Example 2.

Sensitivity of hydraulic head at a point to spatially uniform recharge under steady state flow conditions

0. Forward model

Governing equation

$$K\,b\,\frac{d^2h}{dx^2} + R = 0 \qquad (1)$$
$$(2)$$

Boundary conditions

$$-K\,b\,\frac{dh(x)}{dx} = 0\,, \qquad x = 0 = \Gamma_2 \qquad (3)$$
$$h(x) = h_C\,, \qquad x = L = \Gamma_1 \qquad (4)$$
$$(5)$$

Closed-form solution

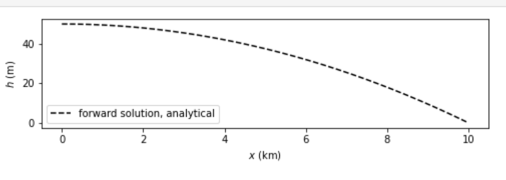
$$h(x) = h_C + \frac{R\,(L^2 - x^2)}{2\,K\,b} \qquad (6)$$
$$(7)$$

Spatial derivatives from differentiation

$$\frac{dh}{dx} = -\frac{R\,x}{K\,b}\,, \qquad \frac{d^2h}{dx^2} = -\frac{R}{K\,b} \qquad (8)$$

```
In [ ]: from IPython.display import HTML, display
        def set_background(color):
            [illegible]
            display(HTML([illegible]))
```

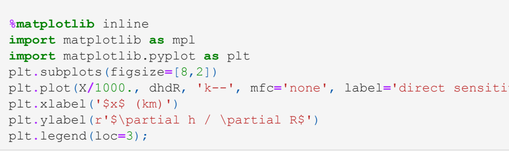
```
In [ ]: from warnings import filterwarnings
        filterwarnings("ignore", category=DeprecationWarning)

        import numpy as np

        def h(x, R, K, b, L, BC1h):
            [illegible]

        [illegible]

        %matplotlib inline
        import matplotlib as mpl
        import matplotlib.pyplot as plt
        plt.subplots(figsize=[8,2])
        plt.plot(X/1000., [illegible], 'k--', mfc='none', label='forward solution, analytical')
        plt.xlabel('$x$ (km)')
        plt.ylabel('$h$ (m)')
        plt.legend(loc=3);
```



1. Direct sensitivity

$$\frac{\partial h(x')}{\partial R} = \frac{L^2 - x'^2}{2\,K\,b} \qquad (9)$$
$$(10)$$
$$(11)$$

```
In [ ]: dhdR = [illegible]
        benchmark = [illegible]

        %matplotlib inline
        import matplotlib as mpl
        import matplotlib.pyplot as plt
        plt.subplots(figsize=[8,2])
        plt.plot(X/1000., dhdR, 'k--', mfc='none', label='direct sensitivity, analytical')
        plt.xlabel('$x$ (km)')
        plt.ylabel(r'$\partial h / \partial R$')
        plt.legend(loc=3);
```




```
In [ ]: set_background('rgba(0, 200, 0, 0.2)')
        print('%.6f (%.6f)'% (dhdR[ocol], benchmark))
```

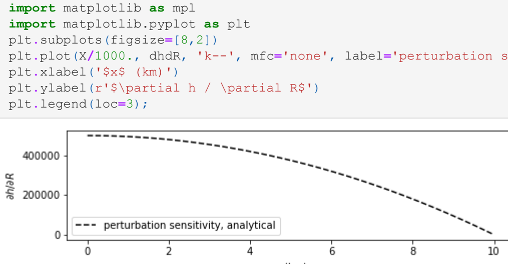
375000.000000 (375000.000000)

2. Perturbation sensitivity

$$\frac{\partial h(x')}{\partial R} \approx \frac{h(x, R + \Delta R) - h(x, R)}{\Delta R} \qquad (12)$$
$$(13)$$
$$(14)$$

2a. Analytical

```
In [ ]: [illegible]

        %matplotlib inline
        import matplotlib as mpl
        import matplotlib.pyplot as plt
        plt.subplots(figsize=[8,2])
        plt.plot(X/1000., dhdR, 'k--', mfc='none', label='perturbation sensitivity, analytical')
        plt.xlabel('$x$ (km)')
        plt.ylabel(r'$\partial h / \partial R$')
        plt.legend(loc=3);
```

