

Multilevel Monte Carlo Methods for UQ

Appendix: Background Material

(based on the notes of Prof. Dr Oliver Ernst, TU Chemnitz)

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A. Probability Theory

- Random Variables
- Random Vectors
- Limit Theorems
- Statistical Estimation

B. Elliptic Boundary Value Problems

- Weak Formulation
- Finite Element Approximation
- Finite Element Convergence

A. Probability Theory

Probability Theory

Probability measure

We denote an abstract **probability space** by $(\Omega, \mathfrak{A}, \mathbb{P})$, in which

Ω is an **abstract set of elementary events**,

\mathfrak{A} is a **σ -algebra** of subsets of Ω containing the measurable events and

\mathbb{P} is a **probability measure** on \mathfrak{A} .

Definition A.1

A measure \mathbb{P} on a measurable space (Ω, \mathfrak{A}) is called a **probability measure** if $\mathbb{P}(\Omega) = 1$.

Definition A.2

An event $A \in \mathfrak{A}$ is said to occur **almost surely** with respect to the measure \mathbb{P} (\mathbb{P} -a.s.) if $\mathbb{P}(A) = 1$.

Probability Theory

Borel-Cantelli lemma

Proposition A.3 (Boole's inequality)

For events $\{A_n\}_{n \in \mathbb{N}}$ there holds

$$\mathbb{P}(\cup_{n=1}^{\infty} A_n) \leq \sum_{n=1}^{\infty} \mathbb{P}(A_n).$$

Definition A.4

The set of all $\omega \in \Omega$ such that $\omega \in A_n$ for infinitely many values of n , i.e., ω occurs infinitely often (i.o.), is defined as

$$\{A_n, \text{ i.o. } \} := \limsup_{n \in \mathbb{N}} A_n := \cap_{k=1}^{\infty} \cup_{n=k}^{\infty} A_n.$$

Theorem A.5 (Borel-Cantelli Lemma)

If $\sum_{n=1}^{\infty} \mathbb{P}(A_n) < \infty$, then $\mathbb{P}\{A_n, \text{ i.o. } \} = 0$. For independent events $\{A_n\}_{n \in \mathbb{N}}$ such that $\sum_{n=1}^{\infty} \mathbb{P}(A_n) = \infty$ there holds $\mathbb{P}\{A_n, \text{ i.o. } \} = 1$.

Probability Theory

Random variables

Definition A.6

Let $(\Omega, \mathfrak{A}, \mathbb{P})$ be a probability space and (E, \mathfrak{E}) a measurable space. A measurable function $X : \Omega \rightarrow E$ is called an **(E-valued) random variable**. Individual values $X(\omega)$ for $\omega \in \Omega$ are called **realisations** of the random variable.

Remark: If E is a topological space then the σ -algebra generated by the open subsets of E is called the Borel σ -algebra $\mathfrak{B}(E)$.

Definition A.7

Let X be an E -valued random variable where (E, \mathfrak{E}) is a measurable space and $(\Omega, \mathfrak{A}, \mathbb{P})$ is the underlying probability space. The **probability distribution** \mathbb{P}_X of X (also called the law of X) is the probability measure on (E, \mathfrak{E}) defined by $\mathbb{P}_X(A) := \mathbb{P}(X^{-1}(A))$ for pre-images $X^{-1}(A) := \{\omega \in \Omega : X(\omega) \in A\}$ of sets $A \in \mathfrak{E}$.

Remark: This construction is sometimes called the **push-forward measure** defined by $(\Omega, \mathfrak{A}, \mathbb{P})$, (E, \mathfrak{E}) and X .

Probability Theory

Expectation, moments

Definition A.8

The **expectation** of a Banach space-valued random variable X is defined as the integral

$$\mathbb{E}[X] := \int_{\Omega} X(\omega) \, d\mathbb{P}(\omega).$$

Definition A.9

The **k -th moment** ($k \in \mathbb{N}$) of a real-valued random variable X is $\mathbb{E}[X^k]$.

The first moment $\mu := \mathbb{E}[X]$ is also called the **mean** or **mean value**.

The **central moments** $\mathbb{E}[(X - \mu)^k]$ measure the deviation of X from its mean.

The second central moment

$$\mathbf{Var} X := \mathbb{E}[(X - \mu)^2] = \mathbb{E}[X^2] - \mu^2$$

of a random variable X is called its **variance**.

Remark: The quantity $\sigma := \sqrt{\mathbf{Var} X}$ is called the **standard deviation** of X .

Probability Theory

Computation of moments

Moments of a random variable are sometimes more easily computed by integrating over the image variable.

Consider a real-valued random variable X from (Ω, \mathfrak{A}) to $(\Gamma, \mathfrak{B}(\Gamma))$ where $\Gamma \subset \mathbb{R}$. For $B \in \mathfrak{B}(\Gamma)$, set $A := X^{-1}(B)$. Then by the definition of the probability distribution \mathbb{P}_X

$$\int_{\Omega} \mathbb{1}_A(\omega) \, d\mathbb{P}(\omega) = \mathbb{P}(A) = \mathbb{P}_X(B) = \int_{\Gamma} \mathbb{1}_B(x) \, d\mathbb{P}_X(x).$$

For measurable functions $f : \Gamma \rightarrow \mathbb{R}$ we have

$$\int_{\Omega} f(X(\omega)) \, d\mathbb{P}(\omega) = \int_{\Gamma} f(x) \, d\mathbb{P}_X(x)$$

and, in particular,

$$\mathbb{E}[X] = \int_{\Omega} X(\omega) \, d\mathbb{P}(\omega) = \int_{\Gamma} x \, d\mathbb{P}_X(x).$$

Probability Theory

Probability density functions

Definition A.10

Let \mathbb{P} be a probability measure on $(\Gamma, \mathfrak{B}(\Gamma))$ for some $\Gamma \subset \mathbb{R}$. If there exists a function $p : \Gamma \rightarrow [0, \infty)$ such that $\mathbb{P}(B) = \int_B p(x) dx$ for any $B \in \mathfrak{B}(\Gamma)$ we say that \mathbb{P} has a density p with respect to Lebesgue measure and we call p its **probability density function (pdf)**. If X is a Γ -valued random variable on $(\Omega, \mathfrak{A}, \mathbb{P})$, the pdf p_X of X (if it exists) is the pdf of the probability distribution \mathbb{P}_X .

For real-valued random variables X from $(\Omega, \mathfrak{A}, \mathbb{P})$ to $(\Gamma, \mathfrak{B}(\Gamma))$ we then have¹

$$\mathbb{E}[X] = \int_{\Omega} X(\omega) d\mathbb{P}(\omega) = \int_{\Gamma} x d\mathbb{P}_X(x) = \int_{\Gamma} xp(x) dx. \quad (\text{A.1})$$

Event probabilities are then easily calculated as

$$\mathbb{P}(X \in (a, b)) = \mathbb{P}(\{\omega \in \Omega : a < X(\omega) < b\}) = \mathbb{P}_X((a, b)) = \int_a^b p(x) dx.$$

¹(where we have omitted the subscript X)

Probability Theory

Uniform distribution

A random variable X is **uniformly distributed** on $D = [a, b] \subset \mathbb{R}$, ($a < b$), denoted

$$X \sim \text{Uni}(a, b),$$

if its pdf is

$$p(x) = \frac{1}{b-a}, \quad x \in [a, b].$$

Using (A.1), we easily obtain

$$\mathbb{E}[X] = \int_a^b \frac{x}{b-a} dx = \frac{a+b}{2}, \quad \mathbb{E}[X^2] = \int_a^b \frac{x^2}{b-a} dx = \frac{b^3 - a^3}{3(b-a)},$$

so that $\mathbf{Var} X = \mathbb{E}[X^2] - \mathbb{E}[X]^2 = \frac{(b-a)^2}{12}$.

Probability Theory

Gaussian distribution

A random variable X is said to follow the **Gaussian** or **normal distribution** on $\Gamma = \mathbb{R}$ if its pdf is given by

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right), \quad x \in \mathbb{R},$$

with two real parameters $\mu \in \mathbb{R}$ and $\sigma > 0$, denoted $X \sim N(\mu, \sigma^2)$.

As is easily verified,

$$\mathbb{E}[X] = \mu, \quad \mathbf{Var} X = \sigma^2.$$

The probability that X is within α of its mean is given by

$$\mathbb{P}(|X - \mu| \leq \alpha) = \operatorname{erf}\left(\frac{\alpha}{\sqrt{2\sigma^2}}\right),$$

with the **error function** erf defined by

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt.$$

Probability Theory

Gaussian distribution

The cumulative distribution function (cdf) of the standard normal distribution $N(0, 1)$ is denoted by

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x e^{-\frac{t^2}{2}} dt = \frac{1}{2} + \frac{1}{2} \operatorname{erf}\left(\frac{x}{\sqrt{2}}\right).$$

Any (finite) linear combination of (jointly) random variables is normally distributed.

Probability Theory

Change of variables formula

Lemma A.11 (Change of variables)

Suppose $Y : \Omega \rightarrow \mathbb{R}$ is a real-valued random variable and $f : (a, b) \rightarrow \mathbb{R}$ is continuously differentiable with inverse function f^{-1} . If p_Y is the pdf of Y , the pdf of the random variable $X : \Omega \rightarrow (a, b)$ defined via $X = f^{-1}(Y)$ is

$$p_X(x) = p_Y(f(x)) |f'(x)| \quad \text{for } a < x < b.$$

Probability Theory

Lognormal distribution

If $Y \sim N(\mu, \sigma^2)$, then the random variable

$$X := \exp(Y)$$

is said to follow a **lognormal distribution**. With $f(x) = \log x$, Lemma A.11 yields the pdf of X as

$$p_X(x) = \frac{1}{\sqrt{2\pi\sigma^2 x^2}} \exp\left(-\frac{[\log(x) - \mu]^2}{2\sigma^2}\right).$$

Moreover, there holds

$$\mathbb{E}[X] = \exp\left(\mu + \frac{\sigma^2}{2}\right), \quad \mathbf{Var} X = (e^{\sigma^2} - 1)e^{2\mu + \sigma^2}.$$

Probability Theory

Covariance

Definition A.12

The **covariance** between two real-valued random variables is defined as

$$\mathbf{Cov}(X, Y) = \mathbb{E}[(X - \mu_X)(Y - \mu_Y)],$$

where $\mu_X := \mathbb{E}[X]$ and $\mu_Y := \mathbb{E}[Y]$. In particular, $\mathbf{Cov}(X, X) = \mathbf{Var} X$.

Note: An equivalent expression is $\mathbf{Cov}(X, Y) = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]$.

Calculation of the covariance requires evaluating the integral

$$\mathbb{E}[XY] = \int_{\Omega} X(\omega)Y(\omega) d\mathbb{P}(\omega) = \int_{X(\Omega) \times Y(\Omega)} xy d\mathbb{P}_{X,Y}(x, y),$$

in which $\mathbb{P}_{X,Y}$ is the **joint probability distribution** of X and Y .

