Scientific Computing:
Interpolation

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Outline

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_2 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):

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

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** $x_i \in \mathcal{X} \subset I$, $i = 0, \ldots, m$, 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 $f(x)$:

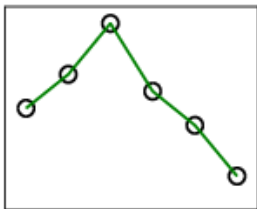$$\tilde{f}(x) = \sum_{i=1}^{n} c_i \phi_i(x)$$

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

$$\mathbf{c}^{\star} = \arg \min_{\mathbf{c}} \left\| f(x) - \tilde{f}(x) \right\|_2,$$
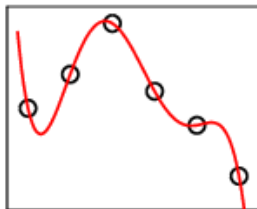
which gives the **orthogonal projection** of $f(x)$ onto the finite-dimensional basis.
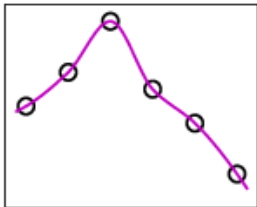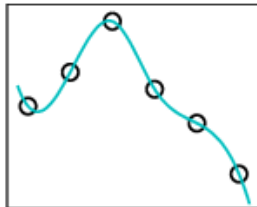
Interpolation in 1D (Cleve Moler)

Figure 3.8. *Four interpolants.*

Interpolation

- The task of interpolation is to find an **interpolating function** $\phi(\mathbf{x})$ which passes through $m+1$ **data points** $(\mathbf{x}_i, y_i)$:

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

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 $\mathbf{a} = \{a_1, \ldots, a_m\}$ are solutions to the square linear system:

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

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

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

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

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

The Vandermonde approach

$$\mathbf{Va} = \mathbf{x}$$

- 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** $\{\phi_0(x), \phi_1(x), \ldots, \phi_m(x)\}$ 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 $\mathbf{a}$ can easily be found by solving the linear system

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

Lagrange basis

- Instead of writing polynomials as sums of monomials, let's consider a more general **polynomial basis** $\{\phi_0(x), \phi_1(x), \ldots, \phi_m(x)\}$:

$$\phi(x) = \sum_{i=0}^{m} a_i \phi_i(x),$$
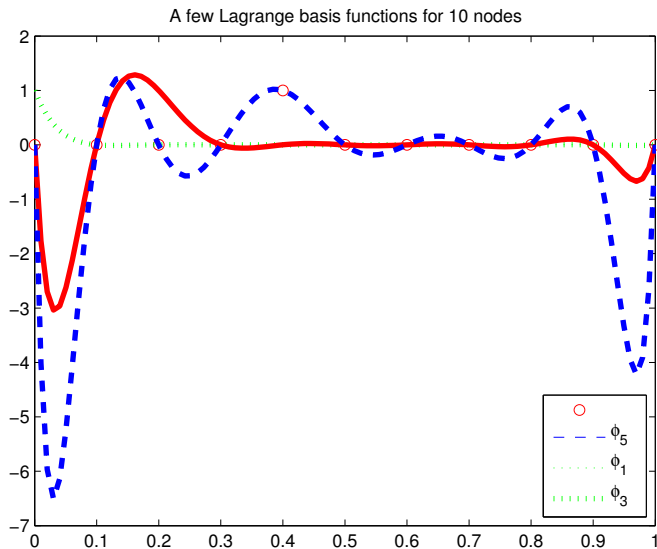
as in $x^2 - 2x + 4 = (x-2)^2$.

- 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:

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

Lagrange basis on 10 nodes

A few Lagrange basis functions for 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**, $x_{i+1} = x_i + h$, where h is a **grid spacing**,

$$\|E_m(x)\|_\infty = max_{x \in I} |f(x) - \phi(x)| \leq \frac{h^{n+1}}{4(m+1)} \left\| f^{(m+1)}(x) \right\|_\infty.$$

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!

