Technical Report (27.08.2012)
Technische Universität München

Probability Distributions for Gradient Directions in Uncertain 3D Scalar Fields

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Abstract

This report introduces a mathematical framework to compute probability density functions for the directions of gradients in Gaussian distributed uncertain 3D scalar fields, and illustrates results by means of several examples.

1 Introduction

The geometry of salient features - prominent structures indicated by strong gradients, such as bounding surfaces, and isocontours - in uncertain 3D scalar fields is stable only to some extent. In order to analyze the stability of the direction of features in scalar fields, we need to investigate the variability of derived vector fields that reveal the uncertainty in direction of these features, such as gradient fields. Gradients at spatial points of a scalar field indicate at every location the direction of the greatest rate of increase of the scalar field, the magnitude giving the rate of increase. A significant change in the values of the scalar field results in a strong gradient magnitude, while the direction of the gradient shows the direction of the greatest change. The gradient direction can thus give further insight into the stability of orientations of features. Nonetheless, in the context of uncertain scalar fields, derived quantities such as gradients are also affected by uncertainty, investigating the gradient variability being thus consequential in addressing the stability of orientations of possible features in uncertain scalar fields.

In situations where the uncertainty of scalar values in scalar fields is completely characterized by the mean and covariance parameters, of which the standard model is the multivariate Gaussian distribution, a closed-form derivation of the probabilty density function of the gradient direction is possible. The gradients at spatial points of a Gaussian distributed scalar field, being obtained by applying a linear operator to stencils of neighbors of the points in the scalar field, can be shown to follow a Gaussian distribution as well. This also holds for any other vector fields that can be obtained similarly. Thus, the uncertainty of the gradients (and other such vector fields) can be modeled via mean and covariance as well. However, such a distribution describes the combined uncertainty of both the gradient magnitude and direction. As we are interested only in the direction uncertainty, we seek to isolate the latter from the gradient strength, by switching from the Cartesian to the spherical coordinate system. This allows us to perform analyses in terms of directions in space, i.e., positions on a sphere, where, by integrating over the radial distance, we are left with positions on the unit sphere, i.e., the direction uncertainty. The rest of the report details the derivation of the probability density functions of gradient directions and uses several examples to illustrate different probability density functions.

2 Derivation

Throughout the paper, we assume a discrete sampling of a 3D domain on a Cartesian grid structure with grid points $\mathbb{S}_{m,n,p} = \{\mathbf{x}_{i,j,k} : 1 \le i \le m, 1 \le j \le n, 1 \le k \le p\}$. The data uncertainty at every point is modeled by a multivariate random variable $\mathbf{Y}$ with scalar-valued components $Y(\mathbf{x}_{i,j,k})$. We further suppose that the random variables follow a *multivariate Gaussian distribution*, so that the distribution at point $\mathbf{x}_{i,j,k}$ is characterized by a mean value $\mu(\mathbf{x}_{i,j,k})$ and a standard deviation $\sigma(\mathbf{x}_{i,j,k})$. Moreover, the correlation values between any pair of random variables, $\rho(Y(\mathbf{x}_{i,j,k}), Y(\mathbf{x}_{u,v,t}))$, can be computed.

The probability density function for the gradient at the grid points of a trivariate Gaussian distributed 3D scalar field can be determined by first approximating the gradient via a linear operator, and then using this operator to approximate the uncertainty parameters from the corresponding uncertainty parameters of the points in the scalar field.

The gradient at a point $\mathbf{x}_{i,j,k}$ can be approximated via central differences (one-sided differences at the domain boundaries) on the random variables as

$$\nabla Y(\mathbf{x}_{i,j,k}) = \mathbf{A}\mathbf{s}(\mathbf{x}_{i,j,k}).$$

Here, the 6-element stencil $\mathbf{s}$ contains the random variables

$$\mathbf{s}(\mathbf{x}_{i,j,k}) = [Y(\mathbf{x}_{i+1,j,k}), Y(\mathbf{x}_{i-1,j,k}), Y(\mathbf{x}_{i,j+1,k}), Y(\mathbf{x}_{i,j-1,k}), Y(\mathbf{x}_{i,j,k+1}), Y(\mathbf{x}_{i,j,k-1})]^\top$$