Sometimes it is useful to scale the covariance to lie in $[-1, 1]$. The resulting quantity is known as the **correlation coefficient**

$$\rho(X, Y) := \frac{\mathbf{Cov}(X, Y)}{\sigma_X \sigma_Y}.$$

Probability Theory

Joint probability distribution

Definition A.13

The **joint probability distribution** of two random variables X and Y is the distribution of the bivariate random variable $\mathbf{X} = (X, Y)$, i.e., for all $B \in \mathfrak{B}(X(\Omega) \times Y(\Omega))$

$$\mathbb{P}_{X,Y}(B) = \mathbb{P}(\{\omega \in \Omega : \mathbf{X}(\omega) \in B\}).$$

If it exists, the density $p_{X,Y}$ of $\mathbb{P}_{X,Y}$ is known as the **joint pdf** and

$$\mathbb{P}_{X,Y} = \int_B p_{X,Y}(x, y) dx dy.$$

Probability Theory

Uncorrelated random variables

Definition A.14

If $\text{Cov}(X, Y) = 0$ the random variables X and Y are said to be **uncorrelated**. A family $\{X_\alpha\}_\alpha$ is said to be **pairwise uncorrelated** if X_α and X_β are uncorrelated for all $\alpha \neq \beta$.

Note: Uncorrelated random variables may still be strongly related. As an example,

$$X \sim N(0, 1), \quad \text{and} \quad Y := \cos X$$

satisfy $\mu_X = 0$ and hence

$$\begin{aligned} \text{Cov}(X, Y) &= \mathbb{E}[X \cos X] = \int_{\mathbb{R}} x \cos(x) \, d\mathbb{P}_X(x) \\ &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} x \cos(x) \exp\left(-\frac{x^2}{2}\right) \, dx = 0. \end{aligned}$$

A stronger notion is that of **independent** random variables.

Probability Theory

Sub σ -algebras, σ -algebras generated by random variables

Definition A.15

A σ -algebra \mathfrak{B} is a **sub σ -algebra** of \mathfrak{A} if $\mathfrak{B} \subset \mathfrak{A}$, i.e., if $A \in \mathfrak{B}$ implies $A \in \mathfrak{A}$.

Definition A.16

Let X be an E -valued random variable on $(\Omega, \mathfrak{A}, \mathbb{P})$ for a measurable space (E, \mathfrak{E}) . The **σ -algebra generated by X** , denoted $\sigma(X)$, is defined as

$$\sigma(X) := \{X^{-1}(A) : A \in \mathfrak{E}\} \subset \mathfrak{A}.$$

Remark: $\sigma(X)$ is the smallest σ -algebra such that X is measurable. It may be considerably smaller than \mathfrak{A} .

Probability Theory

Independence of events, σ -algebras and random variables

Definition A.17

Two events $A, B \in \mathfrak{A}$ are **independent** if $\mathbb{P}(A \cap B) = \mathbb{P}(A)\mathbb{P}(B)$.

Two σ -algebras \mathfrak{A}_1 and \mathfrak{A}_2 are independent if all pairs of events A_1 and A_2 with $A_1 \in \mathfrak{A}_1$ and $A_2 \in \mathfrak{A}_2$ are independent.

Definition A.18

Two random variables X, Y on a probability space $(\Omega, \mathfrak{A}, \mathbb{P})$ are said to be **independent** if the σ -algebras $\sigma(X)$ and $\sigma(Y)$ are independent.

A family $\{X_\alpha\}_\alpha$ of random variables is said to be **pairwise independent** if X_α and X_β are independent for all $\alpha \neq \beta$.

Independence of random variables X and Y can be conveniently determined using their joint distribution $\mathbb{P}_{X,Y}$: X and Y are independent if and only if $\mathbb{P}_{X,Y}$ equals the product measure $\mathbb{P}_X \times \mathbb{P}_Y$. If X and Y are real-valued with densities p_X and p_Y , they are independent if and only if their **joint pdf** is

$$p_{X,Y}(x, y) = p_X(x)p_Y(y).$$

Probability Theory

Independence implies uncorrelatedness

Lemma A.19

If X and Y are independent real-valued random variables and $\mathbb{E}[|X|], \mathbb{E}[|Y|] < \infty$, then X and Y are uncorrelated.

Note: The converse is generally false.

Theorem A.20 (Jensen's inequality)

If X is a real-valued random variable with $\mathbb{E}[|X|] < \infty$ and $\phi : \mathbb{R} \rightarrow \mathbb{R}$ a convex function, then

$$\phi(\mathbb{E}[X]) \leq \mathbb{E}[\phi(X)]. \tag{A.2}$$

Probability Theory

Bochner spaces

Definition A.21

Let $(\Omega, \mathfrak{A}, \mathbb{P})$ be a probability space and let W be a separable Banach space with norm $\|\cdot\|$. We denote by $L^p(\Omega; W)$, $1 \leq p < \infty$, the space of W -valued \mathfrak{A} -measurable random variables $X : \Omega \rightarrow W$ with $\mathbb{E}[\|X\|^p] < \infty$. The resulting space is a Banach space with the norm

$$\|X\|_{L^p(\Omega; W)} := \left(\int_{\Omega} \|X(\omega)\|^p d\mathbb{P}(\omega) \right)^{1/p} = \mathbb{E}[\|X\|^p]^{1/p}.$$

Similarly, $L^\infty(\Omega; W)$ is the Banach space of W -valued random variables $X : \Omega \rightarrow W$ for which

$$\|X\|_{L^\infty(\Omega; W)} = \operatorname{ess\,sup}_{\omega \in \Omega} \|X(\omega)\| < \infty.$$

Probability Theory

Bochner spaces, $p = 2$

The case $p = 2$ when W is a Hilbert space $W = H$ with inner product (\cdot, \cdot) occurs frequently. In this case $L^2(\Omega; H)$ is a Hilbert space with inner product

$$(X, Y)_{L^2(\Omega; H)} := \mathbb{E}[(X, Y)] = \int_{\Omega} (X(\omega), Y(\omega)) d\mathbb{P}(\omega).$$

Random variables in $L^2(\Omega; H)$ are called **mean-square integrable random variables**.

For random variables $X, Y \in L^2(\Omega; H)$ the Cauchy-Schwarz inequality takes on the form

$$|(X, Y)_{L^2(\Omega; H)}| \leq \|X\|_{L^2(\Omega; H)} \|Y\|_{L^2(\Omega; H)}$$

or

$$\mathbb{E}[(X, Y)] \leq \mathbb{E}[\|X\|^2]^{1/2} \mathbb{E}[\|Y\|^2]^{1/2}.$$

Probability Theory

Bochner spaces, $p = 2$, covariance

Definition A.22

Let H be a separable Hilbert space. A linear operator $C : H \rightarrow H$ is the **covariance** of two H -valued random variables X and Y if

$$(C\phi, \psi) = \mathbf{Cov}((\phi, X), (\psi, Y)) \quad \forall \phi, \psi \in H.$$

X and Y are said to be **uncorrelated** if C is the zero operator. If $Y = X$ then C is called the **covariance of X** .

More generally, the covariance of two random variables X and Y with values in a separable Banach space W may be defined as a bilinear map $c : W' \times W' \rightarrow \mathbb{R}$ on the dual space W' of W such that

$$c(\phi, \psi) = \mathbf{Cov}(\langle \phi, X \rangle_{W' \times W}, \langle \psi, Y \rangle_{W' \times W}) \quad \forall \phi, \psi \in W'.$$

Here $\langle \cdot, \cdot \rangle_{W' \times W}$ denotes the duality bracket between W' and W . The bilinear map c may be identified with a linear operator from $C : W' \rightarrow W''$ via the identity

$$\langle C\phi, \psi \rangle_{W'' \times W'} = c(\phi, \psi).$$

Probability Theory

Convergence of random variables

Definition A.23

Let W be a Banach space with norm $\|\cdot\|$ and $\{X_n\}_{n \in \mathbb{N}}$ be a sequence of W -valued random variables. We say X_n converges to $X \in W$

almost surely if $X_n(\omega) \rightarrow X(\omega)$ for almost all $\omega \in \Omega$, i.e., if

$$\mathbb{P}(\|X_n - X\| \rightarrow 0 \text{ for } n \rightarrow \infty) = 1.$$

in probability if $\mathbb{P}(\|X_n - X\| > \epsilon) \rightarrow 0$ for $n \rightarrow \infty$ for any $\epsilon > 0$.

in p -th mean or in $L^p(\Omega; W)$ if $\mathbb{E}[\|X_n - X\|^p] \rightarrow 0$ as $n \rightarrow \infty$. When $p = 2$ this is known as **convergence in mean square**.

in distribution if $\mathbb{E}[\phi(X_n)] \rightarrow \mathbb{E}[\phi(X)]$ as $n \rightarrow \infty$ for any bounded and continuous function $\phi : W \rightarrow \mathbb{R}$.

Probability Theory

Convergence of random variables

Theorem A.24

Let $X_k \rightarrow X$ in p -th mean and, for $r > 0$ and a constant $K = K(p)$, assume that

$$\|X_k - X\|_{L^p(\Omega; W)} := \mathbb{E} [\|X_k - X\|^p]^{1/p} \leq \frac{K(p)}{k^r}. \quad (\text{A.3})$$

Then the following convergence properties apply:

(a) $X_k \rightarrow X$ in probability and, for any $\epsilon > 0$,

$$\mathbb{P} (\|X_k - X\| \geq k^{-r+\epsilon}) \leq \frac{K(p)^p}{k^{p\epsilon}}. \quad (\text{A.4})$$

(b) $\mathbb{E} [\phi(X_k)] \rightarrow \mathbb{E} [\phi(X)]$ for all Lipschitz continuous functions on W and, if L denotes a Lipschitz constant of ϕ ,

$$|\mathbb{E} [\phi(X_k)] - \mathbb{E} [\phi(X)]| \leq L \frac{K(p)}{k^r}.$$

(c) If (A.3) holds for all p sufficiently large, then $X_k \rightarrow X$ a.s. Furthermore, for each $\epsilon > 0$ there exists a nonnegative random variable K such that $\|X_k(\omega) - X(\omega)\| \leq K(\omega)k^{-r+\epsilon}$ for almost all ω .

Probability Theory

Random vectors

Random variables $\mathbf{X} = (X_1, \dots, X_n)^T$ from $(\Omega, \mathfrak{A}, \mathbb{P})$ to $(\Gamma, \mathfrak{B}(\Gamma))$ with $\Gamma \subset \mathbb{R}^n$ are known as **random vectors** or **multivariate random variables** (bivariate for $n = 2$).

