Probability of Detection Curves, Sensitivity Analysis and Kriging

Thomas BROWNE

EDF R&D-MRI Chatou - Université Paris 5

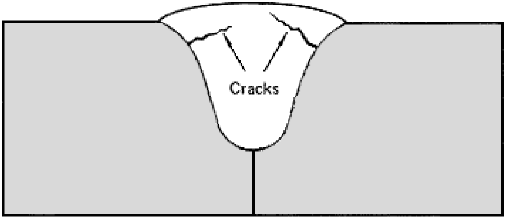
Supervisor: J-C. Fort (Paris 5)

Advisors: B. Iooss & L. Le Gratiet (EDF R&D-MRI Chatou)

Institut Henri Poincarré, Paris, France
March 22nd, 2017

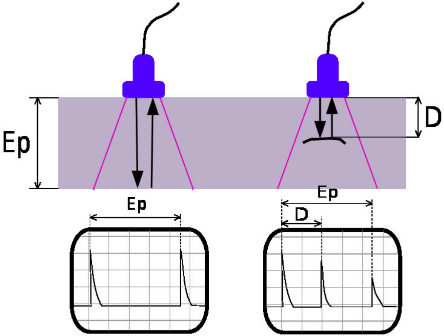
Context : Defect detection

Cracks in a Weld of a Pressurized Water Reactor



- Cracks can appear during the solidification of the weld
  ⇒ We perform Non-Destructive Tests !

Non-Destructive Tests : Ultrasounds



- No defect : record the sending and echo of the ultrasound.
- Defect : reflection of the wave on the defect.

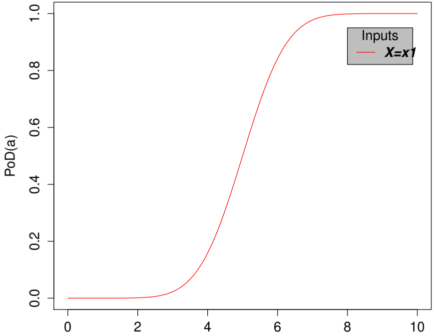
Review of the Influential Parameters

- $Y \in \mathbb{R}$: signal measure after NDT.
- $a > 0$: size of defect. Y is an increasing function of a.
- $X \in \mathbb{R}^d$: structure's geometrical properties, $(X_1, ..., X_d) \perp$.
- t_s : the defect is detected when $Y(a, X = x) > t_s$.
- Presence of an observation noise : $(a, x) \rightarrow Y(a, x)$ is STOCHASTIC !

PoD : Probability of Detection curve

- For a same defect $a > 0$, one can get $Y(a, X = x) > t_s$ and $Y(a, X = x) < t_s$.
- Hence : probability of detection (PoD), *i.e.* for $a > 0$

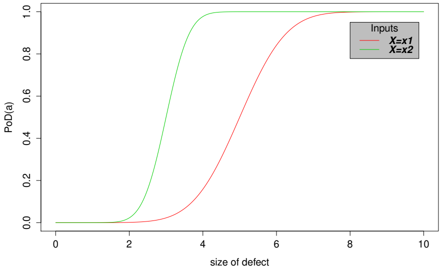
$$\forall a > 0 \quad \pi_{X=x_1}(a) \quad = \mathbb{P}\left(Y(a, X = x_1) > t_s \mid X = x_1\right)$$



PoD : Probability of Detection curve

- For a same defect $a > 0$, one can get $Y(a, X = x) > t_s$ and $Y(a, X = x) < t_s$.
- Hence : probability of detection (PoD), *i.e.* for $a > 0$

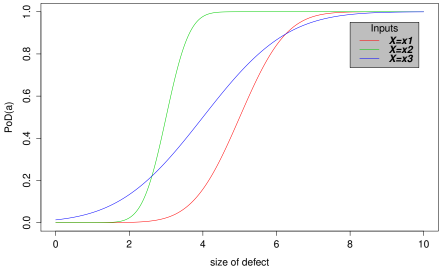
$$\forall a > 0 \quad \pi_{X=x_2}(a) \quad = \mathbb{P}_\delta \left(Y(a, X = x_2) > t_s \mid X = x_2 \right)$$



