Interpolation

CHEN 1703

See also wiki page notes on interpolation.

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Example - Vapor Pressure of Water

What is "vapor pressure?"

- ➡ For our purposes: the pressure at which a liquid will boil at a given temperature.
- ➡ Examples: pressure cooker, high-altitude cooking, etc.

Determine vapor pressure of water at:

- 25 °C
- 92 °C
- 105 °C

T (°C)	P (mm Hg)
0	4.579
10	9.209
20	17.535
30	31.824
40	55.324
50	92.51
60	149.38
70	233.7
80	355.1
85	433.6
90	525.76
95	633.9
98	707.27
100	760
101	787.57

Data could be from experiments, theoretical calculations, etc.

<u>Concept</u>:

Fit a function to the data, and then evaluate the function wherever we need to.

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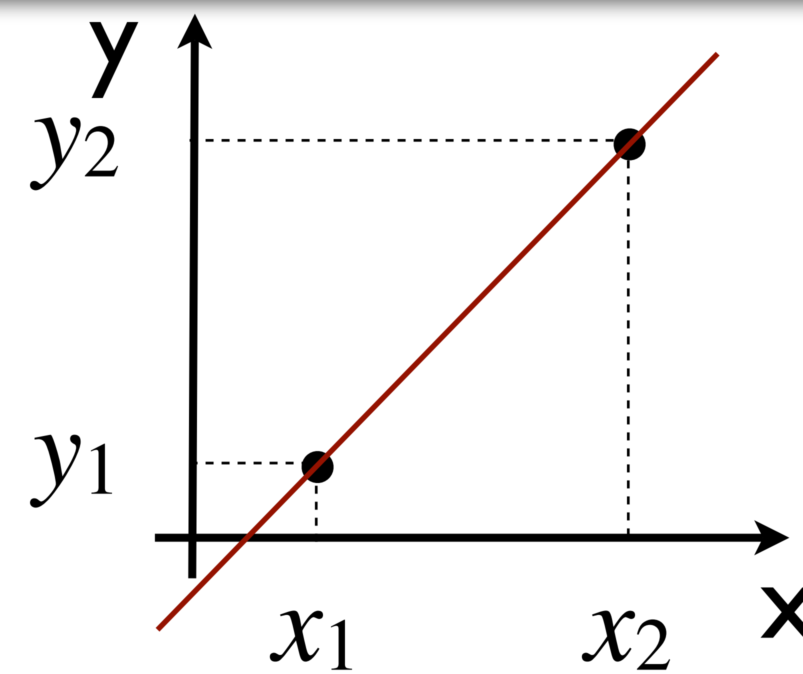
Linear Interpolation

$$y = mx + b \;\rightarrow\; \begin{aligned} y_1 &= mx_1 + b \\ y_2 &= mx_2 + b \end{aligned}$$

Program this into your calculator.

$$y = \left(\frac{y_2 - y_1}{x_2 - x_1}\right)(x - x_1) + y_1$$

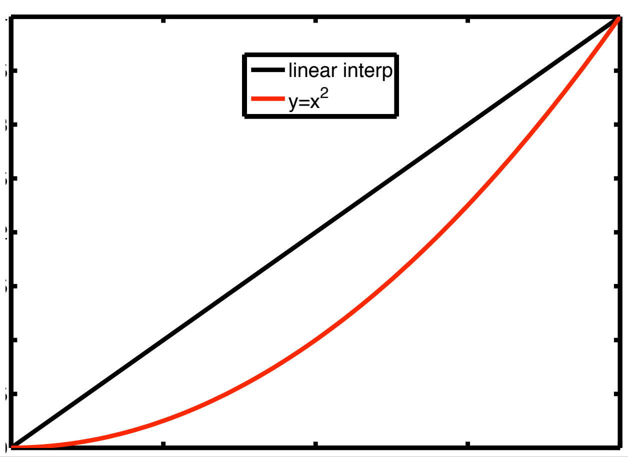


Advantages:

- Easy to use (homework, exams)
- Exact for linear functions

Disadvantages:

- Not very accurate for nonlinear functions



In MATLAB:

```
yi=interp1(x,y,xi,'linear')
```

- `x` - independent variable entries (vector)
- `y` - dependent variable entries (vector)
- `xi` - value(s) where you want to interpolate
- `yi` - interpolated value(s) at `xi`.

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Polynomial Interpolation

$$p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

$$p(x) = \sum_{i=0}^{n} a_i x^i$$

Given n+1 data points, we can fit an n-degree polynomial.