Their expected value

$$\boldsymbol{\mu} = \mathbb{E} [\mathbf{X}] = \int_{\Omega} \mathbf{X}(\omega) d\mathbb{P}(\omega) = [\mathbb{E} [X_1], \dots, \mathbb{E} [X_n]]^T$$

is a vector in \mathbb{R}^n . If \mathbf{X} has a pdf p , then for $B \in \mathfrak{B}(\Gamma)$

$$\mathbb{P}(\mathbf{X} \in B) = \mathbb{P}(\{\omega \in \Omega : \mathbf{X}(\omega) \in B\}) = \mathbb{P}_{\mathbf{X}}(B) = \int_B p(\mathbf{x}) d\mathbf{x}.$$

The components $\{X_j\}_{j=1}^n$ of \mathbf{X} are (pairwise) independent if and only if $\mathbb{P}_{\mathbf{X}}$ is the product measure $\mathbb{P}_{X_1} \times \dots \times \mathbb{P}_{X_n}$. In terms of the pdf, this is equivalent to

$$p(\mathbf{x}) = p_{X_1}(x_1) \cdot p_{X_2}(x_2) \cdot \dots \cdot p_{X_n}(x_n).$$

Probability Theory

Multivariate uniform

A random vector $\mathbf{X} : \Omega \rightarrow \Gamma$ with values in a set $\Gamma \subset \mathbb{R}^n$ with finite Lebesgue measure $|\Gamma|$ follows a **multivariate uniform** distribution on Γ , denoted by

$$\mathbf{X} \sim \text{Uni}(\Gamma)$$

if it has the pdf

$$p(\mathbf{x}) \equiv \frac{1}{|\Gamma|}, \quad \mathbf{x} \in \Gamma.$$

Probability Theory

Covariance matrix

Definition A.25

The covariance of two real-valued random vectors $\mathbf{X} = [X_1, \dots, X_m]^T$ and $\mathbf{Y} = [Y_1, \dots, Y_n]^T$ is given by the $m \times n$ matrix

$$\mathbf{Cov}(\mathbf{X}, \mathbf{Y}) = \mathbb{E} [(\mathbf{X} - \mathbb{E}[\mathbf{X}])(\mathbf{Y} - \mathbb{E}[\mathbf{Y}])^T].$$

\mathbf{X} and \mathbf{Y} are said to be uncorrelated if $\mathbf{Cov}(\mathbf{X}, \mathbf{Y}) = \mathbf{O}$ (the $m \times n$ zero matrix). The matrix $\mathbf{Cov}(\mathbf{X}, \mathbf{X}) \in \mathbb{R}^{n \times n}$ is called the **covariance matrix of \mathbf{X}** .

Proposition A.26

Let \mathbf{X} be an \mathbb{R}^n -valued random variable with mean vector $\boldsymbol{\mu}$ and covariance matrix \mathbf{C} . Then \mathbf{C} is symmetric positive semi-definite and its trace is given by $\mathbb{E} [\|\mathbf{X} - \boldsymbol{\mu}\|_2^2]$.

Probability Theory

Multivariate normal distribution

A random vector with mean vector $\boldsymbol{\mu}$ and positive definite covariance matrix \mathbf{C} is said to follow an n -variate Gaussian distribution if it has the pdf

$$p(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^d \det \mathbf{C}}} \exp\left(-\frac{(\mathbf{x} - \boldsymbol{\mu})^\top \mathbf{C}^{-1}(\mathbf{x} - \boldsymbol{\mu})}{2}\right). \quad (\text{A.5})$$

Definition A.27

An \mathbb{R}^n -valued random vector \mathbf{X} follows a multivariate normal (or Gaussian) distribution, denoted

$$\mathbf{X} \sim N(\boldsymbol{\mu}, \mathbf{C}),$$

where $\boldsymbol{\mu} \in \mathbb{R}^n$ and $\mathbf{C} \in \mathbb{R}^{n \times n}$ is symmetric positive definite, if it has the pdf (A.5).

Note: The case that \mathbf{C} is singular (pos. *semi*-definite) can be handled by characteristic functions.

Probability Theory

Multivariate normal distribution

If $\mathbf{X} \sim N(\boldsymbol{\mu}, \mathbf{C})$ is a multivariate normal random vector, then for any $\mathbf{a} \in \mathbb{R}^n$ the linear combination

$$Y = \mathbf{a}^\top \mathbf{X} = \sum_{k=1}^n a_k X_k$$

follows the normal distribution $Y \sim N(\mathbf{a}^\top \boldsymbol{\mu}, \mathbf{a}^\top \mathbf{C} \mathbf{a})$.

Probability Theory

i.i.d. random variables

Definition A.28

A sequence $\{X_j\}_{j \in \mathbb{N}}$ of random variables is said to be **independent and identically distributed (i.i.d.)** if they all follow the same probability distribution and, in addition, are pairwise independent.

The classical limit theorems of probability theory concern sums of i.i.d. random variables. For an i.i.d. sequence $\{X_j\}_{j \in \mathbb{N}}$, we introduce the notation

$$S_n := X_1 + \cdots + X_n, \quad n \in \mathbb{N}.$$

Probability Theory

Weak Law of Large Numbers

Theorem A.29 (Chebyshev inequality)

A random variable X with finite mean μ and finite variance σ^2 satisfies

$$c^2 \mathbb{P}(|X - \mu| \geq c) \leq \sigma^2.$$

Theorem A.30 (WLLN)

Let $\{X_k\}_{k \in \mathbb{N}}$ be a sequence of i.i.d. random variables on a given probability space $(\Omega, \mathfrak{A}, \mathbb{P})$ with mean μ and finite variance. Then

$$\frac{S_n}{n} \rightarrow \mu \quad \text{in probability, i.e.}$$

for ever fixed $\epsilon > 0$ there holds

$$\mathbb{P}(|S_n/n - \mu| > \epsilon) \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

Probability Theory

Strong Law of Large Numbers

Theorem A.31 (SLLN)

Let $\{X_k\}_{k \in \mathbb{N}}$ be a sequence of i.i.d. real-valued random variables on a given probability space $(\Omega, \mathfrak{A}, \mathbb{P})$. Then S_n/n has a finite limit if and only if $\mathbb{E}[|X_1|] < \infty$, in which case

$$\frac{S_n}{n} \rightarrow \mathbb{E}[X_1] \quad \text{a.s.}$$

If $\mathbb{E}[|X_1|] = \infty$, then $\limsup_{n \rightarrow \infty} |S_n|/n \rightarrow \infty$ a.s.

Probability Theory

Central Limit Theorem

Let the sequence $\{X_k\}_{k \in \mathbb{N}}$ of real-valued random variables be independent, but not necessarily identically distributed. In addition, let $\mathbb{E}[X_k] = 0$ and $\mathbb{E}[X_k^2] < \infty$ for all k .

Besides $S_n = \sum_{k=1}^n X_k$, introduce the quantities

$$\begin{aligned} \sigma_k^2 &:= \mathbf{Var} X_k, \\ \Sigma_n^2 &:= \sum_{j=1}^n \sigma_j^2 = \mathbf{Var} S_n. \end{aligned}$$

The **central limit theorem (CLT)** is the statement that

$$\lim_{n \rightarrow \infty} \frac{S_n}{\Sigma_n} = \lim_{n \rightarrow \infty} \frac{S_n - \mathbb{E}[S_n]}{\sqrt{\mathbf{Var} S_n}} \sim \mathbf{N}(0, 1) \quad \text{in distribution.}$$

Probability Theory

Central Limit Theorem

Definition A.32 (Lyapunov condition)

The sequence $\{X_k\}_{k \in \mathbb{N}}$ satisfies the **Lyapunov condition** if $\mathbb{E}[|X_k|^3] < \infty$ for each k and

$$\lim_{n \rightarrow \infty} \frac{1}{\Sigma_n^2} \sum_{k=1}^n \mathbb{E}[|X_k|^3] = 0.$$

Theorem A.33 (Lyapunov CLT)

If $\{X_k\}_{k \in \mathbb{N}}$ satisfies the Lyapunov condition, then $S_n/\Sigma_n \rightarrow \mathcal{N}(0, 1)$ in distribution.

Note: There exist several variants of the CLT with different assumptions.

Theorem A.34 (Simple CLT)

Let $\{X_k\}_{k \in \mathbb{N}}$ be a sequence of i.i.d. random variables, with $\mathbb{E}[X_k] = \mu$ and $\mathbf{Var} X_k = \sigma^2$ for all $k \in \mathbb{N}$. Then $\sqrt{n}(S_n/n - \mu) \rightarrow \mathcal{N}(0, \sigma^2)$ in distribution.

Probability Theory

Berry-Esseen Theorem

Theorem A.35 (Berry, 1941; Esseen 1942)

Let $\{X_k\}_{k \in \mathbb{N}}$ be i.i.d. random variables such that, for all $k \in \mathbb{N}$,

$$\mu := \mathbb{E}[X_k], \quad \sigma^2 := \mathbf{Var} X_k > 0, \quad \rho := \mathbb{E}[|X_k - \mu|^3] < \infty.$$

If F_n denotes the distribution function of $(S_n - n\mu)/(\sigma\sqrt{n})$ and Φ that of the standard normal distribution $\mathcal{N}(0, 1)$, then, with a universal constant C ,

$$\sup_{x \in \mathbb{R}} |\Phi(x) - F_n(x)| \leq C \cdot \frac{\rho}{\sigma^3 \sqrt{n}}.$$

Note: the constant C is known to satisfy $0.4097 \leq C \leq 0.7056$ [Shevtsova, 2007].

Statistical Estimation

- Estimation theory is concerned with determining an **unknown quantity** θ associated with the probability distribution of a random variable X given n i.i.d. samples $\{X_k\}_{k=1}^n$ of X .
- Typical examples of such quantities θ are **moments** of X 's distribution such as the mean and the variance. Another common situation is the estimation of one or more **parameters** which determine the distribution of X .
- An **estimator** for a scalar quantity θ is a function

$$\phi : \mathbb{R}^n \rightarrow \mathbb{R}, \quad \hat{\theta} = \phi(X_1, \dots, X_n)$$

mapping n i.i.d. realisations of X to the **estimate** $\hat{\theta}$ of θ .

- Note that, since each of the n random samples X_k are random variables, the same is true of

$$\hat{\theta} = \hat{\theta}(\omega) = \phi(X_1(\omega), \dots, X_n(\omega)).$$

Once the samples have been drawn/realised, the estimate $\hat{\theta}$ is a real number.

Statistical Estimation

Sample average, unbiased estimator

- The **sample average**

$$\hat{\mu}_n := \frac{X_1 + \dots + X_n}{n}$$

is an estimate for the mean $\mu = \mathbb{E}[X]$.

- Since the X_k are i.i.d., we conclude from the linearity of expectation that

$$\mathbb{E}[\hat{\mu}_n] = \frac{1}{n} \sum_{k=1}^n \mathbb{E}[X_k] = \frac{1}{n} \cdot n\mu = \mu.$$

- If $\mathbb{E}[|X|] < \infty$ the SLLN tells us that also $\hat{\mu}_n \rightarrow \mu = \mathbb{E}[X]$ a.s. as $n \rightarrow \infty$.
- Since $\mathbf{Var} \hat{\mu}_n = \frac{\sigma^2}{n}$, where $\sigma^2 = \mathbf{Var} X$, we note that the variance $\hat{\mu}_n$ decreases like $1/n$ with growing sample size.

