Maxwellian and Gaussian distributions

by Alec Johnson, February 2011

In this note entropy decreases.

The Maxwellian and Gaussian distributions are the two working examples of Galilean-invariant *entropy-minimizing* closures for the equations of gas dynamics. The Maxwellian distribution is the assumed distribution of hyperbolic five-moment gas-dynamics (the compressible Euler equations). The Gaussian distribution is the assumed distribution of hyperbolic ten-moment gas-dynamics. A Maxwellian distribution is a normal distribution that is isotropic in the reference frame of the fluid. A Gaussian distribution is a distribution that in the reference frame of the fluid is a product of normal distributions with possibly different distribution widths in three principle orthogonal directions.

An entropy-minimizing closure (for a given set of moments) requires that particle distributions minimize entropy over all distributions which share the same given moments. Only variation in velocity is considered, not variation in space. This is consonant with the fact that collision operators ignore variation of particle density in space and only consider variation in velocity space. Thus in this document we ignore variation in space.

Definitions of conserved moments. Let $f(t, \mathbf{v})$ be the distribution of particle mass over velocity space.

$$\begin{aligned}
\rho &:= \int_{\mathbf{v}} f && \text{is mass (density)},\\
\mathbf{M} &:= \int_{\mathbf{v}} f\mathbf{v} && \text{is momentum (density)},\\
\mathcal{E} &:= \int_{\mathbf{v}} f\mathbf{v}^2/2 && \text{is energy (density)},\\
\mathbb{E} &:= \int_{\mathbf{v}} f\mathbf{v}\mathbf{v} && \text{is energy tensor (density)},
\end{aligned}$$

Definitions of statistical averages. Let $\chi(\mathbf{v})$ be a "generic" moment. Denote and define its statistical average by

$$\langle \chi \rangle := \frac{\int_{\mathbf{v}} f\chi}{\rho}.$$

Primitive variables are naturally defined in terms of statistical averages:

$$\begin{aligned}
\mathbf{u} &:= \langle \mathbf{v} \rangle && \text{is bulk velocity},\\
\mathbf{c} &:= \mathbf{v} - \mathbf{u} && \text{is thermal velocity},\\
\Theta &:= \langle \mathbf{c}\mathbf{c} \rangle && \text{is “temperature” tensor, and}\\
\theta &:= \langle c^2/3 \rangle && \text{is “temperature”}.
\end{aligned}$$

Relationships among primitive and conserved variables are

$$\begin{aligned}
\rho\mathbf{u} &= \mathbf{M},\\
\mathcal{E} &= (\rho\mathbf{u}^2 + 3\rho\theta)/2,\\
\mathbb{E} &= \rho\mathbf{u}\mathbf{u} + \rho\Theta,\\
\theta &= \operatorname{tr}\Theta/3,\\
\mathcal{E} &= \operatorname{tr}\mathbb{E}/3.
\end{aligned}$$

Recall that entropy S is defined by

$$\begin{aligned}
\eta &:= f\ln f + \alpha f,\\
S &:= \int_{\mathbf{v}} \eta,
\end{aligned}$$

where α is a constant that can be freely chosen; we will choose $\alpha = 3(\ln(2\pi) + 1)/2$ to make the formula for the gas-dynamic entropy simple. Note that

$$\eta' = \ln f + (1 + \alpha).$$

1 Maxwellian case

In the Maxwellian case we minimize S subject to the constraints that

$$\int_{\mathbf{v}} f = \rho, \qquad \int_{\mathbf{v}} \mathbf{v} f = \mathbf{M}, \qquad \int_{\mathbf{v}} \mathbf{v}^2 f = 2\mathcal{E}.$$

We use the technique of Lagrange multipliers. Define

$$\begin{aligned}
g := \int_{\mathbf{v}} \eta + \lambda\left(\rho - \int_{\mathbf{v}} f\right) + \mu\cdot\left(\mathbf{M} - \int_{\mathbf{v}} \mathbf{v} f\right)\\
+ \nu\left(2\mathcal{E} - \int_{\mathbf{v}} \mathbf{v}^2 f\right).
\end{aligned}$$

