

计算物理第七次作业

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Question 1 ▷ Gumbel Distribution

For random variables x_1, x_2, \dots, x_n ($x_1 < x_2 < \dots < x_n$), find the distribution of

$$\Delta = \max\{x_{i+1} - x_i\}.$$

Solution

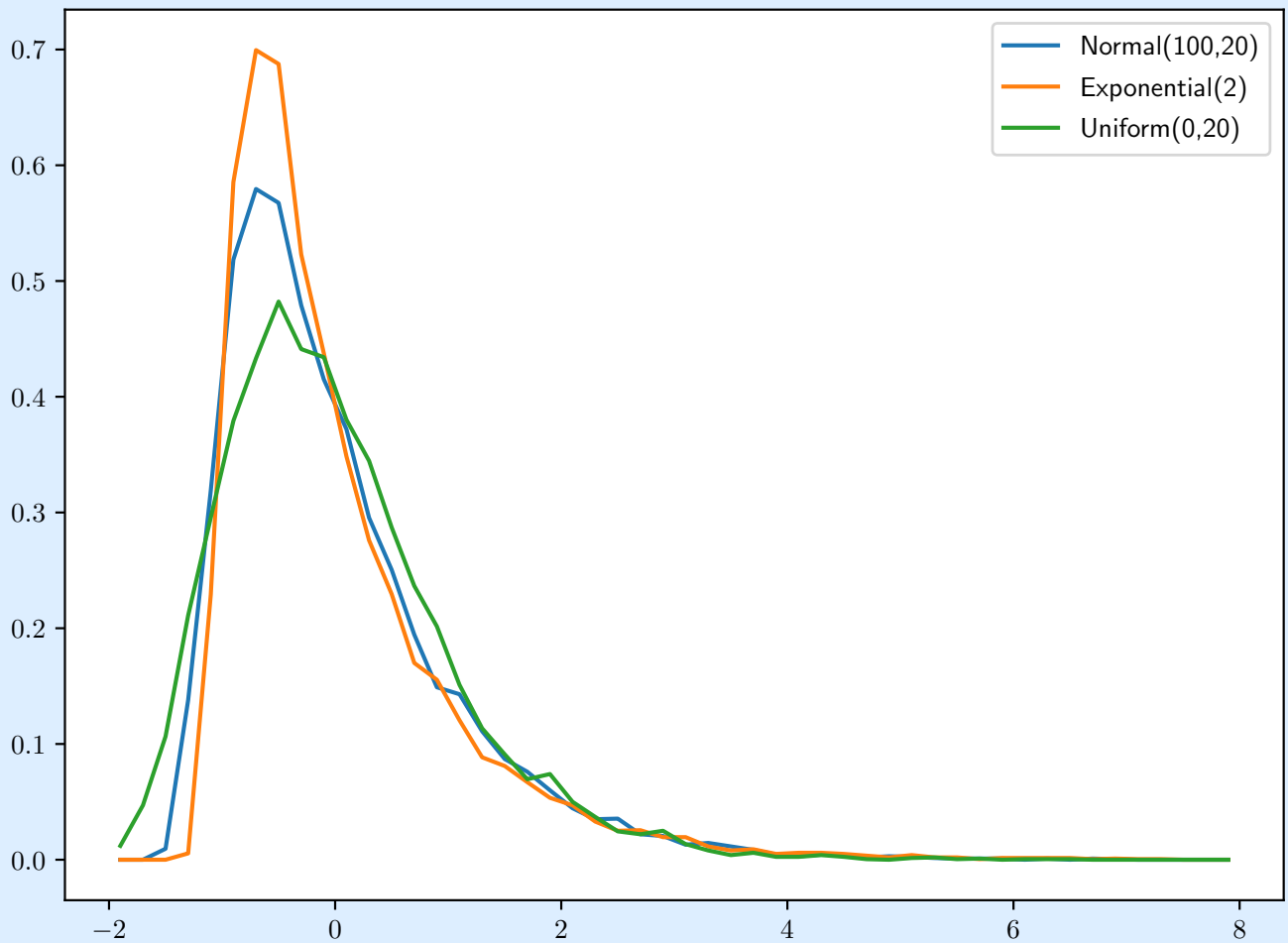
使用Python分别计算 $\{x_i\}$ 分别服从正态分布 $N(100, 20)$ 、指数分布 $Exp(2)$ 和均匀分布 $U(0, 20)$ 的 Δ 分布, 并按照

