

Multivar Gaussians and GMMs

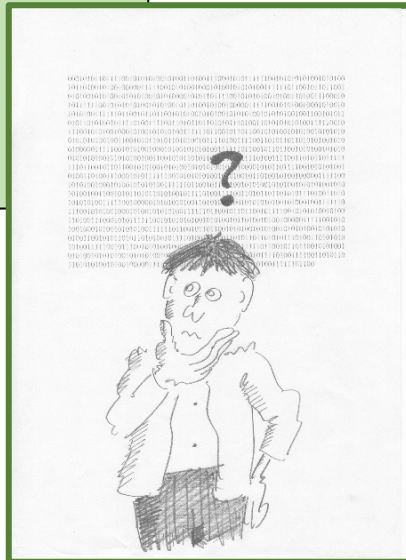
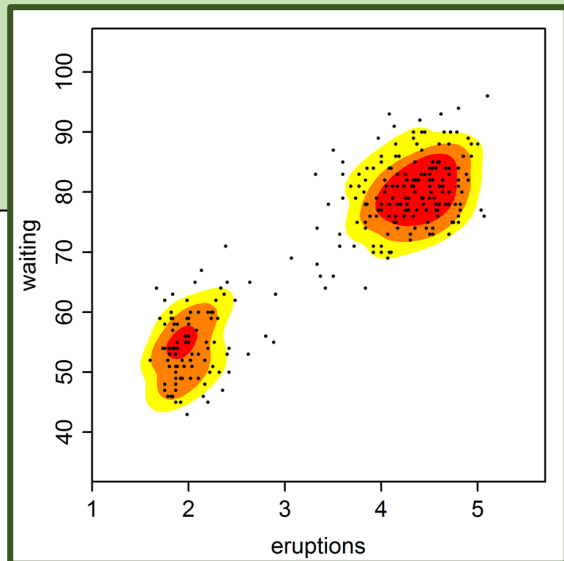
Statistics and data analysis

Ben Galili

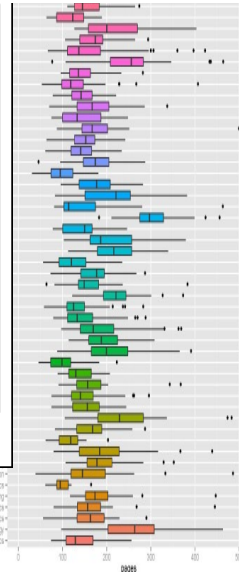
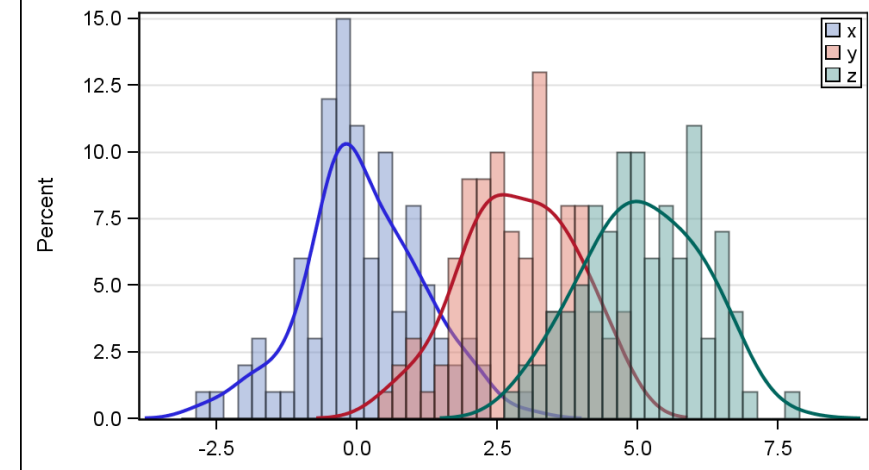
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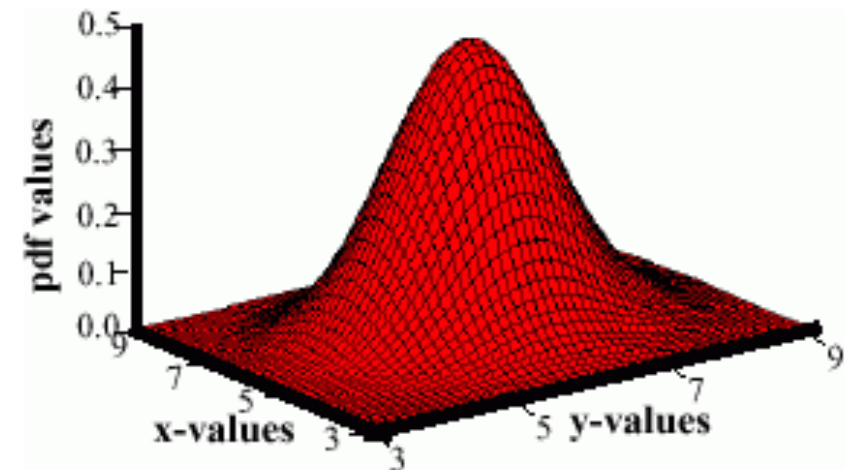
Multivariate Normal Distributions

- A multivariate normal distribution is defined by its pdf:

$$p(\vec{x}) = \frac{1}{\sqrt{(2\pi)^d \cdot \text{Det } \Sigma}} \exp \left(-\frac{1}{2} \cdot \langle \vec{x} - \vec{\mu}, \Sigma^{-1}(\vec{x} - \vec{\mu}) \rangle \right)$$

where μ represents the mean (vector) and Σ represents the covariance matrix.

