Scientific Computing: Interpolation

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# 1 Function spaces

- 2 Polynomial Interpolation in 1D
- 3 Piecewise Polynomial Interpolation
- 4 Higher Dimensions
- 5 Advanced: Orthogonal Polynomials

#### Function spaces

#### Function Spaces

- Function spaces are the equivalent of finite vector spaces for functions (space of polynomial functions  $\mathcal{P}$ , space of smoothly twice-differentiable functions  $\mathcal{C}^2$ , etc.).
- Consider a one-dimensional interval I = [a, b]. Standard norms for functions similar to the usual vector norms:
  - Maximum norm:  $\|f(x)\|_{\infty} = \max_{x \in I} |f(x)|$
  - $L_1$  norm:  $||f(x)||_1 = \int_a^b |f(x)| dx$
  - Euclidian *L*<sub>2</sub> norm:  $||f(x)||_2 = \left[\int_a^b |f(x)|^2 dx\right]^{1/2}$
  - Weighted norm:  $||f(x)||_{w} = \left[\int_{a}^{b} |f(x)|^{2} w(x) dx\right]^{1/2}$
- An inner or scalar product (equivalent of dot product for vectors):

$$(f,g) = \int_a^b f(x)g^*(x)dx$$

#### Function spaces

#### **Finite-Dimensional Function Spaces**

- Formally, function spaces are **infinite-dimensional linear spaces**. Numerically we always **truncate and use a finite basis**.
- Consider a set of m + 1 nodes  $x_i \in \mathcal{X} \subset I$ , i = 0, ..., m, and define:

$$\|f(x)\|_{2}^{\mathcal{X}} = \left[\sum_{i=0}^{m} |f(x_{i})|^{2}\right]^{1/2},$$

which is equivalent to thinking of the function as being the vector  $\mathbf{f}_{\mathcal{X}} = \mathbf{y} = \{f(x_0), f(x_1), \cdots, f(x_m)\}.$ 

- Finite representations lead to semi-norms, but this is not that important.
- A discrete dot product can be just the vector product:

$$(f,g)^{\mathcal{X}} = \mathbf{f}_{\mathcal{X}} \cdot \mathbf{g}_{\mathcal{X}} = \sum_{i=0}^{m} f(x_i)g^{\star}(x_i)$$

#### Function Space Basis

• Think of a function as a vector of coefficients in terms of a set of *n* **basis functions**:

$$\{\phi_0(x),\phi_1(x),\ldots,\phi_n(x)\},\$$

for example, the monomial basis  $\phi_k(x) = x^k$  for polynomials.

• A finite-dimensional approximation to a given function f(x):

$$\tilde{f}(x) = \sum_{i=1}^{n} c_i \phi_i(x)$$

• Least-squares approximation for m > n (usually  $m \gg n$ ):

$$\mathbf{c}^{\star} = \arg\min_{\mathbf{c}} \left\| f(x) - \tilde{f}(x) \right\|_{2},$$

which gives the **orthogonal projection** of f(x) onto the finite-dimensional basis.

Polynomial Interpolation in 1D

# Interpolation in 1D (Cleve Moler)



Full degree polynomial interpolation



Shape-preserving Hermite interpolation





Figure 3.8. Four interpolants.

#### Interpolation

The task of interpolation is to find an interpolating function φ(x) which passes through m + 1 data points (x<sub>i</sub>, y<sub>i</sub>):

$$\phi(\mathbf{x}_i) = y_i = f(\mathbf{x}_i) \text{ for } i = 0, 2, \dots, m,$$

where  $\mathbf{x}_i$  are given **nodes**.

• The type of interpolation is classified based on the form of  $\phi(\mathbf{x})$ :

- Full-degree **polynomial** interpolation if  $\phi(\mathbf{x})$  is globally polynomial.
- **Piecewise polynomial** if  $\phi(\mathbf{x})$  is a collection of local polynomials:
  - Piecewise linear or quadratic
  - Hermite interpolation
  - Spline interpolation
- **Trigonometric** if  $\phi(\mathbf{x})$  is a trigonometric polynomial (polynomial of sines and cosines), leading to the Fast Fourier Transform.
- As for root finding, in dimensions higher than one things are more complicated!