$$\Delta' = \frac{\Delta - \langle \Delta \rangle}{\sigma_{\Delta}} \quad (1)$$

进行标准化, 画出标准化后的 Δ' 分布:

```
1 import numpy as np
2 from numpy import random
3 import matplotlib.pyplot as plt
4
5 def normalize(x):
6     return ( np.array(x) - np.mean(x) ) / np.std(x)
7
8 Nx = int(1e4)
9 Ns = int(1e5)
10
11 spacing_expo = [np.max(np.diff(np.sort(random.exponential(2, Nx)))) for i in range(Ns)]
12 spacing_norm = [np.max(np.diff(np.sort(random.normal(100, 20, Nx)))) for i in range(Ns)]
13 spacing_unif = [np.max(np.diff(np.sort(20*random.rand(Nx)))) for i in range(Ns)]
14
15 nbins=50
16 hist1, binedges = np.histogram(normalize(spacing_norm), nbins, range=(-2, 8), density=True)
17 hist2, binedges = np.histogram(normalize(spacing_expo), nbins, range=(-2, 8), density=True)
18 hist3, binedges = np.histogram(normalize(spacing_unif), nbins, range=(-2, 8), density=True)
19 bins_mean = [0.5 * (binedges[i] + binedges[i+1]) for i in range(nbins)]
20
21 plt.plot(bins_mean, hist1, label='Normal(100, 20)');
22 plt.plot(bins_mean, hist2, label='Exponential(2)');
23 plt.plot(bins_mean, hist3, label='Uniform(0, 20)');
```

得到的数据如下图所示:



Gumble分布的表达式为

$$f(x; \mu, \beta) = \frac{1}{\beta} e^{-(z) + e^{-z}}, \quad \text{where } z = \frac{x - \mu}{\beta}. \quad (2)$$

其中 μ 是众数, 与均值 $\langle x \rangle$ 的关系为

$$\langle x \rangle = \mu + \gamma\beta, \quad \text{where } \gamma \simeq 0.5772 \text{ (Euler-Mascheroni constant)}. \quad (3)$$