- The covariance is always symmetric and positive semidefinite. (invertible, $\text{Det} > 0$)
- Does the covariance matrix Σ represent covariances?
- How does the shape vary as a function of the covariance? – will be discussed



Simple case – diagonal Σ

$$\begin{aligned} p(x; \mu, \Sigma) &= \frac{1}{2\pi \begin{vmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{vmatrix}^{1/2}} \exp \left(-\frac{1}{2} \begin{bmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{bmatrix}^T \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix}^{-1} \begin{bmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{bmatrix} \right) \\ &= \frac{1}{2\pi(\sigma_1^2 \cdot \sigma_2^2 - 0 \cdot 0)^{1/2}} \exp \left(-\frac{1}{2} \begin{bmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{bmatrix}^T \begin{bmatrix} \frac{1}{\sigma_1^2} & 0 \\ 0 & \frac{1}{\sigma_2^2} \end{bmatrix} \begin{bmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{bmatrix} \right) \\ &= \frac{1}{2\pi\sigma_1\sigma_2} \exp \left(-\frac{1}{2\sigma_1^2}(x_1 - \mu_1)^2 - \frac{1}{2\sigma_2^2}(x_2 - \mu_2)^2 \right) \\ &= \frac{1}{\sqrt{2\pi}\sigma_1} \exp \left(-\frac{1}{2\sigma_1^2}(x_1 - \mu_1)^2 \right) \cdot \frac{1}{\sqrt{2\pi}\sigma_2} \exp \left(-\frac{1}{2\sigma_2^2}(x_2 - \mu_2)^2 \right). \end{aligned}$$

An alternative definition

Consider a standard bivariate normal random variable (Z_1, Z_2) .
Note that we can directly define this by defining the joint pdf:

$$\varphi(x, y) = \frac{1}{2\pi} \exp\left(-\frac{1}{2}(x^2 + y^2)\right)$$

Using a set of parameters $\alpha, \beta, \sigma, \tau$ and ρ we now define new random variables as follows:

$$A = \sigma Z_1 + \alpha \quad \text{and} \quad B = \tau\left(\rho Z_1 + \sqrt{1 - \rho^2} \cdot Z_2\right) + \beta$$

Bivar normal – cont ...

We can show (change of variables and some heavy calculus) that the pdf of (A, B) will have the form:

$$p(x, y) = \frac{1}{2\pi \sqrt{\text{Det } \Sigma}} \exp \left(-\frac{1}{2} \cdot \langle (x, y) - \vec{\mu} , \Sigma^{-1} ((x, y) - \vec{\mu}) \rangle \right)$$

What are $\vec{\mu}$ and Σ ?

Bivar normal - cont

$$E(A) = E(\sigma Z_1 + \alpha) = \alpha$$

$$V(A) = V(\sigma Z_1 + \alpha) = \sigma^2$$

Similarly for B

$$E(B) = E\left(\tau\left(\rho Z_1 + \sqrt{1 - \rho^2} \cdot Z_2\right) + \beta\right) = \beta$$

$$V(B) = V\left(\tau\left(\rho Z_1 + \sqrt{1 - \rho^2} \cdot Z_2\right) + \beta\right)$$

$$= \tau^2(\rho^2 V(Z_1) + (1 - \rho^2)V(Z_2))$$

$$= \tau^2$$

Bivar normal – cont ...

We therefore have:

$$E(A) = \alpha \quad , \quad V(A) = \sigma^2 \quad ,$$

$$E(B) = \beta \quad \text{and} \quad V(B) = \tau^2$$

In fact, our construction implies that

$$A \sim \text{Nor}(\alpha, \sigma^2) \quad \text{and} \quad B \sim \text{Nor}(\beta, \tau^2)$$

A useful fact

If $X \sim N(\mu, \sigma^2)$
then
 $Z = (X - \mu)/\sigma$
is standard normal

If $Z \sim N(0, 1)$
then when defining
 $X = \sigma Z + \mu$
we have
 $X \sim N(\mu, \sigma^2)$

Covariance

$$A = \sigma Z_1 + \alpha \quad \text{and} \quad B = \tau \left(\rho Z_1 + \sqrt{1 - \rho^2} \cdot Z_2 \right) + \beta$$

$$\text{Cov}(A, B) = E \left((A - EA) \cdot (B - EB) \right)$$

$$= E \left(\sigma Z_1 \cdot \tau \left(\rho Z_1 + \sqrt{1 - \rho^2} \cdot Z_2 \right) \right)$$

$$= \sigma \tau \cdot E \left(\rho Z_1^2 + \sqrt{1 - \rho^2} Z_1 Z_2 \right)$$

$$= \sigma \tau \cdot \rho$$

Equivalence – the interpretation

Lets use an example to see how this construction reflects our first definition:

$$p(\vec{x}) = \frac{1}{\sqrt{(2\pi)^d \cdot \text{Det } \Sigma}} \exp \left(-\frac{1}{2} \cdot \langle \vec{x} - \vec{\mu}, \Sigma^{-1}(\vec{x} - \vec{\mu}) \rangle \right)$$

In the bivariate case, and assuming a mean at 0:

$$p(x, y) = \frac{1}{2\pi\sqrt{\text{Det } \Sigma}} \exp \left(-\frac{1}{2} \cdot \langle (x, y), \Sigma^{-1}(x, y) \rangle \right)$$

What is Σ ?