# Polynomial interpolation in 1D

• The interpolating polynomial is degree at most m

$$\phi(x) = \sum_{i=0}^{m} a_i x^i = \sum_{i=0}^{m} a_i p_i(x),$$

where the monomials  $p_i(x) = x^i$  form a basis for the space of polynomial functions.

• The coefficients  $\mathbf{a} = \{a_1, \dots, a_m\}$  are solutions to the square linear system:

$$\phi(x_i) = \sum_{j=0}^m a_j x_i^j = y_i \text{ for } i = 0, 2, \dots, m$$

• In matrix notation, if we start indexing at zero:

$$\left[ \mathbf{V}(x_0, x_1, \dots, x_m) 
ight] \mathbf{a} = \mathbf{y}$$

where the **Vandermonde matrix**  $\mathbf{V} = \{v_{i,j}\}$  is given by

$$v_{i,j} = x_i^j$$
.

## The Vandermonde approach

Va = x

• One can prove by induction that

$$\det \mathbf{V} = \prod_{j < k} (x_k - x_j)$$

which means that the Vandermonde system is non-singular and thus: The intepolating polynomial is **unique if the nodes are distinct**.

- Polynomail interpolation is thus equivalent to solving a linear system.
- However, it is easily seen that the Vandermonde matrix can be very ill-conditioned.
- Solving a full linear system is also not very efficient because of the special form of the matrix.

## Choosing the right basis functions

• There are many mathematically equivalent ways to rewrite the unique interpolating polynomial:

$$x^2 - 2x + 4 = (x - 2)^2$$
.

One can think of this as choosing a different polynomial basis
 {φ<sub>0</sub>(x), φ<sub>1</sub>(x),..., φ<sub>m</sub>(x)} for the function space of polynomials of
 degree at most m:

$$\phi(x) = \sum_{i=0}^m a_i \phi_i(x)$$

• For a given basis, the coefficients **a** can easily be found by solving the linear system

$$\phi(x_j) = \sum_{i=0}^m a_i \phi_i(x_j) = y_j \quad \Rightarrow \quad \mathbf{\Phi} \mathbf{a} = \mathbf{y}$$

## Lagrange basis

Instead of writing polynomials as sums of monomials, let's consider a more general polynomial basis {φ<sub>0</sub>(x), φ<sub>1</sub>(x),..., φ<sub>m</sub>(x)}:

$$\phi(x) = \sum_{i=0}^m a_i \phi_i(x),$$

as in  $x^2 - 2x + 4 = (x - 2)^2$ .

• In particular let's consider the **Lagrange basis** which consists of polynomials that vanish at all but exactly one of the nodes, where they are unity:

$$\phi_i(x_j) = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

• The following characteristic polynomial provides the desired basis:

$$\phi_i(x) = \frac{\prod_{j \neq i} (x - x_j)}{\prod_{j \neq i} (x_i - x_j)}$$

Polynomial Interpolation in 1D

#### Lagrange basis on 10 nodes



#### Convergence, stability, etc.

- We have lost track of our goal: How good is polynomial interpolation?
- Assume we have a function f(x) that we are trying to **approximate** over an interval  $I = [x_0, x_m]$  using a polynomial interpolant.
- Using Taylor series type analysis it can be shown that for equi-spaced nodes, x<sub>i+1</sub> = x<sub>i</sub> + h, where h is a grid spacing,

$$\left\| \mathsf{E}_m(x) 
ight\|_\infty = m \mathsf{a}_{x \in I} \left| f(x) - \phi(x) 
ight| \leq rac{h^{n+1}}{4(m+1)} \left\| f^{(m+1)}(x) 
ight\|_\infty$$

Question: Does  $||E_m(x)||_{\infty} \to 0$  as  $m \to \infty$ ?

