Uncertainty Quantification and Quasi-Monte Carlo

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Practical matters

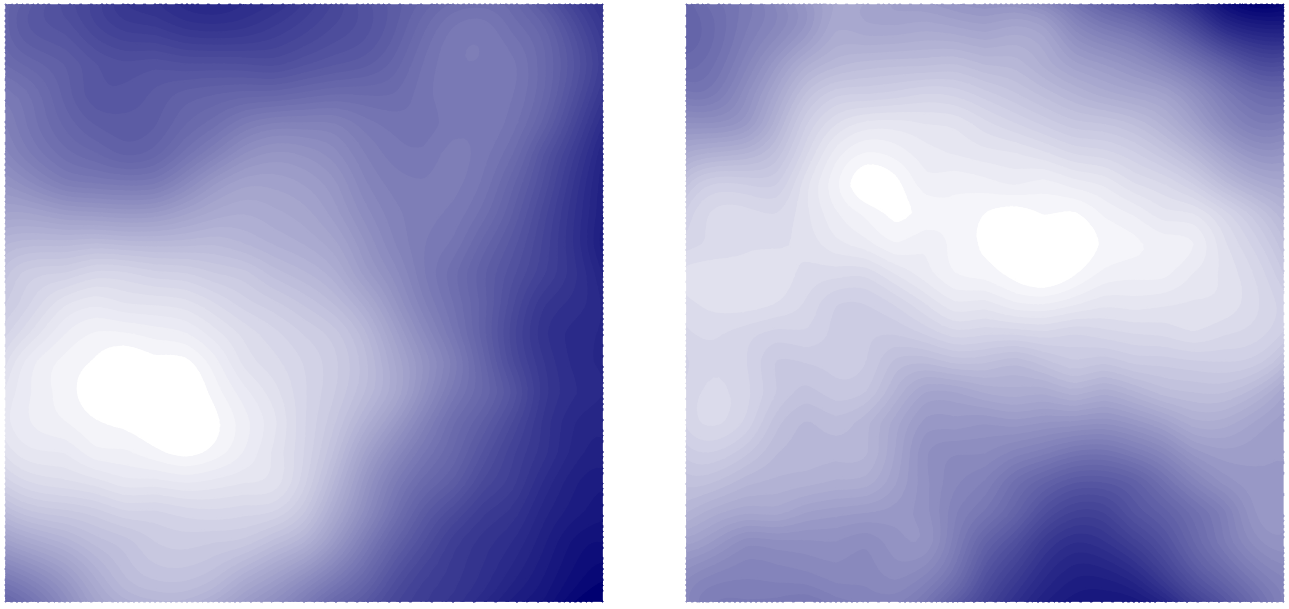
- Lectures on Mondays at 12.15-14.00 in A6/SR009 by Vesa Kaarnioja.
- Exercises on Tuesdays at 12.15-14.00 in A3/SR115 by Vesa Kaarnioja starting next week.
- Weekly exercises published after the lecture. Please return your written solutions to Vesa either by email (vesa.kaarnioja@fu-berlin.de) or at the beginning of the exercise session in the following week.
- The conditions for completing this course are *successfully completing and submitting at least 60% of the course's exercises* and *successfully passing the course exam.*

Uncertainty in groundwater flow

Risk analysis of radwaste disposal or CO_2 sequestration.

Darcy's law	$\boldsymbol{q}(\boldsymbol{x}) + \boldsymbol{a}(\boldsymbol{x})\nabla \boldsymbol{p}(\boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{x})$
mass conservation law	$\nabla \cdot \boldsymbol{q}(\boldsymbol{x}) = 0$

in $D \subset \mathbb{R}^d$, $d \in \{1, 2, 3\}$
together with boundary conditions

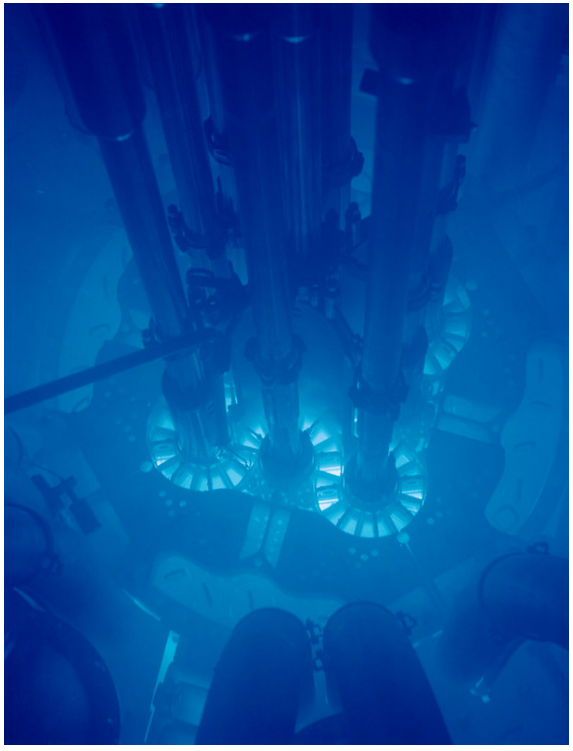


Uncertainty in $\boldsymbol{a}(\boldsymbol{x}, \omega)$ leads to uncertainty in $\boldsymbol{q}(\boldsymbol{x}, \omega)$ and $\boldsymbol{p}(\boldsymbol{x}, \omega)$

