1 Prior System Analysis - Uncertainty Propagation

Consider the mathematical model of a physical process/system represented by the equation

$$\underline{Y} = \underline{g}(\underline{X}, \underline{U}) + \underline{E} \tag{1}$$

where $\underline{X} \in R^n$ are uncertain parameters of the mathematical model of the system, $\underline{Y} \in R^m$ is the output quantity of interest (QoI), $\underline{U} \in R^p$ is the parameter set that defines the input which can also be uncertain, and $\underline{E} \in R^m$ represents the model error which is quantified by a multivariate Gaussian distribution $\underline{E} \sim N(\underline{0}, S)$, where $S \in R^{m \times m}$. Given the uncertainty in the parameters $\underline{X}$ and the input $\underline{U}$, one is interested in the uncertainty in the output QoI $\underline{Y}$. Let $f(\underline{x})$ be the joint PDF that quantifies the uncertainty in the parameter set $\underline{X}$. Let also $\underline{\mu}$ and Σ be the mean and the covariance matrix of the uncertain parameter set $\underline{X}$. Similarly, let $f(\underline{u})$ the joint PDF that quantifies the uncertainty in the input parameter set $\underline{U}$, with $\underline{\mu}_U$ and Σ_U the corresponding mean and covariance matrix. The uncertainty in the output QoI can be quantified by the joint PDF $f(\underline{y})$ or simplified measures of uncertainty such as the mean $\underline{\mu}_Y$ and covariance matrix Σ_Y.

There are special cases of the general mathematical model (1) that will be used to demonstrate the theoretical developments. Specifically, a linear model with a single output QoI is given in the form

$$\underline{Y} = A\underline{X} + \underline{E} \tag{2}$$

where $A \in R^{n \times n}$ is a matrix that defines the system. A special subcase of this model arises for a scalar QoI $Y \in R$ $(m = 1)$ in which case the model error $E \in R$. A nonlinear model with a single output QoI is given by

$$Y = g(\underline{X}) + E \tag{3}$$

where $g(\underline{X})$ is a known nonlinear function of $\underline{X}$ that arises from the mathematical model of the system, $Y \in R$ $(m = 1)$, and the model error $E \in R$. Finally another special case is the mathematical model (1) that does not depend on the input quantities in $\underline{U}$, that is, the system representation

$$\underline{Y} = \underline{g}(\underline{X}) + \underline{E} \tag{4}$$

where $\underline{g}(\underline{X}) \in R^m$ is a known nonlinear vector function of $\underline{X}$ that arises from the mathematical model of the system.

There are a number of methods for propagating the uncertainty in the model parameters and the input through the input-output relationship $\underline{Y} = \underline{g}(\underline{X}, \underline{U})$ to obtain the uncertainty in the output QoI. Exact techniques are only available for linear models of the type (2). For nonlinear model, analytical approximations are also available. Next, we present the formulation for linear models and then we generalize the formulation for nonlinear models using analytical approximate techniques based on the Taylor series expansion of the nonlinear vector function $\underline{g}(\underline{X}, \underline{U})$ in terms of $\underline{X}$ and $\underline{U}$.

1.1 Simple Measures of Uncertainty of QoI – Mean and Covariance

1.1.1 Linear Model

Consider the linear model (2), i.e.

$$\underline{Y} = A\underline{X} + \underline{E}$$

Given any distribution $f(\underline{x})$ of the parameter set $\underline{X}$ with mean $\underline{\mu}$ and covariance matrix Σ, one can proceed to obtain analytical expressions for the mean and the covariance matrix of the QoI $\underline{Y}$. Specifically, the mean of $\underline{Y}$ is given by

$$\underline{\mu}_Y = E[\underline{Y}] = E[A\underline{X} + \underline{E}] = AE[\underline{X}] + E[\underline{E}] = A\underline{\mu} + \underline{0} = A\underline{\mu}$$