and the 3×6 matrix $\mathbf{A}$ contains the inverse point distances

$$\mathbf{A}_{1,1} = \left\|\mathbf{x}_{i+1,j,k} - \mathbf{x}_{i-1,j,k}\right\|^{-1}, \mathbf{A}_{1,2} = -\mathbf{A}_{1,1}, \mathbf{A}_{2,3} = \left\|\mathbf{x}_{i,j+1,k} - \mathbf{x}_{i,j-1,k}\right\|^{-1}, \mathbf{A}_{2,4} = -\mathbf{A}_{2,3}, \mathbf{A}_{3,5} = \left\|\mathbf{x}_{i,j,k+1} - \mathbf{x}_{i,j,k-1}\right\|^{-1},$$
$$\mathbf{A}_{3,6} = -\mathbf{A}_{3,5}, \mathbf{A}_{1,3} = \mathbf{A}_{1,4} = \mathbf{A}_{1,5} = \mathbf{A}_{1,6} = \mathbf{A}_{2,1} = \mathbf{A}_{2,2} = \mathbf{A}_{2,5} = \mathbf{A}_{2,6} = \mathbf{A}_{3,1} = \mathbf{A}_{3,2} = \mathbf{A}_{3,3} = \mathbf{A}_{3,4} = 0.$$

Since the stencil $\mathbf{s}(\mathbf{x}_{i,j,k})$ forms a 6-component subset of the multivariate random variable $\mathbf{Y}$, its probability distribution is multivariate Gaussian as well. Furthermore, due to the linear relation between ∇Y and $\mathbf{s}$, the gradient also follows a *trivariate* Gaussian distribution. In order to fully describe this distribution, we first need to compute the mean gradient μ_∇ and the covariance matrix Σ_∇ of ∇Y, which relate to the means and covariances of the random variables via

$$\mu_\nabla(\mathbf{x}_{i,j,k}) = \mathbf{A}\mu_\mathbf{s}(\mathbf{x}_{i,j,k}), \, \Sigma_\nabla = \mathbf{A}\Sigma_\mathbf{s}\mathbf{A}^\top,$$

where the q-th component of $\mu_\mathbf{s}(\mathbf{x}_{i,j,k})$ contains the mean of the q-th component of $\mathbf{s}(\mathbf{x}_{i,j,k})$, $(\mu_\mathbf{s}(\mathbf{x}_{i,j,k}))_q = \mu(\mathbf{s}(\mathbf{x}_{i,j,k})_q)$, and the covariance matrix of the random stencil vector $\Sigma_\mathbf{s}$ has components $(\Sigma_{\mathbf{s}(\mathbf{x_{i,j,k}})})_{m,n} = \sigma(\mathbf{s}(\mathbf{x}_{i,j,k})_m)\sigma(\mathbf{s}(\mathbf{x}_{i,j,k})_n)\rho(\mathbf{s}(\mathbf{x}_{i,j,k})_m, \mathbf{s}(\mathbf{x}_{i,j,k})_n)$.

From the given mean gradient and covariance matrix, the trivariate probability density function of ∇Y for a vector $\mathbf{g}$ is then derived as

$$p_\nabla(\mathbf{g}) = \frac{1}{\sqrt{(2\pi)^3 \det \Sigma_\nabla}} \exp\left(-0.5(\mathbf{g} - \mu_\nabla)^\top \Sigma_\nabla^{-1}(\mathbf{g} - \mu_\nabla)\right),$$

where expanding the determinant of the gradient covariance matrix yields

$$\det \Sigma_\nabla = \sigma_{\nabla x}^2 \sigma_{\nabla y}^2 \sigma_{\nabla z}^2 \left(1 + 2\rho_{\nabla xy}\rho_{\nabla xz}\rho_{\nabla yz} - (\rho_{\nabla xy}^2 + \rho_{\nabla xz}^2 + \rho_{\nabla yz}^2)\right),$$

