

Machine Learning with Python

MTH786U/P 2023/24

Week 11: Semi-supervised classification with graphs

Nicola Perra, Queen Mary University of London (QMUL)

What is a graph?



What is a graph?

An *undirected graph* is a pair $G = (V, E)$



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V are the *vertices*



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$E = \{x, y \mid (x, y) \in V^2 \wedge x \neq y\}$ are the *edges*

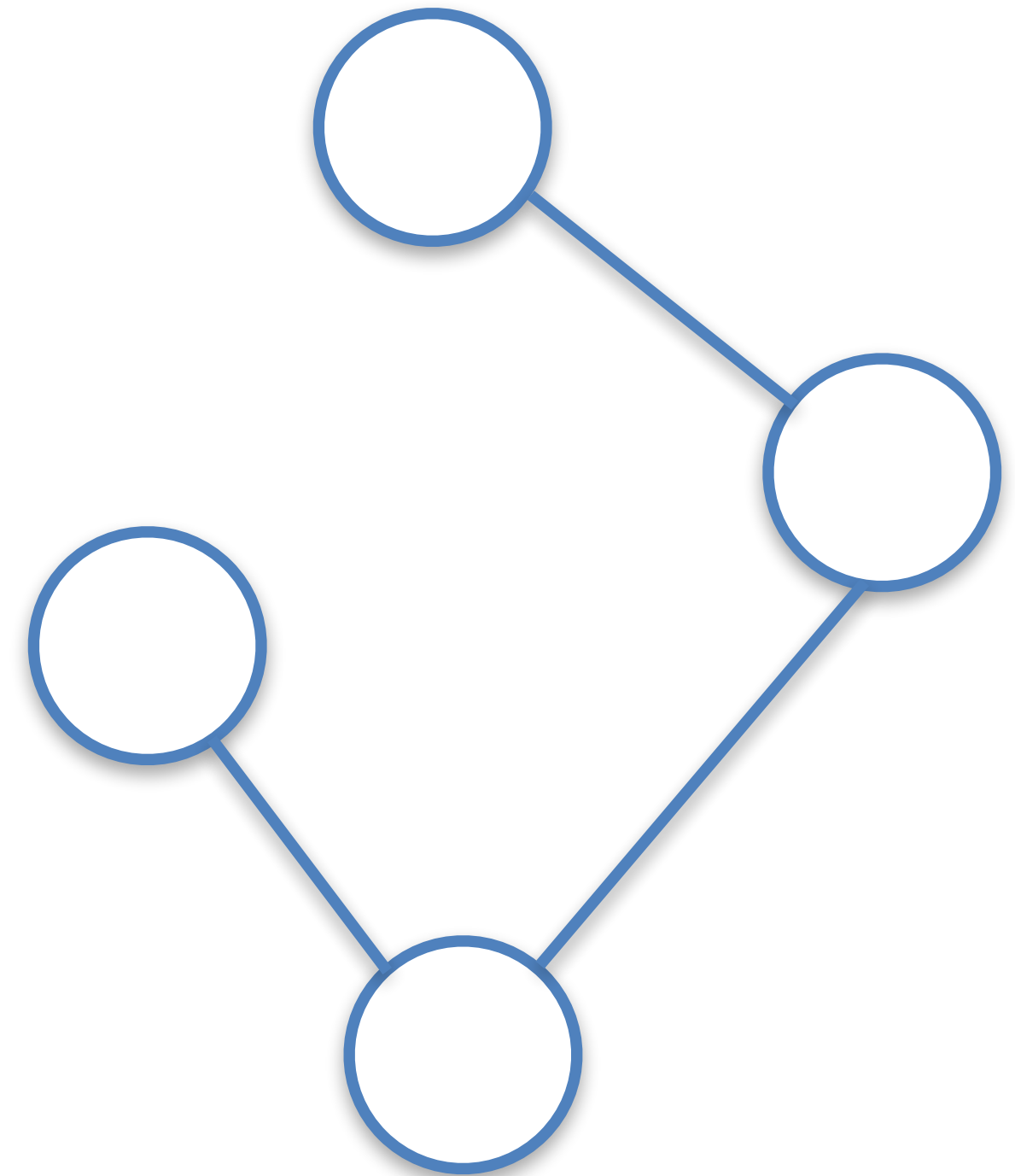


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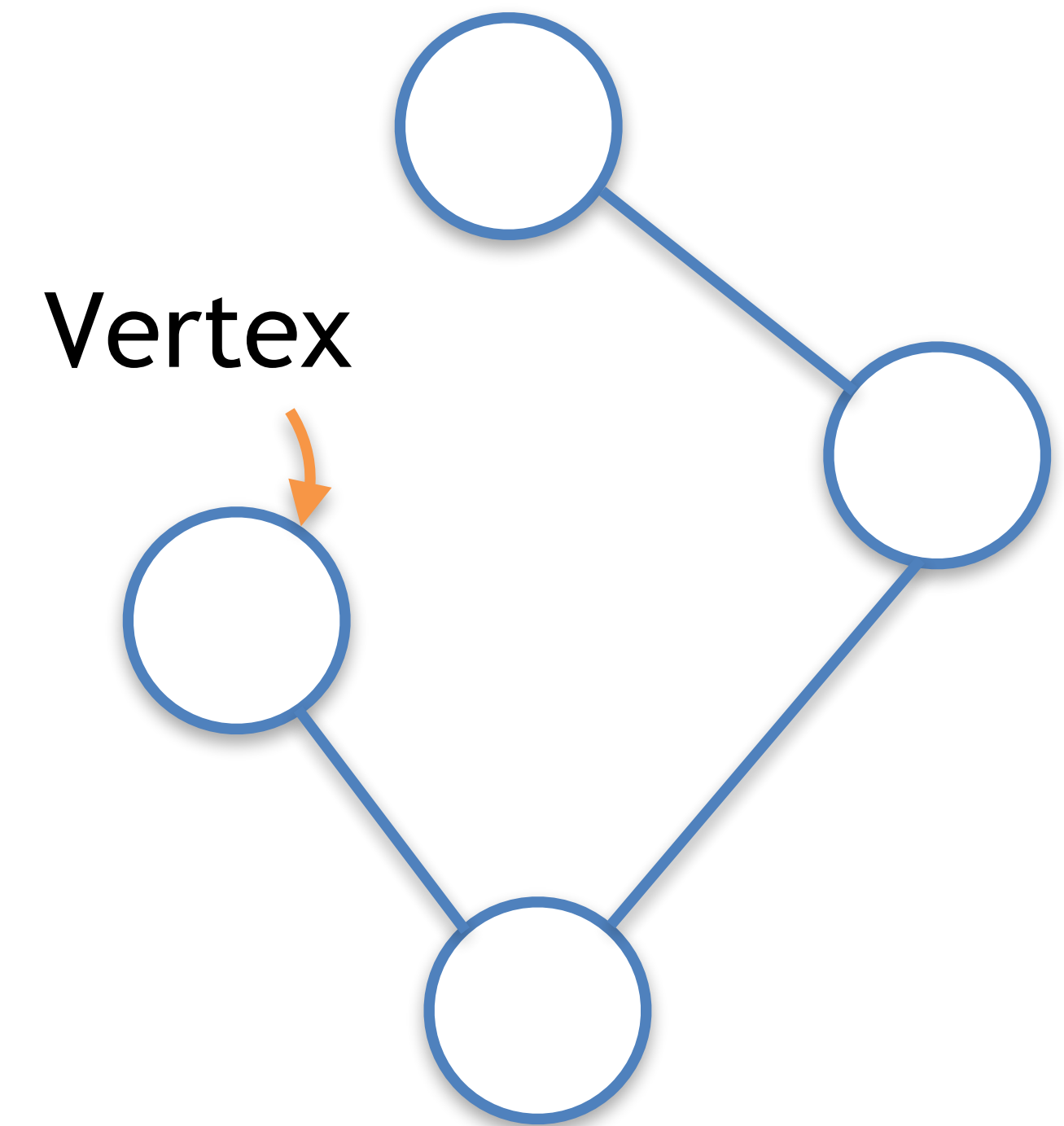


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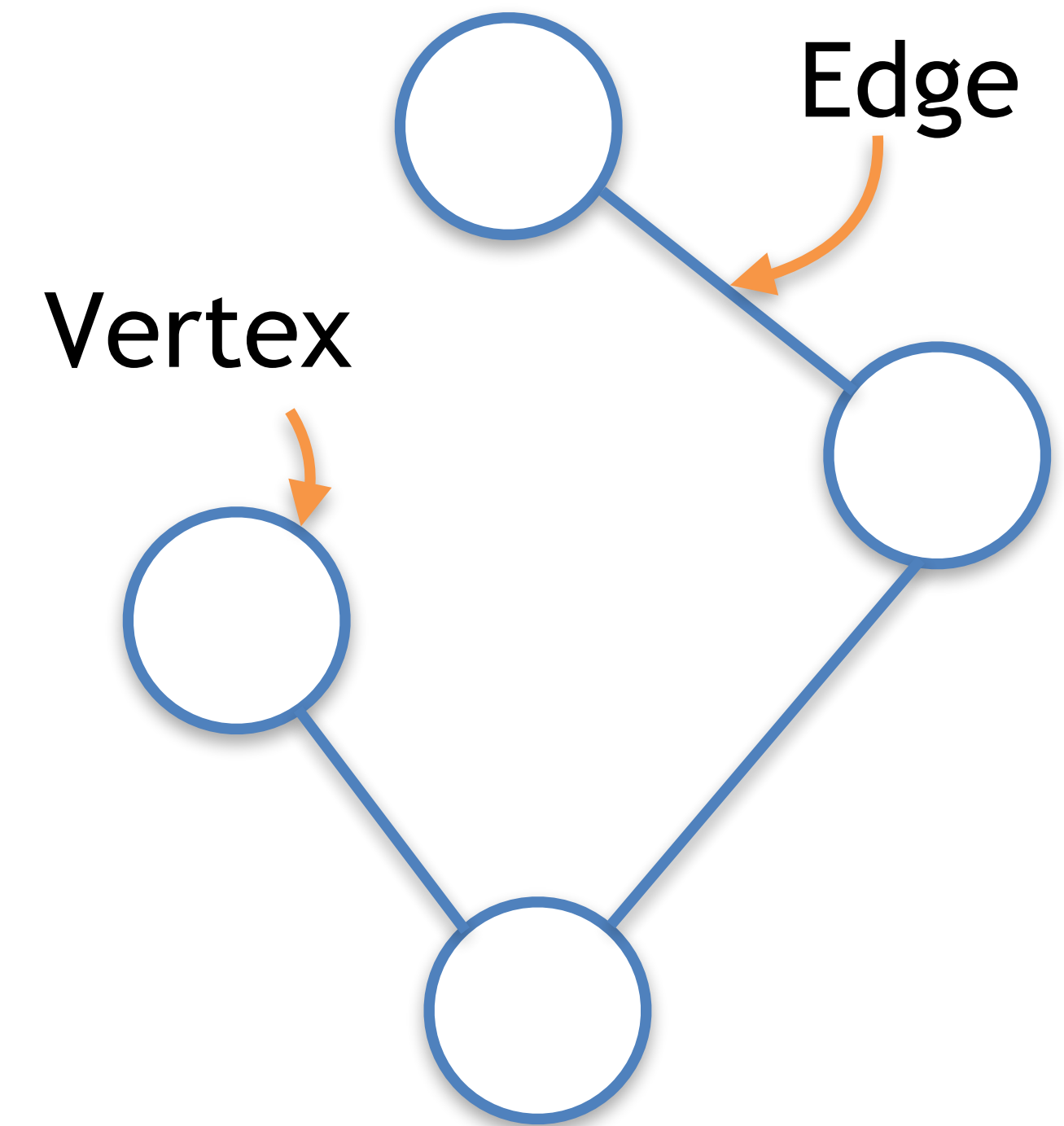


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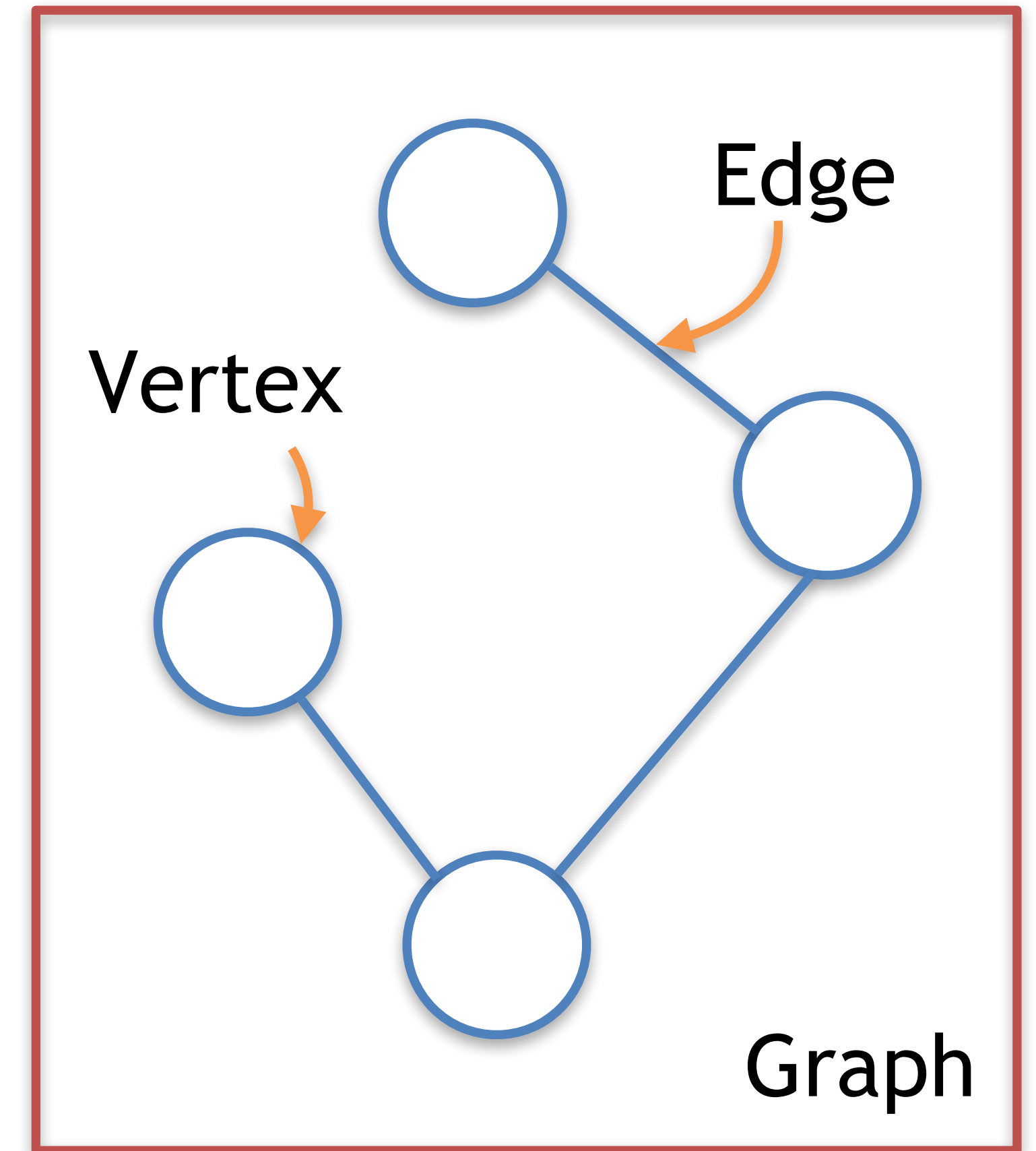


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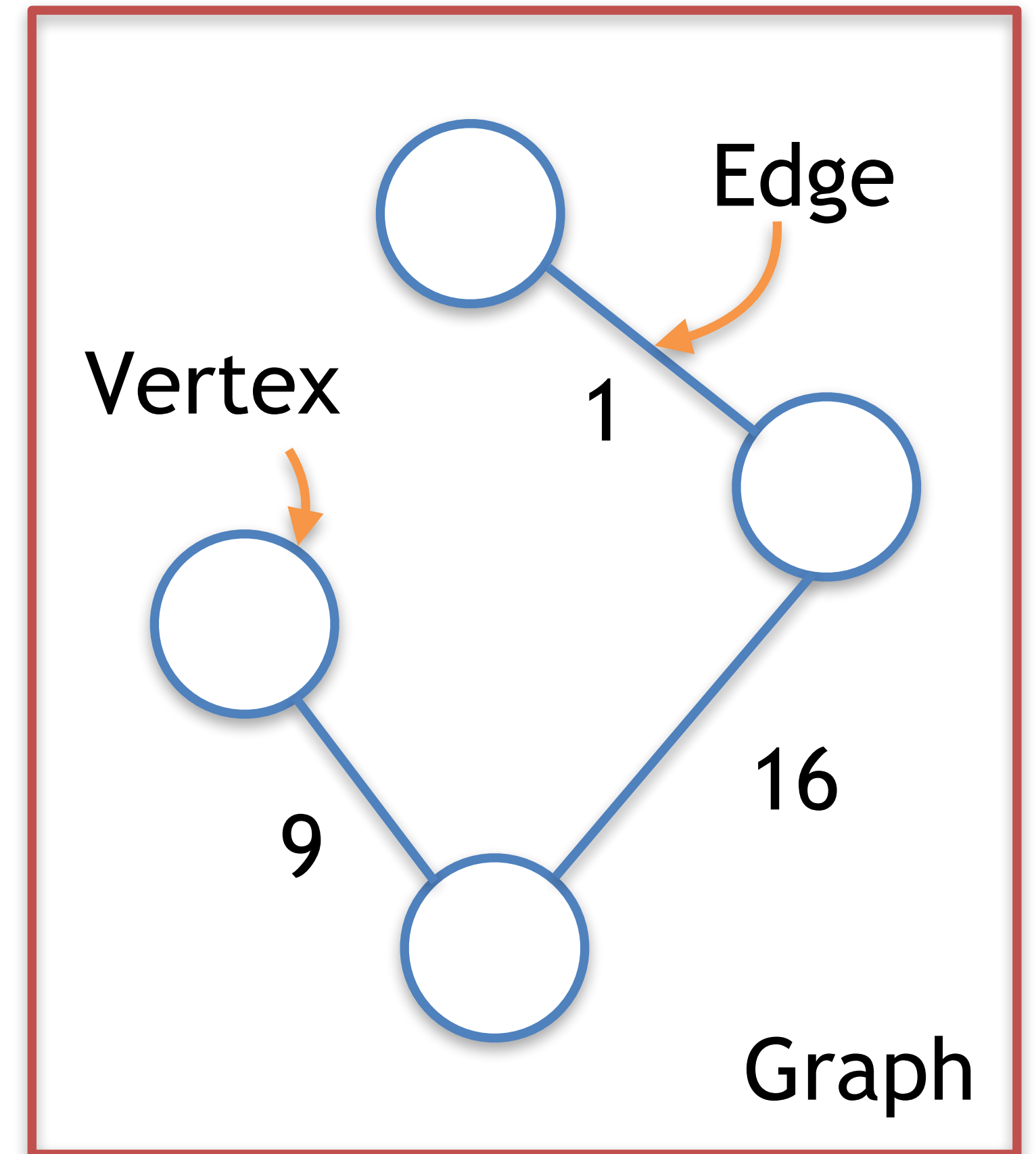
What is a graph?

A *weighted graph* is a pair $G = (V, E)$

V are the *vertices*

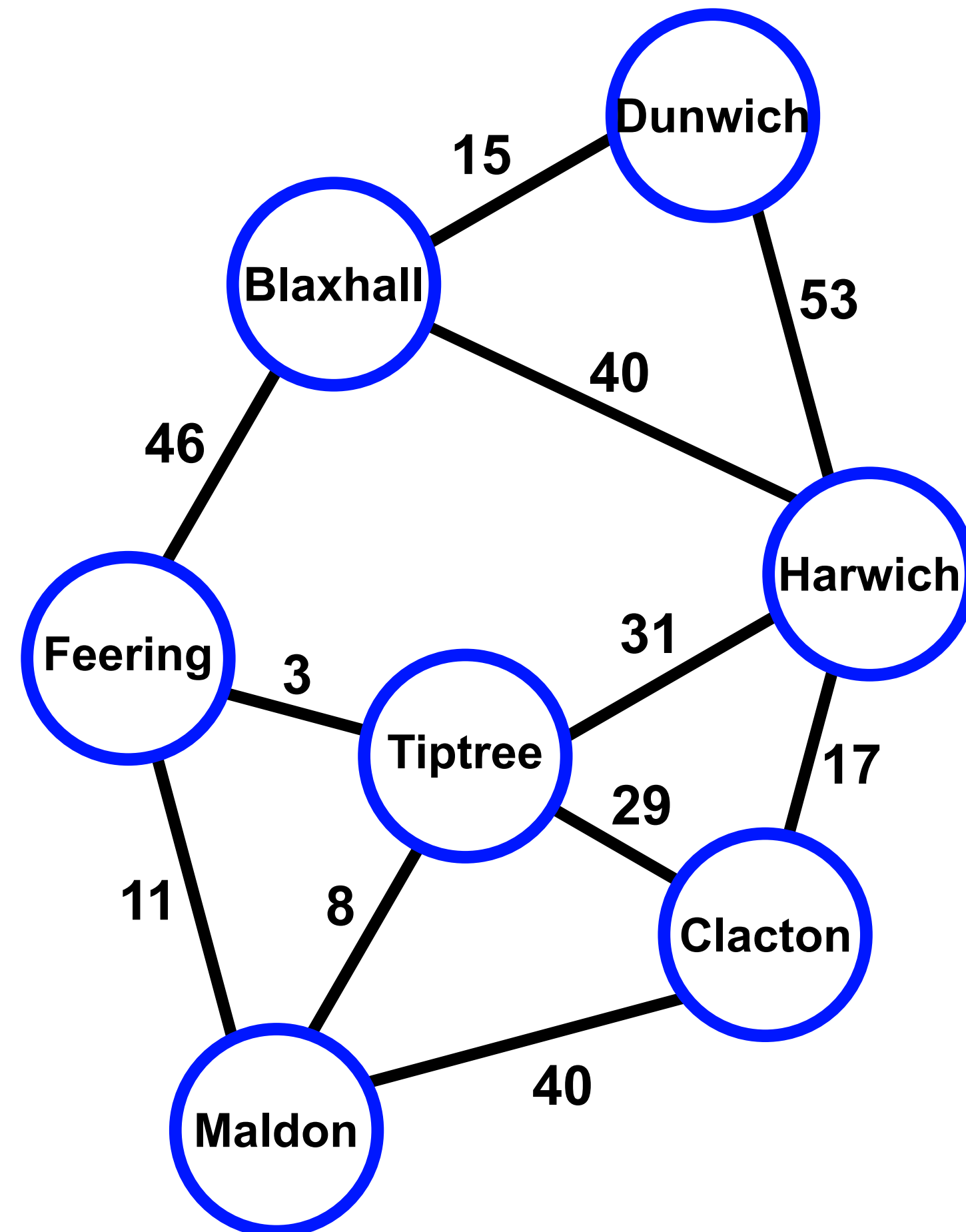
$E = \{x, y \mid (x, y) \in V^2 \wedge x \neq y\}$ are the *edges*

A number called *weight* is assigned to each edge



What is a graph?