由于上面的过程中我们已经进行了标准化使得 Δ' 的均值为0, 故要使用均值为0的Gumble分布进行拟合. 均值为0的Gumble分布有 $\mu = -\gamma\beta$. 使用python进行拟合, 并作出拟合后的Gumble分布与 Δ' 的分布的对比图.

```

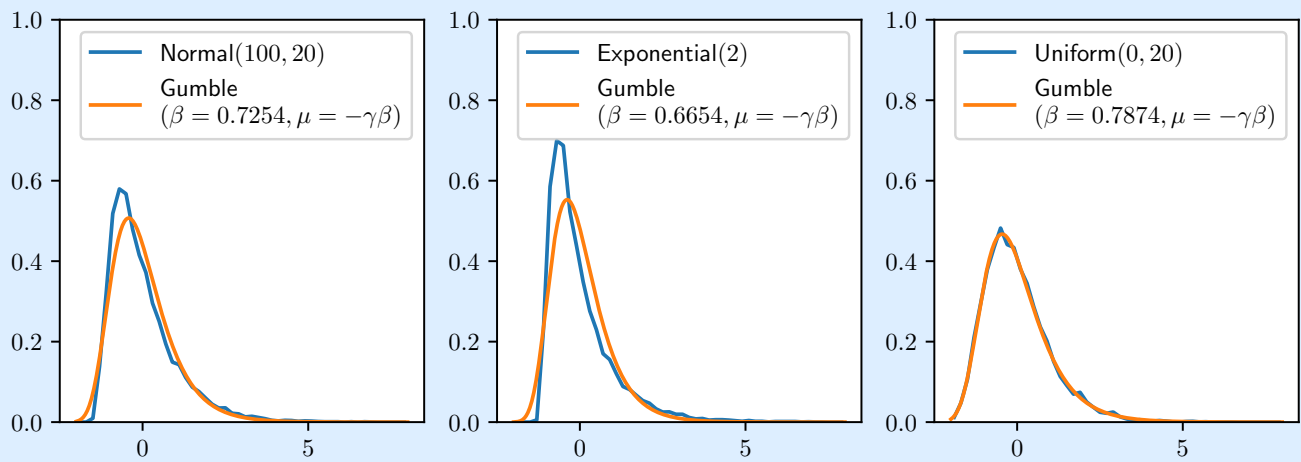
1 def gumble(x,beta):
2     mu = -.5772 * beta # mean = mu + 0.5772 beta = 0
3     z = (x - mu) / beta
4     return np.exp( -(z + np.exp(-z)) ) / beta
5
6 from scipy import optimize
7 beta1 = optimize.curve_fit(gumble, bins_mean[:nbins//2], hist1[:nbins//2])[0][0]
8 beta2 = optimize.curve_fit(gumble, bins_mean[:nbins//2], hist2[:nbins//2])[0][0]
9 beta3 = optimize.curve_fit(gumble, bins_mean[:nbins//2], hist3[:nbins//2])[0][0]
10 xlst = np.linspace(-2,8,1000)
11 fig,axes=plt.subplots(1,3,figsize=(9,3),dpi=200)
12 for i in range(len(axes)):
13     axes[i].set_ylim(0,1)
14 ax = axes[0].

```

```

14 ax.plot(bins_mean,hist1,label=r'Normal$(100,20)$');
15 ax.plot(xlst,gumble(xlst,beta1),label='Gumble\`n'+r'$(\beta=0.4f,\mu=-\gamma\beta)$'%beta1)
16 ax.legend(loc='upper_right')
17 ax = axes[1]
18 ax.plot(bins_mean,hist2,label='Exponential$(2)$');
19 ax.plot(xlst,gumble(xlst,beta2),label='Gumble\`n'+r'$(\beta=0.4f,\mu=-\gamma\beta)$'%beta2)
20 ax.legend(loc='upper_right')
21 ax = axes[2]
22 ax.plot(bins_mean,hist3,label='Uniform$(0,20)$');
23 ax.plot(xlst,gumble(xlst,beta3),label='Gumble\`n'+r'$(\beta=0.4f,\mu=-\gamma\beta)$'%beta3)
24 ax.legend(loc='upper_right')
25 plt.savefig('07q1-f2.pdf',dpi=200,bbox_inches='tight')