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

Runges phenomenon for 10 nodes
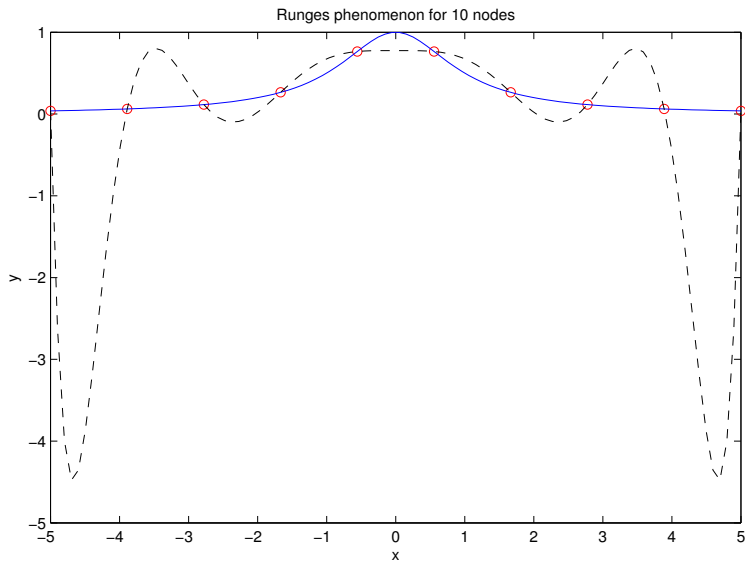
Uniformly-spaced nodes

- 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 $\tilde{\mathbf{y}} = \mathbf{y} + \delta\mathbf{y}$,

$$\|\delta\phi(x)\|_\infty \le \frac{2^{m+1}}{m \log m} \|\delta\mathbf{y}\|_\infty$$

- 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.
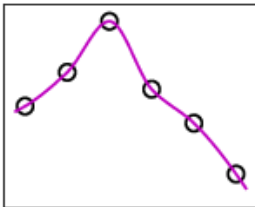
Interpolation in 1D (Cleve Moler)
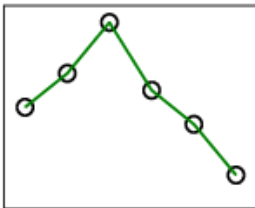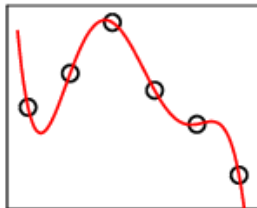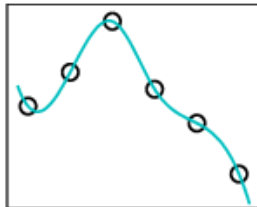

Figure 3.8. *Four interpolants.*

Piecewise interpolants

- The idea is to use a **different low-degree polynomial** function $\phi_i(x)$ in each interval $I_i = [x_i, x_{i+1}]$.

- **Piecewise-constant** interpolation: $\phi_i^{(0)}(x) = y_i$, which is **first-order accurate**:

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

- **Piecewise-linear** interpolation:

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

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, $\phi(x) \in C_I^2$, leads us to **cubic spline interpolation**:

  - The function $\phi_i(x)$ is **cubic** in each interval $I_i = [x_i, x_{i+1}]$ (requires $4m$ coefficients).
  - We **interpolate** the function at the nodes: $\phi_i(x_i) = \phi_{i-1}(x_i) = y_i$. This gives $m + 1$ conditions plus $m - 1$ conditions at **interior nodes**.
  - The **first and second derivatives are continuous** at the interior nodes:

    $$\phi_i'(x_i) = \phi_{i-1}'(x_i) \text{ and } \phi_i''(x_i) = \phi_{i-1}''(x_i) \text{ for } i = 1, 2, \ldots, m - 1,$$

    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 $k \geq 3$, 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):

$$\|f(x) - \phi(x)\|_\infty \leq \frac{5}{384} \cdot h^4 \cdot \left\|f^{(4)}(x)\right\|_\infty$$

$$\left\|f'(x) - \phi'(x)\right\|_\infty \leq \frac{1}{24} \cdot h^3 \cdot \left\|f^{(4)}(x)\right\|_\infty$$

$$\left\|f''(x) - \phi''(x)\right\|_\infty \leq \frac{3}{8} \cdot h^2 \cdot \left\|f^{(4)}(x)\right\|_\infty$$

- 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^n.
- $y = polyval(c, x)$ evaluates the interpolant at new points.
- $y1 = interp1(x, y, x_{new}, 'method')$ or if x is ordered use $interp1q$. Method is one of 'linear', 'spline', 'cubic'.
- The actual piecewise polynomial can be obtained and evaluated using $ppval$.