Definition A.36

An estimator for which $\mathbb{E}[\hat{\theta}] = \theta$ is called **unbiased**.

Statistical Estimation

Sample variance

The **sample variance**

$$\hat{\sigma}_n^2 := \frac{1}{n-1} \sum_{k=1}^n (X_k - \hat{\mu}_n)^2$$

is an unbiased estimator for $\sigma^2 = \mathbf{Var} X$.

In addition, there holds $\hat{\sigma}_n^2 \rightarrow \sigma^2$ a.s. as $n \rightarrow \infty$.

References

- [1] O. Kallenberg. *Foundations of Modern Probability* Springer, Berlin-Heidelberg, 1997.
- [2] I. G. Shevtsova. Sharpening of the upper bound of the absolute constant in the Berry–Esseen inequality. *Theory Probab. Appl.*, **51**, 549–553, 2007.

B. Elliptic Boundary Value Problems

Elliptic Boundary Value Problem

We consider the **elliptic boundary value problem (BVP)** of finding the solution of the partial differential equation with Dirichlet boundary condition

$$-\nabla \cdot (a \nabla u) = f \quad \text{on } D, \tag{B.1a}$$

$$u = g \quad \text{on } \partial D, \tag{B.1b}$$

given a bounded convex domain $D \subset \mathbb{R}^d$, $d = 1, 2, 3$ with sufficiently smooth boundary ∂D , a **coefficient function** $a : D \rightarrow \mathbb{R}^+$, a **source term** $f : D \rightarrow \mathbb{R}$ and **boundary data** in the form of a function $g : \partial D \rightarrow \mathbb{R}$.

The differential operator in (B.1a) is short for

$$\nabla \cdot (a \nabla u) = \sum_{j=1}^d \frac{\partial}{\partial x_j} \left(a(\mathbf{x}) \frac{\partial u(\mathbf{x})}{\partial x_j} \right)$$

Equation (B.1a) is a model for diffusion phenomena occurring in , e.g., heat conduction, electrostatics, potential flow and elasticity. Generalisations of (B.1) involve the addition of lower-order terms, other boundary conditions, a matrix-valued coefficient function and dependence of a on u .

Elliptic Boundary Value Problem

Strong and weak solution

If $f \in C(\bar{D})$ and $a \in C^1(\bar{D})$, then a function $u \in C^2(D) \cap C^1(\bar{D})$ which satisfies (B.1) is called a **classical solution** or a **strong solution** of the boundary value problem.

There are (theoretical and practical) reasons for generalizing the classical solution concept. The key to this generalisation lies in reformulating (B.1) as a **variational problem**. Multiplying both sides of (B.1a) by an arbitrary function $\phi \in C_0^\infty(D)$, in this context known as a **test function**, and integrating by parts, we observe that any (classical) solution of (B.1) also satisfies the equation

$$a(u, \phi) = \ell(\phi) \quad \text{for all } \phi \in C_0^\infty(D), \quad (\text{B.2})$$

with the symmetric bilinear form $a(\cdot, \cdot)$ and linear functional $\ell(\cdot)$ given by

$$a(u, \phi) = \int_D a(\mathbf{x}) \nabla u(x) \cdot \nabla \phi(\mathbf{x}) \, d\mathbf{x}, \quad \ell(\phi) = \int_D f(\mathbf{x}) \phi(\mathbf{x}) \, d\mathbf{x}. \quad (\text{B.3})$$

For (B.2) to make sense, it is sufficient that the integrals and derivatives are well-defined.

Elliptic Boundary Value Problem

Strong and weak solution

This is the case if u and ϕ are taken to lie in the **Sobolev space**

$$H^1(D) := \{v \in L^2(D) : \nabla v \in L^2(D)^2\},$$

which is a Hilbert space with respect to the inner product

$$(u, v)_{H^1(D)} = \int_D (\nabla u \cdot \nabla v + uv) \, d\mathbf{x} = (\nabla u, \nabla v) + (u, v),$$

where we use (\cdot, \cdot) to denote the inner product in $L^2(D)$. The associated norm on $H^1(D)$ is

$$\|u\|_{H^1(D)}^2 = \int_D (|\nabla u|^2 + u^2) \, d\mathbf{x}.$$

The gradients are in terms of **weak derivatives** in the sense of

$$\left(\frac{\partial u}{\partial x_j}, \phi \right) = - \left(u, \frac{\partial \phi}{\partial x_j} \right) \quad \text{for all } \phi \in C_0^\infty(D).$$

Elliptic Boundary Value Problem

Strong and weak solution

Stating the boundary condition (B.1b) requires a well-defined notion of evaluating a function from $H^1(D)$ on the lower-dimensional manifold ∂D .

- Functions in $H^1(D)$ satisfying the BC with homogeneous boundary data $g \equiv 0$ can be characterised as lying in the subspace $H_0^1(D) \subset H^1(D)$, which is defined as the closure of smooth functions with compact support with respect to $\|\cdot\|_{H^1}$:

$$H_0^1(D) := \overline{C_0^\infty(D)} \subset H^1(D).$$

- For inhomogeneous boundary data we define the space

$$W := H_g^1(D) := \{v \in H^1(D) : u|_{\partial D} = g\}.$$

The evaluation on the boundary is understood in the following sense: for a sufficiently smooth boundary there exists a bounded **trace operator** $\gamma : H^1(D) \rightarrow L^2(\partial D)$ such that for all $u \in C^1(\overline{D})$ there holds $\gamma u = u|_{\partial D}$. Since $C^1(\overline{D})$ is dense in $H^1(D)$, we have $\gamma u = \lim_{n \rightarrow \infty} u_n|_{\partial D}$ for any approximating sequence $\{u_n\} \subset C^1(\overline{D})$ converging to u in $H^1(D)$.

Elliptic Boundary Value Problem

Strong and weak solution

Definition B.1

The **trace space** of $H^1(D)$ for a sufficiently smooth domain D is defined as

$$H^{1/2}(\partial D) := \gamma(H^1(D)) = \{\gamma u : u \in H^1(D)\}.$$

$H^{1/2}(\partial D)$ is a Hilbert space with norm

$$\|g\|_{H^{1/2}(\partial D)} := \inf\{\|u\|_{H^1(D)} : \gamma u = g, u \in H^1(D)\}.$$

Since in general $H^{1/2}(\partial D) \subsetneq L^2(\partial D)$, boundary data g in (B.1b) must be chosen from $H^{1/2}(\partial D)$.

Lemma B.2

There exists $C_\gamma > 0$ such that, for all $g \in H^{1/2}(\partial D)$, we can find $u_g \in H^1(D)$ with $\gamma u_g = g$ and

$$\|u_g\|_{H^1(D)} \leq C_\gamma \|g\|_{H^{1/2}(\partial D)}$$

Elliptic Boundary Value Problem

Strong and weak solution

We denote the spaces of **trial** and test functions by

$$W := H_g^1(D), \quad \text{and} \quad V := H_0^1(D).$$

Assumption 1

The coefficient function $a = a(\mathbf{x})$ in (B.1a) satisfies

$$0 < a_{\min} \leq a(\mathbf{x}) \leq a_{\max} < \infty \quad \text{for almost all } \mathbf{x} \in D$$

for positive constants a_{\min} and a_{\max} . In particular, $a \in L^\infty(D)$ and a is uniformly bounded away from zero.

By Assumption 1, the bilinear form $a(\cdot, \cdot)$ is **bounded** on $H^1(D)$, i.e.,

$$|a(u, v)| \leq C \|u\|_{H^1(D)} \|v\|_{H^1(D)}, \quad \text{for all } u, v \in H^1(D)$$

with a constant $C \leq \|a\|_{L^\infty(D)}$.

Elliptic Boundary Value Problem

Strong and weak solution

Definition B.3

A **weak solution** of (B.1) is a function $u \in W$ such that

$$a(u, v) = \ell(v) \quad \text{for all } v \in V, \tag{B.4}$$

with $a(\cdot, \cdot)$ and $\ell(\cdot)$ as defined in (B.3).

Elliptic Boundary Value Problem

Strong and weak solution

Definition B.4

A bilinear form $a : H \times H \rightarrow \mathbb{R}$ on a Hilbert space H is said to be **coercive** if there exists a constant $\alpha > 0$ such that

$$a(u, u) \geq \alpha \|u\|_H^2 \quad \text{for all } u \in H.$$

Lemma B.5 (Lax–Milgram)

Let H be a real Hilbert space with norm $\|\cdot\|_H$ and let ℓ be a bounded linear functional on H . Let $a : H \times H \rightarrow \mathbb{R}$ be a bilinear form that is bounded and coercive. Then there exists a unique $u_\ell \in H$ such that $a(u_\ell, v) = \ell(v)$ for all $v \in H$, and the solution depends continuously on the data

$$\|u_\ell\|_H \leq \frac{1}{\alpha} \|\ell\|.$$

Elliptic Boundary Value Problem

Strong and weak solution

For functions in $H^1(D)$ we introduce the **H^1 semi-norm**

$$|u|_{H^1(D)} := \left(\int_D |\nabla u|^2 \, d\mathbf{x} \right)^{1/2}.$$

as well as the **energy norm** associated with the coefficient function a as

$$|u|_a := a(u, u)^{1/2} = \left(\int_D a \nabla u \cdot \nabla u \, d\mathbf{x} \right)^{1/2}.$$

Theorem B.6 (Poincaré–Friedrichs inequality)

For a bounded domain D there exists a constant $C = C_D > 0$ such that

$$\|u\|_{L^2(D)} \leq C_D |u|_{H^1(D)} \quad \text{for all } u \in H_0^1(D).$$

Elliptic Boundary Value Problem

Strong and weak solution

Lemma B.7

Under Assumption 1 the bilinear form $a : H^1(D) \times H_0^1(D) \rightarrow \mathbb{R}$ is bounded and the energy norm is equivalent to the H^1 semi-norm on $H^1(D)$.

Theorem B.8

Let Assumption 1 hold, $f \in L^2(D)$ and $g \in H^{1/2}(\partial D)$. Then (B.1) has a unique weak solution $u \in W = H_g^1(D)$. Furthermore, the weak solution $u \in W$ satisfies

$$\|u\|_{H^1(D)} \leq C (\|f\|_{L^2(D)} + \|g\|_{H^{1/2}(\partial D)})$$

where $C = \max\{C_D/a_{\min}, C_\gamma(1 + a_{\max}/a_{\min})\}$.

Proof. Lax–Milgram Lemma. □

Finite Element Approximation

Galerkin discretisation

Given: linear variational problem of finding $u \in V$, V a Hilbert space with norm $\|\cdot\|$, such that

$$a(u, v) = \ell(v) \quad \text{for all } v \in V \quad (\text{B.5})$$

with a bilinear form $a(\cdot, \cdot)$ and linear form $\ell(\cdot)$ on V which satisfy the assumptions of the Lax-Milgram lemma.

