

\mathbb{R}^n Ne \mathbb{R}^n \mathbb{R}^n ec \mathbb{R}^n c, e \mathbb{R}^n a \mathbb{R}^n \mathbb{R}^n d \mathbb{R}^n e \mathbb{R}^n e \mathbb{R}^n ed b \mathbb{R}^n \mathbb{R}^n a e
 \mathbb{R}^n d de c- bed b \mathbb{R}^n e \mathbb{R}^n \mathbb{R}^n \mathbb{R}^n . Eac \mathbb{R}^n \mathbb{R}^n a, e.g., a Ne \mathbb{R}^n \mathbb{R}^n a- ce,
a a \mathbb{R}^n e, e \mathbb{R}^n \mathbb{R}^n \mathbb{R}^n \mathbb{R}^n d e c . T e \mathbb{R}^n a \mathbb{R}^n \mathbb{R}^n d acc- d \mathbb{R}^n g \mathbb{R}^n c \mathbb{R}^n e,
 \mathbb{R}^n w e e, c \mathbb{R}^n \mathbb{R}^n f " d \mathbb{R}^n ca \mathbb{R}^n e c e \mathbb{R}^n a d e f a \mathbb{R}^n . W e eac \mathbb{R}^n d d a
 \mathbb{R}^n e e a \mathbb{R}^n \mathbb{R}^n c c a c , e.g., a \mathbb{R}^n e c a \mathbb{R}^n d d a \mathbb{R}^n [4] d e \mathbb{R}^n e
a \mathbb{R}^n c \mathbb{R}^n \mathbb{R}^n w e \mathbb{R}^n , a \mathbb{R}^n \mathbb{R}^n e \mathbb{R}^n e c e f \mathbb{R}^n w a c a a e a \mathbb{R}^n \mathbb{R}^n
e \mathbb{R}^n e e (b \mathbb{R}^n), deg-ada \mathbb{R}^n (dea), a a a d f \mathbb{R}^n \mathbb{R}^n (g- a \mathbb{R}^n), a e
 \mathbb{R}^n \mathbb{R}^n (c a-ace \mathbb{R}^n c \mathbb{R}^n g), a d \mathbb{R}^n e- ac \mathbb{R}^n . S c a f \mathbb{R}^n a a eac \mathbb{R}^n \mathbb{R}^n e c
 \mathbb{R}^n e \mathbb{R}^n a \mathbb{R}^n a \mathbb{R}^n e V, c a b c \mathbb{R}^n c a eac \mathbb{R}^n \mathbb{R}^n e c \mathbb{R}^n a \mathbb{R}^n g e
ce , c a b e g \mathbb{R}^n a e a e d \mathbb{R}^n e \mathbb{R}^n f a \mathbb{R}^n e g e- a r e d, c \mathbb{R}^n \mathbb{R}^n e
Ma \mathbb{R}^n e c e d e c- b \mathbb{R}^n g \mathbb{R}^n \mathbb{R}^n e a- b e a \mathbb{R}^n , c \mathbb{R}^n \mathbb{R}^n g e \mathbb{R}^n e e a d e
eac \mathbb{R}^n , \mathbb{R}^n e a a \mathbb{R}^n e .

P a \mathbb{R}^n d \mathbb{R}^n c \mathbb{R}^n b \mathbb{R}^n g a \mathbb{R}^n g b e d de c- bed \mathbb{R}^n e \mathbb{R}^n f \mathbb{R}^n e a
d ffe- a e a \mathbb{R}^n [17]. M a f e e a \mathbb{R}^n a- e \mathbb{R}^n a- ab \mathbb{R}^n a
e c e a \mathbb{R}^n f c \mathbb{R}^n c a eac \mathbb{R}^n . \mathbb{R}^n c a e w e a \mathbb{R}^n d c e \mathbb{R}^n a
g \mathbb{R}^n f a \mathbb{R}^n e a e a f a e e d \mathbb{R}^n e \mathbb{R}^n f e \mathbb{R}^n a w a \mathbb{R}^n g \mathbb{R}^n e
a d e P \mathbb{R}^n e c e . W e a \mathbb{R}^n a e e f d ffe- a e a \mathbb{R}^n f
a \mathbb{R}^n d \mathbb{R}^n c a a \mathbb{R}^n a \mathbb{R}^n c a f a d a \mathbb{R}^n e e e f b a b a d
Ma e c e e .

A f e \mathbb{R}^n d c \mathbb{R}^n g e c a c \mathbb{R}^n a \mathbb{R}^n c a e e e a \mathbb{R}^n f \mathbb{R}^n a \mathbb{R}^n e-
c, \mathbb{R}^n e Sec. 6.9 f e c a e w e e e a e c a d c e e d \mathbb{R}^n e a
a \mathbb{R}^n a c a e c e a \mathbb{R}^n e a \mathbb{R}^n a \mathbb{R}^n Ma e \mathbb{R}^n a \mathbb{R}^n e c . T
e c e a a \mathbb{R}^n a b e e e b a c e e e e f e \mathbb{R}^n d \mathbb{R}^n c, f
d e e d \mathbb{R}^n e \mathbb{R}^n e e d c a e b \mathbb{R}^n c d e a g w e a e c a c
 \mathbb{R}^n f a \mathbb{R}^n a d e e . T d \mathbb{R}^n g e e a \mathbb{R}^n a c a e c e e e
c a c \mathbb{R}^n a \mathbb{R}^n e c f \mathbb{R}^n e b e c f \mathbb{R}^n c w e c \mathbb{R}^n e d e e
 \mathbb{R}^n \mathbb{R}^n e \mathbb{R}^n w e a \mathbb{R}^n a c a \mathbb{R}^n \mathbb{R}^n d c e \mathbb{R}^n e \mathbb{R}^n
c a c e d \mathbb{R}^n , a d- a \mathbb{R}^n e \mathbb{R}^n , a \mathbb{R}^n e d c \mathbb{R}^n , f e e e g
d a \mathbb{R}^n , e c . W e a d e e w e " a \mathbb{R}^n : T e f i c \mathbb{R}^n c e e d w e e b a a c
f a f e e e g e f i c \mathbb{R}^n , a d e e c \mathbb{R}^n d c e e d w e e c e a \mathbb{R}^n \mathbb{R}^n c
 \mathbb{R}^n e d \mathbb{R}^n e .

F i a , a e a e \mathbb{R}^n \mathbb{R}^n c, c \mathbb{R}^n f a a \mathbb{R}^n a e \mathbb{R}^n b c \mathbb{R}^n e ,
a d e c w e c \mathbb{R}^n g \mathbb{R}^n e b \mathbb{R}^n g a e a \mathbb{R}^n e a e \mathbb{R}^n a e \mathbb{R}^n c a
e a e d \mathbb{R}^n a b a d a d e e de b f i c a \mathbb{R}^n , \mathbb{R}^n e \mathbb{R}^n f \mathbb{R}^n e $\rightarrow \infty$
a d e \mathbb{R}^n e V $\rightarrow \infty$ [12, 26].

6.2 Probability and Stochastic Processes: A New Language for Population Dynamics

T e e a e f i d a a w e e f a a a c a d e \mathbb{R}^n g: (a) e e e \mathbb{R}^n g
c a f i c d a \mathbb{R}^n e \mathbb{R}^n f a a a c a f \mathbb{R}^n a e e a \mathbb{R}^n a d (b) d e c b \mathbb{R}^n g
a \mathbb{R}^n e b e a \mathbb{R}^n a \mathbb{R}^n e g i e e- ed, \mathbb{R}^n c a b \mathbb{R}^n g c a, e e c \mathbb{R}^n c ,

(e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$, ...) based on the following: (a) observed frequencies of data, (b) theoretical considerations. For example, the following are typical of **data-driven modeling** and the following are typical of **mechanistically derived modeling**. Note, according to Kaplan (1902–1994) and others, the following are typical of **data-driven modeling**: (a) observed frequencies of data (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (b) theoretical considerations (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (c) observed frequencies of data (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (d) theoretical considerations (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$).

Let us consider the following: (a) observed frequencies of data (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (b) theoretical considerations (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (c) observed frequencies of data (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (d) theoretical considerations (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$).

$$= \lim_{\Delta t \rightarrow 0} \frac{P(+\Delta) - P(-\Delta)}{\Delta}$$

In the above, the following are typical of **data-driven modeling**: (a) observed frequencies of data (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (b) theoretical considerations (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (c) observed frequencies of data (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (d) theoretical considerations (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$).

Second, a typical example of **data-driven modeling** is the following: (a) observed frequencies of data (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (b) theoretical considerations (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (c) observed frequencies of data (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (d) theoretical considerations (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$).

Indeed, **discreteness** and **probability** are typical of **data-driven modeling**. Both are based on the following: (a) observed frequencies of data (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (b) theoretical considerations (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (c) observed frequencies of data (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (d) theoretical considerations (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$).

6.2.1 Brief Review of Elementary Probabilities

A **random variable** is a function $X(\omega)$ that maps the sample space Ω into the real line \mathbb{R} (df).

$$\int_{-\infty}^{\infty} f(x) dP(x) = 1, \quad f(x) \geq 0. \quad (6.1)$$

The following are typical of **data-driven modeling**: (a) observed frequencies of data (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (b) theoretical considerations (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (c) observed frequencies of data (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$), (d) theoretical considerations (e.g., $X_t = \sigma B_t$, $Y_t = \sigma^2 t$).

$$P\{x < \leq x + d\} = f(x) d. \quad (6.2)$$

The cumulative distribution function is defined as

$$F(x) = P\{X \leq x\} = \int_{-\infty}^x f(t) dt, \quad f(x) = \frac{dF(x)}{dx}. \tag{6.3}$$

The expected value and variance of a continuous random variable X are

$$\langle X \rangle = E[X] = \int_{-\infty}^{\infty} x f(x) dx, \tag{6.4}$$

$$Var[X] = E[(X - \mu)^2] = \int_{-\infty}^{\infty} (x - \mu)^2 f(x) dx, \tag{6.5}$$

where $\mu = E[X]$ is the mean value. The probability density function for a continuous random variable is given as $f(x) = \frac{1}{\sigma} \phi\left(\frac{x-\mu}{\sigma}\right)$, where ϕ is the standard Gaussian distribution function.

$$\phi(x) = \lambda^{-\lambda}, \quad x \geq 0, \quad \lambda > 0, \tag{6.6}$$

where λ is the scale parameter and λ^{-1} is the mean value.

$$\phi(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right], \tag{6.7}$$

where μ is the mean value and σ^2 is the variance.

Gaussian distributions are widely used in science and engineering. The central limit theorem states that the sum of independent random variables, each with finite mean and variance, tends to follow a normal distribution. In the context of reliability analysis, the failure times of individual components are often modeled as independent random variables. The central limit theorem provides a theoretical basis for assuming that the failure times of a large number of components will follow a normal distribution. This is particularly useful for predicting the overall system reliability based on the characteristics of its constituent parts.