 In practice we may be dealing with non-smooth functions, e.g., discontinuous function or derivatives.
 Furthermore, higher-order derivatives of seemingly nice functions can be very large! Polynomial Interpolation in 1D

# Runge's counter-example: $f(x) = (1 + x^2)^{-1}$



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# Uniformly-spaced nodes

- Not all functions can be approximated well by an interpolating polynomial with **equally-spaced nodes** over an interval.
- Interpolating polynomials of higher degree tend to be **very oscillatory** and **peaked**, especially near the endpoints of the interval.
- Even worse, the **interpolation is unstable**, under small perturbations of the points  $\tilde{\mathbf{y}} = \mathbf{y} + \delta \mathbf{y}$ ,

$$\left\|\delta\phi(\mathbf{x})\right\|_{\infty} \leq rac{2^{m+1}}{m\log m} \left\|\delta\mathbf{y}\right\|_{\infty}$$

- It is possible to vastly improve the situation by using **specially-chosen non-equispaced nodes** (e.g., Chebyshev nodes), or by **interpolating derivatives** (Hermite interpolation).
- A true understanding would require developing **approximation theory** and looking into **orthogonal polynomials**, which we will not do here.

# **Chebyshev Nodes**

• A simple but good alternative to equally-spaced nodes are the **Chebyshev nodes**,

$$x_i = \cos\left(\frac{2i-1}{2k}\pi\right), \quad i=1,\ldots,k,$$

which have a simple geometric interpretation as the projection of uniformly spaced points on the unit circle.

- Polynomial interpolation using the Chebyshev nodes eliminates Runge's phenomenon.
- Furthermore, such polynomial interpolation gives **spectral accuracy**, which approximately means that for **sufficiently smooth functions** the error decays **exponentially in the number of points**, faster than any power law (fixed order of accuracy).
- There are very fast and robust numerical methods to actually perform the interpolation (function approximation) on Chebyshev nodes, see for example the package **chebfun** from Nick Trefethen.

Piecewise Polynomial Interpolation

# Interpolation in 1D (Cleve Moler)



Full degree polynomial interpolation



Shape-preserving Hermite interpolation





Figure 3.8. Four interpolants.

#### Piecewise interpolants

- The idea is to use a different low-degree polynomial function φ<sub>i</sub>(x) in each interval I<sub>i</sub> = [x<sub>i</sub>, x<sub>i+1</sub>].
- Piecewise-constant interpolation: \$\phi\_i^{(0)}(x) = y\_i\$, which is first-order accurate:

$$\left\|f(x)-\phi^{(0)}(x)\right\|_{\infty}\leq h\left\|f^{(1)}(x)\right\|_{\infty}$$

• Piecewise-linear interpolation:

$$\phi_i^{(1)}(x) = y_i + \frac{y_{i+1} - y_i}{x_{i+1} - x_i}(x - x_i)$$
 for  $x \in I_i$ 

For node spacing *h* the error estimate is now bounded but only **second-order accurate** 

$$\left\| f(x) - \phi^{(1)}(x) \right\|_{\infty} \le \frac{h^2}{8} \left\| f^{(2)}(x) \right\|_{\infty}$$

# **Cubic Splines**

- One can think about **piecewise-quadratic** interpolants but even better are **piecewise-cubic** interpolants.
- Going after twice continuously-differentiable interpolant,  $\phi(x) \in C_l^2$ , leads us to cubic spline interpolation:
  - The function φ<sub>i</sub>(x) is cubic in each interval l<sub>i</sub> = [x<sub>i</sub>, x<sub>i+1</sub>] (requires 4m coefficients).
  - We interpolate the function at the nodes: φ<sub>i</sub>(x<sub>i</sub>) = φ<sub>i-1</sub>(x<sub>i</sub>) = y<sub>i</sub>. This gives m + 1 conditions plus m - 1 conditions at interior nodes.
  - The first and second derivatives are continuous at the interior nodes:

$$\phi'_i(x_i) = \phi'_{i-1}(x_i)$$
 and  $\phi''_i(x_i) = \phi''_{i-1}(x_i)$  for  $i = 1, 2, \dots, m-1$ ,

which gives 2(m-1) equations.

• Now we have (m + 1) + (m - 1) + 2(m - 1) = 4m - 2 conditions for 4m unknowns.

# Types of Splines

- We need to specify two more conditions arbitrarily (for splines of order k ≥ 3, there are k − 1 arbitrary conditions).
- The most appropriate choice depends on the problem, e.g.:
  - **Periodic** splines, we think of node 0 and node *m* as one interior node and add the two conditions:

$$\phi'_0(x_0) = \phi'_m(x_m) \text{ and } \phi''_0(x_0) = \phi''_m(x_m).$$

- Natural spline: Two conditions  $\phi''(x_0) = \phi''(x_m) = 0$ .
- Once the type of spline is chosen, finding the coefficients of the cubic polynomials requires solving a **sparse tridiagonal linear system**, which can be done very fast (*O*(*m*)).

