid in ρ_1 and ρ_2. We plot some examples

1) Only main diagonal, same f:

$$FCM = \begin{pmatrix} 10 & 0 \\ 0 & 10 \end{pmatrix}$$

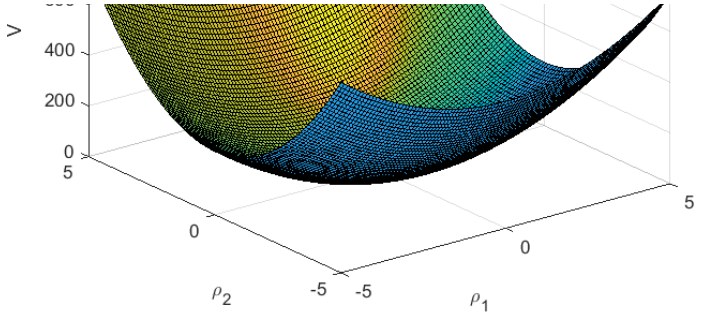
```
fcm=[10 0;0 10];
v1=r1.^2*fcm(1,1)+r2.^2*fcm(2,2)+r1.*r2*fcm(1,2);
[r1 r2]=meshgrid(-5:0.1:5);
surfl(r1,r2,v1); zlim([0 1000]);
xlabel('\rho_1'); ylabel('\rho_2');zlabel('V');
```



2) Only main diagonal, different f:

$$FCM = \begin{pmatrix} 10 & 0 \\ 0 & 20 \end{pmatrix}$$

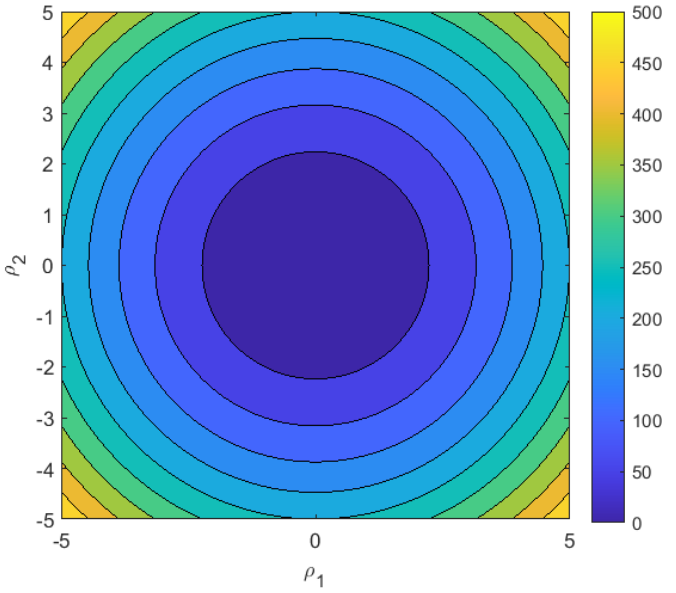
```
fcm=[10 0;0 20];
v2=r1.^2*fcm(1,1)+r2.^2*fcm(2,2)+r1.*r2*fcm(1,2);
[r1 r2]=meshgrid(-5:0.1:5);
surfl(r1,r2,v2); zlim([0 1000]);
xlabel('\rho_1'); ylabel('\rho_2');zlabel('V');
```



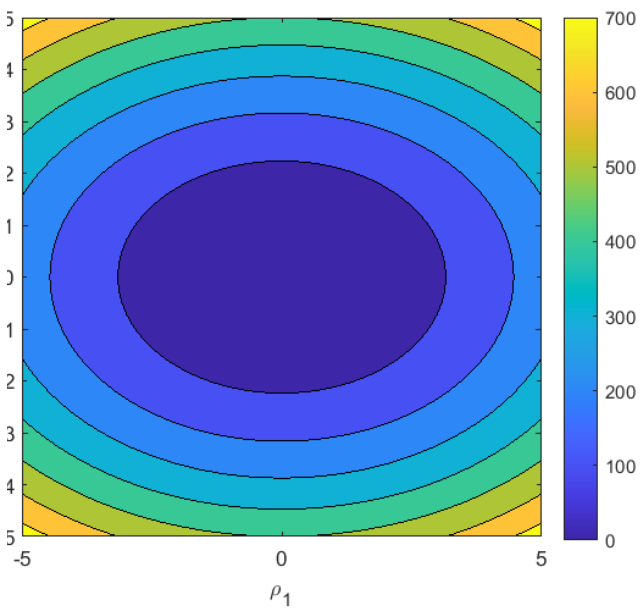
- It turns out that one can see the effect of the terms in the force constant matrix better in contour plots than in 3D plots
- The following page contains several cases
- **One sees that off-diagonal elements cause the paraboloid to rotate !**
- It is still a paraboloid, though, and we are still in the harmonic approximation
- The code for one of the contour plots is given below:

```
fcm=[10 -10;-10 20];
[r1 r2]=meshgrid(-5:0.1:5);
v6=r1.^2*fcm(1,1)+r2.^2*fcm(2,2)+r1.*r2*fcm(1,2);
contourf(r1,r2,v6); axis square; colorbar;
xlabel('\rho_1'); ylabel('\rho_2');
```