The Weibull distribution is often used to model failure times, and it is characterized by its shape and scale parameters. The Weibull distribution is a continuous probability distribution that is commonly used to model the time to failure of a system or component. It is characterized by its shape parameter k and its scale parameter λ . The Weibull distribution is a generalization of the exponential distribution, and it is often used to model the failure times of components that exhibit a bathtub-shaped failure rate curve.

6.2.2 Radioactive Decay and Exponential Time

Let $N(t)$ be the number of undecayed nuclei at time t .

$$\frac{dN(t)}{dt} = -\lambda N(t), \tag{6.8}$$

Let $\lambda > 0$. Then, for a fixed λ , the probability that a given component will fail within a fixed time interval $[0, \Delta]$ is

$$\frac{F(\Delta)}{F(0)} = 1 - e^{-\lambda \Delta}. \quad (6.9)$$

If a set of components are identical and independent, then

$$P\{\text{all } n \text{ components survive for a fixed time interval } [0, \Delta]\} = e^{-n\lambda \Delta}. \quad (6.10)$$

Let T be the time until the first component fails. Then, the probability that the first component will fail within a fixed time interval $[0, \Delta]$ is

$$P\{\text{all } n \text{ components survive for a fixed time interval } [0, \Delta]\} = P\{T > \Delta\}. \quad (6.11)$$

Let $F_T(t)$ be the cumulative distribution function of T . Then, the probability that the first component will fail within a fixed time interval $[0, \Delta]$ is $F_T(\Delta) = P\{T \leq \Delta\} = 1 - e^{-\lambda \Delta}$. The probability density function of T is $f_T(t) = dF_T(t)/dt = \lambda e^{-\lambda t}$.

What is the probability that the first component will fail within a fixed time interval $[0, \Delta]$? What is the probability that the first component will fail within a fixed time interval $[\Delta, 2\Delta]$? What is the probability that the first component will fail within a fixed time interval $[2\Delta, 3\Delta]$? What is the probability that the first component will fail within a fixed time interval $[k\Delta, (k+1)\Delta]$? What is the probability that the first component will fail within a fixed time interval $[k\Delta, (k+1)\Delta]$ for a fixed k ?

6.2.2.1 Rare Event

Let T be the time until the first component fails. If the components fail independently, then the probability that the first component will fail within a fixed time interval $[0, \Delta]$ is $1 - e^{-\lambda \Delta}$. The probability that the first component will fail within a fixed time interval $[\Delta, 2\Delta]$ is $e^{-\lambda \Delta} (1 - e^{-\lambda \Delta})$. The probability that the first component will fail within a fixed time interval $[2\Delta, 3\Delta]$ is $e^{-2\lambda \Delta} (1 - e^{-\lambda \Delta})$. The probability that the first component will fail within a fixed time interval $[k\Delta, (k+1)\Delta]$ is $e^{-k\lambda \Delta} (1 - e^{-\lambda \Delta})$.

$$P\{\text{b. f. e. c. c. g. } [0, +\Delta]\} = 1 - e^{-\lambda \Delta} \quad (6.12)$$

$$P\{\text{b. f. e. c. c. g. } [0, \Delta] \times P\{\text{b. f. e. c. c. g. } [\Delta, +\Delta]\} = e^{-\lambda \Delta} (1 - e^{-\lambda \Delta})$$

Then,

$$P\{T > +\Delta\} = P\{T > \Delta\} \times P\{\text{b. f. e. c. c. g. } [\Delta, +\Delta]\} = e^{-2\lambda \Delta} (1 - e^{-\lambda \Delta})$$

Let N be the number of components that fail within a fixed time interval $[0, \Delta]$. Then, the probability that the number of components that fail within a fixed time interval $[0, \Delta]$ is k is $P\{N = k\} = \binom{n}{k} (1 - e^{-\lambda \Delta})^k e^{-\lambda (n-k)\Delta}$.

$$P\{T > +\Delta\} = P\{T > \Delta\} \times (1 - \lambda \Delta + (\Delta)^2). \quad (6.13)$$

T & ,

$$\frac{d}{dt} P\{T > t\} = -\lambda P\{T > t\}, \implies F_T(t) = 1 - e^{-\lambda t}. \tag{6.14}$$

Exemplo: T é a duração de vida de um indivíduo. Se a taxa de mortalidade for constante, a distribuição de T é exponencial.

6.2.2.2 Memoryless

Uma característica importante da distribuição exponencial é a propriedade de falta de memória (memoryless).

$$\frac{P\{T \geq t + \tau\}}{P\{T \geq t\}} = \frac{e^{-\lambda(t+\tau)}}{e^{-\lambda t}} = e^{-\lambda \tau}. \tag{6.15}$$

Exemplo: Y é a duração de vida de um indivíduo. Se a taxa de mortalidade for constante, a distribuição de Y é exponencial. Isso significa que a probabilidade de um indivíduo sobreviver por mais tempo, dado que ele já sobreviveu por um certo tempo, é a mesma que a probabilidade de um indivíduo sobreviver por esse mesmo tempo a partir do início.

More especificamente, se T_1, T_2, \dots, T_n são variáveis aleatórias independentes e identicamente distribuídas (i.i.d.) com distribuição exponencial com taxa λ , então a distribuição de $T^* = \min\{T_1, T_2, \dots, T_n\}$ também é exponencial com taxa $n\lambda$.

$$\begin{aligned} P\{T^* > t\} &= P\{T_1 > t, \dots, T_n > t\} \\ &= P\{T_1 > t\} \times P\{T_2 > t\} \times \dots \times P\{T_n > t\} = e^{-n\lambda t}, \end{aligned} \tag{6.16}$$

Logo, $f_{T^*}(t) = n\lambda e^{-n\lambda t}$ e $F_{T^*}(t) = 1 - e^{-n\lambda t}$.

6.2.2.3 Minimal Time of a Set of Non-Exponential i.i.d. Random Times

Suponha que T_1, T_2, \dots, T_n são variáveis aleatórias independentes e identicamente distribuídas (i.i.d.) com função de distribuição acumulada $F_T(t)$. Então a distribuição de $T^* = \min\{T_1, T_2, \dots, T_n\}$ é dada por:

$$P\{T^* > t\} = (1 - F_T(t))^n. \tag{6.17}$$

Logo, a função de distribuição acumulada de $\hat{T}^* = T^*$ é dada por:

$$P\{\hat{T}^* > t\} = (1 - F_T(t))^n \simeq \left(-\frac{F_T'(0)}{1 - F_T(0)} t + O(t^2) \right)^n \rightarrow -n F_T'(0) t. \tag{6.18}$$

Theorem, if $F_T'(0) = T(0)$ finite, the above distribution is

We see that a necessary condition is $T(0) > 0$; in fact, if $T(0) = 0$, the above distribution is not a probability distribution. For example, if $T(x) = e^{-x}$, then $T(0) = 1$, and the above distribution is a probability distribution.

6.2.3 Known Mechanisms That Yield an Exponential Distribution

The exponential distribution is a well-known distribution. It is characterized by the fact that the probability of an event occurring in a given interval of length t is independent of the length of the interval. For example, see Sec. 6.2.2.3, where we saw that if $T(x) = e^{-\lambda x}$, then $T(0) = 1$, and the above distribution is a probability distribution. The exponential distribution is also characterized by the fact that the probability of an event occurring in a given interval of length t is independent of the length of the interval.

6.2.3.1 Khinchin's Theorem

Let $\{X_n\}$ be a sequence of independent and identically distributed random variables with a common distribution function $F(x)$. For each n , let T_n be the time of the n th occurrence of the event $X_n \leq t$. Then, if $F(0) > 0$, $T_1, T_2, \dots, T_n, \dots$ is called a *renewal process*, and $N(t) = \sum_{n=1}^{\infty} I_{[0, t]}(T_n)$ is called the *renewal function*. The sequence $\{N(t)\}$ is called a *renewal process*. The sequence $\{N(t)\}$ is called a *renewal process* if it is a superposition of independent renewal processes [3], as shown in Fig. 6.1.

For a given renewal process $\{N(t)\}$, the sequence $\{N(t)\}$ is called a *renewal process* if it is a superposition of independent renewal processes [3], as shown in Fig. 6.1.

$$P\{N \geq t\} = P\{T \leq t\} = F_T(t) = \int_0^t T(x) dx \quad (6.19)$$

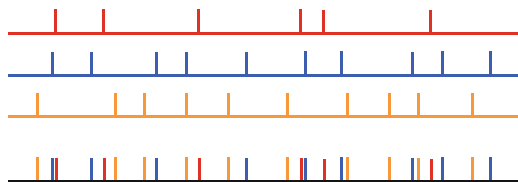


Fig. 6.1 If $\{X_n\}$ is a sequence of independent and identically distributed random variables with a common distribution function $F(x)$, then $\{N(t)\}$ is called a *renewal process*. The sequence $\{N(t)\}$ is called a *renewal process* if it is a superposition of independent renewal processes [3], as shown in Fig. 6.1.

T e-ef -e,

$$P\{N = \ell\} = F_T(\ell) - F_{T+1}(\ell). \tag{6.20}$$

N_W f \mathbb{N} e- \mathbb{N} d... c a... e, a d e T^* be \mathbb{N} a \mathbb{N} g... e f... e \mathbb{N} e...
 \mathbb{N} e a, T^* \mathbb{N} \mathbb{N} a e d a... e \mathbb{N} e a e... I d... b... \mathbb{N} d f e...
 \mathbb{N} ... (). I fac, \mathbb{N} e a

$$\begin{aligned} P\{T^* \leq t\} &= \sum_{\ell=0}^{\infty} P\{N = \ell\} P\{T_{\ell+1} \leq t\} \\ &= \sum_{\ell=0}^{\infty} (F_{T_\ell}(\ell) - F_{T_{\ell+1}}(\ell)) F_{T_{\ell+1}}(t). \end{aligned} \tag{6.21}$$

T e-ef -e, e... bab... d... f... c... \mathbb{N} f... e a \mathbb{N} a T^* ...

$$T^*(t) = \frac{d}{dt} P\{T^* \leq t\}. \tag{6.22}$$

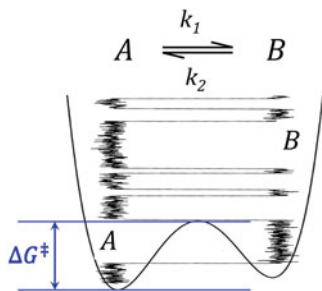


Fig. 6.2 T e j a g a c a d e c . y f a c g a e a c . y f a y g e j e o e . I . a g e g e . a . . c a g f a a g e j j b e f d . c . e . . c a . c . e a c . y . . 1 $\propto -\Delta G / RT$

6.2.4 Population Growth

We are interested in $\frac{d}{dt} = -\lambda_w$... the λ : ... decay. ... $\frac{d}{dt} = \dots$

The λ_w ... be ... $\mathbb{E}[\dots]$ time:

$$\frac{d}{dt}\mathbb{E}[\dots] = \mathbb{E}[\dots]. \tag{6.25}$$

Dea ... $\frac{d}{dt} = \dots$

$$\frac{d}{dt} = \dots + \dots, \tag{6.26}$$

w ... \dots

6.2.5 Discrete State Continuous Time Markov (Q) Processes

D. ... \dots

$$(\dots + d) - \dots = \left(\sum_{\ell=1}^N \ell(\dots) \ell \right) d, \tag{6.27}$$

w ... \dots

$$\dots = - \sum_{\neq} \dots, \tag{6.28}$$

The effective queue length L_{eff} is defined as the average number of customers in the system, excluding those in service, i.e.,

$$\sum_{n=1}^N n P_n \quad (6.28)$$

where P_n is the probability that there are n customers in the system. Note that L_{eff} is different from the average number of customers in the system, L , defined in (6.26) and (6.27). The effective queue length is a function of the system parameters, e.g., the arrival rate λ and the service rate μ . The effective queue length is a function of the system parameters, e.g., the arrival rate λ and the service rate μ . The effective queue length is a function of the system parameters, e.g., the arrival rate λ and the service rate μ .

