Appendix

A Kramers-Moyal expansion

Theorem 2 Let \((X, U)\) define a general bivariate Markov process where \(X\) is described by

\[
U = \frac{dX}{dt}.
\]

The conditional p.d.f. \(p(x, u, t|x_0, u_0, t_0)\) of this process satisfies the Kramers-Moyal expansion

\[
\frac{\partial p}{\partial t} = -u_i \frac{\partial p}{\partial x_i} + \sum_{n=1}^{\infty} (-1)^n \frac{\partial^n D_{jkl}(u, t) p}{\partial u_1^{j} \partial u_2^{k} \partial u_3^{l}}
\]

where \(D_{jkl}(u, t) = \lim_{\tau \to 0} \frac{1}{n!} \left( \frac{\langle (U_1(t+\tau) - U_1(t))^j (U_2(t+\tau) - U_2(t))^k (U_3(t+\tau) - U_3(t))^l \rangle}{\tau} \right)_{U(t)=u} \) and \(\langle \cdot \rangle_{U(t)=u}\) denotes the average over all particles with velocity \(U(t)\) equal to \(u\).

Proof. The derivation of the Kramers-Moyal expansion (KME) for a general N-variable Markov process is given by Risken (Risken, 1989, p. 81 – 84). It is shown that the general form of the KME for a general N-variable Markov process \(Y = (y_1, y_2, \ldots, y_N)\) reads

\[
\frac{\partial f}{\partial t}(y, t|y_0, t_0) = \sum_{n=1}^{\infty} (-1)^n \frac{\partial^n (D_{ji1 \ldots jn}(y, t)f)}{\partial y_{j1} \ldots \partial y_{jn}}
\]

where \(f(y, t|y_0, t_0)\) denotes the p.d.f. of the process \(Y\). The coefficients in the KME for \(j_i = 1, 2, \ldots, N\) and \(i = 1, 2, \ldots, n\) read

\[
D_{j_1 \ldots j_n}(y, t) = \lim_{\tau \to 0} \frac{1}{n!} \left( \frac{\langle (Y_{j_1}(t+\tau) - Y_{j_1}(t)) \ldots (Y_{j_n}(t+\tau) - Y_{j_n}(t)) \rangle_{Y(t)=y}}{\tau} \right)
\]
In the rest of this section, we will use vectors \( x, u \) and \( y = (x, u) \) together. The indices of the vectors \( x \) and \( u \) run from 1 to 3. The indices of \( y \) run from 1 to 6 and \( y_i = x_i \) for \( i = 1, 2, 3 \) and \( y_i = u_{i-3} \) for \( i = 4, 5, 6 \).

The coefficients \( D_{j_1 \ldots j_n}(y, t) \) are invariant to permutations of the indices \( j_i \). The coefficients containing terms \( y_i \) are all equal to the coefficient with first index \( j_1 = i \). The definition of the \( n \)-th moment of the process \( Y \) reads

\[
\begin{align*}
\langle (Y_{j_1}(t + \tau) - Y_{j_1}(t)) \cdots (Y_{j_n}(t + \tau) - Y_{j_n}(t)) \rangle_{Y(t)=y} &= \int_{\mathbb{R}^n} (y'_{j_1}(t + \tau) - y_{j_1}(t))(y'_{j_2}(t + \tau) - y_{j_2}(t)) \cdots (y'_{j_n}(t + \tau) - y_{j_n}(t)) \\
&\quad \times f(y', t + \tau | y, t) \, dy'.
\end{align*}
\]

where \( y'(t + \tau) \) denotes the value of the stochast \( Y \) at time \( t + \tau \). Using this definition we obtain for the KME-coefficients

\[
D_{j_1 \ldots j_n}(y, t) = \frac{1}{n!} \lim_{\tau \to 0} \int_{\mathbb{R}^n} \frac{(y'_{j_1}(t + \tau) - y_{j_1}(t))}{\tau}
\]

\[
(y'_{j_2}(t + \tau) - y_{j_2}(t)) \cdots (y'_{j_n}(t + \tau) - y_{j_n}(t)) f(y', t + \tau | y, t) \, dy'.
\]

