Curve Fitting: Interpolation

CH EN 2450
Numerical Methods
Spring 2022

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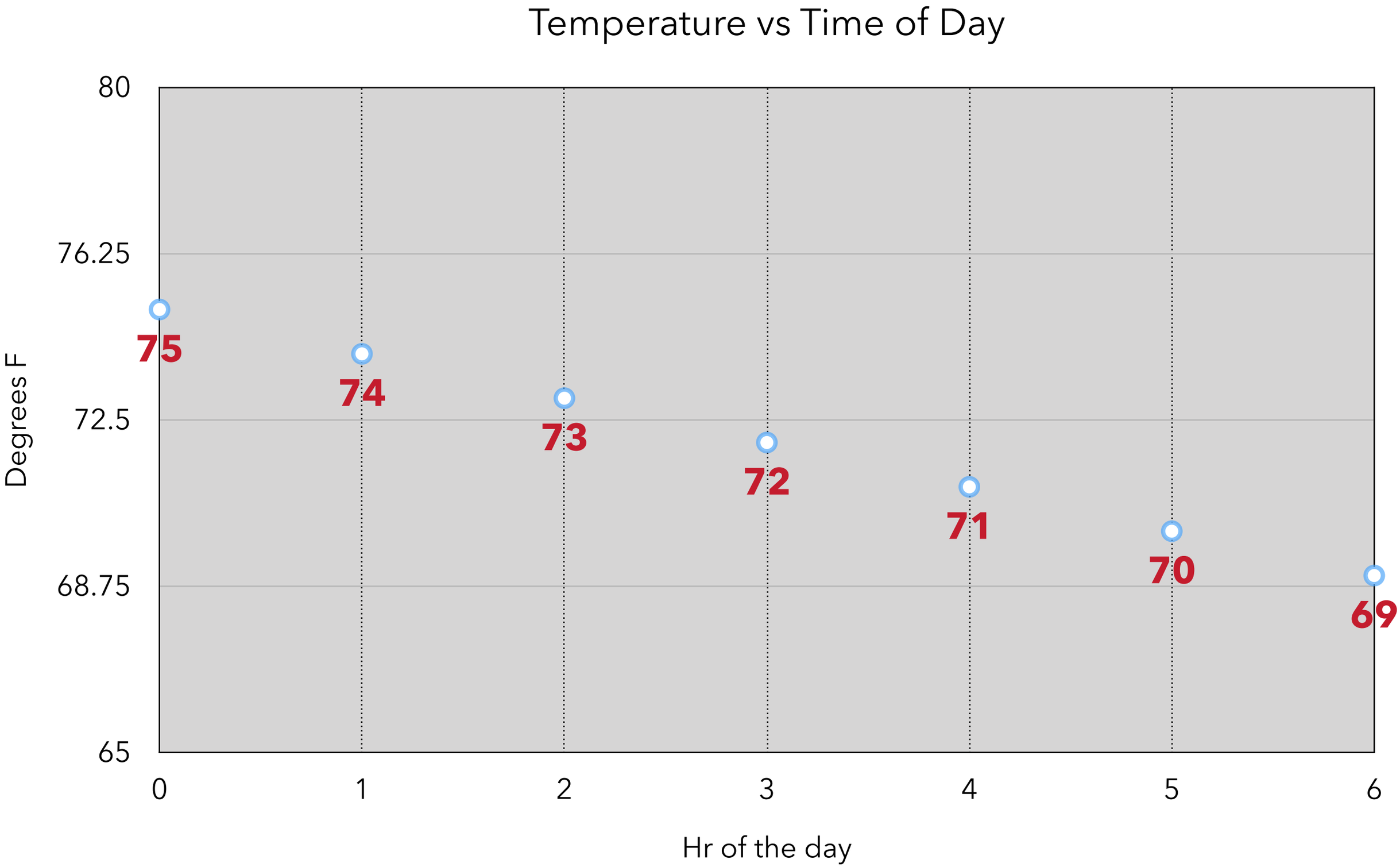
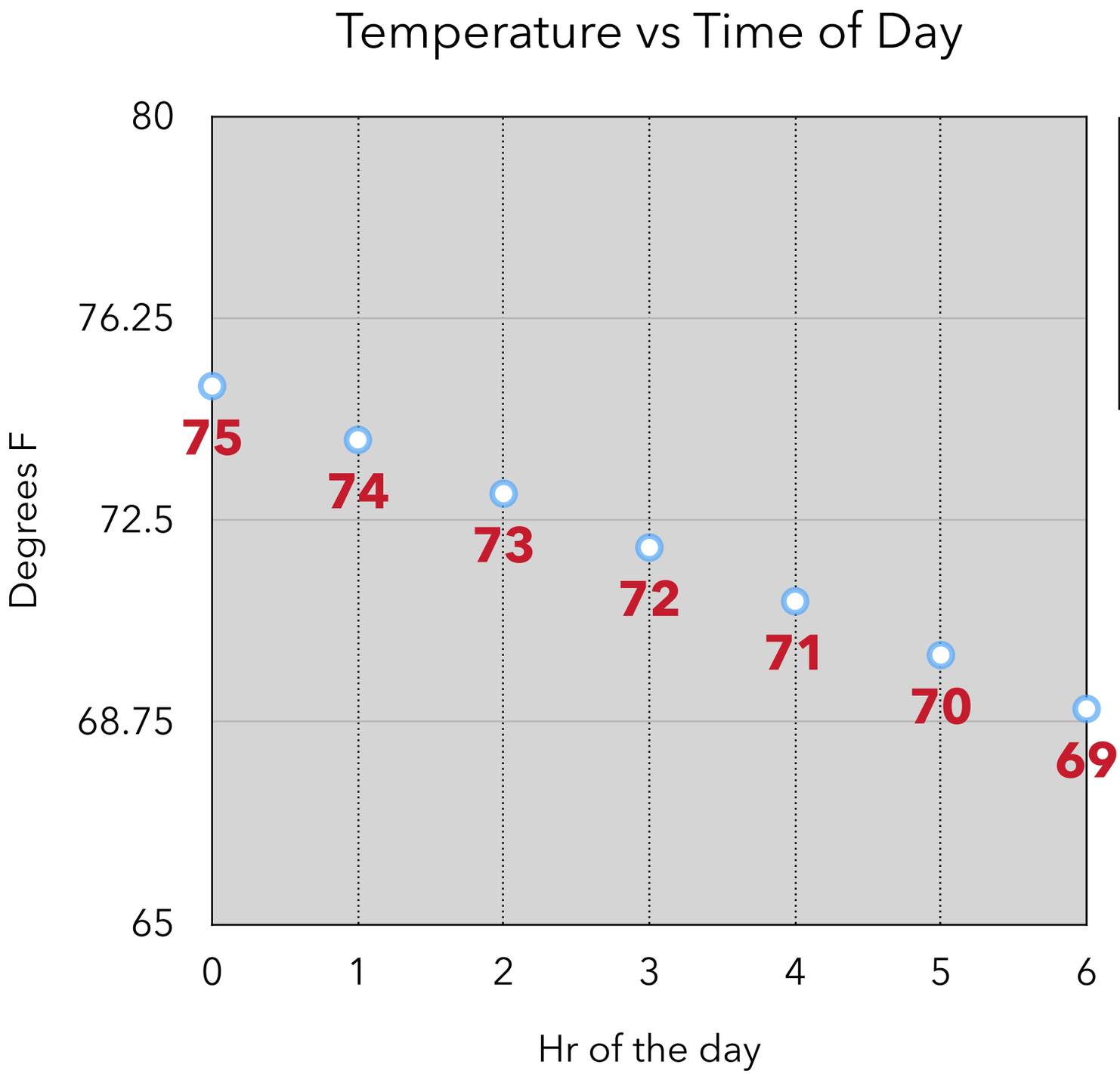
Learning Objectives

At the end of this chapter you should be able to:

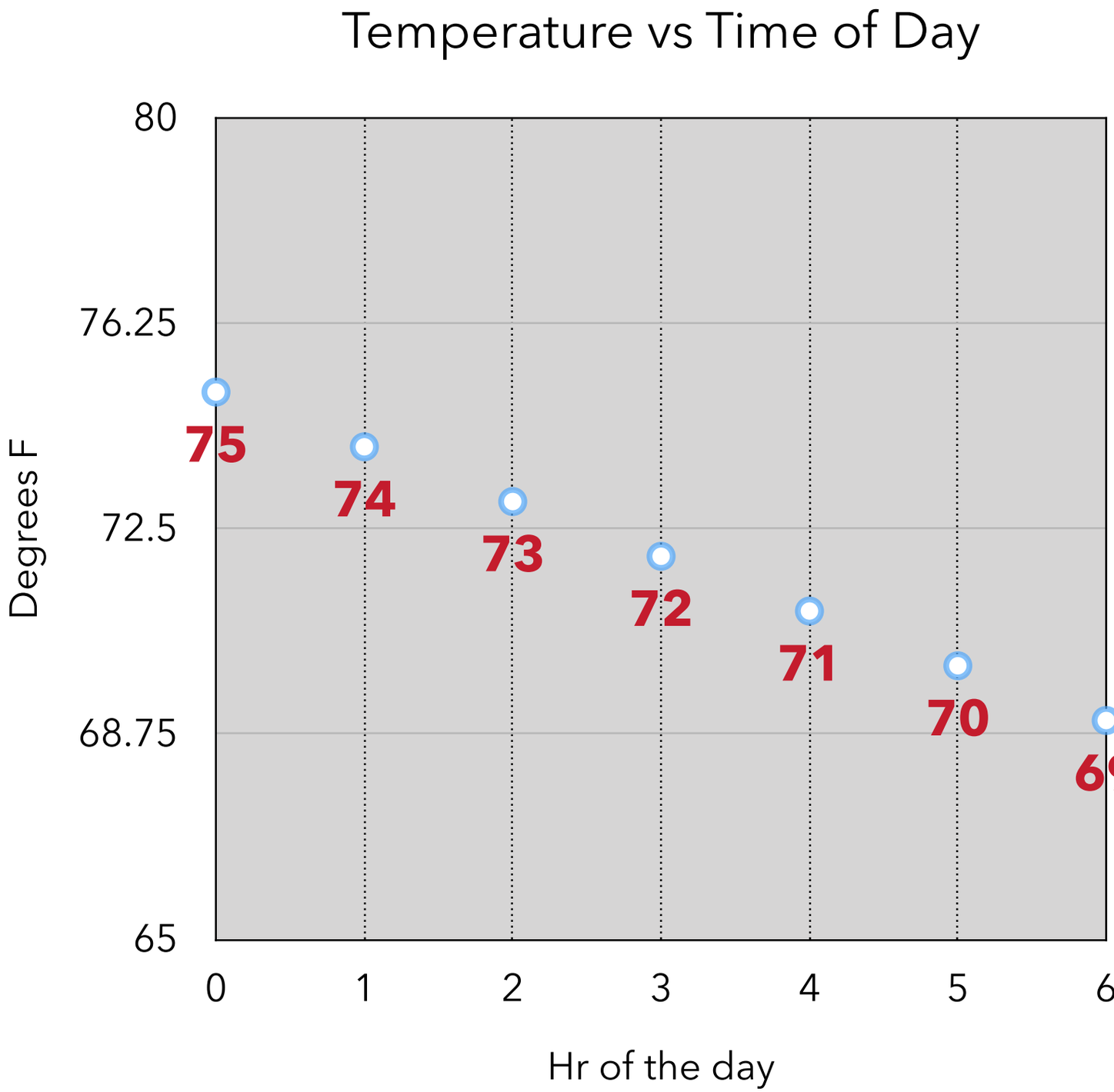
- Define what it means to interpolate data
- Identify the order of the polynomial that interpolates n-data points
- Derive the system of equations that one needs to solve to build a polynomial interpolant
- List the benefits and limitations of first order interpolates
- List the benefits and limitations of high-order polynomial interpolants
- Calculate by hand an interpolated value using a linear interpolant
- Identify which points are best used with a linear and quadratic interpolant
- List the conditions for cubic spline interpolants - only the conditions - and show how many unknowns there are and what the constraints are and be able to list all the constraints
- Use built-in Python functions to perform polynomial and cubic spline interpolation