The covariance matrix is obtained as

$$\begin{aligned}
\Sigma_Y &= E[(\underline{Y} - \mu_Y)(\underline{Y} - \mu_Y)^T] = E[(A\underline{X} + \underline{E} - A\underline{\mu})(A\underline{X} + \underline{E} - A\underline{\mu})^T] \\
&= E[A\underline{X}\underline{X}^T A^T + A\underline{X}\underline{E}^T - A\underline{X}\,\underline{\mu}^T A^T + \underline{E}\underline{X}^T A + \underline{E}\underline{E}^T - \underline{E}\,\underline{\mu}^T A^T - A\underline{\mu}\underline{X}^T A^T - A\underline{\mu}\underline{E}^T + A\underline{\mu}\underline{\mu}^T A^T] \\
&= AE[\underline{X}\underline{X}^T]A^T + AE[\underline{X}\underline{E}^T] - AE[\underline{X}]\underline{\mu}^T A^T + E[\underline{E}\underline{X}^T]A + E[\underline{E}\underline{E}^T] - E[\underline{E}]\underline{\mu}^T A^T - A\underline{\mu}E[\underline{X}^T]A^T \\
&\quad - A\underline{\mu}E[\underline{E}^T] + A\underline{\mu}\underline{\mu}^T A^T \\
&= A(\Sigma + \underline{\mu}\underline{\mu}^T)A^T + 0 - A\underline{\mu}\underline{\mu}^T A^T + 0 + S - 0 - A\underline{\mu}\underline{\mu}^T A^T - 0 + A\underline{\mu}\underline{\mu}^T A^T \\
&= A\Sigma A^T + S
\end{aligned}$$

Assuming further that the parameter set is a multivariate Gaussian vector, one can easily verify from the linear model relationship that the output QoI $\underline{Y}$ is also multivariate Gaussian vector $\underline{Y} \sim N(A\underline{\mu}, A\Sigma A^T + S)$ with joint PDF given by

$$f(\underline{y}) = \frac{1}{\left(\sqrt{2\pi}\right)^m |A\Sigma A^T + S|^{1/2}} \exp\left[-\frac{1}{2}(\underline{y} - A\underline{\mu})^T (A\Sigma A^T + S)^{-1}(\underline{y} - A\underline{\mu})\right]$$

1.1.2 Nonlinear Model

Consider the nonlinear model (2) for a scalar output QoI ($m = 1$), i.e.

$$Y = g(\underline{X}) + E$$

Given any distribution $f(\underline{x})$ of the parameter set $\underline{X}$ with mean $\underline{\mu}$ and covariance matrix Σ, one can proceed to obtain analytical expressions for the mean and the covariance matrix of the scalar QoI Y. Specifically, the mean of Y is given by

$$\underline{\mu}_Y = E[\underline{Y}] = E[g(\underline{X}) + \underline{E}] = E[g(\underline{X})] + E[\underline{E}] = E[g(\underline{X})] \tag{5}$$

The second moment of Y is given by

$$
\begin{aligned}
E[Y^2] &= E[YY^T] = E[\{g(\underline{X})+\underline{E}\}\{g(\underline{X})+\underline{E}\}^T] = \\
&= E[g(\underline{X})g^T(\underline{X}) + g(\underline{X})\underline{E}^T + \underline{E}g^T(\underline{X}) + \underline{E}\underline{E}^T] \\
&= E[g(\underline{X})g^T(\underline{X})] + E[g(\underline{X})\underline{E}^T] + E[\underline{E}g^T(\underline{X})] + E[\underline{E}\underline{E}^T] \\
&= E[g(\underline{X})g^T(\underline{X})] + 0 + 0 + S \\
&= E[g(\underline{X})g^T(\underline{X})] + S
\end{aligned}
\tag{6}
$$

and can be used to obtain the variance of Y by the relationship

$$\sigma_Y^2 = E[Y^2] - \mu_Y^2$$

1.1.3 Analytical Approximations based on Taylor Series Expansion (First and Second-Order Perturbation Techniques)

For a general function $g(\underline{X})$, the expectations $E[g(\underline{X})]$ in (5) and $E[g(\underline{X})g^T(\underline{X})]$ in (6) cannot be computed analytically. Analytical approximations are possible by using a Taylor series approximation of $g(\underline{X})$ about the mean value or the most probable value, say $\underline{x}_0$, of $\underline{X}$. The analytical approximations are first presented for the case of a scalar uncertain parameter X and then are generalized to cover the multidimensional case.

(a) One-Dimensional Case

Assuming that $\underline{X}$ is a scalar X, the Taylor series expansion of the function $g(x)$ about the mean value or the most probable value, say x_0, of X, keeping only up to the quadratic terms is

$$g(x) = g(x_0) + \frac{dg(x_0)}{dx}(x-x_0) + \frac{1}{2}\frac{d^2g(x_0)}{dx^2}(x-x_0)^2$$

The quadratic expansion of $g(x)$ with respect to x is valid only sufficiently close to the point x_0. The accuracy depend on the form of $g(x)$ around this point.