Criticality problem for nuclear reactors

$$-\nabla \cdot (\underbrace{a(\boldsymbol{x})}_{\text{diffusion}} \nabla u(\boldsymbol{x})) + \underbrace{b(\boldsymbol{x})}_{\text{absorption}} u(\boldsymbol{x}) = \lambda \underbrace{c(\boldsymbol{x})}_{\text{fission}} u(\boldsymbol{x})$$

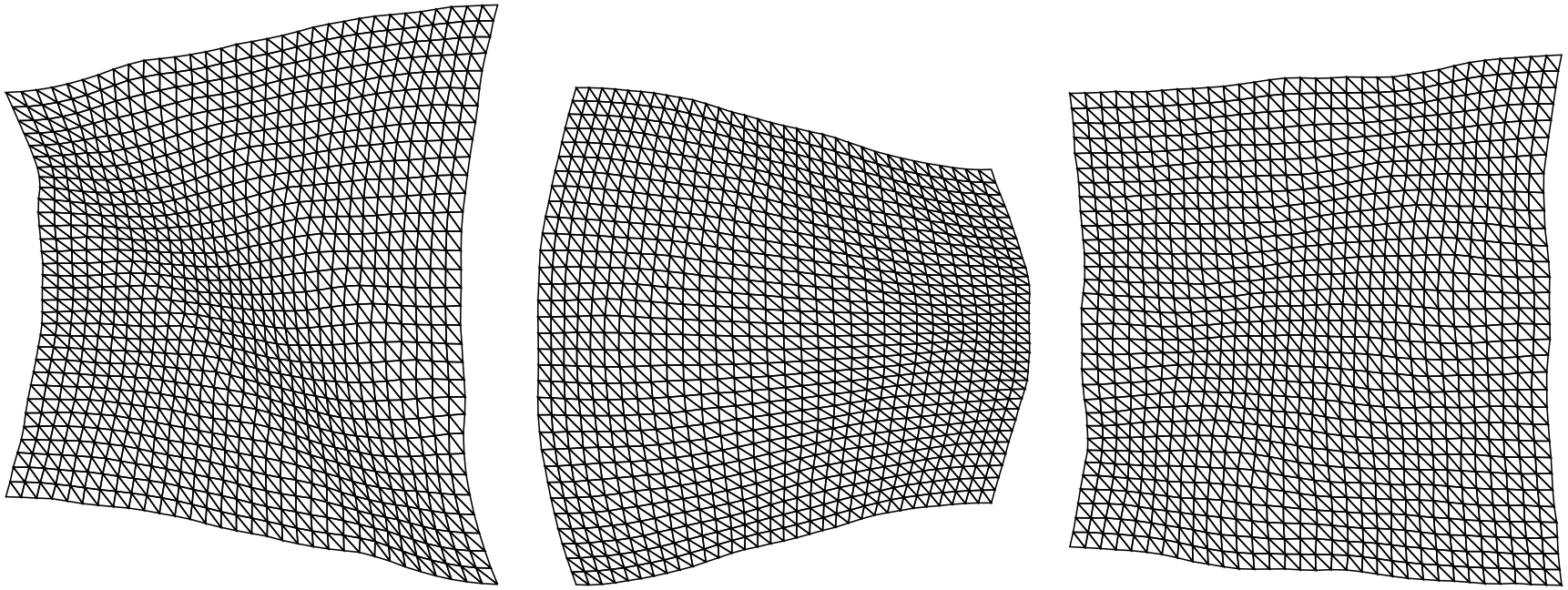
- The smallest eigenvalue $\lambda_1 \in \mathbb{R}$ measures *criticality* of a reactor.
- Eigenfunction $u_1(\boldsymbol{x})$ is the *neutron flux* at the point $\boldsymbol{x}$.