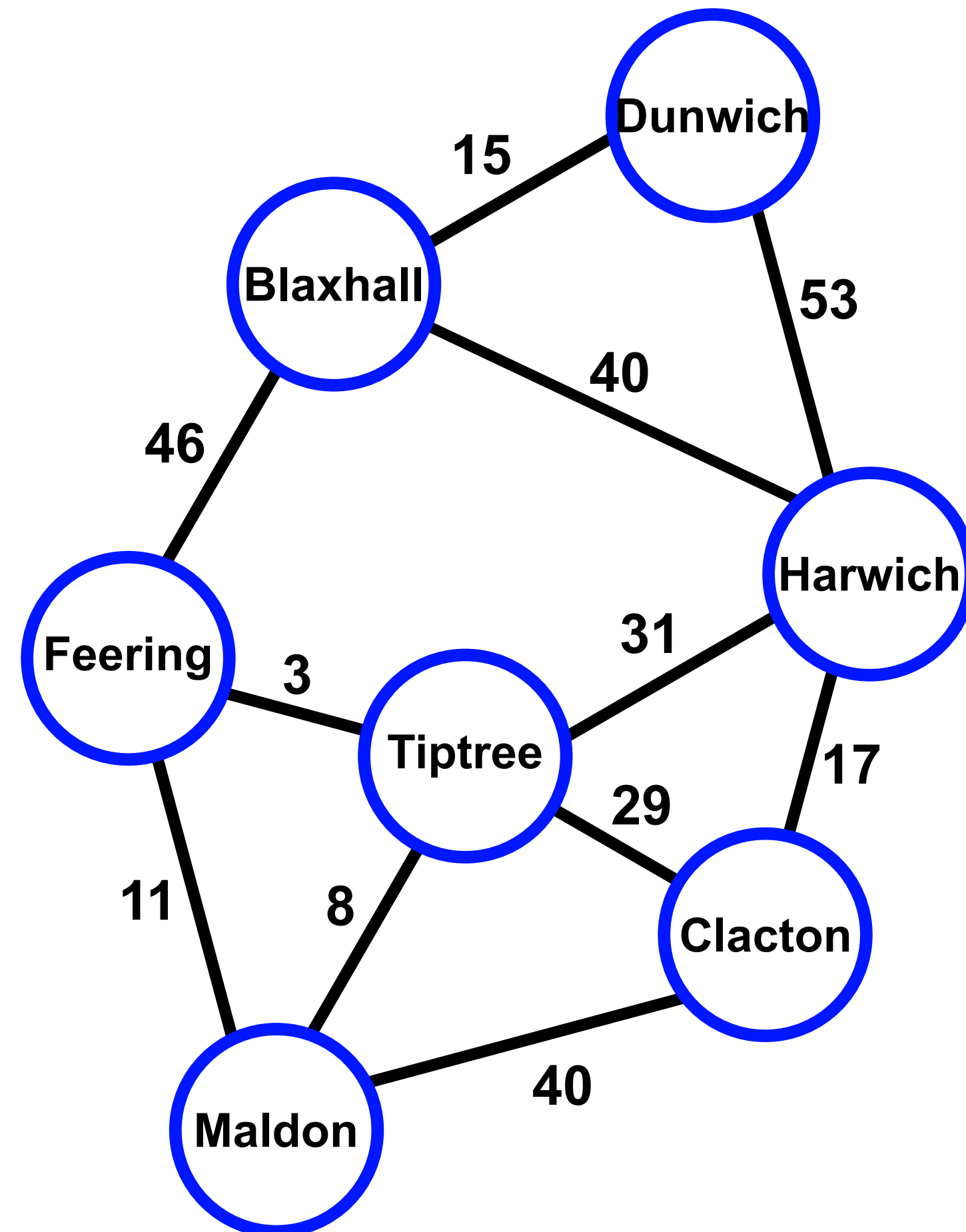
Example



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What is a graph?

Example

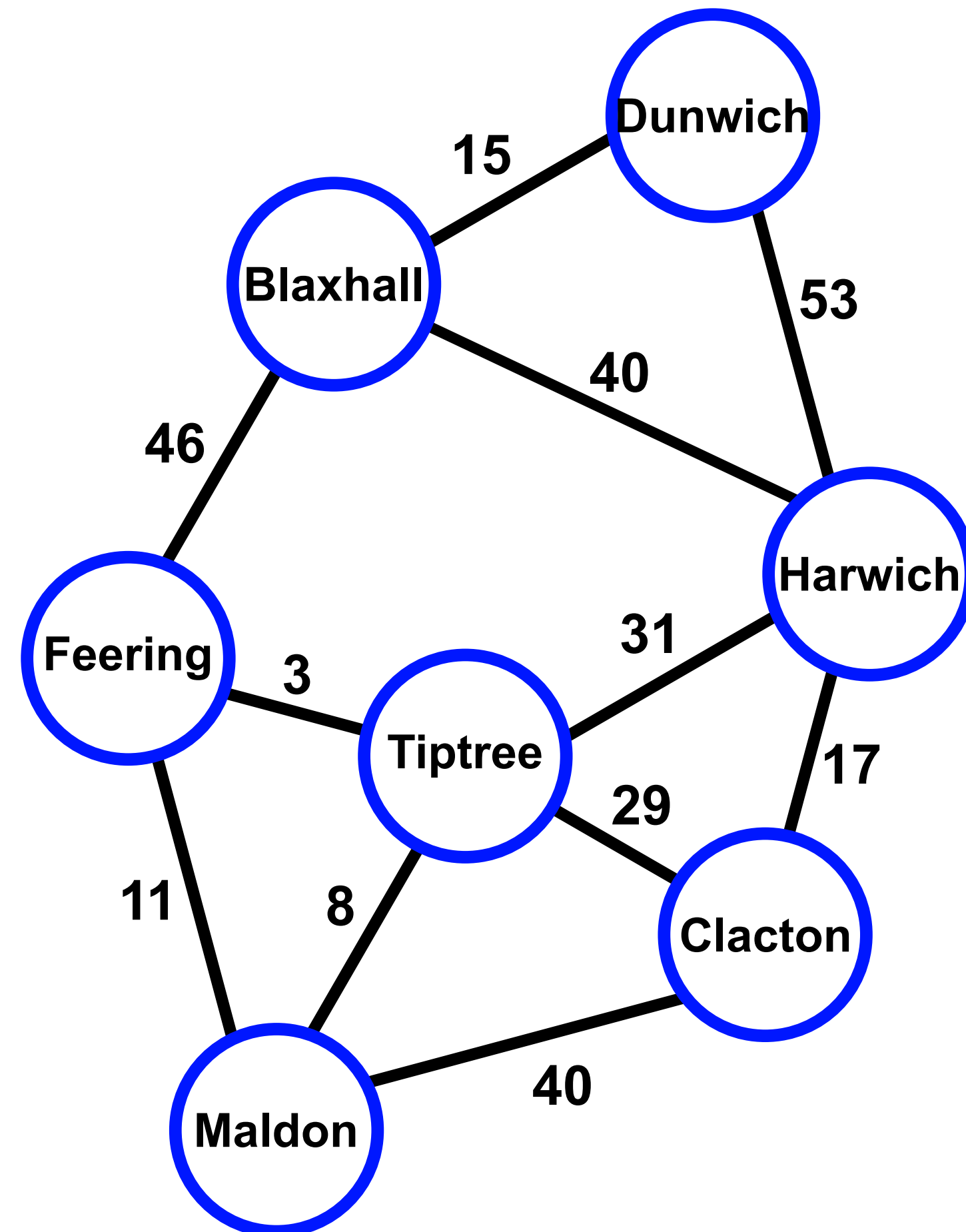


Vertices = towns

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What is a graph?

Example



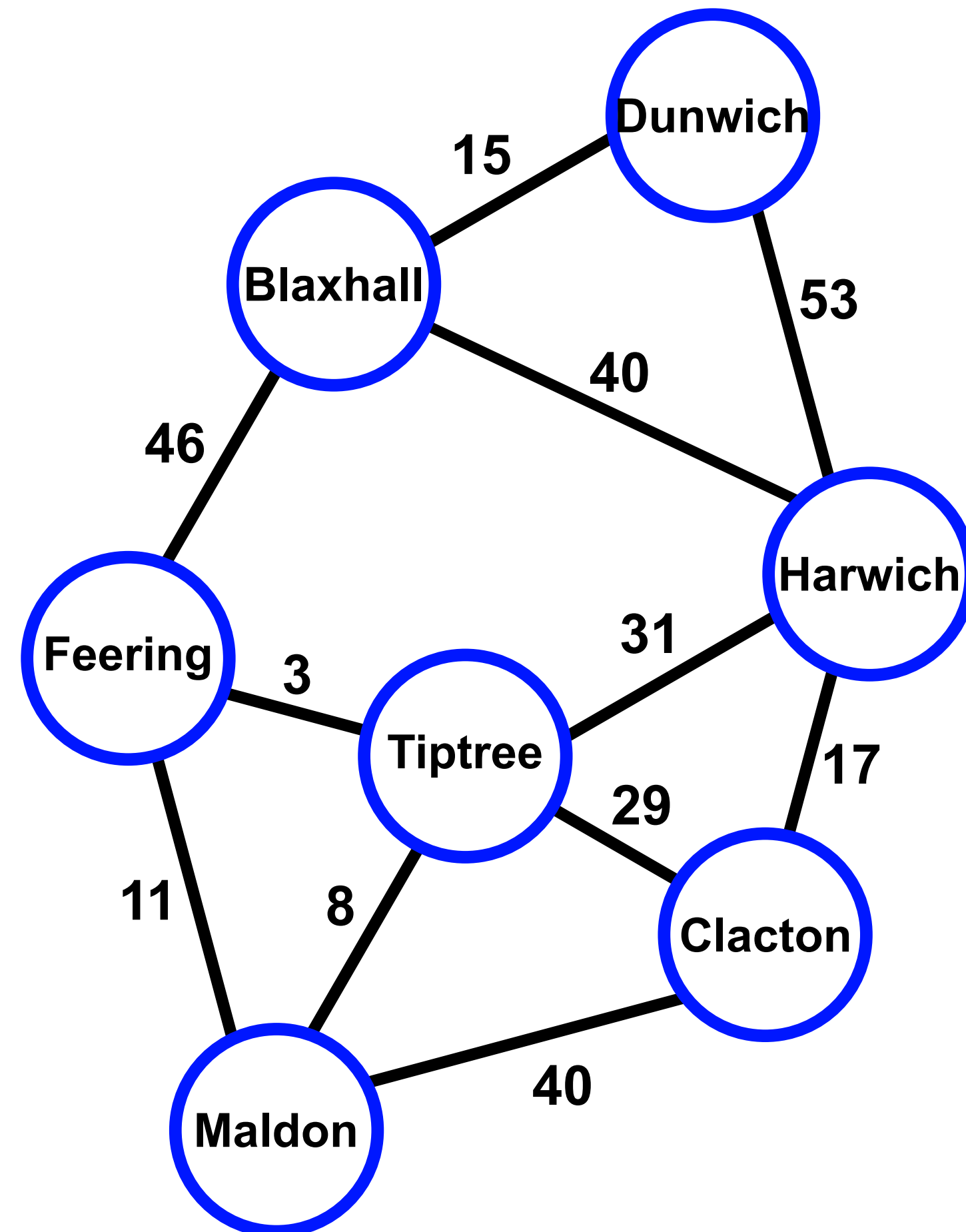
Vertices = towns

Edges = town connections

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What is a graph?

Example



Vertices = towns

Edges = town connections

Weights = distances between towns

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Incidence matrix

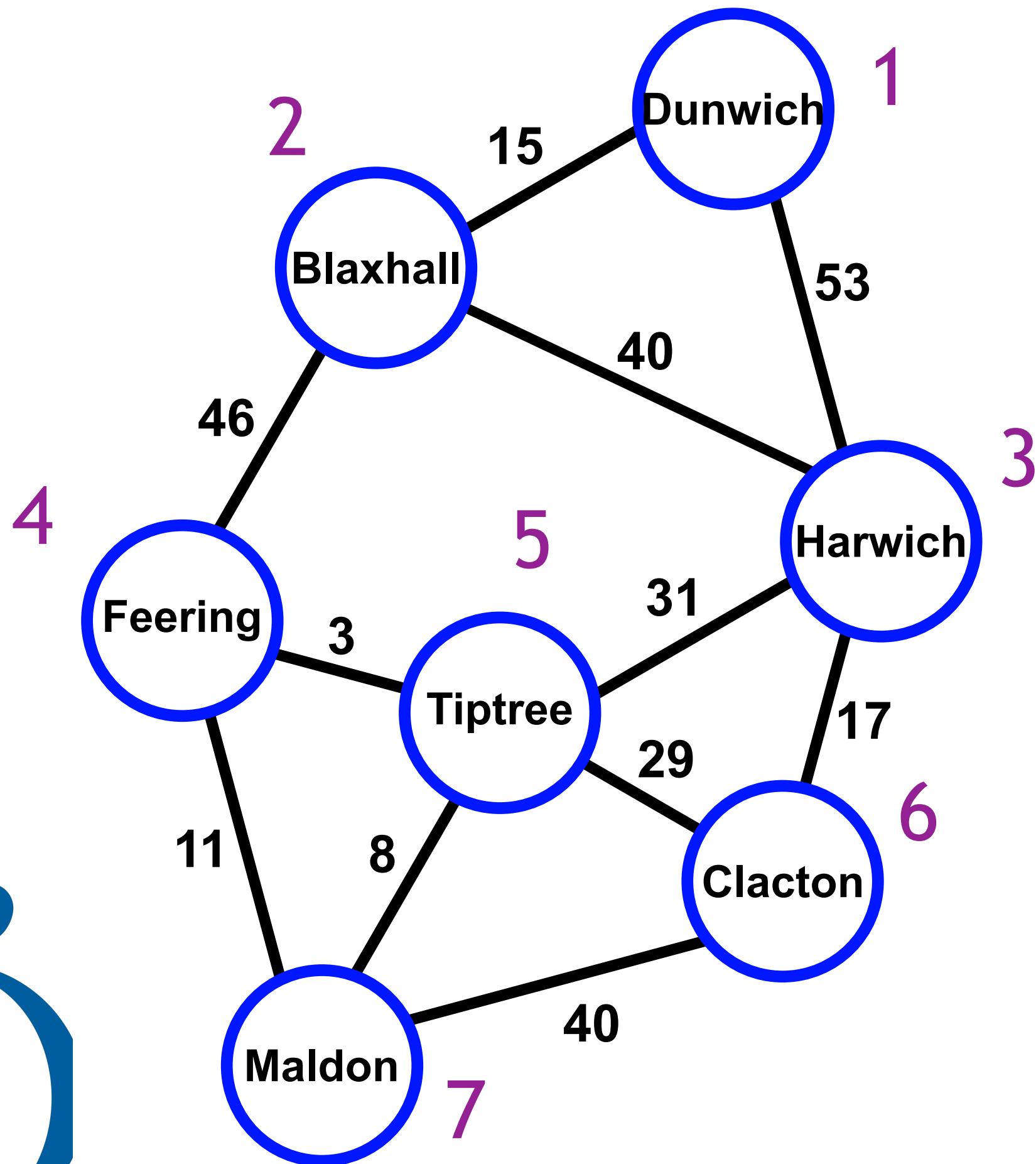
For a (weighted) graph (with weights w) we define a so-called *incidence matrix* $M_w \in \mathbb{R}^{|E| \times |V|}$, where $|E|$ denotes the number of edges and $|V|$ the number of vertices, as

$$(M_w)_{ev} := \begin{cases} \sqrt{w_{ev}} & \text{if } v = i \\ -\sqrt{w_{ev}} & \text{if } v = j \\ 0 & \text{otherwise} \end{cases},$$

where every edge $e = (i, j)$ connects vertices i and j , with $i > j$.



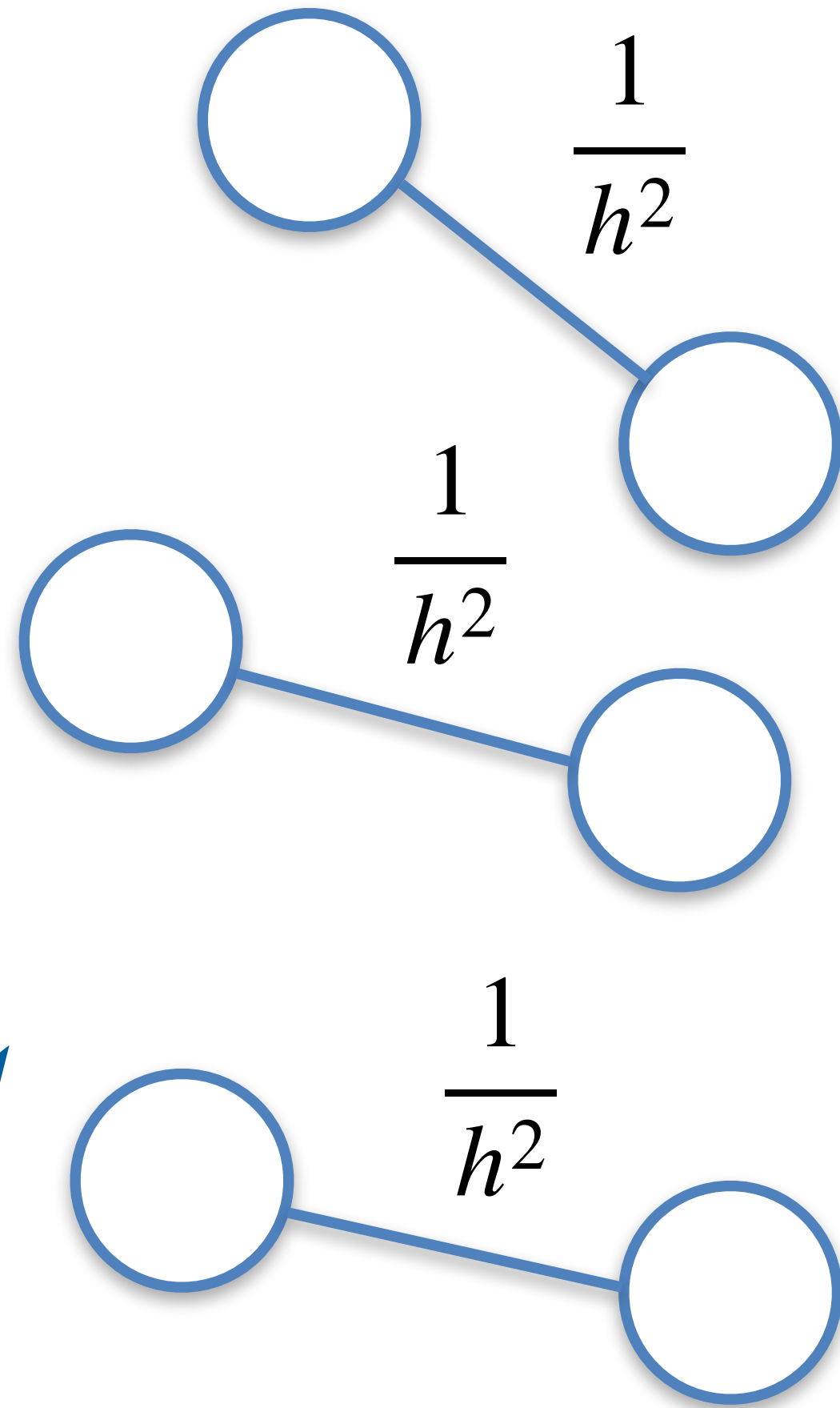
Incidence matrix



$$M_w = \begin{pmatrix} -\sqrt{15} & \sqrt{15} & 0 & 0 & 0 & 0 & 0 \\ -\sqrt{53} & 0 & \sqrt{53} & 0 & 0 & 0 & 0 \\ 0 & -\sqrt{40} & \sqrt{40} & 0 & 0 & 0 & 0 \\ 0 & -\sqrt{46} & 0 & 0 & \sqrt{46} & 0 & 0 \\ 0 & 0 & 0 & -\sqrt{3} & \sqrt{3} & 0 & 0 \\ 0 & 0 & -\sqrt{31} & \sqrt{31} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\sqrt{29} & 0 & \sqrt{29} & 0 \\ 0 & 0 & -\sqrt{17} & 0 & 0 & \sqrt{17} & 0 \\ 0 & 0 & 0 & 0 & -\sqrt{11} & 0 & \sqrt{11} \\ 0 & 0 & 0 & -\sqrt{8} & 0 & 0 & \sqrt{8} \\ 0 & 0 & 0 & 0 & 0 & -\sqrt{40} & \sqrt{40} \end{pmatrix} \begin{matrix} E1 \\ E2 \\ E3 \\ E4 \\ E5 \\ E6 \\ E6 \\ E7 \\ E8 \\ E9 \\ E10 \end{matrix}$$

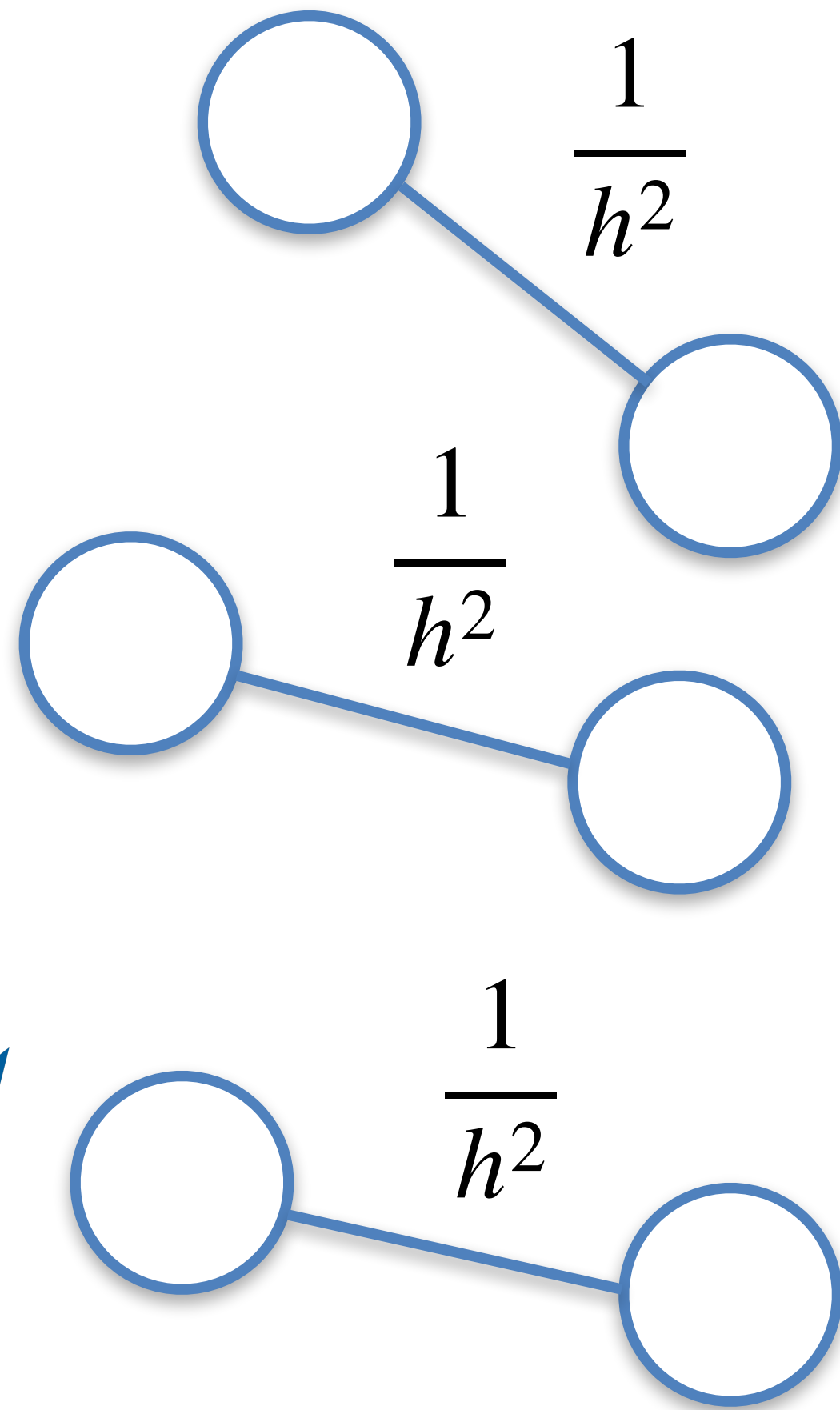
What is a graph?

