Constraint Optimization

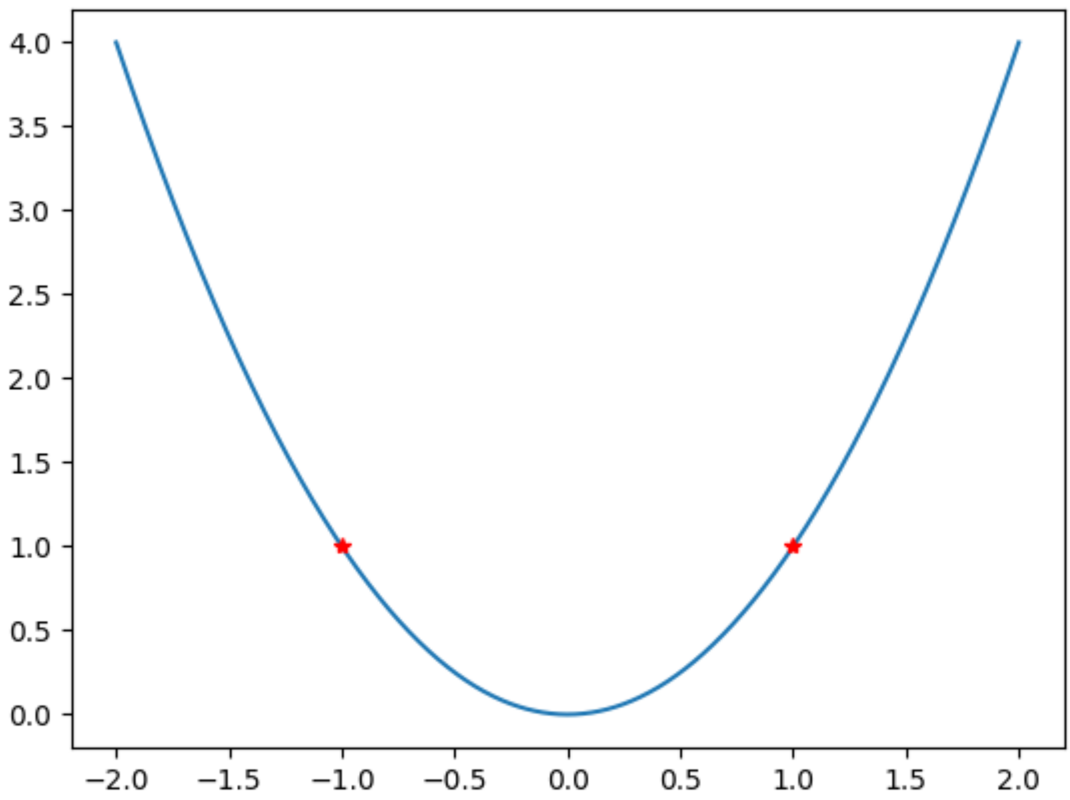
The notebook exercises numerical optimization of problems with equality constraints using Lagrangian multipliers and gradient descent. It implements this idea.

Function and constraint:

$$
\begin{align}
f(x) &= x^2 \tag{1}\\
x^* &= \text{argmin}(f(x)) \tag{2}\\
\text{subject to } x^2 &= 1 \tag{3}
\end{align}
$$

The obviouse solutions are $x_0^* = 1$ and $x_1^* = -1$.

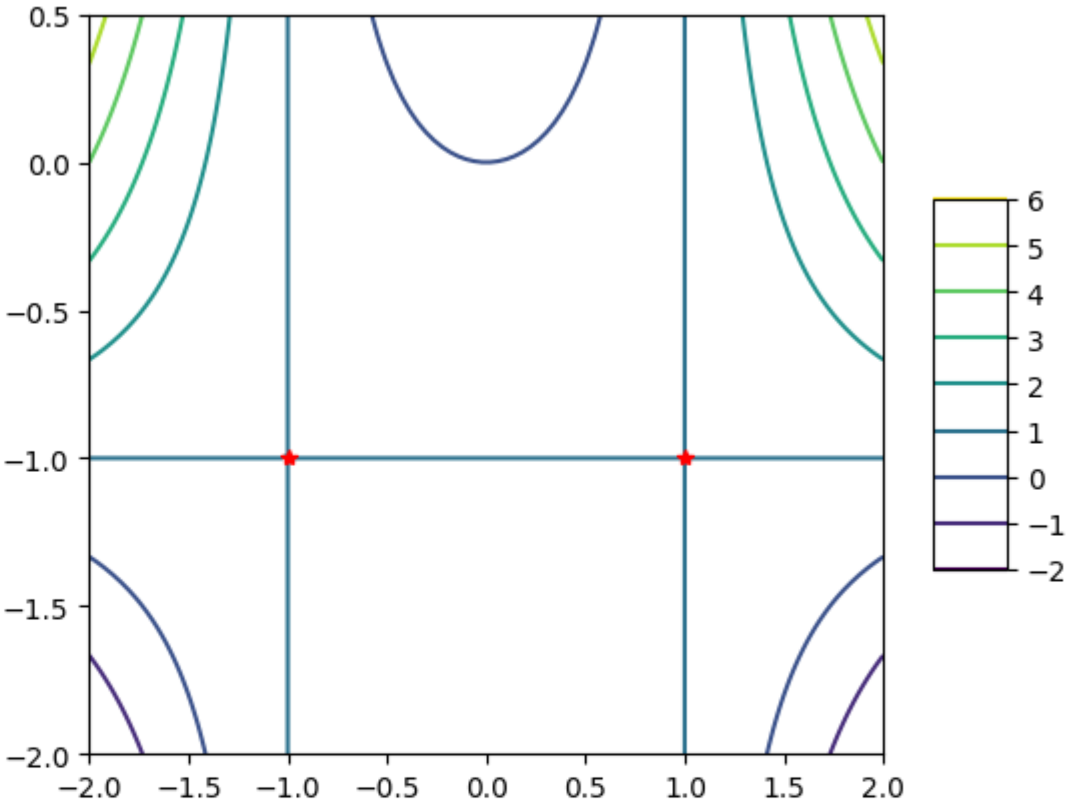
In [ ]:
```
import numpy as np
import matplotlib.pyplot as plt

X = np.linspace(-2,2,1000)
Y = X**2

plt.plot(X,Y)
plt.plot(-1,1, c='r', marker='*')
plt.plot(1,1, c='r', marker='*')
plt.show()
```