We constructed a bivariate random variable that has normal marginal by defining:

$$A = \sigma Z_1 \quad (+ \alpha)$$

$$B = \tau \left(\rho Z_1 + \sqrt{1 - \rho^2} \cdot Z_2 \right) \quad (+ \beta)$$

It can be shown, by a change of variables and setting α and β to 0, that the density function for our constructed bivariate normal is given by:

$$p(x, y) = \frac{1}{2\pi\sqrt{\text{Det } \Sigma}} \exp \left(-\frac{1}{2} \cdot \langle (x, y), \Sigma^{-1}(x, y) \rangle \right)$$

With Σ being:

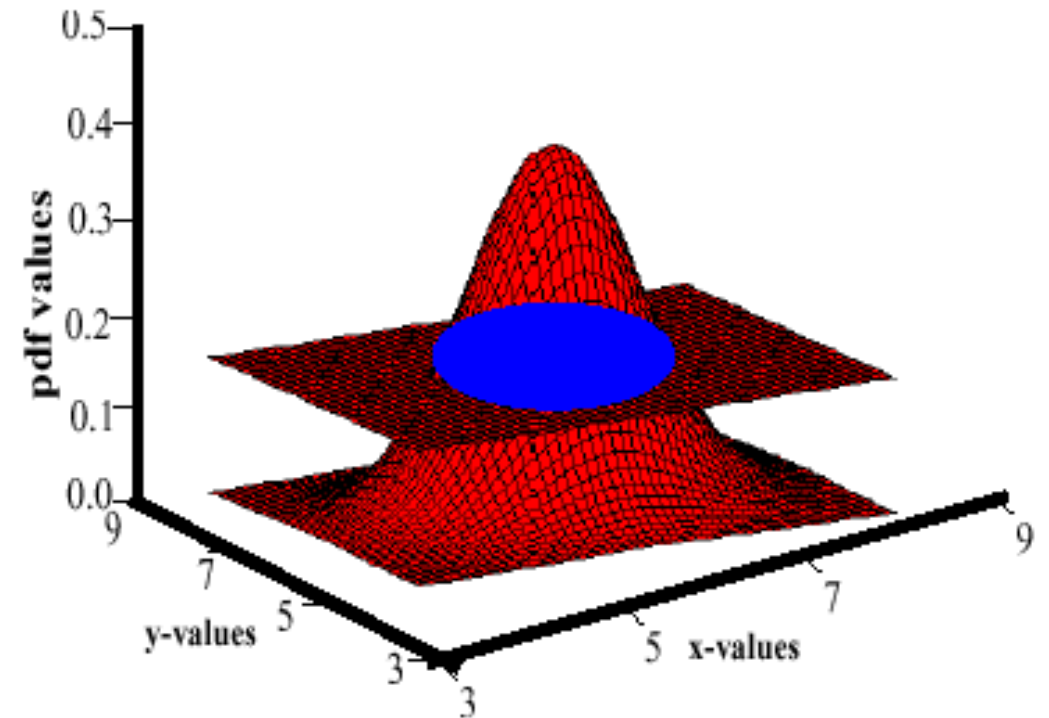
$$\Sigma = \begin{pmatrix} \sigma^2 & \sigma\tau \cdot \rho \\ \sigma\tau \cdot \rho & \tau^2 \end{pmatrix}$$

A third alternative definition

- X is multivariate normal if for any constant vector v , the random variable $W = (v, X)$ has a univariate normal distribution.
- X is multivariate normal with a diagonal Σ iff for any constant vector v , the random variable $W = (v, X)$ has a univariate normal distribution with $\sigma^2 = (v.^2, \text{diag}(\Sigma))$
- In general we have
$$E(W) = (v, E(X)) \text{ and } Var(W) = (v, \Sigma(v))$$

Support Regions or Isocontours

- Horizontal planes cut the pdf graph defining the shapes of ellipses of points that all have equal probability density.
- The shape of these support regions is determined by the covariance matrix.



The diagonal case

What is the shape of isocontours for a diagonal covariance matrix?

Write:

$$c = \frac{1}{2\pi\sigma_1\sigma_2} \exp \left(-\frac{1}{2\sigma_1^2}(x_1 - \mu_1)^2 - \frac{1}{2\sigma_2^2}(x_2 - \mu_2)^2 \right)$$

$$2\pi c\sigma_1\sigma_2 = \exp \left(-\frac{1}{2\sigma_1^2}(x_1 - \mu_1)^2 - \frac{1}{2\sigma_2^2}(x_2 - \mu_2)^2 \right)$$

$$\log(2\pi c\sigma_1\sigma_2) = -\frac{1}{2\sigma_1^2}(x_1 - \mu_1)^2 - \frac{1}{2\sigma_2^2}(x_2 - \mu_2)^2$$

$$\log \left(\frac{1}{2\pi c\sigma_1\sigma_2} \right) = \frac{1}{2\sigma_1^2}(x_1 - \mu_1)^2 + \frac{1}{2\sigma_2^2}(x_2 - \mu_2)^2$$

$$1 = \frac{(x_1 - \mu_1)^2}{2\sigma_1^2 \log \left(\frac{1}{2\pi c\sigma_1\sigma_2} \right)} + \frac{(x_2 - \mu_2)^2}{2\sigma_2^2 \log \left(\frac{1}{2\pi c\sigma_1\sigma_2} \right)}.$$