All functions are continuous and finite hence we may change the order of integration and taking limit to obtain

\[
D_{j_1 \ldots j_n}(y, t) = \frac{1}{n!} \int_{\mathbb{R}^n} \lim_{\tau \to 0} \left[ \frac{(y'_{j_1}(t + \tau) - y_{j_1}(t))}{\tau}
\right.
\]

\[
(y'_{j_2}(t + \tau) - y_{j_2}(t)) \cdots (y'_{j_n}(t + \tau) - y_{j_n}(t)) f(y', t + \tau | y, t) \left. \right] \, dy'.
\]

The time-derivative of \( X \) is prescribed by equation (1); hence the derivative of \( x_i \) with respect to time is equal to the velocity \( u_i \), i.e.

\[
\lim_{\tau \to 0} \frac{(x'_i(t + \tau) - x_i(t))}{\tau} = u_i(t)
\]

For the process \( Y = (X, U) \), the KME-coefficients \( D_{i_1 \ldots i_n}(x, u, t) \) for \( i = 1, 2, 3 \) (and thus all coefficients where at least one term refers to the position \( x \) are equal
Appendix

\[ D_{ij\ldots jn}(y,t) = \frac{1}{n!} u_i(t) \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \lim_{\tau \to 0} \left[ (y'_{j2}(t + \tau) - y_{j2}(t)) \ldots (y'_{jn}(t + \tau) - y_{jn}(t)) \right] p(y', t + \tau | y, t) \, dy'. \]

Accordingly, we find for \( n = 1 \) that

\[ D_i(x, u, t) = u_i(t) \quad \text{for} \quad i = 1, 2, 3 \]
\[ D_i(x, u, t) = D_{i \to 0}(u, t) \quad \text{for} \quad i = 4, 5, 6 \]

For \( n > 1 \), all coefficients including at least one spatial term are equal to zero because

\[ \lim_{\tau \to 0} (y'_{j}(t + \tau) - y_{j}(t)) = 0. \]

Rewriting the KME using these equalities results in the KME (2).

B Generating random vectors \( \Phi \) and \( \Psi \)

In Chapter 4, the motion of two particles in a turbulent flow is described. The particles are transported by the same turbulent flow, thus the trajectories are correlated if the particles are close together. This correlation is expressed in the computation of the particle paths by the vectors \( \Phi(X^{(1)}, X^{(2)}) \) and \( \Psi(X^{(1)}, X^{(2)}) \); the difference and sum of two correlated normally distributed random vectors.

In homogeneous isotropic turbulence the velocity correlation between the two particles is only determined by the distance between the particles, \( r = X^{(1)} - X^{(2)} \). Therefore, the random vectors \( \Phi \) and \( \Psi \) are normally distributed with mean equal to zero and variance equal to

\[ C_\Phi(X^{(1)}, X^{(2)}) = \sigma^2 \cdot I - C_u(r) \]
\[ C_\Psi(X^{(1)}, X^{(2)}) = \sigma^2 \cdot I + C_u(r) \]

where the matrix \( C_u(r) \) denotes the Eulerian velocity correlation between two points at distance \( r \). The elements of this matrix are given by

\[ (C_u(r))_{ij} = \sigma^2 \left( -0.5 \frac{r_i r_j}{r} \frac{\partial f}{\partial r} + \left( f(r) + 0.5 \frac{r_i}{r} \frac{\partial f}{\partial r} \right) \delta_{ij} \right). \]

See Chapter 4 for the derivation.

In general, a random three-dimensional vector from a normal distribution
Generating random vectors $\Phi$ and $\Psi$

with mean equal to $m$ and symmetric covariance equal to $C$, can be generated by computing three random numbers $v_1, v_2$ and $v_3$ from a unitary normal distribution (mean equal to zero, variance equal to one), $v_i \in \mathcal{N}(0,1)$. The vector $\mathbf{v} = (v_1, v_2, v_3)$ is a normally distributed vector with mean zero and variance matrix equal to identity. If the covariance matrix $C$ is symmetric and real-valued, then there is a diagonal matrix $\mathcal{D}$ and an orthogonal matrix $U$ ($U^T U = U U^T = I$), such that $C = U^T \mathcal{D} U$. This is called the orthogonal decomposition of $C$. The vector $\gamma$, resulting from the transformation $\gamma = U^T \sqrt{\mathcal{D}} \, \mathbf{v} + m$, is a random vector following a Gaussian distribution with mean equal to $m$ and covariance $C$.