while the inverse of the matrix can be written as

$$\Sigma_\nabla^{-1} = \frac{\sigma_{\nabla x}\sigma_{\nabla y}\sigma_{\nabla z}}{\det \Sigma_\nabla} \begin{pmatrix} \frac{\sigma_{\nabla y}\sigma_{\nabla z}}{\sigma_{\nabla x}}\left(1 - \rho_{\nabla yz}^2\right) & \sigma_{\nabla z}(\rho_{\nabla xz}\rho_{\nabla yz} - \rho_{\nabla xy}) & \sigma_{\nabla y}(\rho_{\nabla xy}\rho_{\nabla yz} - \rho_{\nabla xz}) \\ \sigma_{\nabla z}(\rho_{\nabla xz}\rho_{\nabla yz} - \rho_{\nabla xy}) & \frac{\sigma_{\nabla x}\sigma_{\nabla z}}{\sigma_{\nabla y}}\left(1 - \rho_{\nabla xz}^2\right) & \sigma_{\nabla x}(\rho_{\nabla xy}\rho_{\nabla xz} - \rho_{\nabla yz}) \\ \sigma_{\nabla y}(\rho_{\nabla xy}\rho_{\nabla yz} - \rho_{\nabla xz}) & \sigma_{\nabla x}(\rho_{\nabla xy}\rho_{\nabla xz} - \rho_{\nabla yz}) & \frac{\sigma_{\nabla x}\sigma_{\nabla y}}{\sigma_{\nabla z}}\left(1 - \rho_{\nabla xy}^2\right) \end{pmatrix}.$$

A similar procedure can be performed for other derived vector fields that can be obtained by applying a linear operator.

In the formula above, p_∇ describes the probability that the gradient takes on a given magnitude and direction, comprising the uncertainty of the gradient in both strength and orientation. For extracting only the *direction uncertainty*, the density function is transformed into spherical coordinates

$$p_\nabla(\theta, \phi, r) = \frac{r^2 \sin\theta}{\sqrt{(2\pi)^3 \det \Sigma_\nabla}} \exp\left(E(\theta, \phi)\right) \;,\; \theta \in [0, \pi], \;\; \phi \in [0, 2\pi], \;\; r \in [0, \infty[$$
$$E(\theta, \phi) = \left(-\frac{1}{2}\left(r\begin{pmatrix}\sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta\end{pmatrix} - \mu_\nabla\right)^\top \Sigma_\nabla^{-1}\left(r\begin{pmatrix}\sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta\end{pmatrix} - \mu_\nabla\right)\right).$$

The probability density function for the gradient direction is given by the θ, ϕ-marginal

$$p_\nabla^{\theta,\phi}(\theta, \phi) = \int_0^\infty p_\nabla(\theta, \phi, r)\,\mathrm{d}r \;,\; \theta \in [0, \pi], \;\; \phi \in [0, 2\pi].$$

For every pair of angles (θ,ϕ), a probability value is obtained by integrating the trivariate gradient density along a line from $r = 0$ to $r = \infty$.

In order to derive the formula for the probability density function of the gradient direction, we first rewrite the θ, ϕ-marginal as

$$p_\nabla^{\theta,\phi}(\theta, \phi) = C\int_0^\infty r^2 \exp\left(-(ar^2 - 2br + c)\right)\mathrm{d}r,$$

with the constants

$$a = \frac{1}{2\det\Sigma_\nabla}\Bigg((\sin\theta)^2\sigma_{\nabla z}^2\left((\cos\phi)^2\sigma_{\nabla y}^2(1-\rho_{\nabla yz}^2)+(\sin\phi)^2\sigma_{\nabla x}^2(1-\rho_{\nabla xz}^2)\right)+(\cos\theta)^2\sigma_{\nabla x}^2\sigma_{\nabla y}^2(1-\rho_{\nabla xy}^2)+2\sigma_{\nabla x}\sigma_{\nabla y}\sigma_{\nabla z}\cdot$$
$$\Big(\sin\theta\cos\theta\big(\cos\phi\,\sigma_{\nabla y}(\rho_{\nabla xy}\rho_{\nabla yz}-\rho_{\nabla xz})+\sin\phi\,\sigma_{\nabla x}(\rho_{\nabla xy}\rho_{\nabla xz}-\rho_{\nabla yz})\big)+(\sin\theta)^2\sin\phi\cos\phi\,\sigma_{\nabla z}(\rho_{\nabla xz}\rho_{\nabla yz}-\rho_{\nabla xy})\Big)\Bigg),$$