Given: (x_i,y_i), solve for a_i

Two steps:

- obtain polynomial coefficients
- evaluate the value of the polynomial at the desired location (x_i)

Example: vapor pressure data...

For 4 data points, we can produce a third order polynomial to interpolate them.

$$\begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ 1 & x_3 & x_3^2 & x_3^3 \\ 1 & x_4 & x_4^2 & x_4^3 \end{bmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix}$$

In MATLAB:

- `a=polyfit(x,y,n)`
  - requires at least n+1 points
  - if you supply more than n+1 points, then *regression* will be performed (more later).
- `yi=polyval(a,xi)`
  - evaluates polynomial at point(s) given by `xi`.

Cubic Spline Interpolation

Concept: use cubic polynomial and "hook" them together over a wide range of data...

Advantages:

- Provides a "smooth" interpolant.
- Usually more accurate than linear interpolation.
- Doesn't get "wiggly" like higher-order polynomial interpolation can.

Disadvantages:

- Requires a bit more work than linear interpolation to implement (we won't discuss this).

```
yi=interp1(x,y,xi,'spline')
```

- `x` - independent variable entries (vector)
- `y` - dependent variable entries (vector)
- `xi` - value(s) where you want to interpolate
- `yi` - interpolated value(s) at `xi`.

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2-D Linear Interpolation

Bilinear interpolation

If you have "structured" (tabular) data:

1. Interpolate in one direction (two 1-D interpolations)
2. Interpolate in second direction.

Use this for simple homework assignments, in-class exams, etc.

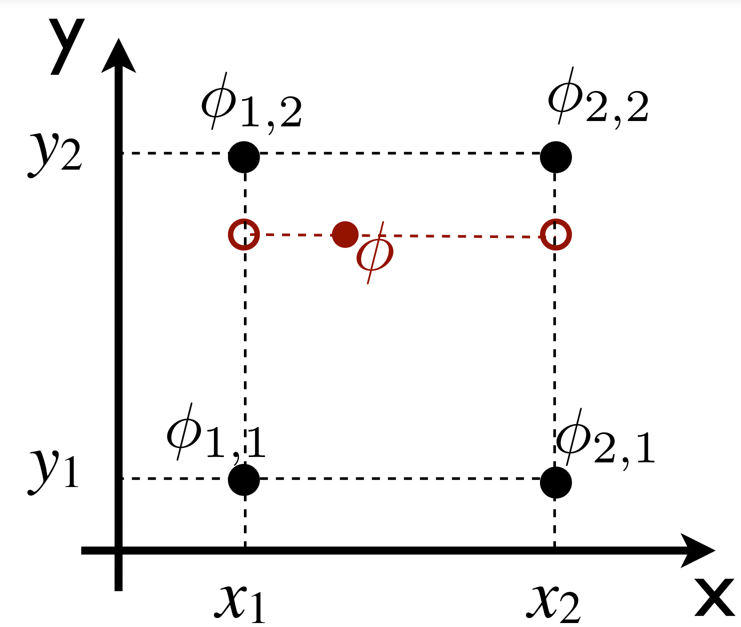
$$
\begin{aligned}
\phi(x,y) \approx\ & \frac{\phi_{1,1}}{(x_2-x_1)(y_2-y_1)}(x_2-x)(y_2-y) \\
+\ & \frac{\phi_{2,1}}{(x_2-x_1)(y_2-y_1)}(x-x_1)(y_2-y) \\
+\ & \frac{\phi_{1,2}}{(x_2-x_1)(y_2-y_1)}(x_2-x)(y-y_1) \\
+\ & \frac{\phi_{2,2}}{(x_2-x_1)(y_2-y_1)}(x-x_1)(y-y_1)
\end{aligned}
$$