Lagrange multipliers:

$$\mathcal{L}(x, \lambda) = x^2 + \lambda(x^2 - 1)$$

In [ ]:
```
L = lambda x, l: x**2 + l*(x**2-1)
xs = np.linspace(-2,2,100)
ls = np.linspace(-2,0.5,100)

A, B = np.meshgrid(xs, ls)

fig = plt.figure()
ax = fig.add_subplot()
surf = ax.contour(A, B, L(A,B), cmap='viridis')
ax.plot(-1,-1, c='r', marker='*')
ax.plot(1,-1, c='r', marker='*')
fig.colorbar(surf, shrink=0.5, aspect=5)
plt.show()
```

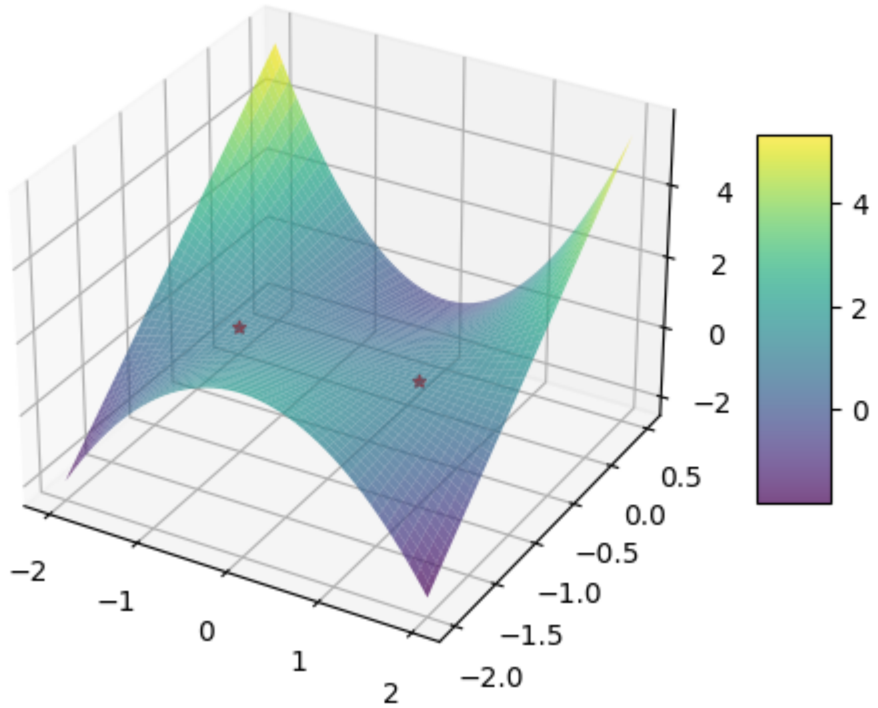


Partials:

$$\frac{\partial \mathcal{L}}{\partial x} = 2x + 2x\lambda \tag{4}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda} = x^2 - 1 \tag{5}$$

In [ ]:
```
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
surf = ax.plot_surface(A, B, L(A,B), cmap='viridis', alpha=0.7)
ax.scatter(-1,-1, L(-1,-1), c='r', marker='*')
ax.scatter(1,-1, L(1,-1), c='r', marker='*')
fig.colorbar(surf, shrink=0.5, aspect=5)
plt.show()
```



In [ ]:
```
def grad_L(x,l):
    grad_x = 2*x+2*x*l
    grad_l = x**2-1
    return np.array([grad_x, grad_l])
```