The expectation $E[g(X)]$ in (5) takes the form

$$
\begin{aligned}
E[g(x)] &= g(x_0) + \frac{dg(x_0)}{dx}E[(x-x_0)] + \frac{1}{2}\frac{d^2g(x_0)}{dx^2}E[(x-x_0)^2] \\
&= g(x_0) + \frac{dg(x_0)}{dx}(\mu-x_0) + \frac{1}{2}\frac{d^2g(x_0)}{dx^2}[\Sigma + (\mu-x_0)^2]
\end{aligned}
$$

where the expressions were simplified using that $E[(x-x_0)] = E[x] - E[x_0] = \mu - x_0$ and

$$
\begin{aligned}
E[(x-x_0)^2] &= E[(x-\mu+\mu-x_0)^2] = E[(x-\mu)^2 + (\mu-x_0)^2 + 2(x-\mu)(\mu-x_0)] \\
&= E[(x-\mu)^2] + E[(\mu-x_0)^2] = \Sigma + (\mu-x_0)^2
\end{aligned}
$$

Similarly, the $E[g^2(X)]$ in (6) takes the form

$$E[g^2(x)] = E[g^2(x_0)] + 2g(x_0)\frac{dg(x_0)}{dx}E[(x-x_0)] + \left[\frac{dg(x_0)}{dx}\right]^2 E[(x-x_0)^2]$$
$$+ g(x_0)\frac{d^2g(x_0)}{dx^2}E[(x-x_0)^2]$$
$$= E[g^2(x_0)] + 2g(x_0)\frac{dg(x_0)}{dx}(\mu - x_0) + \left[\frac{dg(x_0)}{dx}\right]^2 [\Sigma + (\mu - x_0)^2]$$
$$+ g(x_0)\frac{d^2g(x_0)}{dx^2}[\Sigma + (\mu - x_0)^2]$$
$$= g^2(x_0) + 2g(x_0)\frac{dg(x_0)}{dx}(\mu - x_0) + \left\{\left[\frac{dg(x_0)}{dx}\right]^2 + g(x_0)\frac{d^2g(x_0)}{dx^2}\right\}[\Sigma + (\mu - x_0)^2]$$

Both the expectations depend on the first and second-order derivatives of the function $g(x)$ with respect to the parameters in x and the first two moments, mean μ and variance Σ, of the uncertain parameter X.

For the case for which x_0 is chosen to be the mean value μ of X, the aforementioned expectations simplify to

$$E[g(x)] = g(\mu) + \frac{1}{2}\frac{d^2g(\mu)}{dx^2}\Sigma \tag{7}$$

and

$$E[g^2(x)] = g^2(\mu) + \left\{\left[\frac{dg(\mu)}{dx}\right]^2 + g(\mu)\frac{d^2g(\mu)}{dx^2}\right\}\Sigma \tag{8}$$

Note that in this case the first and second-order derivatives of the function $g(x)$ with respect to the parameters in x are evaluated at the mean μ, while the expressions also depend on the variance Σ of the uncertain parameter X.

(b) Multi-dimensional Case

For the multidimensional uncertain parameter case, keeping the first three terms in the Taylor series, one has that

$$g(\underline{x}) = g(\underline{x}_0) + \underline{\nabla}^T g(\underline{x}_0)(\underline{x} - \underline{x}_0) + \frac{1}{2}(\underline{x} - \underline{x}_0)^T \underline{\nabla}.\underline{\nabla}^T g(\underline{x}_0)(\underline{x} - \underline{x}_0)$$
$$= g(\underline{x}_0) + \underline{\nabla}^T g(\underline{x}_0)(\underline{x} - \underline{x}_0) + \frac{1}{2}(\underline{x} - \underline{x}_0)^T H(\underline{x}_0)(\underline{x} - \underline{x}_0)$$
$$= g(\underline{x}_0) + \underline{\nabla}^T g(\underline{x}_0)(\underline{x} - \underline{x}_0) + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} H_{ij}(\underline{x}_0)(x_i - x_{0,i})(x_j - x_{0,j})$$

where $H(\underline{x}_0) = \underline{\nabla}.\underline{\nabla}^T g(\underline{x}_0)$ is the Hessian of the function $g(\underline{x})$ and $H_{ij}(\underline{x}_0)$ is the (i, j) component of the Hessian matrix $H(\underline{x}_0)$. The quadratic expansion of $g(\underline{x})$ with respect to $\underline{x}$ is valid only sufficiently close to the point $\underline{x}_0$. The accuracy depend on the form of $g(\underline{x})$ around this point.