Isocontours - continued

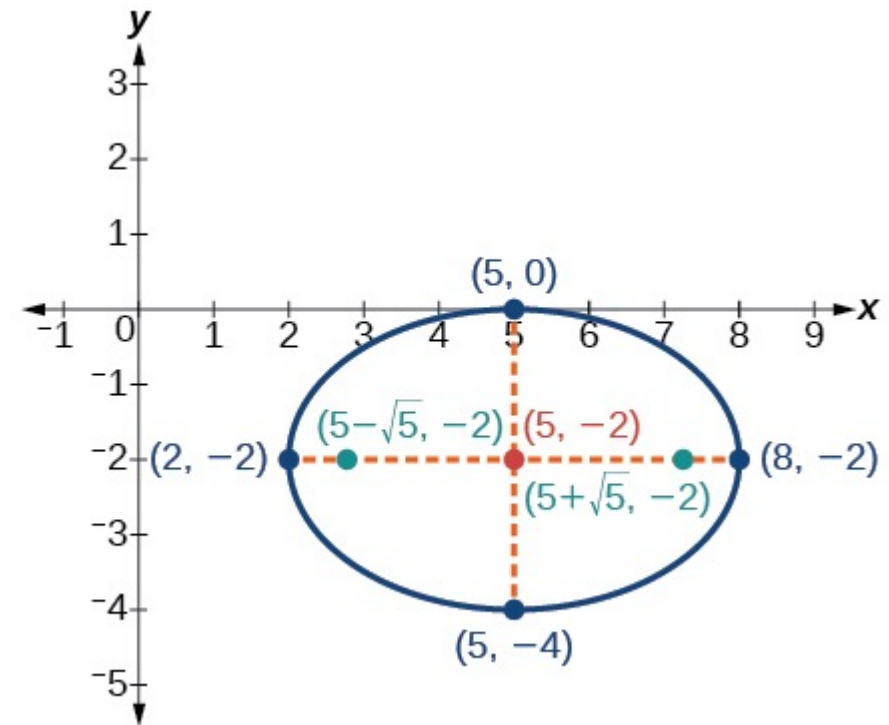
Setting

$$r_1 = \sqrt{2\sigma_1^2 \ln \left(\frac{1}{2\pi c \sigma_1 \sigma_2} \right)}$$

$$r_2 = \sqrt{2\sigma_2^2 \ln \left(\frac{1}{2\pi c \sigma_1 \sigma_2} \right)}$$

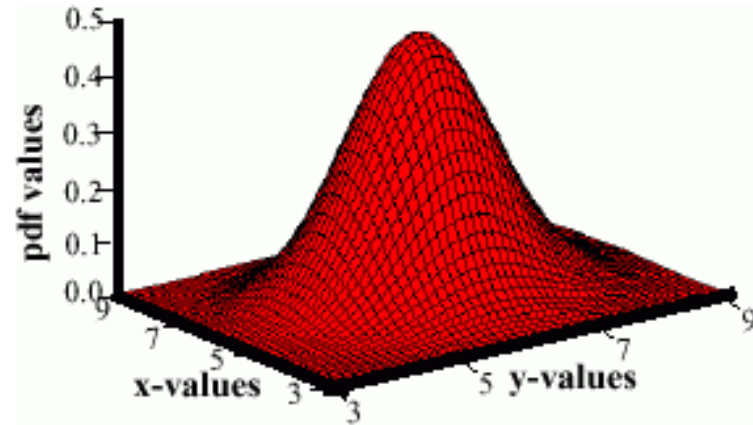
We get that (x_1, x_2) on the contour satisfies

$$\left(\frac{x_1 - \mu_1}{r_1} \right)^2 + \left(\frac{x_2 - \mu_2}{r_2} \right)^2 = 1$$

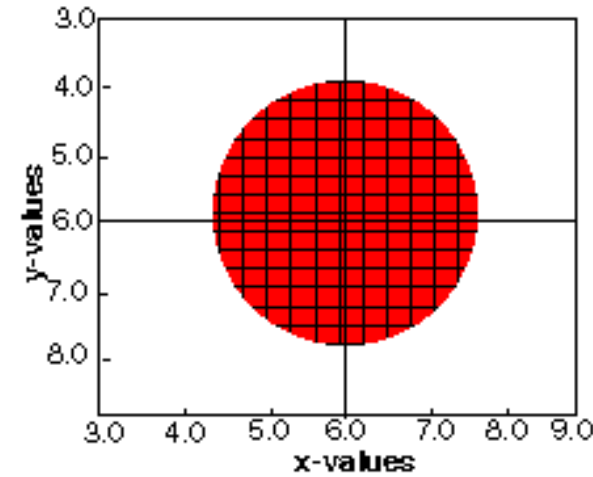


Identity Covariance

Gaussian distribution



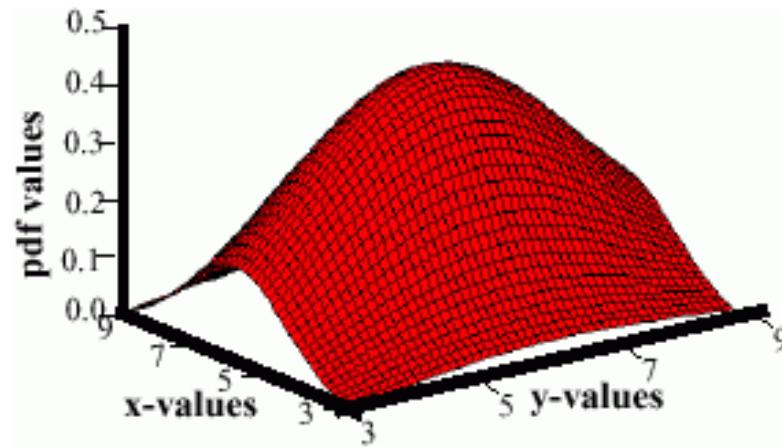
Support Region



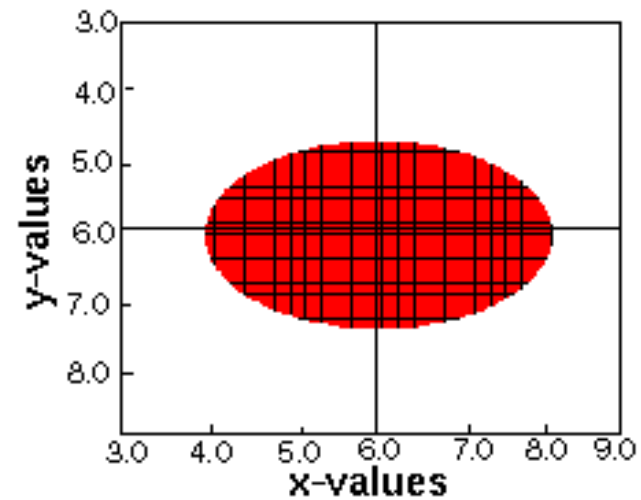
- Gaussian distribution with identity covariance matrix has equal variances in all directions
- Support region for a Gaussian distribution with identity covariance matrix $C = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ is a circle