$$b = \frac{1}{2\det\Sigma_\nabla}\Bigg(\sigma_{\nabla x}\sigma_{\nabla y}\sigma_{\nabla z}\Big(\sin\theta\,\sigma_{\nabla z}(\rho_{\nabla xz}\rho_{\nabla yz}-\rho_{\nabla xy})(\sin\phi\,\mu_{\nabla x}+\cos\phi\,\mu_{\nabla y})+\sigma_{\nabla y}(\rho_{\nabla xy}\rho_{\nabla yz}-\rho_{\nabla xz})(\sin\theta\cos\phi\,\mu_{\nabla z}+$$
$$\cos\theta\,\mu_{\nabla x})+\sigma_{\nabla x}(\rho_{\nabla xy}\rho_{\nabla xz}-\rho_{\nabla yz})(\cos\theta\,\mu_{\nabla y}+\sin\theta\sin\phi\,\mu_{\nabla z})\Big)+\cos\theta\,\mu_{\nabla z}\sigma_{\nabla x}^2\sigma_{\nabla y}^2(1-\rho_{\nabla xy}^2)+\sin\theta\,\sigma_{\nabla z}^2\Big(\cos\phi\,\mu_{\nabla x}\sigma_{\nabla y}^2\cdot$$
$$(1-\rho_{\nabla yz}^2)+\sin\phi\,\mu_{\nabla y}\sigma_{\nabla x}^2(1-\rho_{\nabla xz}^2)\Big)\Bigg),$$

$$c = \frac{1}{2\det\Sigma_\nabla}\Bigg(2\sigma_{\nabla x}\sigma_{\nabla y}\sigma_{\nabla z}\Big(\mu_{\nabla x}\mu_{\nabla y}\sigma_{\nabla z}(\rho_{\nabla xz}\rho_{\nabla yz}-\rho_{\nabla xy})+\mu_{\nabla x}\mu_{\nabla z}\sigma_{\nabla y}(\rho_{\nabla xy}\rho_{\nabla yz}-\rho_{\nabla xz})+\mu_{\nabla y}\mu_{\nabla z}\sigma_{\nabla x}(\rho_{\nabla xy}\rho_{\nabla xz}-\rho_{\nabla yz})\Big)+$$
$$\sigma_{\nabla z}^2\left(\mu_{\nabla x}^2\sigma_{\nabla y}^2(1-\rho_{\nabla yz}^2)+\mu_{\nabla y}^2\sigma_{\nabla x}^2(1-\rho_{\nabla xz}^2)\right)+\mu_{\nabla z}^2\sigma_{\nabla x}^2\sigma_{\nabla y}^2(1-\rho_{\nabla xy}^2)\Bigg),$$

$$C = \frac{\sin\theta}{\sqrt{(2\pi)^3\det\Sigma_\nabla}}.$$

It follows that

$$p_\nabla^{\theta,\phi}(\theta,\phi) = C\int_0^\infty r^2\exp\left(-(ar^2-2br+c)\right)\mathrm{d}r = C\exp\left(\frac{b^2}{a}-c\right)\int_0^\infty r^2\exp\left(-\left(\sqrt{a}r-\frac{b}{\sqrt{a}}\right)^2\right)\mathrm{d}r,$$

whereby the change of variables $\sqrt{a}r-b/\sqrt{a}=u$ gives

$$p_\nabla^{\theta,\phi}(\theta,\phi) = \frac{C}{a\sqrt{a}}\exp\left(\frac{b^2}{a}-c\right)\int_{-\frac{b}{\sqrt{a}}}^\infty\left(u+\frac{b}{\sqrt{a}}\right)^2\exp(-u^2)\mathrm{d}u = \frac{C}{a\sqrt{a}}\exp\left(\frac{b^2}{a}-c\right)\left(I_1+\frac{b}{\sqrt{a}}I_2+\frac{b^2}{a}I_3\right),$$

the three integrals I_1, I_2, and I_3 resulting from expanding the quadratic expression:

$$I_1 = \int_{-\frac{b}{\sqrt{a}}}^\infty u^2\exp(-u^2)\mathrm{d}u = -0.5\left(u\exp(-u^2)|_{-\frac{b}{\sqrt{a}}}^\infty - I_3\right) = -0.5\left(\frac{b}{\sqrt{a}}\exp\left(-\frac{b^2}{a}\right)-I_3\right),$$
$$I_2 = \int_{-\frac{b}{\sqrt{a}}}^\infty 2u\exp(-u^2)\mathrm{d}u = -\exp(-u^2)|_{-\frac{b}{\sqrt{a}}}^\infty = \exp\left(-\frac{b^2}{a}\right),$$
$$I_3 = \int_{-\frac{b}{\sqrt{a}}}^\infty \exp(-u^2)\mathrm{d}u = \frac{\sqrt{\pi}}{2}\left(1-\mathrm{erf}\left(-\frac{b}{\sqrt{a}}\right)\right).$$

Putting everything together yields

$$p_\nabla^{\theta,\phi}(\theta,\phi) = \frac{C}{a\sqrt{a}}\exp\left(\frac{b^2}{a}-c\right)\left(\frac{b}{2\sqrt{a}}\exp\left(-\frac{b^2}{a}\right)+\left(\frac{1}{2}+\frac{b^2}{a}\right)\frac{\sqrt{\pi}}{2}\left(1-\mathrm{erf}\left(-\frac{b}{\sqrt{a}}\right)\right)\right).$$

3 Illustration

This section illustrates by means of several examples the previously derived formula. The following figures have been done using Matlab.

We start with the simplest case, that of a null mean vector and identity covariance matrix, as shown by the unit sphere centered at the origin in Figure 1.

In Cartesian coordinates, this results in a uniformly distributed gradient. However, in spherical coordinates, due to the $\sin\theta$ term present in the Jacobian when performing the coordinate transformation, the probability density function of the gradient yields the paraboloidal shape in Figure 2 (a), where the plotting is done with respect to the angles θ and ϕ. A more suitable visualization for the marginal probability when expressed in spherical coordinates is by means of the unit sphere, as indicated in Figure 2 (b). The figure also hints why the probability density function is no longer uniform, since the surface elements on the sphere do not have an equal area, as for regular grids, but are larger at the equator than at the poles.

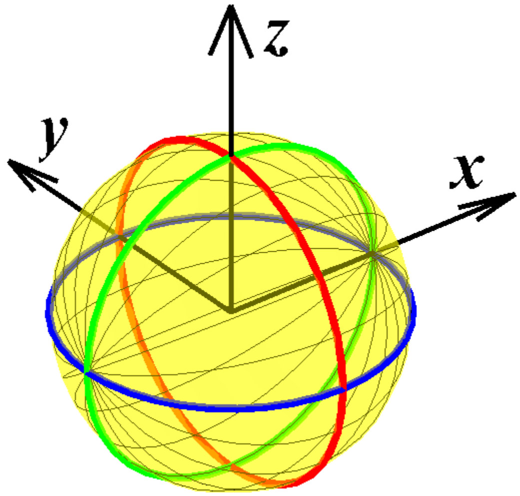

Figure 1: 3D Gaussian uniform probability density of the gradient vector. The mean vector is zero and thus not displayed, while the yellow sphere indicates the confidence region.

Nonetheless, Figure 2 (a) shows that, but for the $\sin\theta$ term, the probability density function in spherical coordinates would also be uniform. Dividing each point at which the function is given by the corresponding $\sin\theta$ value, gives indeed a uniform probability density function, as illustrated in Figure 2 (c) and (d). The following examples will only present the probability density function mapped onto the sphere after the division by $\sin\theta$.

The second example translates the mean with one unit to the right on the x-axis and modifies the diagonal of the covariance matrix, so that σ_x^2 becomes 1.5 and σ_y^2 becomes 0.5. This is reflected in Figure 3 (a), where the sphere has turned into an ellipsoid that is centered on the x-axis, rather than at the origin, and has the largest semi-axis on the x-axis, where the standard deviation is largest. The probability density function, shown in Figure 3 (b), is symmetric and has a strong mode at $\theta = \pi/2$ and $\phi = 0$, i.e., in the direction of the mean, on the x-axis.

