# Numerical Methods I
# Polynomial 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.

# Least-Squares Approximation

- Discrete case: Think of **fitting** a straight line or quadratic through experimental data points.
- The function becomes the vector $\mathbf{y} = \mathbf{f}_{\mathcal{X}}$, and the approximation is

$$y_i = \sum_{j=1}^{n} c_j \phi_j(x_i) \quad \Rightarrow \quad \mathbf{y} = \mathbf{\Phi} \mathbf{c},$$

$$\mathbf{\Phi}_{ij} = \phi_j(x_i).$$

- This means that finding the approximation consists of solving an **overdetermined linear system**

$$\mathbf{\Phi} \mathbf{c} = \mathbf{y}$$

- Note that for $m = n$ this is equivalent to interpolation. MATLAB's *polyfit* works for $m \geq n$.

# Normal Equations

- Recall that one way to solve this is via the normal equations:

$$\left(\mathbf{\Phi}^{\star}\mathbf{\Phi}\right)\mathbf{c}^{\star}=\mathbf{\Phi}^{\star}\mathbf{y}$$

- A basis set is an **orthonormal basis** if

$$(\phi_i,\phi_j)=\sum_{k=0}^{m}\phi_i(x_k)\phi_j(x_k)=\delta_{ij}=\begin{cases}1 & \text{if } i=j\\ 0 & \text{if } i\neq j\end{cases}$$

$$\mathbf{\Phi}^{\star}\mathbf{\Phi}=\mathbf{I}\text{ (unitary or orthogonal matrix)}\quad\Rightarrow$$

$$\mathbf{c}^{\star}=\mathbf{\Phi}^{\star}\mathbf{y}\quad\Rightarrow\quad c_i=\phi_i^{\mathcal{X}}\cdot\mathbf{f}_{\mathcal{X}}=\sum_{k=0}^{m}f(x_k)\phi_i(x_k)$$

# Interpolation in 1D (Cleve Moler)

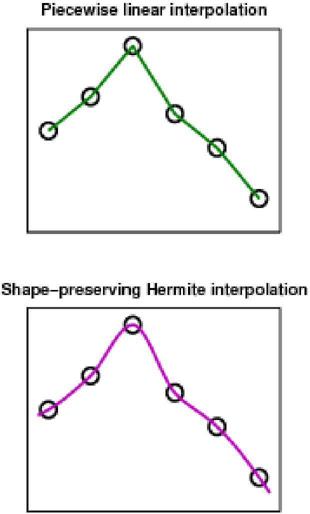



**Figure 3.8.** *Four interpolants.*

# 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).
  - **Orthogonal polynomial** intepolation (Chebyshev, Legendre, etc.).
- 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

$$\mathbf{V}\mathbf{a} = \mathbf{x}$$

- 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 **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

$$\mathbf{\Phi a} = \mathbf{y}$$

- This linear system will be trivial to solve if $\mathbf{\Phi} = \mathbf{I}$, i.e., if

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

- The $\phi_i(x)$ is itself a polynomial interpolant on the same nodes but with function values $\delta_{ij}$, and is thus unique.
- Note that the **nodal polynomial**

$$w_{m+1}(x) = \prod_{i=0}^{m} (x - x_i)$$

vanishes at all of the nodes but has degree $m + 1$.

# Lagrange interpolant

- It can easily be seen that the following **characteristic polynomial** provides the desired basis:

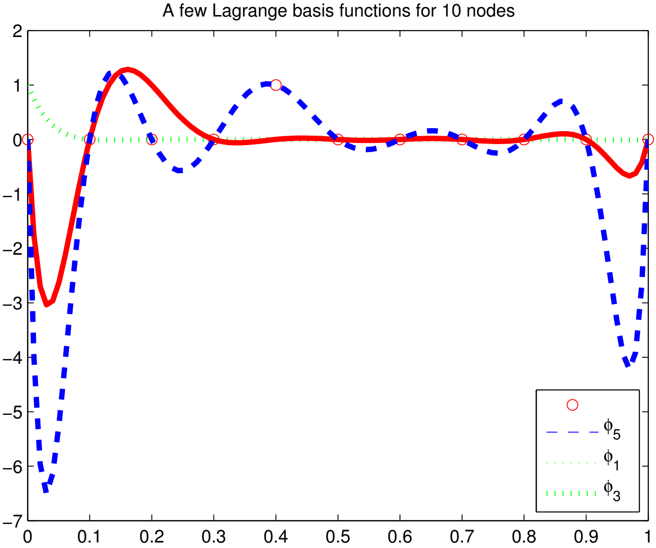
$$\phi_i(x) = \frac{\prod_{j\neq i}(x - x_j)}{\prod_{j\neq i}(x_i - x_j)} = \frac{w_{m+1}(x)}{(x - x_i)\,w'_{m+1}(x_i)}$$

- The resulting **Lagrange interpolation formula** is

$$\phi(x) = \sum_{i=0}^{m} y_i \phi_i(x) = \sum_{i=0}^{m} \left[\frac{y_i}{\prod_{j\neq i}(x_i - x_j)}\right] \prod_{j\neq i}(x - x_j)$$

- This is useful analytically but **expensive and cumbersome** to use computationally!

# Lagrange basis on 10 nodes



# Newton's interpolation formula

- By choosing a different basis we get different representations, and Newton's choice is:

$$\phi_i(x) = w_i(x) = \prod_{j=0}^{i-1} (x - x_j)$$

- There is a simple recursive formula to calculate the coefficients **a** in this basis, using Newton's **divided differences**

$$D_i^0 f = f(x_i) = y_i$$

$$D_i^k = \frac{D_{i+1}^{k-1} - D_i^{k-1}}{x_{i+1} - x_i}.$$

- Note that the first divided difference is

$$D_i^1 = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} \approx f'(x_i),$$

  and $D_i^2$ corresponds to second-order derivatives, etc.

# Convergence and stability

- 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 is not hard to show that

$$\exists \xi \in I \text{ such that } E_m(x) = f(x) - \phi(x) = \frac{f^{(m+1)}(\xi)}{(m+1)!}\left[\prod_{i=0}^{m}(x - x_i)\right].$$

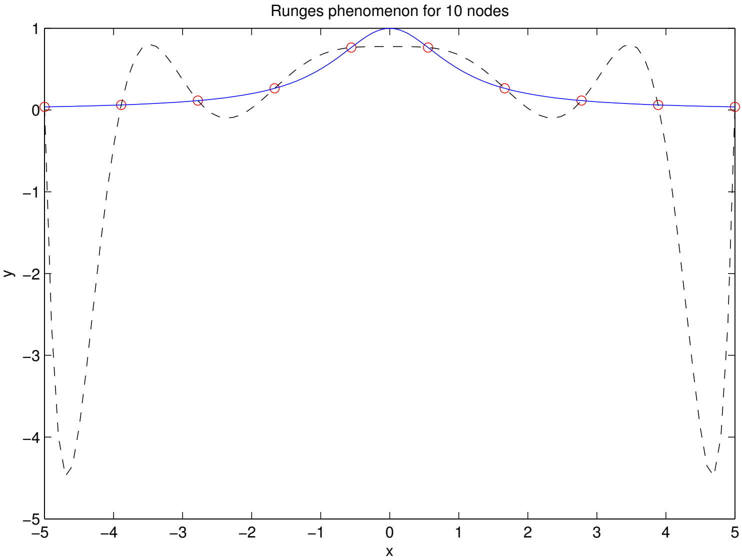
Question: Does $\|E_m(x)\|_\infty = max_{x \in I}|f(x)| \to 0$ as $m \to \infty$.