Source: Argonne National Laboratory on Flickr

- $\lambda_1 \approx 1 \Rightarrow$ operating efficiently
- $\lambda_1 > 1 \Rightarrow$ not self-sustaining
- $\lambda_1 < 1 \Rightarrow$ supercritical

Domain uncertainty quantification

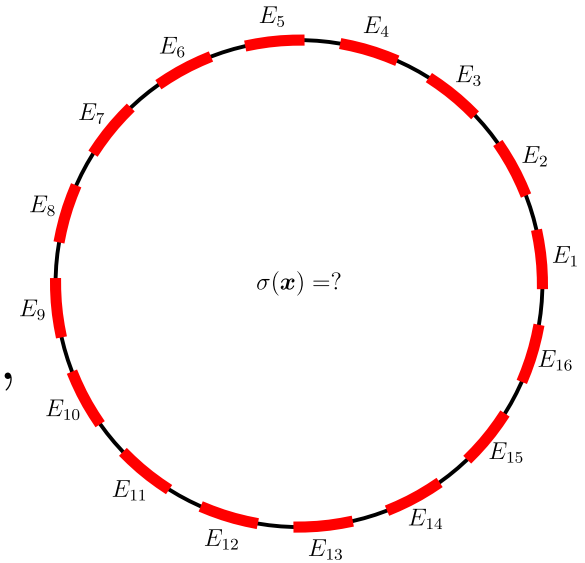


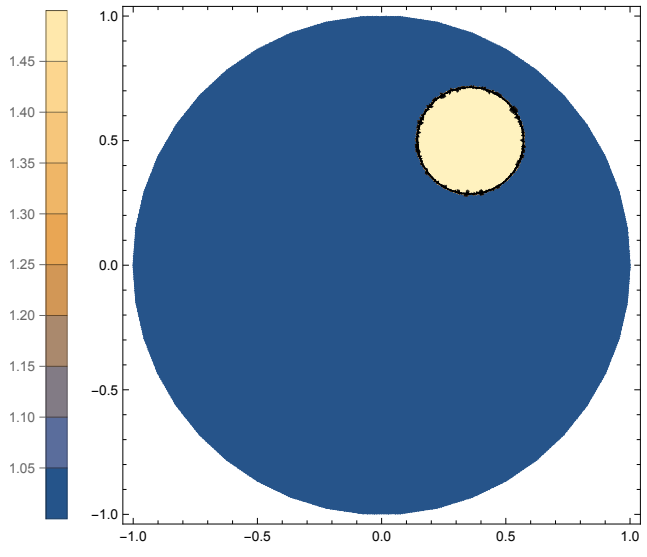
Three realizations of a random spatial domain

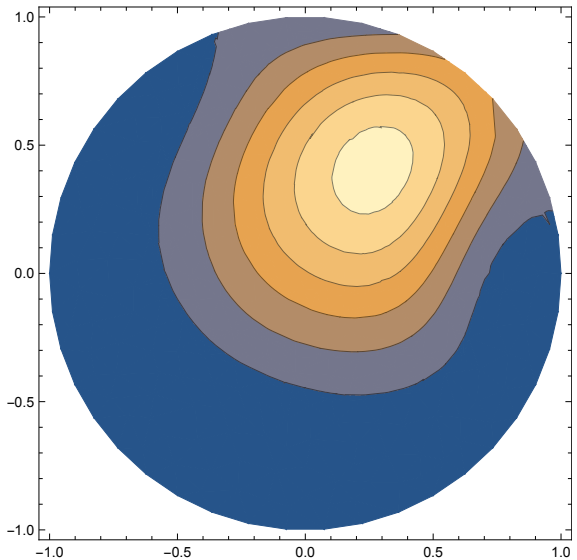
Electrical impedance tomography

Use measurements of current and voltage collected at electrodes covering part of the boundary to infer the interior conductivity of an object/body.

$$\begin{cases} \nabla \cdot (\sigma \nabla u) = 0 & \text{in } D, \\ \sigma \frac{\partial u}{\partial \boldsymbol{n}} = 0 & \text{on } \partial D \setminus \bigcup_{k=1}^{L} \overline{E_k}, \\ u + z_k \sigma \frac{\partial u}{\partial \boldsymbol{n}} = U_k & \text{on } E_k, \ k \in \{1, \ldots, L\}, \\ \int_{E_k} \sigma \frac{\partial u}{\partial \boldsymbol{n}} \, \mathrm{d}S = I_k, & k \in \{1, \ldots, L\}, \end{cases}$$







Consider the elliptic PDE problem:

$$\begin{cases} -\nabla \cdot \big(a(\boldsymbol{x}) \nabla u(\boldsymbol{x})\big) = f(\boldsymbol{x}) \quad \text{for } \boldsymbol{x} \in D, \\ +\text{boundary conditions.} \end{cases}$$

In practice, one or several of the material/system parameters may be uncertain or incompletely known and modeled as random fields:

- PDE coefficient a may be uncertain;
- Source term f may be uncertain;
- Boundary conditions may be uncertain;
- The domain D itself may be uncertain.

In forward uncertainty quantification, one is interested in assessing how uncertainties in the inputs of a mathematical model affect the output.
$\Rightarrow$ If the uncertain inputs are modeled as random fields, then the output of the PDE is also a random field. One may be interested in assessing the statistical response of the system, for example, the expectation or variance of the PDE solution (or some other quantity of interest thereof).