Another example: finite differences



What is a graph?

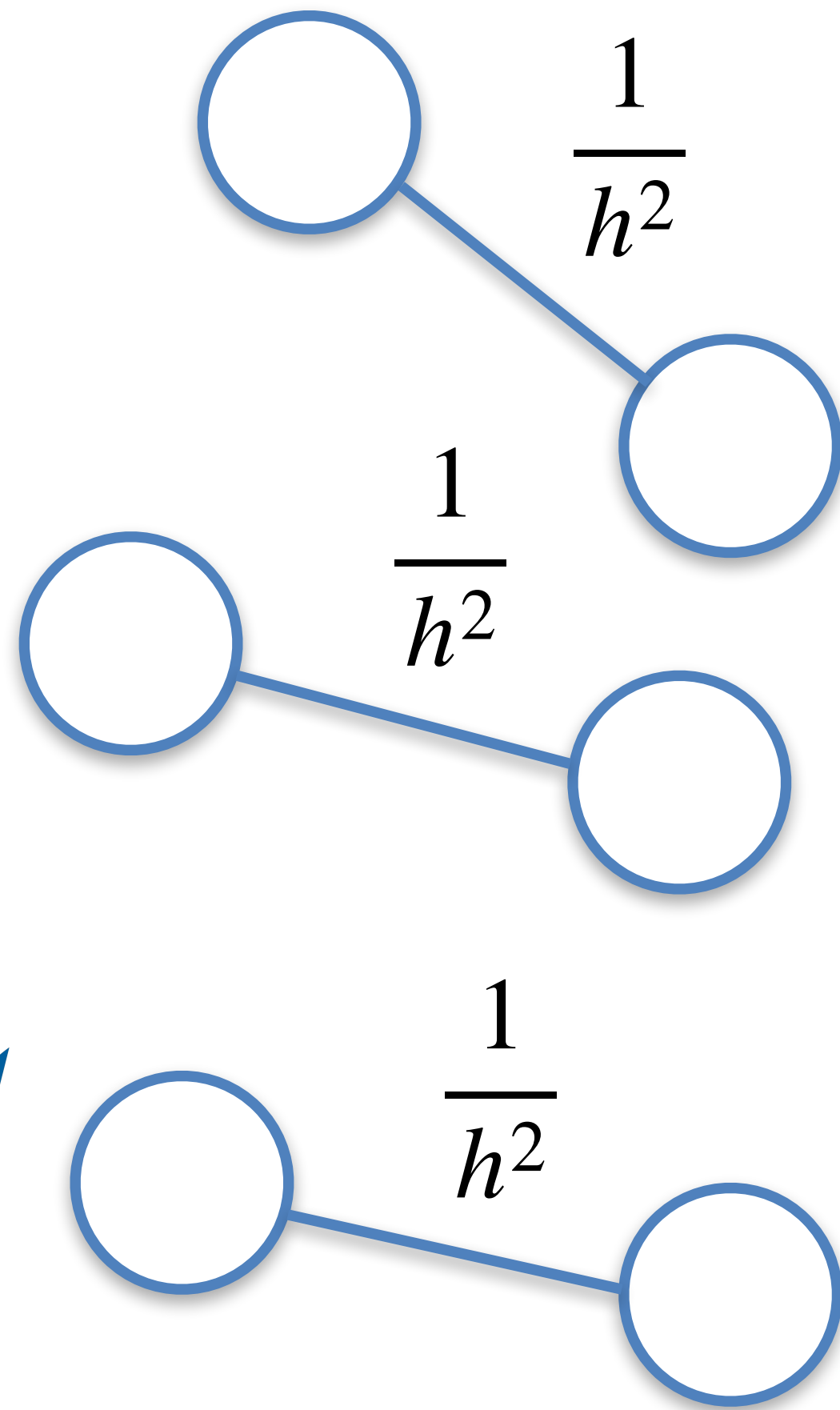
Another example: finite differences



Every vertex is connected only to one other vertex

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Another example: finite differences

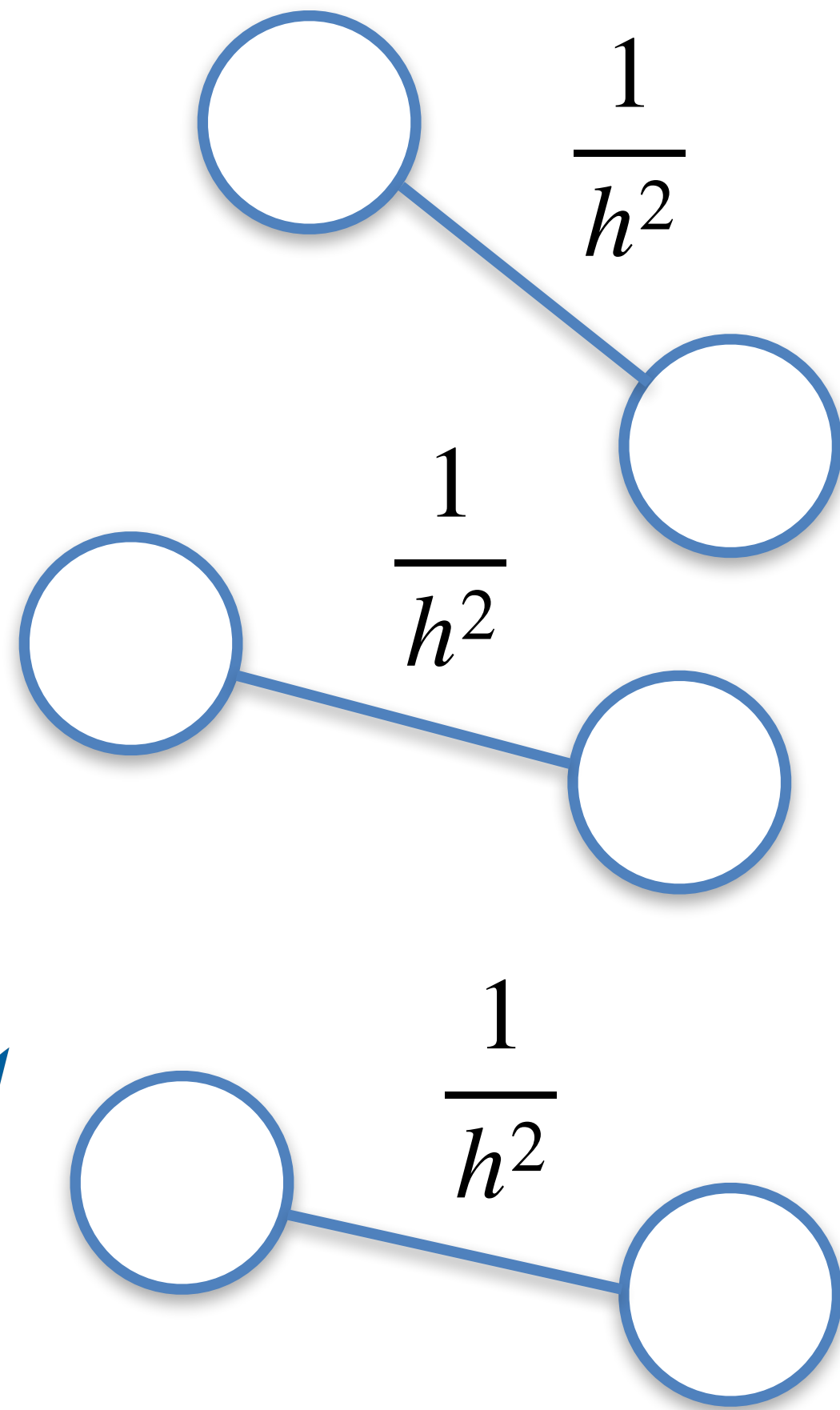


Every vertex is connected only to one other vertex

The weight is a constant factor $(1/h)^2$

What is a graph?

Another example: finite differences



Every vertex is connected only to one other vertex

The weight is a constant factor $(1/h)^2$

Suppose every vertex represents $f(x_i)$:

What is a graph?

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{h}$$

can be written as matrix-vector multiplication

$$\begin{pmatrix} f'(x_1) \\ f'(x_2) \\ \vdots \\ f'(x_d) \end{pmatrix} \approx \frac{1}{h} \begin{pmatrix} -1 & 1 & 0 & \dots & 0 & 0 \\ 0 & -1 & 1 & \dots & 0 & 0 \\ \vdots & & \ddots & & \vdots & \\ 0 & 0 & \dots & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_{d+1}) \end{pmatrix}$$



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This is our *incidence matrix*

Graph Laplacian

Based on the finite difference approximation

$$M_{\frac{1}{h}} = \frac{1}{h} \begin{pmatrix} -1 & 1 & 0 & \dots & 0 & 0 \\ 0 & -1 & 1 & \dots & 0 & 0 \\ \vdots & & \ddots & & & \vdots \\ 0 & 0 & \dots & 0 & -1 & 1 \end{pmatrix},$$

it is natural to define second-order finite differences (or *Laplacians* in higher dimensions) as

$$L_{\frac{1}{h}} = M_{\frac{1}{h}}^{\top} M_{\frac{1}{h}}$$



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We can define the same for arbitrary graphs!

Graph Laplacian

The *graph-Laplacian* $L_w \in \mathbb{R}^{|\mathcal{V}| \times |\mathcal{V}|}$ is defined as

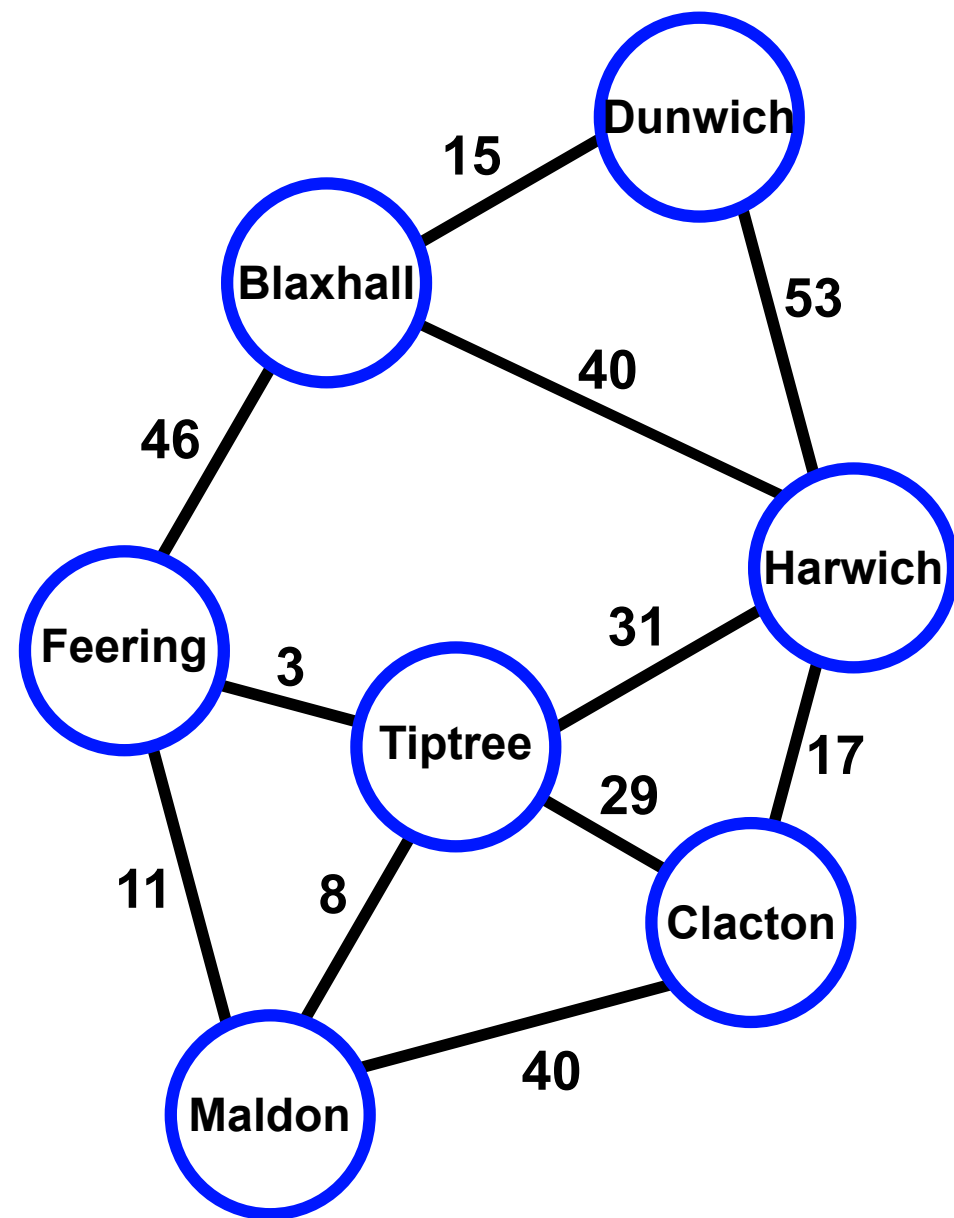
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Graph Laplacian

The *graph-Laplacian* $L_w \in \mathbb{R}^{|V| \times |V|}$ is defined as

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$$L_w = M_w^\top M_w = \begin{pmatrix} 68 & -15 & -53 & 0 & 0 & 0 & 0 \\ -15 & 101 & -40 & 0 & -46 & 0 & 0 \\ -53 & -40 & 141 & -31 & 0 & -17 & 0 \\ 0 & 0 & -31 & 71 & -3 & -29 & -8 \\ 0 & -46 & 0 & -3 & 60 & 0 & -11 \\ 0 & 0 & -17 & -29 & 0 & 86 & -40 \\ 0 & 0 & 0 & -8 & -11 & -40 & 59 \end{pmatrix}$$

Graph Laplacian

The *graph-Laplacian* $L_w \in \mathbb{R}^{|V| \times |V|}$ is defined also as

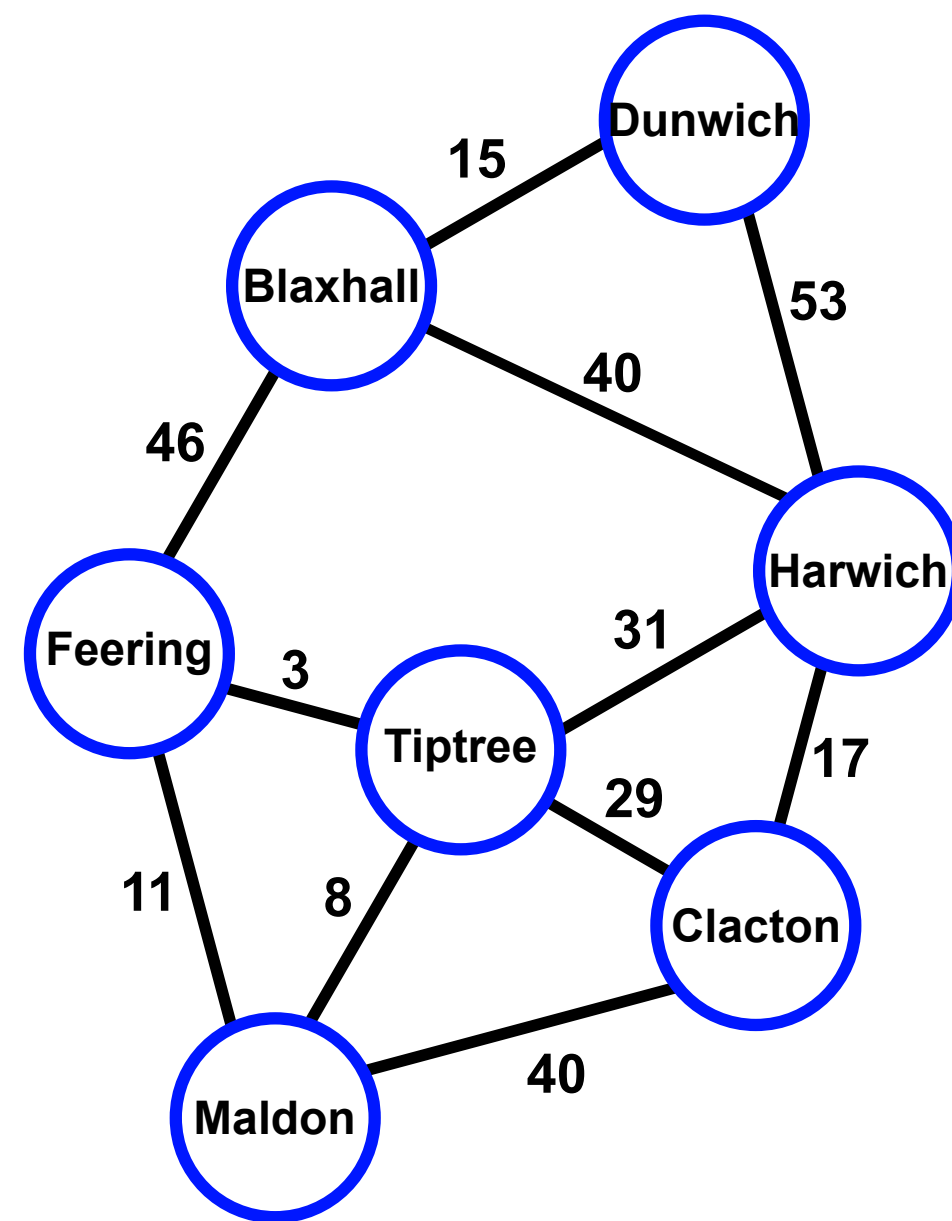
Degree matrix

Adjacency matrix



Graph Laplacian

The *graph-Laplacian* $L_w \in \mathbb{R}^{|V| \times |V|}$ is defined also as $L_w = D_w - A_w$



$$D = \begin{pmatrix} 68 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 101 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 141 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 71 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 60 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 86 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 59 \end{pmatrix} \quad \text{Degree matrix}$$

$$A = \begin{pmatrix} 0 & 15 & 53 & 0 & 0 & 0 & 0 \\ 15 & 0 & 40 & 0 & 46 & 0 & 0 \\ 53 & 40 & 0 & 31 & 0 & 17 & 0 \\ 0 & 0 & 31 & 0 & 3 & 29 & 8 \\ 0 & 46 & 0 & 3 & 0 & 0 & 11 \\ 0 & 0 & 17 & 29 & 0 & 0 & 40 \\ 0 & 0 & 0 & 8 & 11 & 40 & 0 \end{pmatrix} \quad \text{Adjacency matrix}$$

Semi-supervised learning

We can use incidence matrices and graph-Laplacians to model and exploit similarities in a dataset



Interpolation

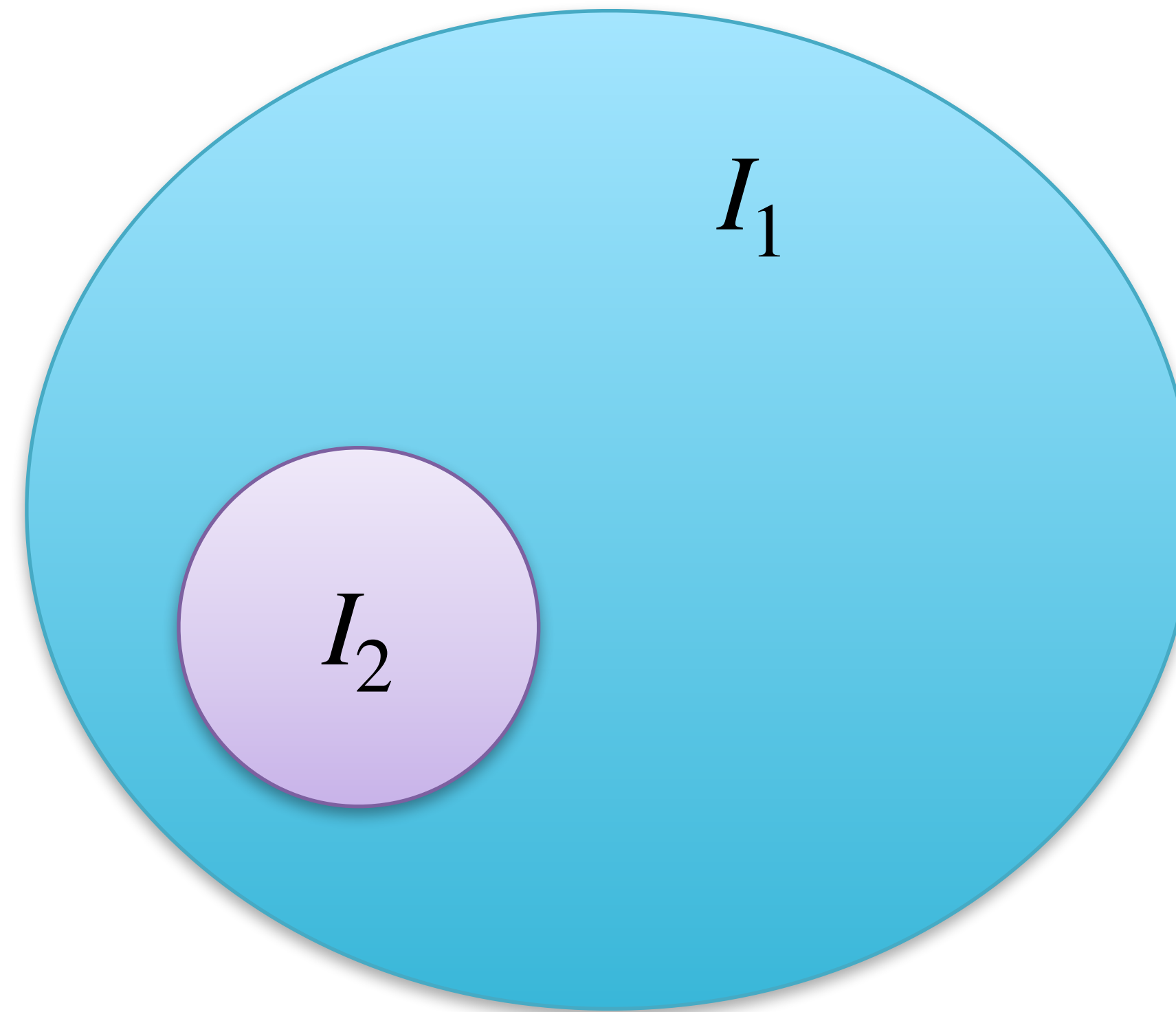
Suppose we are given data points $\{x_i\}_{i \in I_1}$ and pairs $\{(x_j, y_j)\}_{j \in I_2}$ with $I_2 \subset I_1$;

How do we find $\{(x_i, y_i)\}_{i \in I_1}$?