- For equi-spaced nodes, $x_{i+1} = x_i + h$, a bound is

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

- The problem is that **higher-order derivatives** of seemingly nice functions **can be unbounded**!

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



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

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

- It is possible to improve the situation by using **specially-chosen nodes** (e.g., Chebyshev nodes), or by **interpolating derivatives** (Hermite interpolation).
- In general however, we conclude that **interpolating using high-degree polynomials is a bad idea**!

# Interpolation in 1D (Cleve Moler)

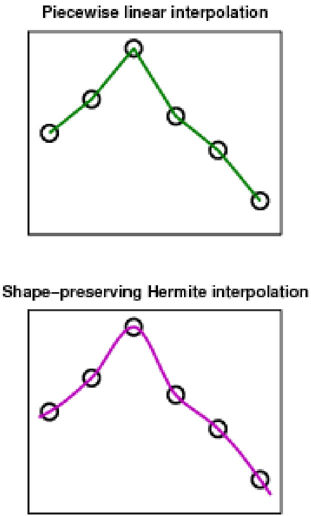



**Figure 3.8.** *Four interpolants.*

# Piecewise Lagrange 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: $\phi_i^{(0)}(x) = y_i$.
- **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 and stable:

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

# Piecewise Hermite interpolants

- If we are given not just the function values but also the first derivatives at the nodes:
$$z_i = f'(x_i),$$
we can find a cubic polynomial on every interval that interpolates both the function and the derivatives at the endpoints:
$$\phi_i(x_i) = y_i \text{ and } \phi_i'(x_i) = z_i$$
$$\phi_i(x_{i+1}) = y_{i+1} \text{ and } \phi_i'(x_{i+1}) = z_{i+1}.$$
- This is called the **piecewise cubic Hermite interpolant**.
- If the derivatives are not available we can try to estimate $z_i \approx \phi_i'(x_i)$ (see MATLAB's *pchip*).

# Splines

- Note that in piecewise Hermite interpolation $\phi(x)$ has is continuously differentiable, $\phi(x) \in C_I^1$:
  Both $\phi(x)$ and $\phi'(x)$ are continuous across the **internal nodes**.
- We can make this even stronger, $\phi(x) \in C_I^2$, leading to **piecewise 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 continous** 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, for a total of $4m-2$ conditions.

# 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 **tridiagonal linear system**, which can be done very fast ($O(m)$).

# Nice properties of splines

- Minimum curvature property:

$$\int_I \left[\phi''(x)\right]^2 dx \leq \int_I \left[f''(x)\right]^2 dx$$

- The spline approximation converges for zeroth, first and second derivatives (also third for uniformly-spaced nodes):

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

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

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

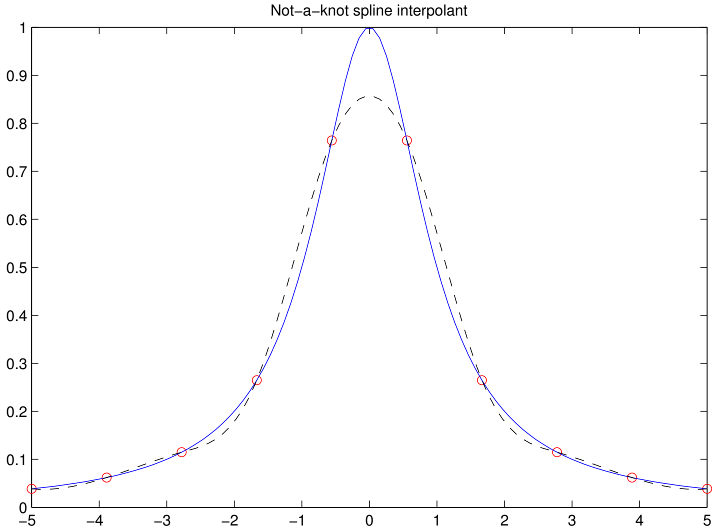
# In MATLAB

- $c = polyfit(x, y, n)$ 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*.