Galerkin method for finding approximate solutions of (B.5) proceeds by restricting the problem to a finite-dimensional subspace $V_n \subset V$: denote by $u_n \in V_n$ the solution of

$$a(u_n, v_n) = \ell(v_n) \quad \text{for all } v_n \in V_n. \quad (\text{B.6})$$

Note: The **Galerkin approximation** u_n of u with respect to the space V_n is uniquely determined since the conditions of the Lax-Milgram Lemma are satisfied for Problem (B.6) by inclusion.

Finite Element Approximation

C a's lemma

Galerkin orthogonality

The Galerkin solution $u_n \in V_n$ satisfies

$$a(u - u_n, v_n) = 0, \quad \text{for all } v_n \in V_n.$$

The simple structure of a linear variational problem allows its reduction to a problem of best approximation.

Lemma B.9 (C a)

If the assumptions of the Lax-Milgram lemma apply to Problem (B.5) with solution $u \in V$, then the Galerkin approximation u_n , i.e., the solution of (B.6), satisfies

$$\|u - u_n\| \leq \frac{C}{\alpha} \inf_{v_n \in V_n} \|u - v_n\|. \quad (\text{B.7})$$

Finite Element Approximation

C a's lemma, symmetric case

- If the bilinear form $a(\cdot, \cdot)$ is, in addition, symmetric (Hermitian) then, because of coercivity, it defines an inner product on V .
- Galerkin orthogonality then implies u_n is the a -orthogonal projection of u onto V_n and therefore the best approximation to u from V_n with respect to the associated (energy) norm.
- In the energy norm (B.7) is therefore satisfied with $C = \alpha = 1$.
- Coercivity and boundedness also imply that the energy norm is equivalent to $\|\cdot\|$, i.e.,

$$\sqrt{\alpha}\|v\| \leq |v|_a \leq \sqrt{C}\|v\| \quad \text{for all } v \in V,$$

which leads to the improved estimate over (B.7)

$$\|u - u_n\| \leq \sqrt{\frac{C}{\alpha}} \inf_{v \in V_n} \|u - v\|.$$

Finite Element Approximation

Application to elliptic BVP

We have seen that, for the elliptic BVP (B.1), we have the equivalences

$$\|\cdot\|_{H^1(D)} \asymp |\cdot|_{H^1(D)} \asymp |\cdot|_a.$$

Corollary B.10

Under Assumption 1, the Galerkin approximation u_n to the solution of the elliptic boundary value problem (B.1), with respect to any subspace V_n of $V = H_0^1(D)$, satisfies

$$|u - u_n|_a = \inf_{v \in V_n} |u - v|_a,$$
$$|u - u_n|_{H^1(D)} \leq \sqrt{\frac{a_{\min}}{a_{\max}}} |u - v|_{H^1(D)} \quad \text{for all } v \in V_n.$$

Finite Element Approximation

Galerkin system

Given a basis $\{v_1, \dots, v_n\}$ of V_n and the solution $u_n = \sum_{j=1}^n \xi_j v_j$, then the Galerkin variational equation (B.6) is equivalent to

$$\sum_{j=1}^n \xi_j a(v_j, v_i) = \ell(v_i), \quad i = 1, \dots, n,$$

which, when rewritten as a linear system of equation, becomes the **Galerkin system**

$$\mathbf{Ax} = \mathbf{b} \tag{B.8}$$

with **Galerkin matrix** $[\mathbf{A}]_{i,j} = a(v_j, v_i)$, unknown vector $[\mathbf{x}]_i = \xi_i$ and right-hand side vector $[\mathbf{b}]_i = \ell(v_i)$.

- If $a(\cdot, \cdot)$ is symmetric, then so is \mathbf{A} .
- If $a(\cdot, \cdot)$ is coercive, then \mathbf{A} is (uniformly) positive definite.

Finite Element Approximation

The finite element method

- Different Galerkin methods result from different choices of subspaces.
- Wavelets.
- Trigonometric functions, global polynomials (spectral methods).
- Radial basis functions.
- The **finite element method** employs finite dimensional subspaces of the variational spaces (trial and test spaces) consisting of **piecewise polynomials** with respect to a partition of D .
- We shall assume in the following that D is a polygon (polyhedron), but the finite element method can also be applied to domains with curved boundaries.
- For the remainder of this section we consider the case where $D \subset \mathbb{R}^2$, i.e., $d = 2$. The concepts can easily be extended to different d .

Finite Element Approximation

Triangulations

Assumptions on the partition of the domain D , denoted by \mathcal{T}_h with elements K :

$$(Z_1) \quad \bar{D} = \cup_{K \in \mathcal{T}_h} K.$$

$$(Z_2) \quad \text{Each } K \in \mathcal{T}_h \text{ is a closed set with nonempty interior } \overset{\circ}{K}.$$

$$(Z_3) \quad \text{For two distinct } K_1, K_2 \in \mathcal{T}_h \text{ there holds } \overset{\circ}{K}_1 \cap \overset{\circ}{K}_2 = \emptyset.$$

$$(Z_4) \quad \text{Each } K \in \mathcal{T}_h \text{ has a Lipschitz-continuous boundary } \partial K.$$

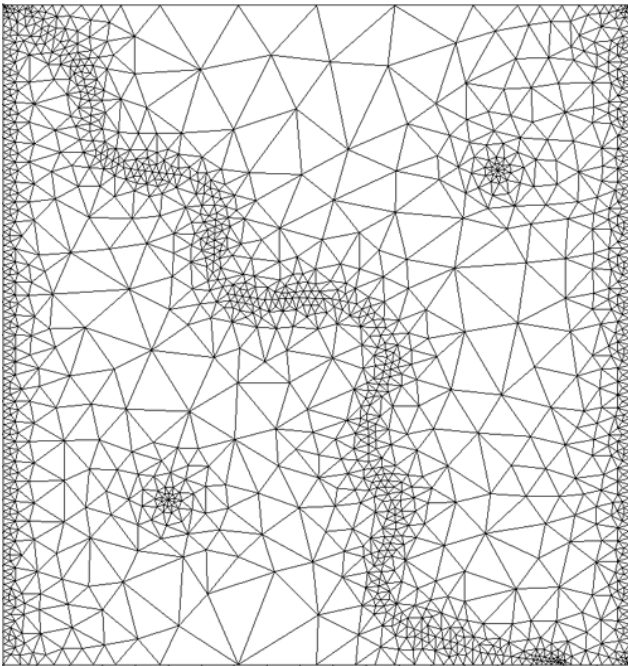
The partition is usually assigned a **discretisation parameter** $h > 0$ given by

$$h := \max_{K \in \mathcal{T}_h} \text{diam}K,$$

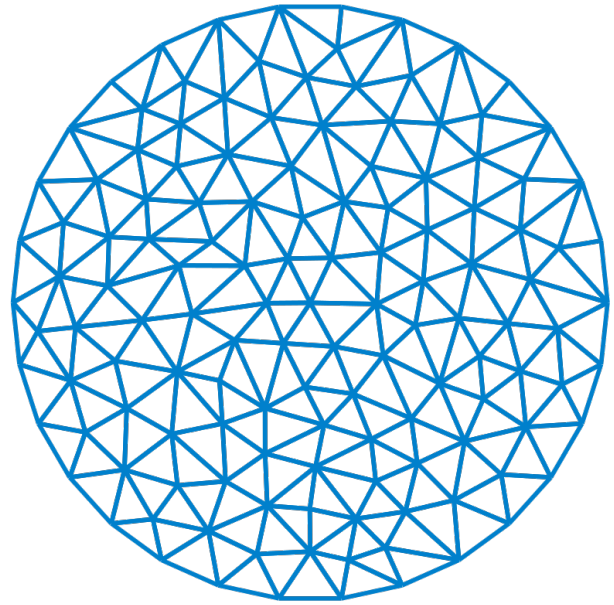
which is a measure of how fine the partition is.

Finite Element Approximation

Triangulations



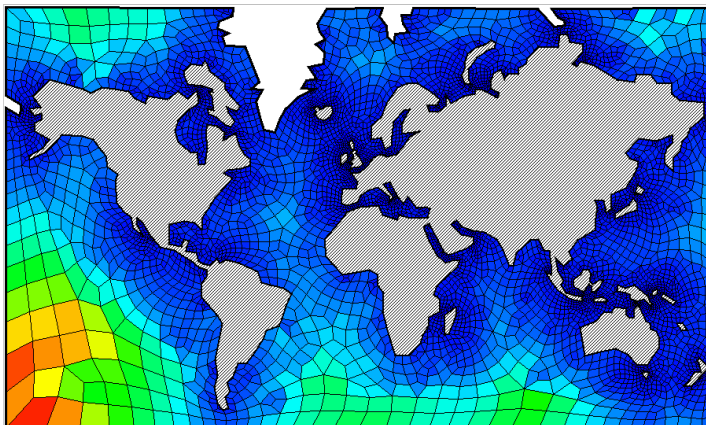
Triangular mesh on a square domain.



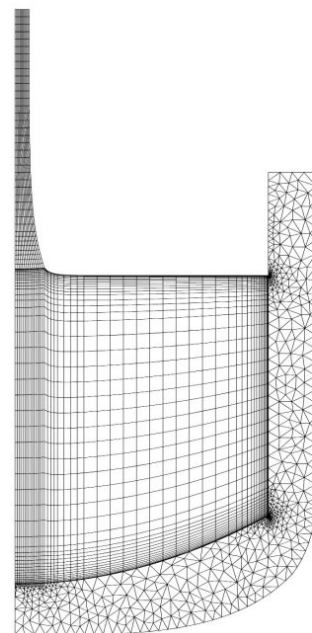
Triangular mesh on a polygonal approximation of a circle.

Finite Element Approximation

Triangulations



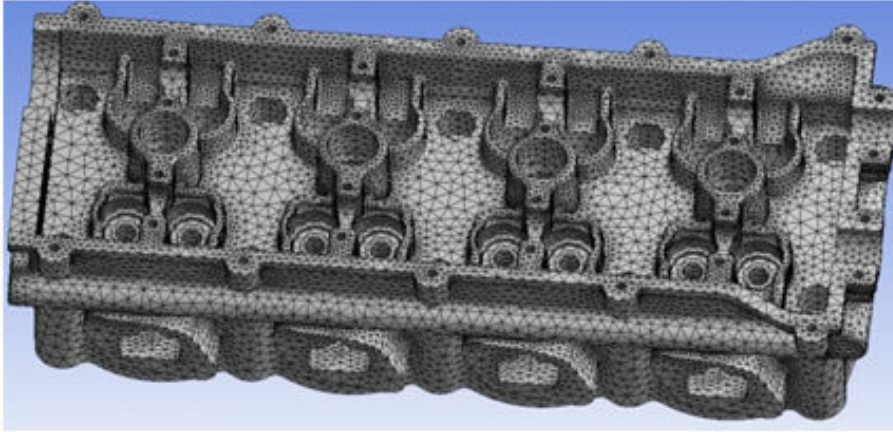
Quadrilateral mesh on a rectangular (exterior) domain.