Activity:

What is the temperature at 5:30 AM?

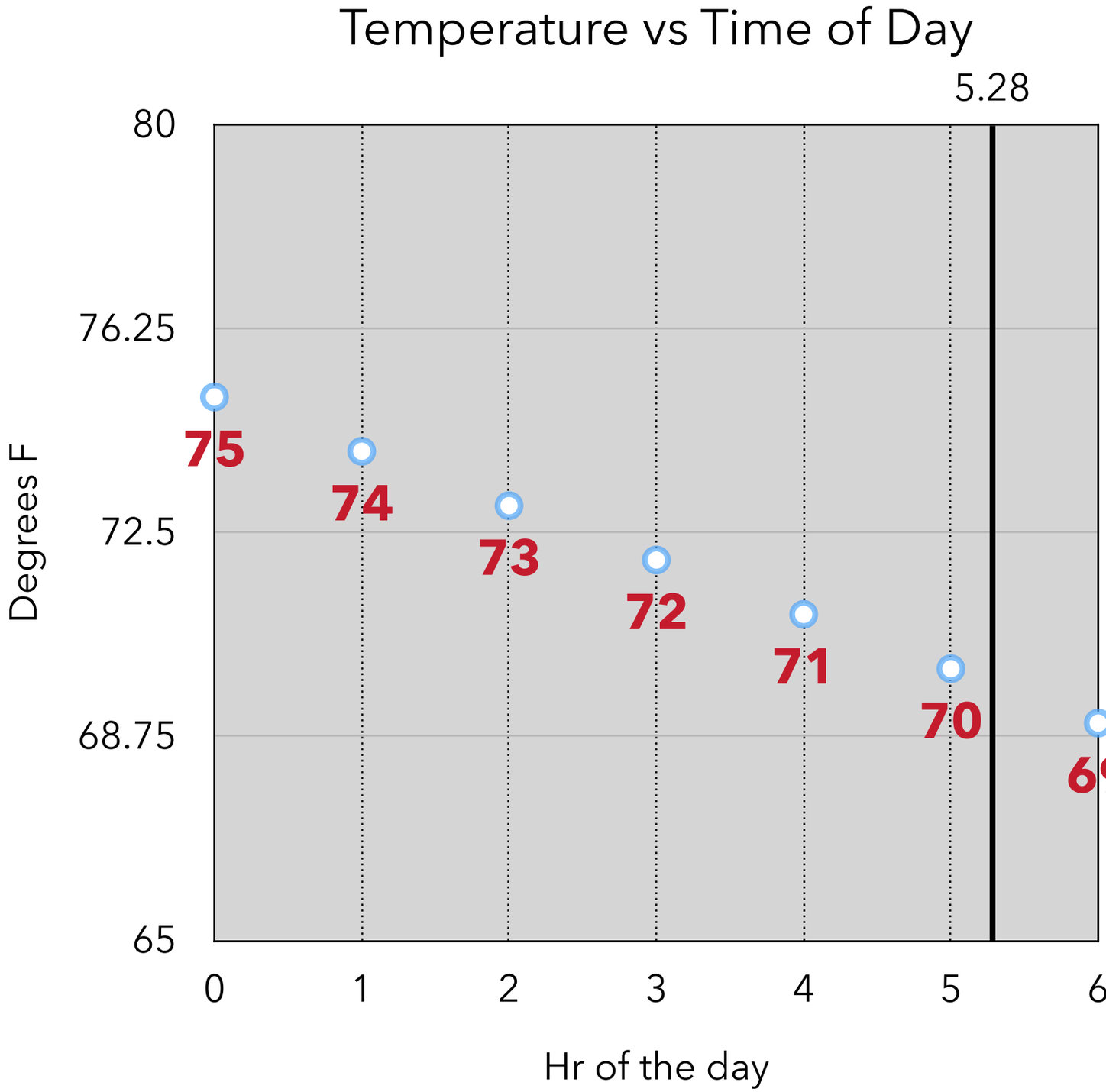


Activity:

What is the temperature at 5:30 AM?

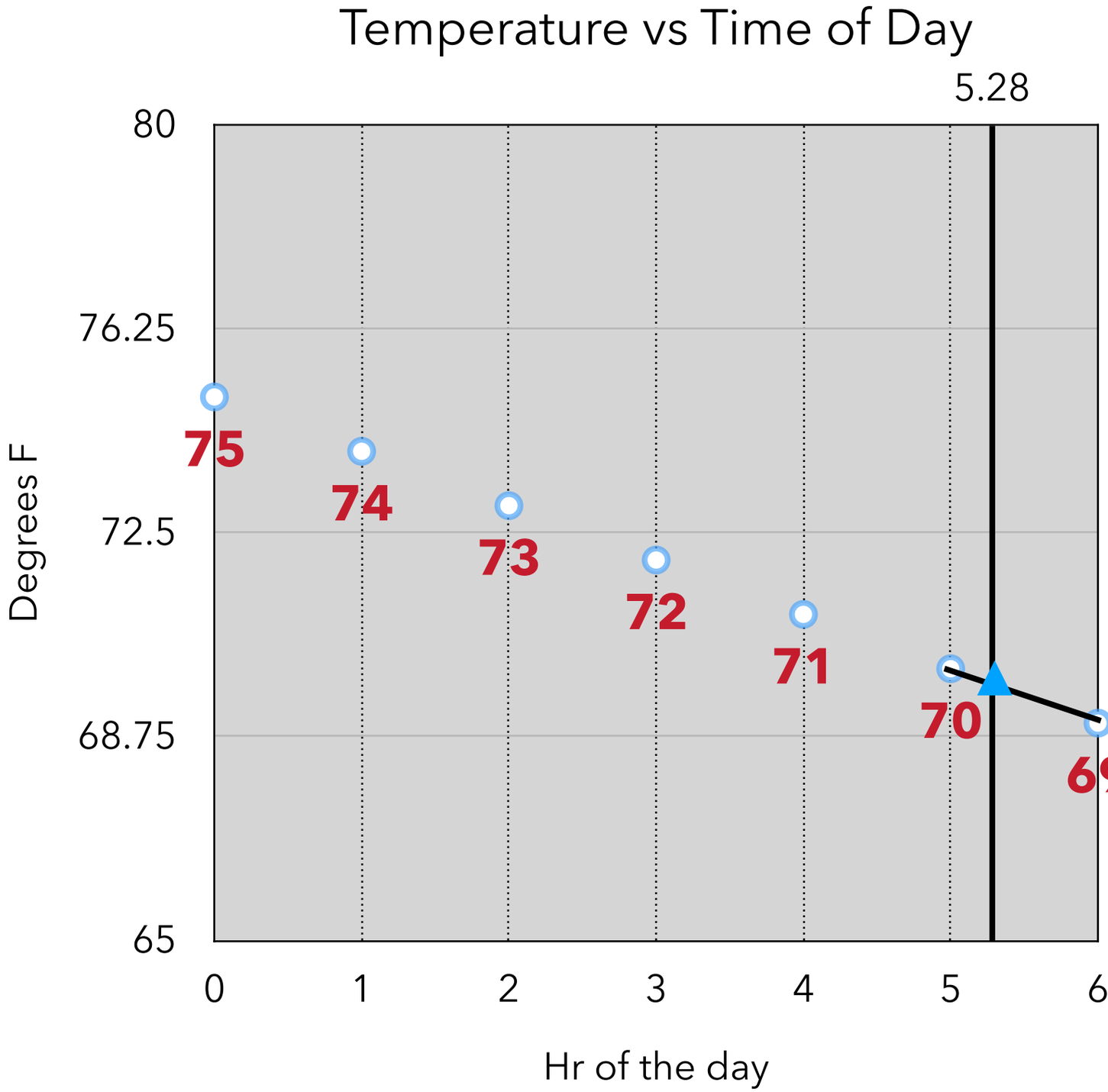
At 5:30 AM, the temperature is likely to be the average between 70 and 69:

T(5:30AM) = 69.5 F



Activity:

What is the temperature at 5:17 AM? (That's at hr 5.28). You only need to describe how you would find that temperature.