PoD : Probability of Detection curve

- For a same defect $a > 0$, one can get $Y(a, X = x) > t_s$ and $Y(a, X = x) < t_s$.
- Hence : probability of detection (PoD), *i.e.* for $a > 0$

$$\forall a > 0 \quad \pi_{X=x_3}(a) \quad = \mathbb{P}_\delta\left(Y(a, X = x_3) > t_s \mid X = x_3\right)$$



Random cumulative distribution functions

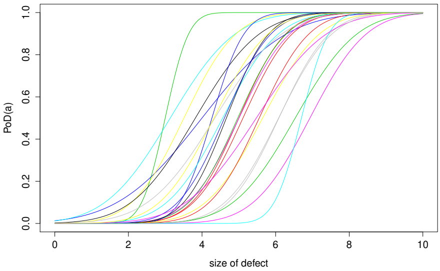


FIGURE: 20 realizations of π_X.

- π_X is a random curve - random CDF, function of X.
- Need to define tools to quantify a CDF random distribution.
- Wish to perform Sensitivity Analysis.

Contrast Functions

Y's feature : $\theta_\varphi(Y) := \arg\min_{\theta\in\mathbb{R}} \mathbb{E}_Y[\varphi(Y-\theta)]$.

- Simple contrasts : φ convex, $\forall (y,\theta) \in \mathbb{R}^2 \quad \varphi(y-\theta) \geq 0$

$\varphi(y-\theta) = m(y-\theta) = \mid y-\theta \mid^2$:

$\longrightarrow \theta_\varphi(Y) = \mathbb{E}[Y]$.

If, for $\alpha \in]0;1[$,
$\varphi(y-\theta) = c_\alpha(y-\theta) = (y-\theta)(\alpha - 1_{y\leq\theta})$:

$\longrightarrow \theta_\varphi(Y) = q^\alpha(Y)$, α-quantile of Y.

Contrast Extension to CDF's

$$\pi_X\textbf{'s feature : } \Theta_\varphi(\pi_X) := \arg\min_{F\in\mathcal{F}^2} \ \mathbb{E}_X[\psi_\varphi(\pi_X - F)].$$

- Real simple contrasts : $\forall y, \theta \in \mathbb{R} \quad \varphi(y-\theta)$

$\longrightarrow$ Simple CDF-contrasts :

$$\forall F, G \in \mathcal{F}^2 \quad \boxed{\psi_\varphi(F-G) = \min_{\substack{(X,Y)\ r.r.v.\\ X\sim F,\, Y\sim G}} \mathbb{E}_{(X,Y)}[\varphi(X-Y)].}$$

- Theorem(Cambanis) : for the simple contrasts m et c_α

$$\forall F, G \in \mathcal{F}^2 \quad \psi_\varphi(F-G) = \mathbb{E}_U[\varphi\left(F^{-1}(U) - G^{-1}(U)\right)] \quad U \sim \mathcal{U}([0,1])$$

$$= \int_0^1 \varphi\left(F^{-1}(u) - G^{-1}(u)\right) du.$$

N.B. : $F^{-1}(U) \sim F$!

CDF-Contrasts

π_X**'s feature :** $\Theta_\varphi(\pi_X) := \arg\min_{F \in \mathcal{F}^2} \mathbb{E}_X[\psi_\varphi(\pi_X - F)]$.

$$\forall u \in]0,1[, \quad \Theta_\varphi(\pi_X)^{-1}(u) = \arg\min_{\theta \in \mathbb{R}} \mathbb{E}[\varphi(\pi_X^{-1}(u) - \theta)] = \theta_\varphi\left(\pi_X^{-1}(u)\right)$$

PoD-mean :

$\varphi = m : \mathbb{E}[Y] \to \mathcal{E}(\pi_X)$

$\mathcal{E}(\pi_X)^{-1}(u) = \mathbb{E}_X\left[\pi_X^{-1}(u)\right]$

PoD-α-quantiles :

$\varphi = c_\alpha : q^\alpha(Y) \to \mathcal{Q}^\alpha(\pi_X)$

$\mathcal{Q}^\alpha(\pi_X)^{-1}(u) = q_X^\alpha\left(\pi_X^{-1}(u)\right)$.