Mesh consisting of triangles and quadrilaterals.

Finite Element Approximation

Triangulations



Tetrahedral mesh of complex 3D geometry (engine block).

Finite Element Approximation

H^1 -conforming finite element spaces

A **conforming** Galerkin approximation is one which employs finite-dimensional spaces V_n such that $V_n \subset V$.

Let V_h denote a space of piecewise continuous functions $v : \bar{D} \rightarrow \mathbb{R}$ with respect to an admissible triangulation \mathcal{T}_h of D , i.e., such that each restriction $v|_K$ to any $K \in \mathcal{T}_h$ is continuous on K .

Theorem B.11

With the notation defined above, there holds $V_h \subset H^1(D)$ if, and only if,

$$V_h \subset C(\bar{D}) \quad \text{and} \quad \{v|_K : v \in V_h\} \subset H^1(K).$$

In this case $\{v \in V_h : v = 0 \text{ on } \partial D\} \subset H_0^1(D)$.

Finite Element Approximation

Finite elements

According to [Ciarlet, 1978], a **finite element** is a triple (K, P_K, Ψ_K) such that

- (1) K is a nonempty set
- (2) P_K is a finite-dimensional space of functions defined on K and
- (3) Ψ_K is a set of linearly independent linear functionals ψ on P_K with the property that, for any $p \in P_K$,

$$\psi(p) = 0 \text{ for all } \psi \in \Psi_K \quad \Rightarrow \quad p = 0.$$

We shall consider a single finite element, the so-called **linear triangle**, where

- (1) $K \in \mathbb{R}^2$ is a triangle with (non-collinear) vertices \mathbf{x}_1 , \mathbf{x}_2 and \mathbf{x}_3 ,
- (2) P_K is the space of all affine functions on K and
- (3) Ψ_K consists of the three functionals

$$\Psi_K = \{\psi_j : P_K \rightarrow \mathbb{R}, \psi_j(p) = p(\mathbf{x}_j), j = 1, 2, 3\}.$$

Finite Element Approximation

Trianglular finite elements

- To construct a (global) finite element space V_h based on linear triangle elements consider a triangulation \mathcal{T}_h of D consisting of (closed) triangles K which satisfy properties **(Z1)**–**(Z4)**.
- The functions in V_h will also lie in $H^1(D)$ if they are continuous on \bar{D} , which, for piecewise linear (polynomial) functions, is equivalent to their being **continuous** across triangle boundaries.
- We thus obtain the space

$$V_h := \{v \in C(\bar{D}) : v|_K \in \mathcal{P}_1 \text{ for all } K \in \mathcal{T}_h\},$$

where \mathcal{P}_k denotes the space of (multivariate) polynomials of (complete) degree k .

- Define the subspace $V_{h,0}$ of V_h by

$$V_{h,0} := \{v \in V_h : v|_{\partial D} = 0\} \subset H_0^1(D).$$

Finite Element Approximation

Degrees of freedom, nodal basis

- A continuous piecewise linear function in V_h is completely determined by its values at all triangle vertices.
- Such a (finite) set of parameters which uniquely determine a finite element function is called a set of **degrees of freedom (DOF)**.
- In $V_{h,0}$ these are the values at all nodes which do not lie on ∂D ; denote their number by n .
- A particularly convenient basis $\{\phi_1, \dots, \phi_n\}$ of $V_{h,0}$ is the so-called **nodal basis** characterised by

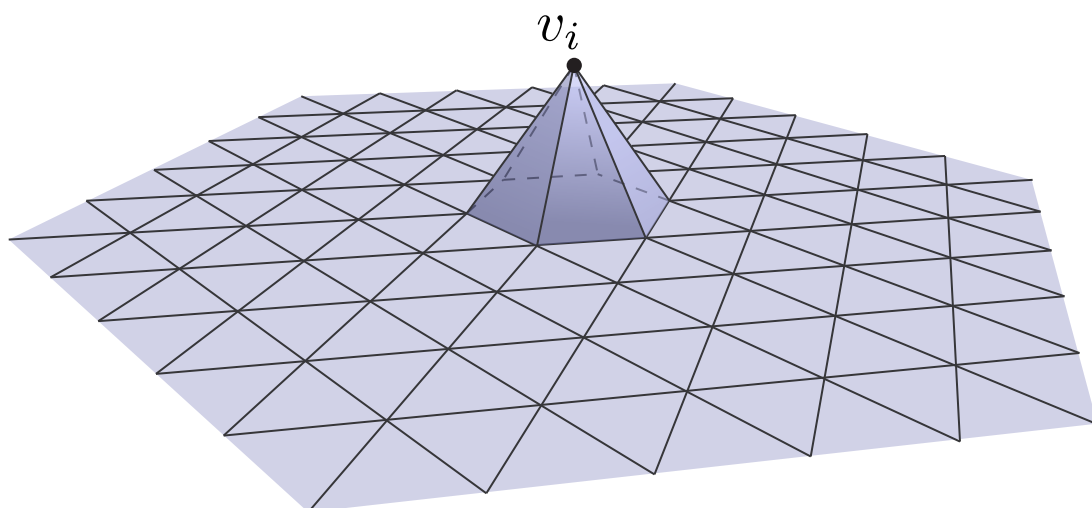
$$\phi_j(\mathbf{x}_i) = \delta_{i,j} \quad i, j = 1, \dots, n.$$

- If $\mathcal{N}_h = \{x_1, \dots, x_n\}$ denotes the set of vertices $x_j \notin \partial D$, then

$$\text{supp } \phi_j = \bigcup_{\substack{K \in \mathcal{T}_h \\ \mathbf{x}_j \in K}} K.$$

Finite Element Approximation

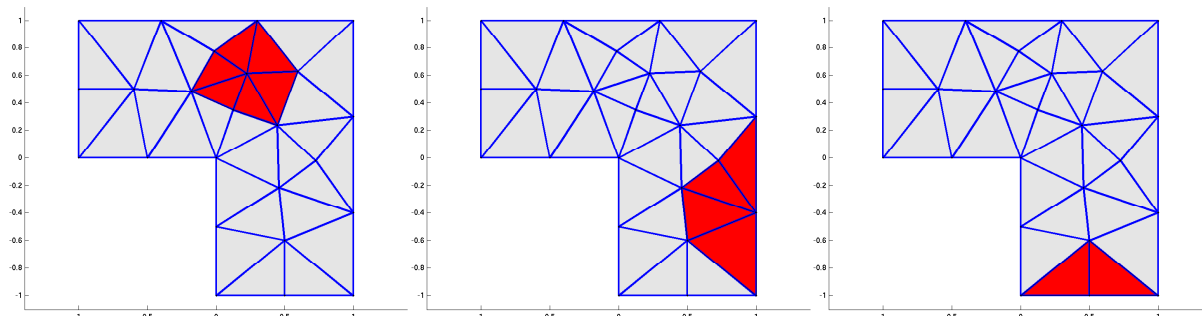
Nodal basis for linear triangles



A nodal basis function with its support.

Finite Element Approximation

Nodal basis for linear triangles



Triangulation of an L-shaped domain with the supports of several basis functions.

Finite Element Approximation

Galerkin matrix, linear triangles

Implications for Galerkin system (B.8):

$$[\mathbf{b}]_i = \ell(\phi_i) = \int_D f \phi_i \, d\mathbf{x} = \int_{\text{supp } \phi_i} f \phi_i \, d\mathbf{x},$$

$$\begin{aligned} [\mathbf{A}]_{i,j} &= a(\phi_j, \phi_i) = \int_D a(\mathbf{x}) \phi_i(\mathbf{x}) \cdot \nabla \phi_j(\mathbf{x}) \, d\mathbf{x} \\ &= \int_{\text{supp } \phi_i \cap \text{supp } \phi_j} a(\mathbf{x}) \nabla \phi_i(\mathbf{x}) \cdot \nabla \phi_j(\mathbf{x}) \, d\mathbf{x}. \end{aligned}$$

In particular, the Galerkin matrix \mathbf{A} is **sparse**.

Finite Element Approximation

Finite element assembly

Common procedure in **assembling** the Galerkin system:

(1) Ignore boundary condition initially, i.e., consider all of V_h with nodal basis

$$\{\phi_1, \phi_2, \dots, \phi_n, \phi_{n+1}, \dots, \phi_{\tilde{n}}\},$$

$\tilde{n} - n$ the number of vertices on the boundary ∂D .

Yields matrix $\tilde{\mathbf{A}} \in \mathbb{R}^{\tilde{n} \times \tilde{n}}$, vector $\tilde{\mathbf{b}} \in \mathbb{R}^{\tilde{n}}$.

(2) Then eliminate the DOF associated with boundary vertices.

Yields matrix \mathbf{A} , vector \mathbf{b} .

Note:

- Initial approach for step (1): compute $\tilde{\mathbf{A}}, \tilde{\mathbf{b}}$, entry by entry, i.e., basis function by basis function
- But: shape and connectivity of supports typically very different.
- Simpler: compute \mathbf{A}, \mathbf{b} element by element.

Finite Element Approximation

Finite element assembly

$K \in \mathcal{T}_h$: then for $i, j = 1, 2, \dots, \tilde{n}$:

$$a(\phi_j, \phi_i) = \int_D a \nabla \phi_j \cdot \nabla \phi_i \, d\mathbf{x} = \sum_{K \in \mathcal{T}_h} \int_K a \nabla \phi_j \cdot \nabla \phi_i \, d\mathbf{x} =: \sum_{K \in \mathcal{T}_h} a_K(\phi_j, \phi_i),$$

$$\ell(\phi_i) = \int_D f \phi_i \, d\mathbf{x} = \sum_{K \in \mathcal{T}_h} \int_K f \phi_i \, d\mathbf{x} =: \sum_{K \in \mathcal{T}_h} \ell_K(\phi_i).$$

Setting

$$\begin{aligned} [\tilde{\mathbf{A}}_K]_{i,j} &:= a_K(\phi_j, \phi_i) & i, j &= 1, 2, \dots, \tilde{n}, \\ [\tilde{\mathbf{b}}_K]_i &:= \ell_K(\phi_i), & i &= 1, 2, \dots, \tilde{n}, \end{aligned}$$

we obtain

$$\tilde{\mathbf{A}} = \sum_{K \in \mathcal{T}_h} \tilde{\mathbf{A}}_K, \quad \tilde{\mathbf{b}} = \sum_{K \in \mathcal{T}_h} \tilde{\mathbf{b}}_K.$$

Finite Element Approximation

Finite element assembly: element table

Since each element belongs to the support of exactly three basis functions, only (at most) nine entries of $\tilde{\mathbf{A}}_K$ and three entries of $\tilde{\mathbf{b}}_K$ are nonzero.