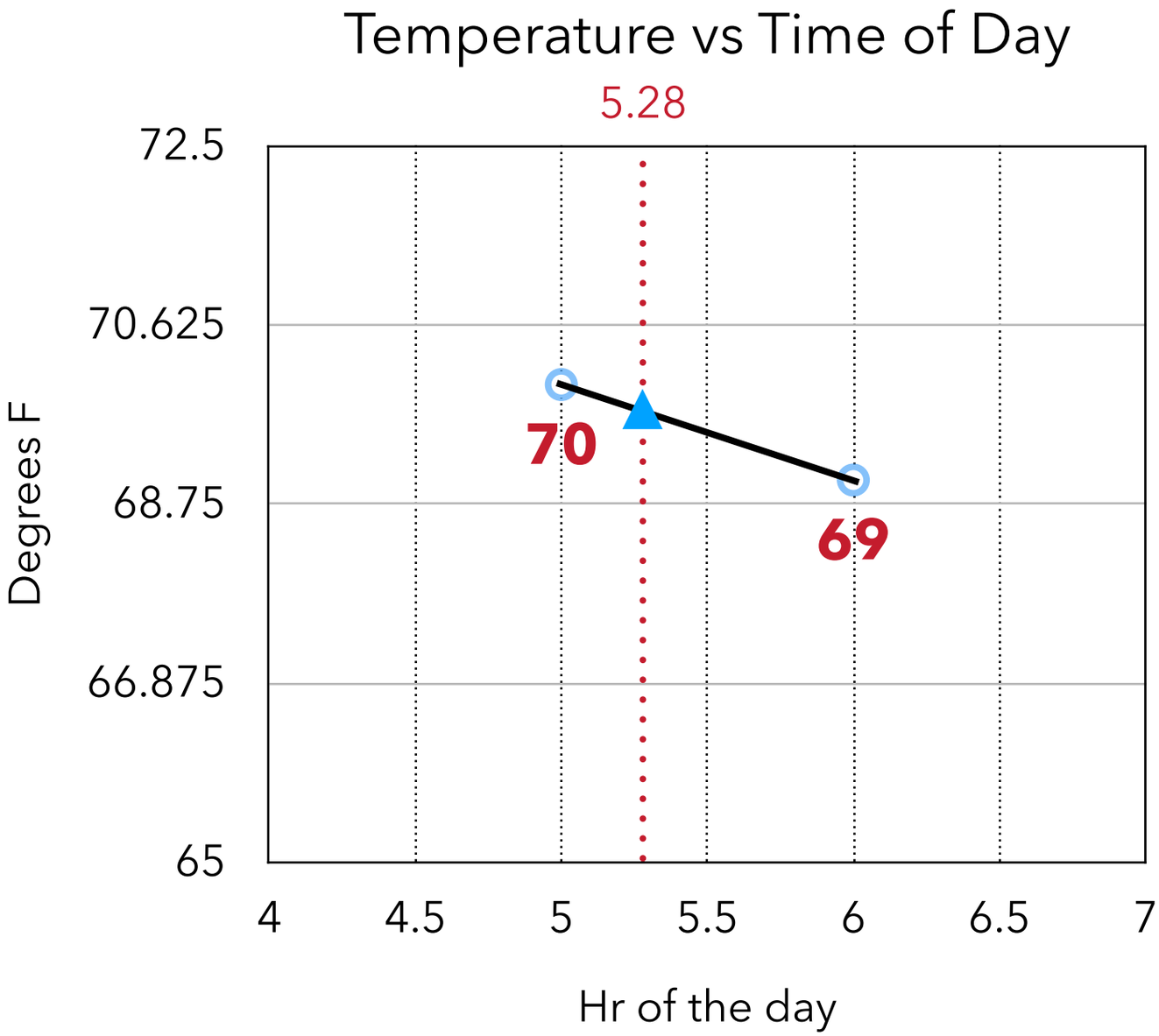
Activity:

What is the temperature at 5:17 AM? (That's at hr 5.28). You only need to describe how you would find that temperature.

Draw a straight line between 70 and 69 and intersect it with the vertical line at 5.28

Activity:

Go ahead and do that



We need an equation for the line connecting the points (5,70) and (6,69).

Equation for a straight line is: $T(x) = mx + b$ **T is temperature and x is hr of day**

Slope is: $m = \dfrac{69 - 70}{6 - 5} = -1$

To find the intercept, evaluate the equation of the line at one of the known points, $T(5) = 70$ or $T(6) = 69$

$$T(5) = 70 = m \times 5 + b = -5 + b \implies b = 75$$

Finally, the temperature at 5:17 AM (x = 5.28 hr) is:

$$T(5.28) = -5.28 + 75 = 69.72F$$

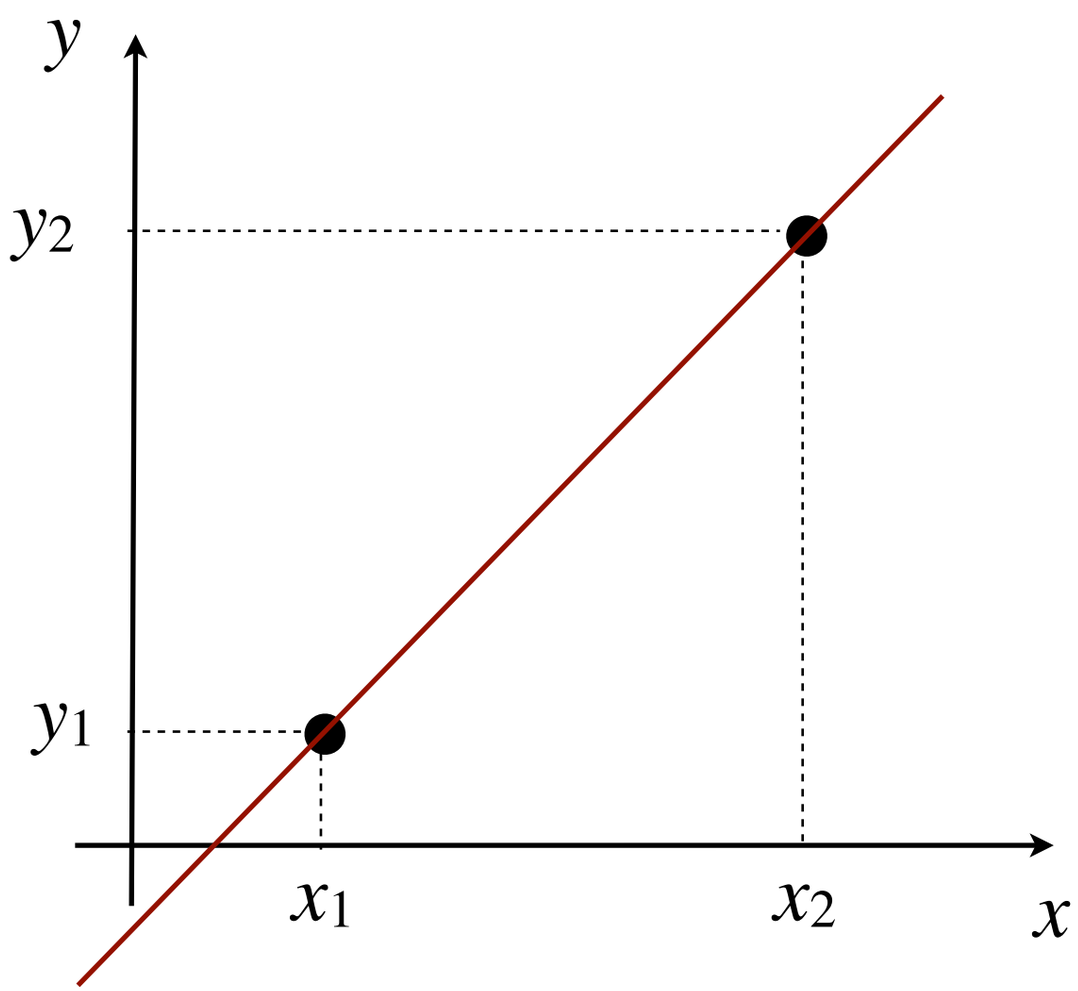
You just did linear interpolation!

Let us Generalize

Linear Interpolation

given: $(x_1, y_1) \quad (x_2, y_2)$

find: $y(x) = mx + b$



Activity:

Given two points (x_1, y_1) and (x_2, y_2), find the general formula for a straight line (linear interpolant) between these two points.