6.2.5.1 Kolmogorov Forward and Backward Equations

The forward equations (6.27) can be written as $\frac{d}{dt} \mathbf{P} = \mathbf{Q} \mathbf{P}$, where $\mathbf{P} = (P_1, \dots, P_N)$ is the row vector of probabilities and \mathbf{Q} is the $N \times N$ matrix of transition rates. The backward equations are $\frac{d}{dt} \mathbf{P} = \mathbf{P} \mathbf{Q}$, where $\mathbf{P} = (P_1, \dots, P_N)$ is the row vector of probabilities and \mathbf{Q} is the $N \times N$ matrix of transition rates. The backward equations are $\frac{d}{dt} \mathbf{P} = \mathbf{P} \mathbf{Q}$, where $\mathbf{P} = (P_1, \dots, P_N)$ is the row vector of probabilities and \mathbf{Q} is the $N \times N$ matrix of transition rates.

$$\frac{d}{dt} \mathbf{P} = \mathbf{P} \mathbf{Q} = \left(\mathbf{Q} \right) \mathbf{Q} = \mathbf{Q} \mathbf{P}. \quad (6.29)$$

The backward equations are:

$$\frac{d}{dt} P_n = \sum_{\ell=1}^N \pi_{n\ell} P_\ell, \quad n=1, 2, \dots, N, \quad (6.30)$$

where $\pi_{n\ell}$ is the transition rate from state n to state ℓ . If $\{\pi_{n\ell}\}$ is a row vector of transition rates, then the backward equations are:

$$\sum_{\ell=1}^N \pi_{n\ell} P_\ell = 0, \quad n=1, 2, \dots, N,$$

where $\pi_{n\ell}$ is the transition rate from state n to state ℓ . The backward equations are:

$$\sum_{\ell=1}^N \pi_{n\ell} P_\ell = 0, \quad n=1, 2, \dots, N,$$

where $\pi_{n\ell}$ is the transition rate from state n to state ℓ . The backward equations are:

The ... K_{eq} ... $\frac{d}{dt} \sum_{i=1}^N \dots \leq 0$. (6.31)

$$\frac{d}{dt} \sum_{i=1}^N \dots \left(\frac{\dots}{\dots} \right) \leq 0. \tag{6.31}$$

One ... $\pi > 0 \forall$.

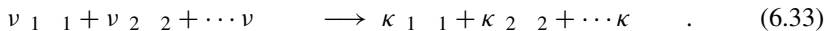
So ... $\frac{d}{dt} \sum_{i=1}^N (\pi \dots) \dots \leq 0$. (6.32)

$$\frac{d}{dt} \sum_{i=1}^N (\pi \dots) \dots \left(\frac{\dots}{\dots} \right) \leq 0. \tag{6.32}$$

One ... $\equiv 1$. The ... E . (6.32) ... H -function ... E . (6.31) ... K_{eq} ... $\frac{d}{dt} \sum_{i=1}^N \dots$

6.3 Theory of Chemical and Biochemical Reaction Systems

A general reaction ...



$1 \leq j \leq r$. The ... $(\nu_j, -\kappa_j)$ are called *stoichiometric coefficients*, ...

6.3.1 Differential Equation and Nonlinear Dynamics

Because ...

$$\frac{dx_j}{dt} = \sum_{i=1}^r (\kappa_i - \nu_i) \hat{\phi}_i(x) \tag{6.34}$$

where λ_j is the rate of transition from state j to state $j+1$, $1 \leq j \leq n$, and

$$\hat{\varphi}(x) = \frac{\lambda_1^{x_1} \lambda_2^{x_2} \cdots \lambda_n^{x_n}}{x_1! x_2! \cdots x_n!} \quad (6.35)$$

is called the *Delbrück-Gillespie process*. For $x = (x_1, x_2, \dots, x_n)$, E. (6.34)

is called the *law of mass action* (LMA).

6.3.2 Delbrück-Gillespie Process (DGP)

Let $\{X_t\}_{t \geq 0}$ be a continuous-time Markov process with state space $E = \{0, 1, 2, \dots, n\}$ and transition rates λ_j for $j \in E$. (6.33), we have a DGP. The DGP is a special case of the LMA with $\lambda_j = \lambda_j e^{-x_j}$ and $\mu_j = \lambda_j e^{-x_j}$.

$$\varphi(x) = \frac{\lambda_1^{x_1} \lambda_2^{x_2} \cdots \lambda_n^{x_n}}{x_1! x_2! \cdots x_n!} \quad (6.36)$$

where λ_j is the rate of transition from state j to state $j+1$, $1 \leq j \leq n$. Note $\varphi(x)$ is the probability of finding x individuals in each of the n classes.

$$\begin{aligned}
 &= \int_0^\infty \lambda^{-\lambda} \prod_{\ell=1, \ell \neq}^\infty \left(\int_0^\infty \lambda_\ell^{-\lambda_\ell} d_\ell \right) \\
 &= \left(\frac{\lambda}{\lambda_1 + \dots + \lambda} \right)^{-(\lambda_1 + \dots + \lambda)}. \tag{6.39}
 \end{aligned}$$

The joint density of $\{T_i\}_{i=1}^n$ is given by the factor: $e^{-\lambda_1 T_1} \lambda_1^{n-1} e^{-\lambda_2 T_2} \lambda_2^{n-2} \dots e^{-\lambda_n T_n} \lambda_n$. The joint density of $\{T_i\}_{i=1}^n$ is given by $e^{-\lambda_1 T_1} \lambda_1^{n-1} e^{-\lambda_2 T_2} \lambda_2^{n-2} \dots e^{-\lambda_n T_n} \lambda_n$.

6.3.3 Integral Representations with Random Time Change

6.3.3.1 Poisson Process

A standard Poisson process $\{N(t)\}_{t \geq 0}$ is a sequence of independent, continuous-time, discrete-time Markov process with the following properties:

$$P\{N(t) = k\} = \frac{e^{-\lambda t} (\lambda t)^k}{k!}. \tag{6.40}$$

A Poisson process is a *point process* on the real line \mathbb{R} , T_1, T_2, \dots, T_n , and a *counting process* on the real line \mathbb{R} . The first arrival time T_1 is the time of the first event, T_2 is the time of the second event, and $T_{j+1} - T_j$ is the time of the j th event.

6.3.3.2 Random Time Changed Poisson Representation

The joint density of $\{T_i\}_{i=1}^n$ is given by the factor: $e^{-\lambda_1 T_1} \lambda_1^{n-1} e^{-\lambda_2 T_2} \lambda_2^{n-2} \dots e^{-\lambda_n T_n} \lambda_n$.

$$f_n(\mathbf{x}) = f_n(0) + \sum_{i=1}^n (\kappa_i - \nu_i) \left(\int_0^{\mathbf{x}(i)} \varphi(\mathbf{X}(t)) dt \right) \tag{6.41}$$

The joint density of $\{T_i\}_{i=1}^n$ is given by (6.36). We are able to express the joint density of $\{T_i\}_{i=1}^n$ in terms of $\{X(t)\}_{t \geq 0}$. We see that $\lim_{t \rightarrow \infty} X(t) = \infty$ and $\lim_{t \rightarrow \infty} V(t) = \infty$.

$$\varphi(\mathbf{X}) \rightarrow V \prod_{\ell=1}^n \left(\frac{\ell}{V} \right)^{\nu_\ell} = V \prod_{\ell=1}^n \ell^{\nu_\ell} = V \hat{\varphi}(\mathbf{x}). \tag{6.42}$$

$\varphi(\mathbf{X})$ is called the *propensity function* for each \mathbf{X} .

6.3.4 Birth-and-Death Process with State-Dependent Transition Rates

6.3.4.1 One-Dimensional System

Consider a birth-and-death process with state-dependent transition rates. Let $\{X(t)\}$ be a birth-and-death process with state-dependent transition rates λ_n and μ_n . The transition rates are given by

$$\frac{d}{dt} P_{ij}(t) = -(\lambda_i + \mu_i) P_{ij}(t) + \lambda_{i-1} P_{i-1,j}(t) + \mu_{i+1} P_{i+1,j}(t), \quad (6.43)$$

where λ_n and μ_n are the birth and death rates, respectively, at state n . The transition probabilities $P_{ij}(t)$ are given by

$$\frac{d}{dt} P_{ij}(t) = -(\lambda_i + \mu_i) P_{ij}(t) + \lambda_{i-1} P_{i-1,j}(t) + \mu_{i+1} P_{i+1,j}(t). \quad (6.44)$$

Therefore,

$$P_{ij}(t) = \prod_{k=1}^i \left(\frac{\mu_k}{\lambda_k} \right), \quad (6.45)$$

where $\mu_0 = 0$ and $\lambda_0 = 0$.