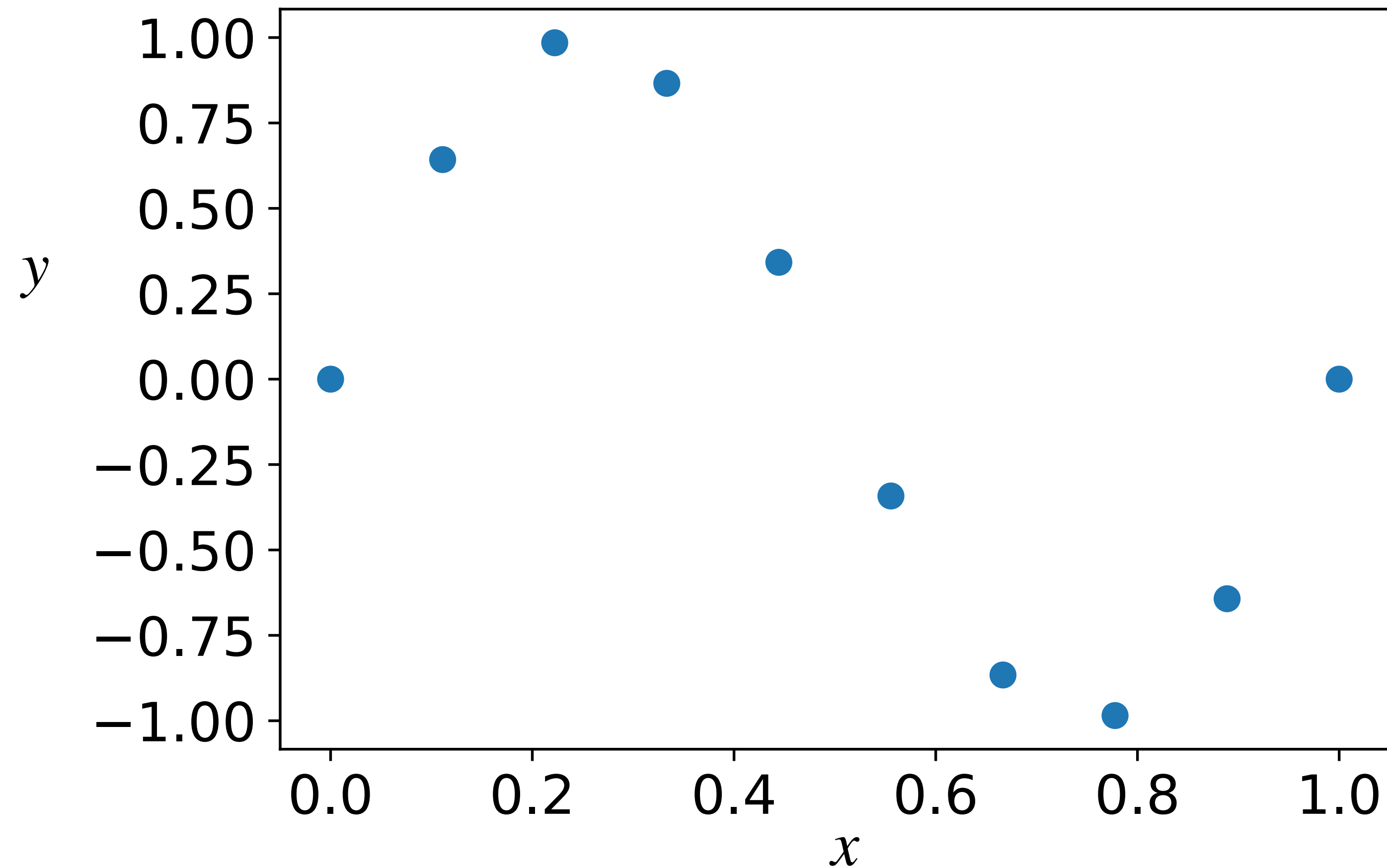
Interpolation

For each x_i in I_2 we know
the correspondent y_i



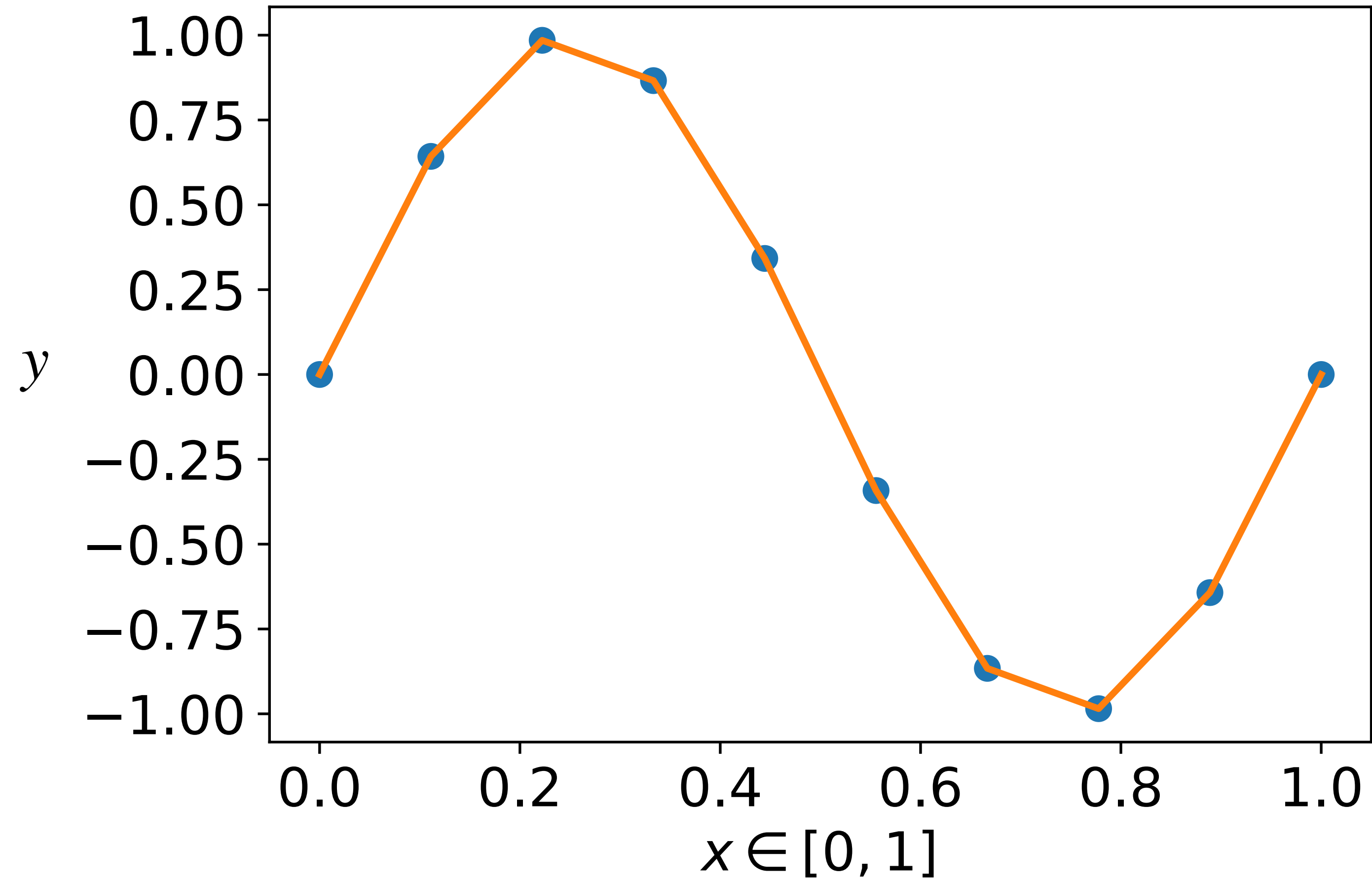
Interpolation

In general we don't know the underlying function, how can we connect the dots?



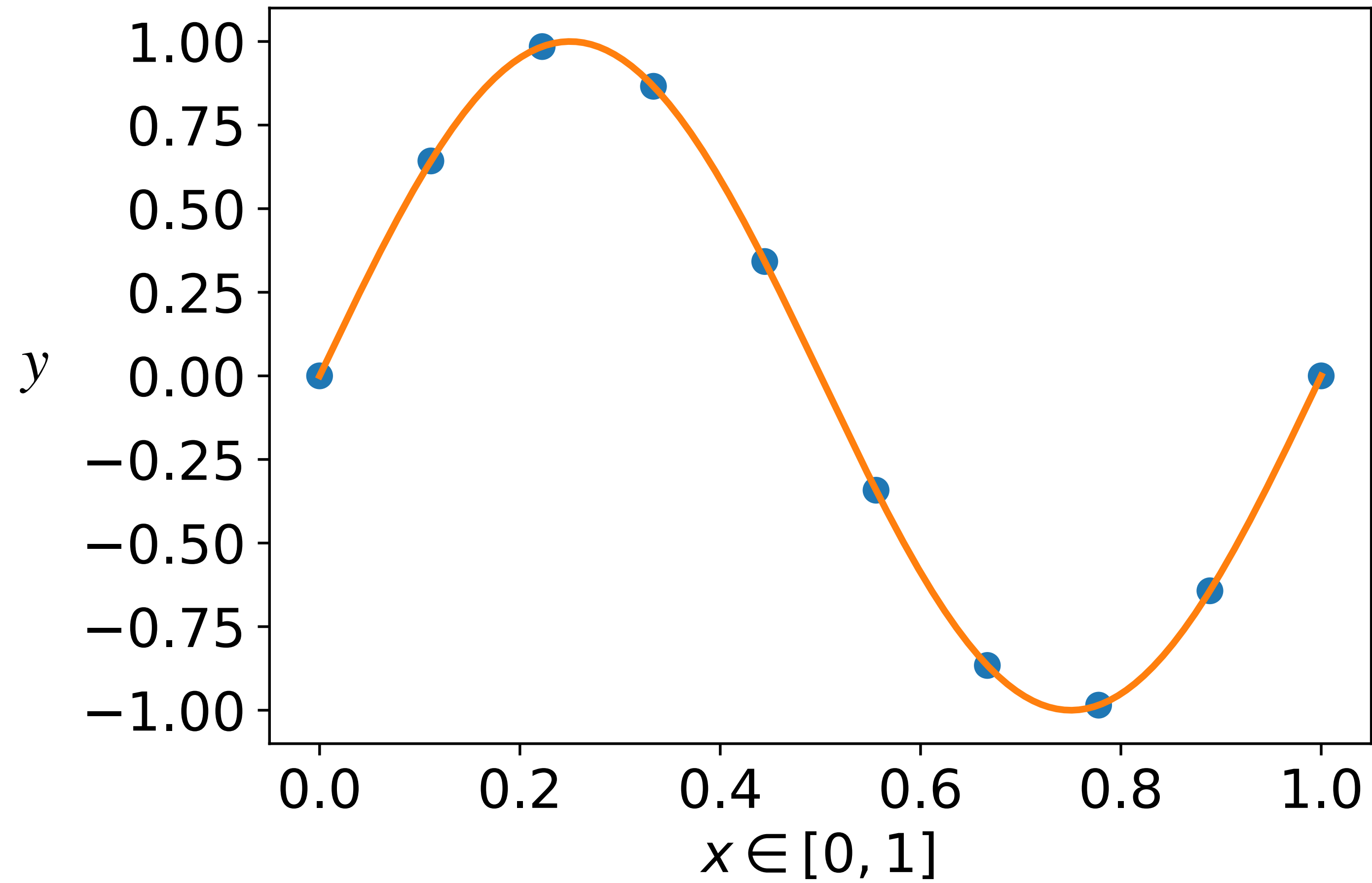
Interpolation

Linear interpolation



Interpolation

Smoother interpolation



Interpolation

One way of formulating this problem mathematically uses the ideas of optimization:

$$\min_{\{y_i\}_{i \in I_1}} E(\mathbf{y}) \quad \text{subject to} \quad (\mathbf{P}_{I_2} \mathbf{y})_j = y_j \quad \forall j \in I_2$$



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We can find the new points by minimizing a certain energy function, subject to the constraints of the points y we know



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Here, \mathbf{P}_{I_2} denotes the projection of a vector with indices in I_1 onto a vector with indices in I_2



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How to choose E to interpolate?



Interpolation

We cannot use the MSE ! Since, we miss the ground truth for the new \mathbf{y}



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We want to ensure that the values we are trying to estimate (interpolate) do not have strange behaviors (i.e., oscillation, large variations)



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Proposal:



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Proposal:

$$E(\mathbf{y}) = \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{y} \right\|^2$$



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Interpolation



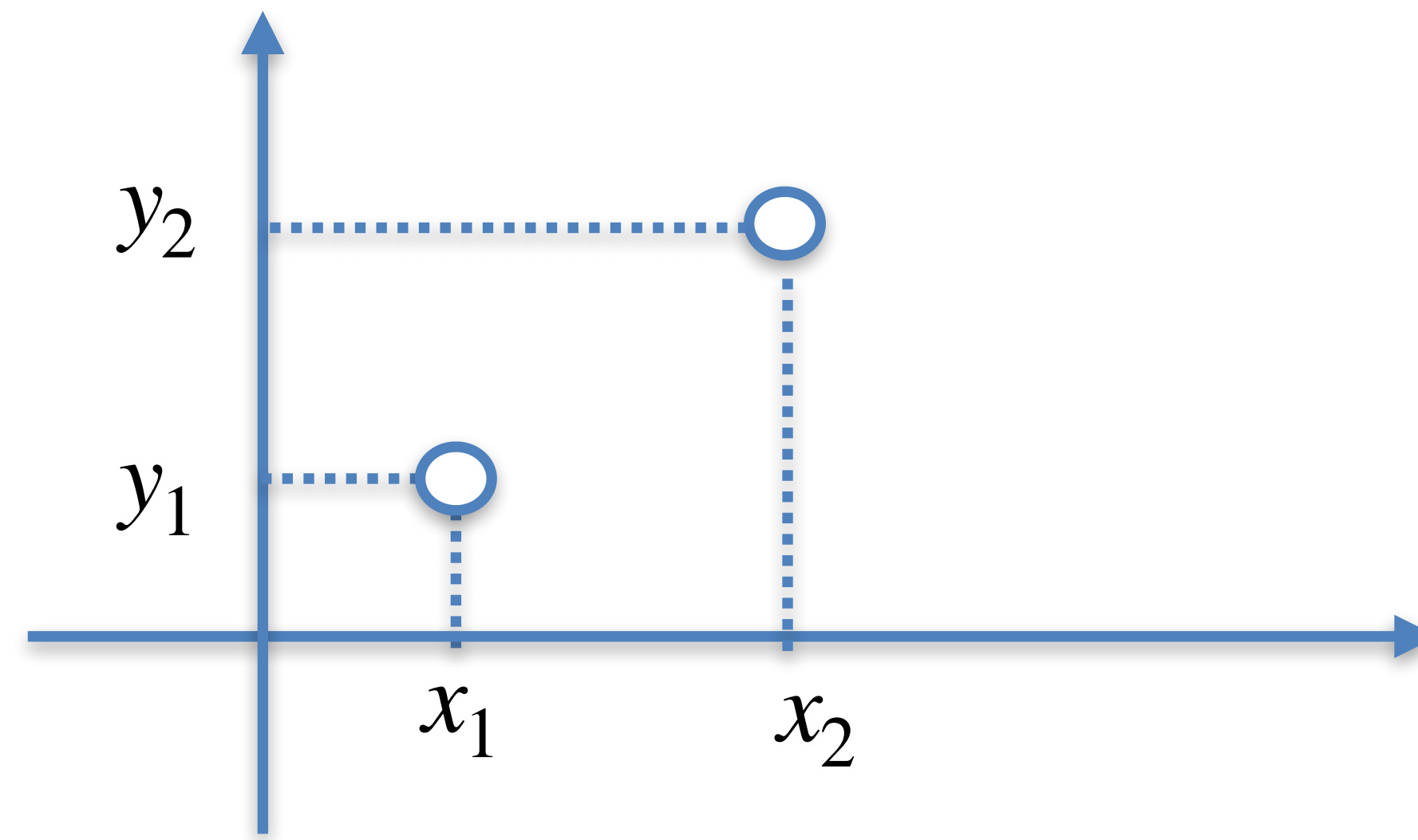
Interpolation

A simple example might help us understand why this is a good idea



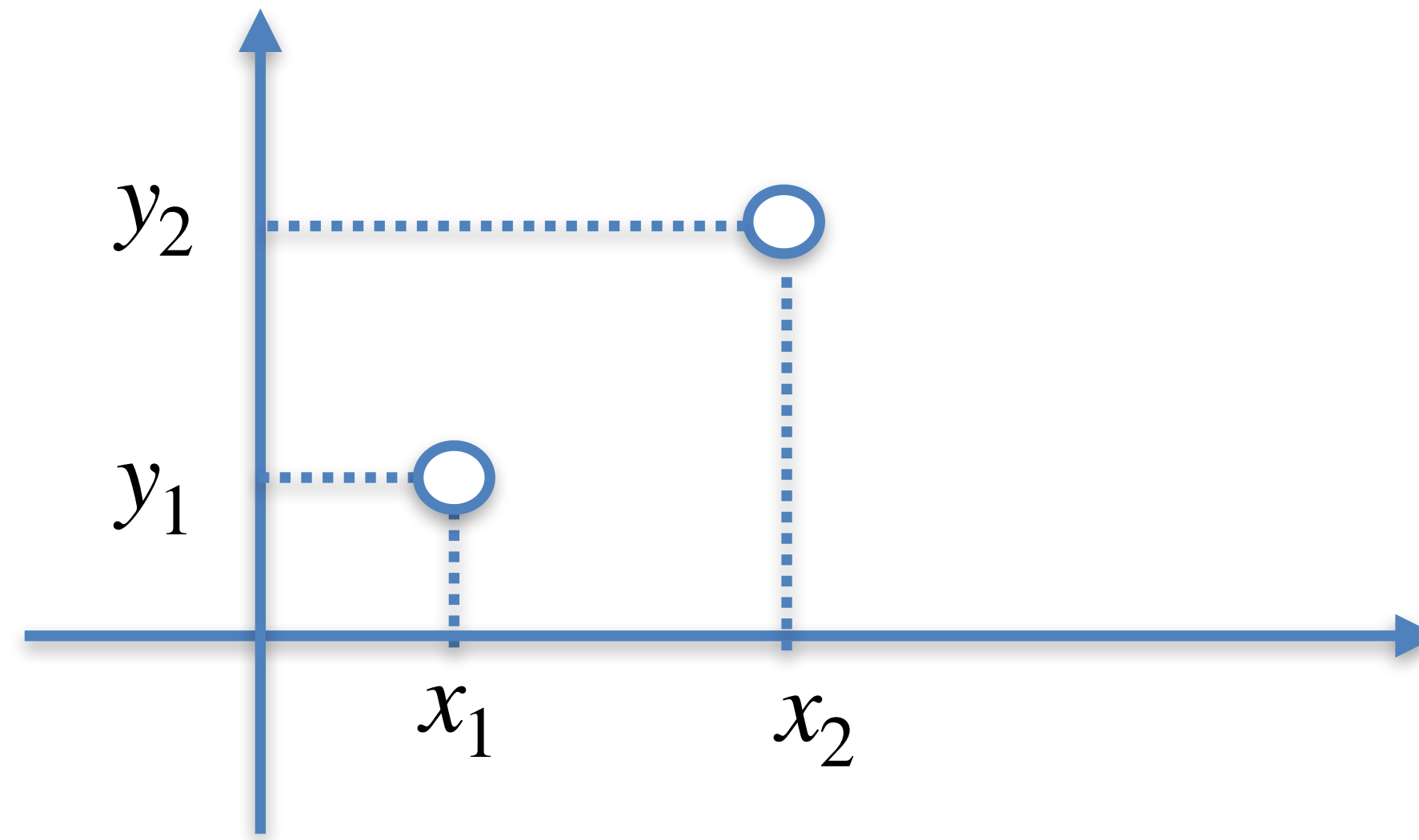
Interpolation

Imagine that we are given these two points



Interpolation

Imagine that we are given these two points



We would add another point, between x_1 and x_3 , thus interpolating

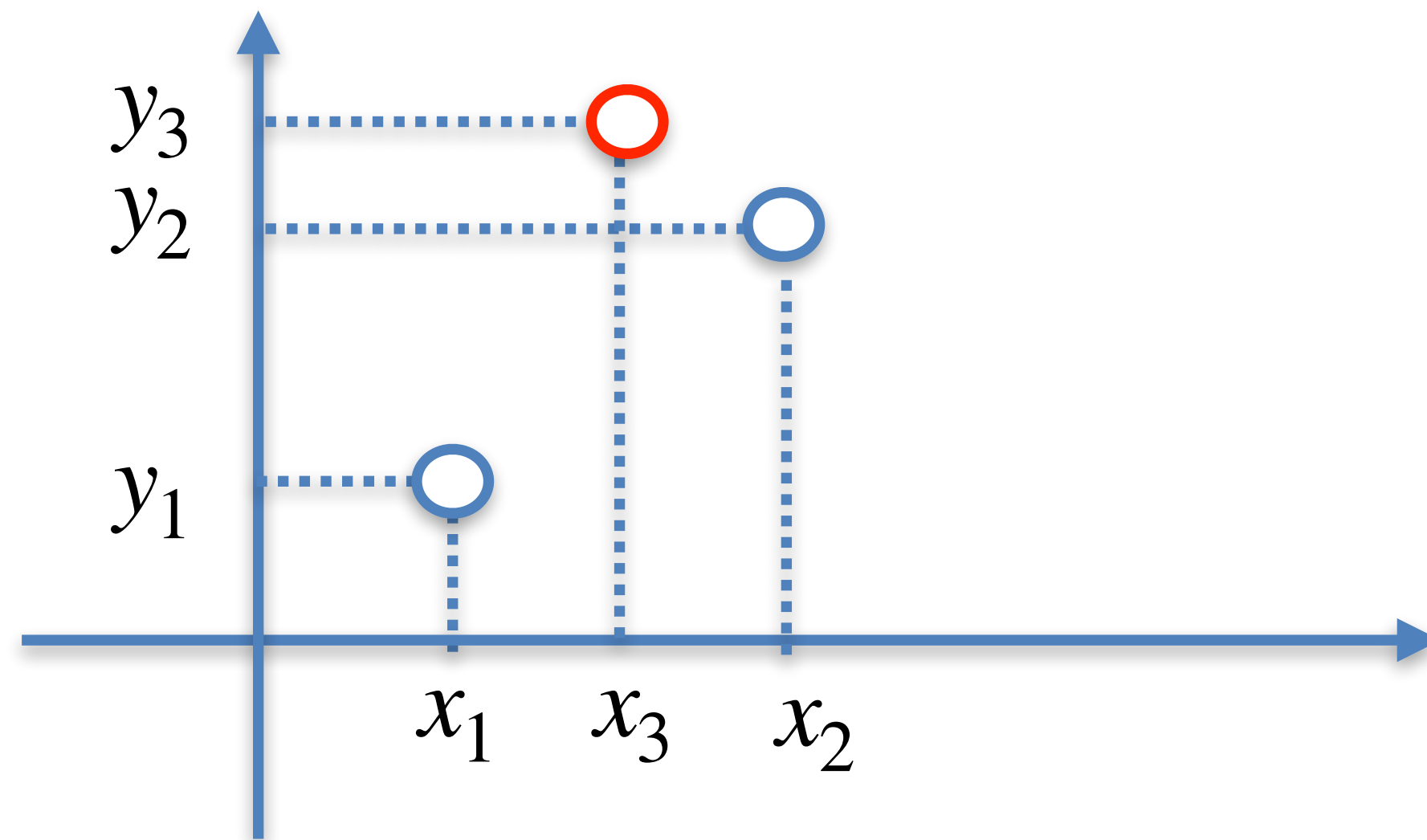
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The goal is to find y_3 (in interpolation x_3 is in the middle between the other two points)