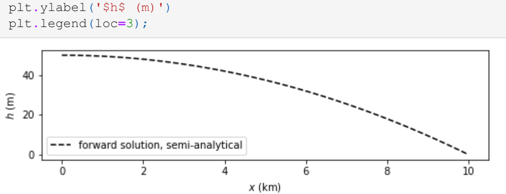



```
In [ ]: set_background('rgba(0, 200, 0, 0.2)')
        print('%.6f (%.6f)'% (dhdR[ocol], benchmark))
```

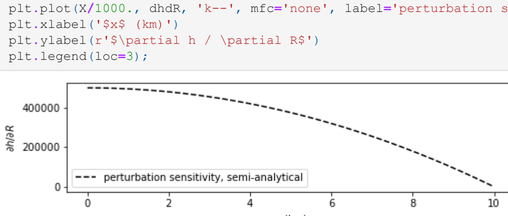
[illegible] (375000.000000)

2b. Semi-analytical

```
In [ ]: from ttim import [illegible]
        [illegible]

        %matplotlib inline
        import matplotlib as mpl
        import matplotlib.pyplot as plt
        plt.subplots(figsize=[8,2])
        plt.plot(X/1000., [illegible], 'k--', mfc='none', label='forward solution, semi-analytical')
        plt.xlabel('$x$ (km)')
        plt.ylabel('$h$ (m)')
        plt.legend(loc=3);
```




```
In [ ]: [illegible]

        %matplotlib inline
        import matplotlib as mpl
        import matplotlib.pyplot as plt
        plt.subplots(figsize=[8,2])
        plt.plot(X/1000., dhdR, 'k--', mfc='none', label='perturbation sensitivity, semi-analytical')
        plt.xlabel('$x$ (km)')
        plt.ylabel(r'$\partial h / \partial R$')
        plt.legend(loc=3);
```

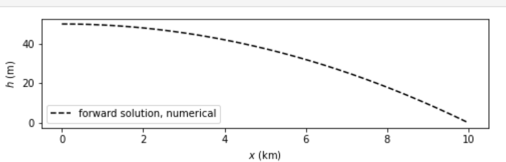



```
In [35]: set_background('rgba(0, 200, 0, 0.2)')
         print('%.6f (%.6f)'% (dhdR[ocol], benchmark))
```

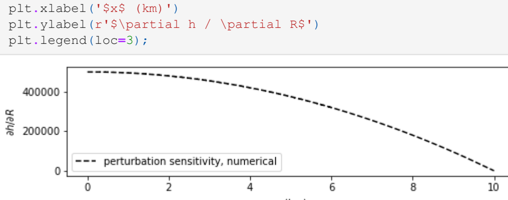
375000.000000 (375000.000000)

2c. Numerical

```
In [36]: import flopy

         nrow, ncol = 1, int(L)
         M0 = flopy.modflow.Modflow(modelname='model', exe_name='../mf2005.exe')
         flopy.modflow.ModflowDis(M0, nlay=1, nrow=nrow, ncol=ncol, nper=1, delr=1., delc=1., top=0., botm=-b, steady=Tr
                                  perlen=1., nstp=1)
         flopy.modflow.ModflowBas(M0, ibound=np.hstack([np.ones([nrow, ncol-1], dtype=int), -1*np.ones([1,1])]),
                                  strt=BC1h*np.ones([nrow, ncol], dtype=float))
         flopy.modflow.ModflowLpf(M0, hk=K, vka=-999., ss=-999., sy=-999., ipakcb=53)
         flopy.modflow.ModflowRch(M0, nrchop=1, rech=R, ipakcb=53)
         flopy.modflow.ModflowPcg(M0, hclose=1e-6, rclose=1e-6)
         flopy.modflow.ModflowOc(M0, stress_period_data={(0,0): ['save head', 'save budget']})
         M0.write_input()
         success, buff = M0.run_model(silent=True)
         H0 = flopy.utils.binaryfile.HeadFile('model.hds').get_data()[0,0,:]

         %matplotlib inline
         import matplotlib as mpl
         import matplotlib.pyplot as plt
         plt.subplots(figsize=[8,2])
         plt.plot(X/1000., H0, 'k--', mfc='none', label='forward solution, numerical')
         plt.xlabel('$x$ (km)')
         plt.ylabel('$h$ (m)')
         plt.legend(loc=3);
```




```
In [37]: M1 = M0
         flopy.modflow.ModflowRch(M1, nrchop=1, rech=R+R*dpar, ipakcb=53)
         M1.write_input()
         success, buff = M1.run_model(silent=True)
         H1 = flopy.utils.binaryfile.HeadFile('model.hds').get_data()[0,0,:]
         dhdR = (H1-H0)/(R*dpar)

         %matplotlib inline
         import matplotlib as mpl
         import matplotlib.pyplot as plt
         plt.subplots(figsize=[8,2])
         plt.plot(X/1000., dhdR, 'k--', mfc='none', label='perturbation sensitivity, numerical')
         plt.xlabel('$x$ (km)')
         plt.ylabel(r'$\partial h / \partial R$')
         plt.legend(loc=3);
```




```
In [38]: set_background('rgba(0, 200, 0, 0.2)')
         print('%.6f (%.6f)'% (dhdR[ocol], benchmark))
```