```



Question 2 ▷ Langevin Equation

For $U(x) = ax^2 + bx^4$ ($a < 0$), $m = 1$, solve

$$m\ddot{x} = -\alpha\dot{x} - \nabla U + \xi(t),$$

where

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = D\delta(t - t').$$

Solution

运动方程为

$$\dot{x} = v, \tag{4}$$

$$\dot{v} = -\alpha - 2ax - 4bx^3 - \xi(t).$$

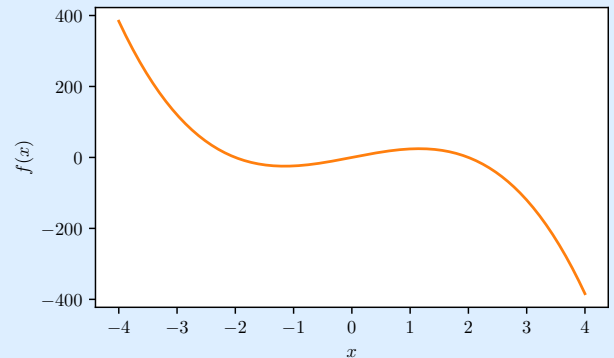
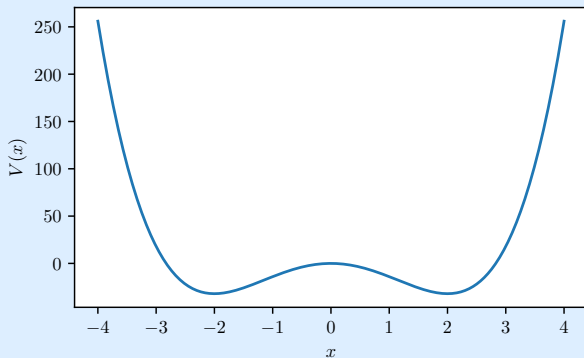
离散化后为

$$\begin{aligned} x_{n+1} &= x_n + v_n dt, \\ v_{n+1} &= v_n + \left[-\alpha v_n + f(x_n) + \sqrt{\frac{D}{dt}} \xi_n \right] dt, \end{aligned} \tag{5}$$

with

$$f(x) = -2ax^2 - 4bx^4 \quad \text{and} \quad \xi_n \sim N(0, 1). \tag{6}$$

取 $a = -16b = 2$, $V(x), f(x)$ 的图像如下图所示, 两个平衡位置为 $\pm x_b$ ($x_b = 2$)



使用python进行计算, 代码如下:

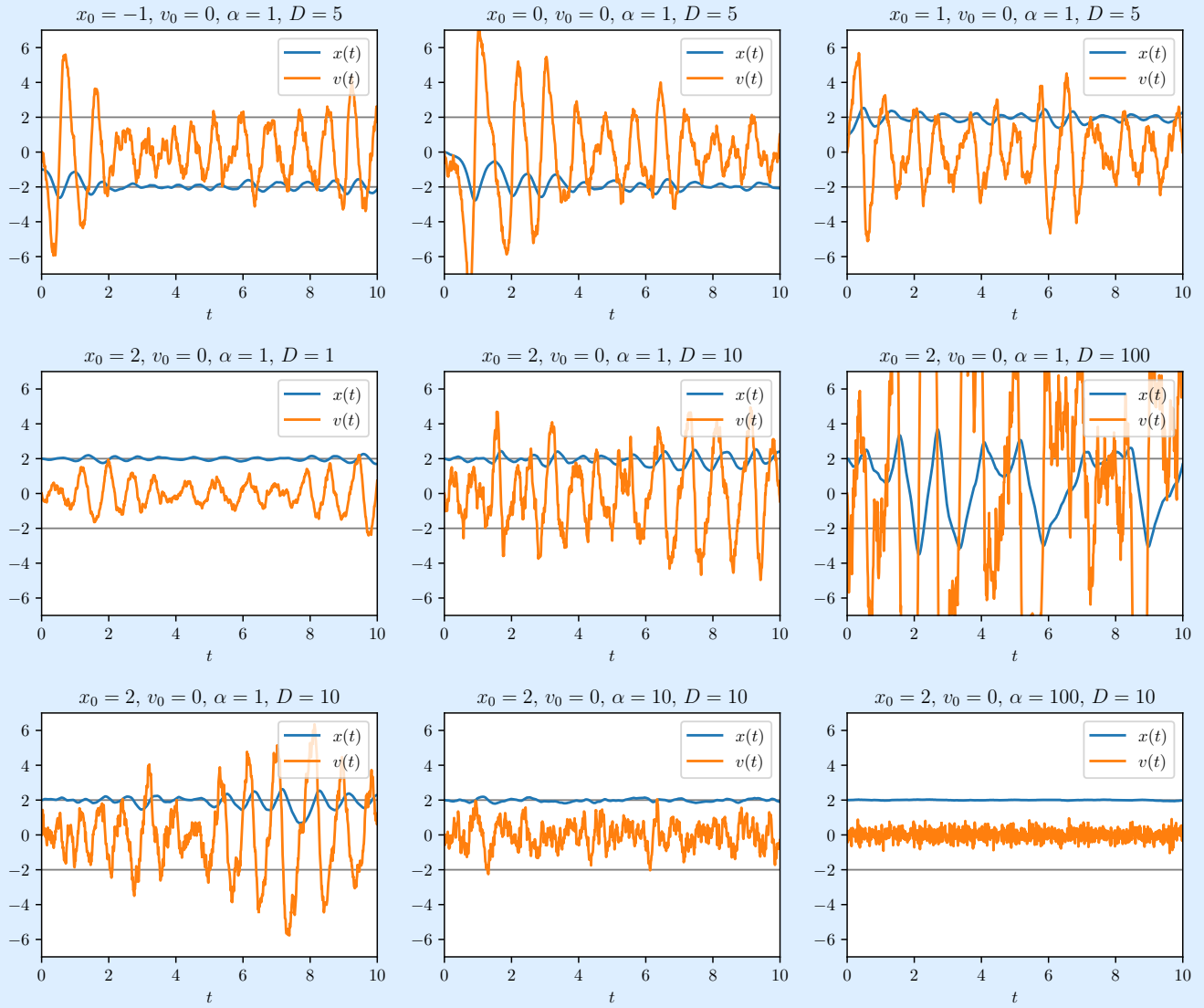
```
1 import numpy as np
2 from numpy import random
3 import matplotlib.pyplot as plt
4
5 a = -16; b = 2;
6
7 def f(x):
8     return - 2*a*x - 4*b*(x**3)
9
10 def evolve(x0, v0, alpha, D):
11     xi = random.normal(size = N)
12     x = x0; v = v0;
13     xs = [x]; vs = [v];
14     for i in range(N):
```

```

15     x += v * dt
16     v += ( - alpha*v + f(x) + (D/dt)**.5 * xi[i] ) * dt
17     xs.append(x)
18     vs.append(v)
19     return xs, vs
20
21 fig, axes = plt.subplots(3, 3, figsize=(12, 10), dpi=200)
22
23 v0 = 0; alpha = 1; D = 5;
24 for i in range(3):
25     ax = axes[0, i]
26     x0 = 1 * (i-1)
27     xs, vs = evolve(x0, v0, alpha, D)
28     ax.plot(ts, xs, label='$x(t)$');
29     ax.plot(ts, vs, label='$v(t)$');
30
31 x0 = 2; v0 = 0; alpha = 1;
32 for i in range(3):
33     ax = axes[1, i]
34     D = 10**i
35     xs, vs = evolve(x0, v0, alpha, D)
36     ax.plot(ts, xs, label='$x(t)$');
37     ax.plot(ts, vs, label='$v(t)$');
38
39 x0 = 2; v0 = 0; D = 10;
40 for i in range(3):
41     ax = axes[2, i]
42     alpha = 10**i
43     xs, vs = evolve(x0, v0, alpha, D)
44     ax.plot(ts, xs, label='$x(t)$');
45     ax.plot(ts, vs, label='$v(t)$');

```

计算结果如下图所示:



首先固定其他参数而改变初始位置 x_0 . 可以看到, 当 D 不太大时, 在两个势阱的其中一个中释放粒子, 粒子将在这个阱中运动. 而当在 $x = 0$ 处静止释放粒子时, 粒子则会随机地进入其中一个势阱.

然后固定其他参数而改变随机力大小 D . 当 D 不太大时, 粒子将始终在初始时刻所在的势阱中运动, 且震荡幅度随 D 增大而增大. 而当 D 足够大时, 粒子将有可能在随机力的作用下在两个势阱之间跃迁.

最后固定其他参数而改变阻尼大小 α . 可见粒子的震荡幅度随 α 增大而减小.