Assume f minimizes entropy. Consider a perturbation $\tilde{f} = f + \epsilon f_1$. Then

$$\begin{aligned}
0 &= d_\epsilon g|_{\epsilon=0}\\
&= \int_{\mathbf{v}} \eta' f_1 - \lambda \int_{\mathbf{v}} f_1 - \mu\cdot\int_{\mathbf{v}} \mathbf{v} f_1 - \nu \int_{\mathbf{v}} \mathbf{v}^2 f_1\\
&= \int_{\mathbf{v}} f_1 \left(\log f - \tilde{\lambda} - \mu\cdot\mathbf{v} - \nu\mathbf{v}^2\right),
\end{aligned}$$

where $\tilde{\lambda} := \lambda - \alpha - 1$. Since the integral must be zero for arbitrary perturbation f_1 the multiplier of f_1 in the integrand must be zero. Thus, f must be an exponential of an "isotropic" quadratic polynomial in $\mathbf{v}$:

$$f = \exp\left(\tilde{\lambda} + \mu\cdot\mathbf{v} + \nu\mathbf{v}^2\right). \tag{1}$$

We impose the finiteness requirement that $\int_{\mathbf{v}} f < \infty$; that is, $\nu < 0$.

It remains to compute the moments of such a polynomial so that we can match them up with the constrained moments. We will show that

$$\boxed{f = \frac{\rho}{(2\pi\theta)^{3/2}} \exp\left(\frac{-|\mathbf{v}-\mathbf{u}|^2}{2\theta}\right)}.$$

It is evident by completing the square that any exponential of a quadratic polynomial in $\mathbf{v}$ of the form (1) can be put in this form. The issue is whether we indeed have that $\rho = \int_{\mathbf{v}} f$, $\rho\mathbf{u} := \int_{\mathbf{v}} \mathbf{v}f$, and $\rho\theta := \int_{\mathbf{v}} f\mathbf{c}^2/2$. So it remains to confirm these moments by computation.

Shifting into the reference from of the fluid,

$$f = \frac{\rho}{(2\pi\theta)^{3/2}} \exp\left(\frac{-\mathbf{c}^2}{2\theta}\right).$$

It will be enough to show that:

$$\int_{\mathbf{c}} f = \rho,$$
$$\int_{\mathbf{c}} \mathbf{c}f = 0,$$
$$\int_{\mathbf{c}} c^2 f = 3\rho\theta.$$

Recall how to integrate a Gaussian normal distribution:

$$\begin{aligned}
&\int_{-\infty}^{\infty} e^{-x^2/2}\,dx \int_{-\infty}^{\infty} e^{-y^2/2}\,dy \\
&= \int_0^{2\pi}\int_0^{\infty} e^{-r^2/2} r\,dr\,d\theta \\
&= 2\pi\left[e^{-r^2/2}\right]_{\infty}^{0} \\
&= 2\pi,
\end{aligned}$$

so

$$\int_{-\infty}^{\infty} e^{-x^2/2}\,dx = \sqrt{2\pi}$$

so

$$\boxed{\int_{-\infty}^{\infty} \exp\left(\frac{-x^2}{2T}\right)\,dx = \sqrt{2\pi T}}.$$

The first moment is zero by even-odd symmetry:

$$\boxed{\int_{-\infty}^{\infty} x\exp\left(\frac{-x^2}{2T}\right)\,dx = 0}.$$

For the temperature we will need second moments. Integrating by parts,

$$\begin{aligned}
&\int_{-\infty}^{\infty} x^2\exp\left(\frac{-x^2}{2}\right)\,dx \\
&= \int_{-\infty}^{\infty} x\left(x\exp\left(\frac{-x^2}{2}\right)\right)\,dx \\
&= \int_{-\infty}^{\infty} \exp\left(\frac{-x^2}{2}\right)\,dx \\
&= \sqrt{2\pi}
\end{aligned}$$