# Nice properties of splines

• The spline approximation converges for zeroth, first and second derivatives and even third derivatives (for equi-spaced nodes):

$$\|f(x) - \phi(x)\|_{\infty} \le \frac{5}{384} \cdot h^{4} \cdot \|f^{(4)}(x)\|_{\infty}$$
$$\|f'(x) - \phi'(x)\|_{\infty} \le \frac{1}{24} \cdot h^{3} \cdot \|f^{(4)}(x)\|_{\infty}$$
$$\|f''(x) - \phi''(x)\|_{\infty} \le \frac{3}{8} \cdot h^{2} \cdot \|f^{(4)}(x)\|_{\infty}$$

• We see that cubic spline interpolants are **fourth-order accurate** for functions. For **each derivative** we **loose one order of accuracy** (this is typical of all interpolants).

## In MATLAB

- c = polyfit(x, y, n) does least-squares polynomial of degree n which is interpolating if n = length(x).
- Note that MATLAB stores the coefficients in reverse order, i.e., c(1) is the coefficient of x<sup>n</sup>.
- y = polyval(c, x) evaluates the interpolant at new points.
- y1 = interp1(x, y, x<sub>new</sub>,' method') or if x is ordered use interp1q. Method is one of 'linear', 'spline', 'cubic'.
- The actual piecewise polynomial can be obtained and evaluated using *ppval*.

Piecewise Polynomial Interpolation

# Interpolating $(1 + x^2)^{-1}$ in MATLAB

Piecewise Polynomial Interpolation

#### Runge's function with spline



# Two Dimensions



# Regular grids

- Now x = {x<sub>1</sub>,...,x<sub>n</sub>} ∈ R<sup>n</sup> is a multidimensional data point. Focus on two-dimensions (2D) since three-dimensions (3D) is similar.
- The easiest case is when the data points are all inside a rectangle

$$\Omega = [x_0, x_{m_x}] \times [y_0, y_{m_y}]$$

where the  $m = (m_x + 1)(m_y + 1)$  nodes lie on a regular grid

$$\mathbf{x}_{i,j} = \{x_i, y_j\}, \quad f_{i,j} = f(\mathbf{x}_{i,j}).$$

• Just as in 1D, one can use a different interpolation function  $\phi_{i,j}: \Omega_{i,j} \to \mathbb{R}$  in each rectangle of the grid (pixel)

$$\Omega_{i,j} = [x_i, x_{i+1}] \times [y_j, y_{j+1}].$$

## **Bilinear Interpolation**

• The equivalent of piecewise linear interpolation for 1D in 2D is the **piecewise bilinear interpolation** 

$$\phi_{i,j}(x,y) = (\alpha x + \beta) (\gamma y + \delta) = a_{i,j} xy + b_{i,j} x + c_{i,j} y + d_{i,j}.$$

- There are 4 unknown coefficients in  $\phi_{i,j}$  that can be found from the 4 data (function) values at the corners of rectangle  $\Omega_{i,j}$ . This requires solving a small  $4 \times 4$  linear system inside each pixel independently.
- Note that the pieces of the interpolating function \$\phi\_{i,j}(x, y)\$ are not linear (but also not quadratic since no \$x^2\$ or \$y^2\$) since they contain quadratic product terms \$xy\$: bilinear functions. This is because there is not a plane that passes through 4 generic

points in 3D.

#### Piecewise-Polynomial Interpolation

• The key distinction about **regular grids** is that we can use **separable basis** functions:

$$\phi_{i,j}(\mathbf{x}) = \phi_i(x)\phi_j(y).$$

- Furthermore, it is sufficient to look at a **unit reference rectangle**  $\hat{\Omega} = [0,1] \times [0,1]$  since any other rectangle or even **parallelogram** can be obtained from the reference one via a linear transformation.
- Consider one of the corners (0,0) of the reference rectangle and the corresponding basis  $\hat{\phi}_{0,0}$  restricted to  $\hat{\Omega}$ :

$$\hat{\phi}_{0,0}(\hat{x},\hat{y}) = (1-\hat{x})(1-\hat{y})$$

• Generalization of bilinear to 3D is trilinear interpolation

$$\phi_{i,j,k} = a_{i,j,k}xyz + b_{i,j,k}xy + c_{i,j,k}xz + d_{i,j,k}yz + e_{i,j,k}x + f_{i,j,k}y + g_{i,j,k}z + h_{i,j,k}yz + g_{i,j,k}yz + g_{i$$

which has 8 coefficients which can be solved for given the 8 values at the vertices of the cube.