High-dimensional numerical integration

$$\int_{[0,1]^s} f(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \approx \sum_{i=1}^{n} w_i f(\boldsymbol{t}_i)$$

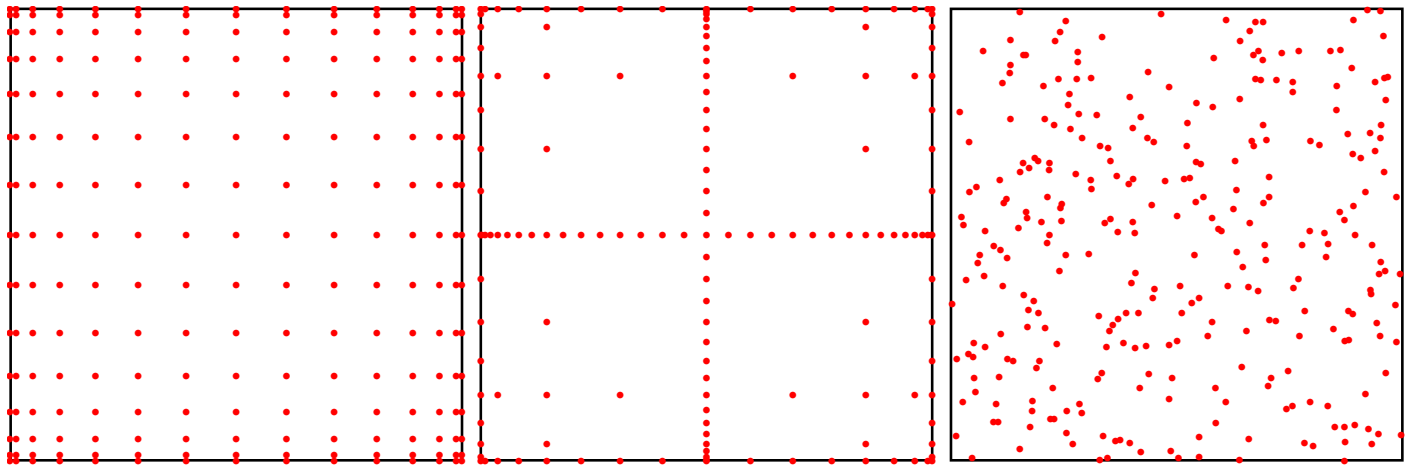


Figure: Tensor product grid, sparse grid, Monte Carlo nodes (not QMC rules)

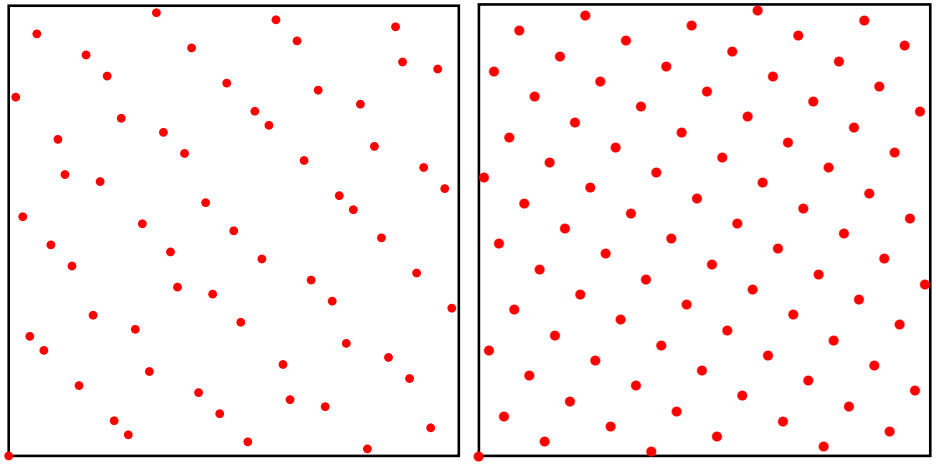


Figure: Sobol′ points, lattice rule (examples of QMC rules)

Quasi-Monte Carlo (QMC) methods are a class of *equal weight* cubature rules

$$\int_{[0,1]^s} f(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \approx \frac{1}{n}\sum_{i=1}^{n} f(\boldsymbol{t}_i),$$

where $(\boldsymbol{t}_i)_{i=1}^n$ is an ensemble of *deterministic* nodes in $[0,1]^s$.

The nodes $(\boldsymbol{t}_i)_{i=1}^n$ are NOT random! Instead, they are *deterministically chosen*.

QMC methods exploit the smoothness and anisotropy of an integrand in order to achieve better-than-Monte Carlo rates.