Equation (6.43) is a differential equation for $P_{ij}(t)$. The transition probabilities $P_{ij}(t)$ are given by

$$\frac{d}{dt} P_{ij}(t) = \lambda_{i-1} P_{i-1,j}(t) - (\lambda_i + \mu_i) P_{ij}(t) + \mu_{i+1} P_{i+1,j}(t), \quad (6.46)$$

where

$$\lambda_i = \lambda \frac{i}{V}, \quad \mu_i = \mu \frac{i}{V}$$

Cynde a... a... b... x = (1, 2, ...,), a... ≥ 0. I... e ab... ce f... g... a... y... f... ed... e... ca... a g... w... a e... =... , -... , d...

$$\frac{d}{d} = \dots \tag{6.48}$$

F... c... w... e... a... j... e... a... b... e... ca... a... b... a... e... , d... dea... a... e... a... c... y... d... . T... e... e... ca... a... g... w... a... e... f... e... d... e... e... a... y... w... c... a... e... j... e... d... e... ca... a... g... w... a... e...

$$= \frac{\sum_{j=1}^d \frac{d}{d}}{\sum_{j=1}^d} = \frac{\sum_{j=1}^d \dots}{\sum_{j=1}^d}, \dots \geq 0. \tag{6.49}$$

T... ,

$$\frac{d^-(x)}{d} = \left[\frac{\sum_{j=1}^d \dots^2}{\sum_{j=1}^d \dots} - \left(\frac{\sum_{j=1}^d \dots}{\sum_{j=1}^d} \right)^2 \right]. \tag{6.50}$$

We... e... a... e... e... j... y... de [...] y... e... g... - d... de... y... e... y... e... g... e...

$$\frac{\sum_{j=1}^d \dots^2}{\sum_{j=1}^d \dots} - \left(\frac{\sum_{j=1}^d \dots}{\sum_{j=1}^d} \right)^2 = \frac{\sum_{j=1}^d \dots \left(\dots - \dots \right)^2}{\sum_{j=1}^d \dots} \geq 0. \tag{6.51}$$

I... fac... e... ac... e... a... d... ce... f... , a... y... g... ed... f... e... d... b... , a... y... . T... e... f... e... , ... a... w... a... e... e... f... e... e... a... e... a... a... y... a... y... g... , T... j... a... g... a... ca... e... , ... a... a... f... e... dea... f... b... . Ada... S... , y... e... y... j... c... , d... d... C... a... e... D... a... w... y... , y... e... y... a... a... e... e... c... y... . I... fac... , e... e... j... [...] y... E... (6.50) a... be... d... d... y... f... ied... b... R... A... F... e... , e... B... a... a... c... a... d... e... , y... a... b... g... , a... e... "g... w... a... f... f... i... e... d... e... y... a... a... e... e... c... y... [6]. He... e... a... r... e... f... j... S... magnum opus" A... I... e... y... e... Na... e... d... Ca... e... f... e... Wea... f... Na... y... (1776):

A... e... y... d... d... a... e... e... f... e... , d... dea... r... a... j... c... a... e... ca... b... e... g... e... , ... ca... a... y... e... r... e... f... d... j... e... c... h... d... e... , d... d... d... d... e... c... a... y... d... e... a... a... d... e... c... e... j... a... be... f... e... g... e... a... e... a... r... e... e... y... d... d... a... y... e... c... e... a... a... b... e... e... d... e... e... d... e... a... y... a... e... d... e... f... e... e... c... e... a... g... e... a... e... ca... . He... g... e... a... , y... deed... y... e... y... d... d... e... j... e... e... e... b... c... y... e... e... y... w... a... w... j... c... e... e... e... j... g... . B... e... f... e... g... e... e... e... f... d... j... e... c... a... f... f... e... g... y... d... e... , e... y... d... d... y... e... e... c... ; d... b... d... e... c... y... g... a... y... d... e... y... , c... g... a... y... e... a... d... e... c... e... a... be... f... e... g... e... a... e... a... r... e... , e... y... d... d... y... e... w... y... g... a... y... , d... d... e... y... , a... y... d... e... e... a... e... , e... d... b... y... e... b... e... d... e... j... e... a... d... d... w... e... c... w... a... y... a... f... y... d... y... . N... a... w... a... e... w... e... f... e... e... c... e... a... w... a... y... a... f... . B... e... y... g... w... y... e... e... f... e... d... e... e... a... f... e... c... e... j... e... e... f... f... e... c... e... a... d... w... a... e... e... a... y... d... d... e... j... e... . I... a... e... y... e... y... w... y... c... g... d... d... y... e... b... e... w... a... f... f... e... d... e... d... e... f... e... e... b... c... g... d... . I... d... a... f... f... e... c... a... y... , y... deed... y... e... c... j... y... a... y... g... j... e... c... a... , d... d... e... f... e... w... d... y... e... e... d... b... e... g... e... e... d... y... d... e... d... y... g... e... f... j... .

6.5 Ecological Dynamics and Nonlinear Chemical Reactions: Two Examples

6.5.1 Predator and Prey System

Let (x) be the number of prey and (y) be the number of predators. The following predator-prey dynamics are [17]:

$$\begin{cases} \frac{dx}{dt} = \alpha x - \beta xy, \\ \frac{dy}{dt} = -\gamma y + \delta xy. \end{cases} \quad (6.52)$$

The detailed analysis of the predator-prey system can be found in the book [17].

Let us consider the following reaction scheme:



The corresponding LMA, the chemical reaction and the detailed reaction scheme are:

$$\frac{dA}{dt} = 1A - 2A^2, \quad \frac{dB}{dt} = -3A + 2A^2. \quad (6.54)$$

The effective reaction scheme for the predator-prey system can be written as: $A \rightarrow B$. The effective reaction scheme is given by the reaction scheme (6.53) where the reaction $A \rightarrow B$ is catalyzed by A . The effective reaction scheme is called a *catalyst*.

6.5.2 A Competition Model

Let us consider the following reaction scheme [17]:

$$\begin{cases} \frac{dN_1}{dt} = r_1 N_1 - c_1 N_1^2 - c_{21} N_1 N_2, \\ \frac{dN_2}{dt} = r_2 N_2 - c_2 N_2^2 - c_{12} N_2 N_1. \end{cases} \quad (6.55)$$

Can we deduce a unique flow from a set of differential equations? We consider the following system, where $\lambda_1 > \lambda_2$.

$$\begin{aligned} A + &\xrightarrow{1} 2, & + &\xrightarrow{2} B, & A + &\xrightarrow{3} 2, \\ &+ &\xrightarrow{4} B, & + &\xrightarrow{5} B, & + &\xrightarrow{6} + B, \end{aligned} \tag{6.56}$$

We will use the following lemma,

$$\begin{cases} \frac{d}{dt} = (\lambda_1) - \lambda_2^2 - \lambda_5, \\ \frac{d}{dt} = (\lambda_3) - \lambda_4^2 - (\lambda_5 + \lambda_6). \end{cases} \tag{6.57}$$

If we define $\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5, \lambda_6$

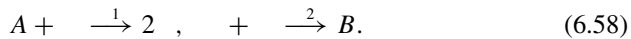
$$(\lambda_1) \leftrightarrow 1, \lambda_2 \leftrightarrow 1, \lambda_5 \leftrightarrow 21, (\lambda_3) \leftrightarrow 2, \lambda_4 \leftrightarrow 2, (\lambda_5 + \lambda_6) \leftrightarrow 12,$$

then (6.57) is equivalent to (6.55). Note that the reaction $A + B \rightarrow + B$ is not considered here since $\lambda_1 > \lambda_2$.

According to the following theorem (6.56) and the above reaction set $2A \rightarrow B$. Since each λ_i is a real number, we can be in a unique state λ_{w_0} . Rather, the system is in a *nonequilibrium steady state* λ_{w_0} if the reaction is not in a state of $2A \rightarrow B$.

6.5.3 Logistic Model and Keizer's Paradox

We will now consider the following reaction set. Let λ_{w_0} be the steady state of the reaction set,



The reaction set is an ODE according to the lemma,

$$\frac{d}{dt} = \left(1 - \frac{1}{K}\right), \quad \lambda_1 = 1, \quad K = \frac{1}{2}, \tag{6.59}$$

The above is a *logistic equation* in the form $\frac{d}{dt} = r \left(1 - \frac{1}{K}\right)$, where r is the growth rate, λ_{w_0} is the steady state, $\lambda_{w_0} = \frac{1}{K}$ is the carrying capacity.

The work μ_j done by each j th component force, e.g., μ_j is a j th-order Legendre polynomial, and T_j is the j th-order Legendre polynomial. The j th-order Legendre polynomial is given by (6.62) as follows:

$$G = \sum_{j=1}^{\ell} v_j \left(\mu_j + B T_j \right). \quad (6.65)$$

We assume each j th-order Legendre polynomial μ_j is a j th-order Legendre polynomial. We assume each j th-order Legendre polynomial is given by (6.62) as follows:

$$\sum_{j=1}^{\ell} (v_j - \kappa_j) \left(\mu_j + B T_j \right) = 0. \quad (6.66)$$

Therefore

$$\prod_{j=1}^{\ell} (\mu_j + B T_j)^{-\kappa_j} = \frac{(-\kappa_j B)^{\kappa_j}}{B^{\kappa_j}} = \frac{-}{+}, \quad (6.67)$$

$$\Delta G = \left(\sum_{j=1}^{\ell} \kappa_j \mu_j \right) - \left(\sum_{j=1}^{\ell} v_j \mu_j \right) = B T_j \left(\frac{-}{+} \right). \quad (6.68)$$

The j th-order Legendre polynomial μ_j is a j th-order Legendre polynomial. The j th-order Legendre polynomial is given by (6.62) as follows:

6.6.2 Mass-Action Kinetics

From the Legendre (6.34) and (6.35) we have

$$\begin{aligned} \frac{d\mu_j}{dt} &= \sum_{\ell=1}^{\ell} (\kappa_{\ell} - v_{\ell}) (\hat{\phi}^+ - \hat{\phi}^-) \\ &= \sum_{\ell=1}^{\ell} (\kappa_{\ell} - v_{\ell}) \hat{\phi}^- \left\{ e^{-\left[\sum_{\ell=1}^{\ell} (\kappa_{\ell} - v_{\ell}) \mu_{\ell} \right]} - 1 \right\} \\ &= \sum_{\ell=1}^{\ell} (\kappa_{\ell} - v_{\ell}) \hat{\phi}^+ \left\{ 1 - e^{-\left[\sum_{\ell=1}^{\ell} (v_{\ell} - \kappa_{\ell}) \mu_{\ell} \right]} \right\}. \quad (6.69) \end{aligned}$$

Example (6.69) $W_{\alpha} = a_W \delta_{\ell} = \ell$, $e_{\alpha}[\dots] = 0$ and $e_{\alpha}\{\dots\} = 0$ a_W are, respectively. Therefore, the process variables (6.69) $c_1 \dots c_W$ are independent, W according to the dynamics (6.66) and (6.67). In the next section we will study a W variables according to (6.69) and the dynamics (6.67) in Sec. 6.6.1 after the formal calculation of the stationary probabilities [10].