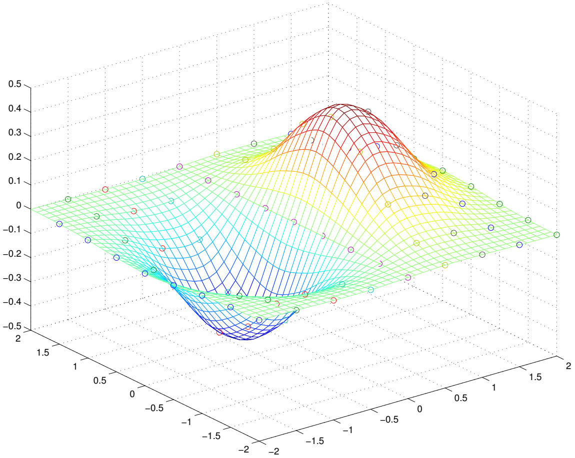
# Interpolating $(1+x^2)^{-1}$ in MATLAB

```
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



# Two Dimensions



# Regular grids

- Now $\mathbf{x} = \{x_1, \ldots, x_n\} \in \mathbf{R}^n$ is a multidimensional data point. Focus on 2D since 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**

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

- We can use **separable basis** functions:

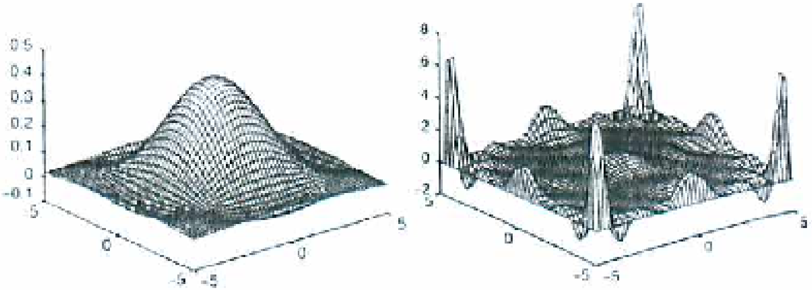
$$\phi_{i,j}(\mathbf{x}) = \phi_i(x)\phi_j(y).$$

# Full degree polynomial interpolation

We can directly apply Lagrange interpolation to each coordinate separately:

$$\phi(x) = \sum_{i,j} f_{i,j}\phi_{i,j}(x,y) = \sum_{i,j} f_{i,j}\phi_i(x)\phi_j(y),$$

but this still suffers from **Runge's phenomenon**:



# Piecewise-Polynomial Interpolation

- Juse as in 1D, one can use a different interpolation function $\phi_{i,j}: \; \Omega_{i,j} \rightarrow \mathbb{R}$ in each rectange of the grid

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

- For separable polynomials, the equivalent of piecewise linear interpolation in 1D is the **piecewise bilinear interpolation**

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

- There are 4 unknown coefficients in $\phi_{i,j}$ that can be found from the 4 data (function) values at the corners of rectangle $\Omega_{i,j}$.
- 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.