Course contents

- Preliminaries: Hilbert spaces, Sobolev spaces, elliptic partial differential equations (PDEs)
- Finite element (FE) method
- Modeling random field inputs
- Elliptic PDEs with random coefficients
- Quasi-Monte Carlo (QMC) methods
- QMC-FE methods for forward and inverse uncertainty quantification for elliptic PDEs with random coefficients
- Additional topics: multilevel methods and variance reduction, higher-order QMC, domain UQ, ...

Preliminary functional analysis

Inner product space

A real vector space X is an *inner product space* if there exists a mapping $\langle \cdot, \cdot \rangle : X \times X \to \mathbb{R}$ satisfying

- $\langle ax_1 + bx_2, y \rangle = a\langle x_1, y \rangle + b\langle x_2, y \rangle$ for all $x_1, x_2, y \in X$ and $a, b \in \mathbb{R}$;
- $\langle x, y \rangle = \langle y, x \rangle$ for all $x, y \in X$;
- $\langle x, x \rangle \geq 0$ for all $x \in X$, where equality holds iff $x = 0$.

A mapping $\langle \cdot, \cdot \rangle$ satisfying these conditions is called an *inner product*.

Example

i) $\mathbb{R}^n = \{(x_1, \ldots, x_n) \mid x_k \in \mathbb{R}\}$. Then the inner product is the Euclidean dot product

$$\langle x, y \rangle = \sum_{k=1}^{n} x_k y_k, \quad x = (x_1, \ldots, x_n),\ y = (y_1, \ldots, y_n).$$

ii) Let $X = C([a, b]) = \{f \mid f : [a, b] \to \mathbb{R} \text{ is continuous}\}$ and define

$$\langle f, g \rangle = \int_a^b f(x)g(x)\,\mathrm{d}x.$$

Then this is an inner product on $C([a, b])$.

iii) Let $X = \ell^2(\mathbb{R}) = \left\{(z_k)_{k=1}^{\infty} \mid \sum_{k=1}^{\infty} |z_k|^2 < \infty\right\}$. Then $\ell^2(\mathbb{R})$ is an inner product space when

$$\langle x, y \rangle = \sum_{k=1}^{\infty} x_k y_k, \quad x = (x_1, x_2, \ldots),\ y = (y_1, y_2, \ldots).$$

Definition

A real vector space X is a *normed space* if there exists a mapping $\|\cdot\| : X \to \mathbb{R}$ satisfying

- $\|ax\| = |a|\|x\|$ for all $a \in \mathbb{R}$ and $x \in X$;
- $\|x\| \geq 0$ for all $x \in X$, where equality holds iff $x = 0$.
- $\|x + y\| \leq \|x\| + \|y\|$ for all $x, y \in X$ (triangle inequality).

If X is an inner product space, then it is a normed space in a canonical way with the induced norm $\|\cdot\| : X \to \mathbb{R}$ defined by

$$\|x\| = \sqrt{\langle x, x \rangle}, \quad x \in X.$$

The first two postulates follow immediately from the properties of inner product spaces, the triangle inequality follows from the Cauchy–Schwarz inequality.

Proposition (Cauchy–Schwarz inequality)

If $(X, \langle \cdot, \cdot \rangle)$ *is an inner product space, then*

$$|\langle x, y \rangle| \leq \|x\|\|y\| \quad \textit{for all } x, y \in X.$$

Proof. Let $x, y \in X$ and $t \in \mathbb{R}$. If $x = 0$ or $y = 0$, then the claim is trivial. Suppose that $x \neq 0 \neq y$. Then

$$0 \leq \langle x + ty, x + ty \rangle = \|x\|^2 + 2t\langle x, y \rangle + t^2\|y\|^2.$$

This is a second degree polynomial w.r.t. t with at most 1 real root. Hence,

$$\begin{aligned} \text{discriminant} \leq 0 \quad &\Leftrightarrow \quad 4|\langle x, y \rangle|^2 - 4\|x\|^2\|y\|^2 \leq 0 \\ &\Leftrightarrow \quad |\langle x, y \rangle|^2 \leq \|x\|^2\|y\|^2. \end{aligned}$$

Note that if $y = ax$, $a \in \mathbb{R}$, then discriminant $= 0$ and Cauchy–Schwarz holds with equality. □

The triangle inequality is an immediate consequence of Cauchy–Schwarz:

$$\begin{aligned} \|x + y\|^2 &= \langle x + y, x + y \rangle = \|x\|^2 + \|y\|^2 + 2\langle x, y \rangle \\ &\leq \|x\|^2 + \|y\|^2 + 2|\langle x, y \rangle| \leq \|x\|^2 + \|y\|^2 + 2\|x\|\|y\| \\ &= (\|x\| + \|y\|)^2 \quad \text{for all } x, y \in X. \end{aligned}$$

For our purposes, having an inner product is not enough. We need to know that these spaces are also *complete* normed spaces.