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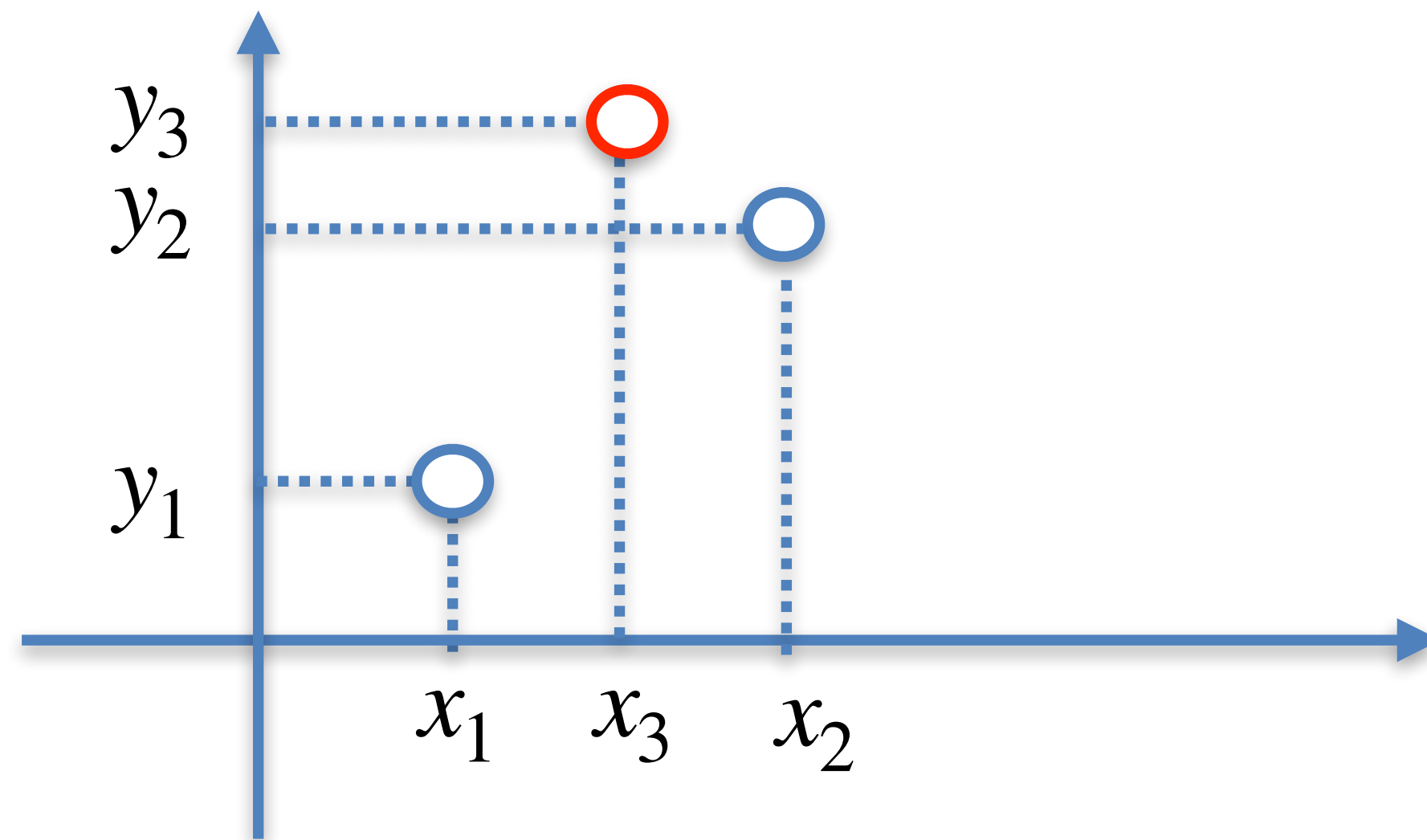


Is it here?

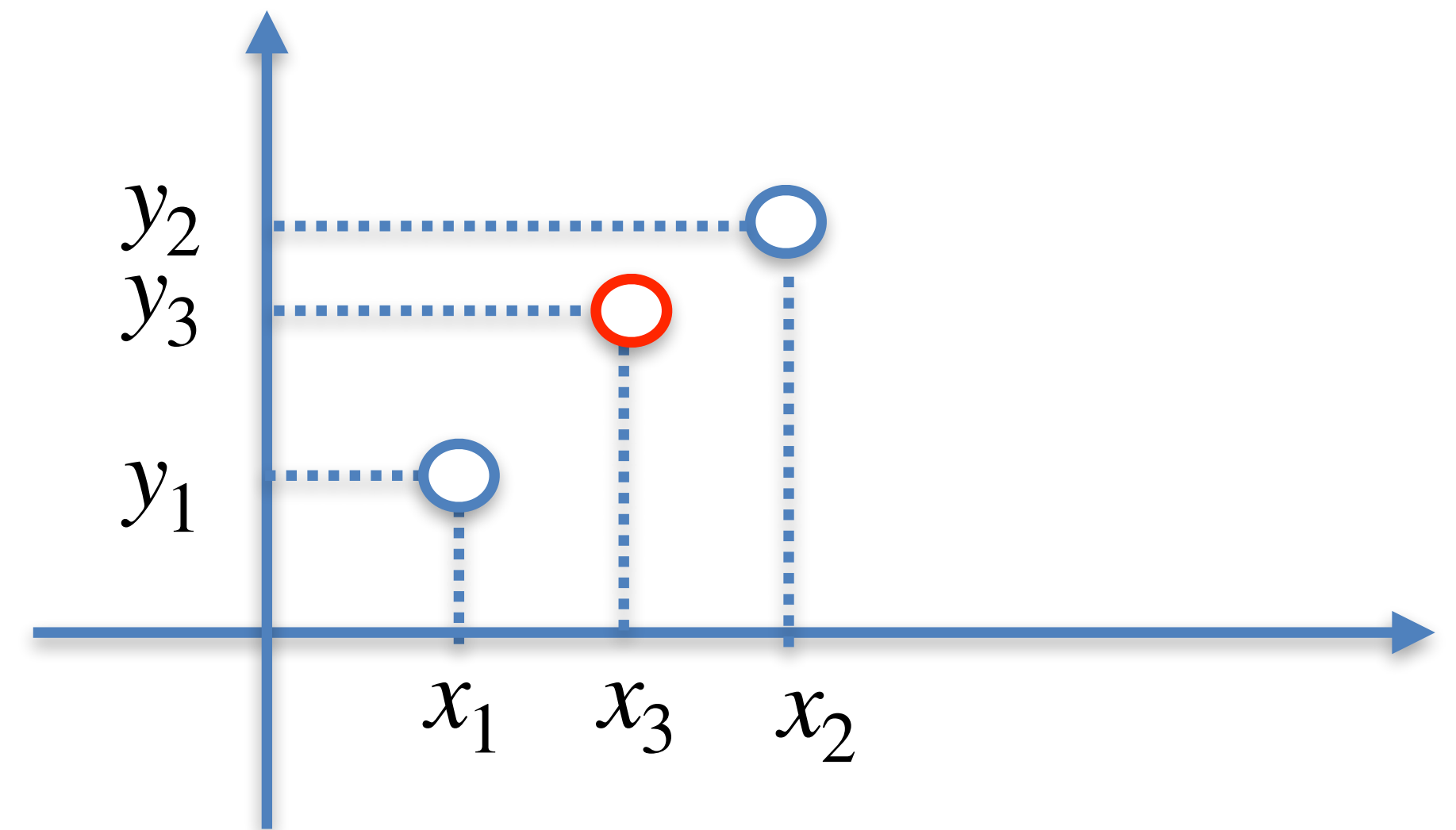


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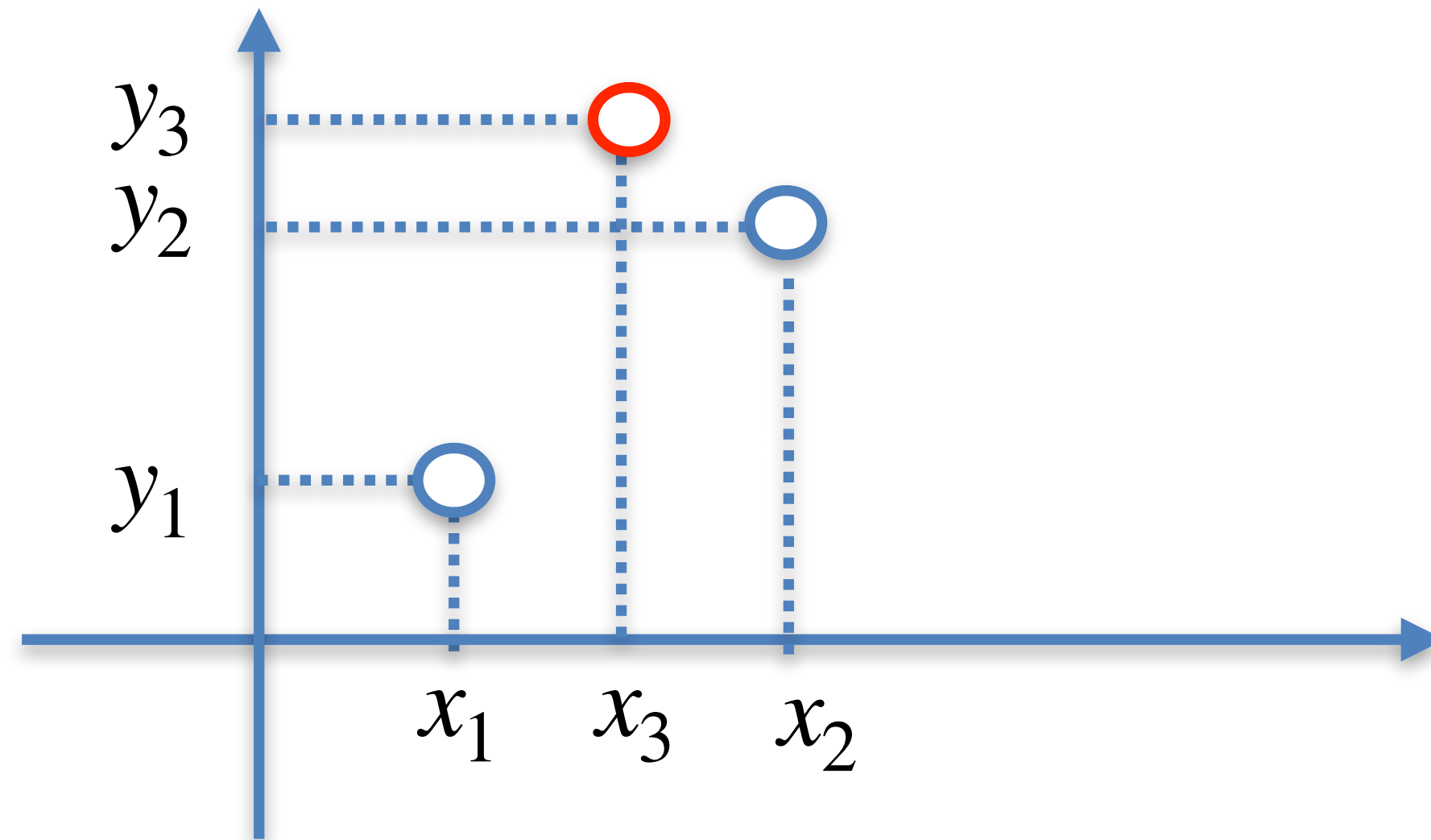


Or here?

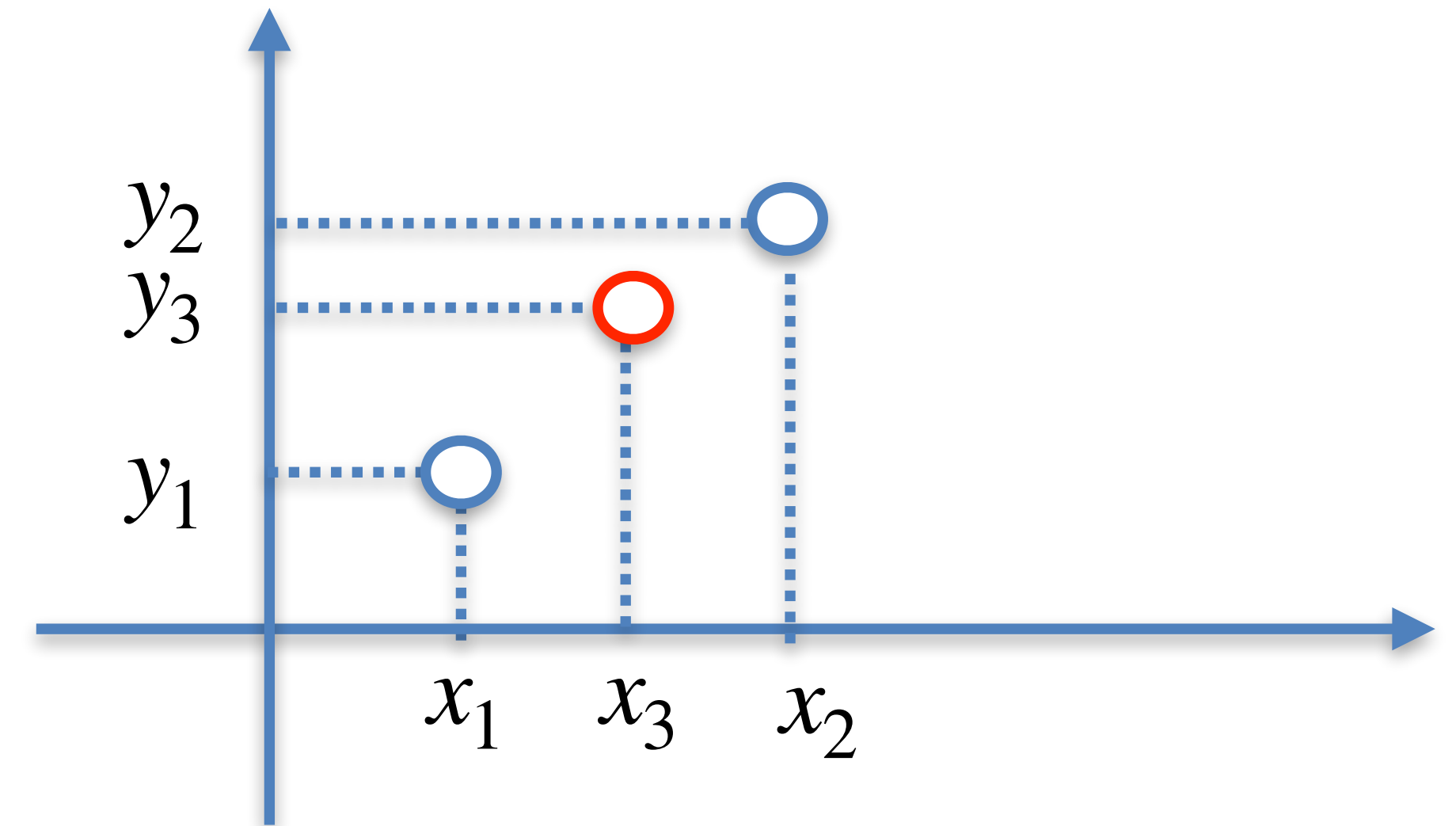


Interpolation

The goal is to find y_3 (in interpolation x_3 is in the middle between the other two points)



Is it here?



Or here?

Hence, $y_3 = ?$



Interpolation

We can now see how using the incidence matrix and minimising E might help



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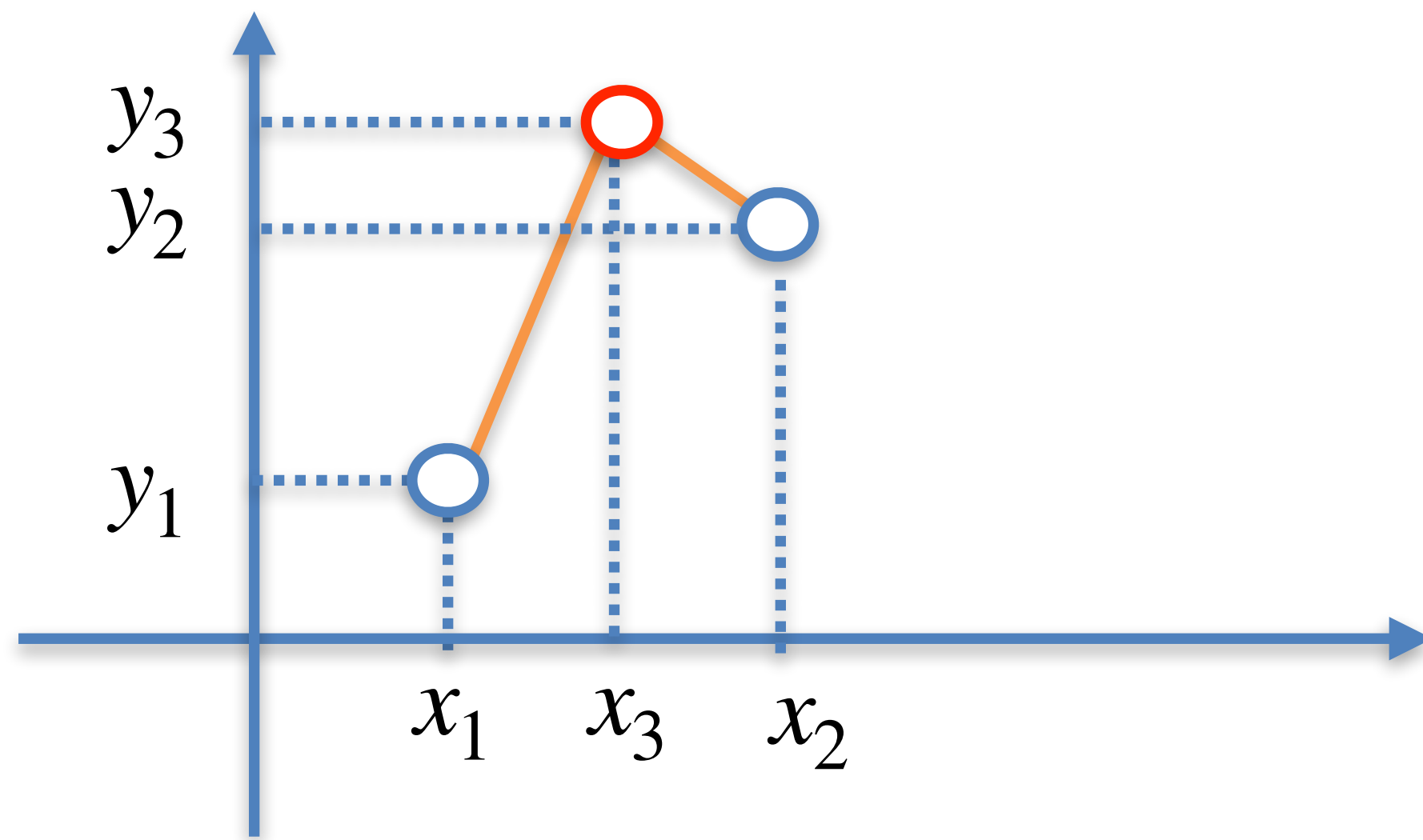
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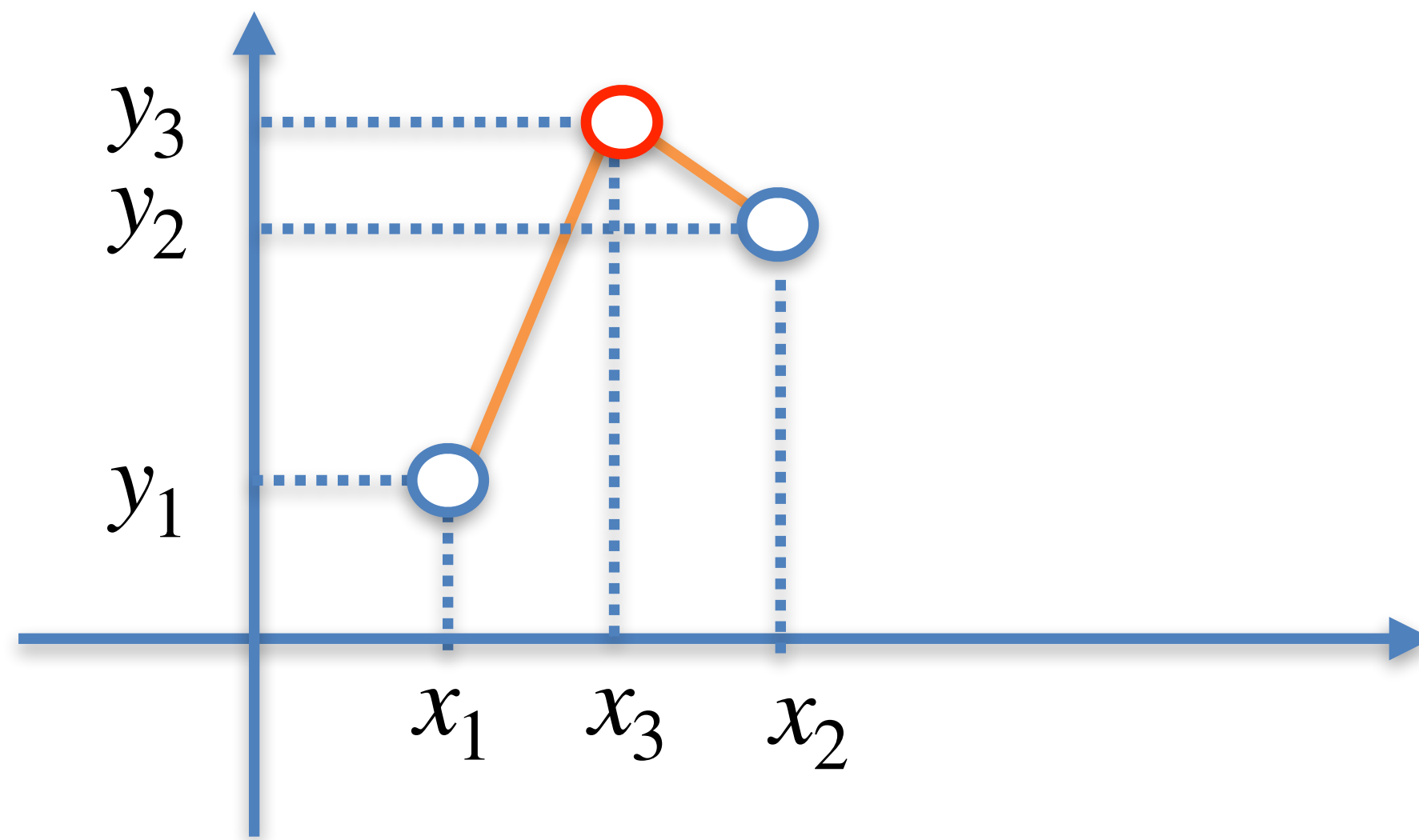
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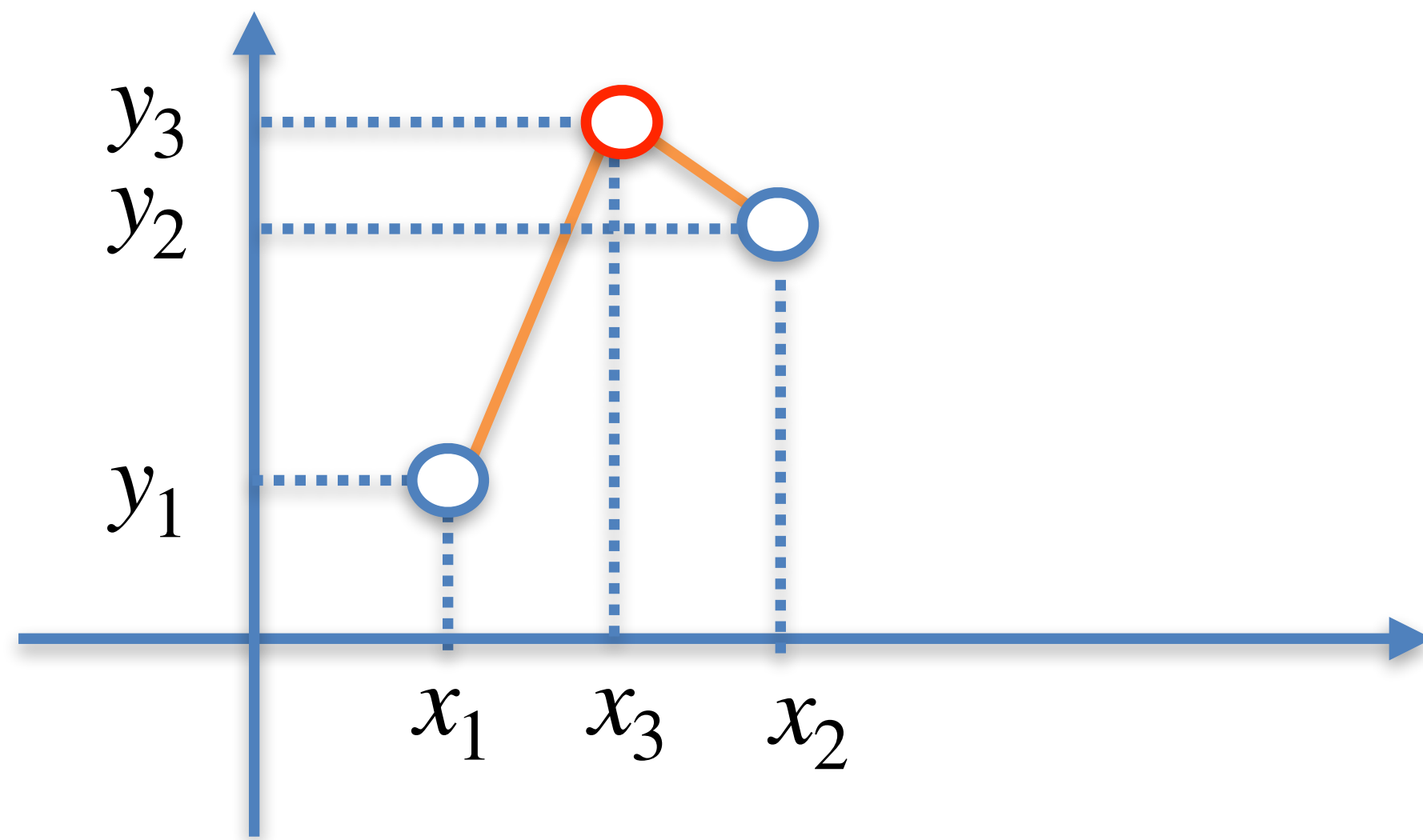


$$M_{\frac{1}{h}} = \frac{1}{h} \begin{pmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix}$$

Interpolation

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What is the incidence matrix here?