So

$$\boxed{\int_{-\infty}^{\infty} x^2\exp\left(\frac{-x^2}{2T}\right)\,dx = T\sqrt{2\pi T}}.$$

For density we verify that

$$\int_{\mathbf{c}} \exp\left(\frac{-\mathbf{c}^2}{2\theta}\right) d^3\mathbf{c} = (2\pi\theta)^{3/2}.$$

For momentum we compute that

$$\int_{\mathbf{c}} c_1 \exp\left(\frac{-\mathbf{c}^2}{2\theta}\right) d^3\mathbf{c} = 0$$

by even/odd symmetry.

For temperature we compute that

$$\begin{aligned}
&\int_{\mathbf{c}} c^2\exp\left(\frac{-c^2}{2\theta}\right) \\
&= \int_{c_1} c_1^2\exp\left(\frac{-c_1^2}{2\theta}\right)\int_{c_2} c_2^2\exp\left(\frac{-c_2^2}{2\theta}\right)\int_{c_3} c_3^2\exp\left(\frac{-c_3^2}{2\theta}\right) \\
&= 3\theta\sqrt{2\pi\theta}.
\end{aligned}$$

Maxwellian distributions have the property that the heat flux $\mathbf{q} := \int_{\mathbf{c}} \mathbf{c}c^2 f$ is zero. Indeed,

$$\mathbf{q} = \int_{\mathbf{c}} \mathbf{c}c^2\exp\left(\frac{-c^2}{2\theta}\right) = 0,$$

because the integrand is odd.

2 Gaussian case

In the Gaussian case we minimize S subject to the constraints that

$$\int_{\mathbf{v}} f = \rho, \qquad \int_{\mathbf{v}} \mathbf{v}f = \mathbf{M}, \qquad \int_{\mathbf{v}} \mathbf{v}\mathbf{v}f = \mathbb{E}.$$

We use the technique of Lagrange multipliers. Define

$$\begin{aligned}
g := \int_{\mathbf{v}} \eta + \lambda\left(\rho - \int_{\mathbf{v}} f\right) + \mu\cdot\left(\mathbf{M} - \int_{\mathbf{v}} \mathbf{v}f\right) \\
+ \nu\left(\mathbb{E} - \int_{\mathbf{v}} \mathbf{v}\mathbf{v}f\right).
\end{aligned}$$

Assume f minimizes entropy. Consider a perturbation $\tilde{f} = f + \epsilon f_1$. Then

$$\begin{aligned}
0 &= d_\epsilon g|_{\epsilon=0} \\
&= \int_{\mathbf{v}} \eta' f_1 - \lambda\int_{\mathbf{v}} f_1 - \mu\cdot\int_{\mathbf{v}} \mathbf{v}f_1 - \nu : \int_{\mathbf{v}} \mathbf{v}\mathbf{v}f_1 \\
&= \int_{\mathbf{v}} f_1\left(\log f - \tilde{\lambda} - \mu\cdot\mathbf{v} - \nu : \mathbf{v}\mathbf{v}\right).
\end{aligned}$$

Since the integral must be zero for arbitrary perturbation f_1 the multiplier of f_1 in the integrand must be zero. Thus, f must be an exponential of a quadratic polynomial in $\mathbf{v}$:

$$f = \exp\left(\lambda + \mu \cdot \mathbf{v} + \nu : \mathbf{vv}\right). \tag{2}$$

We may require that ν is symmetric. We impose the finiteness requirement that $\int_{\mathbf{v}} f < \infty$; that is, $\nu < 0$, i.e., ν is negative definite.