PoD-mean & PoD-quantiles

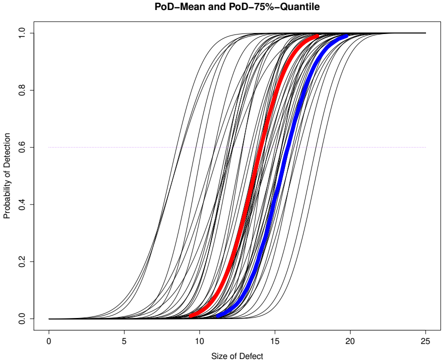


FIGURE: 25 realizations of π_X in black, $\mathcal{E}(\pi_X)$, and $\mathcal{Q}^{0.75}(\pi_X)$.

- PoD-mean : $\forall u \in]0,1[$

  $\mathcal{E}(\pi_X)^{-1}(u) = \mathbb{E}_X\left[\pi_X^{-1}(u)\right]$

- PoD-α-quantile : $\forall u \in]0,1[$

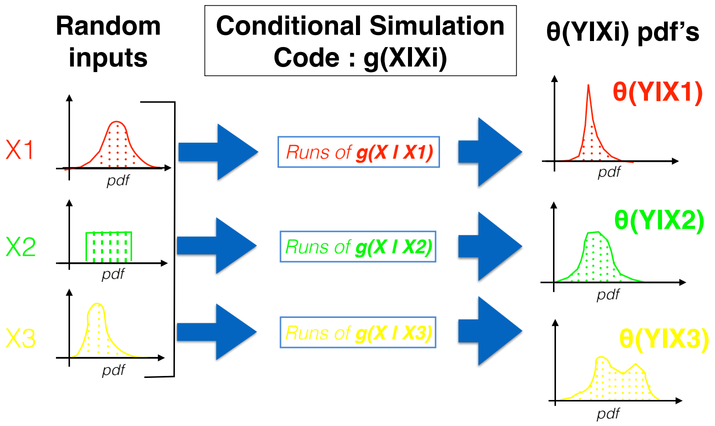
  $\mathcal{Q}^{\alpha}(\pi_X)^{-1}(u) = q_X^{\alpha}\left(\pi_X^{-1}(u)\right),$

  $\alpha = 0.75.$

1. PoD-Curve Definition
2. PoD-mean & PoD-quantiles
3. Sensitivity Analysis over PoD-Curves
4. PoD-Curves & Kriging

Goal-Oriented Sensitivity Analysis [N. Rachdi, 2011]

Respective Influence of Each Input over θ(Y)



Sensitivity Analysis with Respect to a Contrast

Need to quantify the variability of $\theta_\varphi(Y \mid X_i)$!

- Sensitivity indices based on contrasts [Fort et al., 2016]

$$
\begin{aligned}
S_\varphi^{X_i}(Y) &= \min_{\theta \in \mathbb{R}} \mathbb{E}\left[\varphi\left(Y, \theta\right)\right] - \mathbb{E}\left[\min_{\theta \in \mathbb{R}} \mathbb{E}\left[\varphi\left(Y, \theta\right) \mid X_i\right]\right] \\
&= \mathbb{E}\left[\varphi\left(Y, \theta(Y)\right)\right] - \mathbb{E}_{X_i}\left[\varphi\left(Y, \theta(Y \mid X_i)\right)\right].
\end{aligned}
$$

$\longrightarrow$ quantifies the variability of $\theta_\varphi(Y \mid X_i)$.