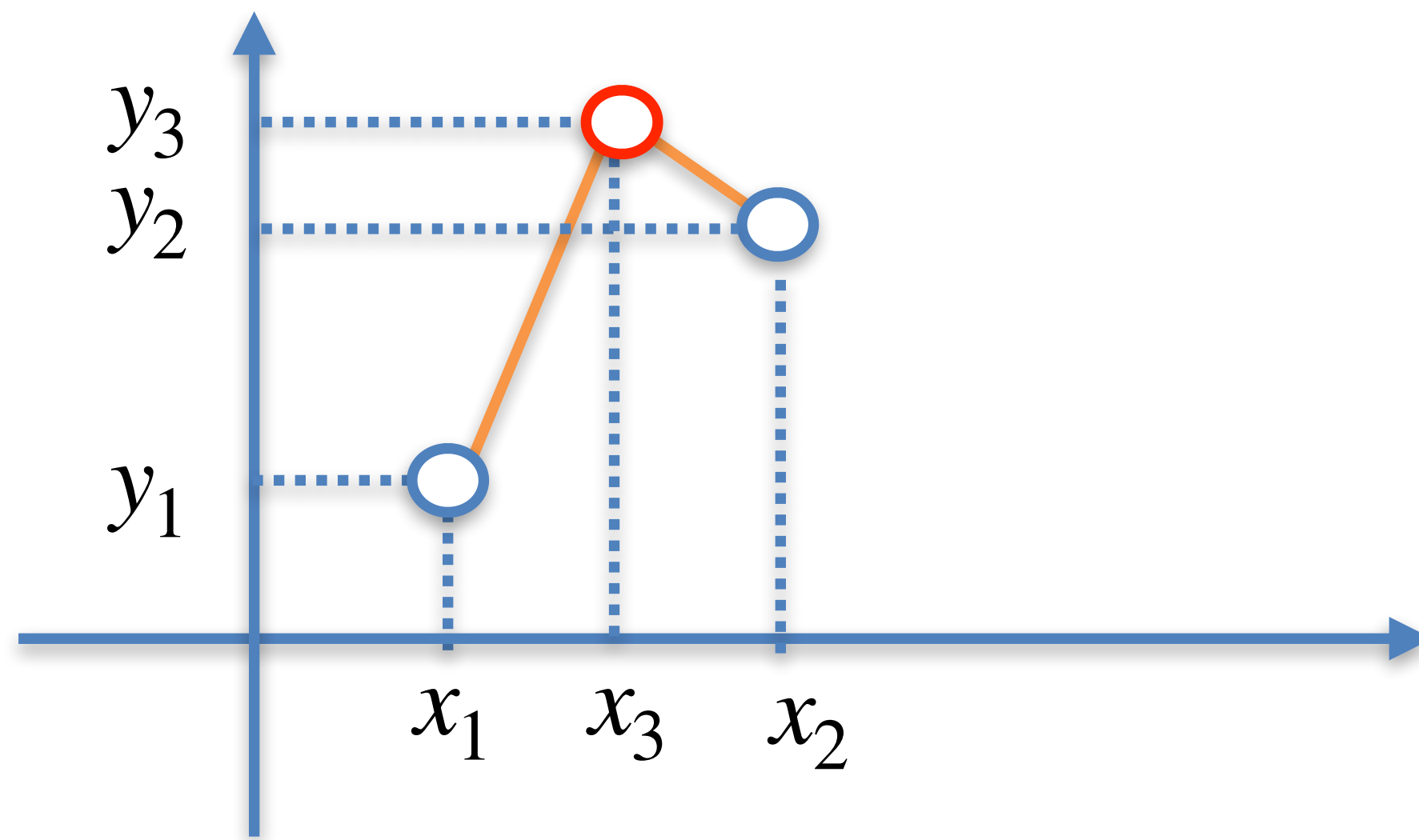
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What is the incidence matrix here?



What is \mathbf{y} ?

$$M_{\frac{1}{h}} = \frac{1}{h} \begin{pmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix}$$

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_3 \\ y_2 \end{pmatrix}$$

Interpolation

Given

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Interpolation

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Interpolation

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Hence, the proposed energy function becomes



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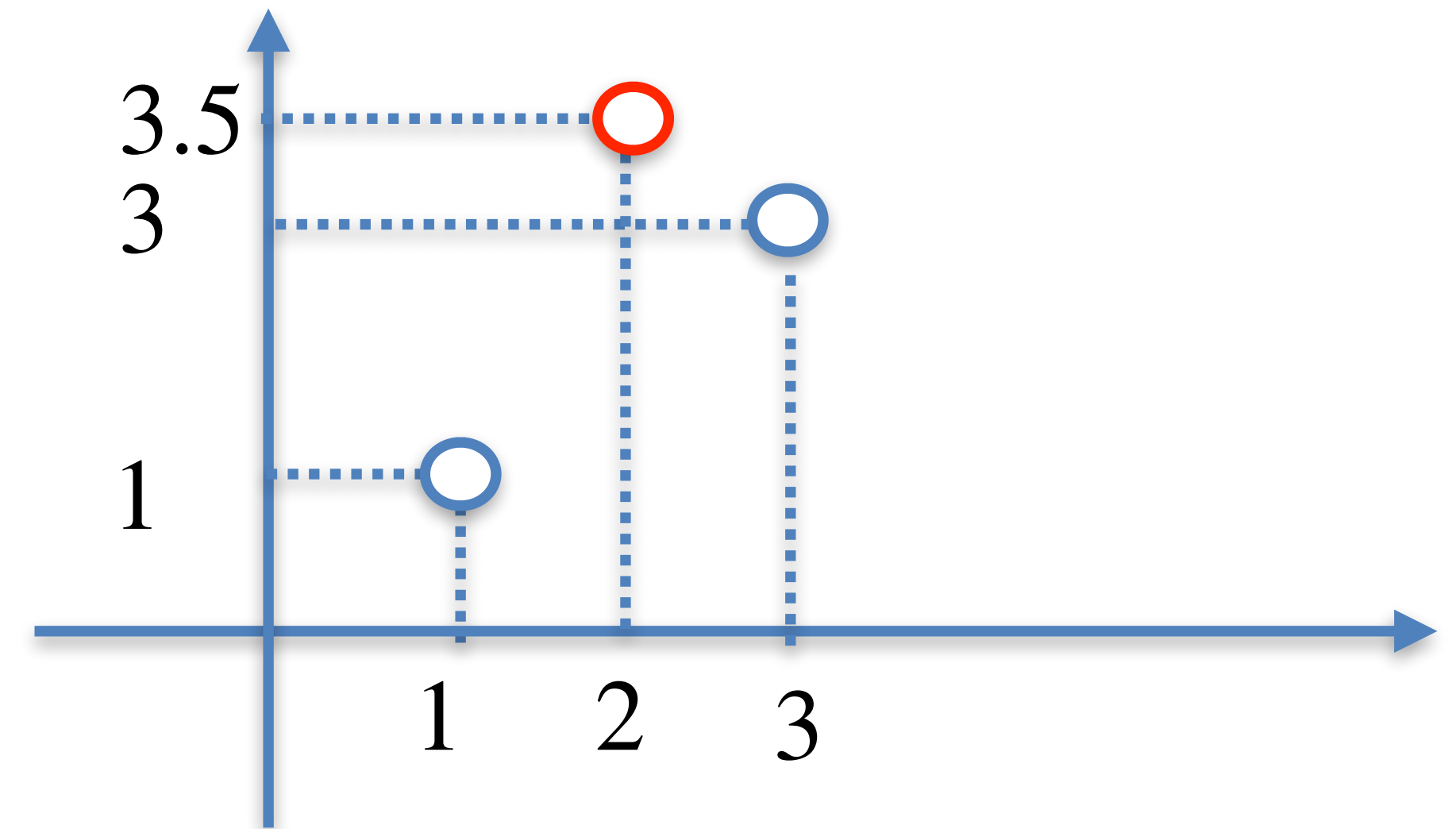
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Hence, the proposed energy function becomes

$$E(\mathbf{y}) = \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{y} \right\|^2 = \frac{1}{h^2} \left[(y_3 - y_1)^2 + (y_2 - y_3)^2 \right]$$

Interpolation

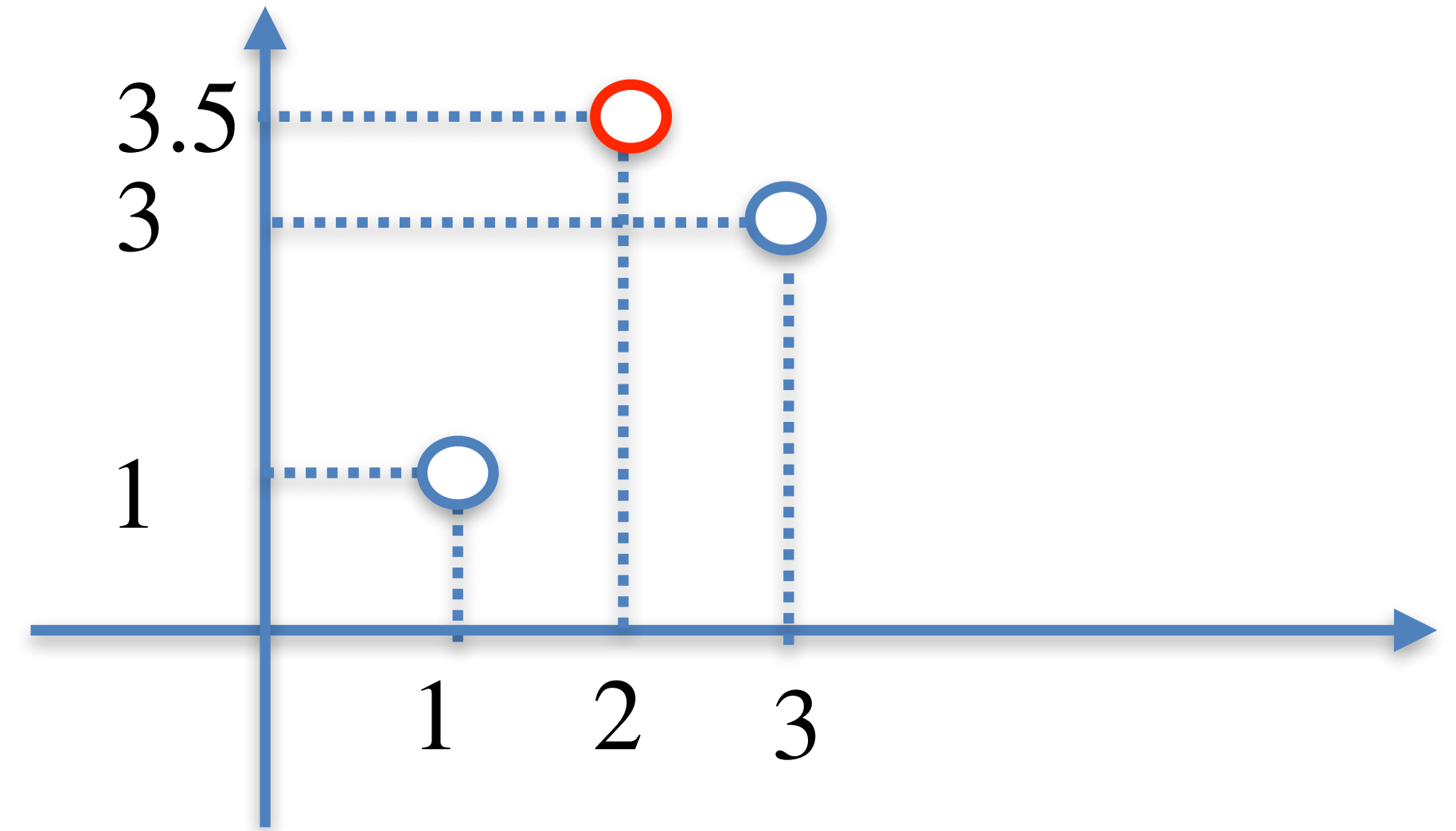
Let's put some numbers considering this scenario



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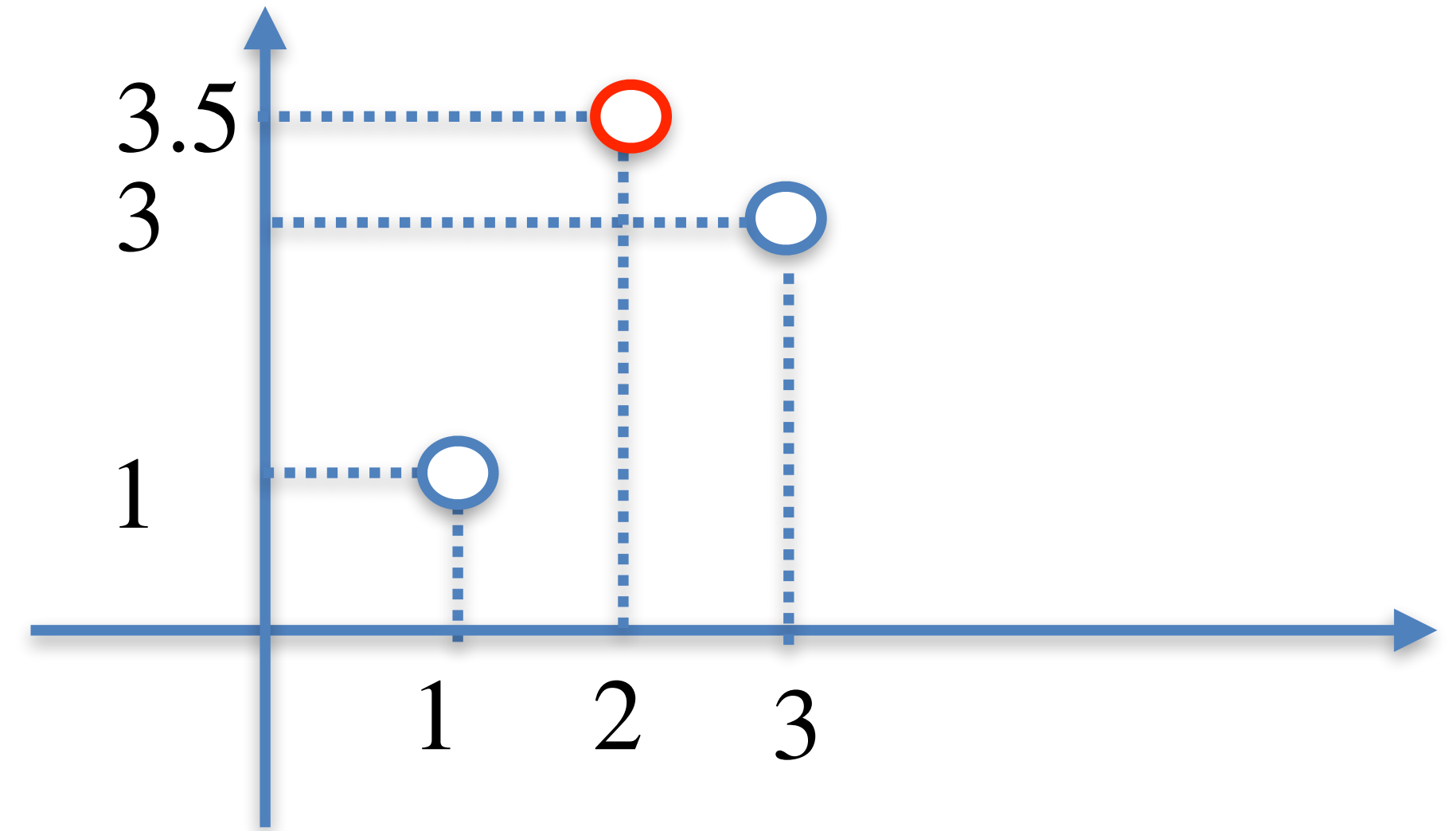


Interpolation

Let's put some numbers considering this scenario

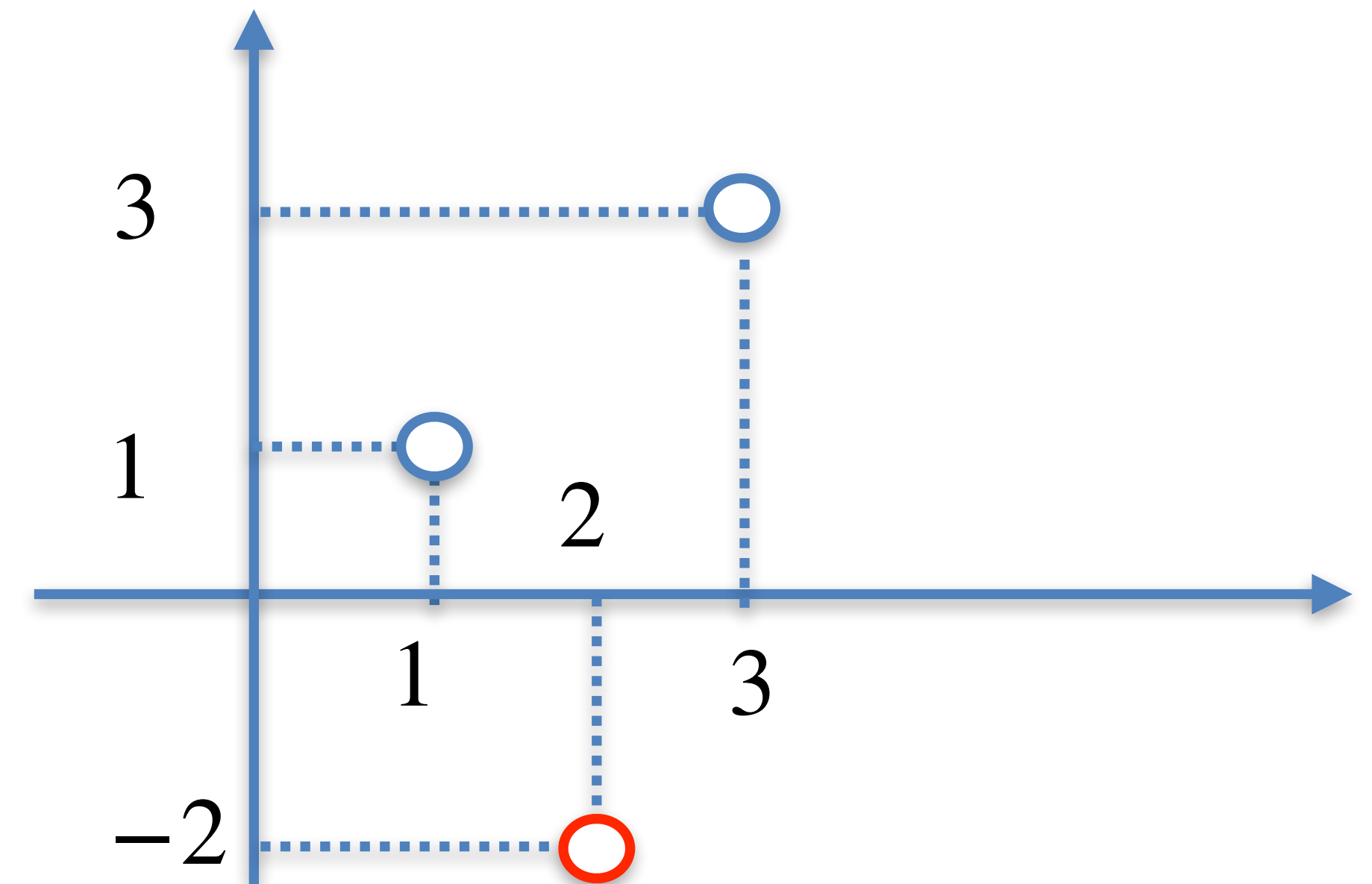
$$E(\mathbf{y}) = \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{y} \right\|^2 = \frac{1}{h^2} [(y_3 - y_1)^2 + (y_2 - y_3)^2]$$

$$E(\mathbf{y}) = \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{y} \right\|^2 \sim \frac{25}{4} + \frac{1}{4} = \frac{13}{2}$$