# Bilinear Interpolation

- It is better to think in terms of a basis set $\{\phi_{i,j}(x,y)\}$, where each basis function $\phi_{i,j}$ is itself piecewise bilinear, one at the node $(i,j)$-th node of the grid, zero elsewhere:

$$\phi(x) = \sum_{i,j} f_{i,j}\phi_{i,j}(x,y).$$

- 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:

$$\mathbf{B}_{i,j}\hat{\Omega} + \mathbf{b}_{i,j} = \Omega_{i,j},$$

and the same transformation can then be applied to the interpolation function:

$$\phi_{i,j}(\mathbf{x}) = \hat{\phi}(\mathbf{B}_{i,j}\hat{\mathbf{x}} + \mathbf{b}_{i,j}).$$

# Bilinear Basis Functions

- Consider one of the corners $(0,0)$ of the reference rectangle and the corresponding basis $\hat{\phi}_{0,0}$ restricted to $\hat{\Omega}$:

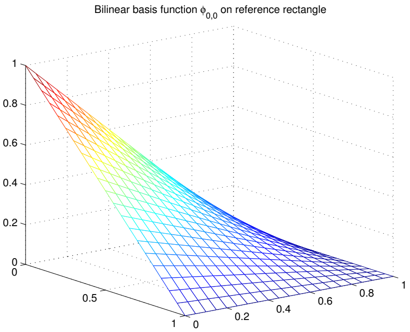
$$\hat{\phi}_{0,0}(\hat{x},\hat{y}) = (1-\hat{x})(1-\hat{y})$$

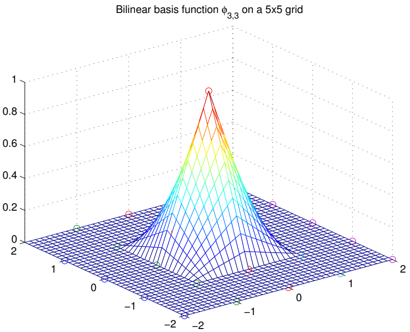
- For an actual grid, the basis function corresponding to a given interior node is simply a composite of 4 such bilinear terms, one for each rectangle that has that interior node as a vertex: Often called a **tent function**.
- If higher smoothness is required one can consider, for example, **bicubic Hermite interpolation** (when derivatives $f_x$, $f_y$ and $f_{xy}$ are known at the nodes as well).
- Generalization of bilinear to 3D is **trilinear interpolation**

$$\phi(x,y,z) = axyz + bxy + cxz + dyz + ex + fy + gz + h,$$

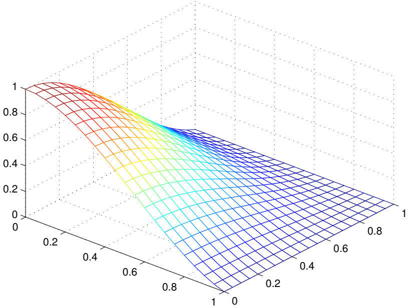