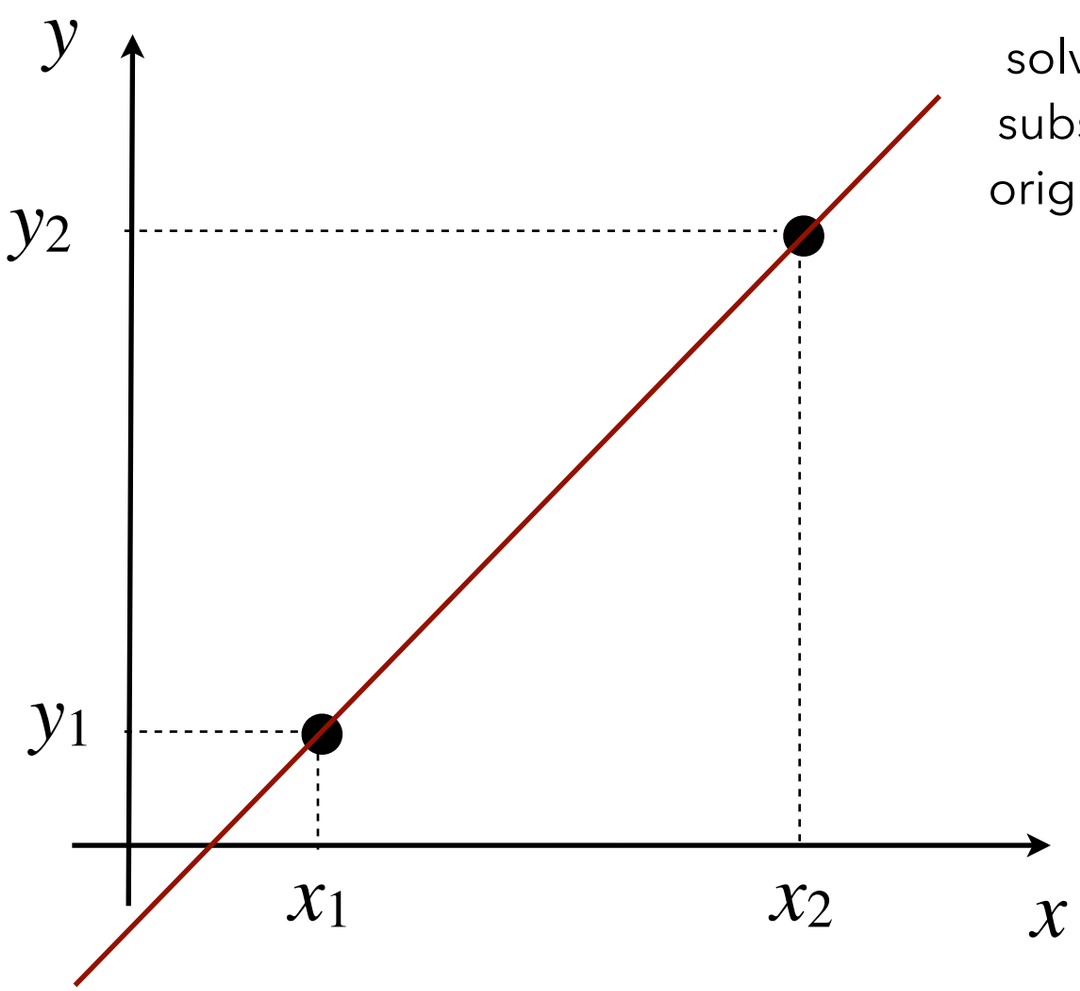
Linear Interpolation

given: (x_1, y_1) (x_2, y_2)

find: $y(x) = mx + b$

$$y_1 = mx_1 + b$$
$$y_2 = mx_2 + b$$

$$\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \end{bmatrix} \begin{pmatrix} m \\ b \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$



solve for m, b and substitute into the original equation...

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

Advantages:

- Easy to use (homework, exams)

Disadvantages:

- Not very accurate for nonlinear functions

Motivation & Concept

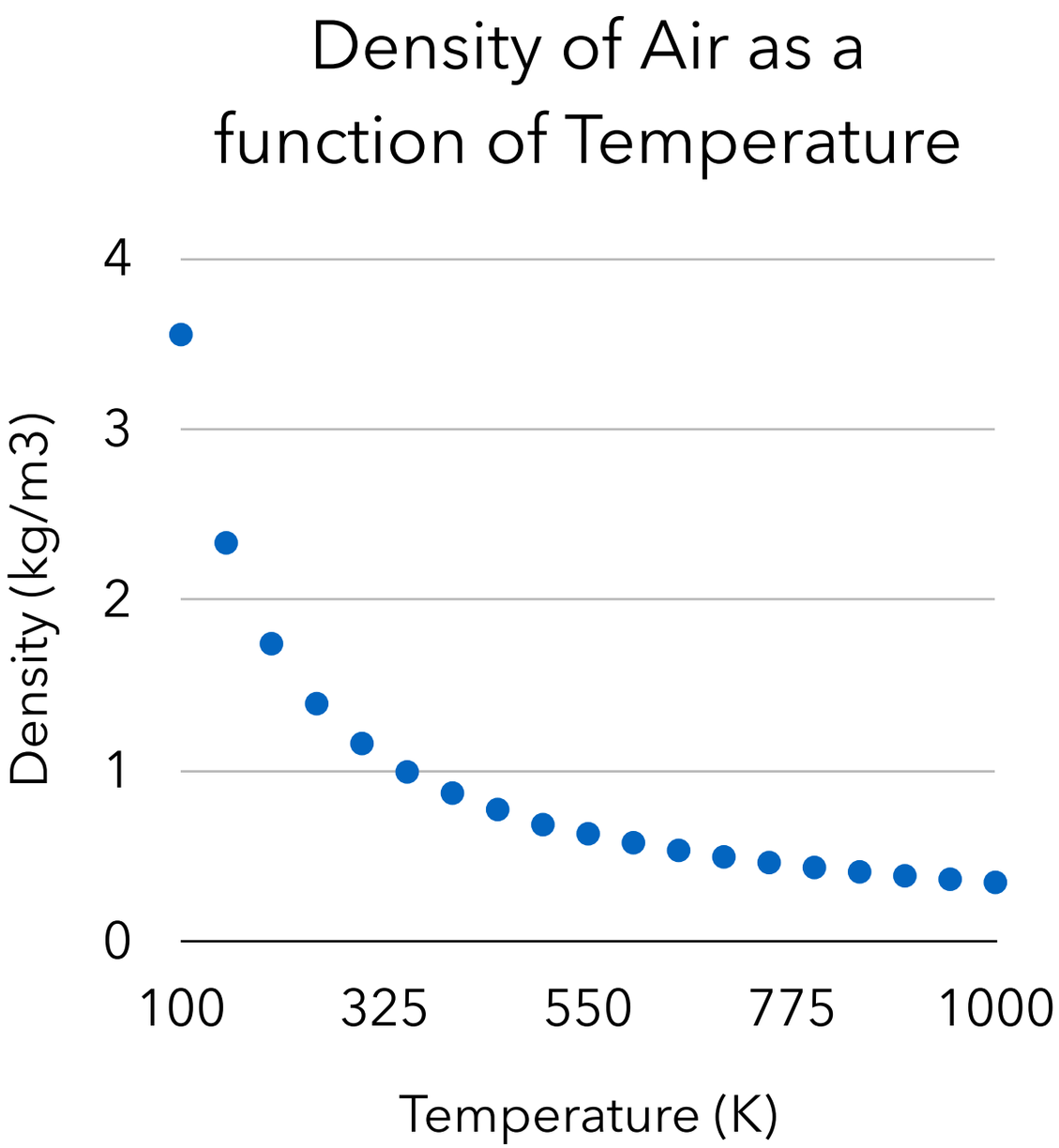
- Motivation:
  - Often we have discrete data (tabulated, from experiments, etc) that we need to interpolate.
- Concept:
  - Choose a polynomial function to fit to the data (connect the dots)
  - Solve for the coefficients of the polynomial
  - Evaluate the polynomial wherever you want (interpolation)

Properties of air at atmospheric pressure

T K	ρ kg/m³	λ W/(m K)	μ N s/m²
100	3.5562	0.0093	7.110e-06
150	2.3364	0.0138	1.034e-05
200	1.7458	0.0181	1.325e-05
250	1.3947	0.0223	1.596e-05
300	1.1614	0.0263	1.846e-05
350	0.9950	0.0300	2.082e-05
400	0.8711	0.0338	2.301e-05
450	0.7750	0.0373	2.507e-05
500	0.6864	0.0407	2.701e-05
550	0.6329	0.0439	2.884e-05
600	0.5804	0.0469	3.058e-05
650	0.5356	0.0497	3.225e-05
700	0.4975	0.0524	3.388e-05
750	0.4643	0.0549	3.546e-05
800	0.4354	0.0573	3.698e-05
850	0.4097	0.0596	3.843e-05
900	0.3868	0.0620	3.981e-05
950	0.3666	0.0643	4.113e-05
1000	0.3482	0.0667	4.244e-05

Incropera & DeWitt, *Fundamentals of Heat and Mass Transfer*, 4th ed.