In [ ]:
```
grad_L(0.5,0.5)
```

Out[ ]:
```
array([ 1.5 , -0.75])
```

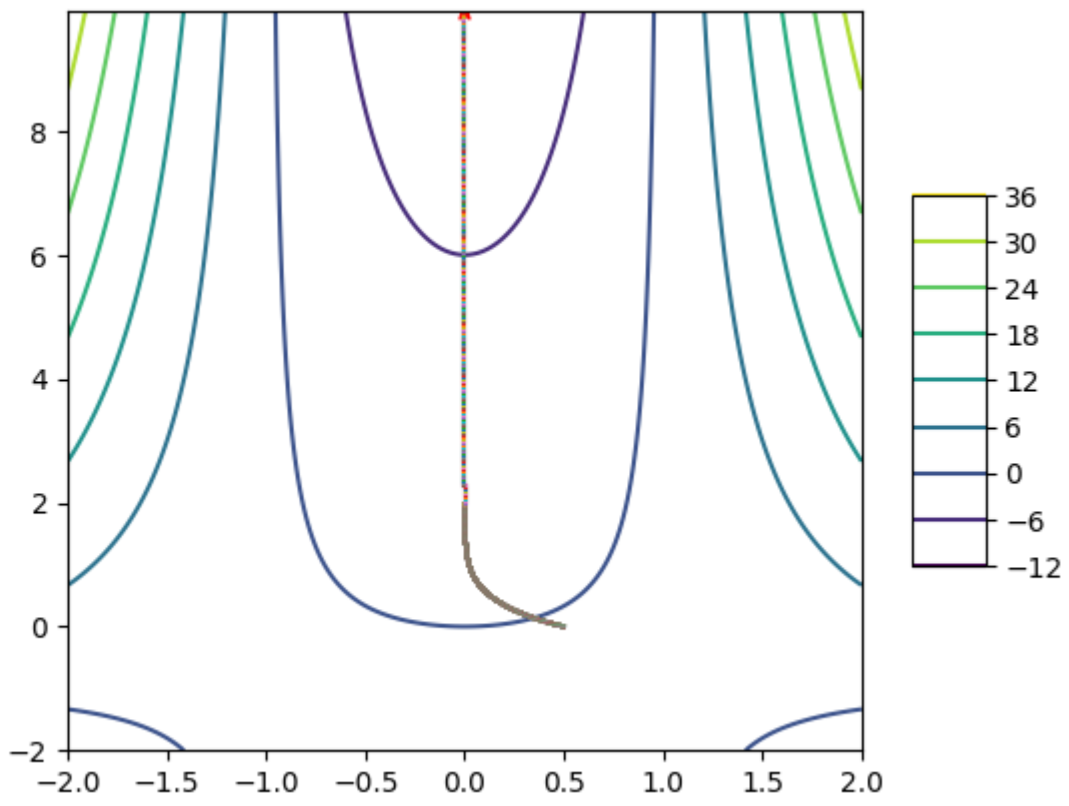
In [ ]:
```
def plot3d(f,A,B,real3d):
    Z = f(A,B)
    if real3d:
        fig = plt.figure()
        ax = fig.add_subplot(111, projection='3d')
        surf = ax.plot_surface(A, B, Z, cmap='viridis')
        fig.colorbar(surf, shrink=0.5, aspect=5)
    else:
        fig = plt.figure()
        ax = fig.add_subplot(111)
        surf = ax.contour(A, B, Z, cmap='viridis')
        fig.colorbar(surf, shrink=0.5, aspect=5)
    return fig, ax
```

In [ ]:
```
def grad_desc(K, x0, l0, learning_eps, f, ff, verbose):
    xs = np.zeros((K+1))
    ls = np.zeros((K+1))
    xs[0] = x0
    ls[0] = l0
    for k in range(K):
        grad = ff(xs[k], ls[k])
        grad_x = grad[0]
        grad_l = grad[1]
        xs[k+1] = xs[k] - learning_eps * grad_x
        ls[k+1] = ls[k] - learning_eps * grad_l
```

```
    if verbose:
        xlow = min(-2, np.min(xs))
        xhigh = max(+2, np.max(xs))
        llow = min(-2, np.min(ls))
        lhigh = max(+0.5, np.max(ls))
        x_sequence = np.linspace(xlow, xhigh, 300)
        l_sequence = np.linspace(llow, lhigh, 300)

        A, B = np.meshgrid(x_sequence, l_sequence)
        fig, ax = plot3d(L, A, B, False)
        for k in range(K):
            ax.plot([xs[k], xs[k+1]], [ls[k], ls[k+1]])
    return xs, ls
```

In [ ]:
```
ff = lambda x,l: grad_L(x,l)

K = 10000
learning_eps = 0.001
xs, ls = grad_desc(K, 0.5,0, learning_eps, L, ff, True)
print(f'{xs[-1]}, {ls[-1]}')
plt.scatter(xs[-1], ls[-1], marker='*', c='r')
plt.show()
```

```
4.596488233240132e-53, 9.946226665273938
```



Gradient descent does not seam to converge to a solution.

The reason is that the critical points of Lagrangians occur at saddle points, rather than at local minima. Therefore, we must modify the problem formulation to ensure that it's a minimization problem. Below we do this by minimizing the square of the Lagrangian gradient's magnitude.