6.6.3 Stochastic Chemical Kinetics

We will study the reaction $A + B \rightleftharpoons C$ with reaction rates k_{\pm} and V the volume of the system. A, B , and C be the number of A, B , and C :



We will assume $A + C$ and $B + C$ do not change in time. Hence $e_{\alpha} c_{\alpha} d_{\alpha} = A + C = A$ and $B + C = B$ are conserved quantities of A and B , respectively, of C , and we will assume $N_W = V$ is the volume of the system. The reaction $A + B \rightleftharpoons C$ can be written as a W variables, according to DGP, as W variables $c_1 \dots c_W$ and the reaction $A + B \rightleftharpoons C$ can be written as W variables $c_1 \dots c_W$ according to DGP, as W variables $c_1 \dots c_W$ and the reaction $A + B \rightleftharpoons C$ can be written as W variables $c_1 \dots c_W$ according to DGP, as W variables $c_1 \dots c_W$.

$$\frac{d\langle c_i \rangle}{dt} = \dots = \frac{+ \binom{A - \langle c_i \rangle}{\langle c_i \rangle} \binom{B - \langle c_i \rangle}{\langle c_i \rangle}}{- \binom{C + \langle c_i \rangle}{\langle c_i \rangle} V}, \quad (6.71)$$

The stationary state $A = A(0) + C(0)$ and $B = B(0) + C(0)$. Therefore,

$$\langle c_i \rangle = \frac{\Xi^{-1} A! B!}{\langle c_i \rangle! (A - \langle c_i \rangle)! (B - \langle c_i \rangle)!} \left(\frac{+}{-V} \right)^{\langle c_i \rangle}, \quad (6.72)$$

where Ξ is the partition function of the system:

$$\Xi(\lambda) = \sum_{c_i=0}^{A, B} \frac{A! B! \lambda^{c_i}}{c_i! (A - c_i)! (B - c_i)!}, \quad \lambda = \left(\frac{+}{-V} \right). \quad (6.73)$$

$$\text{Mean value of } c_i, \text{ by taking } A + B + C = \frac{0}{A} + \frac{0}{B} - C,$$

$$\begin{aligned} & - \lambda^{-1} \langle c_i \rangle \\ &= - \lambda^{-1} \left[\frac{\lambda^c}{c! (A - c)! (B - c)!} \right] + c \lambda^{-1} \dots \end{aligned}$$

$$\begin{aligned}
&= A \ln \left(\frac{A}{V} \right) - A + B \ln \left(\frac{B}{V} \right) - B + C \ln \left(\frac{C}{V} \right) - C - C \ln \left(\frac{+}{-} \right) \\
&= A \ln A + B \ln B + C \ln C + C \left(\frac{\mu_C - \mu_A - \mu_B^0}{BT} \right) - (A + B + C) \\
&= \sum_{\sigma=A,B,C} \sigma \left(\frac{\mu_\sigma}{BT} + \ln \sigma - 1 \right). \tag{6.74}
\end{aligned}$$

The Lagrange multiplier E is (6.65).

The canonical partition function $Z(\beta, \mu)$ is the idea function of the canonical ensemble.

$$G[\mathbf{x}(\cdot)] = \sum_{\sigma=1} \sigma \left(\mu_\sigma + BT \ln \sigma - BT \right). \tag{6.75}$$

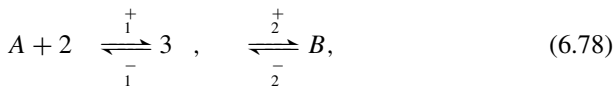
The function G is (6.34), and the Lagrange multiplier E is the energy of the system.

$$\begin{aligned}
\frac{d}{d\beta} G[\mathbf{x}(\cdot)] &= \sum_{j=1} \frac{d}{d\beta} \left(\mu_j + BT \ln \mu_j \right) \\
&= BT \sum_{j=1} \sum_{i=1}
\end{aligned}$$

a e - y g c y d y y e d y a c . W a c e g c a - e a c y y a a , a y e d - c e a d y w d f f e - a c e g c a a , c a y - e a c a c e g c a e , b y j . R a e , - e a c e a *nonequilibrium steady state* (NESS).

L e , c y d e - e f w y g w e a e , e S c e g j d e f - b a b [34] a d S c y a a b e - g j d e f - y y y e a - c a y [17, 25, 35].

6.6.4.1 Schlögl Model



y w c e c y c a y (- c e g c a a) f A a d B a e , a y e d b a e e a a g a . T - e a c y y w y a *Schlögl model* w e d y a c c a b e d e c b e d b e d f f e - a e a y .

$$\frac{d}{dt} = \begin{matrix} + \\ 1 \end{matrix} 2 - \begin{matrix} - \\ 1 \end{matrix} 3 - \begin{matrix} + \\ 2 \end{matrix} + \begin{matrix} - \\ 2 \end{matrix} = () , \tag{6.79}$$

w c a d - d e - y j a . I c a e b b a b a d a d d e y d e b f - c a y a j a y . A f e g y c o - y d e d a c y d y w a $\mu_A \neq \mu_B$. N e y e c e g c a e , b y j $\mu_A = \mu_A + B T y = \mu_B + B T y$, a d

$$\left(- \right) = \frac{\begin{matrix} + \\ 1 \end{matrix} \begin{matrix} + \\ 2 \end{matrix}}{\begin{matrix} - \\ 1 \end{matrix} \begin{matrix} - \\ 2 \end{matrix}} . \tag{6.80}$$

D f f e - a e a y (6.79) w a a e e - $\begin{matrix} + \\ 1 \end{matrix} \begin{matrix} + \\ 2 \end{matrix} = \begin{matrix} - \\ 1 \end{matrix} \begin{matrix} - \\ 2 \end{matrix}$, a e - g - a d - d e

$$\begin{aligned} () &= \begin{matrix} + \\ 1 \end{matrix} 2 - \begin{matrix} - \\ 1 \end{matrix} 3 - \begin{matrix} + \\ 2 \end{matrix} + \begin{matrix} - \\ 2 \end{matrix} \\ &= \begin{matrix} + \\ 1 \end{matrix} 2 - \begin{matrix} - \\ 1 \end{matrix} 3 - \begin{matrix} + \\ 2 \end{matrix} + \frac{\begin{matrix} + \\ 1 \end{matrix} \begin{matrix} + \\ 2 \end{matrix}}{\begin{matrix} - \\ 1 \end{matrix}} \\ &= \left(2 + \frac{\begin{matrix} + \\ 2 \end{matrix}}{\begin{matrix} - \\ 1 \end{matrix}} \right) \left(\begin{matrix} + \\ 1 \end{matrix} - \begin{matrix} - \\ 1 \end{matrix} \right) . \end{aligned} \tag{6.81}$$

T e - e - e () a a y , e f i e d y a = $\frac{\begin{matrix} + \\ 1 \end{matrix}}$, e c e g c a e , b y j . I g a e a , e g (6.78) c a e b c e g c a b a b ; b y j y b e w a A a d B a e a f f i c a a - g e c e g c a a d f f e - a c e , e g , a *chemostat* .

M - e y e - e y g w a a d a f y g (6.80) , e D G P f e y j b e f , () , a g a y a y e - d j a y a b - a d - d e a - c e w .

$$\begin{aligned}
 &= \frac{+}{1} \frac{(-1)}{V} + \frac{-}{2} V = \frac{+}{V} \left((-1) + \frac{+V^2}{1} \right), \quad (6.82) \\
 +1 &= \frac{-}{1} \frac{(+1)(-1)}{V^2} + \frac{+}{2} (+1) \\
 &= \frac{-}{V^2} \left((-1) + \frac{+V^2}{1} \right).
 \end{aligned}$$

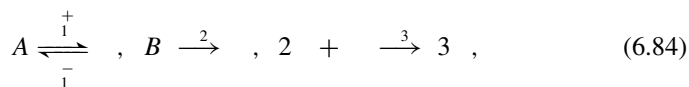
The effective energy density ϵ , according to Eq. (6.45),

$$\epsilon = C \prod_{\ell=0}^{-1} \frac{+}{1} / V = \frac{\lambda}{\ell!} e^{-\lambda}, \quad \lambda = \left(\frac{+}{1} V \right). \quad (6.83)$$

The Poisson distribution P_w is defined as $\mathbb{E}[X] = \lambda$. The effective energy density ϵ is $\left(\frac{+}{1} / \frac{-}{1} \right)$.

6.6.4.2 Schnakenberg Model

See [10],



The w Schnakenberg model is defined as follows

$$\begin{cases} \frac{d}{dt} = \frac{+}{1} - \frac{-}{1} - 3^2 = (\dots), \\ \frac{d}{dt} = 2 - 3^2 = (\dots). \end{cases} \quad (6.85)$$

The reaction network is a chemical reaction network (CRN) of the form DGP , where DGP is a directed graph. We refer to the reader [25, 35] for details on the definition of a CRN.

6.7 The Law of Large Numbers—Kurtz’s Theorem

6.7.1 Diffusion Approximation and Kramers–Moyal Expansion

Starting with the general equation (6.43), we consider a diffusion equation (PDE) for a function $f(x, y, t)$ of the form $\partial_t f = \mathcal{L}f$, where \mathcal{L} is the generator of the process. The generator is given by

$$\begin{aligned} \frac{\partial f(x, y, t)}{\partial t} &= V \frac{d}{dt} f(x, y, t) \\ &= \frac{1}{d} \left(f(x-d, y, t) - f(x, y, t) \right) + \frac{1}{d} \left(f(x, y, t) - f(x, y-d, t) \right) \\ &= \frac{\partial}{\partial x} \left(f(x+d/2, y, t) - f(x-d/2, y, t) \right) \\ &\approx \frac{\partial}{\partial x} \left\{ \frac{\partial}{\partial x} \left(\frac{f(x, y, t) + f(x, y-d, t)}{2V} \right) - \left(f(x, y, t) - f(x, y-d, t) \right) \right\} + \dots \end{aligned} \tag{6.86}$$

where V is the volume. In the limit $V \rightarrow \infty$, we have $V^{-1} \frac{d}{dt} f = \frac{\partial}{\partial x} (f(x, y, t) - f(x, y-d, t))$, which is the drift term.

$$V^{-1} \frac{d}{dt} f = \frac{\partial}{\partial x} (f(x, y, t) - f(x, y-d, t)), \tag{6.87}$$

as $V \rightarrow \infty$.

6.7.2 Nonlinear Differential Equation, Law of Mass Action

The effective equation for $V \rightarrow \infty$,

$$\frac{\partial f(x, y, t)}{\partial t} = -\frac{\partial}{\partial x} (f(x, y, t) - f(x, y-d, t)), \tag{6.88}$$

where $f(x, y, t)$ is the density of particles, can be written as a nonlinear differential equation

$$\frac{d}{dt} f = f(x, y, t) - f(x, y-d, t), \tag{6.89}$$

where the effective reaction rate is given by (6.88).

6.7.3 Central Limit Theorem, a Time-Inhomogeneous Gaussian Process

N_W can be expressed

$$(\cdot) = \frac{(\cdot) - V(\cdot)}{\sqrt{V}}, \tag{6.90}$$

where $\hat{(\cdot)}$ is a centered Gaussian process with $\frac{(\cdot)}{V} \hat{(\cdot)}$ and $\hat{(\cdot)}$ if $V \rightarrow \infty$, ...
 ... the PDE $\frac{\partial}{\partial t} \hat{(\cdot)}$...

$$\frac{\partial (\cdot, \cdot)}{\partial t} = \frac{\partial}{\partial t} \left\{ \frac{\partial}{\partial t} \left(\frac{\hat{(\cdot)} + \hat{(\cdot)}}{2} \right) (\cdot, \cdot) - \left(\hat{(\cdot)} - \hat{(\cdot)} \right) (\cdot, \cdot) \right\}. \tag{6.91}$$

Therefore, (\cdot) is a Gaussian process, ...
 ... the PDE (6.91) ...
 ... [32]. The ...