- If $\varphi(y-\theta) = (y-\theta)^2$, $S_\varphi^{X_i}(Y)$ is the Sobol index !

Indices' Properties

$$S_{\varphi}^{X_i}(Y) = \min_{\theta\in\mathbb{R}} \mathbb{E}\left[\varphi\left(Y,\theta\right)\right] - \mathbb{E}\left[\min_{\theta\in\mathbb{R}} \mathbb{E}\left[\varphi\left(Y,\theta\right) \mid X_i\right]\right]$$

- $S_{\varphi}^{X_i}(Y) \geq 0$.
- We divide $S_{\varphi}^{X_i}(Y)$ by $\min_{\theta\in\mathbb{R}} \mathbb{E}\left[\varphi\left(Y,\theta\right)\right]$ so that $0 \leq S_{\varphi}^{X_i}(Y) \leq 1$.
- We proved [Browne et al., 2017] :

  $S_{\varphi}^{X_i}(Y) = 0 \Leftrightarrow \theta_{\varphi}(Y \mid X_i) = \theta_{\varphi}(Y)$ *a.s.*

  $S_{\varphi}^{X_i}(Y) = 1 \Leftrightarrow (Y \mid X_i = x) = constant(x)$ *a.s.*

Sensitivity Analysis : Extension to Random CDF's

Need to quantify the variability of $\Theta_\varphi(\pi_X \mid X_i)$!

- Substitution : $\psi_\varphi \to \varphi$, $\pi_X \to Y$.
- $\mathcal{T}_\varphi^{Xi}(\pi_X) = \min_{G\in\mathcal{F}^2} \mathbb{E}\left[\psi_\varphi\left(\pi_X, G\right)\right] - \mathbb{E}\left[\min_{G\in\mathcal{F}^2} \mathbb{E}\left[\psi_\varphi\left(\pi_X, G\right) \mid X_i\right]\right].$
  - $\boxed{\mathcal{T}_\varphi^{Xi}(\pi_X) = \int_0^1 S_\varphi^{Xi}\left(\pi_X^{-1}\left(u\right)\right) du.}$

$\longrightarrow \mathcal{T}_\varphi^{Xi}(\pi_X)$ quantifies the variability of $\Theta_\varphi(\pi_X \mid X_i)$.

Numerical Experiments : Toy-Function

For $(X_1, X_2, X_3) \sim \mathcal{U}(-\pi, \pi)$ iid :

$$\boxed{Y(a, X) := a + \frac{3}{2}\left(\sin(X_1) + 7\sin(X_2)^2 + 0.1X_3^4\sin(X_1)\right) + \varepsilon(X),}$$

with $\varepsilon(x) \sim \mathcal{N}\left(0, \delta(x)^2\right)$, $\delta(x) := 2 + \frac{x_1+x_2+x_3}{6}$ and $t_s = 15$.

- PoD-mean-oriented Sensitivity Analysis
- PoD-quantiles-oriented Sensitivity Analysis

Toy-Function : SA over PoD-mean

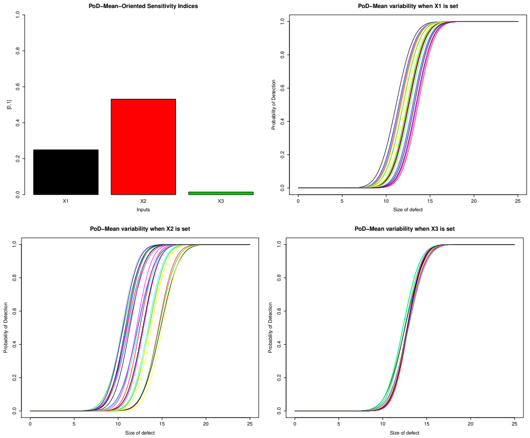


FIGURE: Sensitivity Analysis over $\mathcal{E}(\pi_X)$: Barplot of $\mathcal{T}_{\varphi}^{Xi}(\pi_X)$ and $\mathcal{E}(\pi_X \mid X_i)$, $i = 1, 2, 3$.