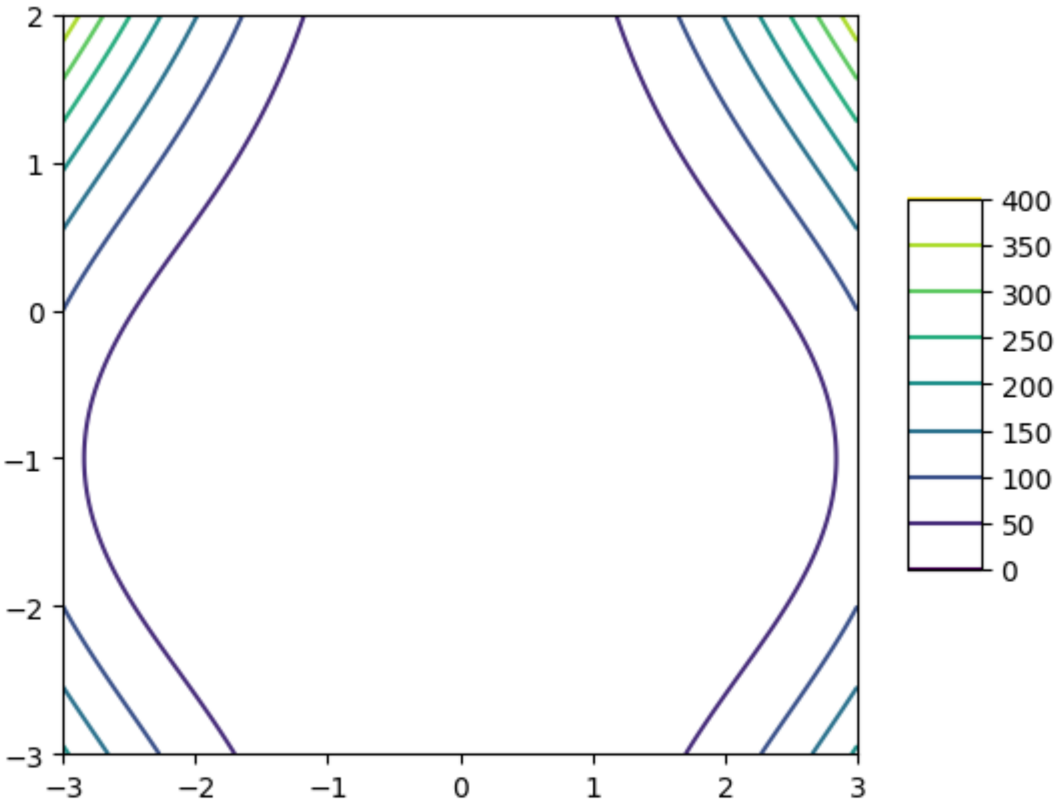
(Squared) magnitude of the gradient of the Lagrangian:

$$h^2(x, \lambda) = (2x + 2x\lambda)^2 + (x^2 - 1)^2$$

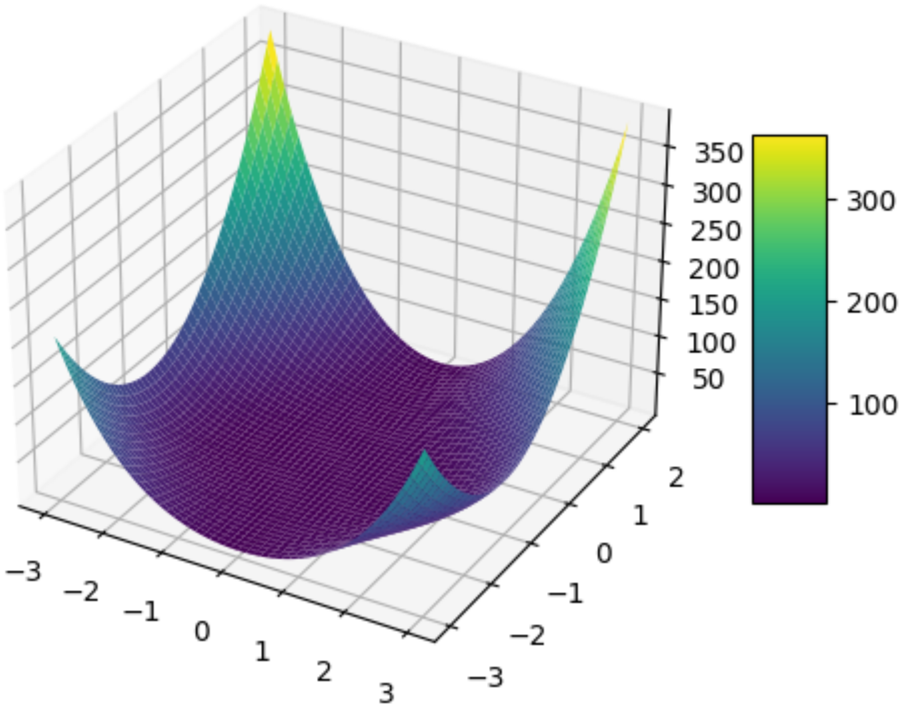
$$h(x, \lambda) = \sqrt{(2x + 2x\lambda)^2 + (x^2 - 1)^2}$$

In [ ]:
```
h2 = lambda x, l: (2*x+2*x*l)**2 + (x**2-1)**2
h = lambda x, l: np.sqrt(h2(x,l))

x_sequence = np.linspace(-3, 3, 300)
l_sequence = np.linspace(-3, 2, 300)

A,B = np.meshgrid(x_sequence, l_sequence)
```