Motivation & Concept



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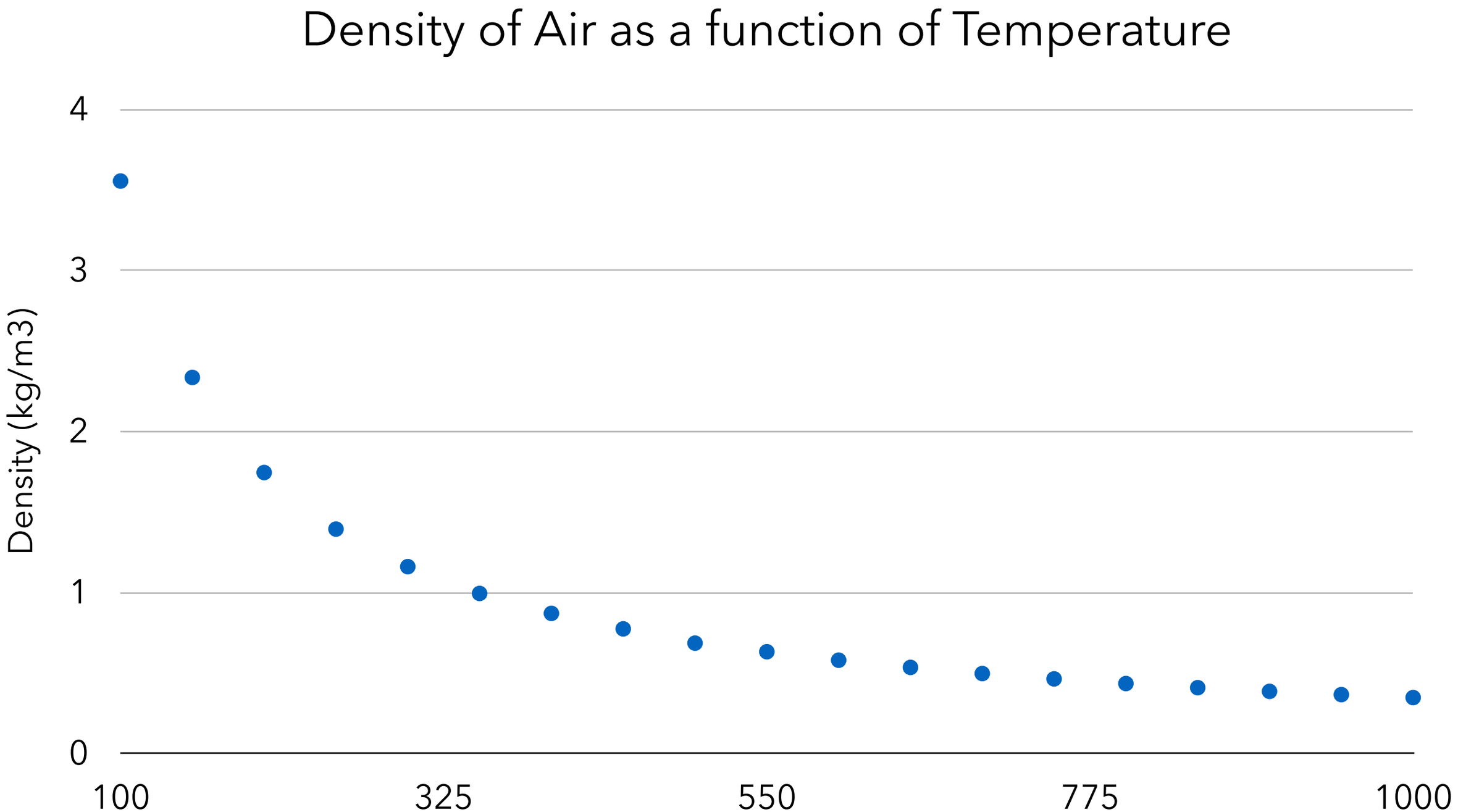
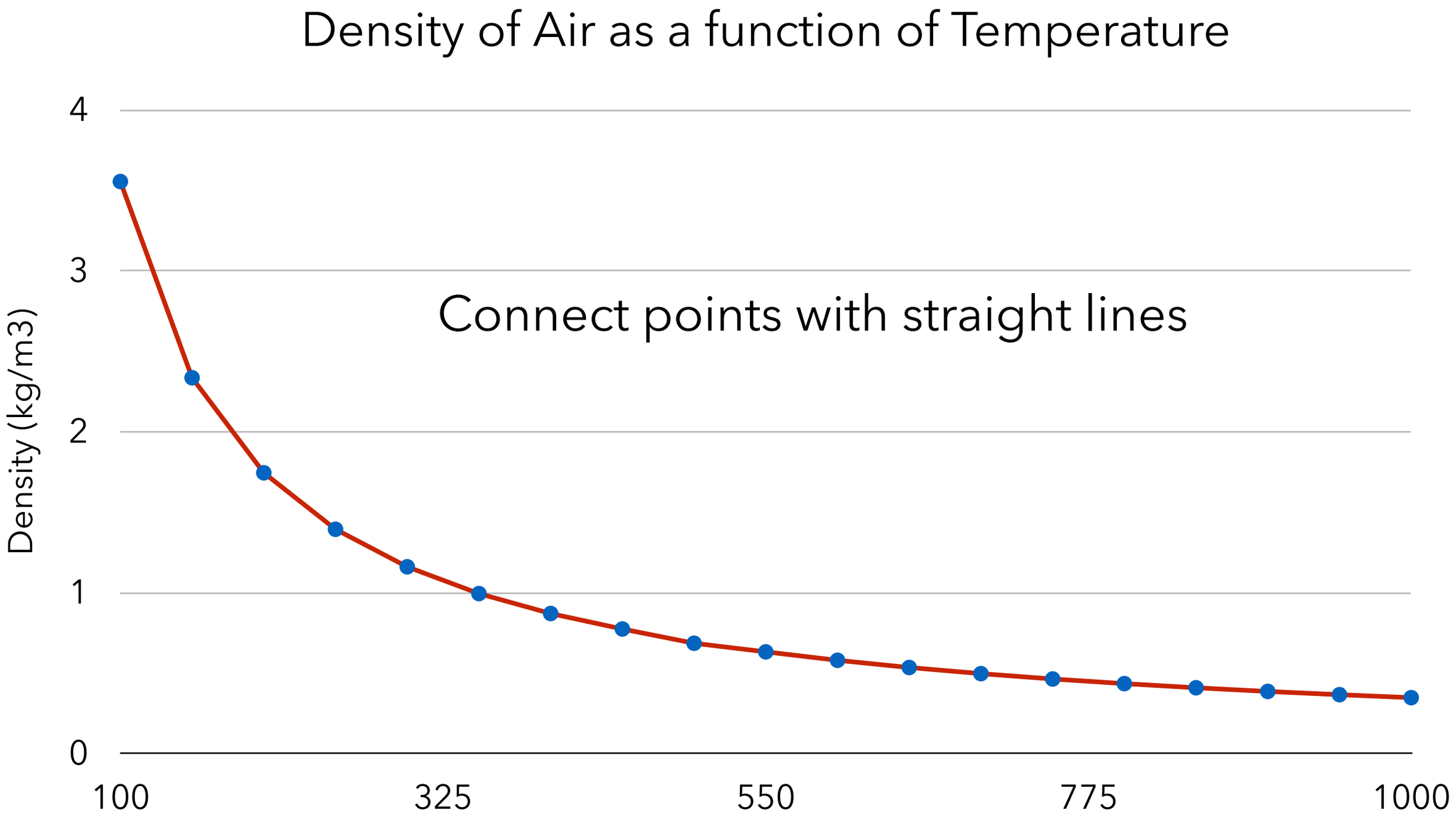
Linear Interpolation

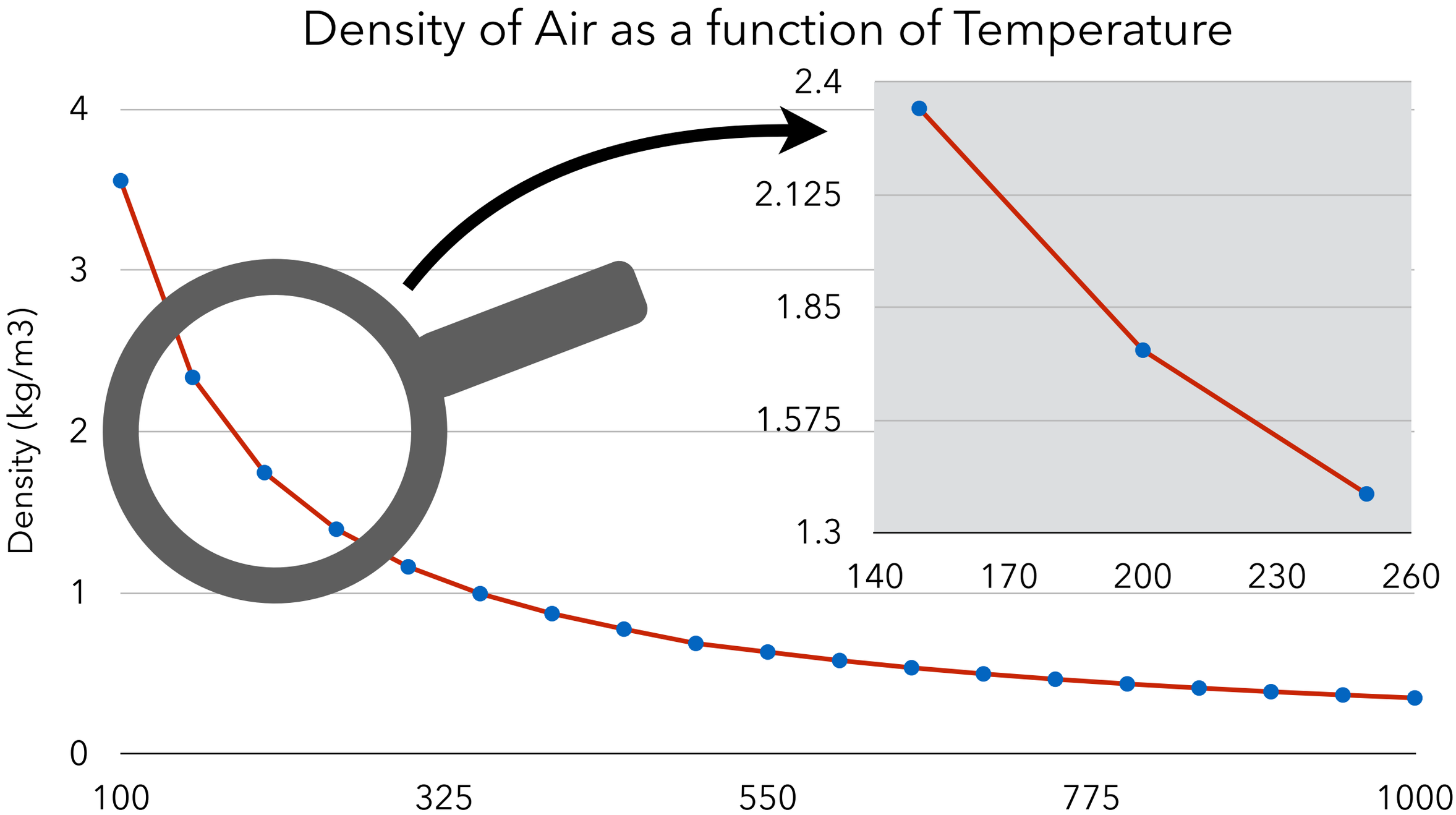
Linear Interpolation



Linear Interpolation



Linear Interpolation



Linear Interpolation

In Python:

```
ye = numpy.interp(xe,xi,yi)
```

- `xi` - (known) independent variable entries (vector)
- `yi` - (known) dependent variable entries (vector)
- `xe` - (known) value(s) where you want to interpolate
- `ye` - interpolated value(s) at `xe`

Coding Activity:
Download the notebook **Interp-activity-1-with-gaps.ipynb** from the Interpolation module on Canvas.

Linear Interpolation

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Achtung! The abscissae (xi) need to be sorted in increasing order!