Unequal Variances

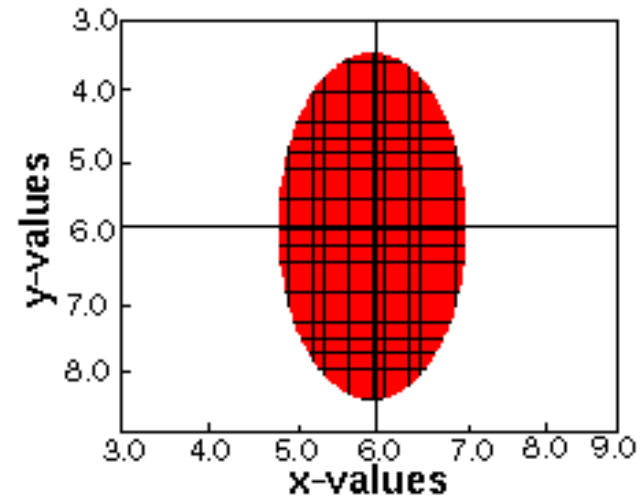
Gaussian distribution



Support Region

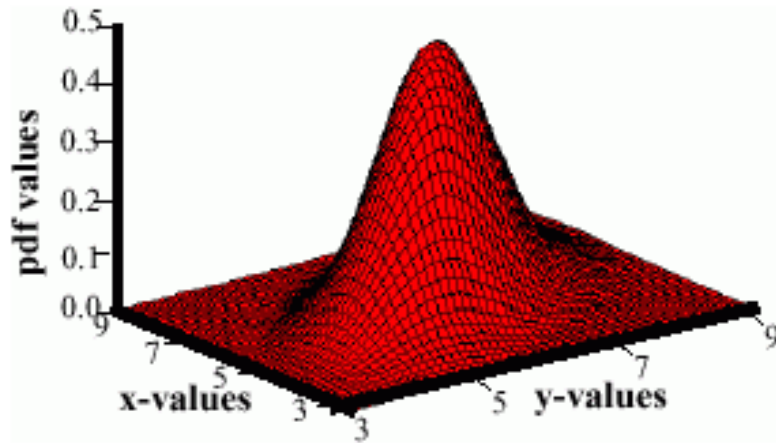


Support region for a Gaussian distribution with covariance matrix $C = \begin{bmatrix} 5 & 0 \\ 0 & 2 \end{bmatrix}$ is an ellipse aligned with respect to the original axes

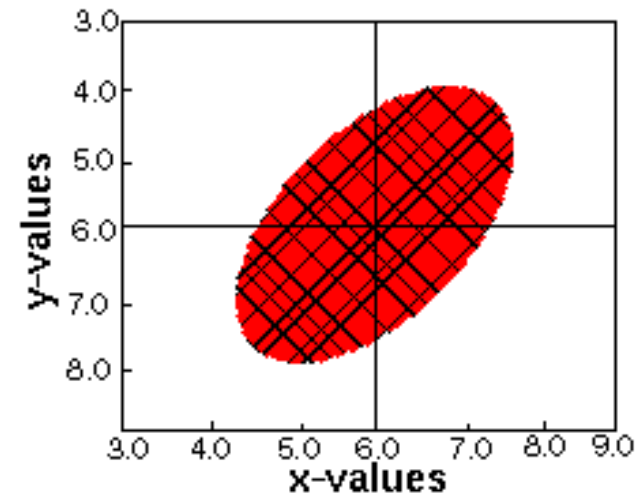


Nonzero Off-Diagonal Elements

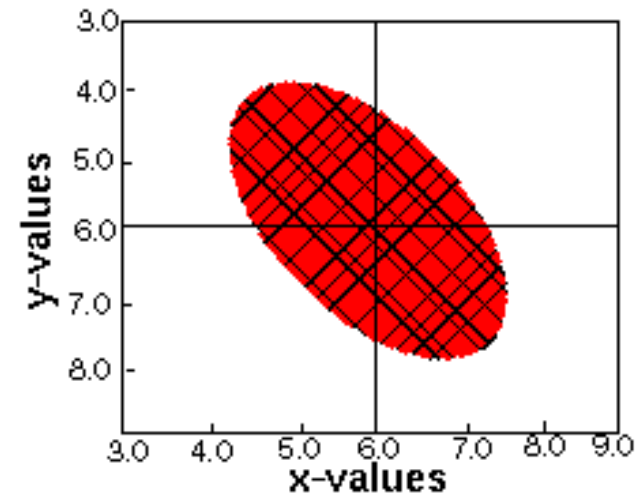
Gaussian distribution



Support Region

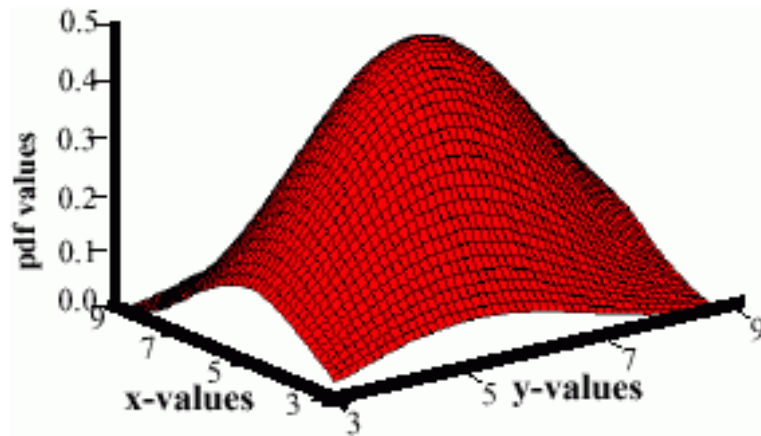


Support region for a Gaussian distribution with covariance matrix $C = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}$ is an ellipse rotated at an angle of 45 degree with respect to the original axes