#### Bilinear basis functions



## Bicubic basis functions



# Irregular (Simplicial) Meshes

Any polygon can be triangulated into arbitrarily many **disjoint triangles**. Similarly **tetrahedral meshes** in 3D.



#### Basis functions on triangles

- For irregular grids the x and y directions are no longer separable.
- But the idea of using basis functions \(\phi\_{i,j}\), a reference triangle, and piecewise polynomial interpolants still applies.
- For a piecewise constant function we need one coefficient per triangle, for a linear function we need 3 coefficients (x, y, const), for quadratic 6 (x, y, x<sup>2</sup>, y<sup>2</sup>, xy, const), so we choose the reference nodes:





Fig. 8.8. Local interpolation nodes on  $\hat{T}$  for k=0 (ieft), k=1 (center), k=2 (right)

#### In MATLAB

• For regular grids the function

$$qz = interp2(x, y, z, qx, qy,' linear')$$

will evaluate the piecewise bilinear interpolant of the data x, y, z = f(x, y) at the points (qx, qy).

- Other method are 'spline' and 'cubic', and there is also *interp*3 for 3D.
- For irregular grids one can use the old function *griddata* which will generate its own triangulation or there are more sophisticated routines to manipulate triangulations also.

# Regular grids

$$[x, y] = meshgrid(-2:.5:2, -2:.5:2); z = x.*exp(-x.^2-y.^2);$$

```
mesh(qx,qy,qz); hold on;
plot3(x,y,z,'o'); hold off;
```

# MATLAB's *interp*2



## Irregular grids

```
mesh(qx,qy,qz); hold on;
plot3(x,y,z,'o'); hold off;
```

# MATLAB's griddata



Advanced: Orthogonal Polynomials

#### Advanced optional material: Orthogonal Polynomials

- Any finite interval [a, b] can be transformed to I = [-1, 1] by a simple transformation.
- Using a weight function w(x), define a function dot product as:

$$(f,g) = \int_a^b w(x) \left[ f(x)g(x) \right] dx$$

 For different choices of the weight w(x), one can explicitly construct basis of orthogonal polynomials where φ<sub>k</sub>(x) is a polynomial of degree k (triangular basis):

$$(\phi_i,\phi_j) = \int_a^b w(x) \left[\phi_i(x)\phi_j(x)\right] dx = \delta_{ij} \|\phi_i\|^2.$$

• For Chebyshev polynomials we set  $w = (1 - x^2)^{-1/2}$  and this gives

$$\phi_k(x) = \cos\left(k \arccos x\right).$$

# Legendre Polynomials

• For equal weighting w(x) = 1, the resulting triangular family of of polynomials are called **Legendre polynomials**:

$$\begin{aligned} \phi_0(x) &= 1\\ \phi_1(x) &= x\\ \phi_2(x) &= \frac{1}{2}(3x^2 - 1)\\ \phi_3(x) &= \frac{1}{2}(5x^3 - 3x)\\ \phi_{k+1}(x) &= \frac{2k+1}{k+1}x\phi_k(x) - \frac{k}{k+1}\phi_{k-1}(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\left[\left(x^2 - 1\right)^n\right]\end{aligned}$$

• These are orthogonal on I = [-1, 1]:

$$\int_{-1}^{-1}\phi_i(x)\phi_j(x)dx=\delta_{ij}\cdot\frac{2}{2i+1}.$$

#### Interpolation using Orthogonal Polynomials

Let's look at the interpolating polynomial φ(x) of a function f(x) on a set of m + 1 nodes {x<sub>0</sub>,..., x<sub>m</sub>} ∈ I, expressed in an orthogonal basis:

$$\phi(x) = \sum_{i=0}^{m} a_i \phi_i(x)$$

• Due to orthogonality, taking a dot product with  $\phi_j$  (weak formulation):

$$(\phi, \phi_j) = \sum_{i=0}^m a_i (\phi_i, \phi_j) = \sum_{i=0}^m a_i \delta_{ij} \|\phi_i\|^2 = a_j \|\phi_j\|^2$$