Which entries these are can be determined by maintaining an **element table**:

$$[G(i, j)]_{i=1,2,3; j=1, \dots, n_K} :$$

Element	K_1	K_2	\dots	K_{n_K}
first vertex	$i_1^{(1)}$	$i_1^{(2)}$	\dots	$i_1^{(n_K)}$
second vertex	$i_2^{(1)}$	$i_2^{(2)}$	\dots	$i_2^{(n_K)}$
third vertex	$i_3^{(1)}$	$i_3^{(2)}$	\dots	$i_3^{(n_K)}$

Here n_K denotes the number of triangles in \mathcal{T}_h .

Besides the **global vertex numbering**

$$x_1, x_2, \dots, x_{\tilde{n}},$$

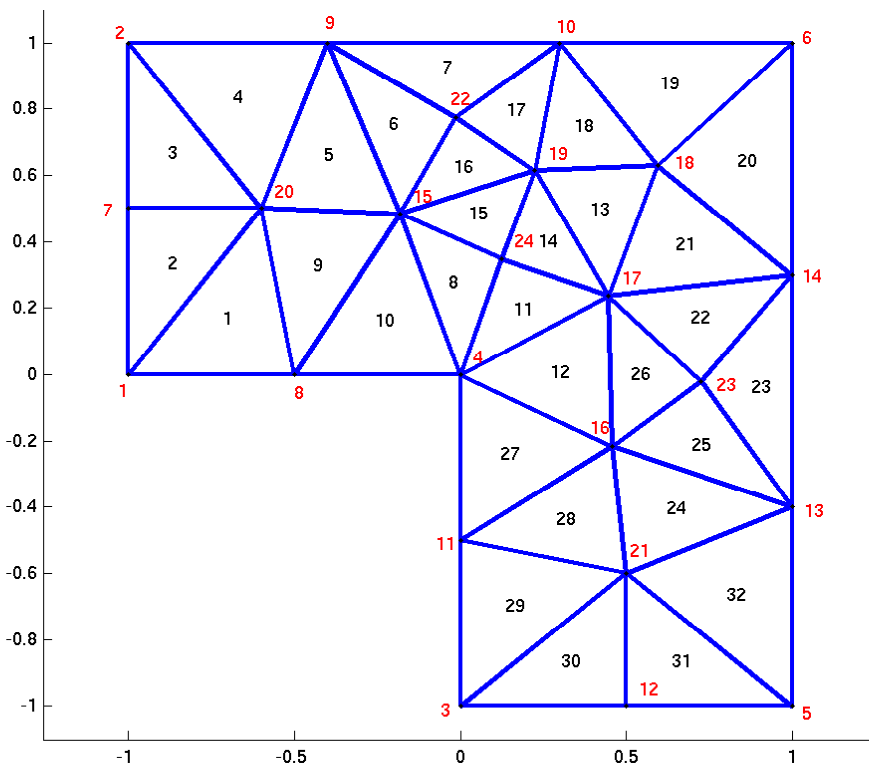
the element table introduces a second, **local vertex numbering**

$$x_1^{(K)}, x_2^{(K)}, x_3^{(K)}$$

of the vertices (DOFs) associated with K . G is the local to global mapping of the DOFs.

Finite Element Approximation

Finite element assembly



Global numbering of vertices (red) and elements (black) in a triangulation of an L-shaped domain.

Finite Element Approximation

Finite element assembly

With this notation the nonzero submatrix \mathbf{A}_K of $\tilde{\mathbf{A}}_K$ and nonzero subvector \mathbf{b}_K of $\tilde{\mathbf{b}}_K$ are given by

$$\mathbf{A}_K := \begin{bmatrix} a_K(\phi_1^{(K)}, \phi_1^{(K)}) & a_K(\phi_2^{(K)}, \phi_1^{(K)}) & a_K(\phi_3^{(K)}, \phi_1^{(K)}) \\ a_K(\phi_1^{(K)}, \phi_2^{(K)}) & a_K(\phi_2^{(K)}, \phi_2^{(K)}) & a_K(\phi_3^{(K)}, \phi_2^{(K)}) \\ a_K(\phi_1^{(K)}, \phi_3^{(K)}) & a_K(\phi_2^{(K)}, \phi_3^{(K)}) & a_K(\phi_3^{(K)}, \phi_3^{(K)}) \end{bmatrix}, \quad \mathbf{b}_K := \begin{bmatrix} \ell_K(\phi_1^{(K)}) \\ \ell_K(\phi_2^{(K)}) \\ \ell_K(\phi_3^{(K)}) \end{bmatrix}.$$

If K has number k in the enumeration of the elements, then the association of the local numbering $\{\phi_i^{(K)}\}_{i=1,2,3}$ of the three basis functions whose support contains K with the global numbering $\{\phi_j\}_{j=1}^{\tilde{n}}$ of all basis functions is given by

$$\phi_i^{(K)} = \phi_j, \quad j = G(i, k), \quad i = 1, 2, 3.$$

\mathbf{A}_K and \mathbf{b}_K are sometimes called the **element stiffness matrix** and **element load vector**.

Finite Element Approximation

Finite element assembly

We summarise phase (1) of the finite element assembly process in the following algorithm²

Algorithm 1 Phase (1) of finite element assembly.

- 1: Initialise $\tilde{\mathbf{A}} := \mathbf{O}$, $\tilde{\mathbf{b}} := \mathbf{0}$.
 - 2: **for** $K \in \mathcal{T}_h$ **do**
 - 3: Compute \mathbf{A}_K and \mathbf{b}_K
 - 4: $k \leftarrow$ [index of element K]
 - 5: $i_1 \leftarrow G(1, k)$, $i_2 \leftarrow G(2, k)$, $i_3 \leftarrow G(3, k)$
 - 6: $\tilde{\mathbf{A}}([i_1 i_2 i_3], [i_1 i_2 i_3]) \leftarrow \tilde{\mathbf{A}}([i_1 i_2 i_3], [i_1 i_2 i_3]) + \mathbf{A}_K$
 - 7: $\tilde{\mathbf{b}}([i_1 i_2 i_3]) \leftarrow \tilde{\mathbf{b}}([i_1 i_2 i_3]) + \mathbf{b}_K$
 - 8: **end for**
-

²We use the following MATLAB-inspired notation:

$$\mathbf{A}([i_1 i_2 i_3], [i_1 i_2 i_3]) = \begin{bmatrix} a_{i_1, i_1} & a_{i_1, i_2} & a_{i_1, i_3} \\ a_{i_2, i_1} & a_{i_2, i_2} & a_{i_2, i_3} \\ a_{i_3, i_1} & a_{i_3, i_2} & a_{i_3, i_3} \end{bmatrix}, \quad \mathbf{b}([i_1 i_2 i_3]) = \begin{bmatrix} b_{i_1} \\ b_{i_2} \\ b_{i_3} \end{bmatrix}.$$

Finite Element Approximation

Reference element

Both the numerical integration as well as the error analysis benefit from a change of variables to a **reference element** $\hat{K} \subset \mathbb{R}^2$. Each element $K \in \mathcal{T}_h$ then has a parametrisation $K = \mu_K(\hat{K})$, where

$$\mu_K : \hat{K} \rightarrow K, \quad \hat{K} \ni \xi \mapsto \mathbf{x} \in K, \quad \mathbf{x} = \mu_K(\xi) = B_K \xi + \mathbf{b}_K.$$

Most common for triangular elements: **unit simplex**

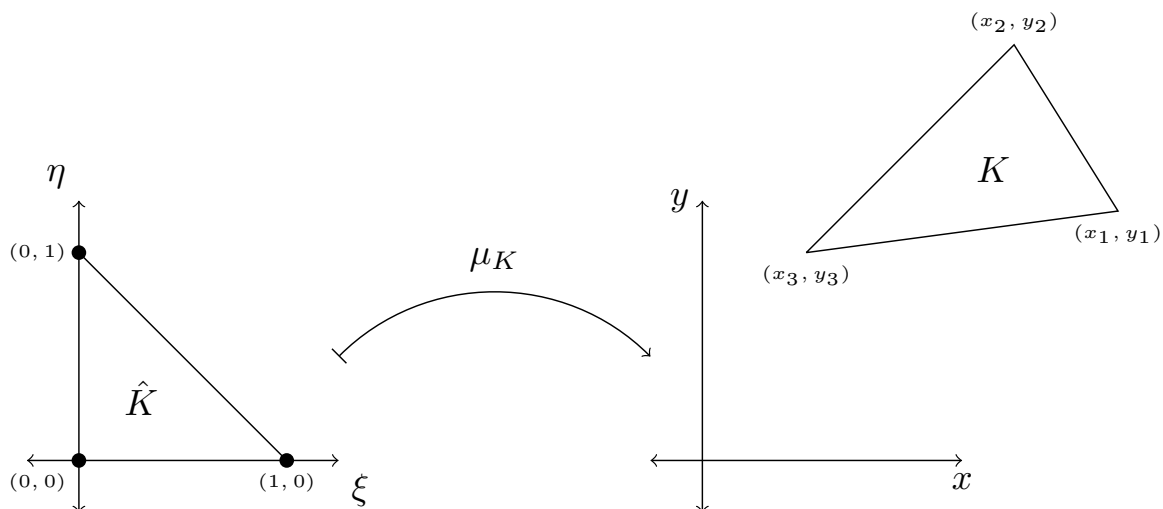
$$\hat{K} = \{(\xi, \eta) \in \mathbb{R}^2 : 0 \leq \xi \leq 1, 0 \leq \eta \leq 1 - \xi\}.$$

For each triangle $K \in \mathcal{T}_h$ the **affine** mapping μ_K is determined by prescribing, e.g.,

$$\begin{aligned} (1, 0) &\mapsto (x_1, y_1), \\ (0, 1) &\mapsto (x_2, y_2), \\ (0, 0) &\mapsto (x_3, y_3), \quad \text{i.e.} \end{aligned}$$

Finite Element Approximation

Reference element



$$\begin{bmatrix} x \\ y \end{bmatrix} = \underbrace{\begin{bmatrix} x_1 - x_3 & x_2 - x_3 \\ y_1 - y_3 & y_2 - y_3 \end{bmatrix}}_{B_K} \begin{bmatrix} \xi \\ \eta \end{bmatrix} + \underbrace{\begin{bmatrix} x_3 \\ y_3 \end{bmatrix}}_{\mathbf{b}_K}$$

Finite Element Approximation

Reference element

Local (nodal) basis on \hat{K} : (dual basis of DOF)

$$\hat{\phi}_1(\xi, \eta) = \xi, \quad \hat{\phi}_2(\xi, \eta) = \eta, \quad \hat{\phi}_3(\xi, \eta) = 1 - \xi - \eta, \quad (\xi, \eta) \in \hat{K}.$$

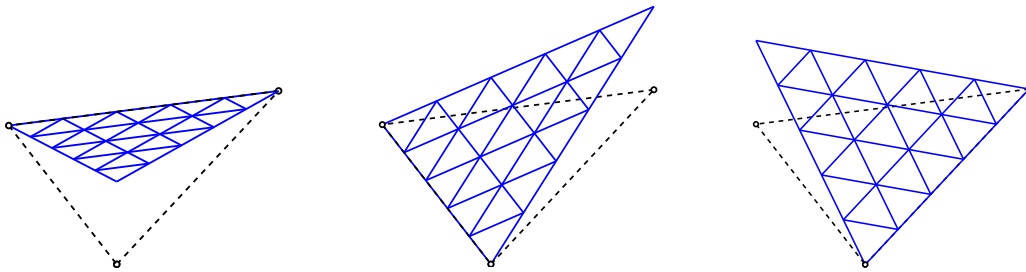
The correspondence

$$\hat{\phi} \mapsto \phi := \hat{\phi} \circ \mu_K^{-1}, \quad \text{d.h.} \quad \phi(\mathbf{x}) := \hat{\phi}(\boldsymbol{\xi}(\mathbf{x})) = \hat{\phi}(\mu_K^{-1}(\mathbf{x}))$$

assigns to $\hat{\phi}$ on \hat{K} a unique function ϕ on K .