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

```
n=10;
x=linspace(-5,5,n);
y=(1+x.^2).^(-1);
plot(x,y,'ro'); hold on;

x_fine=linspace(-5,5,100);
y_fine=(1+x_fine.^2).^(-1);
plot(x_fine,y_fine,'b-');

c=polyfit(x,y,n);
y_interp=polyval(c,x_fine);
plot(x_fine,y_interp,'k--');

y_interp=interp1(x,y,x_fine,'spline');
plot(x_fine,y_interp,'k--');
% Or equivalently:
pp=spline(x,y);
y_interp=ppval(pp,x_fine)
```
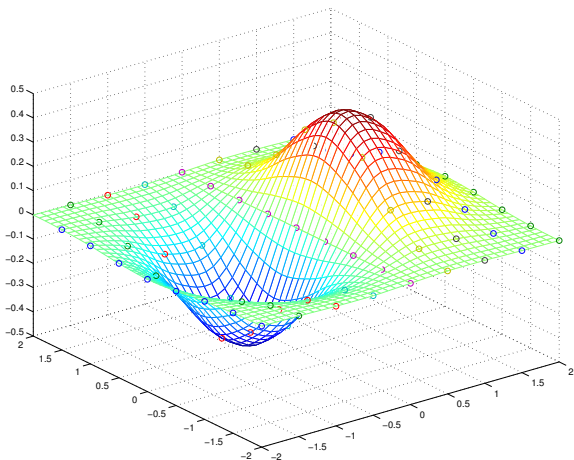
Runge's function with spline

Not-a-knot spline interpolant
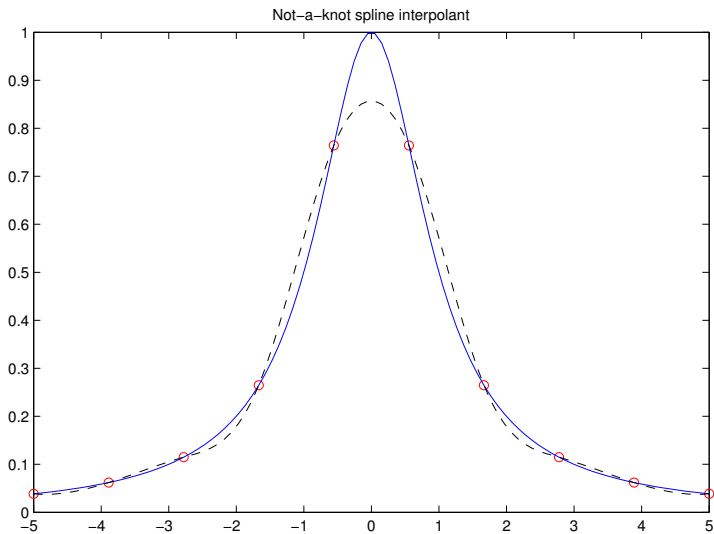
Two Dimensions

Regular grids

- Now $\mathbf{x} = \{x_1, \ldots, x_n\} \in \mathbf{R}^n$ 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 4×4 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**

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

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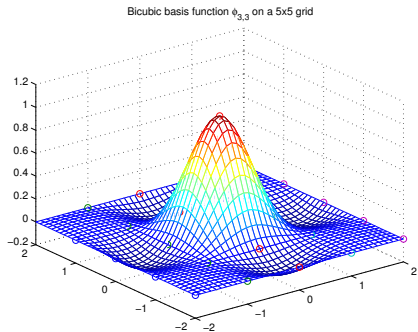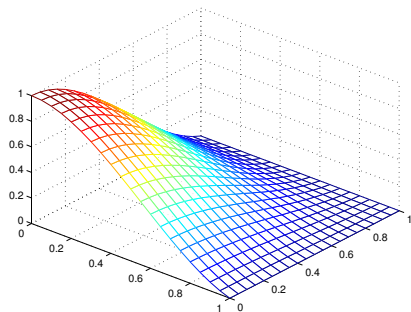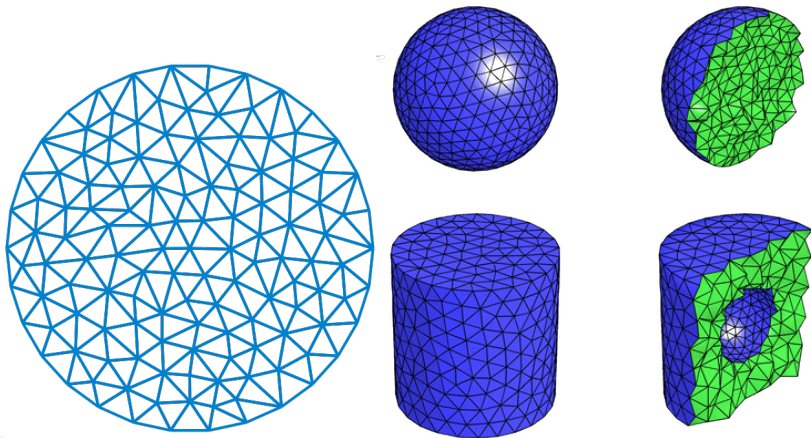
Bilinear basis functions
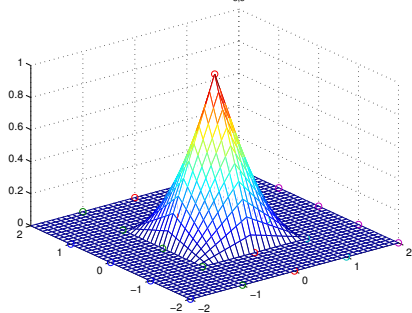
Bicubic basis functions