374984.750000 (375000.000000)

3. Adjoint sensitivity

$$\frac{\partial h(x')}{\partial R} = \int_X \psi_1^*(x)\,dx \qquad (15)$$

Governing equation:

$$K\,b\,\frac{d\psi_1^*}{dx} + \frac{1}{2\,K\,b}\delta(x - x') = 0 \qquad (16)$$
$$(17)$$

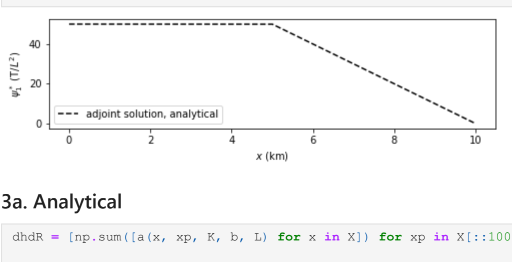
Boundary conditions:

$$-K\,b\,\frac{d\psi_1^*(x)}{dx} = 0\,, \qquad x = 0 = \Gamma_2 \qquad (18)$$
$$\psi_1^*(x) = 0\,, \qquad x = L = \Gamma_1 \qquad (19)$$
$$(20)$$

Closed-form solution:

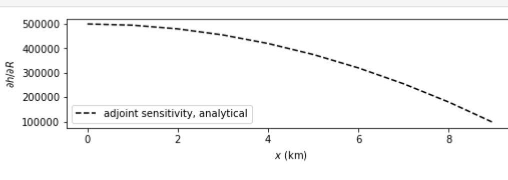
$$\psi_1^*(x) = \frac{1}{2\,K\,b}\left[H\left(x' - x\right)\left(L - x'\right) + H\left(x - x'\right)\left(L - x\right)\right] \qquad (21)$$

```
In [39]: def a(x, xp, K, b, L):
             if x>xp:
                 a = L-x
             else:
                 a = L-xp
             return a/K/b
         A = np.array([a(x, float(ocol), K, b, L) for x in X])

         %matplotlib inline
         import matplotlib as mpl
         import matplotlib.pyplot as plt
         plt.subplots(figsize=[8,2])
         plt.plot(X/1000., A, 'k--', mfc='none', label='adjoint solution, analytical')
         plt.xlabel('$x$ (km)')
         plt.ylabel(r'$\psi^*_1$ (T/$L^2$)')
         plt.legend(loc=3);
```



3a. Analytical

```
In [40]: dhdR = [np.sum([a(x, xp, K, b, L) for x in X]) for xp in X[::1000]]

         %matplotlib inline
         import matplotlib as mpl
         import matplotlib.pyplot as plt
         plt.subplots(figsize=[8,2])
         plt.plot(X[::1000]/1000., dhdR, 'k--', mfc='none', label='adjoint sensitivity, analytical')
         plt.xlabel('$x$ (km)')
         plt.ylabel(r'$\partial h / \partial R$')
         plt.legend(loc=3);
```

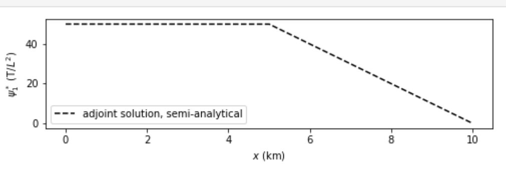



```
In [41]: set_background('rgba(0, 200, 0, 0.2)')
         print('%.6f (%.6f)'% (dhdR[int(np.where(X[::1000]==float(ocol))[0])], benchmark))
```

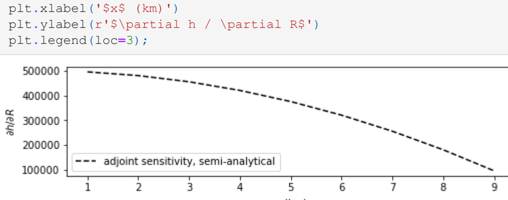
375025.000000 (375000.000000)