 This is equivalent to normal equations if we use the right dot product:

$$(\mathbf{\Phi}^{\star}\mathbf{\Phi})_{ij} = (\phi_i, \phi_j) = \delta_{ij} \|\phi_i\|^2$$
 and  $\mathbf{\Phi}^{\star}\mathbf{y} = (\phi, \phi_j)$ 

#### Gauss Integration

$$a_j \|\phi_j\|^2 = (\phi, \phi_j) \quad \Rightarrow \quad a_j = \left(\|\phi_j\|^2\right)^{-1} (\phi, \phi_j)$$

#### • Question: Can we easily compute

$$(\phi,\phi_j) = \int_a^b w(x) \left[\phi(x)\phi_j(x)\right] dx = \int_a^b w(x)p_{2m}(x) dx$$

for a polynomial  $p_{2m}(x) = \phi(x)\phi_j(x)$  of degree at most 2m?

#### Gauss nodes

If we choose the nodes to be zeros of φ<sub>m+1</sub>(x), then we can quickly project any polynomial onto the basis of orthogonal polynomials:

$$(\phi,\phi_j)=\sum_{i=0}^m w_i\phi(x_i)\phi_j(x_i)=\sum_{i=0}^m w_if(x_i)\phi_j(x_i)$$

where the Gauss weights w are given by

$$w_i = \int_a^b w(x)\phi_i(x)dx.$$

 The orthogonality relation can be expressed as a sum instead of integral:

$$(\phi_i, \phi_j) = \sum_{i=0}^m w_i \phi_i(x_i) \phi_j(x_i) = \delta_{ij} \|\phi_i\|^2$$

# Gauss-Legendre polynomials

- For any weighting function the polynomial  $\phi_k(x)$  has k simple zeros all of which are in (-1, 1), called the (order k) **Gauss nodes**,  $\phi_{m+1}(x_i) = 0$ .
- The interpolating polynomial φ(x<sub>i</sub>) = f(x<sub>i</sub>) on the Gauss nodes is the Gauss-Legendre interpolant φ<sub>GL</sub>(x).
- We can thus define a new weighted discrete dot product

$$\mathbf{f} \cdot \mathbf{g} = \sum_{i=0}^{m} w_i f_i g_i$$

The Gauss-Legendre interpolant is thus easy to compute:

$$\phi_{GL}(x) = \sum_{i=0}^{m} \frac{\mathbf{f} \cdot \phi_i}{\phi_i \cdot \phi_i} \phi_i(x).$$

#### Discrete spectral approximation

- Using orthogonal polynomails has many advantages for function approximation: **stability**, **rapid convergence**, and **computational efficiency**.
- The convergence, for sufficiently smooth (nice) functions (analytic in the neighborhood of [-1,1] in the complex plane), is **more rapid** than any power law

$$\|f(x)-\phi_{GL}(x)\|\sim C^{-m},$$

• This so-called **spectral accuracy** (limited by smoothness only) cannot be achived by piecewise, i.e., local, approximations (limited by order of local approximation).

Advanced: Orthogonal Polynomials

#### Gauss-Legendre Interpolation



Advanced: Orthogonal Polynomials

# Global polynomial interpolation error



# Conclusions/Summary

- Interpolation means approximating function values in the interior of a domain when there are **known samples** of the function at a set of **interior and boundary nodes**.
- Given a **basis set** for the **interpolating functions**, interpolation amounts to solving a linear system for the coefficients of the basis functions.
- Polynomial interpolants in 1D can be constructed using several basis.
- Using polynomial interpolants of **high order is a bad idea**: Not accurate and not stable!
- Instead, it is better to use **piecewise polynomial** interpolation: constant, linear, Hermite cubic, cubic spline interpolant on each **interval**.
- In higher dimensions one must be more careful about how the domain is split into disjoint elements (analogues of intervals in 1D): regular grids (separable basis such as bilinear), or simplicial meshes (triangular or tetrahedral).