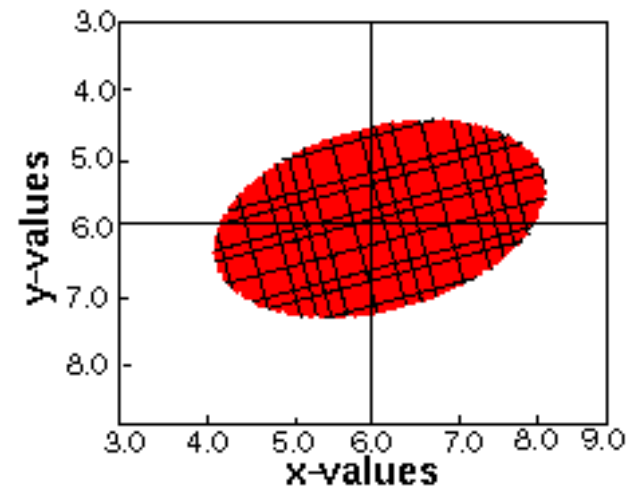


Unconstrained or “Full” Covariance

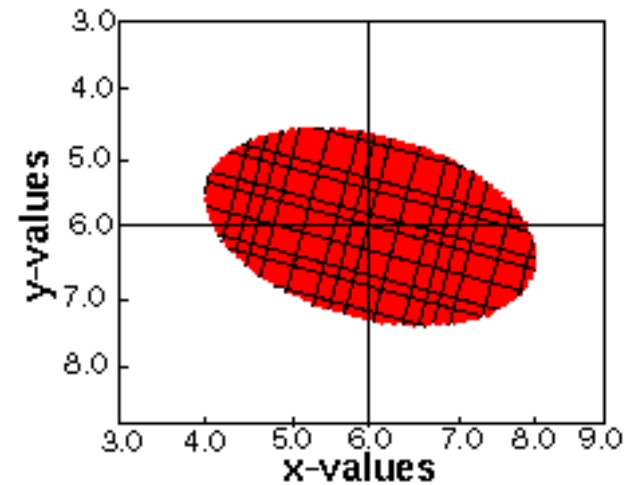
Gaussian distribution

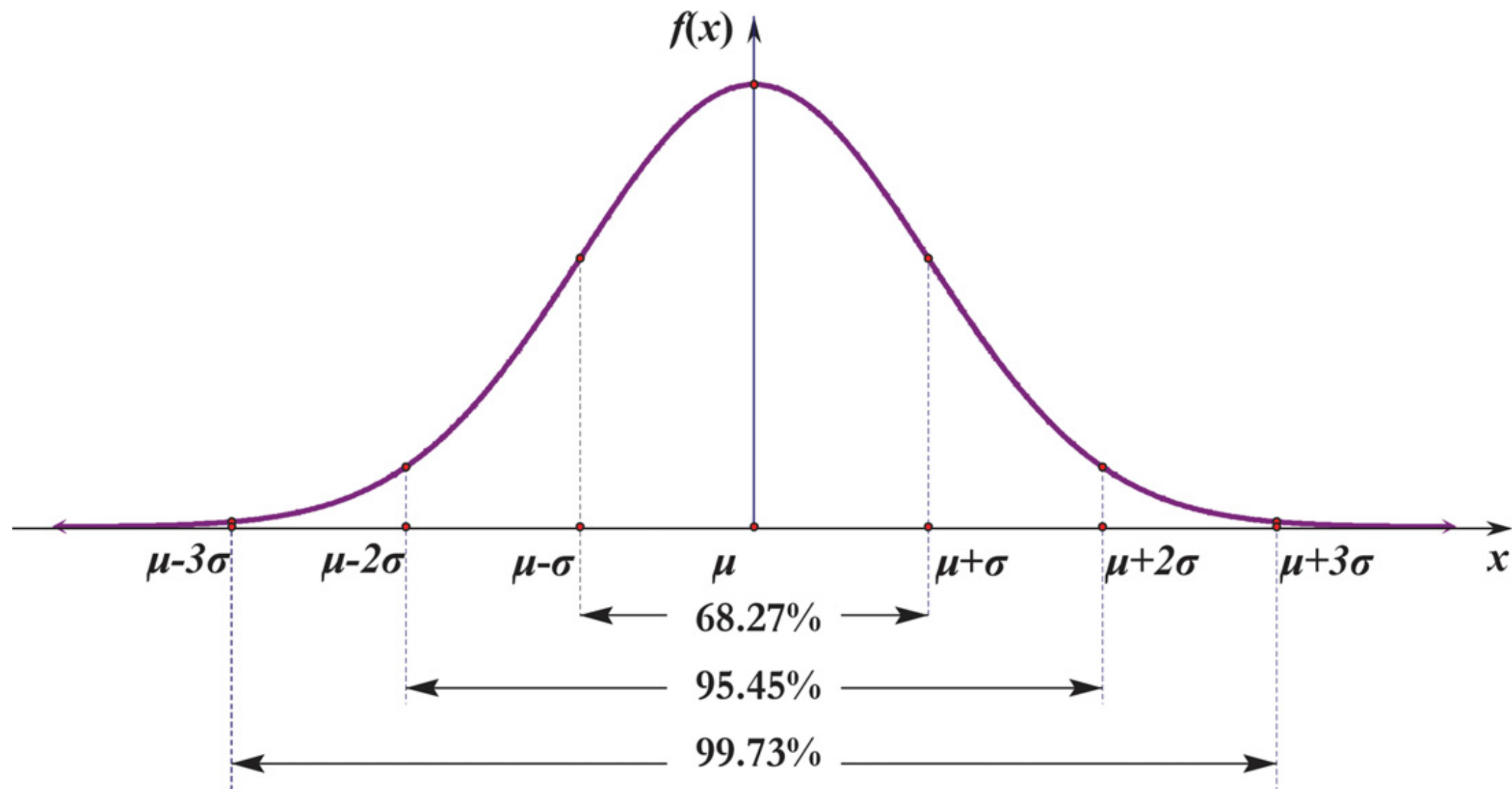


Support Region



Support region for a Gaussian distribution with covariance matrix $C = \begin{bmatrix} 5 & 0.5 \\ 0.5 & 2 \end{bmatrix}$ is an ellipse rotated at an angle of 9 degrees and -81 degrees with respect to the original axes