The expectation $E[g(\underline{X})]$ in (5) takes the form

$$E[g(\underline{x})] = g(\underline{x}_0) + \underline{\nabla}^T g(\underline{x}_0) E[(\underline{x} - \underline{x}_0)] + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} H_{ij}(\underline{x}_0) E[(x_i - x_{0,i})(x_j - x_{0,j})]$$

$$= g(\underline{x}_0) + \underline{\nabla}^T g(\underline{x}_0)(\underline{\mu} - \underline{x}_0) + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} H_{ij}(\underline{x}_0)[\Sigma_{ij} + (\mu_i - x_{0,i})(\mu_j - x_{0,j})]$$

which depends on the first and second-order derivatives of the function $g(\underline{x})$ with respect to the parameters in $\underline{x}$ and the first two moments of the uncertain parameter $\underline{X}$. Similarly, the $E[g(\underline{X})g^T(\underline{X})]$ in (6) takes the form

$$E[g(\underline{x})g(\underline{x})] = E[g(\underline{x}_0)g(\underline{x}_0)] + 2g(\underline{x}_0)\underline{\nabla}^T g(\underline{x}_0)E[(\underline{x} - \underline{x}_0)] + \underline{\nabla}^T g(\underline{x}_0)E[(\underline{x} - \underline{x}_0)(\underline{x} - \underline{x}_0)^T]\underline{\nabla} g(\underline{x}_0)$$

$$+ g(\underline{x}_0)\sum_{i=1}^{n} H_{ij}(\underline{x}_0)E[(x_i - x_{0,i})(x_j - x_{0,j})]$$

$$= g^2(\underline{x}_0) + 2g(\underline{x}_0)\underline{\nabla}^T g(\underline{x}_0)(\underline{\mu} - \underline{x}_0) + \underline{\nabla}^T g(\underline{x}_0)[\Sigma + (\underline{\mu} - \underline{x}_0)(\underline{\mu} - \underline{x}_0)^T]\underline{\nabla} g(\underline{x}_0)$$

$$+ g(\underline{x}_0)\sum_{i=1}^{n}\sum_{j=1}^{n} H_{ij}(\underline{x}_0)[\Sigma_{ij} + (\mu_i - x_{0,i})(\mu_j - x_{0,j})]$$

Both the expectations depend on the first and second-order derivatives of the function $g(\underline{x})$ with respect to the parameters in $\underline{x}$ and the first two moments of the uncertain parameter set $\underline{X}$.

For the case for which $\underline{x}_0$ is chosen to be the mean value $\underline{\mu}$ of X, the aforementioned expectations simplify to

$$E[g(\underline{x})] = g(\underline{\mu}) + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} H_{ij}(\underline{\mu})\Sigma_{ij} \tag{9}$$

$$E[g(\underline{x})g(\underline{x})] = g^2(\underline{\mu}) + \underline{\nabla}^T g(\underline{\mu})\Sigma\underline{\nabla} g(\underline{\mu}) + g(\underline{\mu})\sum_{i=1}^{n}\sum_{j=1}^{n} H_{ij}(\underline{\mu})\Sigma_{ij} \tag{10}$$

A similar Taylor series analysis can be used to handle the multi-dimensional QoI $\underline{Y} \in R^m$ defined in (4).

1.2 Reliability Measures

Often in systems one is interested in finding the probability an uncertain output QoI $\underline{Y}$ exceeds a level $\underline{y}_0$ which is usually associated with unacceptable performance of the system. Using the fact that $\underline{Y} = \underline{g}(\underline{X})$ where $\underline{Y}$ is a general function of the uncertain model parameters $\underline{X}$, this problem is mathematically stated

$$F = \Pr[g(\underline{X}) \geq y_0]$$

where F is known as the probability of unacceptable performance or failure probability. Introducing the limit state function $h(\underline{x}) = y_0 - g(\underline{x})$, the aforementioned failure probability problem is stated and represented as

$$F = \Pr[h(\underline{X}) \le 0] = \int I_f(\underline{x}) f(\underline{x}) d\underline{x} \\ = \int_{h(\underline{x}) \le 0} f(\underline{x}) d\underline{x} \tag{11}$$

where $I_f(\underline{x})$ is the indicator function given by

$$\begin{aligned} I_f(\underline{x}) &= 1 \quad \text{if} \quad h(\underline{x}) \le 0 \\ &= 0 \quad \text{if} \quad h(\underline{x}) > 0 \end{aligned}$$

The equation $h(\underline{x}) = 0$ is called the limit state equation which is represented by a hypersurface, called the limit state surface, in the multidimensional space of parameters and divides the space into two domains, the failure domain and the safe domain. A graphical representation in the two-dimensional case is shown in Figure 1.