The last example translates the mean with one unit in both the x- and z-axes, and modifies the covariance matrix to have $\sigma_y^2 = 2$ on the diagonal. Then, the covariance matrix has further non-diagonal elements different from zero, taking correlations into account by setting $\rho_{xy} = 0.5$ and $\rho_{yz} = -0.7$. Figure 4 (a) shows the corresponding ellipsoid. The effect of correlations can be noticed in the change in orientation of the ellipsoid, whose semi-axes are no longer parallel to those of the Cartesian grid. Figure 4 (b) reveals an almost symmetric bimodal density function, with a right slightly stronger mode, and a left slightly lower mode. The direction of the mean is rather unlikely.

4 Conclusion

In this report, we introduced a mathematical framework to compute probability density functions for directions of vectors in Gaussian distributed uncertain 3D scalar fields that can be obtained by applying a linear operator, and derived appropriate formulae for gradients at Gaussian distributed 3D scalar fields. We showed that performing a coordinate transformation from Cartesian to spherical coordinates and computing in the spherical coordinate system is better suited to convey the probability density for gradient directions, and illustrated various direction probability density functions in several examples.

5 Acknowledgments

This work was supported by the European Union under the ERC Advanced Grant 291372 SaferVis - Uncertainty Visualization for Reliable Data Discovery.