Definition (Cauchy sequence)

A sequence $(x_k)_{k=1}^{\infty}$ of elements of $(X, \|\cdot\|)$ is called a *Cauchy sequence* if for all $\varepsilon > 0$, there exists $N \in \mathbb{N}$ such that

$$m, n > N \quad \Rightarrow \quad \|x_m - x_n\| < \varepsilon.$$

Definition (Complete space)

A normed space $(X, \|\cdot\|)$ is *complete* if all Cauchy sequences in X converge to an element of X.

Definition (Banach space)

A normed space $(X, \|\cdot\|)$ which is complete with respect to $\|\cdot\|$ is a *Banach space*.

Definition (Hilbert space)

An inner product space $(H, \langle\cdot,\cdot\rangle)$ which is complete with respect to $\|\cdot\| = \sqrt{\langle\cdot,\cdot\rangle}$ defined by the inner product is a *Hilbert space*.

Example

i) $\mathbb{R}^n$ and $\ell^2(\mathbb{R})$ are complete.

ii) $C([a,b])$ is *not* complete w.r.t. the norm

$$\|f\|^2 = \int_a^b |f(x)|^2 \,\mathrm{d}x.$$

Let $a = -1$, $b = 1$, and define

$$f_n(x) := \begin{cases} 0, & -1 \le x < 0, \\ nx, & 0 \le x \le \frac{1}{n}, \\ 1, & \frac{1}{n} < x \le 1. \end{cases}$$

Then f_n is continuous, and if $H(x) = \chi_{[0,1]}(x) = \begin{cases} 0, & -1 \le x \le 0, \\ 1, & 0 < x \le 1, \end{cases}$ we have

$$\int_{-1}^1 |f_n(x) - H(x)|^2 \,\mathrm{d}x = \int_0^{1/n} |nx - 1|^2 \,\mathrm{d}x = \int_0^{1/n} (n^2x^2 - 2nx + 1) \,\mathrm{d}x$$

$$= \left[\frac{n^2x^3}{3} - nx^2 + x \right]_{x=0}^{x=1/n} = \frac{1}{3n} - \frac{1}{n} + \frac{1}{n} = \frac{1}{3n} \xrightarrow{n\to\infty} 0.$$

We have $\|f_n - H\| \to 0$, but $H \notin C([-1,1])$.

However, note that $C([a,b])$ *is* complete w.r.t. the sup-norm $\|f\|_\infty = \sup_{a\le x\le b} |f(x)|$, but $\|\cdot\|_\infty \neq \|\cdot\|$ and *there is no inner product inducing* $\|\cdot\|_\infty$*-norm* (Exercise).

If one wishes to consider function spaces equipped with inner product norms, one is led to L^2 spaces.

Definition

Let $D \subset \mathbb{R}^n$ be a Lebesgue measurable set. Then

$$L^2(D) := \{[f] \mid f : D \to \mathbb{R} \text{ measurable}, \int_D |f(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} < \infty\}.$$

Here, $[f]$ is the equivalence class of all measurable functions g s.t. $f = g$ a.e. We define the inner product

$$\langle f, g \rangle_{L^2(D)} = \int_D f(\boldsymbol{x}) g(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}. \qquad \text{(well-defined in equivalence classes)}$$

This is a Hilbert space with norm

$$\|f\|_{L^2(D)} = \left(\int_D |f(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} \right)^{1/2}.$$

Remark. In practice, we treat the elements of $L^2(D)$ (resp. $L^p(D)$) as functions. For example, if the class $[f]$ contains a continuous function, we can choose it as a representer of the class. However, in general, the values of L^2-functions (resp. $L^p(D)$) are not pointwise well-defined – making inferences about the class $[f]$ should therefore be independent of the pointwise behavior of a chosen representative of this class!

Bounded linear operators in Hilbert spaces

Definition

Let X and Y be normed spaces with norms $\|\cdot\|_X$ and $\|\cdot\|_Y$. A linear operator $A\colon X \to Y$ is said to be *bounded* if there exists $C > 0$ such that

$$\|Ax\|_Y \leq C\|x\|_X \quad \text{for all } x \in X.$$

Lemma

Let $(X, \|\cdot\|_X)$ and $(Y, \|\cdot\|_Y)$ be normed spaces. Then a linear operator $A\colon X \to Y$ is bounded iff

$$\|A\| := \|A\|_{X\to Y} := \sup_{\|x\|_X \leq 1} \|Ax\|_Y < \infty. \qquad \text{(operator norm)}$$

Proof. "$\Rightarrow$" If there is $C > 0$ s.t. $\|Ax\|_Y \leq C\|x\|_X$ for all $x \in X$, then clearly $\|A\| = \sup_{\|x\|_X \leq 1} \|Ax\|_Y \leq C$.
"$\Leftarrow$" Let $\|A\| < \infty$. Since $\|\frac{x}{\|x\|_X}\|_X = 1$ for all $x \neq 0$, from the linearity of A we infer

$$\frac{\|Ax\|_Y}{\|x\|_X} = \|A(\tfrac{x}{\|x\|_X})\|_Y \leq \|A\| \quad \text{for all } x \in X.$$

This implies the important estimate

$$\|Ax\|_Y \leq \|A\|\|x\|_X \quad \text{for all } x \in X.$$

A linear operator is continuous precisely when it is bounded.