Interpolation

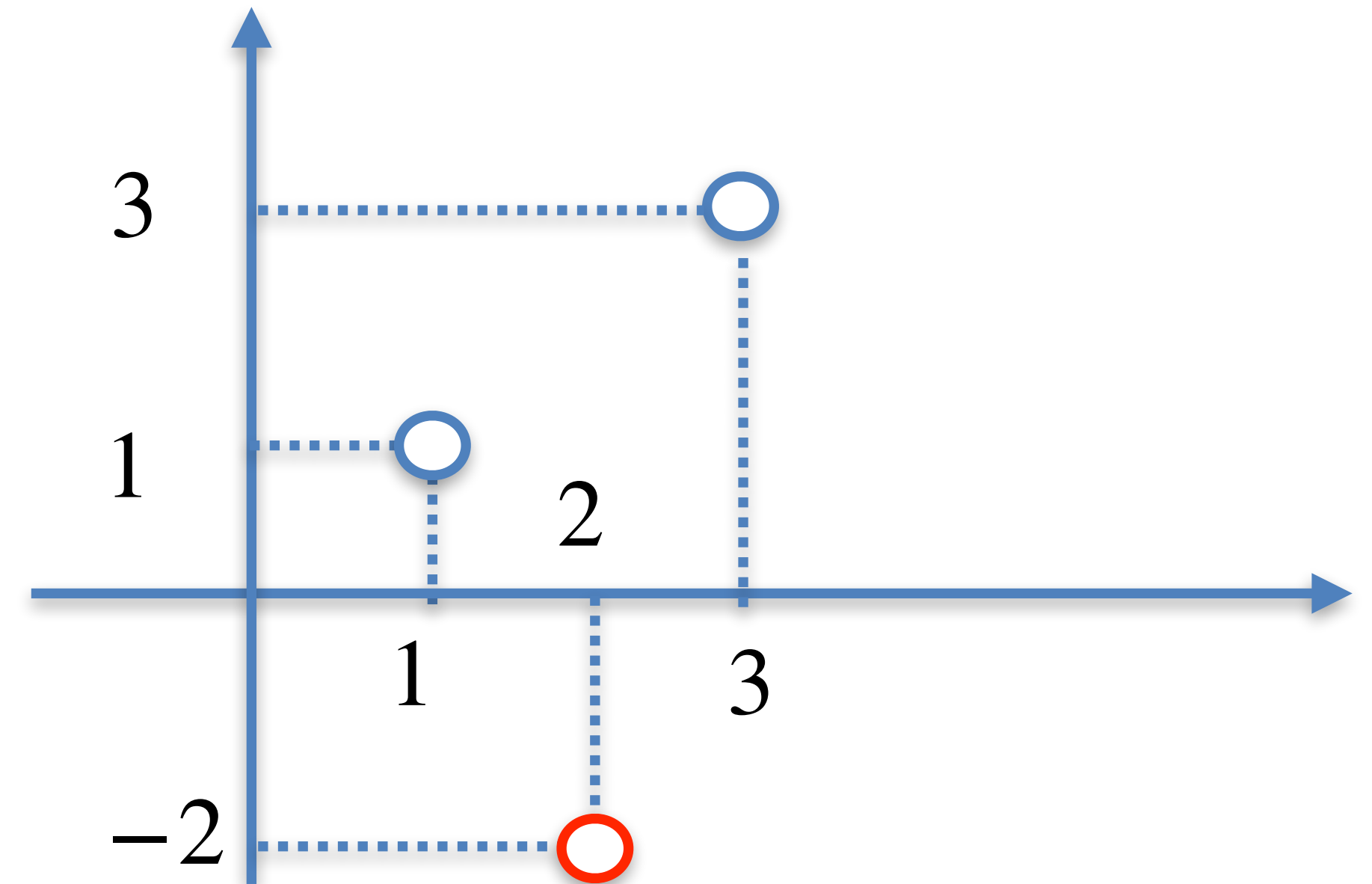
Let's put some numbers in this other scenario



Interpolation

Let's put some numbers in this other scenario

$$E(\mathbf{y}) = \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{y} \right\|^2 = \frac{1}{h^2} \left[(y_3 - y_1)^2 + (y_2 - y_3)^2 \right]$$

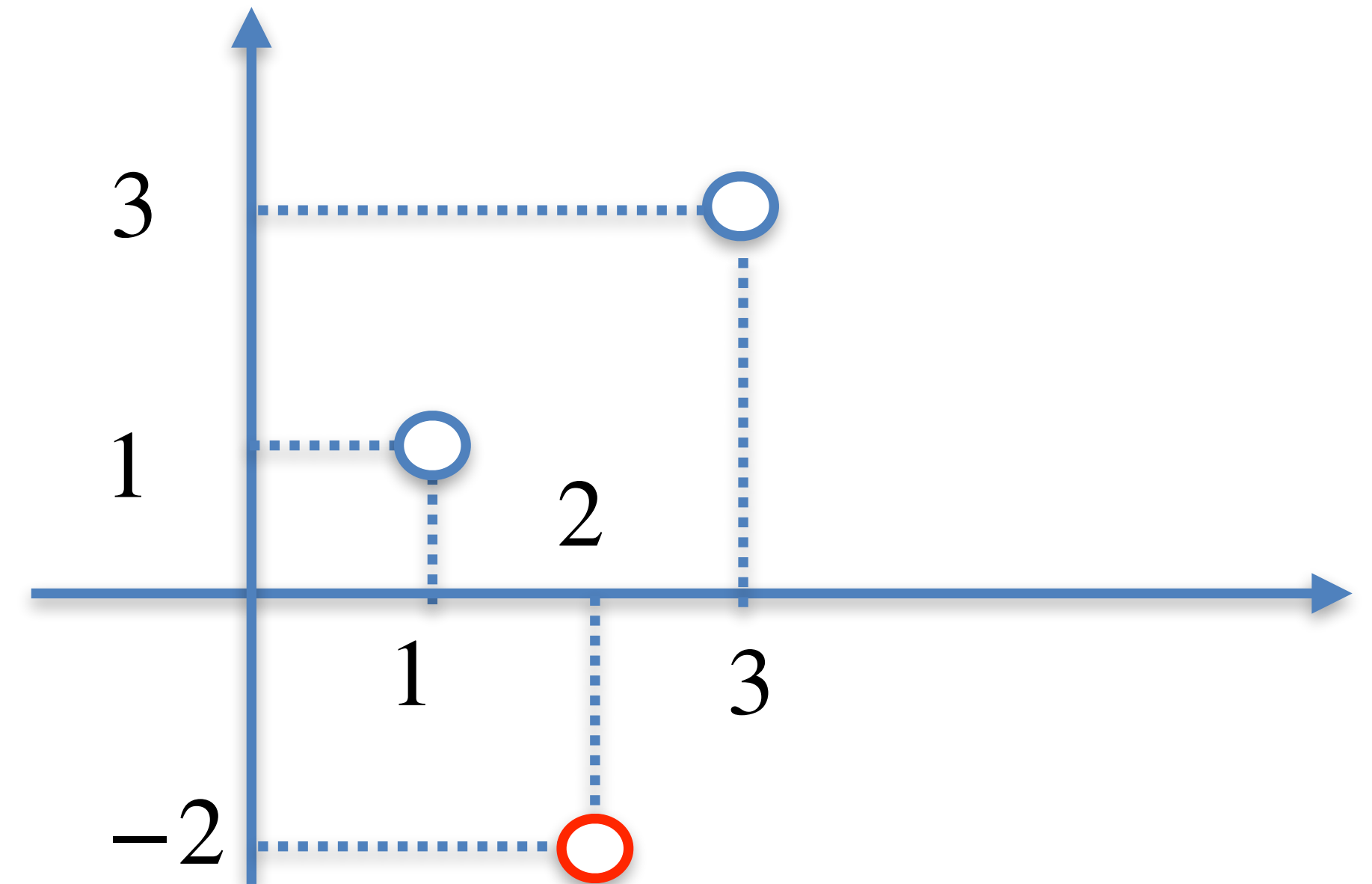


Interpolation

Let's put some numbers in this other scenario

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$$E(\mathbf{y}) = \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{y} \right\|^2 \sim 9 + 25 = 34$$

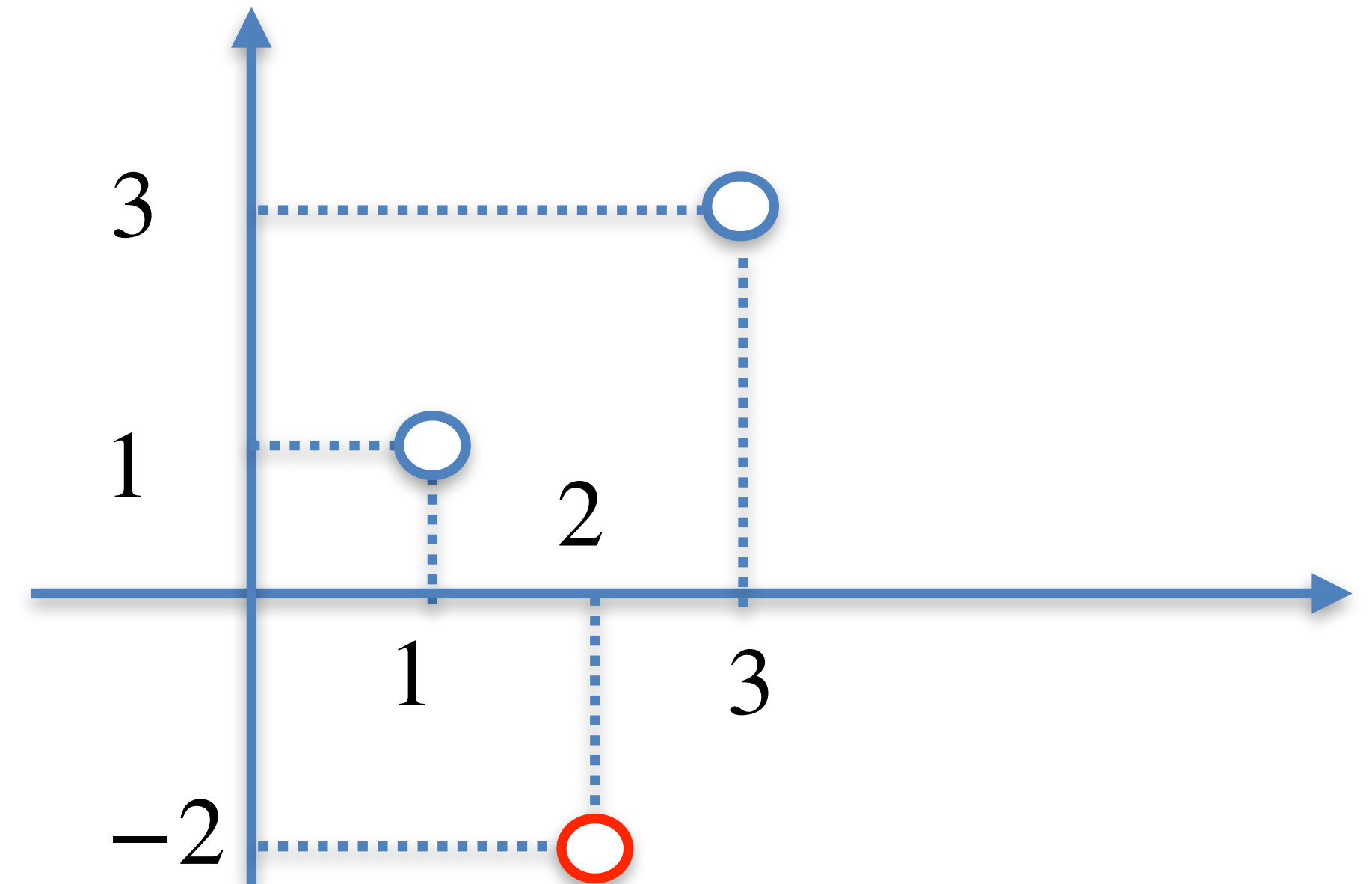


Interpolation

Let's put some numbers in this other scenario

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$$E(\mathbf{y}) = \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{y} \right\|^2 \sim 9 + 25 = 34$$



What is the minimum value?



Interpolation

The min can be found getting the derivative and setting to zero!



Interpolation

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Interpolation

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$$\nabla E(\mathbf{y}_3) = 2(y_3 - y_1) - 2(y_3 - y_2) = 0$$



Interpolation

The min can be found getting the derivative and setting to zero!

$$E(\mathbf{y}) = \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{y} \right\|^2 = \frac{1}{h^2} [(y_3 - y_1)^2 + (y_2 - y_3)^2]$$

$$\nabla E(\mathbf{y}_3) = 2(y_3 - y_1) - 2(y_3 - y_2) = 0$$

$$y_3 = \frac{y_1 + y_2}{2}$$



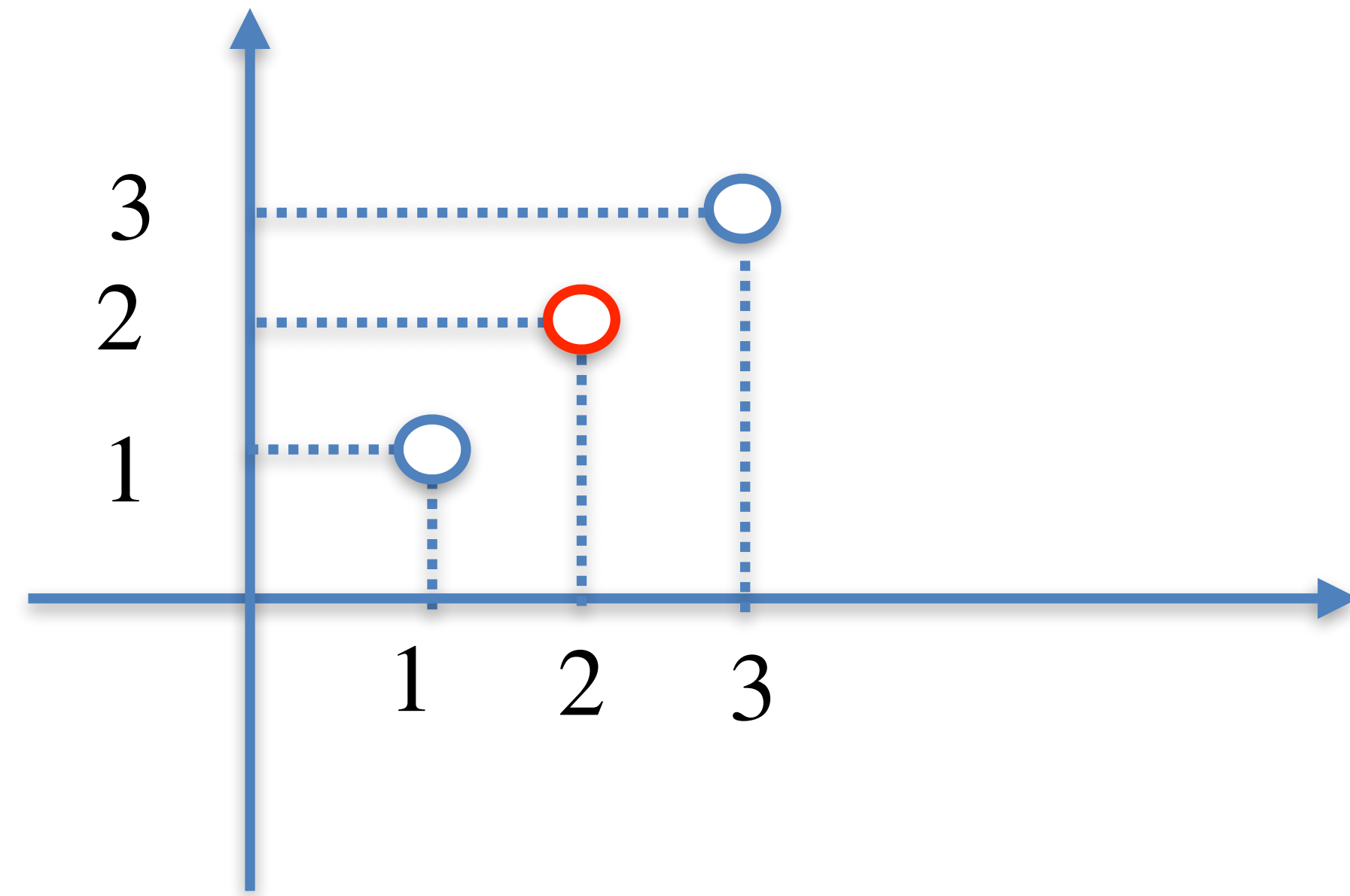
Interpolation

The min can be found getting the derivative and setting to zero!

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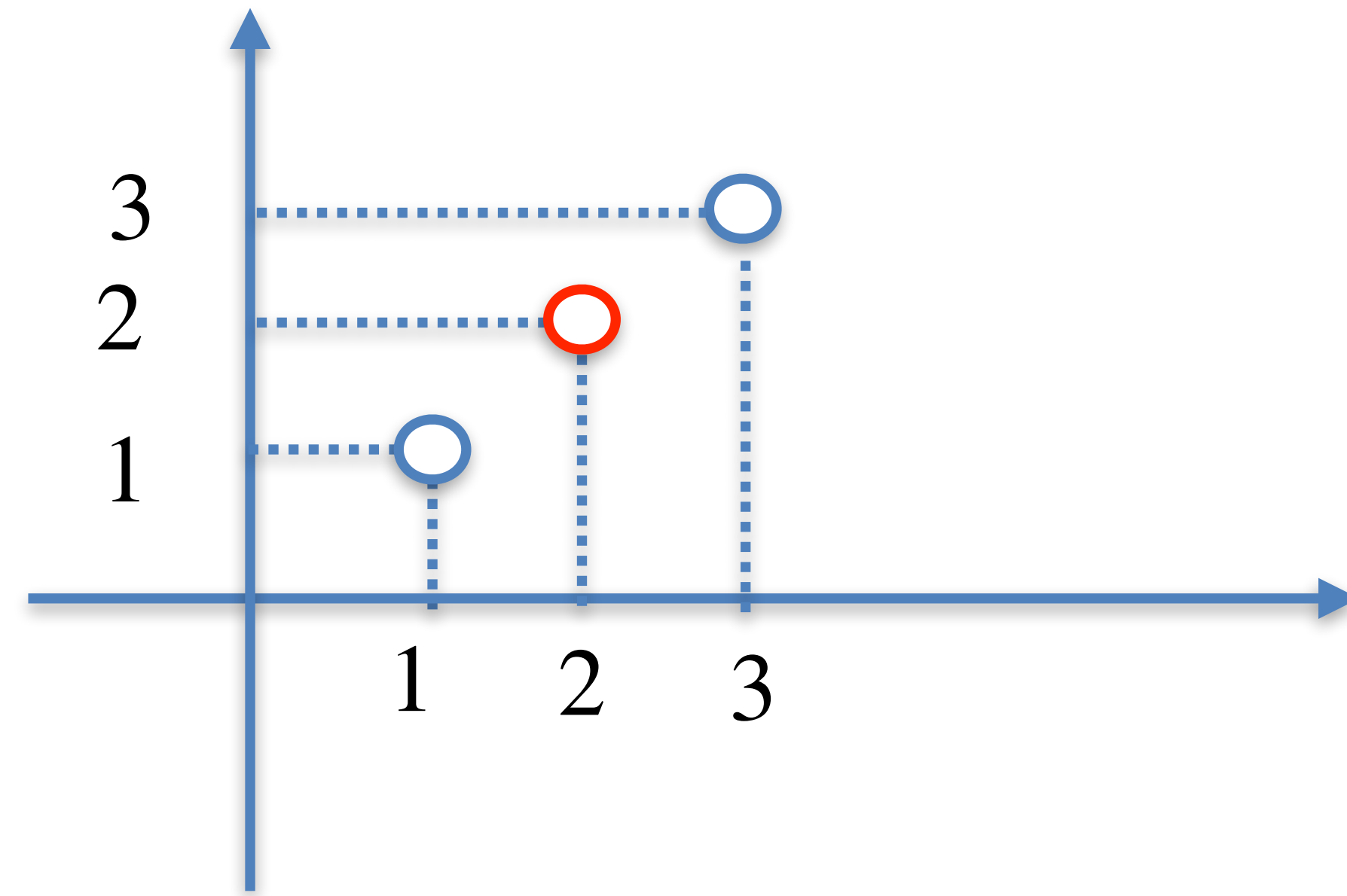
Interpolation

The min can be found getting the derivative and setting to zero!

$$E(\mathbf{y}) = \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{y} \right\|^2 = \frac{1}{h^2} [(y_3 - y_1)^2 + (y_2 - y_3)^2]$$

$$\nabla E(\mathbf{y}_3) = 2(y_3 - y_1) - 2(y_3 - y_2) = 0$$

$$y_3 = \frac{y_1 + y_2}{2}$$



The min is, not surprisingly, the point laying in the middle between the two! This is why it is called interpolation!

Interpolation

So, it looks like that this energy function does the job!

$$E(\mathbf{y}) = \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{y} \right\|^2 \quad \text{with} \quad \mathbf{M}_{\frac{1}{h}} = \frac{1}{h} \begin{pmatrix} -1 & 1 & 0 & \dots & 0 & 0 \\ 0 & -1 & 1 & \dots & 0 & 0 \\ \vdots & & \ddots & & & \vdots \\ 0 & 0 & \dots & 0 & -1 & 1 \end{pmatrix},$$



Interpolation

So, it looks like that this energy function does the job!

$$E(\mathbf{y}) = \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{y} \right\|^2 \quad \text{with} \quad \mathbf{M}_{\frac{1}{h}} = \frac{1}{h} \begin{pmatrix} -1 & 1 & 0 & \dots & 0 & 0 \\ 0 & -1 & 1 & \dots & 0 & 0 \\ \vdots & & \ddots & & & \vdots \\ 0 & 0 & \dots & 0 & -1 & 1 \end{pmatrix},$$

How can we use this to solve the problem in general?



Interpolation

We can write $\mathbf{y} = \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \underbrace{\mathbf{P}_{I_2} \mathbf{v}}_{= \text{known}}$.



Interpolation

We can write $\mathbf{y} = \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \underbrace{\mathbf{P}_{I_2} \mathbf{v}}_{= \text{known}}$.

Thus we split the vector \mathbf{y} in two parts, the first of unknown the second of known



Interpolation

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Thus we split the vector \mathbf{y} in two parts, the first of unknown the second of known

The two \mathbf{P} are projectors



Interpolation

Consider a simple case where we have only 2 known y s out of 5



Interpolation

Consider a simple case where we have only 2 known y s out of 5

$$\mathbf{y} = \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v}$$

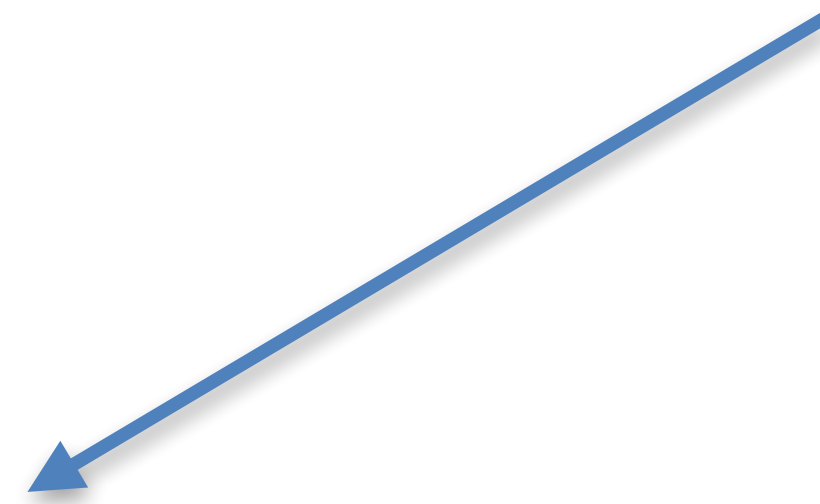


Interpolation

Consider a simple case where we have only 2 known ys out of 5

$$\mathbf{y} = \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v}$$

$$\begin{pmatrix} y_1 \\ y_2 \\ ? \\ ? \\ ? \end{pmatrix}$$



Interpolation

Consider a simple case where we have only 2 known ys out of 5

$$\mathbf{y} = \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v}$$

The diagram illustrates the decomposition of the vector equation. Two blue arrows point from the terms in the equation to their respective matrix representations:

- The left arrow points from $\mathbf{P}_{I_1 \setminus I_2}$ to the matrix $\begin{pmatrix} y_1 \\ y_2 \\ ? \\ ? \\ ? \end{pmatrix}$.
- The right arrow points from \mathbf{P}_{I_2} to the matrix $\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$.