3b. Semi-analytical

```
In [42]: M0 = timml.Model3D(kaq=K, z=[0., -b])
         timml.ImpLineDoublet1D(M0, xld=0.)
         timml.HeadLineSink1D(M0, xls=L, hls=0.)
         timml.LineSink1D(M0, xls=float(ocol), sigls=-1.)
         M0.solve(silent=True)
         A = M0.headalongline(X, 0.).flatten()

         %matplotlib inline
         import matplotlib as mpl
         import matplotlib.pyplot as plt
         plt.subplots(figsize=[8,2])
         plt.plot(X/1000., A, 'k--', mfc='none', label='adjoint solution, semi-analytical')
         plt.xlabel('$x$ (km)')
         plt.ylabel(r'$\psi^*_1$ (T/$L^2$)')
         plt.legend(loc=3);
```




```
In [43]: dhdR = np.empty(0)
         for xp in X[::1000]:
             M0 = timml.Model3D(kaq=K, z=[0., -b])
             timml.ImpLineDoublet1D(M0, xld=0.)
             timml.HeadLineSink1D(M0, xls=L, hls=0.)
             timml.LineSink1D(M0, xls=xp, sigls=-1.)
             M0.solve(silent=True)
             A = M0.headalongline(X, 0.).flatten()
             dhdR = np.append(dhdR, np.sum(A))

         %matplotlib inline
         import matplotlib as mpl
         import matplotlib.pyplot as plt
         plt.subplots(figsize=[8,2])
         plt.plot(X[::1000][1:]/1000., dhdR[1:], 'k--', mfc='none', label='adjoint sensitivity, semi-analytical')
         plt.xlabel('$x$ (km)')
         plt.ylabel(r'$\partial h / \partial R$')
         plt.legend(loc=3);
```

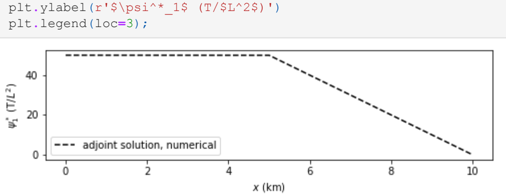



```
In [44]: set_background('rgba(0, 200, 0, 0.2)')
         print('%.6f (%.6f)'% (dhdR[int(np.where(X[::1000]==float(ocol))[0])], benchmark))
```

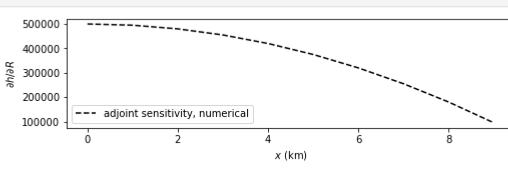
375025.000000 (375000.000000)

3c. Numerical

```
In [45]: M0 = flopy.modflow.Modflow(modelname='model', exe_name='../mf2005.exe')
         flopy.modflow.ModflowDis(M0, nlay=1, nrow=1, ncol=ncol, nper=1, delr=1., delc=1., top=0., botm=-b, steady=True,
                                  perlen=1., nstp=1)
         flopy.modflow.ModflowBas(M0, ibound=np.hstack([np.ones([nrow, ncol-1], dtype=int), -1*np.ones([1,1])]),
                                  strt=np.zeros([nrow, ncol], dtype=float))
         flopy.modflow.ModflowLpf(M0, hk=K, vka=-999., ss=-999., sy=-999., ipakcb=53)
         flopy.modflow.ModflowWel(M0, stress_period_data={0: [0, 0, ocol, 1.]})
         flopy.modflow.ModflowPcg(M0, hclose=1e-6, rclose=1e-6)
         flopy.modflow.ModflowOc(M0, stress_period_data={(0,0): ['save head', 'save budget']})
         M0.write_input()
         success, buff = M0.run_model(silent=True)
         A = flopy.utils.binaryfile.HeadFile('model.hds').get_data()[0,0,:]

         %matplotlib inline
         import matplotlib as mpl
         import matplotlib.pyplot as plt
         plt.subplots(figsize=[8,2])
         plt.plot(X/1000., A, 'k--', mfc='none', label='adjoint solution, numerical')
         plt.xlabel('$x$ (km)')
         plt.ylabel(r'$\psi^*_1$ (T/$L^2$)')
         plt.legend(loc=3);
```




```
In [46]: dhdR = np.empty(0)
         for oc,xp in enumerate(X[::1000]):
             M1 = M0
             flopy.modflow.ModflowWel(M1, stress_period_data={0: [0, 0, oc*1000, 1.]})
             M1.write_input()
             success, buff = M1.run_model(silent=True)
             A = flopy.utils.binaryfile.HeadFile('model.hds').get_data()[0,0,:]
             dhdR = np.append(dhdR, np.sum(A))

         %matplotlib inline
         import matplotlib as mpl
         import matplotlib.pyplot as plt
         f,s = plt.subplots(figsize=[8,2])
         plt.plot(X[::1000]/1000., dhdR, 'k--', mfc='none', label='adjoint sensitivity, numerical')
         plt.xlabel('$x$ (km)')
         plt.ylabel(r'$\partial h / \partial R$')
         plt.legend(loc=3);
```




```
In [47]: set_background('rgba(0, 200, 0, 0.2)')
         print('%.6f (%.6f)'% (dhdR[int(np.where(X[::1000]==float(ocol))[0])], benchmark))
```