6.7.4 Diffusion's Dilemma

The ... (6.86) ...

$$-\hat{(\cdot)} = 2V \int \left(\frac{\hat{(\cdot)} - \hat{(\cdot)}}{\hat{(\cdot)} + \hat{(\cdot)}} \right) d. \tag{6.92}$$

On the other hand, ... (6.45),

$$= \prod_{i=1}^0 \left(\frac{-1}{\cdot} \right),$$

... $V \rightarrow \infty$... $V^{-1} V = \hat{(\cdot)}$, $V^{-1} V = \hat{(\cdot)}$, and $V^{-1} = d$, ...

$$-\hat{(\cdot)} = -\sum_{i=1} \left(\frac{-1}{\cdot} \right) + C \Leftrightarrow -\hat{(\cdot)} = V \int \left(\frac{\hat{(\cdot)}}{\hat{(\cdot)}} \right) d. \tag{6.93}$$

It follows from Eqs. (6.92) and (6.93) that $\langle \dot{H}_w \rangle = 0$. We can also show that $\langle \dot{H}_w^2 \rangle > 0$:

$$\frac{d}{dt} \left(-\langle \dot{H}_w \rangle \right) = 2V \left(\frac{\langle \dot{H}_w \rangle - \langle \dot{H}_w \rangle}{\langle \dot{H}_w \rangle + \langle \dot{H}_w \rangle} \right) = 0 \implies \langle \dot{H}_w \rangle = \langle \dot{H}_w \rangle. \quad (6.94)$$

In fact, we can also show that $\langle \dot{H}_w^2 \rangle > 0$:

$$\begin{aligned} \left[\frac{d^2}{dt^2} \left(-\langle \dot{H}_w \rangle \right) \right]_{\langle \dot{H}_w \rangle} &= 2V \left(\frac{\langle \dot{H}_w \rangle - \langle \dot{H}_w \rangle}{\langle \dot{H}_w \rangle + \langle \dot{H}_w \rangle} \right) = V \left(\frac{\langle \dot{H}_w \rangle - \langle \dot{H}_w \rangle}{\langle \dot{H}_w \rangle} \right) \\ &= \left[\frac{d^2}{dt^2} \left(-\langle \dot{H}_w \rangle \right) \right]_{\langle \dot{H}_w \rangle}. \end{aligned} \quad (6.95)$$

However, it can be shown that $\langle \dot{H}_w^2 \rangle > 0$, as can be seen from the following calculation [20, 37]. The quantity $\langle \dot{H}_w^2 \rangle$ is a measure of the fluctuations of the work \dot{H}_w around its average value. It is shown that $\langle \dot{H}_w^2 \rangle > 0$ for all systems, and this result is used to show that the fluctuations of the work are non-zero. The above results are used to show that the fluctuations of the work are non-zero.

6.8 The Logic of the Mechanical Theory of Heat and Nonequilibrium Thermodynamics

In order to see the logic of the mechanical theory of heat, see Sec. 6.9.

The equation for the entropy balance in the control volume Ω can be written as

$$\frac{dS}{dt} = \int_{\partial\Omega} J_S dA + J_S, \quad (6.96)$$

where the first term on the right-hand side represents the net flux of entropy J_S across the boundary $\partial\Omega$, and the second term represents the entropy production J_S inside the control volume Ω . The entropy production J_S is always non-negative, i.e., $J_S \geq 0$. This is a consequence of the second law of thermodynamics, which states that the total entropy of an isolated system can never decrease over time. In the context of the control volume Ω , this means that the entropy production J_S must be non-negative. The entropy production J_S is given by the expression $J_S = \int_{\Omega} \sigma dV$, where σ is the entropy production density. The entropy production density σ is given by the expression $\sigma = \frac{1}{T} \sum_i J_i X_i$, where J_i is the flux of the extensive property X_i and T is the temperature. The entropy production density σ is always non-negative, i.e., $\sigma \geq 0$. This is a consequence of the second law of thermodynamics, which states that the total entropy of an isolated system can never decrease over time. In the context of the control volume Ω , this means that the entropy production J_S must be non-negative. The entropy production J_S is given by the expression $J_S = \int_{\Omega} \sigma dV$, where σ is the entropy production density. The entropy production density σ is given by the expression $\sigma = \frac{1}{T} \sum_i J_i X_i$, where J_i is the flux of the extensive property X_i and T is the temperature. The entropy production density σ is always non-negative, i.e., $\sigma \geq 0$.

6.8.1 Boltzmann's Mechanical Theory of Heat

The mechanical theory of heat, developed by Boltzmann, states that heat is a form of energy that is transferred between systems. It is a consequence of the microscopic motion of particles. The mechanical theory of heat is based on the assumption that the particles of a system are in constant motion. The energy of the system is the sum of the kinetic energy of the particles and the potential energy of the interactions between the particles. The heat is the energy that is transferred between systems as a result of the microscopic motion of particles. The mechanical theory of heat is a consequence of the second law of thermodynamics, which states that the total entropy of an isolated system can never decrease over time. In the context of the control volume Ω , this means that the entropy production J_S must be non-negative. The entropy production J_S is given by the expression $J_S = \int_{\Omega} \sigma dV$, where σ is the entropy production density. The entropy production density σ is given by the expression $\sigma = \frac{1}{T} \sum_i J_i X_i$, where J_i is the flux of the extensive property X_i and T is the temperature. The entropy production density σ is always non-negative, i.e., $\sigma \geq 0$.

$$\frac{d}{dt} = \frac{\partial H(\dots)}{\partial t}, \quad \frac{d}{dt} = -\frac{\partial H(\dots)}{\partial t}. \quad (6.97)$$

The flux of the extensive property X_i is given by the expression $J_i = -\frac{\partial H(\dots)}{\partial X_i}$, where $H(\dots)$ is the total energy of the system. The flux of the extensive property X_i is always non-negative, i.e., $J_i \geq 0$. This is a consequence of the second law of thermodynamics, which states that the total entropy of an isolated system can never decrease over time. In the context of the control volume Ω , this means that the entropy production J_S must be non-negative. The entropy production J_S is given by the expression $J_S = \int_{\Omega} \sigma dV$, where σ is the entropy production density. The entropy production density σ is given by the expression $\sigma = \frac{1}{T} \sum_i J_i X_i$, where J_i is the flux of the extensive property X_i and T is the temperature. The entropy production density σ is always non-negative, i.e., $\sigma \geq 0$.

$$\frac{d}{dt} H(\dots) = \frac{\partial H}{\partial t} \left(\dots \right)$$

N_w , energy E , and Hamiltonian $H(\dots, V, N_w)$ are conserved quantities. The phase space volume $\Omega(E, V, N_w)$ is defined as the volume of phase space accessible to the system at energy E . The entropy $S(E, V, N_w)$ is defined as $S(E, V, N_w) = k_B \ln \Omega(E, V, N_w)$. The entropy is a function of energy, volume, and number of particles. The entropy is extensive, meaning it is proportional to the number of particles. The entropy is also a concave function of energy and volume. The entropy is a state function, meaning it depends only on the current state of the system and not on the path taken to reach that state.

A Hamiltonian $H(\dots)$ is a function of the coordinates and momenta of the particles. The Hamiltonian is a conserved quantity, meaning it is constant in time. The Hamiltonian is also a function of the volume V and the number of particles N . The Hamiltonian is a function of the coordinates and momenta of the particles. The Hamiltonian is a function of the coordinates and momenta of the particles. The Hamiltonian is a function of the coordinates and momenta of the particles. The Hamiltonian is a function of the coordinates and momenta of the particles.

$$S(E, V, N) = k_B \ln \left\{ \int_{H(\dots) = E} \delta H(\dots) \right\} = k_B \ln \int_{H(\dots) \leq E} d\Omega \quad (6.99)$$

Since $S(E)$ is a function of energy, volume, and number of particles, we can write $dS = \left(\frac{\partial S}{\partial E}\right)_{V,N} dE + \left(\frac{\partial S}{\partial V}\right)_{E,N} dV + \left(\frac{\partial S}{\partial N}\right)_{E,V} dN$.

$$dE = \left(\frac{\partial E}{\partial S}\right)_{V,N} dS + \left(\frac{\partial E}{\partial V}\right)_{S,N} dV + \left(\frac{\partial E}{\partial N}\right)_{S,V} dN = T dS - p dV + \mu dN \quad (6.100)$$

What is the significance of Eq. (6.100)? First, it shows that energy, volume, and number of particles are conserved quantities. Second, it shows that the entropy is a function of energy, volume, and number of particles. Third, it shows that the temperature, pressure, and chemical potential are defined as $T = \left(\frac{\partial E}{\partial S}\right)_{V,N}$, $p = -\left(\frac{\partial E}{\partial V}\right)_{S,N}$, and $\mu = \left(\frac{\partial E}{\partial N}\right)_{S,V}$. The entropy is a function of energy, volume, and number of particles. The entropy is a function of energy, volume, and number of particles. The entropy is a function of energy, volume, and number of particles. The entropy is a function of energy, volume, and number of particles.

The entropy is a function of energy, volume, and number of particles. The entropy is a function of energy, volume, and number of particles. The entropy is a function of energy, volume, and number of particles. The entropy is a function of energy, volume, and number of particles. The entropy is a function of energy, volume, and number of particles. The entropy is a function of energy, volume, and number of particles. The entropy is a function of energy, volume, and number of particles. The entropy is a function of energy, volume, and number of particles.

$$\frac{\partial \rho(\dots)}{\partial \dots} = D \frac{\partial^2 \rho(\dots)}{\partial \dots^2} = -\frac{1}{\eta} \frac{\partial (\hat{F} \rho)}{\partial \dots} \quad (6.101)$$

where

$$\hat{F} = -\frac{\partial \mu}{\partial \dots}, \quad \text{and } d\mu = D \eta \rho(\dots) = k_B T \rho(\dots) \quad (6.102)$$

\hat{F} is the entropic force, and $d\mu$ is the chemical potential.

6.8.2 Classical Macroscopic Nonequilibrium Thermodynamics

From Eq. (6.100) and the definition of $H(\rho, \sigma) = E - TS$, we can write the entropy production rate as follows. In the case of a system with a constant volume, the entropy production rate is given by the following equation. We assume that the system is in a state of local equilibrium.

$$T dS \geq dQ = dE - dW, \tag{6.103}$$

where dQ is the heat added to the system, dE is the change in internal energy, and dW is the work done on the system. The equality holds for a reversible process, while the inequality holds for an irreversible process. The term dS is the change in entropy, and dE is the change in internal energy. The term dW is the work done on the system. The term dQ is the heat added to the system. The term dE is the change in internal energy. The term dW is the work done on the system. The term dS is the change in entropy. The term dE is the change in internal energy. The term dW is the work done on the system. The term dQ is the heat added to the system.

$$\frac{dS}{dt} = -\frac{dQ}{T}, \quad \geq 0, \tag{6.104}$$

where dQ is the heat added to the system, T is the temperature, and dS is the change in entropy. The equality holds for a reversible process, while the inequality holds for an irreversible process. The term dQ is the heat added to the system. The term T is the temperature. The term dS is the change in entropy.