We will show that

$$f = \frac{\rho}{\sqrt{\det(2\pi\Theta)}} \exp\left(-(\mathbf{v}-\mathbf{u})\cdot\Theta^{-1}\cdot(\mathbf{v}-\mathbf{u})/2\right).$$

That is (shifting into the reference frame of the fluid),

$$\boxed{f = \frac{\rho}{\sqrt{\det(2\pi\Theta)}} \exp\left(-\mathbf{c}\cdot\Theta^{-1}\cdot\mathbf{c}/2\right)},$$

where recall that $\mathbf{c} := \mathbf{v} - \mathbf{u}$.

By substituting the expansion $(\mathbf{v}-\mathbf{u})\cdot\Theta^{-1}\cdot(\mathbf{v}-\mathbf{u}) = \Theta^{-1} : \mathbf{vv} - 2\mathbf{u}\cdot\Theta^{-1}\cdot\mathbf{v} + \mathbf{u}\cdot\Theta^{-1}\cdot\mathbf{u}$ and matching up with the terms in (2), it is evident that we can complete the square to put any entropy-minimizing closure in this form.

The issue is whether we indeed have that $\rho = \int_{\mathbf{v}} f$, $\rho\mathbf{u} := \int_{\mathbf{v}} \mathbf{v}f$, and $\rho\theta := \int_{\mathbf{v}} f\mathbf{cc}$.

It will be enough to show that

$$\int_{\mathbf{c}} f = \rho, \qquad \int_{\mathbf{c}} \mathbf{c}f = 0, \qquad \int_{\mathbf{c}} \mathbf{cc}f = \rho\Theta.$$

Since Θ is positive definite we may choose orthogonal coordinates in which it is diagonal. So without loss of generality $\Theta = \operatorname{diag}(T_1, T_2, T_3)$.

For the momentum we compute that

$$\begin{aligned}
&\int_{\mathbf{c}} c_1 \exp\left(-\mathbf{c}\cdot\Theta^{-1}\cdot\mathbf{c}/2\right) \\
&= \int_{c_1} c_1 \exp\left(\frac{-c_1^2}{2T_1}\right) \int_{c_2} \exp\left(\frac{-c_2^2}{2T_2}\right) \int_{c_3} \exp\left(\frac{-c_3^2}{2T_3}\right) \\
&= 0.
\end{aligned}$$

For the density we compute that

$$\begin{aligned}
&\int_{\mathbf{c}} \exp\left(-\mathbf{c}\cdot\Theta^{-1}\cdot\mathbf{c}/2\right) \\
&= \int_{c_1} \exp\left(\frac{-c_1^2}{2T_1}\right) \int_{c_2} \exp\left(\frac{-c_2^2}{2T_2}\right) \int_{c_3} \exp\left(\frac{-c_3^2}{2T_3}\right) \\
&= \sqrt{2\pi T_1}\sqrt{2\pi T_2}\sqrt{2\pi T_3} \\
&= \sqrt{\det(2\pi\Theta)}.
\end{aligned}$$

For the temperature we compute that

$$\begin{aligned}
&\int_{\mathbf{c}} c_1^2 \exp\left(-\mathbf{c}\cdot\Theta^{-1}\cdot\mathbf{c}/2\right) \\
&= \int_{c_1} c_1^2 \exp\left(\frac{-c_1^2}{2T_1}\right) \int_{c_2} \exp\left(\frac{-c_2^2}{2T_2}\right) \int_{c_3} \exp\left(\frac{-c_3^2}{2T_3}\right) \\
&= T_1\sqrt{2\pi T_1}\sqrt{2\pi T_2}\sqrt{2\pi T_3} \\
&= T_1\sqrt{\det(2\pi\Theta)}
\end{aligned}$$

and that

$$\begin{aligned}
&\int_{\mathbf{c}} c_1 c_2 \exp\left(-\mathbf{c}\cdot\Theta^{-1}\cdot\mathbf{c}/2\right) \\
&= \int_{c_1} c_1 \exp\left(\frac{-c_1^2}{2T_1}\right) \int_{c_2} c_2 \exp\left(\frac{-c_2^2}{2T_2}\right) \int_{c_3} \exp\left(\frac{-c_3^2}{2T_3}\right) \\
&= 0.
\end{aligned}$$

Gaussian distributions have the property that the heat flux tensor $\mathbf{q} := \int_{\mathbf{c}} \mathbf{ccc}f$ is zero (because for any component at least one of the three independent integrals has an odd integrand). (A trivial corrolary is that for both Maxwellian and Guassian distributions both the heat flux tensor and the heat flux are zero.)