Local basis functions on K :

$$\phi_j = \hat{\phi}_j \circ \mu_K^{-1} : K \rightarrow \mathbb{R}, \quad j = 1, 2, 3.$$



Finite Element Approximation

Reference element, change of variables

The chain rule³ applied to $\phi(\mathbf{x}) = \hat{\phi}(\boldsymbol{\xi}(\mathbf{x}))$ gives

$$\nabla \phi = \begin{bmatrix} \phi_x \\ \phi_y \end{bmatrix} = \begin{bmatrix} \hat{\phi}_\xi \xi_x + \hat{\phi}_\eta \eta_x \\ \hat{\phi}_\xi \xi_y + \hat{\phi}_\eta \eta_y \end{bmatrix} = \begin{bmatrix} \xi_x & \eta_x \\ \xi_y & \eta_y \end{bmatrix} \begin{bmatrix} \hat{\phi}_\xi \\ \hat{\phi}_\eta \end{bmatrix} = (D\mu_K^{-1})^\top \hat{\nabla} \hat{\phi}.$$

Since $\mathbf{x} = \mu_K(\boldsymbol{\xi}) = B_K \boldsymbol{\xi} + \mathbf{b}_K$, i.e. $D\mu_K \equiv B_K$,

$\boldsymbol{\xi} = \mu_K^{-1}(\mathbf{x}) = B_K^{-1}(\mathbf{x} - \mathbf{b}_K)$, i.e. $D\mu_K^{-1} \equiv B_K^{-1}$

we obtain

$$\nabla \phi = B_K^{-\top} \hat{\nabla} \hat{\phi}.$$

³ $\hat{\nabla}$ indicates differentiation with respect to the variables ξ and η .

Finite Element Approximation

Reference element, element integrals

This finally gives the element integrals ($\phi_i = \phi_i^{(K)}$, $i = 1, 2, 3$)

$$\begin{aligned} a_K(\phi_j, \phi_i) &= \int_K a(\mathbf{x}) \nabla \phi_j(\mathbf{x}) \cdot \nabla \phi_i(\mathbf{x}) \, d\mathbf{x} \\ &= \int_{\hat{K}} a(\mathbf{x}(\boldsymbol{\xi})) \left(B_K^{-\top} \hat{\nabla} \hat{\phi}_j(\boldsymbol{\xi}) \right) \cdot \left(B_K^{-\top} \hat{\nabla} \hat{\phi}_i(\boldsymbol{\xi}) \right) |\det B_K| \, d\boldsymbol{\xi}. \end{aligned} \tag{B.9}$$

The determinant is given by (note K is a triangle)

$$|\det B_K| = 2|K|,$$

$$B_K^{-\top} = \frac{1}{2|K|} \begin{bmatrix} y_2 - y_3 & x_3 - x_2 \\ y_3 - y_1 & x_1 - x_3 \end{bmatrix},$$

$$[\hat{\nabla} \hat{\phi}_1 \quad \hat{\nabla} \hat{\phi}_2 \quad \hat{\nabla} \hat{\phi}_3] = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \end{bmatrix}.$$

Finite Element Approximation

Eliminate constrained boundary DOF

To impose the Dirichlet boundary condition we require that the Galerkin approximation $u_h \in V_h$ satisfy

$$u_h(\mathbf{x}_j) = g(\mathbf{x}_j) \quad \text{at all boundary vertices } \{\mathbf{x}_j\}_{j=n+1}^{\tilde{n}}. \tag{B.10}$$

- We partition the coefficient vector $\mathbf{u} \in \mathbb{R}^{\tilde{n}}$ into a first block $\mathbf{u}_I \in \mathbb{R}^n$ containing the coefficients associated with the interior vertices $\{\mathbf{x}_j\}_{j=1}^n$ and a second block $\mathbf{u}_B \in \mathbb{R}^{\tilde{n}-n}$ containing the constrained coefficients associated with boundary vertices.
- For the assembled matrix $\tilde{\mathbf{A}}$ and vector $\tilde{\mathbf{b}}$ this induces the partitionings

$$\tilde{\mathbf{A}} = \begin{bmatrix} \tilde{\mathbf{A}}_{II} & \tilde{\mathbf{A}}_{IB} \\ \tilde{\mathbf{A}}_{BI} & \tilde{\mathbf{A}}_{BB} \end{bmatrix}, \quad \tilde{\mathbf{b}} = \begin{bmatrix} \tilde{\mathbf{b}}_I \\ \tilde{\mathbf{b}}_B \end{bmatrix}.$$

- The constraint (B.10) now reads $\mathbf{u}_B = \mathbf{g}$, where $\mathbf{g} \in \mathbb{R}^{\tilde{n}-n}$ contains the boundary data $\{g(\mathbf{x}_j)\}_{j=n+1}^{\tilde{n}}$.

Finite Element Approximation

Eliminate constrained boundary DOF

This constraint is characterised by there being no coupling of the boundary DOF to either interior DOF or among themselves, resulting in the modified linear system of equations

$$\begin{bmatrix} \tilde{\mathbf{A}}_{II} & \tilde{\mathbf{A}}_{IB} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{u}_I \\ \mathbf{u}_B \end{bmatrix} = \begin{bmatrix} \mathbf{b}_I \\ \mathbf{g} \end{bmatrix},$$

which gives the reduced system

$$\mathbf{A}\mathbf{u}_I = \mathbf{b}, \quad \mathbf{A} = \tilde{\mathbf{A}}_{II}, \quad \mathbf{b} = \mathbf{b}_I - \tilde{\mathbf{A}}_{IB}\mathbf{g}$$

for the interior DOF.

Note that this procedure is a discrete variant of the reformulation of the BVP with inhomogeneous Dirichlet boundary conditions to an equivalent one with homogeneous Dirichlet boundary conditions.

Finite Element Convergence

Summary

- C a's lemma characterises the Galerkin error as one of best approximation from the FE subspace V_h .
- An upper bound for this error is the distance of the true solution from its **interpolant** from the FE subspace. This is the uniquely determined function from V_h which possesses the same global DOF as the exact solution.
- The asymptotic behavior of the interpolant is then analyzed on a **sequence of meshes** $\{\mathcal{T}_{h_n}\}_{n \in \mathbb{N}}$ with $\lim_{n \rightarrow \infty} h_n = 0$.
- For the interpolation error to become small, the mesh sequence has to be **shape-regular**: if ρ_K denotes the radius of the inscribed circle in K and $h_K = \text{diam}K$, then a sequence of meshes is shape-regular provided the ratio

$$\frac{\rho_K}{h_K}, \quad K \in \mathcal{T}_h$$

is bounded below uniformly for all $\{\mathcal{T}_{h_n}\}$.

- A priori convergence bounds are obtained by relating the smoothness of the exact solution to the convergence rate h^α of the interpolation error as $h \rightarrow 0$.

Finite Element Convergence

Extra regularity

Interpolation estimates for u that is only in $H^1(D)$ do not yield a useful rate h^α with an $\alpha > 0$. As such one looks for solutions that possess higher regularity.

Definition B.12

For $r \in \mathbb{N}$ and $D \subset \mathbb{R}^d$ bounded, we denote by $H^r(D)$ the Sobolev space

$$H^r(D) := \{v \in L^2(D) : D^\alpha v \in L^2(D) \text{ for all } \alpha \in \mathbb{N}_0^d, |\alpha| \leq r\}.$$

$H^r(D)$ is a Hilbert space with the inner product

$$(u, v)_{H^r(D)} = \sum_{|\alpha| \leq r} \int_D (D^\alpha u)(D^\alpha v) \, dx,$$

and the induced norm given by

$$\|u\|_{H^r(D)}^2 = (u, u)_{H^r(D)} = \sum_{|\alpha| \leq r} \|D^\alpha u\|_{L^2(D)}^2.$$

Note: the vector $\alpha \in \mathbb{N}_0^d$ is called a *multiindex*, and $|\alpha| := \sum_{j=1}^d \alpha_j$.

Finite Element Convergence

Interpolation error of linear FE for H^2 -regular functions

- Let V_h denote the space of piecewise linear functions subject to a shape-regular, admissible triangulation \mathcal{T}_h of D .
- Denote by $I_h : C(\overline{D}) \rightarrow V_h$ the (global) interpolation operator assigning to each continuous function v the interpolant $v_h \in V_h$ determined by the condition that v_h agrees with v at all vertices of \mathcal{T}_h .
- Then the error of best approximation of $u \in C(\overline{D})$ is bounded by the interpolation error

$$\inf_{v \in V_h} |u - v|_{H^1(D)} \leq |u - I_h u|_{H^1(D)}.$$

- If the solution u of (B.4) has additional regularity $u \in H^2(D)$, then the **Sobolev imbedding theorem** assures that u agrees a.e. with a function in $C(\overline{D})$, so that pointwise evaluation of u and thus the interpolant is well-defined.
- In this case a scaling argument can be used to show

$$|u - I_h u|_{H^1(D)} \leq C h |u|_{H^2(D)}$$

with a constant C independent of h and u .

Finite Element Convergence

Model problem

Assumption 2 (H^2 /elliptic regularity)

There exists a constant $C_2 > 0$ such that, for every $f \in L^2(D)$, the solution of (B.4) belongs to $H^2(D)$ and satisfies

$$|u|_{H^2(D)} \leq C_2 \|f\|_{L^2(D)}.$$

Theorem B.13

Under Assumptions 1 and 2, the solution u of (B.4) with $f \in L^2(D)$ and the piecewise linear finite element approximation u_h on a sequence of shape-regular meshes satisfy

$$|u - u_h|_a \leq C \sqrt{a_{\max}} |u|_{H^2(D)} h \leq CC_2 \sqrt{a_{\max}} \|f\|_{L^2(D)} h, \quad (\text{B.11})$$

with a constant C independent of h .

Corollary B.14

Under the assumptions of Theorem B.13 there holds

$$|u - u_h|_{H^1(D)} \leq C \sqrt{\frac{a_{\max}}{a_{\min}}} |u|_{H^2(D)} h \leq CC_2 \sqrt{\frac{a_{\max}}{a_{\min}}} \|f\|_{L^2(D)} h.$$

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