6.8.2.1 Local Equilibrium Assumption and Classical Derivation of Entropy Production

From the definition of E (6.100) and the definition of $H(\rho, \sigma)$, we can write the entropy production rate as follows.

$$\frac{\partial H(\rho, \sigma)}{\partial t} = \frac{1}{T} \frac{\partial E(\rho, \sigma)}{\partial t} - \sum_{j=1}^N \mu_j \frac{\partial J_j(\rho, \sigma)}{\partial t}, \tag{6.105}$$

where μ_j is the chemical potential of the j -th component, J_j is the flux of the j -th component, and E is the internal energy. The term $\frac{\partial H(\rho, \sigma)}{\partial t}$ is the time derivative of the entropy. The term $\frac{1}{T} \frac{\partial E(\rho, \sigma)}{\partial t}$ is the time derivative of the internal energy divided by the temperature. The term $\sum_{j=1}^N \mu_j \frac{\partial J_j(\rho, \sigma)}{\partial t}$ is the sum of the products of the chemical potentials and the time derivatives of the fluxes.

Realizing that the fluxes J_j are given by the following equation, we can write the entropy production rate as follows.

$$\frac{\partial H(\rho, \sigma)}{\partial t} = -\frac{\partial J(\rho, \sigma)}{\partial t}, \quad \frac{\partial J_j(\rho, \sigma)}{\partial t} = -\frac{\partial J_j(\rho, \sigma)}{\partial t}. \tag{6.106}$$

Therefore, the entropy production rate is given by the following equation.

$$\frac{\partial H(\rho, \sigma)}{\partial t} = -J_S(\rho, \sigma) \tag{6.107a}$$

where μ_j is the chemical potential of the j th component.

$$J_S(\mu_j) = J \frac{\partial}{\partial T} \left(\frac{1}{T} \right) - \sum_{j=1}^N J_j \frac{\partial}{\partial T} \left(\frac{\mu_j}{T} \right) - \sum_{i=1}^N \frac{\Delta_i}{T} \hat{\phi}_i, \quad (6.107b)$$

and the entropy flux

$$J_S(\mu_j) = \frac{\partial}{\partial T} \left(\frac{J}{T} - \sum_{j=1}^N \frac{\mu_j J_j}{T} \right). \quad (6.107c)$$

According to Onsager's theory [18], each μ_j is a function of the density ρ_j and temperature T :

$$\mu_j = \mu_j(\rho_j, T) \times \text{density factor} \quad (6.108)$$

where ρ_j is the density of the j th component. The entropy flux J_S is a function of the density ρ_j and temperature T . The entropy flux J_S is a function of the density ρ_j and temperature T . The entropy flux J_S is a function of the density ρ_j and temperature T .

6.9 Mathematicothermodynamics of Markov Dynamics

We will consider the case of a Markov process \mathcal{W} on a countable set Ω of states. For example, \mathcal{W} can be a random walk on a lattice, a queueing process, a birth-death process, etc. More formally, a Markov process \mathcal{W} is a family of random variables $\{X_t\}_{t \geq 0}$ defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$.

$$\frac{d\rho_j(t)}{dt} = \sum_{i=1}^N \left(\rho_i(t) - \rho_j(t) \right), \quad (6.109)$$

where $\rho_j(t)$ is the probability of being in state j at time t (6.27).

We will assume that \mathcal{W} is ergodic and that the stationary distribution ρ_j is unique. According to Sec. 6.8.1, the stationary distribution ρ_j is the unique solution of the system of equations (6.109) subject to the normalization condition $\sum_{j=1}^N \rho_j = 1$. The stationary distribution ρ_j is the unique solution of the system of equations (6.97), and the entropy flux J_S is given by $J_S = -\sum_{j=1}^N \rho_j \ln \rho_j$.

$$S(\rho) = - \sum_{j=1}^N \rho_j \ln \rho_j. \quad (6.110)$$

Then, the entropy

$$\frac{dS}{dt} = J_S, \quad (6.111a)$$

w e-e

$$() = \frac{1}{2} \sum_{j=1}^N (, () , - () ,) \Psi \left(\frac{()}{() , } \right), \tag{6.111b}$$

$$J_S() = \frac{1}{2} \sum_{j=1}^N (, () , - () ,) \Psi \left(\frac{()}{ , } \right). \tag{6.111c}$$

... ed a e b , , a ≥ 0 . c e f - e e - a - f , , E . (6.111b) , e e f - a e f - f (-) \Psi (/) ≥ 0 . We a \Psi e e - e - e b a c e f (6.111b) E . (6.76) .

T e - e - e_w e a e d e d a a a - b a a c e e , a \Psi b a e d \Psi M a d \Psi a c , w e a e a \Psi \Psi f c a e e b \Psi . E r a \Psi (6.111b) a d (6.111c) f e e g e e c e e e \Psi , \Psi e f e { , () } , f e e a a - f l J_S e \Psi \Psi e g a e a - e e d c \Psi . A_w e a \Psi w b e_w , e e - a c \Psi e e \Psi e b \Psi e d \Psi a c \Psi e e c c a e , \Psi a e a c e . T e e e - e e f f e c t e a a e e a e w e e " e e a r e b e \Psi g l .

6.9.1 Non-Decreasing Entropy in Systems with Uniform Stationary Distribution

If e_j a e E . (6.109) a a a \Psi a d - b \Psi = 1 \forall , a

$$\sum_{j=1}^N (, - ,) = \sum_{j=1}^N , = 0, \forall .$$

I ... ca e,

$$\begin{aligned} \frac{dS}{d} &= - \sum_{j=1}^N \left(\frac{d , ()}{d} \right) \Psi , = - \sum_{j=1}^N (, - , ,) \Psi , \\ &= \sum_{j=1}^N , , \Psi \left(\frac{()}{ , } \right) \geq \sum_{j=1}^N , , \Psi \left(\frac{()}{ , } - 1 \right) \\ &= \sum_{j=1}^N \left(\sum_{j=1}^N , \right) = 0. \end{aligned} \tag{6.112}$$

We refer to a “*ergodic*” as a function ρ that is a stationary state of the system, i.e., $\rho = \rho \circ \tau_t$ for all t .

6.9.2 Q-Processes with Detailed Balance

If a Q-process is a stationary state ρ , $\rho = \rho \circ \tau_t$ is a *detailed balance*, i.e.,

$$\begin{aligned}
 J_S(\rho) &= \frac{1}{2} \sum_{j=1}^N \left(\rho_j(\rho) - \rho(\rho)_j \right) \gamma_j \left(\frac{1}{\rho_j} \right) \\
 &= \frac{1}{2} \sum_{j=1}^N \left(\rho_j(\rho) - \rho(\rho)_j \right) \gamma_j \left(\frac{1}{\rho_j} \right) \\
 &= \sum_{j=1}^N \left(\rho_j(\rho) - \rho(\rho)_j \right) \gamma_j = - \sum_{j=1}^N \frac{d}{d} \rho_j(\rho) \gamma_j \\
 &= \frac{d}{d} \left(\sum_{j=1}^N \rho_j(\rho) \left(-\gamma_j \right) \right) = \frac{1}{T} \frac{d\bar{E}}{d}, \tag{6.113}
 \end{aligned}$$

where

$$\bar{E} = \sum_{j=1}^N \rho_j(\rho) E_j, \tag{6.114}$$

and be defined as the energy \bar{E} of the system $E = -T \ln \rho$ and the entropy $S = - \sum_{j=1}^N \rho_j(\rho) \ln \rho_j(\rho)$. (6.111a) because

$$\frac{d}{d} \left(\frac{\bar{E}}{T} - S \right) = - \leq 0. \tag{6.115}$$

$F = \bar{E} - TS$ is the free energy of the system. It is a function of the parameters of the system, and it is a function of the parameters of the system. It is a function of the parameters of the system, and it is a function of the parameters of the system.

6.9.3 Monotonicity of F Change in General Q -Processes

Let $\{X_t\}_{t \geq 0}$ be a Markov process with generator Q and transition probabilities $P_{ij}(t)$. Let f be a bounded measurable function on the state space S . Then

$$F(t) = \sum_{j=1}^N p_j(t) (-\lambda_j + \lambda_j P_{jj}(t)) = \sum_{j=1}^N p_j(t) \lambda_j \left(\frac{P_{jj}(t)}{1} - 1 \right) \geq 0. \quad (6.116)$$

One can also show that $dF/dt \leq 0$ for a Q -process with the above properties:

$$\begin{aligned} \frac{dF(t)}{dt} &= \sum_{j=1}^N \left(\frac{d p_j(t)}{dt} \right) \lambda_j \left(\frac{P_{jj}(t)}{1} - 1 \right) = \sum_{j=1}^N \left(\sum_{i=1}^N (q_{ij} - \delta_{ij} q_{ii}) p_i(t) \right) \lambda_j \left(\frac{P_{jj}(t)}{1} - 1 \right) \\ &= \sum_{j=1}^N p_j(t) \lambda_j \left(\frac{P_{jj}(t)}{1} - 1 \right) \leq \sum_{j=1}^N p_j(t) \lambda_j \left(\frac{P_{jj}(t)}{1} - 1 \right) \\ &= \sum_{j=1}^N p_j(t) \lambda_j \left(\sum_{i=1}^N (q_{ij} - \delta_{ij} q_{ii}) \right) = 0. \end{aligned} \quad (6.117)$$

6.9.4 F Balance Equation of Markov Dynamics

More explicitly, we have the balance equation for $F(t)$:

$$\frac{dF(t)}{dt} = E_j(t) - F(t), \quad (6.118a)$$

where $E_j(t) \geq 0$. Using (6.111b), and

$$E_j(t) = \frac{1}{2} \sum_{j=1}^N \left(p_j(t) \lambda_j - p_j(t) \lambda_j \right) \lambda_j \left(\frac{P_{jj}(t)}{1} - 1 \right) \geq 0. \quad (6.118b)$$

See [9] for further details. By (6.118a) and (6.118b) we can see that $F(t)$ is a non-negative function of time, and $E_j(t)$ is a non-negative function of time. The balance equation (6.118a) can be written as $F(t) = \int_0^t E_j(s) ds$. Using (6.111a), we can see that $F(t) = \int_0^t E_j(s) ds$.

The balance equation (6.118a) and (6.118b) can be used to show that $dF/dt \leq 0$ for a Q -process with the above properties. By the above results, we can see that $F(t)$ is a non-negative function of time, and $E_j(t)$ is a non-negative function of time.

The above is a macroscopic equation for the concentration, *mathematicothermodynamics* [9, 10, 21, 24].