3 Expressions for entropy.

Now that we have found the distribution that minimizes entropy, what is the entropy?

Recall the Gaussian distribution,

$$\mathcal{G} = \frac{\rho}{\sqrt{\det(2\pi\Theta)}} \exp\left(\frac{-\mathbf{c}\cdot\Theta^{-1}\cdot\mathbf{c}}{2}\right).$$

By definition the entropy of the Gaussian distribution is

$$S = \int_{\mathbf{c}} \mathcal{G}\ln\mathcal{G} + \alpha\mathcal{G}.$$

By definition,

$$\int_{\mathbf{c}} \mathcal{G} = \rho.$$

Observe that

$$\ln\mathcal{G} = \ln\left(\frac{\rho}{\sqrt{\det(2\pi\Theta)}}\right) + \frac{-\mathbf{c}\cdot\Theta^{-1}\cdot\mathbf{c}}{2}.$$

To compute $\int_{\mathbf{c}} \mathcal{G}\ln\mathcal{G}$ the main result we need is:

$$\int_{\mathbf{c}} \left(\mathbf{c}\cdot\Theta^{-1}\cdot\mathbf{c}\right)\mathcal{G} = 3\rho.$$

To verify this claim, choose coordinates in which Θ is diagonal. By definition of θ_i,

$$\int_{\mathbf{c}} (c_i)^2\mathcal{G} = \theta_i\rho, \quad \text{i.e.,} \quad \int_{\mathbf{c}} \left(c_i\theta_i^{-1}c_i\right)\mathcal{G} = \rho.$$

Summing over all three dimensions yields the claim.

We now compute the entropy:

$$\begin{aligned} S &= \int_{\mathbf{c}} \mathcal{G} \ln \mathcal{G} + \alpha \mathcal{G} \\ &= \rho \ln \left(\frac{\rho}{\sqrt{\det(2\pi\Theta)}} \right) - \frac{3}{2}\rho + \alpha\rho. \\ &= -\rho \ln \left(\frac{\sqrt{\det(\Theta)}}{\rho} \right) + \rho \left(\alpha - \frac{3}{2} - \frac{3}{2}\ln(2\pi) \right). \end{aligned}$$

That is,

$$\boxed{S = -\rho \ln \left(\frac{\sqrt{\det(\Theta)}}{\rho} \right)}$$

if we choose $\alpha = 3\,(1 + \ln(2\pi))\,/2$.

The five-moment formula is a special case:

$$\boxed{S = -\rho \ln \left(\frac{\theta^{3/2}}{\rho} \right)}.$$

4 Number density

Hitherto f has represented mass density. Let $\widetilde{f}$ denote particle number density. Then $\widetilde{f} = f/m$, where m is particle mass. We define $n := \int_{\mathbf{v}} \widetilde{f} = \rho/m$ to be the number density. So the boxed expressions for particle distributions become

$$\boxed{\widetilde{\mathcal{G}} = \frac{n}{(2\pi\theta)^{3/2}} \exp\left(\frac{-|\mathbf{v}-\mathbf{u}|^2}{2\theta} \right)}$$

for the 5-moment distribution and

$$\boxed{\widetilde{\mathcal{G}} = \frac{n}{\sqrt{\det(2\pi\Theta)}} \exp\left(\frac{-\mathbf{c}\cdot\Theta^{-1}\cdot\mathbf{c}}{2} \right)}$$

for the 10-moment distribution.