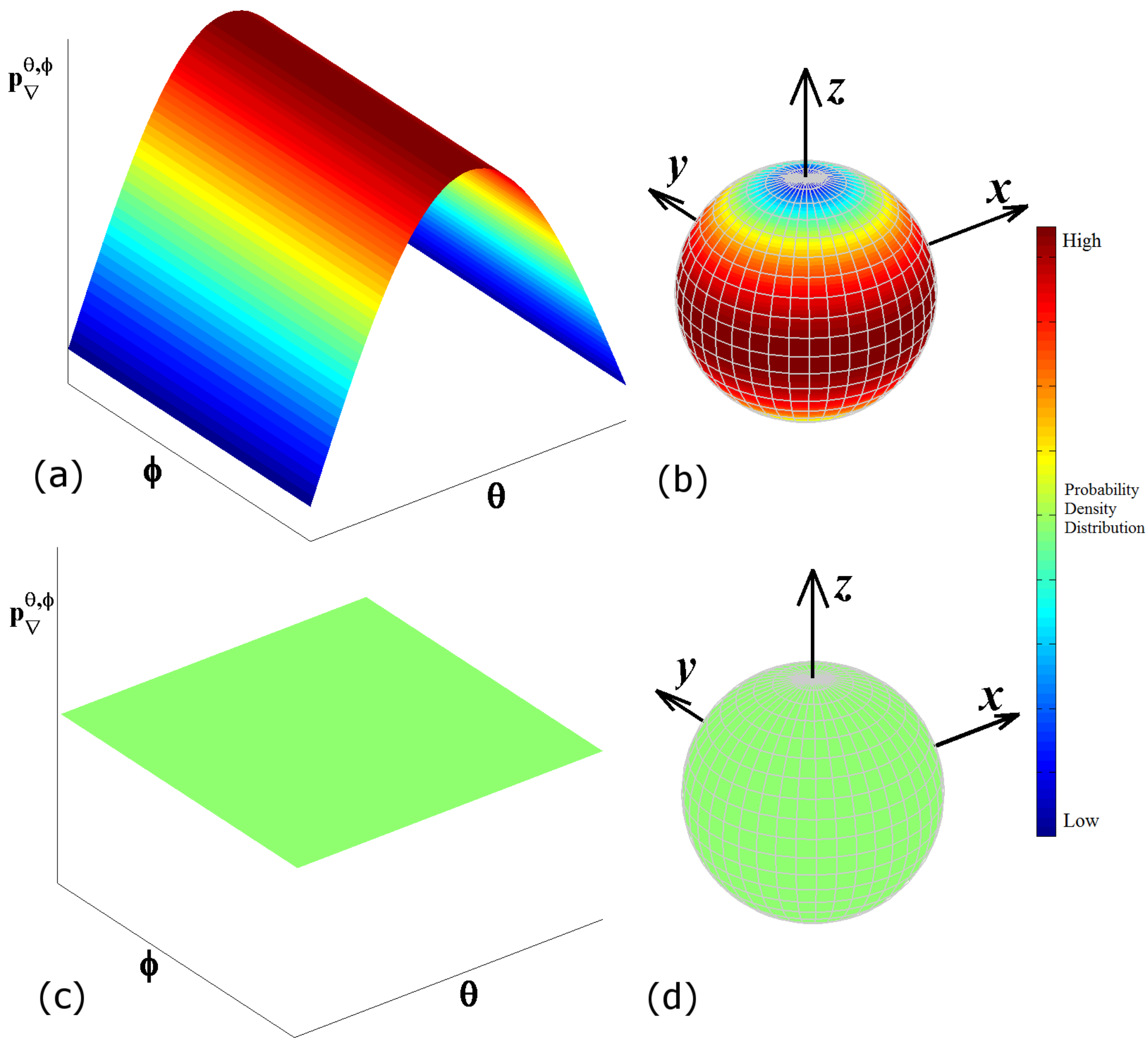

Figure 2: (a) The previous probability density expressed in spherical coordinates on a regular grid having angles θ and ϕ as coordinates. (b) The same probability density as in (a), mapped onto the unit sphere. It can be noticed that the probability density is no longer uniform, as the surface elements on the sphere no longer occupy the same area. (c) The probability density after division expressed in spherical coordinates on a regular grid having angles θ and ϕ as coordinates. (d) The probability density after division, mapped onto the unit sphere. It can be noticed that the probability density is now uniform.