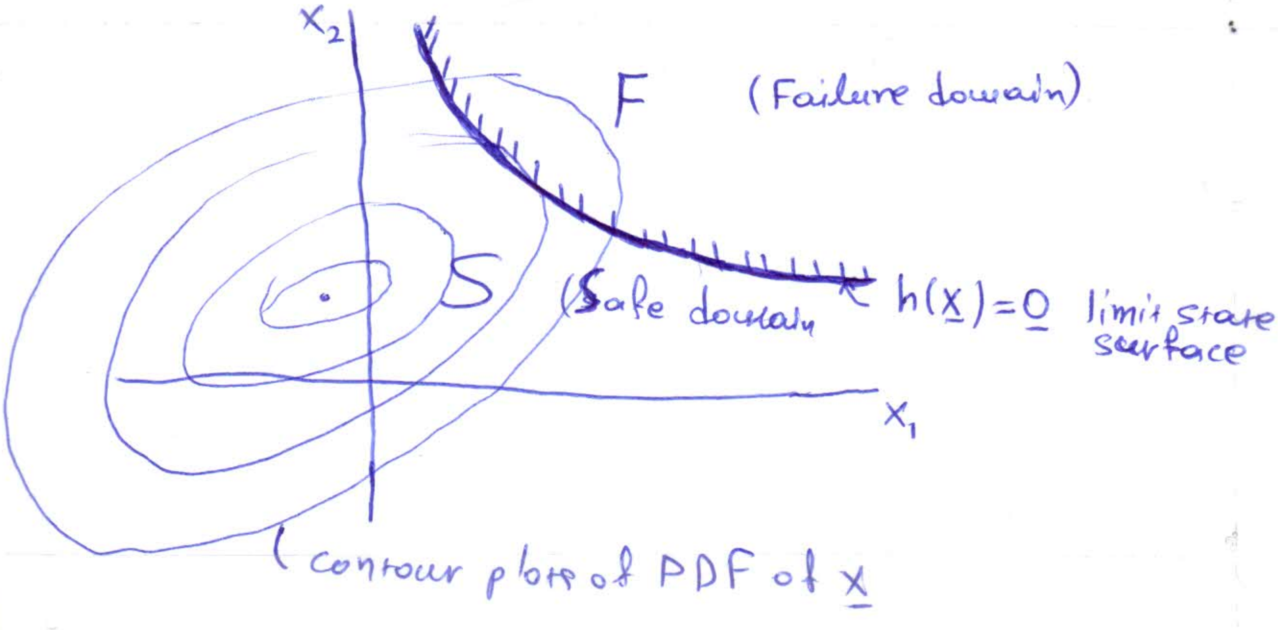

Figure 1: Failure and safe domains in two-dimensional space of parameters

Exact analytical values of the probability of failure can be obtained for the case where the limit state function $h(\underline{x})$ is linear in $\underline{x}$. Otherwise, the probability of failure can only be approximated using techniques such as first-order and second-order reliability methods (FORM and SORM).

(a) Linear Limit State Function and Standard Gaussian Parameters

An exact estimate of the probability of failure is next provided for the case where $h(\underline{Z})$ is a linear function of standard Gaussian (normal) parameters $\underline{Z} \in R^n$, i.e.

$$h(\underline{z}) = a + \underline{b}^T \underline{z}$$

The limit state surface is a hyper-plane in the n-dimensional space of standard Gaussian variables $\underline{Z}$. A two-dimensional representation with the limit state function, the failure and safe domains is shown in Figure 2.