The true temperature $T = m\langle \mathbf{c}^2 \rangle/3$ is related to the scalar pressure $p = \rho\langle \mathbf{c}^2 \rangle/3$ and to the pseudo-temperature $\theta := \langle \mathbf{c}^2 \rangle/3$ by the relations

$$nT = p = \rho\theta, \qquad \text{i.e.,} \qquad \theta = T/m.$$

The true temperature tensor $\mathbb{T} := m\langle \mathbf{cc} \rangle$ is related to the pressure tensor $\mathbb{P} = \rho\langle \mathbf{cc} \rangle$ and to the pseudo temperature tensor $\Theta := \langle \mathbf{cc} \rangle$ by the relations

$$n\mathbb{T} = \mathbb{P} = \rho\Theta, \qquad \text{i.e.,} \qquad \Theta = \mathbb{T}/m.$$

Note that

$$\langle \chi \rangle = \frac{\int_{\mathbf{v}} f\chi}{\rho} = \frac{\int_{\mathbf{v}} \widetilde{f}\chi}{n}.$$

5 Consistent entropy for interacting species

For a gas with multiple species we should define the entropy of each species consistently so that the total entropy obeys an entropy inequality when species interact. For such a consistent entropy we define the true entropy of each species in terms of the number density rather than the mass density:

$$\widetilde{\eta} := \widetilde{f} \ln \widetilde{f} + \widetilde{\alpha}\widetilde{f}, \qquad \widetilde{S} := \int_{\mathbf{v}} \widetilde{\eta}.$$

(In this section the casual reader may regard blue text as an arbitrary irrelevant constant.) Since $\widetilde{f} = m^{-1} f$,

$$\begin{aligned} \widetilde{\eta} &= \widetilde{f} \ln(m^{-1} f) + \widetilde{\alpha}\widetilde{f} \\ &= m^{-1}\eta + (\ln m^{-1} + \widetilde{\alpha} - \alpha)\widetilde{f}. \end{aligned}$$

So

$$\begin{aligned} \widetilde{S} &= \int_{\mathbf{v}} \widetilde{\eta} = \int_{\mathbf{v}} m^{-1}\eta + (\ln m^{-1} + \widetilde{\alpha} - \alpha)\widetilde{f} \\ &= m^{-1} S + (\ln m^{-1} + \widetilde{\alpha} - \alpha) n. \end{aligned}$$

Recall that for $f = \mathcal{G}$,

$$S = -\rho \ln \left(\frac{\sqrt{\det(\Theta)}}{\rho} \right) + \rho \left(\alpha - \frac{3}{2} - \frac{3}{2}\ln(2\pi) \right).$$

So for $\widetilde{f} = \widetilde{\mathcal{G}}$,

$$\begin{aligned} \widetilde{S} &= -\,n \ln \left(\frac{\sqrt{\det(\Theta)}}{\rho} \right) + n \left(\alpha - \frac{3}{2} - \frac{3}{2}\ln(2\pi) \right) \\ &\quad + n \left(\ln m^{-1} + \widetilde{\alpha} - \alpha \right) \\ &= -\,n \ln \left(\frac{\sqrt{\det(\mathbb{T})}}{n} \right) \\ &\quad + n \left(\widetilde{\alpha} + \frac{3}{2}\ln m - \frac{3}{2} - \frac{3}{2}\ln(2\pi) \right). \end{aligned}$$

That is, a consistently defined ten-moment entropy is

$$\boxed{S_{\mathcal{G}} := -n \ln \left(\frac{\sqrt{\det(\mathbb{T})}}{n} \right)},$$

where we define the ten-moment entropy of a distribution to be the entropy it would have if it were relaxed to minimum entropy without changing the first 10 gas-dynamic moments and where we have chosen $\widetilde{\alpha} = \frac{3}{2}\,(1 + \ln(2\pi/m))$.

As a special case a consistently defined five-moment entropy is:

$$\boxed{S_{\mathcal{M}} = -n \ln \left(\frac{T^{3/2}}{n} \right)},$$

where we define the five-moment entropy of a distribution to be the entropy it would have if it were relaxed to minimum entropy without changing the five conserved moments.