which has 8 coefficients which can be solved for given the 8 values at the vertices of the cube.

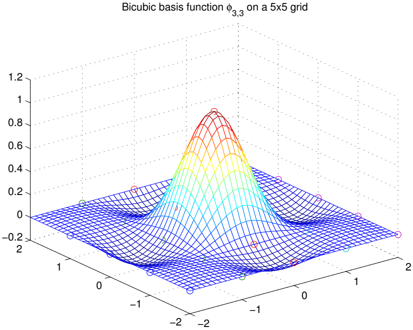
# Bilinear basis functions



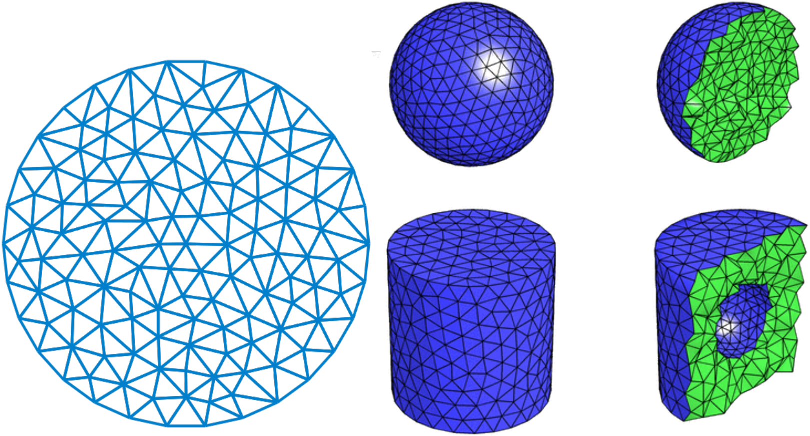
# Bicubic basis functions



# 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 linear function we need 3 coefficients $(x, y, \text{const})$, for quadratic 6 $(x, y, x^2, y^2, xy, \text{const})$:

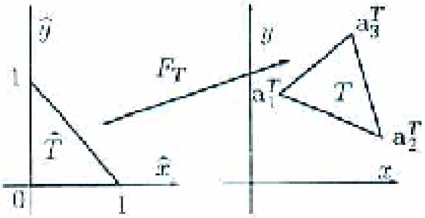



Fig. 8.8. Local interpolation nodes on $\hat{T}$ for $k = 0$ (*left*), $k = 1$ (*center*), $k = 2$ (*right*)

# Piecewise constant / linear basis functions

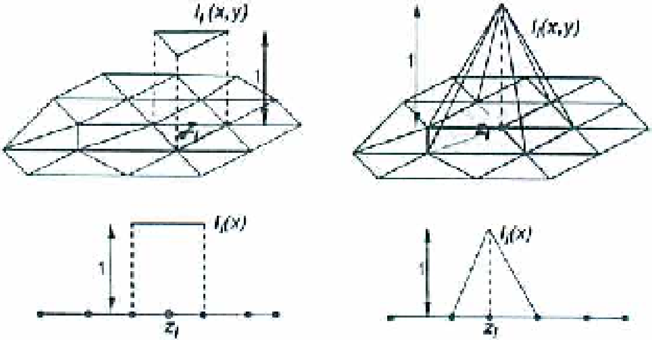



Fig. 8.7. Characteristic piecewise Lagrange polynomial, in two and one space dimensions. Left, $k = 0$; right, $k = 1$

# In MATLAB

- For regular grids the function

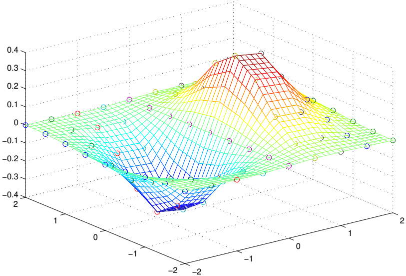
$$qz = interp2(x, y, z, qx, qy,' \, linear')$$

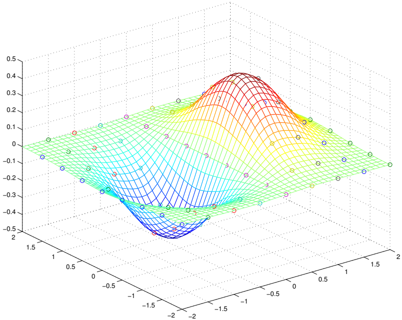
  will evaluate the piecewise bilinear interpolant of the data $x, y, z = f(x, y)$ at the points $(qx, qy)$.
- Other method are 'spline' and 'cubic', and there is also *interp*3 for 3D.
- For irregular grids one can use the old function *griddata* which will generate its own triangulation or there are 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);

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 *interp2*

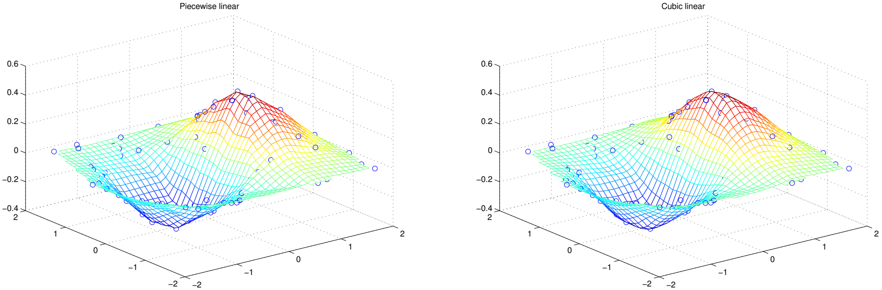


# Irregular grids

```
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).