Toy-Function : SA over PoD-quantiles

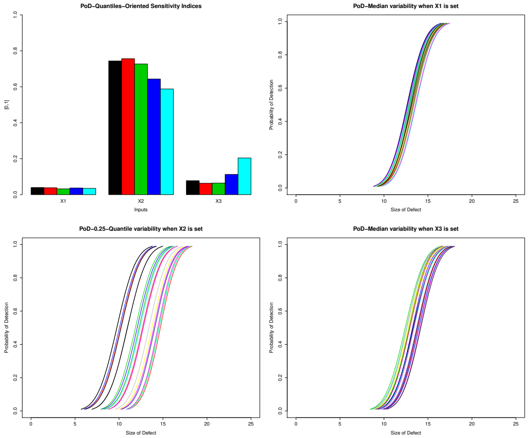


FIGURE: Sensitivity Analysis over $\mathcal{Q}^{\alpha}(\pi_X)$: Barplot of $\mathcal{T}_{\varphi}^{Xi}(\pi_X)$ with $\alpha = 0.1, 0.25, 0.5, 0.75$ and 0.9 and $\mathcal{Q}^{0.5}(\pi_X \mid X_i)$, $i = 1, 2, 3$.

PoD-curves & Kriging

Hypothesis :

$$Y(a,x) = \alpha_0 + \alpha_1 a + m(x) + \varepsilon(x),$$

with $\varepsilon(x) \sim \mathcal{N}\left(0, \delta^2(x)\right)$ the observation noise.

- Linear contribution of a
- Additive Gaussian Noise ε
- ε depends only on x.

PoD-curves & Kriging

Hypothesis :

$$\boxed{Y(a,x) = \alpha_0 + \alpha_1 a + m(x) + \varepsilon(x),}$$

with $\varepsilon(x) \sim \mathcal{N}\left(0, \delta^2(x)\right)$ the observation noise.

$$\begin{aligned} \forall a > 0 \qquad \pi_X(a) &= \mathbb{P}\left(\alpha_0 + \alpha_1 a + m(X) + \varepsilon(X) > t_s \mid X\right) \\ &= \Phi\left(\frac{\alpha_0 + \alpha_1 a + m(X) - t_s}{\delta(X)} \mid X\right), \quad \Phi \quad \text{CDF} \sim \mathcal{N}(0,1), \\ \forall u \in]0,1[\quad \pi_X^{-1}(u) &= \frac{t_s + \Phi^{-1}(u)\delta(X) - \alpha_0 - m(X)}{\alpha_1} \quad wrt\ X. \end{aligned}$$

PoD-curves & Kriging

Hypothesis :

$$\boxed{Y(a,x) = \alpha_0 + \alpha_1 a + m(x) + \varepsilon(x),}$$

with $\varepsilon(x) \sim \mathcal{N}\left(0, \delta^2\left(x\right)\right)$ the observation noise.

$$\begin{aligned}
\forall u \in]0,1[\quad \mathcal{E}\left(\pi_X\right)^{-1}(u) &= \mathbb{E}_X\left[\pi_X^{-1}(u)\right] \\
&= \frac{t_s + \Phi^{-1}(u)\mathbb{E}_X[\delta(X)] - \alpha_0 - \mathbb{E}_X[m(X)]}{\alpha_1} \\
\mathcal{Q}^\alpha\left(\pi_X\right)^{-1}(u) &= q_X^\alpha\left(\pi_X^{-1}(u)\right) \\
&= \frac{t_s - \alpha_0 + q_X^\alpha\left(\Phi^{-1}(u)\delta(X) - m(X)\right)}{\alpha_1}
\end{aligned}$$

PoD-Curves & Kriging

Hypothesis :

$$\boxed{Y(a,x) = \alpha_0 + \alpha_1 a + m(x) + \varepsilon(x),}$$

with $\varepsilon(x) \sim \mathcal{N}\left(0, \delta^2(x)\right)$ the observation noise.