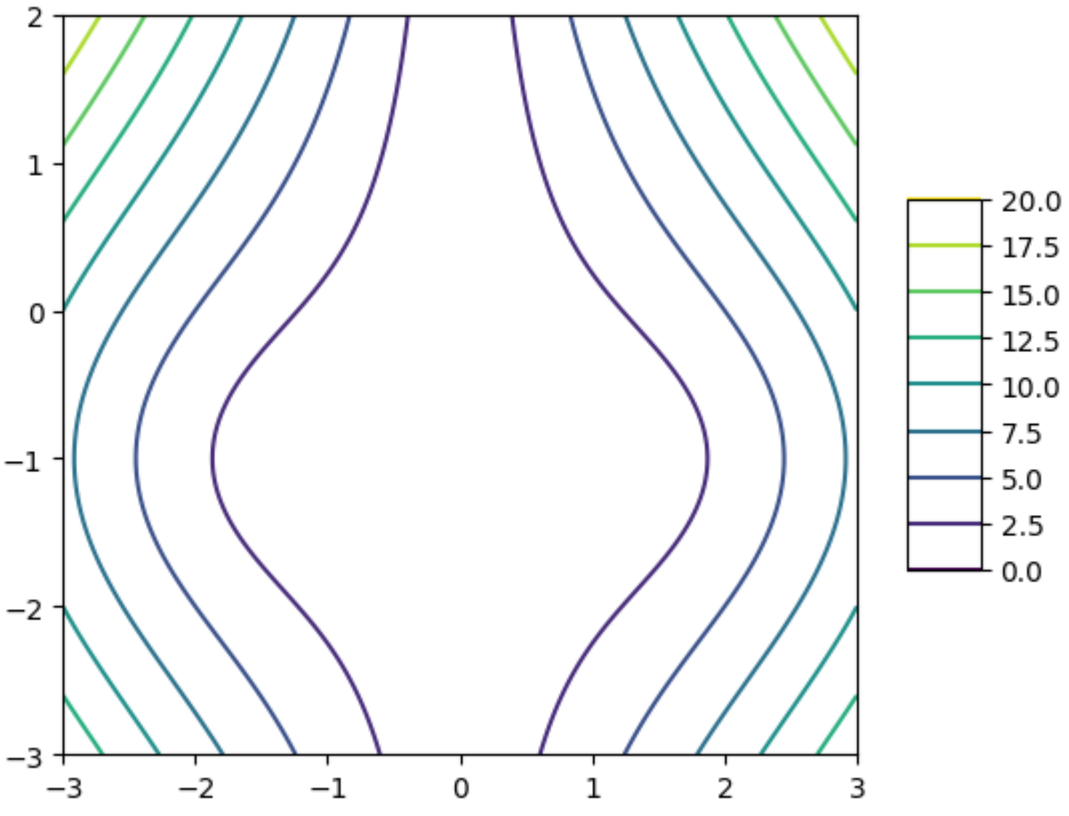
In [ ]:
```
plot3d(h2, A, B, False)
plt.show()
```



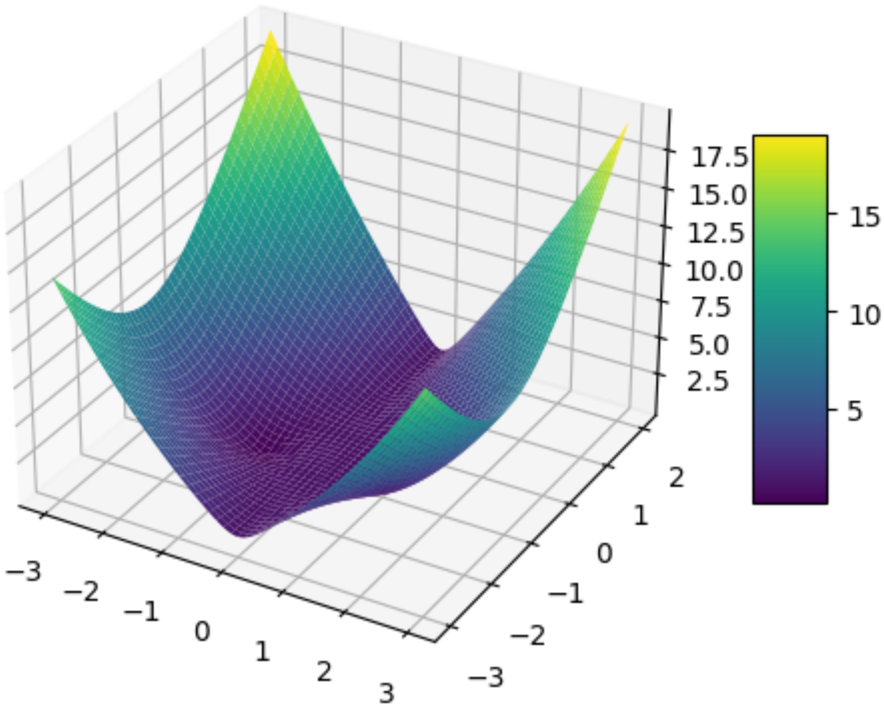
In [ ]:
```
plot3d(h2, A, B, True)
plt.show()
```



In [ ]:
```
plot3d(h, A, B, False)
plt.show()
```



In [ ]:
```
plot3d(h, A, B, True)
plt.show()
```



Gradient of squared magnitude

$$\begin{bmatrix} \frac{\partial h^2}{\partial x} \\ \frac{\partial h^2}{\partial \lambda} \end{bmatrix} = \begin{bmatrix} 4x(x^2 + 2\lambda^2 + 4\lambda + 1) \\ 8x^2(\lambda + 1) \end{bmatrix}$$

