# Stability of BRDFs Gaussian Process Kriging

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February 1, 2018

## 1 Notations and summary

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|---|---|
| $\mathbf{e}_i$ | $i^{\text{th}}$ vector of the canonical basis |
| $\{\mathbf{x}_0,\dots,\mathbf{x}_n\}$ | latent variables |
| $\mathbf{z}_*(\mathbf{x})$ | interpolated BRDF at latent point $\mathbf{x}$ |
| $\mathbf{z}_*(\mathbf{x}_i),\mathbf{z}_i$ | input BRDF at latent point $\mathbf{x}_i$ |
| $\mathbf{K}$ | covariance matrix |
| $\kappa(\mathbf{K})$ | condition number of the covariance matrix |
| $\mathbf{k}_i^\intercal$ | $i^{th}$ line of matrix $\mathbf{K}$ |
| $\mathbf{k}_*(\mathbf{x})$ | covariance vector with $i^{th}$ component $c(\mathbf{x},\mathbf{x}_i)$ |
| $\delta\mathbf{k}_i(\mathbf{x})$ | defined as the difference $\mathbf{k}_*(\mathbf{x})-\mathbf{k}_i$ |
| $\mathbf{Z}$ | matrix of input BRDF data, with lines $\mathbf{z}_i$ |
| $\|\mathbf{x}\|$ | $L_2$ norm of vector $\mathbf{x}$ |
| $\|\mathbf{Z}\|$ | Frobenius norm of matrix $\mathbf{Z}$ |

We study the krigging value of the Gaussian Process defined by:

$$\mathbf{z}_*(\mathbf{x}) = \mathbf{k}_*^\intercal(\mathbf{x})\mathbf{K}^{-1}\mathbf{Z} \tag{1}$$

and prove the following two theorems:

**Theorem 1.** *For every point* $\mathbf{x}$ *in the latent space, we have*

$$\forall \mathbf{x}\ \ \exists \beta(\mathbf{x}) \in \{1,\dots,n\}\ \ \|\mathbf{z}_*(\mathbf{x})-\mathbf{z}_{\beta(\mathbf{x})}\| \leq \kappa(\mathbf{K})\|\mathbf{Z}\|\min_i \|\delta\mathbf{k}_i(\mathbf{x})\|. \tag{2}$$

*This bound expresses that the value of $f$ at any $x$ in between the latent variables stays in the vicinity of the value $\mathbf{z}_i$ for at least one latent point $\mathbf{x}_i$. In practice this point is the data point in the latent space that is closest to $\mathbf{x}$.*

**Theorem 2.** *Supposing that the covariance function $c$ is a Gaussian with variance $\ell$ defined by*

$$c(\mathbf{x},\mathbf{y}) = e^{-\|\mathbf{x}-\mathbf{y}\|/\ell^2},$$

*the bound in theorem 1 becomes*

$$\|\mathbf{z}_*(\mathbf{x})-\mathbf{z}_{\beta(\mathbf{x})}\| \leq \kappa(\mathbf{K})\|\mathbf{Z}\|\frac{\sqrt{2n}}{\ell}e^{-1/2}\|\mathbf{x}-\mathbf{x}_{\beta(\mathbf{x})}\|. \tag{3}$$

## 2 Derivation of inequality 2

We examine the behavior of the interpolant defined by Equation 1 in the region around a particular training data point $\mathbf{x}_i$. In order to derive an argument for stability, we study how much $\mathbf{k}_*(\mathbf{x})\mathbf{K}^{-1}$ depends on $\mathbf{x} = \mathbf{x}_i + \delta\mathbf{x}$ around $\mathbf{x}_i$.

Following the definition of $\mathbf{K}$ we have

$$\mathbf{k}_*(\mathbf{x}_i) = \mathbf{k}_i.$$

And consequently

$$\begin{aligned} \mathbf{z}_*(\mathbf{x}_i+\delta\mathbf{x}) - \mathbf{z}_*(\mathbf{x}_i) &= \mathbf{k}_*^{\intercal}(\mathbf{x}_i+\delta\mathbf{x})\mathbf{K}^{-1}\mathbf{Z} - \mathbf{k}_*(\mathbf{x}_i)\mathbf{K}^{-1}\mathbf{Z} \\ &= (\mathbf{k}_*^{\intercal}(\mathbf{x}_i+\delta\mathbf{x}) - \mathbf{k}_*^{\intercal}(\mathbf{x}_i))\mathbf{K}^{-1}\mathbf{Z} \end{aligned} \tag{4}$$

We denote the perturbation $\delta\mathbf{k}$ of $\mathbf{k}_*(\mathbf{x}_i)$ around $k_i$, that is defined by

$$\mathbf{k}_*(\mathbf{x}_i+\delta\mathbf{x}) = \mathbf{k}_i + \delta\mathbf{k}.$$

Since $\mathbf{k}_i^{\intercal}\mathbf{K}^{-1} = \mathbf{e}_i$, we define $\delta\mathbf{e}$ as:

$$(\delta\mathbf{k} + \mathbf{k}_i)^{\intercal}\mathbf{K}^{-1} = \delta\mathbf{e} + \mathbf{e}_i \tag{5}$$

We use the following theorem:

**Theorem 3** (Atkinson'1989)**.** *Let* $\mathbf{x}$ *be the solution to a non degenerate linear system* $\mathbf{A}\mathbf{x} = b$*. The solution of the perturbated linear system* $(\mathbf{A}+\delta\mathbf{A})(\mathbf{x}+\delta\mathbf{x}) = (\mathbf{b}+\delta b)$ *verifies:*

$$\frac{\|\delta\mathbf{x}\|}{\|\mathbf{x}\|} \leq \frac{\kappa(\mathbf{A})}{1-\kappa(\mathbf{A})\frac{\|\delta\mathbf{A}\|}{\|\mathbf{A}\|}}\left(\frac{\|\delta\mathbf{A}\|}{\|\mathbf{A}\|} + \frac{\|\delta\mathbf{b}\|}{\|\mathbf{b}\|}\right)$$

*where* $\kappa(\mathbf{A})$ *is the condition number of* $\mathbf{A}$ *induced by the norm* $\|.\|$*, and defined by* $\kappa(\mathbf{A}) = \|\mathbf{A}\|\|\mathbf{A}^{-1}\|$.