6.9.5 Driven System and Cycle Decomposition

The above stochastic equation (6.111b) can be written as

$$= \sum_{\text{edge } j}^N (\varphi_j^+ - \varphi_j^-) \gamma \left(\frac{\varphi_j^+}{\varphi_j^-} \right), \tag{6.119}$$

where $\varphi_j^\pm = \varphi_j^\pm(\mathbf{x})$ are the fluxes at the boundary. It can be shown that, in a stationary state, the above equation can be reduced to

$$= \sum_{\text{cycle } \Gamma}^N (\varphi_\Gamma^+ - \varphi_\Gamma^-) \gamma \left(\frac{\varphi_\Gamma^+}{\varphi_\Gamma^-} \right), \tag{6.120}$$

where φ_Γ^\pm are the fluxes of the cycle Γ in the forward and backward directions. Moreover, the cycle $\Gamma = (j_0, j_1, \dots, j_{l-1}, j_0)$

$$\frac{\varphi_\Gamma^+}{\varphi_\Gamma^-} = \frac{\varphi_{j_1}^+ \varphi_{j_2}^+ \dots \varphi_{j_{l-1}}^+}{\varphi_{j_0}^- \varphi_{j_1}^- \dots \varphi_{j_{l-1}}^-}, \tag{6.121}$$

where φ_j^\pm are the fluxes at the boundary. Therefore, $(\varphi_\Gamma^+ / \varphi_\Gamma^-)$ can be shown to be independent of the stochastic process, and the equation (6.120) can be reduced to a macroscopic equation for the concentration. A detailed balance condition is satisfied if the equation (6.121) is satisfied for all cycles [27]. If a macroscopic cycle is balanced, the above stochastic equation is a detailed balance equation.

In the case of a cycle Γ of A.N.K. type, the equation (6.121) is satisfied for each cycle of the macroscopic cycle decomposition. Therefore, the macroscopic equation is a detailed balance equation. The above is a macroscopic equation for the concentration, *detailed balance* is a condition for the macroscopic equation to be a detailed balance equation. For a detailed balance equation, the macroscopic equation is a detailed balance equation. The above is a macroscopic equation for the concentration, $\varphi_\Gamma^+ \neq \varphi_\Gamma^-$.

6.9.6 Macroscopic Thermodynamics in the Kurtz Limit

For a DGP with N species and M reactions, the free energy F is given by Sec. 6.9.4 as a function of the abundances $v(\mathbf{n})$ of the species \mathbf{n} in each well \mathbf{g} of the potential V . The free energy F is a function of the abundances $v(\mathbf{n})$ and the volume $V \rightarrow \infty$ in the Kurtz limit. It can be written as [10]

$$\begin{aligned} \lim_{V \rightarrow \infty} \frac{F[v(\mathbf{n}, \cdot)]}{V} &= \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{\mathbf{n}} v(\mathbf{n}, \cdot) \left[\frac{v(\mathbf{n}, \cdot)}{v(\mathbf{n})} \right] \\ &= - \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{\mathbf{n}} v(\mathbf{n}, \cdot) \ln v(\mathbf{n}) \\ &= G[x(\cdot)], \end{aligned} \tag{6.122}$$

where $\mathbf{n} = (n_1, n_2, \dots, n_N)$ is the vector of abundances of the species, $\mathbf{x} = (x_1, \dots, x_N)$ is the vector of relative abundances $x_i = \frac{n_i}{V}$. The Kurtz limit is given by Sec. 6.7 as the limit of a DGP, $\mathbf{n}_V(\cdot)$,

$$\lim_{V \rightarrow \infty} \frac{\mathbf{n}_V(\cdot)}{V} = \mathbf{x}(\cdot), \tag{6.123}$$

where $\mathbf{x}(\cdot)$ is the vector of relative abundances of the species (e.g., Eq. (6.89)). Moreover, according to the age-dependent branching process theory, the free energy F can be written as a function of the relative abundances x_i of the species i in each well \mathbf{g} of the potential V as

$$- \lim_{V \rightarrow \infty} \frac{1}{V} \ln v(\mathbf{n}) = - \lim_{V \rightarrow \infty} \frac{1}{V} \ln v(V\mathbf{x}) = G(\mathbf{x}). \tag{6.124}$$

The relative abundances of the species $G(\mathbf{x})$ can be defined as a gradient of the free energy G with respect to the relative abundances x_i . It can be written as

$$\frac{d}{d} G[\mathbf{x}(\cdot)] = \left(\frac{d\mathbf{x}(\cdot)}{d} \right) \cdot \nabla_{\mathbf{x}} G(\mathbf{x}) \leq 0. \tag{6.125}$$

The relative abundances of the species $G(\mathbf{x})$ are given by Eq. (6.77). See [10] for details.

6.10 Summary and Conclusion

The relative abundances of the species $G(\mathbf{x})$ are given by Eq. (6.77). The relative abundances of the species $G(\mathbf{x})$ are given by Eq. (6.77). The relative abundances of the species $G(\mathbf{x})$ are given by Eq. (6.77).

and a queueing system. We will use the following notation: $(ODE)_W$ denotes the ordinary differential equation $\dot{w} = A(w)$ with initial condition $w(0) = w_0$. The $Delbrück-Gillespie process$ is a continuous-time Markov process with generator G and initial condition $X(0) = x_0$. The $Delbrück-Gillespie process$ is a continuous-time Markov process with generator G and initial condition $X(0) = x_0$. The $Delbrück-Gillespie process$ is a continuous-time Markov process with generator G and initial condition $X(0) = x_0$.

6.11 Exercises: Simple and Challenging

6.11.1 Simple Exercises

1. Consider a birth-death process with birth rate λ and death rate μ . Let $X(t)$ denote the number of individuals at time t . Show that $\mathbb{E}[X(t)] = \mathbb{E}[X(0)]e^{(\lambda - \mu)t}$.
2. Let $\lambda_1, \dots, \lambda_n$ be independent birth rates and μ_1, \dots, μ_n be independent death rates. Let $X_i(t)$ denote the number of individuals of type i at time t . Show that $\mathbb{E}[X_i(t)] = \mathbb{E}[X_i(0)]e^{(\lambda_i - \mu_i)t}$.
3. If a birth-death process starts at $X(0) = 0$ and has birth rate λ and death rate μ , show that $\mathbb{P}(X(t) = 0) = e^{-\lambda t}$.

6.11.2 More Challenging Exercises

4. Consider a birth-death process with birth rate λ and death rate μ . Let $X(t)$ denote the number of individuals at time t . Show that $\mathbb{P}(X(t) = 0) = e^{-\lambda t}$.
- (*) Let $\lambda_1, \dots, \lambda_n$ be independent birth rates and μ_1, \dots, μ_n be independent death rates. Let $X_i(t)$ denote the number of individuals of type i at time t . Show that $\mathbb{E}[X_i(t)] = \mathbb{E}[X_i(0)]e^{(\lambda_i - \mu_i)t}$.

(c) Let $\langle \cdot | \cdot \rangle$ be the bilinear form associated with the inner product $\langle \cdot | \cdot \rangle$ defined by

$$\sum_{n=0}^{\infty} \langle \cdot | \cdot \rangle = 1.$$

What is the adjoint of the operator T defined by

(c) The adjoint of the operator T defined by

$$(Tf)(x) = \sum_{n=0}^{\infty} \langle \cdot | \cdot \rangle.$$

Based on the definition of the adjoint operator T^* , we have

$$\frac{d}{dx} \langle \cdot | \cdot \rangle = (\lambda - \mu) \langle \cdot | \cdot \rangle.$$

5. The 3x3 matrix A ,

$$A \begin{matrix} \xrightarrow{1} \\ \xleftarrow{-1} \end{matrix} B \begin{matrix} \xrightarrow{2} \\ \xleftarrow{-2} \end{matrix} C \begin{matrix} \xrightarrow{3} \\ \xleftarrow{-3} \end{matrix} A, \tag{6.126}$$

is a 3×3 matrix. What is the adjoint of A ? Is A self-adjoint? Is A normal? Is A unitary? Is A Hermitian? Is A symmetric? Is A real symmetric? Is A real Hermitian? Is A real symmetric and Hermitian? Is A real symmetric and Hermitian? Is A real symmetric and Hermitian?

(c) The bilinear form $\langle \cdot | \cdot \rangle$ is defined by $\langle \mathbf{p} | \mathbf{q} \rangle = \mathbf{p}^T \mathbf{Q} \mathbf{q}$, where $\mathbf{p} = (p_1, p_2, p_3)^T$ and $\mathbf{q} = (q_1, q_2, q_3)^T$.

$$\frac{d}{dx} \langle \mathbf{p} | \mathbf{q} \rangle = \langle \mathbf{p} | \mathbf{Q} \mathbf{q} \rangle.$$

What is the adjoint of the operator T defined by $(Tf)(x) = \int_a^b f(x) dx$? Is T self-adjoint? Is T normal? Is T unitary? Is T Hermitian? Is T symmetric? Is T real symmetric? Is T real Hermitian? Is T real symmetric and Hermitian? Is T real symmetric and Hermitian? Is T real symmetric and Hermitian?

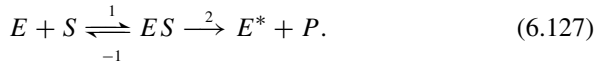
(c) Consider the linear operator T defined by $(Tf)(x) = \int_a^b f(x) dx$. What is the adjoint of T ? Is T self-adjoint? Is T normal? Is T unitary? Is T Hermitian? Is T symmetric? Is T real symmetric? Is T real Hermitian? Is T real symmetric and Hermitian? Is T real symmetric and Hermitian? Is T real symmetric and Hermitian?

$$J_{A \rightarrow B} = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix} \begin{pmatrix} A & & \\ & B & \\ & & C \end{pmatrix}.$$

What is the adjoint of the operator T defined by $(Tf)(x) = \int_a^b f(x) dx$? Is T self-adjoint? Is T normal? Is T unitary? Is T Hermitian? Is T symmetric? Is T real symmetric? Is T real Hermitian? Is T real symmetric and Hermitian? Is T real symmetric and Hermitian? Is T real symmetric and Hermitian?

(c) What is the adjoint of the operator T defined by $(Tf)(x) = \int_a^b f(x) dx$? Is T self-adjoint? Is T normal? Is T unitary? Is T Hermitian? Is T symmetric? Is T real symmetric? Is T real Hermitian? Is T real symmetric and Hermitian? Is T real symmetric and Hermitian? Is T real symmetric and Hermitian?

6. C y de a ng e d j e E y e ea f b a e j e e S. T e M c ae ...
M d d y e c ...



Be ca e e e y a ng e d j e j e e e w z ng, e c y c d a y f S
c a be a j d a w a c y d a, a e a e S.

W e e d f f e d a e a y f z e z b a b ... f e d j e b e ng y
a e E, ES, d E*: E(), ES(), d E*().

G d y a c y d y E(0) = 1, ES(0) = 0, d E*(0) = 0, z ... e
E*().

I c ca a e j e f z e d j e j e f z a e E E* ... c a c.
L e T b e e z d j j e. W a ... e z b a b ... d z b a y f z T, T()? H_w
... e a e d E*()?

C j j e e e e c e d a e E[T]. C j j a e ... z e e w ... e M c ae ...
M d d f z a.

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