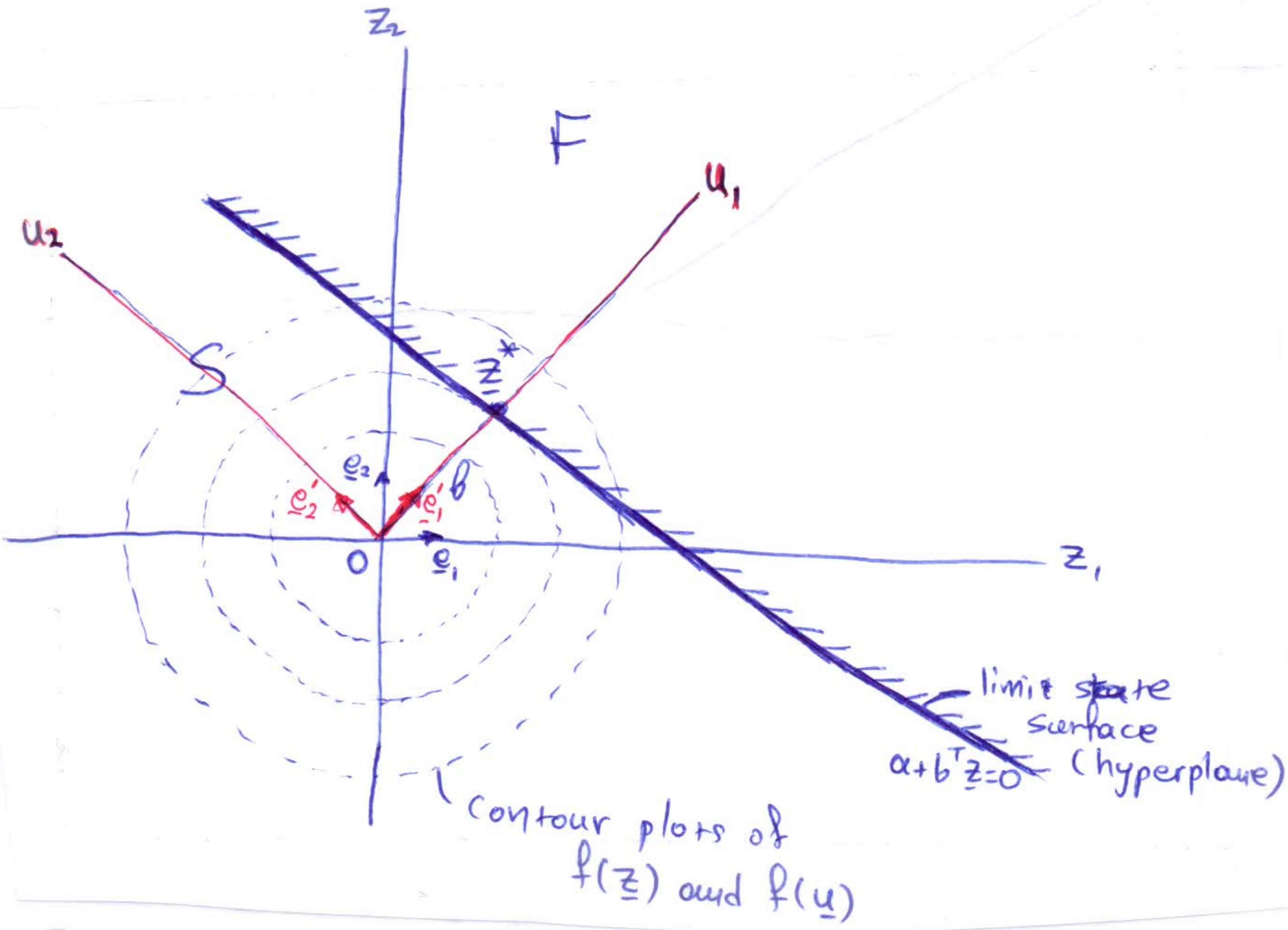

Figure 2: Hyper-plane and failure/safe domains for the two-dimensional space of standard Gaussian variables. Original and new coordinate system. Point on the hyperplane closest to origin.