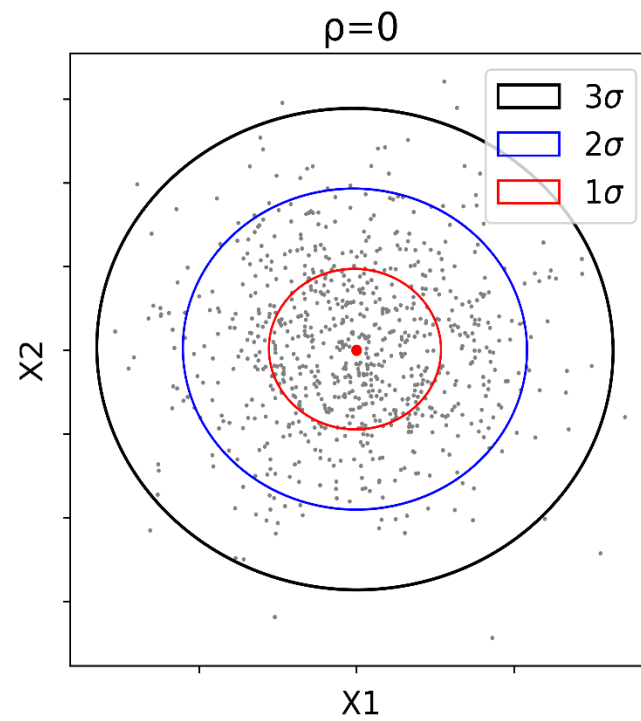
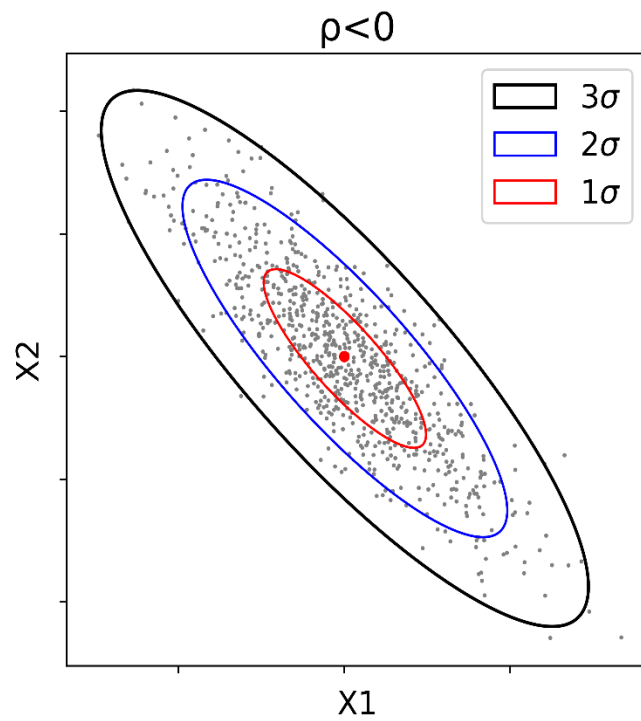
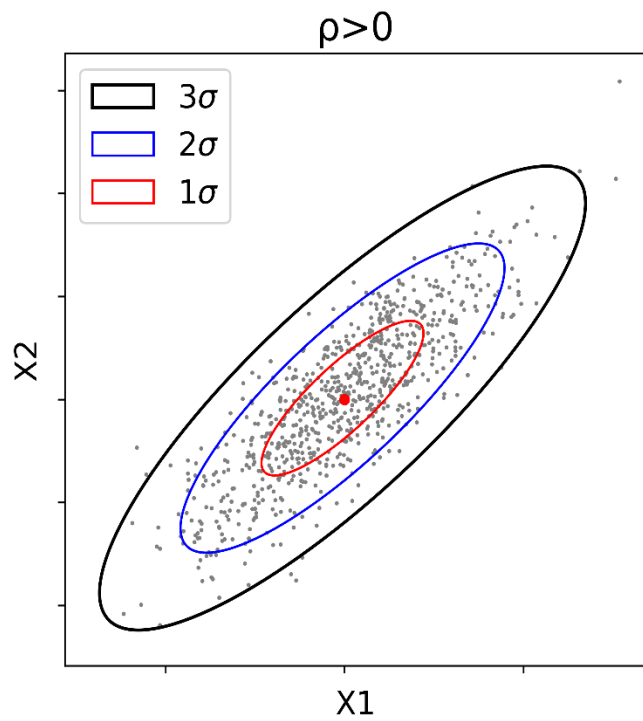