Applying this theorem to Equation 5, taking $\mathbf{A} = \mathbf{K}, b = \mathbf{k}_i, \delta b = \delta\mathbf{k}_i, \mathbf{x} = \mathbf{e}_i$ and $\delta\mathbf{x} = \delta\mathbf{e}$, we have:

$$\frac{\|\delta\mathbf{e}\|}{\|\mathbf{e}_i\|} \leq \kappa(\mathbf{K})\frac{\|\delta\mathbf{k}_i\|}{\|\mathbf{k}_i\|}$$

Using this in Equation 4, we use the fact that $\mathbf{K}^{-1}\mathbf{Z}$ is a vector, and that $\|\mathbf{e}_i\| = 1$, in order to get:

$$\begin{aligned} |\mathbf{z}_*(\mathbf{x}_i+\delta\mathbf{x}) - \mathbf{z}_*(\mathbf{x}_i)| &\leq \|\underbrace{(\mathbf{k}_*^{\intercal}(\mathbf{x}_i+\delta\mathbf{x}) - \mathbf{k}_*^{\intercal}(\mathbf{x}_i))\,\mathbf{K}^{-1}}_{\delta\mathbf{e}}\|\|\mathbf{Z}\| \\ &\leq \kappa(\mathbf{K})\frac{\|\delta\mathbf{k}_i\|}{\|\mathbf{k}_i\|}\|\mathbf{Z}\| \end{aligned}$$

Now if we consider a point $\mathbf{x}$ in the latent space and denote $\mathbf{x}_{\beta(\mathbf{x})}$ the training point for which the right member is the smallest (in practice, this is likely to happen for the point $\mathbf{x}_i$ that is closest to $\mathbf{x}$), we have

$$|\mathbf{z}_*(\mathbf{x}) - \mathbf{z}_*(\mathbf{x}_{\beta(\mathbf{x})})| \leq \kappa(\mathbf{K}) \|\mathbf{Z}\| \min_i \frac{\|\delta \mathbf{k}_i(\mathbf{x})\|}{\|\mathbf{k}_i\|}.$$

Combining this with the fact that $\|\mathbf{k}_i\| \geq 1$, and noting that $\mathbf{z}_*(\mathbf{x}_{\beta(\mathbf{x})}) = \mathbf{z}_{\beta(\mathbf{x})}$, completes the proof.

# 3 Derivation of inequality 3

Using the continuity of the interpolant, if we bound the first derivative of $\delta\mathbf{k}_i(x)$ over the entire domain, we obtain

$$\|\delta \mathbf{k}_i(x)\| \leq \|\mathbf{x} - \mathbf{x}_i\| \sup_{\mathbf{x}} \|\nabla \mathbf{k}_*(\mathbf{x})\|.$$

Similarly, if we can bound the second derivative of $\delta\mathbf{k}_i(x)$ over the entire domain, we obtain

$$\|\delta \mathbf{k}_i(x)\| \leq \|\mathbf{x} - \mathbf{x}_i\| \|\nabla \mathbf{k}_*(\mathbf{x}_i)\| + \|\mathbf{x} - \mathbf{x}_i\|^2 \sup_{\mathbf{x}} \|\mathrm{tr}(H(\mathbf{k}_*)(\mathbf{x}))\|,$$

where $H$ is the Heassian of $\mathbf{k}_*$. Since the covariance $c$ is defined using a Gaussian as

$$c(\mathbf{x}, \mathbf{y}) = g(\|\mathbf{x} - \mathbf{y}\|) \quad \text{with} \quad g(x) = e^{-x^2/\ell^2},$$

the first and second derivatives of $g$ are bounded over the entire domain by:

$$-\frac{\sqrt{2}}{\ell} e^{-1/2} \leq g'(x) \leq \frac{\sqrt{2}}{\ell} e^{-1/2} \quad \text{and} \quad -\frac{2}{\ell^2} \leq g''(x) \leq \frac{4}{\ell^2} e^{-3/2}$$

We have consequently for all $i$

$$\|\delta \mathbf{k}_i(\mathbf{x})\| \leq \sqrt{2n} \frac{1}{\ell} e^{-1/2} \|\mathbf{x} - \mathbf{x}_i\|, \tag{6}$$

which completes the proof. Similarly we can use the bound over the second derivative to obtain a much tighter bound, that necessitates to compute $\|\nabla \mathbf{k}_*(\mathbf{x}_i)\|$:

$$\|\delta \mathbf{k}_i(\mathbf{x})\| \leq \|\mathbf{x} - \mathbf{x}_i\| \|\nabla \mathbf{k}_*(\mathbf{x}_i)\| + \frac{4}{\ell^2} e^{-3/2} \|\mathbf{x} - \mathbf{x}_i\|^2. \tag{7}$$