The coordinates of the points in the n-dimensional space of parameters $\underline{z}$ are given with respect to the orthonormal basis (orthogonal unit vectors) $\{\underline{e}_1,\ldots,\underline{e}_n\}$. Introduce next a new orthonormal basis $\{\underline{e}_1',\ldots,\underline{e}_n'\}$ and let $\{u_1,\ldots,u_n\}$ be the coordinates of a point of the space in the new orthonormal basis. This basis is obtained by rotating the original orthonormal basis such that the unit vector $\underline{e}_1'$ and the axis u_1 is perpendicular to the hyperplane $h(\underline{z}) = a + \underline{b}^T \underline{z} = \underline{0}$. The subspace defined by the orthonormal basis $\{\underline{e}_2',\ldots,\underline{e}_n'\}$ belongs to this hyperplane. It is known from linear algebra that the coordinates $\underline{u}$ of a point in the space with respect to the new coordinate system (basis) are related to the coordinates $\underline{z}$ of the same point with respect to the original system by the transformation $\underline{u} = Q\underline{z}$, where Q is an orthonormal matrix satisfying $QQ^T = Q^T Q = I$ and $\det Q = |Q| = 1$. The transformation $\underline{u} = Q\underline{z}$ results in standard Gaussian variables $\underline{u} \sim N(0, I)$ since the transformation is linear, the mean $\underline{u}$ is $E[\underline{u}] = QE[\underline{z}] = Q\underline{0} = \underline{0}$ and the covariance matrix of $\underline{u}$ is $E[\underline{u}\underline{u}^T] = QE[\underline{z}\underline{z}^T]Q^T = QIQ^T = QQ^T = I$.

Let β be the minimum distance of the origin of the space from the hyperplane. A two-dimensional representation of the new system and the distance β is shown in Figure 2. It can easily be verified that the failure domain given by the points in space that satisfy $h(\underline{z}) = a + \underline{b}^T \underline{z} \geq \underline{0}$ can also by expressed in the new coordinate system by the points in space that satisfy $u_1 \geq \beta$ for any values of the other coordinates $u_2, \ldots, u_n$. Thus the probability of failure in (11) simplifies to

$$
\begin{aligned}
F &= \Pr[h(\underline{z}) \leq 0] = \int_{h(\underline{z}) \leq 0} f(\underline{z}) d\underline{z} = \int_{\substack{u_1 \geq \beta, \\ -\infty < u_i < \infty,\ i \geq 2}} f(\underline{u}) \det(Q) d\underline{u} \\
&= \int_{\substack{u_1 \geq \beta, \\ -\infty < u_i < \infty,\ i \geq 2}} \phi(u_1) \cdots \phi(u_n) du_1 \cdots du_n \\
&= \int_{u_1 \geq \beta} \phi(u_1) du_1 \left[\int \phi(u_2) du_2 \cdots \int \phi(u_n) du_n \right] = \int_{u_1 \geq \beta} \phi(u_1) du_1 = 1 - \Phi(\beta) \\
&= \Phi(-\beta)
\end{aligned}
\tag{12}
$$

Thus the failure probability in this case depends on the minimum distance β of the origin in the parameter space from the hyperplane. The variable β related to the safety of the system and is called the safety index. The point $\underline{z}^*$ (see Figure 2) on the hyperplane that is closest to the origin is obtained by minimizing the distance $\underline{z}\underline{z}^T$ of a point $\underline{z}$ in the parameter space subject to the constraint that the point $\underline{z}$ lies on the hyperplane. Specifically, introducing the Lagrange multiplier λ, this constrained optimization problem is formulated as unconstrained optimization problem of minimizing the augmented function

$$
J(\underline{z}, \lambda) = \underline{z}\underline{z}^T + \lambda(a + \underline{b}^T \underline{z})
$$

with respect to $\underline{z}$ and λ. The conditions for minimum are that

$$
\underline{\nabla} J(\underline{z}, \lambda) = \underline{z}^* + \lambda^* \underline{b} = \underline{0}
$$

and

$$
\frac{\partial J(\underline{z}, \lambda)}{\partial \lambda} = a + \underline{b}^T \underline{z}^* = \underline{0}
$$

Solving the first condition gives that $\underline{z}^* = -\lambda^* \underline{b}$ and substituting in the second condition one derives that $a + \underline{b}^T(-\lambda^* \underline{b}) = \underline{0}$ or equivalently that $\lambda^* = a/(\underline{b}^T \underline{b}) = a/|\underline{b}|^2$. As a result the point $\underline{z}^*$ of the hyperplane closest to the origin is $\underline{z}^* = -\lambda^* \underline{b} = -(a/|\underline{b}|^2)\underline{b}$. Thus the safety index β is given by

$$
\beta = |\underline{z}^*| = \frac{a}{|\underline{b}|^2} |\underline{b}| = \frac{a}{|\underline{b}|}
\tag{13}
$$