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 $(x, y, x^2, y^2, xy, \text{const})$, so we choose the **reference nodes**:
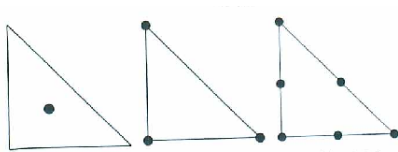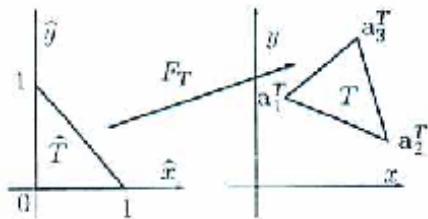

Fig. 8.8. Local interpolation nodes on $\hat{T}$ for $k = 0$ (left), $k = 1$ (center), $k = 2$ (right)

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 *interp3* for 3D.

- For irregular grids one can use the old function *griddata* which will
generate its own triangulation or there are more sophisticated routines
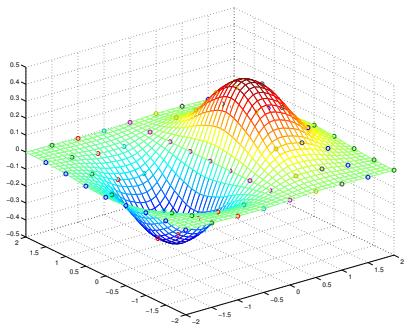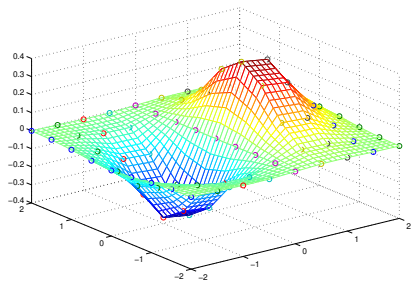to manipulate triangulations also.

Regular grids

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

ti = -2:.1:2;
[qx,qy] = meshgrid(ti,ti);

qz= interp2(x,y,z,qx,qy,'cubic');

mesh(qx,qy,qz); hold on;
plot3(x,y,z,'o'); hold off;
```
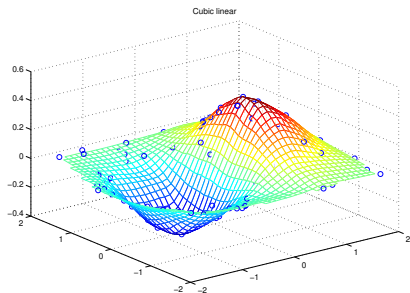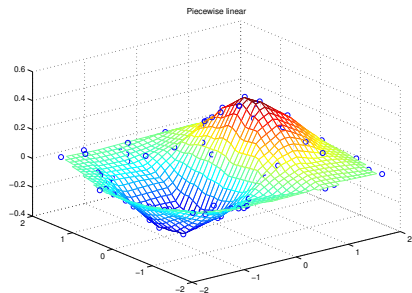
MATLAB's *interp*2

Irregular grids

```
x = rand(100,1)*4-2; y = rand(100,1)*4-2;
z = x.*exp(-x.^2-y.^2);

ti = -2:.1:2;
[qx,qy] = meshgrid(ti,ti);

qz= griddata(x,y,z,qx,qy,'cubic');

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

MATLAB's *griddata*

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).