- `np.argsort()` - Returns the indices that would sort an array. Useful when you need to sort multiple related arrays
- `np.sort()` - sorts array
- `np.flipud()` - flips array upside down

Higher Order

Polynomial Interpolants

Higher Order Interpolants

2 points
(x_1, y_1)
(x_2, y_2)

straight line $y(x) = a_0 + a_1 x$

$$y_1 = a_0 + a_1 x_1$$
$$y_2 = a_0 + a_1 x_2$$

$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \end{bmatrix} \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

3 points
(x_1, y_1)
(x_2, y_2)
(x_3, y_3)

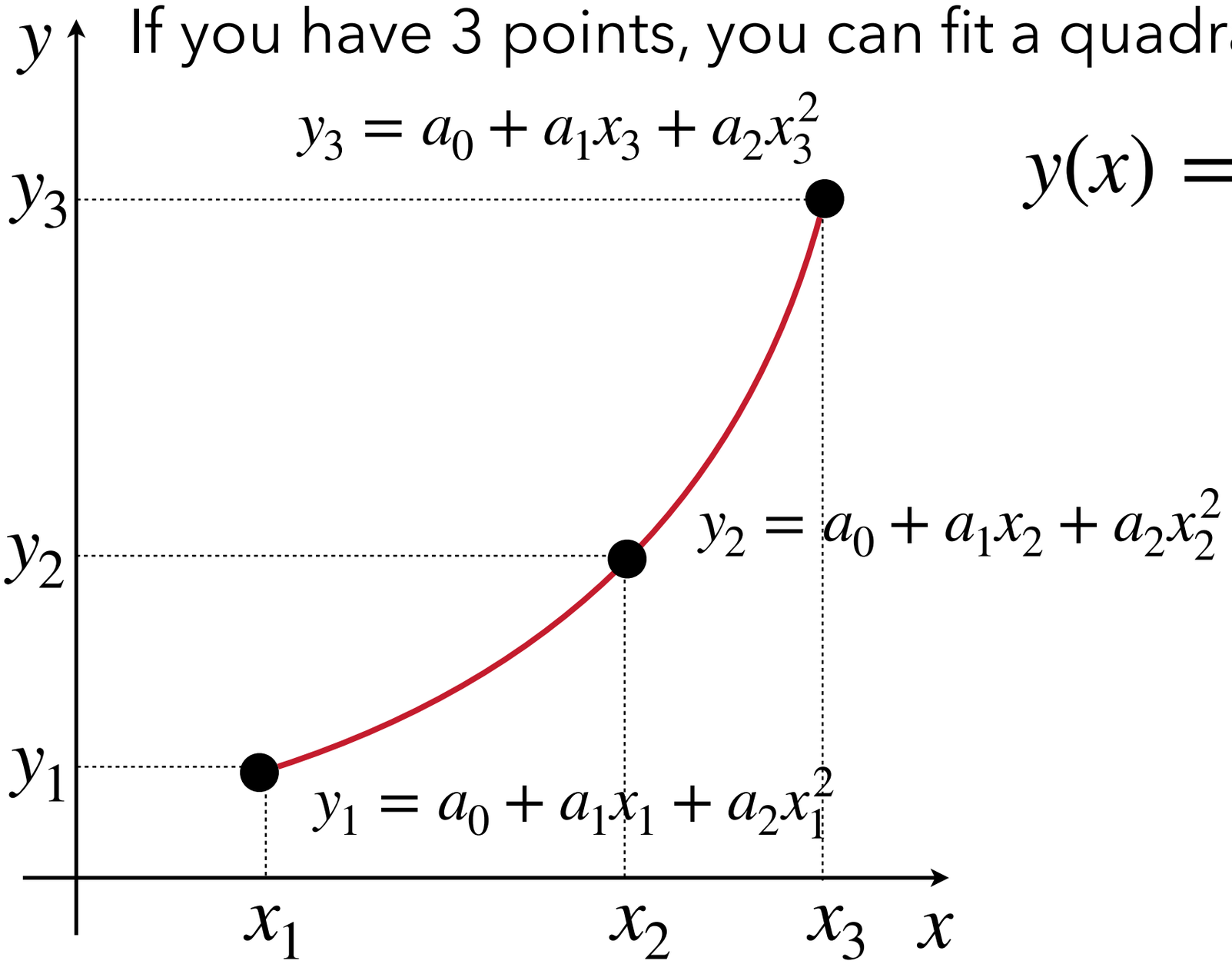
quadratic $y(x) = a_0 + a_1 x + a_2 x^2$

Activity:

Find the system of equations that we need to solve in order to find a_0, a_1, and a_2.

Higher Order Interpolants

If you have 3 points, you can fit a quadratic (parabola)



$$y(x) = a_0 + a_1 x + a_2 x^2$$

Higher Order Interpolants

$$y_1 = a_0 + a_1 x_1 + a_2 x_1^2$$

$$y_2 = a_0 + a_1 x_2 + a_2 x_2^2$$

$$y_3 = a_0 + a_1 x_3 + a_2 x_3^2$$

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

Higher Order Interpolants

# data points	fit	equation
2 points	straight line	$a_0 + a_1 x$
3 points	quadratic	$a_0 + a_1 x + a_2 x^2$
4 points	cubic	$a_0 + a_1 x + a_2 x^2 + a_3 x^3$
$n+1$ points	n-th order	$a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n$

Polynomial Interpolation

Fit polynomial through part of/entire dataset:

$$a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n$$

$a_0, a_1, \ldots, a_n$ are the unknowns

We have $n+1$ unknowns

We need $n+1$ equations

We need $n+1$ points

Polynomial Interpolation

For $n+1$ data points,
we can fit a polynomial of order n,
at most

Remember: An interpolating polynomial, by definition, MUST go through each and every point of the data used to build the polynomial.

Polynomial Interpolation

$$p(x) = \sum_{k=0}^{n} a_k x^k$$

Given n+1 data points, we can fit an n^{th}-degree polynomial.

$$\begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^n \\ 1 & x_2 & x_2^2 & \cdots & x_2^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n+1} & x_{n+1}^2 & \cdots & x_{n+1}^n \end{bmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{n+1} \end{pmatrix}$$

Given: (x_i, y_i), solve for a_i

Two steps:

1. Obtain polynomial coefficients by solving the system of linear equations
2. Evaluate the polynomial at the desired location(s) (x_i)

Pythonification

```
from numpy import polyfit, polyval
p  = polyfit(xi,yi,deg)
ye = polyval(p,xe)
```

- `p` - vector of coefficients of the polynomial, $a_n, a_{n-1}, \ldots, a_0$
- `xi` - vector of independent variable entries (known input values)
- `yi` - vector of dependent variable entries (known input values)
- `deg` - is the degree of the polynomial. Degree n Requires $n+1$ points (input)
- `polyfit(xi,yi,deg)` - returns the coefficients of the polynomial fit
- `ye = polyval(p,xe)`: evaluates polynomial at point(s) `xe`
- For $n+1$ points, if you choose a degree less than n, then regression will be performed (more later)

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- `ye = polyval(p,xe)`: evaluates polynomial at point(s) `xe`
- For $n+1$ points, if you choose a degree less than n, then regression will be performed (more later)

Coding Activity:

Perform polynomial interpolation on the Density-vs-Temperature dataset in the notebook **interp-activity-1-with-gaps.ipynb** from the Interpolation module on Canvas.

Best Practices for Polynomial Interpolants

- Polynomial Interpolants can be oscillatory, especially high order ones
- Apply a low-order polynomial interpolant (2nd or 3rd locally)
- Unfortunately, it is not straightforward in Python to apply local `polyfit`
- Instead, resort to splines (discussed next)