374924.968750 (375000.000000)

3d. Numerical, discrete

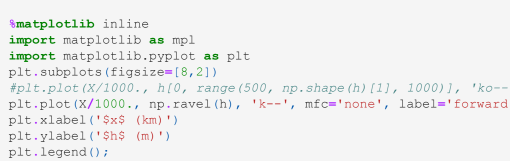
Re-run adjoint model to obtain the adjoint state vector, ψ_1^*:

```
In [48]: M1 = M0
         flopy.modflow.ModflowWel(M1, stress_period_data={0: [0, 0, ocol, 1.]})
         M1.write_input()
         success, buff = M1.run_model(silent=True)
         psi = np.atleast_2d(flopy.utils.binaryfile.HeadFile('model.hds').get_data()[0,0,:])
         np.shape(psi)
```

```
Out[48]: (1, 10000)
```

Re-run forward model to obtain vectors of output heads, h, cell-by-cell conductances, CR, and RHS terms, RHS :

```
In [49]: import flopy
         from os import system

         nrow, ncol = 1, int(L)
         M0 = flopy.modflow.Modflow(modelname='model', exe_name='../mf2005.exe')
         flopy.modflow.ModflowDis(M0, nlay=1, nrow=nrow, ncol=ncol, nper=1, delr=1., delc=1., top=0., botm=-b, steady=Tr
                                  perlen=1., nstp=1)
         flopy.modflow.ModflowBas(M0, ibound=np.hstack([np.ones([nrow, ncol-1], dtype=int), -1*np.ones([1,1])]),
                                  strt=BC1h*np.ones([nrow, ncol], dtype=float))
         flopy.modflow.ModflowLpf(M0, hk=K, vka=-999., ss=-999., sy=-999., ipakcb=53)
         flopy.modflow.ModflowRch(M0, nrchop=1, rech=R, ipakcb=53)
         flopy.modflow.ModflowPcg(M0, hclose=1e-6, rclose=1e-6)
         flopy.modflow.ModflowOc(M0, stress_period_data={(0,0): ['save head', 'save budget']})
         M0.write_input()
         #success, buff = M0.run_model(silent=True)
         system('mf2005_stream.exe < model.in')
         h = np.atleast_2d(flopy.utils.binaryfile.HeadFile('model.hds').get_data()[0,0,:])

         %matplotlib inline
         import matplotlib as mpl
         import matplotlib.pyplot as plt
         plt.subplots(figsize=[8,2])
         #plt.plot(X/1000., h[0, range(500, np.shape(h)[1], 1000)], 'ko--', mfc='none', label='forward solution, numeric
         plt.plot(X/1000., np.ravel(h), 'k--', mfc='none', label='forward solution, numerical')
         plt.xlabel('$x$ (km)')
         plt.ylabel('$h$ (m)')
         plt.legend();
```



Import RHS vector:

```
In [50]: RHS = np.atleast_2d(np.loadtxt('RHS.arr').flatten())
         print(np.shape(RHS))
```

(1, 10000)

Assemble d(RHS)/dR vector analytically:

```
In [51]: dRHSdR = RHS/R
```

```
In [52]: set_background('rgba(0, 200, 0, 0.2)')
         print('%.6f (%.6f)'% (np.float(-psi@dRHSdR.T), benchmark))
```

374925.008392 (375000.000000)

```
In [53]: dRHSdR
```

```
Out[53]: array([[-1., -1., -1., ..., -1., -1.,  0.]])
```

```
In [ ]:
```