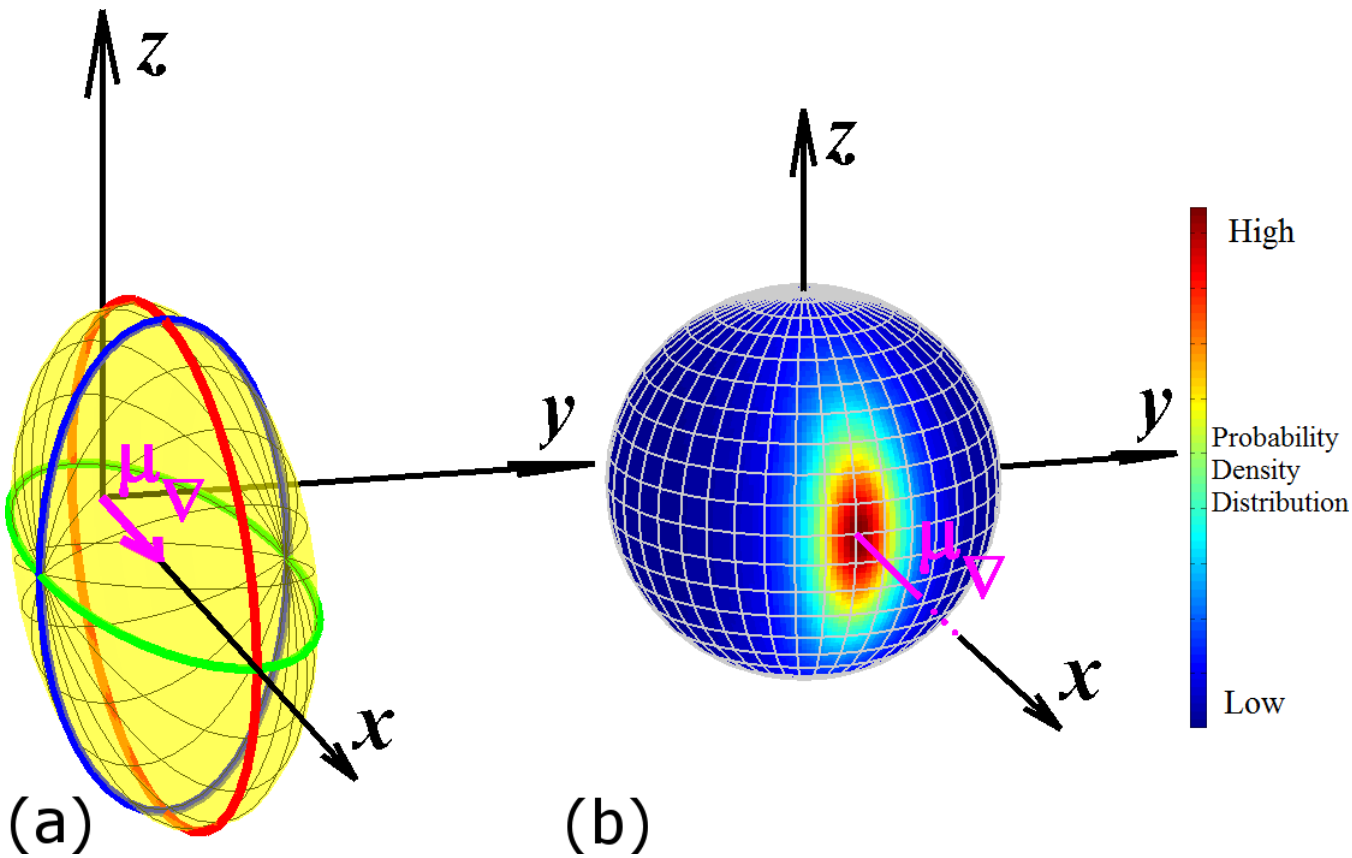

Figure 3: (a) 3D Gaussian probability density of the gradient vector, with the mean vector drawn in magenta along the x-axis, and the yellow ellipsoid indicating the confidence region. The three ellipses colored in red, green, and blue, respectively, are the corresponding ellipses having as semi-major and semi-minor axes the semi-axes of the ellipsoid. (b) The symmetric probability density mapped onto the unit sphere, where the magenta-colored line extending to infinity has the direction of the mean vector.

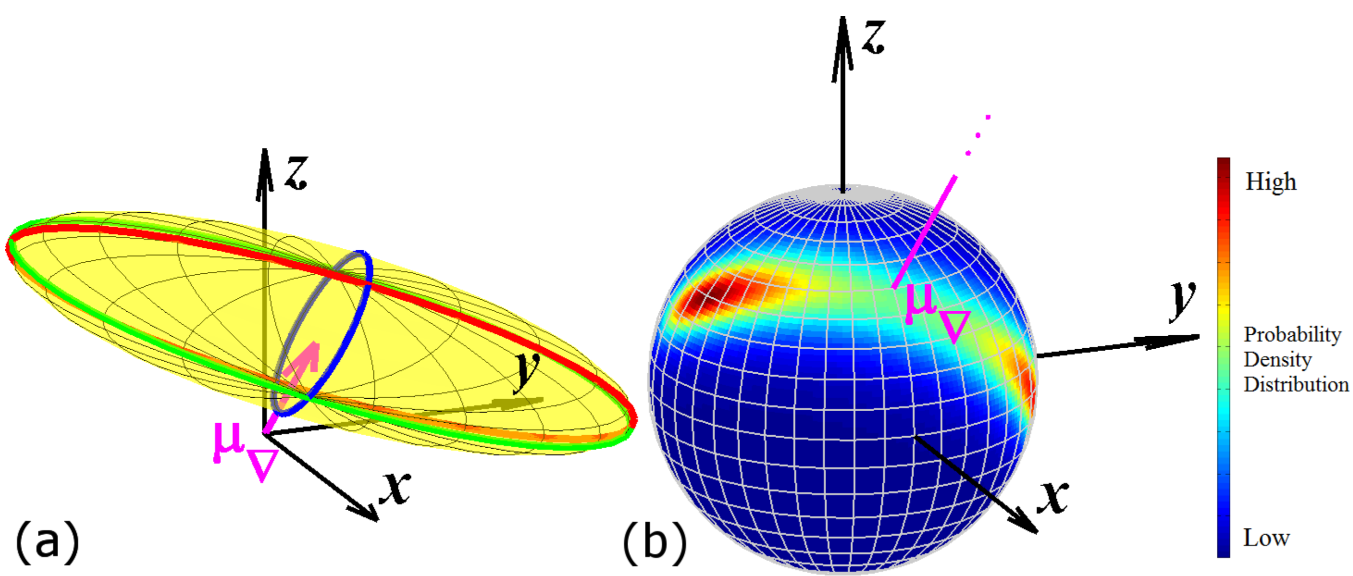

Figure 4: (a) 3D Gaussian probability density of the gradient vector, with the mean vector drawn in magenta in the XZ-plane and the tilted yellow ellipsoid indicating the confidence region. (b) The bimodal probability density, mapped onto the unit sphere, where the magenta-colored line has the direction of the mean vector.