This formula corresponds to x (first) then y interpolation

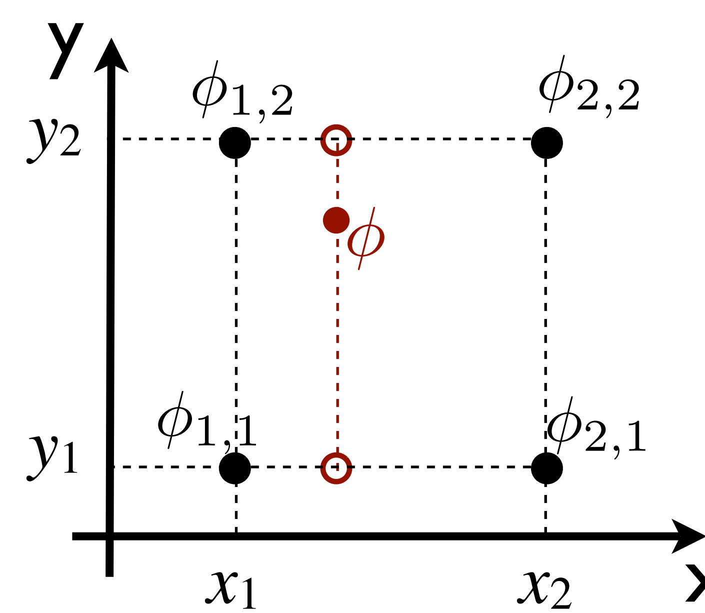
```
ϕ=interp2(x,y,ϕ,xi,yi,'method')
```

- `'linear'` - linear interpolation (default)
- `'spline'` - spline interpolation

Interpolate y first



Interpolate x first



x,y may be **vectors** (matlab assumes tabular form), ϕ must be a **matrix**.

Example - "Real" Gases

$$p\bar{V} = zRT$$

z - "compressibility factor" (1 for ideal gas)

p - pressure
z - compressibility factor
R - gas constant
T - temperature
$\bar{V}$ - Molar volume

z as a function of T and P

T (K)	Pressure (bar)			
	1	5	10	20
300	0.9983	0.9915	0.9830	0.9667
400	0.9995	0.9977	0.9953	0.9912
600	1.0000	1.0009	1.0020	1.0039
1000	1.0004	1.0014	1.0035	1.0071

Source: Perry's Chemical Engineer's Handbook (7th ed.)

MATLAB

```
interp2(x,y,ϕ,xi,yi,'method')
```

Assumes that x is in columns and y is in rows of the table.

Find z at T=725 K and p=8 bar.

$$\phi = \left(\frac{\phi_2 - \phi_1}{x_2 - x_1}\right)(x - x_1) + \phi_1$$

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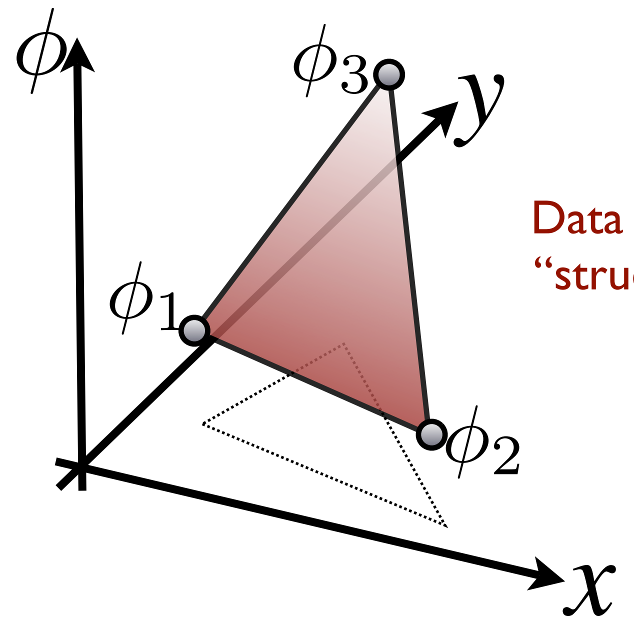
General 2-D Linear Interpolation

$$\phi = ax + by + c$$

$$\begin{aligned}\phi_1 &= ax_1 + by_1 + c\\ \phi_2 &= ax_2 + by_2 + c\\ \phi_3 &= ax_3 + by_3 + c\end{aligned}$$



Data is NOT "structured"

$$a = \frac{\phi_3(y_1 - y_2) + \phi_2(y_3 - y_1) + \phi_1(y_2 - y_3)}{x_3(y_1 - y_2) + x_2(y_3 - y_1) + x_1(y_2 - y_3)},$$

$$b = \frac{\phi_3(x_2 - x_1) + \phi_2(x_1 - x_3) + \phi_1(x_3 - x_2)}{y_3(x_2 - x_1) + y_2(x_1 - x_3) + y_1(x_3 - x_2)},$$

$$c = \frac{\phi_3(x_1 y_2 - x_2 y_1) + \phi_2(x_3 y_1 - x_1 y_3) + \phi_1(x_2 y_3 - x_3 y_2)}{x_1(y_2 - y_3) + x_2(y_3 - y_1) + x_3(y_1 - y_2)}$$

```
ϕ=interp2(x,y,ϕ,xi,yi,'method')
```

- `'linear'` - linear interpolation
- `'spline'` - spline interpolation

x, y, ϕ are **matrices** (unique x, y for each ϕ).

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