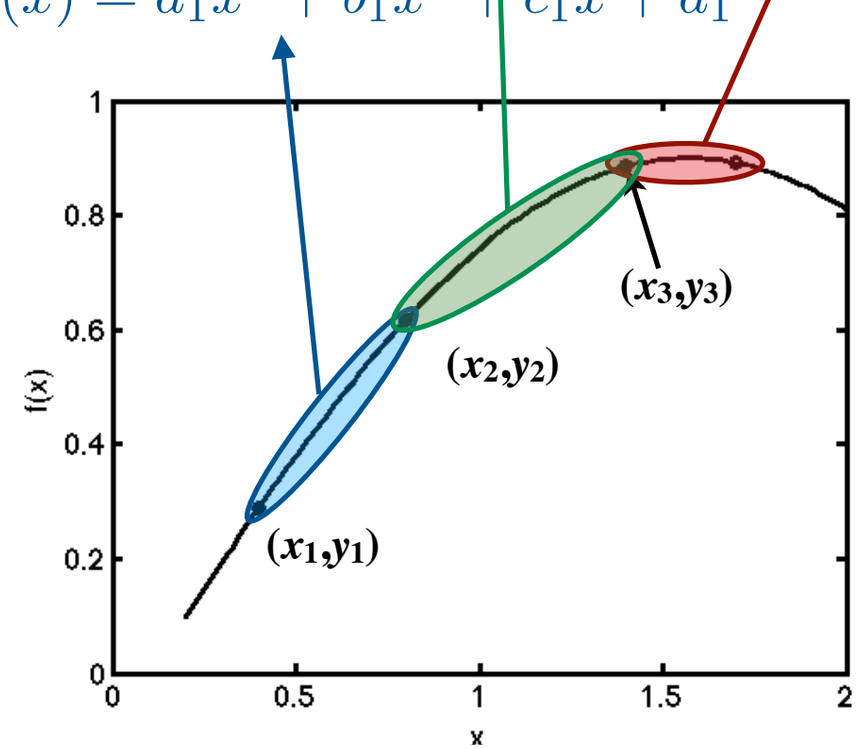
Cubic Spline Interpolation

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

$$f_3(x) = a_3x^3 + b_3x^2 + c_3x + d_3$$

$$f_2(x) = a_2x^3 + b_2x^2 + c_2x + d_2$$

$$f_1(x) = a_1x^3 + b_1x^2 + c_1x + d_1$$

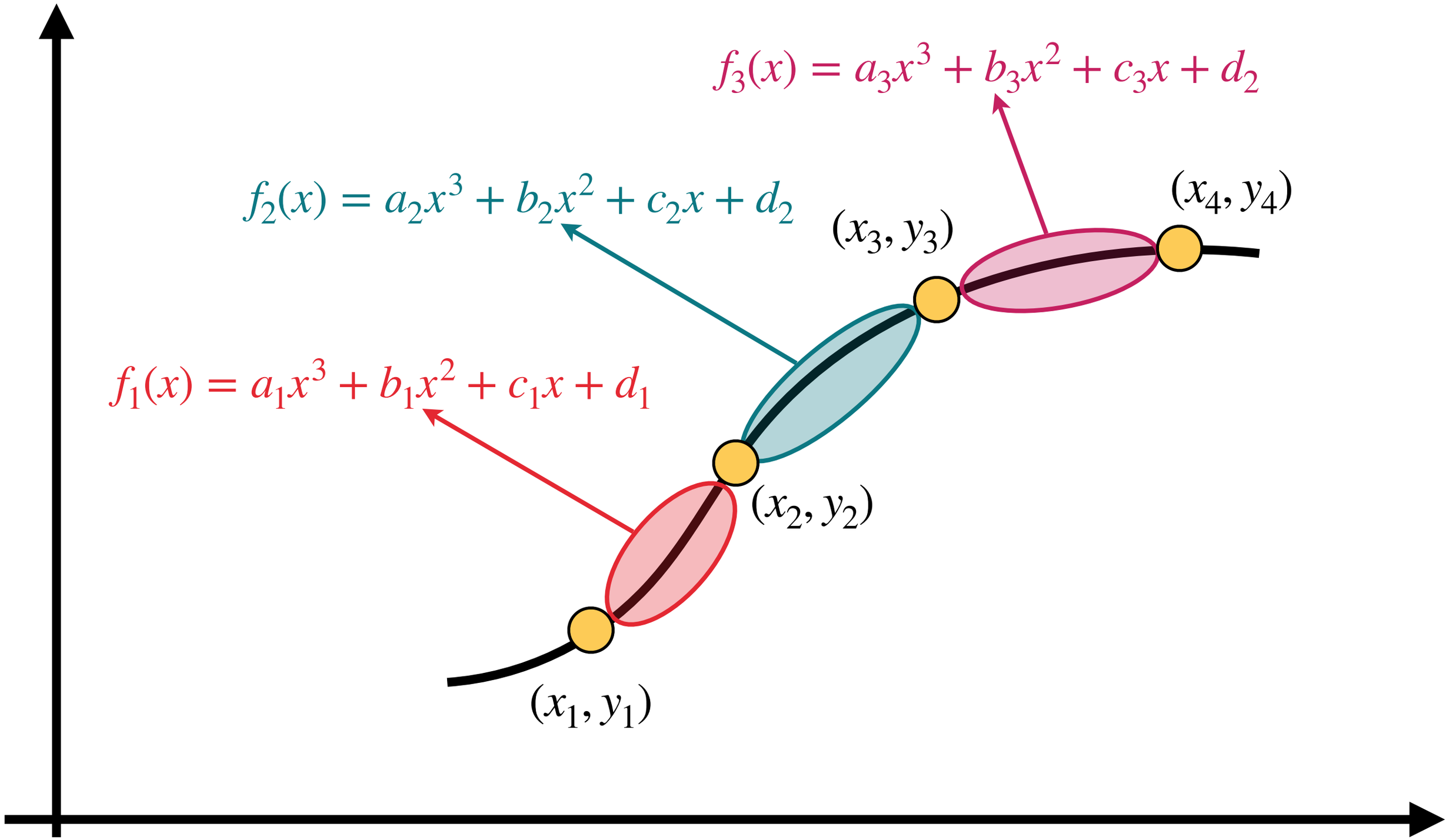


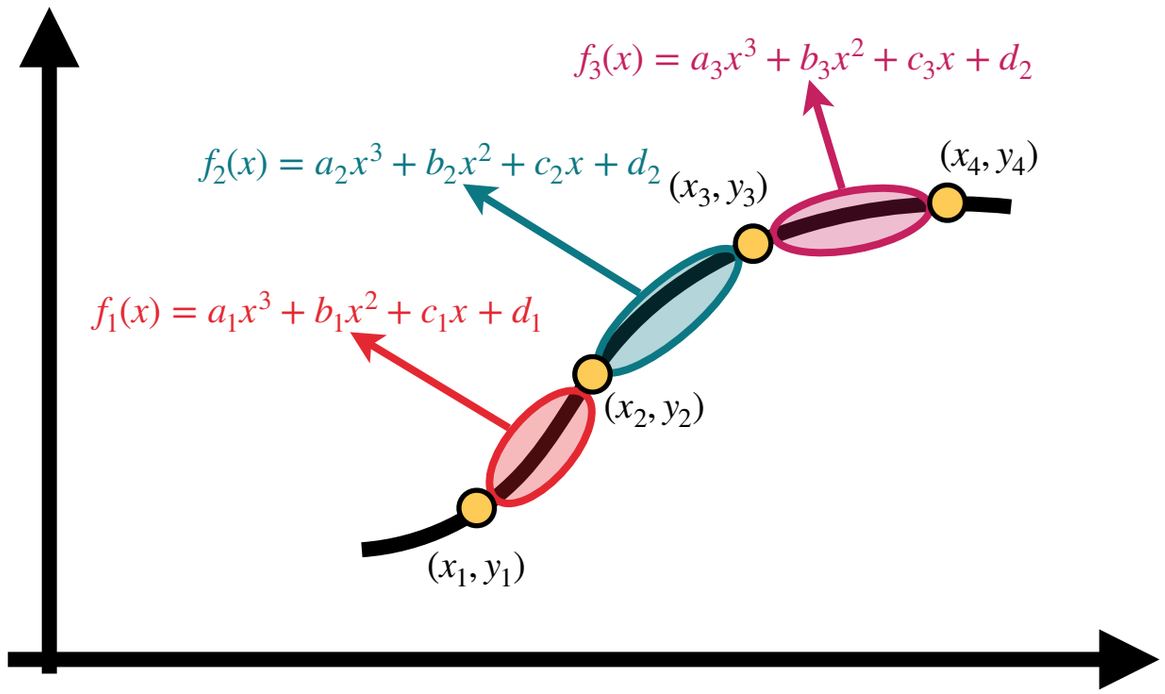
For n+1 points, we form n splines.

We must specify 4 variables per spline ⇒ we need **4*n* equations**.

1. At each data point, the values of adjacent splines must be the same. This applies to all interior points (where two functions meet) ⇒ 2(n-1) constraints.
2. At each point, the *first* derivatives of adjacent splines must be equal (applies to all interior points) ⇒ (n-1) constraints.
3. At each point, the *second* derivative of adjacent splines must be equal (applies to all interior points) ⇒ (n-1) constraints.
4. The first and last splines must pass through the first and last points, respectively ⇒ 2 constraints.
5. The curvature (d^2f / dx^2) must be specified at the end points ⇒ 2 constraints.
   - $d^2f / dx^2 = 0$ ⇒ "natural spline"

4*n* constraints





$$f_1(x_1) = y_1$$
$$f_1(x_2) = y_2$$
$$f_2(x_2) = y_2$$
$$f_2(x_3) = y_3$$
$$f_3(x_3) = y_3$$
$$f_3(x_4) = y_4$$

$$f_1'(x_2) = f_2'(x_2)$$

$$f_2'(x_3) = f_3'(x_3)$$

$$f_1''(x_2) = f_2''(x_2)$$

$$f_2''(x_3) = f_3''(x_3)$$

- natural spline

$$f_1''(x_1) = 0$$
$$f_3''(x_4) = 0$$

Cubic Spline Interpolation

Advantages:

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

Disadvantages:

- Requires a bit more work than linear interpolation to implement.

Cubic Spline Interpolation

Python Implementation:

```
from scipy.interpolate import CubicSpline
cs = CubicSpline(xi,yi)
ye = cs(xe)
```

- `xi` - independent variable entries (vector)
- `yi` - dependent variable entries (vector)
- `xe` - value(s) where you want to interpolate
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Coding Activity:
Perform cubic-spline interpolation on the Density-vs-Temperature dataset in the notebook **interp-activity-1-with-gaps.ipynb** from the Interpolation module on Canvas.

2-D Linear Interpolation

Example: Specific volume (m^3/kg) of water at various temperatures and pressures.

p (bar) \ T (C)	75.0	100.0	150.0	200.0	250.0	300.0	350.0	400.0	450.0	500.0
0.1	16.000	17.200	19.500	21.800	24.200	26.500	28.700	30.100	33.300	35.700
0.5	**0.001**	3.410	3.890	4.350	4.830	5.290	5.750	6.210	6.670	7.140
1.0	**0.001**	1.690	1.940	2.170	2.400	2.640	2.870	3.110	3.330	3.570
5.0	**0.001**	**0.001**	**0.001**	0.425	0.474	0.522	0.571	0.617	0.664	0.711
10.0	**0.001**	**0.001**	**0.001**	0.206	0.233	0.258	0.282	0.307	0.330	0.353

2-D Linear Interpolation

Example: Specific volume (m^3/kg) of water at various temperatures and pressures.