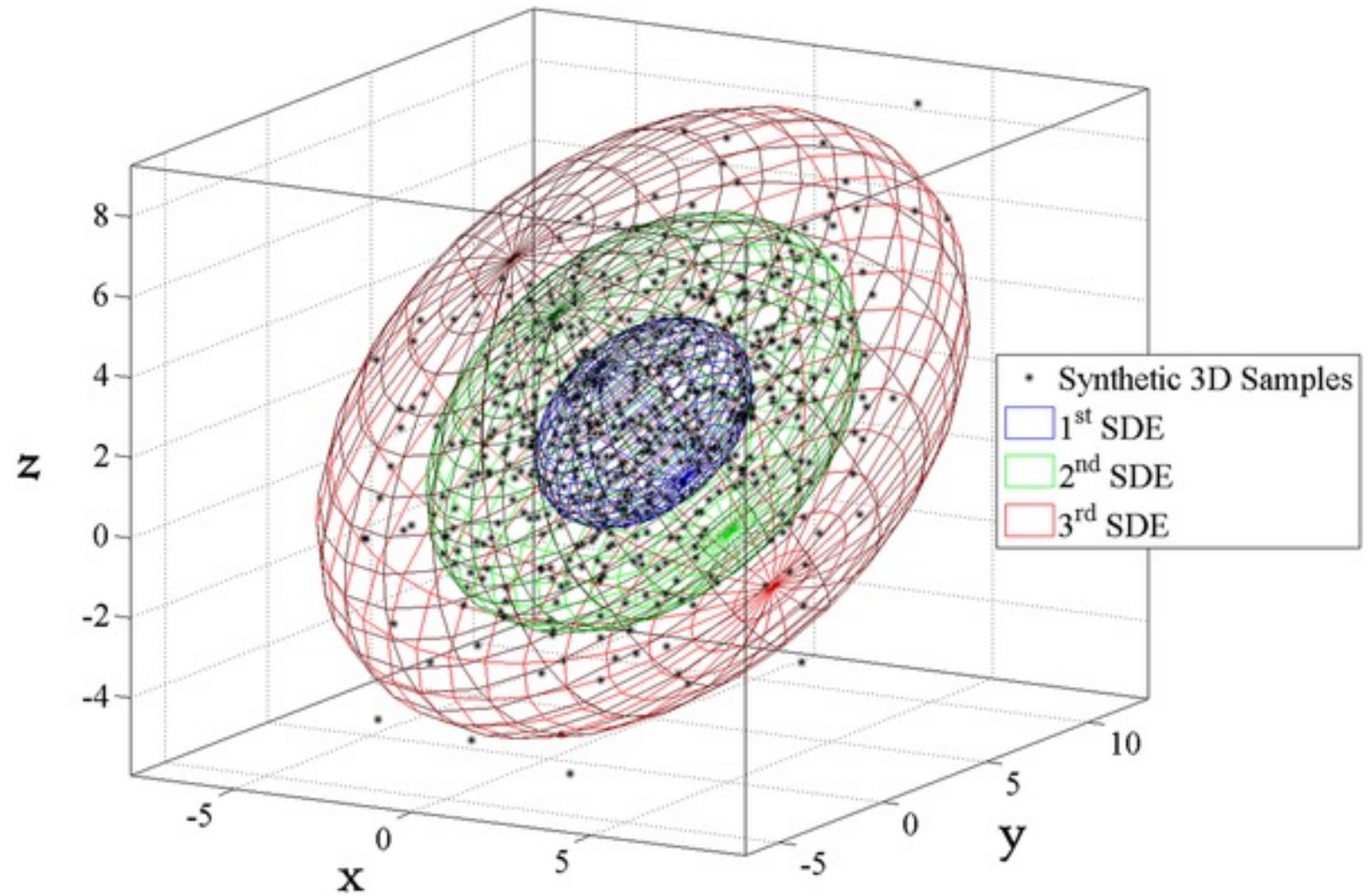
Table 2. Magnification ratios of scaled SDHE corresponding to different specified confidence levels with space dimensionality not exceeding 10.

| Dimensionality | Confidence Level (%) | | | | | |
|----------------|----------------------|--------|--------|--------|--------|--------|
| | 80.0 | 85.0 | 90.0 | 95.0 | 99.0 | 99.9 |
| 1 | 1.2816 | 1.4395 | 1.6449 | 1.9600 | 2.5758 | 3.2905 |
| 2 | 1.7941 | 1.9479 | 2.1460 | 2.4477 | 3.0349 | 3.7169 |
| 3 | 2.1544 | 2.3059 | 2.5003 | 2.7955 | 3.3682 | 4.0331 |
| 4 | 2.4472 | 2.5971 | 2.7892 | 3.0802 | 3.6437 | 4.2973 |
| 5 | 2.6999 | 2.8487 | 3.0391 | 3.3272 | 3.8841 | 4.5293 |
| 6 | 2.9254 | 3.0735 | 3.2626 | 3.5485 | 4.1002 | 4.7390 |
| 7 | 3.1310 | 3.2784 | 3.4666 | 3.7506 | 4.2983 | 4.9317 |
| 8 | 3.3212 | 3.4680 | 3.6553 | 3.9379 | 4.4822 | 5.1112 |
| 9 | 3.4989 | 3.6453 | 3.8319 | 4.1133 | 4.6547 | 5.2799 |
| 10 | 3.6663 | 3.8123 | 3.9984 | 4.2787 | 4.8176 | 5.4395 |

doi:10.1371/journal.pone.0118537.t002

Wang B, Shi W, Miao Z (2015) Confidence Analysis of Standard Deviation Ellipse and Its Extension into Higher Dimensional Euclidean Space. PLOS ONE 10(3): e0118537. <https://doi.org/10.1371/journal.pone.0118537>
<https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0118537>

Wang et al 2015 –
Std ellipses in higher dimension



Wang B, Shi W, Miao Z (2015) Confidence Analysis of Standard Deviation Ellipse and Its Extension into Higher Dimensional Euclidean Space. PLOS ONE 10(3): e0118537. <https://doi.org/10.1371/journal.pone.0118537>
<https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0118537>

Summary of Gauss related topics

- The normal distribution
- Central limit theorem – characterizing the distribution of averages.
- Approximately normal natural phenomena
- Multi D Gaussians and its defining characteristics and quantities.
- Log Normal distribution – next time