Proposition

Let $(X, \|\cdot\|_X)$ and $(Y, \|\cdot\|_Y)$ be normed spaces and $A\colon X \to Y$ a linear operator. Then the following are equivalent:

(i) *A is a bounded operator;*

(ii) *A is continuous (in X);*

(iii) *A is continuous at one point $x_0 \in X$.*

Proof. (i) $\Rightarrow$ (ii): if $x, y \in X$ and $\varepsilon > 0$, then

$$\|x - y\|_X \leq \frac{\varepsilon}{\|A\|} =: \delta \quad \Rightarrow \quad \|Ax - Ay\|_Y \overset{A \text{ linear}}{=} \|A(x-y)\|_Y \leq \|A\|\|x-y\|_X \leq \varepsilon.$$

(ii) $\Rightarrow$ (iii): trivial.
(iii) $\Rightarrow$ (i): let A be continuous at $x_0 \in X$. By definition, there exists $\delta > 0$ such that

$$\|y - x_0\|_X \leq \delta \quad \Rightarrow \quad \|Ay - Ax_0\|_Y \leq 1.$$

If $x \in X$ is such that $\|x\|_X \leq \delta$, then by taking $y = x + x_0$:

$$\|Ax\|_Y = \|A(x + x_0) - Ax_0\|_Y \leq 1.$$

On the other hand, for any $\|x\|_X \leq 1$, there holds $\|\delta x\|_X = \delta\|x\|_X \leq \delta$ and thus

$$\delta\|Ax\|_Y = \|A(\delta x)\|_Y \leq 1, \quad \text{i.e.,} \quad \|Ax\|_Y \leq \frac{1}{\delta} \quad \text{for all } \|x\|_X \leq 1.$$

Therefore $\|A\| \leq \frac{1}{\delta}$, meaning that A is bounded. □

Let H be a real Hilbert space.

Definition

Two elements $x, y \in H$ are said to be *orthogonal* if $\langle x, y \rangle = 0$.

Let $M \subset H$ be a subset. The orthogonal complement of M in H is defined as

$$M^{\perp} := \{y \in H \mid \langle x, y \rangle = 0 \quad \text{for all } x \in M\}.$$

We state the following easy consequences.

Lemma

For any subset $M \subset H$, $M^{\perp}$ is a closed subspace of H and $M \subset (M^{\perp})^{\perp}$.

Lemma

If M is a non-closed subspace, then $(M^{\perp})^{\perp} = \overline{M}$.

Proof. Exercise. □

Proposition (Hilbert projection theorem)

Let M be a nonempty, closed, and convex[†] subset of a real Hilbert space H. Then there exists a unique element $x_0 \in M$ satisfying

$$\|x_0\| \leq \|x\| \quad \textit{for all } x \in M.$$

Proof. Let $\delta = \inf\{\|x\| \mid x \in M\}$. We use the parallelogram identity $\|u+v\|^2 + \|u-v\|^2 = 2\|u\|^2 + 2\|v\|^2$ (Exercise) applied to vectors $u = \frac{1}{2}x$ and $v = \frac{1}{2}y$, $x, y \in M$, to obtain

$$\frac{1}{4}\|x-y\|^2 = \frac{1}{2}\|x\|^2 + \frac{1}{2}\|y\|^2 - \left\|\frac{x+y}{2}\right\|^2.$$

Due to convexity $\frac{1}{2}(x+y) \in M$, so

$$\|x-y\|^2 \leq 2\|x\|^2 + 2\|y\|^2 - 4\delta^2 \quad \text{for all } x, y \in M. \tag{1}$$

Existence: let $(x_k)_{k=1}^{\infty} \subset M$ s.t. $\|x_k\| \xrightarrow{k\to\infty} \delta$. Substituting $x \leftarrow x_n$ and $y \leftarrow x_m$ in (1) yields $\|x_n - x_m\|^2 \leq 2\|x_n\|^2 + 2\|x_m\|^2 - 4\delta^2$, since $\frac{1}{2}(x_n + x_m) \in M$ for all n, m. Thus $\|x_n - x_m\| \to 0$ as $n, m \to \infty$. $(x_k)_{k=1}^{\infty}$ is Cauchy in the Hilbert space H, so there exists $x_0 := \lim_{k\to\infty} x_k \in H$. Since $\|\cdot\|$ is continuous, $\|x_0\| = \lim_{k\to\infty} \|x_k\| = \delta$. Since M is closed and $(x_k)_{k=1}^{\infty} \subset M$, the limit $x_0 \in M$.