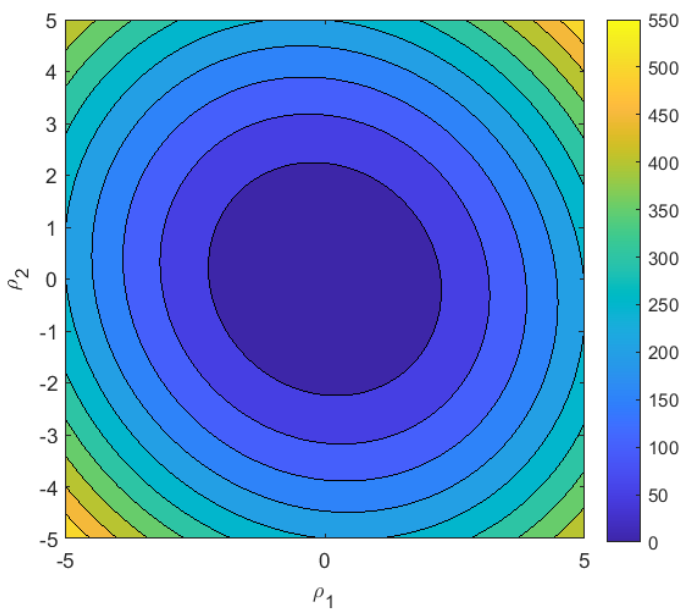
FCM=$\begin{pmatrix} 10 & 0 \\ 0 & 10 \end{pmatrix}$



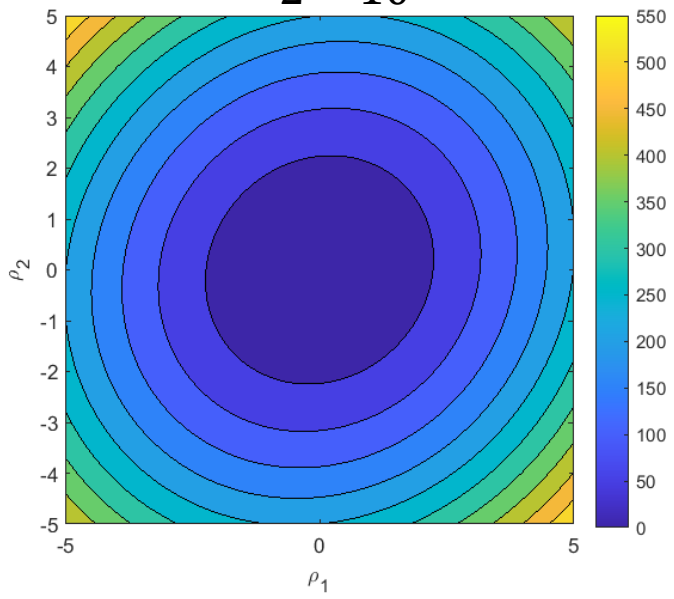
FCM=$\begin{pmatrix} 10 & 0 \\ 0 & 20 \end{pmatrix}$



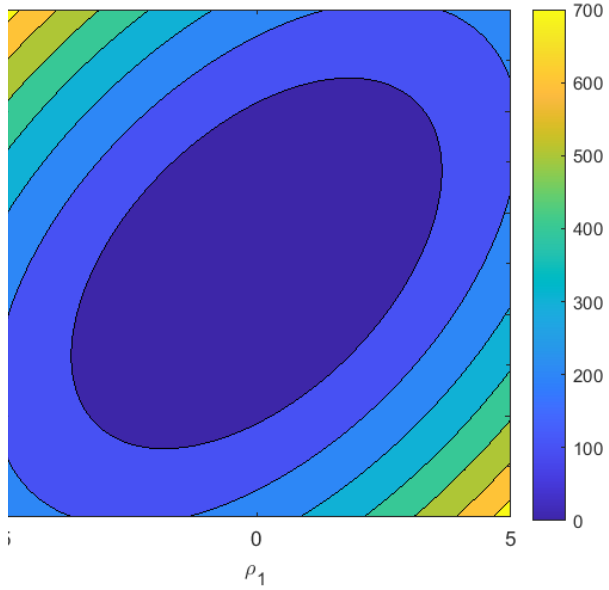
FCM=$\begin{pmatrix} 10 & 2 \\ 2 & 10 \end{pmatrix}$



FCM=$\begin{pmatrix} 10 & -2 \\ -2 & 10 \end{pmatrix}$



FCM=$\begin{pmatrix} 10 & -10 \\ -10 & 10 \end{pmatrix}$



FCM=$\begin{pmatrix} 10 & -10 \\ -10 & 10 \end{pmatrix}$