In [ ]:
```
def grad_h2(x,l):
    grad_x = 4*x*(x**2+2*l**2+4*l+1)
    grad_l = 8*x**2*(l+1)
    return np.array([grad_x, grad_l])
```

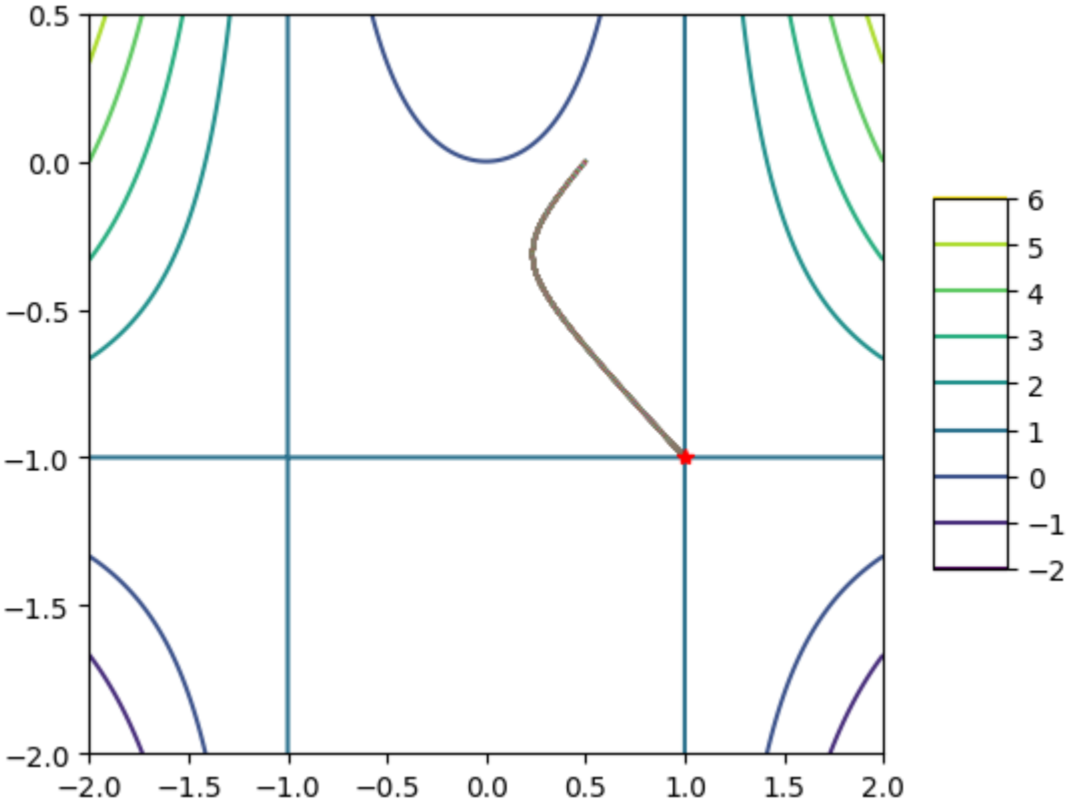
In [ ]:
```
grad_h2(0,0)
```

Out[ ]:
```
array([0, 0])
```

We should not start at the saddle points $(0, \lambda_0)$

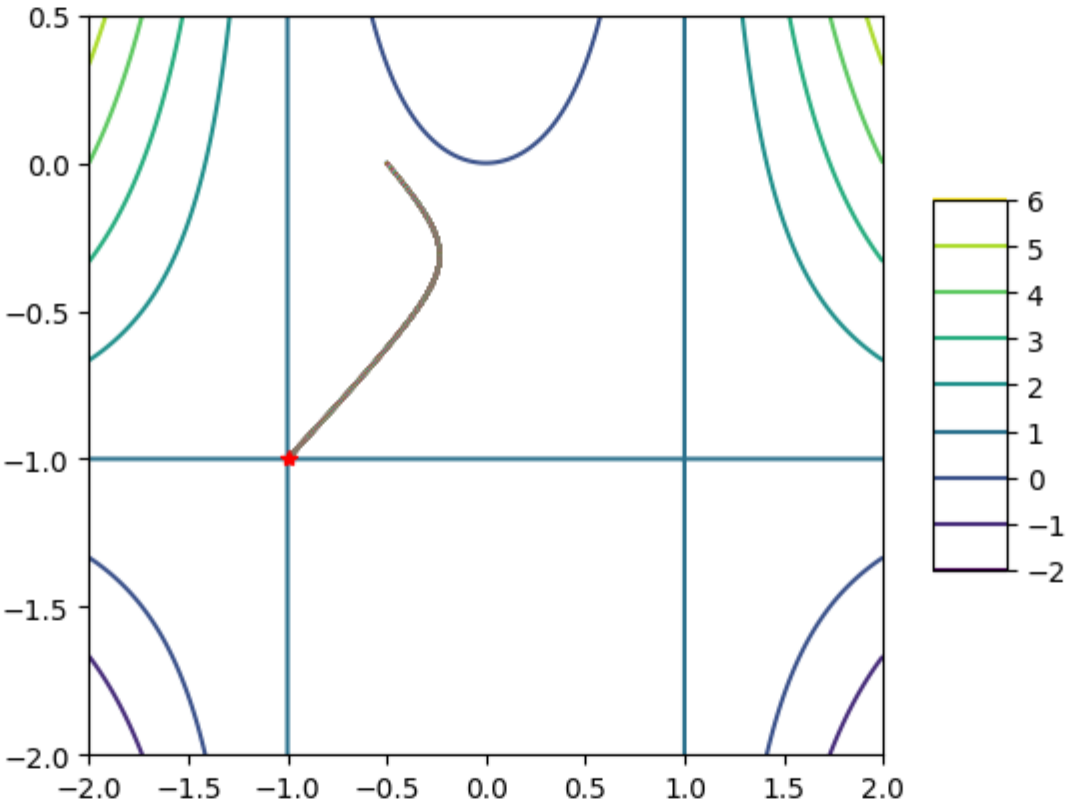
In [ ]:
```
ff = lambda x,l : grad_h2(x,l)

K = 10000
learning_eps = 0.001
xs, ls = grad_desc(K, 0.5, 0, learning_eps, h2, ff, True)
print(f'{xs[-1]}, {ls[-1]}')
plt.plot([xs[-1]], [ls[-1]], marker='*', c='r')
plt.show()
```

```
0.9999999999999931, -0.9999999999999931
```