Uniqueness: If $\|x\| = \|y\| = \delta \Rightarrow \|x-y\|^2 \leq 0$ by (1) and so $x = y$. □

[†] $tx + (1-t)y \in M$ for all $x, y \in M$, $t \in (0,1)$.

Corollary

Let H be a real Hilbert space, M a nonempty, closed, and convex subset of H, and $x \in H$. Then there exists a unique element $y_0 \in M$ such that

$$\|x - y_0\| = \inf\{\|x - y\| \mid y \in M\}.$$

Proof. The set $x - M := \{x - y \mid y \in M\}$ is closed and convex, and $\min\{\|x - y\| \mid x - y \in x - M\} = \min\{\|x - y\| \mid y \in M\}$. The claim follows from the previous result. □

Proposition (Orthogonal decomposition)

If M is a closed subspace of a real Hilbert space H, then

$$H = M \oplus M^{\perp},$$

which means that every element $y \in H$ can be uniquely represented as

$$y = x + x^{\perp}, \quad x \in M,\ x^{\perp} \in M^{\perp}.$$

Proof. It suffices to prove that $M \cap M^{\perp} = \{0\}$ and $M + M^{\perp} = H$.
• If $x \in M \cap M^{\perp}$, then $0 = \langle x, x \rangle = \|x\|^2$ (i.e., $x \perp x$) so $x = 0$.
$\therefore$ $M \cap M^{\perp} = \{0\}$.
• Let $x \in H$. The Hilbert projection theorem guarantees that there exists a unique $y_0 \in M$ such that

$$\|x - y_0\| \leq \|x - y\| \quad \text{for all } y \in M. \tag{2}$$

Let $x_0 = x - y_0$ so that $x = y_0 + x_0 \in M + x_0$. It remains to show that $x_0 \in M^{\perp}$.
The inequality (2) can be written as

$$\|x_0\| \leq \|z\| \quad \text{for all } z \in x - M.$$

Since $y_0 \in M$ and M is a vector space, $y_0 + M = M$ and $M = -M$ which implies $x - M = x + M = y_0 + x_0 + M = x_0 + M$. The previous inequality can be recast as

$$\|x_0\| \leq \|z\| \quad \text{for all } z \in x_0 + M \quad \Leftrightarrow \quad \|x_0\| \leq \|x_0 + z\| \quad \text{for all } z \in M.$$

This statement is true if and only if $\langle x_0, z \rangle = 0$ for all $z \in M$. Therefore $x_0 \in M^{\perp}$.

Let M be a closed subspace. The orthogonal decomposition implies that every element $y \in H$ can be uniquely represented as

$$y = x + x^{\perp},\ x \in M,\ x^{\perp} \in M^{\perp}.$$

Lemma

Let $M \subset H$ be a closed subspace. The mapping $P_M : H \to M$, $y \mapsto x$, is an orthogonal projection, i.e., $P_M^2 = P_M$ and $\mathrm{Ran}(P_M) \perp \mathrm{Ran}(I - P_M)$. It satisfies the following properties:

- *P_M is linear;*
- *$\|P_M\| = 1$ if $M \neq \{0\}$;*
- *$I - P_M = P_{M^{\perp}}$;*
- *$\|y - P_M y\| \leq \|y - z\|$ for all $z \in M$;*
- *$y \in M \ \Rightarrow\ P_M y = y,\ (I - P_M)y = 0$;*
  $y \in M^{\perp} \Rightarrow\ P_M y = 0,\ (I - P_M)y = y$.
- *$\|y\|^2 = \|P_M y\|^2 + \|(I - P_M)y\|^2$ (Pythagoras)*

Proof. Omitted; see for example [Rudin, Real and Complex Analysis, pp. 34–35]. □

Example

Let H_1 and H_2 be real Hilbert spaces and let $A\colon H_1 \to H_2$ be a continuous linear operator.

The kernel (or null space) of operator A is defined as

$$\mathrm{Ker}(A) := \{x \in H_1 \mid Ax = 0\}.$$

The range (or image) of operator A is defined as

$$\mathrm{Ran}(A) := \{y \in H_2 \mid y = Ax,\ x \in H_1\}.$$

Then we have the following:

- $\mathrm{Ker}(A)$ is a *closed* subspace of H_1, and $\mathrm{Ran}(A)$ is a subspace of H_2.
- $H_1 = \mathrm{Ker}(A) \oplus (\mathrm{Ker}(A))^{\perp}$.
- $H_2 = \overline{\mathrm{Ran}(A)} \oplus (\mathrm{Ran}(A))^{\perp}$.