- Assumptions : $(x \to m(x)) \sim \mathcal{GP}\left(\mu_m(\cdot), \sigma_m(\cdot,\cdot)\right)$, with $\sigma_m(x,x') = \Delta_m^2 K_m(x,x')$ and $K_m(x,x) = 1$.
- Assumptions : $(x \to \delta(x)) \sim \mathcal{GP}\left(\mu_\delta(\cdot), \sigma_\delta(\cdot,\cdot)\right)$, with $\sigma_\delta(x,x') = \Delta_\delta^2 K_\delta(x,x')$ and $K_\delta(x,x) = 1$.
- Assumptions : $Z_m \perp Z_\delta$.

Joint Metamodels Approach [Marrel et al., 2012]...

PoD-curves & Kriging : Predicators

$$\boxed{Y(a,x) = \alpha_0 + \alpha_1 a + m(x) + \varepsilon(x),}$$

with $\varepsilon(x) \sim \mathcal{N}\left(0, \delta^2(x)\right)$ the observation noise.

- Deterministic Kriging : $(\delta(\cdot) \mid \mathcal{D}) \sim \mathcal{GP}\left(\hat{\delta}(\cdot), \hat{\sigma}_\delta(\cdot,\cdot)\right)$,

  with $\hat{\delta}(x) = \mathbb{E}\left[Z_\delta(x) \mid \mathcal{D}\right]$, $\hat{\sigma}_\delta(x,x') = \mathrm{Cov}\left[Z_\delta(x), Z_\delta(x') \mid \mathcal{D}\right]$.

- Stochastic Kriging : $(m(\cdot) \mid \mathcal{D}) \sim \mathcal{GP}\left(\hat{m}(\cdot), \hat{\sigma}(\cdot,\cdot)\right)$,

  with $\hat{m}(x) = \mathbb{E}\left[Z_m(x) \mid \mathcal{D}\right]$, $\hat{\sigma}_m(x,x') = \mathrm{Cov}\left[Z_m(x), Z_m(x') \mid \mathcal{D}\right]$.

PoD-curve Estimates

$$\boxed{Y(a,x) = \alpha_0 + \alpha_1 a + m(x) + \varepsilon(x).}$$

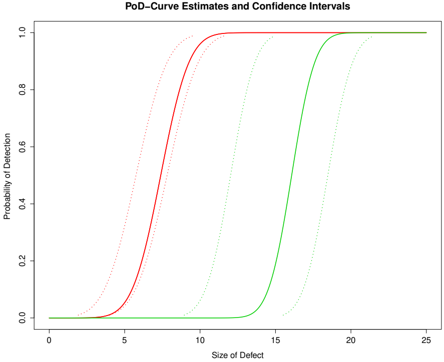
Kriging PoD-Curve Estimators :

$$\forall u \in]0,1[\quad \hat{\pi}_X^{-1}(u) = \frac{t_s + \Phi^{-1}(u)\hat{\delta}(X) - \alpha_0 - \hat{m}(X)}{\alpha_1} \quad wrt\ X.$$

$$\widehat{\mathcal{E}}_X\left(\pi_X\right)^{-1}(u) = \frac{t_s + \Phi^{-1}(u)\bar{\hat{\delta}}(X) - \alpha_0 - \bar{\hat{m}}(X)}{\alpha_1}.$$

$$\widehat{\mathcal{Q}}^{\alpha}\left(\pi_X\right)^{-1}(u) = \frac{t_s - \alpha_0 + \hat{q}^{\alpha}\left(\Phi^{-1}(u)\hat{\delta}(X) - \hat{m}(X)\right)}{\alpha_1}.$$

PoD-curve Estimates



- Kriging prediction :

$$\forall x \in \chi \quad \forall u \in]0,1[$$

$$\pi_x^{-1}(u) =$$

$$\frac{t_s + \Phi^{-1}(u)\delta(X) - \alpha_0 - m(X)}{\alpha_1}$$

$$\sim \mathcal{N}\left(\hat{\pi}_x^{-1}(u), \frac{\Phi^{-1}(u)^2\hat{\sigma}_\delta^2 + \hat{\sigma}_m^2}{\alpha_1^2}\right).$$

- x_1, x_2 realizations of X :

π_{x_1} and π_{x_2}.