Let us assume that the matrix $C$ can be written as sum of a diagonal matrix $\alpha I$ and a symmetric matrix, $\beta \mathcal{R}$, thus

$$C = \alpha I + \beta \mathcal{R}.$$  

If the orthogonal decomposition of the symmetric matrix $\mathcal{R}$ reads $\mathcal{R} = U^T \mathcal{D} U$ then the orthogonal decomposition of $C$ is given by

$$C = U^T (\alpha I + \beta \mathcal{D}) \, U. \quad (4)$$

Accordingly a normally distributed random vector $\gamma$ with mean $m$ and covariance $C$ which can be written as in equation (4), is computed from a vector $\mathbf{v} \in \mathcal{N}(0,1)$ by

$$\gamma = U^T \sqrt{\alpha I + \beta \mathcal{D}} \, \mathbf{v} + m.$$  

The covariance matrices of $\Phi$ and $\Psi$ can be written in the form

$$C_{\Phi} = \sigma^2 \left[ \left( 1 - f(r) - 0.5 \frac{\partial f}{\partial r} \right) I + 0.5 \frac{\partial f}{r \partial r} \mathcal{Q} \right]$$

$$C_{\Psi} = \sigma^2 \left[ \left( 1 + f(r) + 0.5 \frac{\partial f}{\partial r} \right) I - 0.5 \frac{\partial f}{r \partial r} \mathcal{Q} \right]$$

where $\mathcal{Q}$ is a symmetric matrix with elements

$$Q_{ij} = r_i \, r_j.$$  

An orthogonal decomposition of $\mathcal{Q}$ is given by the orthogonal matrix

$$U = \begin{pmatrix} -\frac{\hat{r}_2}{\hat{r}} & \frac{\hat{r}_1 \hat{r}_3}{\hat{r}} & \frac{\hat{r}_1}{\hat{r}} \\ \frac{\hat{r}_3}{\hat{r}} & \frac{\hat{r}_1 \hat{r}_2}{\hat{r}} & \frac{\hat{r}_2}{\hat{r}} \\ 0 & -\frac{\hat{r}_3}{\hat{r}} & \frac{\hat{r}_1 \hat{r}_3}{\hat{r}} \end{pmatrix}$$

where $\hat{r}$ stands for $\sqrt{(r_1)^2 + (r_2)^2}$. The diagonal matrix $\mathcal{D}$ of the decomposition consists of elements equal to the eigenvalues of $\mathcal{Q}$. The matrix $\mathcal{Q}$ has a double
eigenvalue equal to zero and the other eigenvalue is equal to $r^2$.

The orthogonal decompositions of $C_\psi$ and $C_\phi$ are thus given by

$$C_\phi = \sigma^2 u^T \left[ \left( 1 - f(r) - 0.5 r \frac{\partial f}{\partial r} \right) I + 0.5 \frac{1}{r} \frac{\partial f}{\partial r} D \right] u$$

$$C_\psi = \sigma^2 u^T \left[ \left( 1 + f(r) + 0.5 r \frac{\partial f}{\partial r} \right) I - 0.5 \frac{1}{r} \frac{\partial f}{\partial r} D \right] u.$$

In summary, the random vectors $\Phi$ and $\Psi$ can be generated from two random vectors $v_\phi \in N(0, 1)$ and $v_\psi \in N(0, 1)$. The vectors $\Psi$ and $\Phi$ are computed using

$$\Phi = u^T \sqrt{D_\phi} \ v_\phi$$

$$\Psi = u^T \sqrt{D_\psi} \ v_\psi$$

where $D_\phi$ and $D_\psi$ are diagonal matrices with elements equal to

$$(D_\phi)_{11} = (D_\phi)_{22} = \sigma^2 \left( 1 - f(r) - 0.5 r \frac{\partial f}{\partial r} \right)$$

$$(D_\phi)_{33} = \sigma^2 \left( 1 - f(r) \right)$$

and

$$(D_\psi)_{11} = (D_\psi)_{22} = \sigma^2 \left( 1 + f(r) + 0.5 r \frac{\partial f}{\partial r} \right)$$

$$(D_\psi)_{33} = \sigma^2 \left( 1 + f(r) \right).$$