175

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0.75

2-D Linear Interpolation

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175

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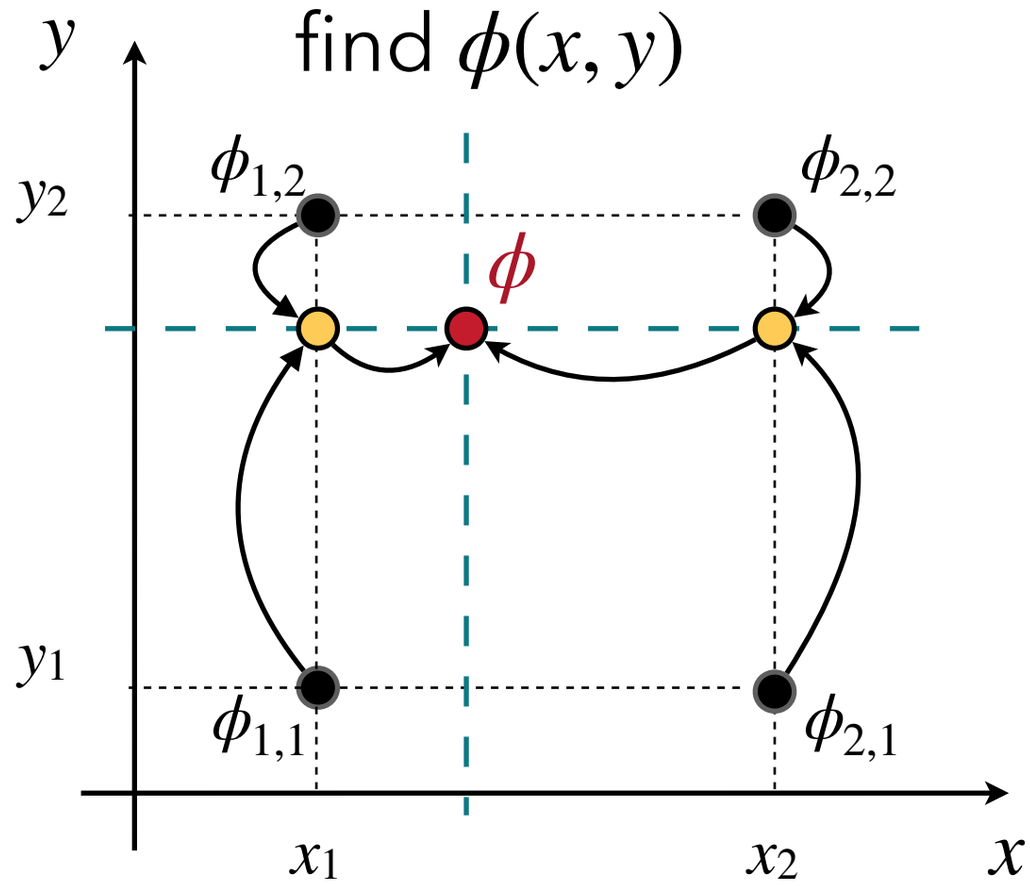
0.1	16.000	17.200	19.500	21.800	24.200	26.500	28.700	30.100	33.300	35.700
0.5	**0.001**	3.410	3.890	4.350	4.830	5.290	5.750	6.210	6.670	7.140
1.0 (0.75)	**0.001**	1.690	1.940	2.170	2.400	2.640	2.870	3.110	3.330	3.570
5.0	**0.001**	**0.001**	**0.001**	0.425	0.474	0.522	0.571	0.617	0.664	0.711
10.0	**0.001**	**0.001**	**0.001**	0.206	0.233	0.258	0.282	0.307	0.330	0.353

2-D Linear Interpolation

Bilinear Interpolation
If you have "structured" (tabular) data, you can do two 1-D interpolations:
1. Interpolate in one direction
2. Interpolate in second direction.

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



Interpolate in y first

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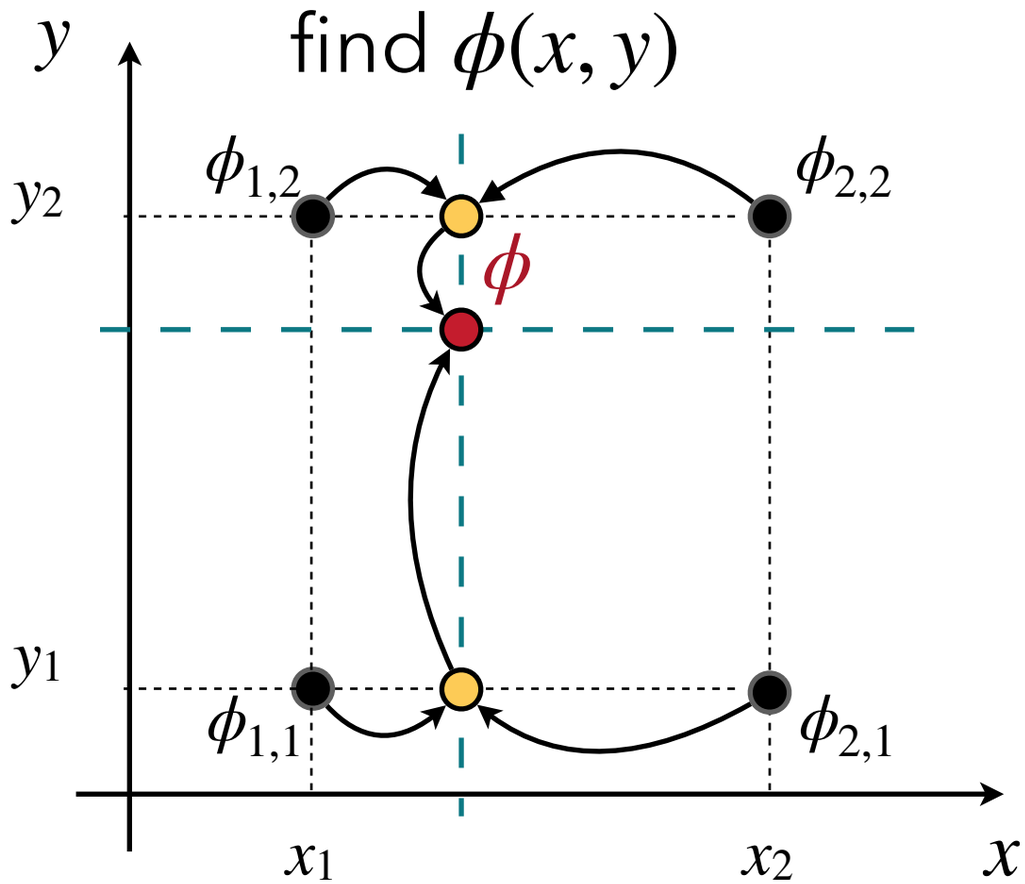
p (bar)	75.0	100.0	150.0	200.0	250.0
0.1	16.000	17.200	19.500	21.800	24.200
0.5	**0.001**	3.410	3.890	4.350	4.830
1.0	**0.001**	1.690	1.940	2.170	2.400
5.0	**0.001**	**0.001**	**0.001**	0.425	0.474
10.0	**0.001**	**0.001**	**0.001**	0.206	0.233

0.75

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.



Interpolate in x first

Either way, you get this:

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

p	250.0
0	24.200
0	4.830
1	2.400
5	0.474
10	0.233

Pythonification

```
from scipy.interpolate import interp2d
f2d = interp2d(xi,yi,zi,method)
ze = f2d(xe,ye)
```

- **xi** - independent variable entries (vector)
- **yi** - independent variable entries (vector)
- **zi** - dependent variable entires (2d vector)
- **method** = ‘linear’, ‘cubic’, ‘quintic’
- **xe, ye** - value(s) where you want to interpolate
- **ze** - interpolated value(s) at **xe** and **ye**

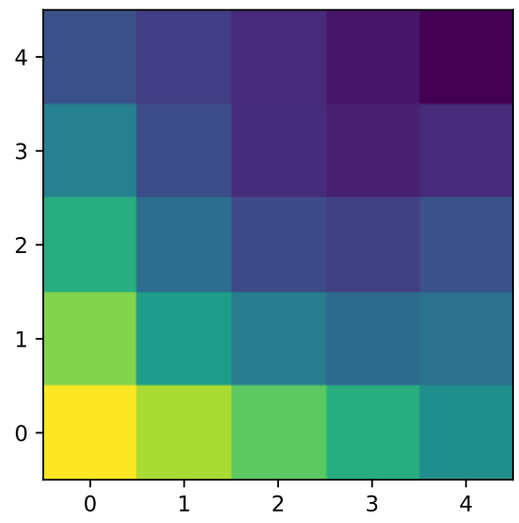
2-D Interpolation Example

Temperatures are measured at various points on a heated plate (Table P18.30). Estimate the temperature at **(a)** $x = 4$, $y = 3.2$, and **(b)** $x = 4.3$, $y = 2.7$.

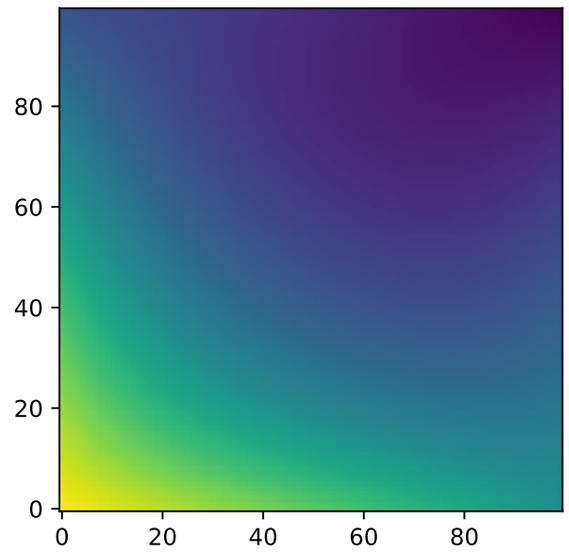
TABLE P18.30 Temperature (°C) at various points on a square heated plate.

	$x = 0$	$x = 2$	$x = 4$	$x = 6$	$x = 8$
$y = 0$	100.00	90.00	80.00	70.00	60.00
$y = 2$	85.00	64.49	53.50	48.15	50.00
$y = 4$	70.00	48.90	38.43	35.03	40.00
$y = 6$	55.00	38.78	30.39	27.07	30.00
$y = 8$	40.00	35.00	30.00	25.00	20.00

```python
import numpy as np
import matplotlib.pyplot as plt
from scipy import interpolate
x = [0.0,2.0,4.0,6.0,8.0]
y = [0.0,2.0,4.0,6.0,8.0]
T = [[100,90,80,70,60],
     [85,64.49,53.50,48.15,50.0],
    [70,48.9,38.43,35.03,40.0],
    [55.00,38.78,30.39,27.07,30.0],
    [40.00,35,30,25,20]]
f = interpolate.interp2d(x, y, T, kind='cubic')
plt.imshow(f(x,y),origin='lower')
plt.show()
xnew = np.linspace(0,8,100)
ynew = np.linspace(0,8,100)
fnew = f(xnew,ynew)
plt.imshow(f(xnew,ynew),origin='lower')
```



Original data



Interpolated data