In [ ]:
```
xs, ls = grad_desc(K, -0.5, 0, learning_eps, h2, ff, True)
print(f'{xs[-1]}, {ls[-1]}')
plt.plot([xs[-1]], [ls[-1]], marker='*', c='r')
plt.show()
```

```
-0.9999999999999931, -0.9999999999999931
```



Gradient of magnitude

$$\begin{bmatrix} \frac{\partial h}{\partial x} \\ \frac{\partial h}{\partial \lambda} \end{bmatrix} = \frac{1}{\sqrt{x^4 + x^2(4\lambda^2 + 8\lambda + 2) + 1}} \begin{bmatrix} 2x(x^2 + 2\lambda^2 + 4\lambda + 1) \\ 4x^2(\lambda + 1) \end{bmatrix}$$

In [ ]:
```
import math

def grad_h(x,l):
    grad_x = 2*x*(x**2+2*l**2+4*l+1)
    grad_l = 4*x**2*(l+1)
    factor = 1/math.sqrt(x**4+x**2*(4*l**2+8*l+2)+1)
    return np.array([grad_x * factor, grad_l * factor])
```

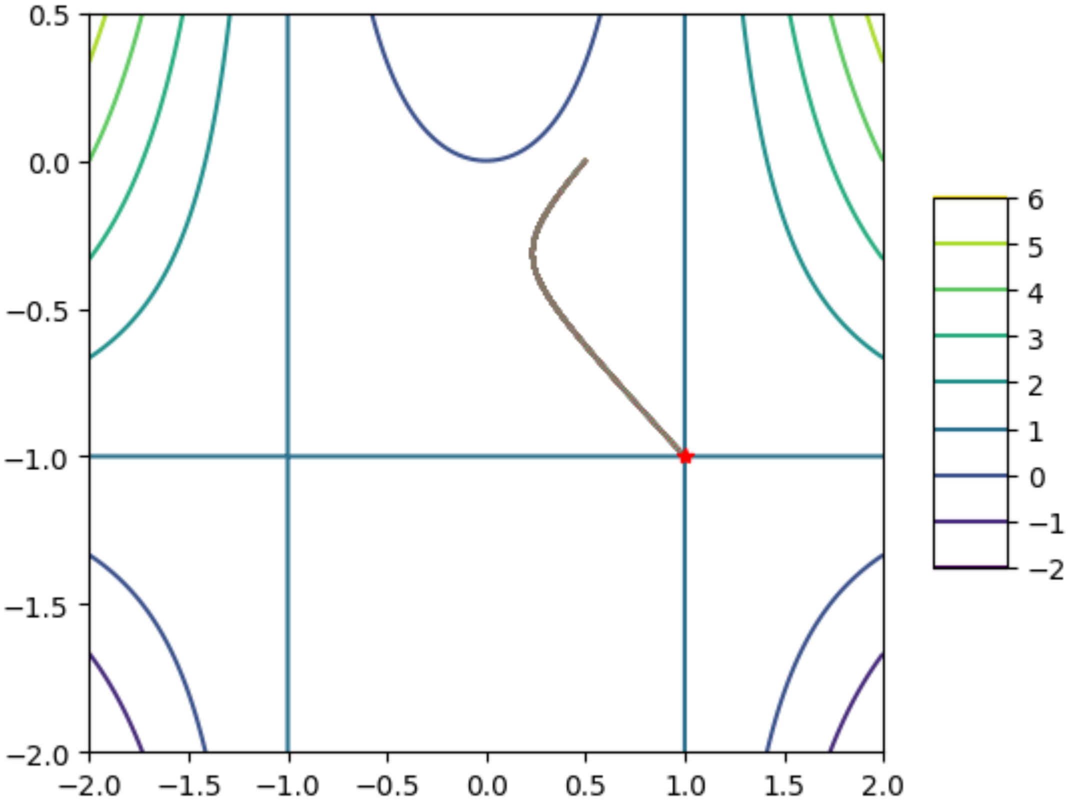
In [ ]:
```
grad_h(0,0)
```

Out[ ]:
```
array([0., 0.])
```

Mind that $(0, \lambda_0)$ are saddle points in h as well. We should not start at any of them.