- 95%-Pointwise Confidence Bounds

Conclusion

PoD-curves are fun !

- Kriging $\times$ Sensitivity Analysis
- Applications to an industrial simulator : ATHENA_2D
- Kriging $\longrightarrow$ Sequential Design, Optimization Problems...

Browne, T., Fort, J. C., Iooss, B., & Le Gratiet, L. (2017).
Estimate of quantile-oriented sensitivity indices.
Submitted, 2017

Browne T., Iooss B., Le Gratiet L., Lonchampt J., Remy E. (2017).
Stochastic simulators based optimization by Gaussian process metamodels - Application to maintenance investments planning issues
Quality and Reliability Engineering International, 32(6), 2067-2080.

J. C. Fort, T. Klein, N. Rachdi (2016).
New sensitivity analysis subordinated to a contrast
Communication in Statistics : Theory and Methods, 45(15), 4349-4364.

N. Rachdi
Statistical Learning and Computer Experiments
PhD thesis, Université Paul Sabatier, France, 2011.

Marrel A., Iooss B., Da Veiga S., Ribatet M. (2012).
Global Sensitivity Analysis of Stochastic Computer Models with Joint Metamodels
Statistics and Computing, 22(3), 833-847, Springer.

Kanishcheva K. (2014).
Statistical estimation of the PoD in a numerical experiments context
Master's degree thesis, Airbus Group.

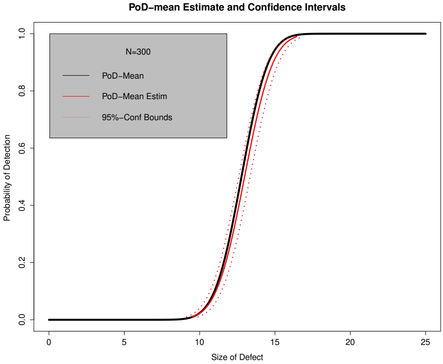
Le Gratiet L., Iooss B., Blatman G., Browne T., Cordeiro S., Goursaud B. (2017).
Model Assisted Probability of Detection curves : New statistical tools and progressive methodology
Journal of Nondestructive Evaluation, 36, 1 : 8, Springer.

Thank you for your attention !

PoD-curves & Kriging

- Numerical Experiments : $n \in \mathbb{N}$ inputs $\{(a^1, x^1), \ldots, (a^n, x^n)\}$.
- Noise : $\forall j = 1, \ldots, n$, $M \in \mathbb{N}$ replicates on $Y\left(a^j, x^j\right)_{j=1,\ldots,n}$: $\left(Y^{j,k}\right)_{1 \leq k \leq M}$.
- Estimator for $m(x^j)$: $\tilde{m}(x^j) := \frac{1}{M}\sum_{k=1}^{M} Y^{j,k} - \alpha_0 - \alpha_1 a^j$.
- Noise Standard Deviation : $\delta(x^j) \simeq \text{sd}\left(\left(Y^{j,k}\right)_{1 \leq k \leq M}\right)$.

PoD-mean & Confidence Bounds



- 2 sources of error
- Kriging Error : $\hat{\delta}$, $\hat{m}$.
- Monte-Carlo Error :
  $\bar{\hat{\delta}}(X) \simeq \mathbb{E}[\hat{\delta}(X)]$ and $\bar{\hat{m}}(X) \simeq \mathbb{E}[\hat{m}(X)]$.
- Bootstrap over the Confidence Bounds.