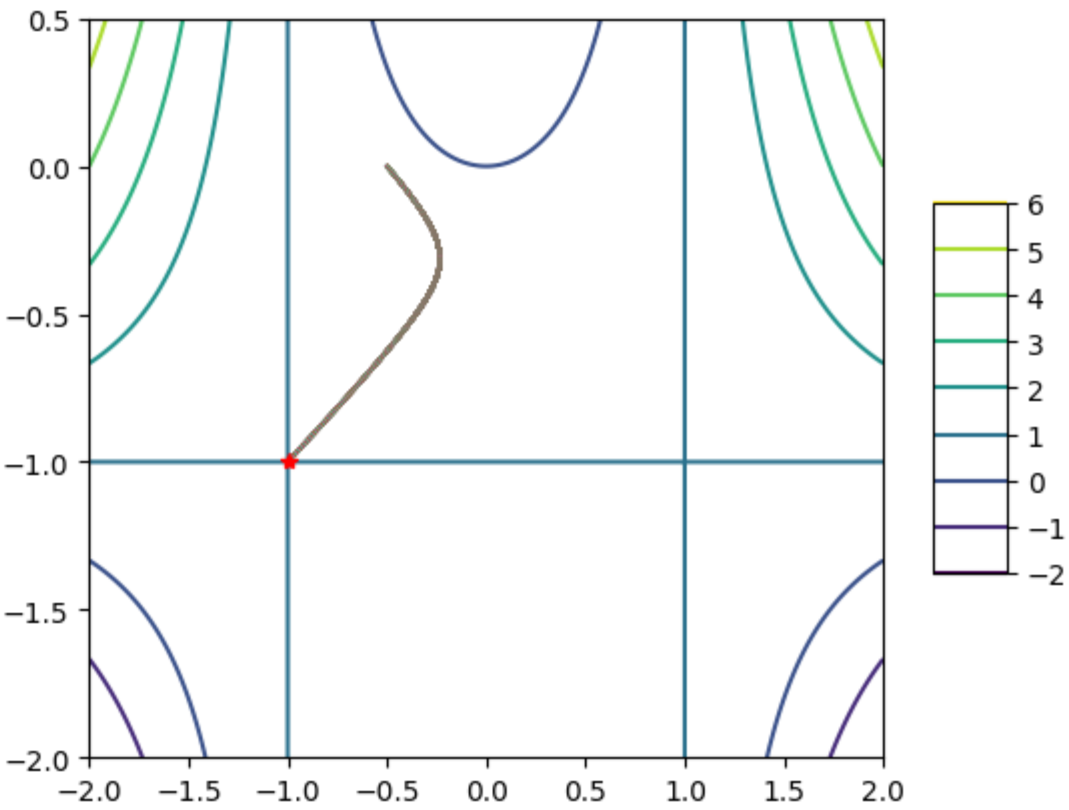
In [ ]:
```
ff = lambda x,l: grad_h(x,l)
xs, ls = grad_desc(K, 0.5, 0, learning_eps, h, ff, True)
print(f'{xs[-1]}, {ls[-1]}')
plt.plot([xs[-1]], [ls[-1]], marker='*', c='r')
plt.show()
```

```
0.999186474261779, -0.9994251028655677
```



In [ ]:
```
xs, ls = grad_desc(K, -0.5, 0, learning_eps, h, ff, True)
print(f'{xs[-1]}, {ls[-1]}')
plt.plot([xs[-1]], [ls[-1]], marker='*', c='r')
plt.show()
```

```
-0.999186474261779, -0.9994251028655677
```



In [ ]:
```
grad_factor = lambda x,l: 1/math.sqrt(x**4+x**2*(4*l**2+8*l+2)+1)
grad_factor(1,-1)
```

```
---------------------------------------------------------------------------
ZeroDivisionError                         Traceback (most recent call last)
Cell In[22], line 2
      1 grad_factor = lambda x,l: 1/math.sqrt(x**4+x**2*(4*l**2+8*l+2)+1)
----> 2 grad_factor(1,-1)

Cell In[22], line 1, in <lambda>(x, l)
----> 1 grad_factor = lambda x,l: 1/math.sqrt(x**4+x**2*(4*l**2+8*l+2)+1)
      2 grad_factor(1,-1)

ZeroDivisionError: float division by zero
```

In my case, I got an ZeroDevisionError. This is based on the interpretation of the denominator of the grad_factor:

In [ ]:
```
grad_factor_denom = lambda x,l: math.sqrt(x**4+x**2*(4*l**2+8*l+2)+1)
grad_factor_denom(1,-1)
```

Out[ ]: 0.0

Although the minima are more pronounced in h than in h^2, gradient descent converges better in h^2. This is due to problems of calculating the factor

$$\frac{1}{\sqrt{x^4 + x^2(4\lambda^2 + 8\lambda + 2) + 1}}$$

of the gradient of h near the solutions. This factor is actually not defined at the solution (division by zero).