The resulting equation is:

$$\begin{pmatrix} y_1 \\ y_2 \\ ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Interpolation

Consider a simple case where we have only 2 known ys out of 5

$$\mathbf{y} = \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v}$$
$$\begin{pmatrix} y_1 \\ y_2 \\ ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} ? \\ ? \\ ? \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ ? \\ ? \\ ? \end{pmatrix}$$
$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Interpolation

Consider a simple case where we have only 2 known ys out of 5

$$\mathbf{y} = \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v}$$
$$\begin{pmatrix} y_1 \\ y_2 \\ ? \\ ? \\ ? \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ ? \\ ? \\ ? \end{pmatrix}$$
$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$
$$\mathbf{w} \in \mathbb{R}^3 \rightarrow \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} \in \mathbb{R}^6$$

Interpolation

Consider a simple case where we have only 2 known ys out of 5

$$\mathbf{y} = \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v}$$
$$\begin{pmatrix} y_1 \\ y_2 \\ ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} ? \\ ? \\ ? \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$
$$\mathbf{w} \in \mathbb{R}^3 \rightarrow \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} \in \mathbb{R}^6 \qquad \mathbf{v} \in \mathbb{R}^2 \rightarrow \mathbf{P}_{I_2} \mathbf{v} \in \mathbb{R}^6$$

Interpolation

Now, from $\mathbf{y} = \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \underbrace{\mathbf{P}_{I_2} \mathbf{v}}_{= \text{known}}$.



Interpolation

Now, from $\mathbf{y} = \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \underbrace{\mathbf{P}_{I_2} \mathbf{v}}_{= \text{known}}$.

The missing indices can be computed via

$$\min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \left(\mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v} \right) \right\|^2$$



Interpolation

$$\min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \left(\mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v} \right) \right\|^2$$



Interpolation

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This is a least-squares problem, for which we know the solution. Indeed we can re-write



Interpolation

$$\min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \left(\mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v} \right) \right\|^2$$

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$$\min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \left(\mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v} \right) \right\|^2 = \min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{M}_{\frac{1}{h}} \mathbf{P}_{I_2} \mathbf{v} \right\|^2 = \min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{X} \mathbf{w} + \mathbf{r} \right\|^2$$

Interpolation

$$\min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \left(\mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v} \right) \right\|^2$$

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Matrices are different but the form is the same of the usual MSE (except for the +!!)

Interpolation

The solution is then the normal equation with a minus on the right hand side

$$\min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \left(\mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v} \right) \right\|^2 = \min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{M}_{\frac{1}{h}} \mathbf{P}_{I_2} \mathbf{v} \right\|^2 = \min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{X} \mathbf{w} + \mathbf{r} \right\|^2$$



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$$\min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \left(\mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v} \right) \right\|^2 = \min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{M}_{\frac{1}{h}} \mathbf{P}_{I_2} \mathbf{v} \right\|^2 = \min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{X} \mathbf{w} + \mathbf{r} \right\|^2$$

Normal equation



Interpolation

The solution is then the normal equation with a minus on the right hand side

$$\min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \left(\mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v} \right) \right\|^2 = \min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{M}_{\frac{1}{h}} \mathbf{P}_{I_2} \mathbf{v} \right\|^2 = \min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{X} \mathbf{w} + \mathbf{r} \right\|^2$$

Normal equation

$$\mathbf{X}^\top \mathbf{X} \hat{\mathbf{w}} = -\mathbf{X}^\top \mathbf{r}$$



Interpolation

The solution is then the normal equation with a minus on the right hand side

$$\min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \left(\mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v} \right) \right\|^2 = \min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{M}_{\frac{1}{h}} \mathbf{P}_{I_2} \mathbf{v} \right\|^2 = \min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{X} \mathbf{w} + \mathbf{r} \right\|^2$$

Normal equation

$$\mathbf{X}^\top \mathbf{X} \hat{\mathbf{w}} = -\mathbf{X}^\top \mathbf{r}$$

$$\mathbf{X}^\top \mathbf{X} = \mathbf{P}_{I_1 \setminus I_2}^\top \mathbf{M}_{\frac{1}{h}}^\top \mathbf{M}_{\frac{1}{h}} \mathbf{P}_{I_1 \setminus I_2} = \mathbf{P}_{I_1 \setminus I_2}^\top \mathbf{L}_{\frac{1}{h}} \mathbf{P}_{I_1 \setminus I_2}$$



Interpolation

The solution is then the normal equation with a minus on the right hand side

$$\min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \left(\mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{P}_{I_2} \mathbf{v} \right) \right\|^2 = \min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{M}_{\frac{1}{h}} \mathbf{P}_{I_1 \setminus I_2} \mathbf{w} + \mathbf{M}_{\frac{1}{h}} \mathbf{P}_{I_2} \mathbf{v} \right\|^2 = \min_{\{w_i\}_{i \in I_1 \setminus I_2}} \left\| \mathbf{X} \mathbf{w} + \mathbf{r} \right\|^2$$

Normal equation

$$\mathbf{X}^\top \mathbf{X} \hat{\mathbf{w}} = -\mathbf{X}^\top \mathbf{r}$$

$$\mathbf{X}^\top \mathbf{X} = \mathbf{P}_{I_1 \setminus I_2}^\top \mathbf{M}_{\frac{1}{h}}^\top \mathbf{M}_{\frac{1}{h}} \mathbf{P}_{I_1 \setminus I_2} = \mathbf{P}_{I_1 \setminus I_2}^\top \mathbf{L}_{\frac{1}{h}} \mathbf{P}_{I_1 \setminus I_2}$$

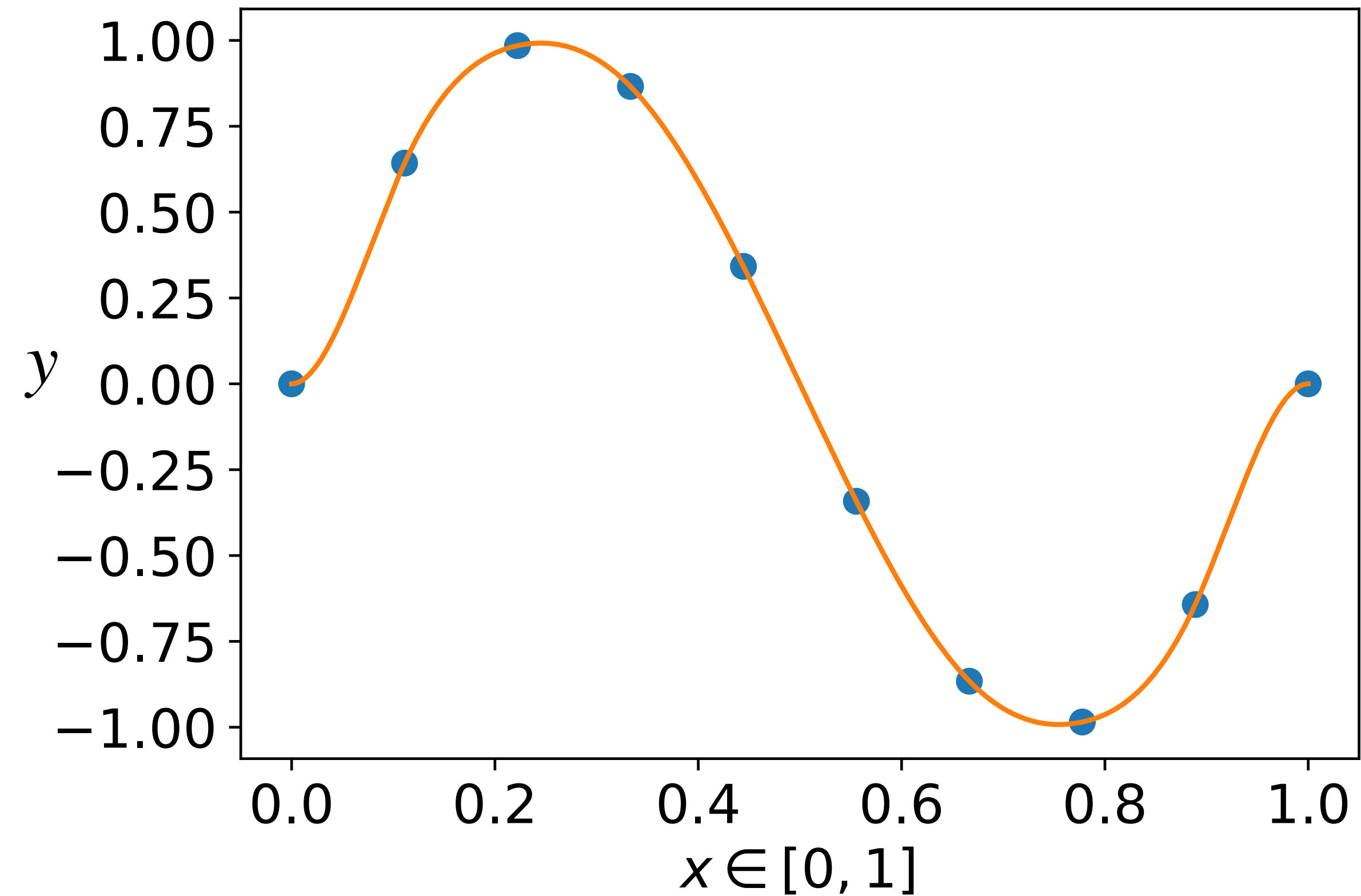
$$\mathbf{P}_{I_1 \setminus I_2}^\top \mathbf{L}_{\frac{1}{h}} \mathbf{P}_{I_1 \setminus I_2} \hat{\mathbf{w}} = \underbrace{-\mathbf{P}_{I_1 \setminus I_2}^\top \mathbf{M}_{\frac{1}{h}}^\top \mathbf{M}_{\frac{1}{h}} \mathbf{P}_{I_2} \mathbf{v}}_{\text{known}} = -\mathbf{P}_{I_1 \setminus I_2}^\top \mathbf{L}_{\frac{1}{h}} \mathbf{P}_{I_2} \mathbf{v},$$

Interpolation

Example

I_1 has 10000 points

I_2 has 10 points



“Training” set is very small, and since we don’t know the ground truth for the others this a semi-supervised problem

Applications

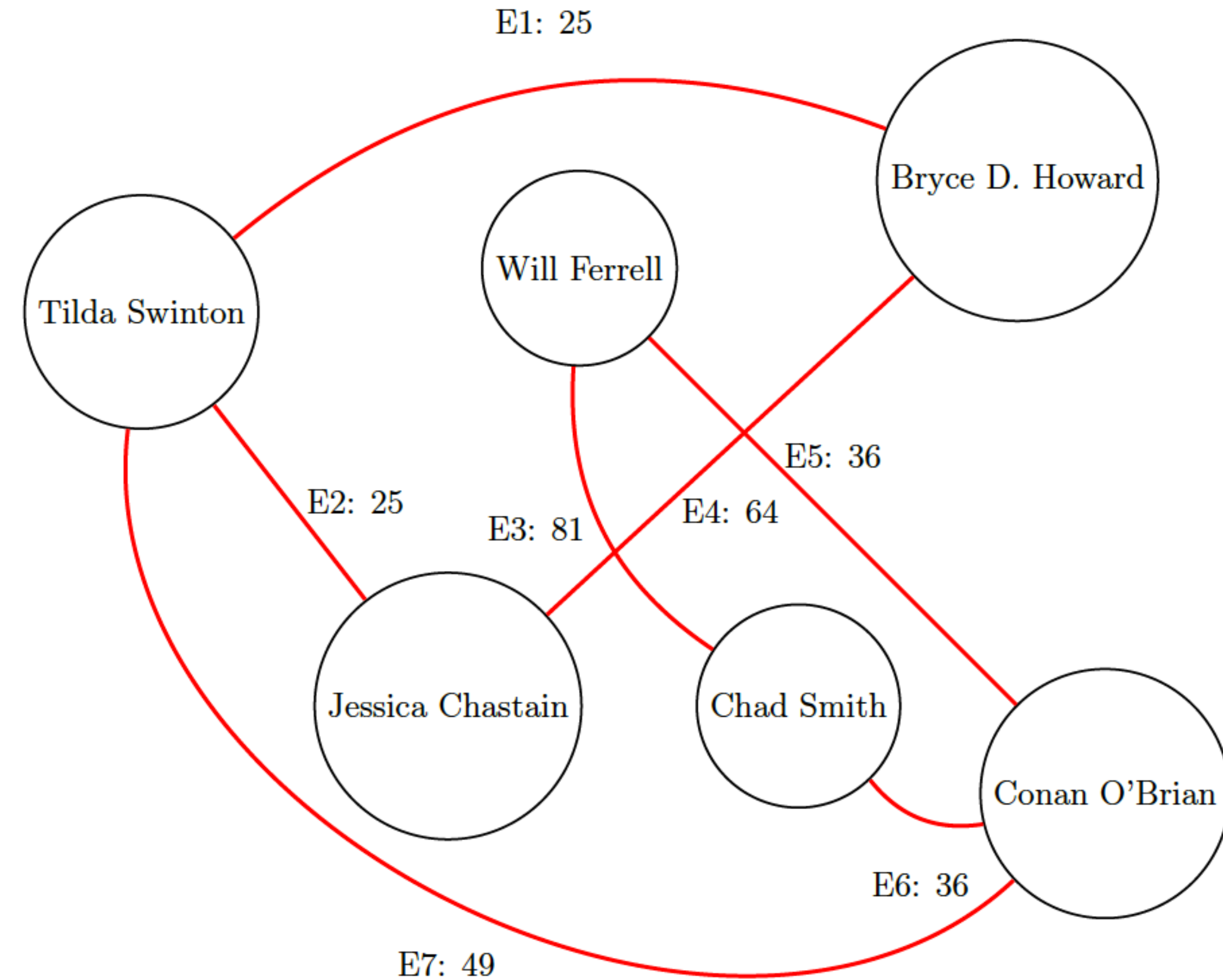
The advantages of using this formulation is that it can be applied to points like we just did, but also to data point for which you can define a similarity



Actors similarity

Incidence matrix

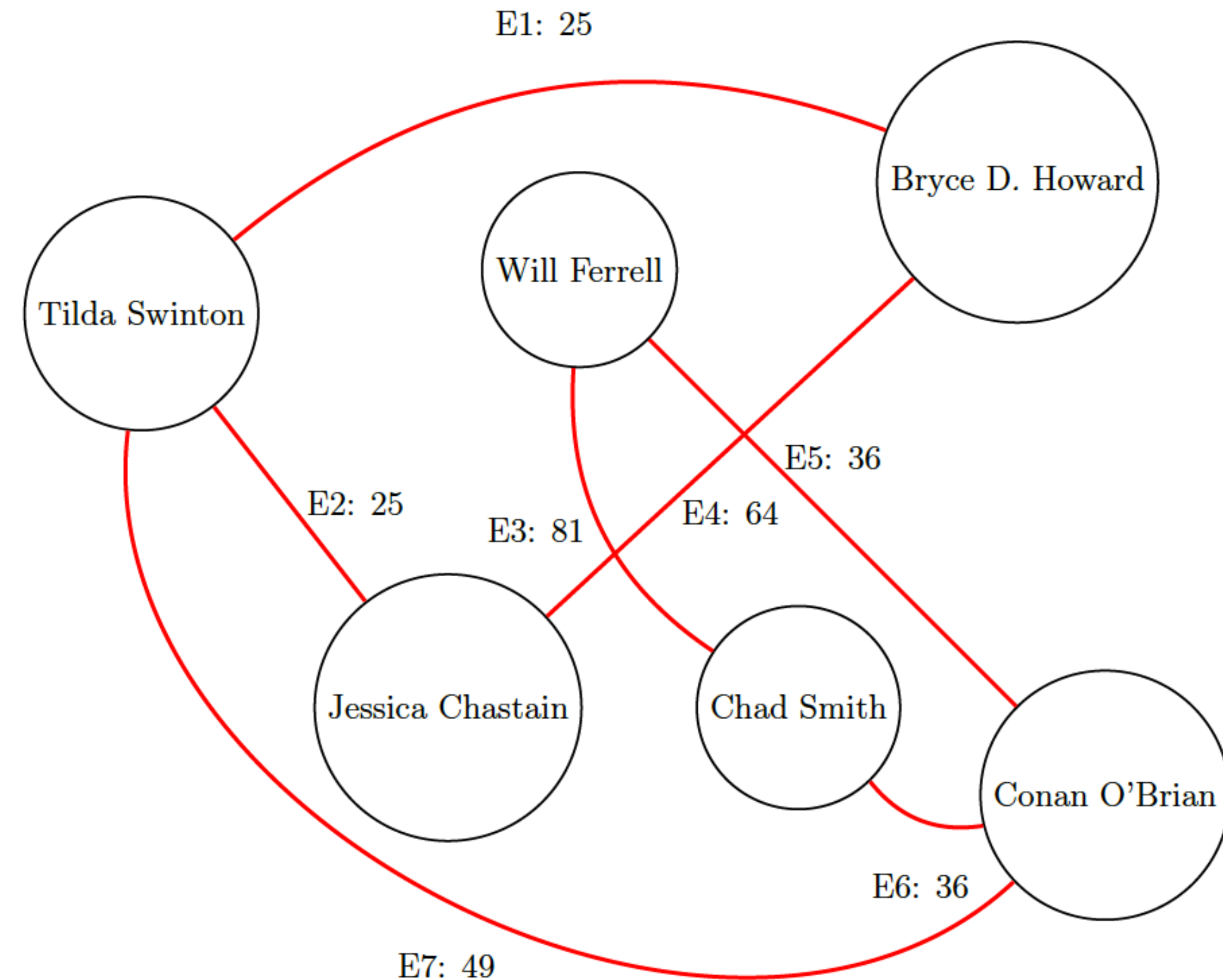
E1	-5	0	0	0	5	0
E2	0	0	0	-5	5	0
E3	0	-9	0	0	0	9
E4	-8	0	0	8	0	0
E5	0	0	-6	0	0	6
E6	0	-6	6	0	0	0
E7	0	0	-7	0	7	0
	B. D. Howard	C. Smith	C. O' Brian	J. Chastain	T. Swinton	W. Ferrell



Actors similarity

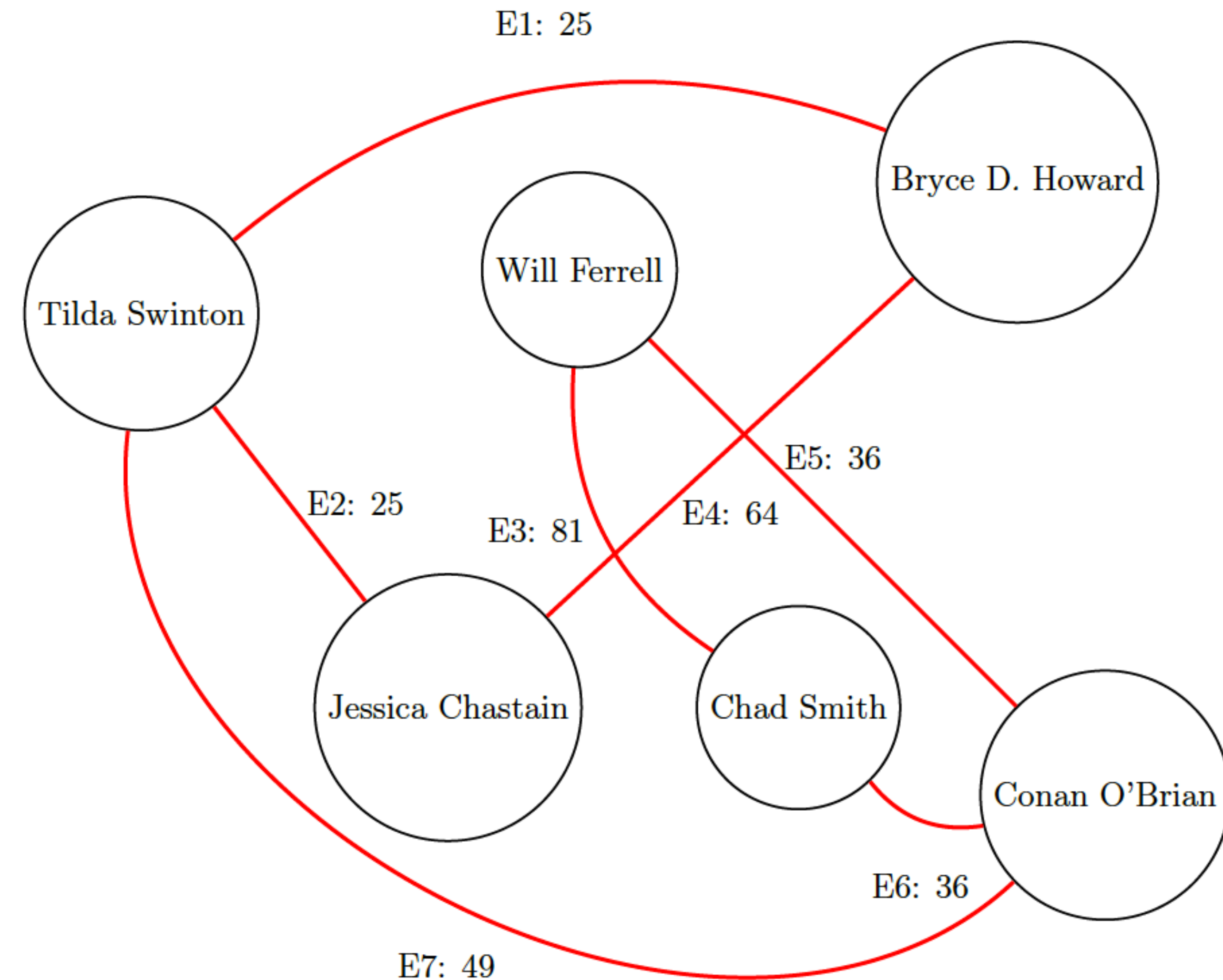
Laplacian matrix

$$L_w = M_w^T M_w = \begin{pmatrix} 89 & 0 & 0 & -64 & -25 & 0 \\ 0 & 117 & -36 & 0 & 0 & -81 \\ 0 & -36 & 121 & 0 & -49 & -36 \\ -64 & 0 & 0 & 89 & -25 & 0 \\ -25 & 0 & -49 & -25 & 99 & 0 \\ 0 & -81 & -36 & 0 & 0 & 117 \end{pmatrix}.$$



Actors similarity

The task is: knowing the biological sex of a small set of actors, and using their similarity, predict the biological sex of the others



Actors similarity

Assume that we know that Jessica Chastain is female (label 1) and Will Ferrel male (label 0)

$$\mathbf{y}_{known} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$



Actors similarity

Assume that we know that Jessica Chastain is female (label 1) and Will Ferrel male (label 0)

$$\mathbf{y}_{known} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\mathbf{P}_{I_1 \setminus I_2}^\top \mathbf{L}_w \mathbf{P}_{I_1 \setminus I_2} \mathbf{y}_{unknown} = - \mathbf{P}_{I_1 \setminus I_2}^\top \mathbf{L}_w \mathbf{P}_{I_2} \mathbf{y}_{known},$$



Actors similarity

Assume that we know that Jessica Chastain is female (label 1) and Will Ferrel male (label 0)

$$\mathbf{y}_{known} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

2x1

$$\mathbf{P}_{I_1 \setminus I_2}^\top \mathbf{L}_w \mathbf{P}_{I_1 \setminus I_2} \mathbf{y}_{unknown} = - \mathbf{P}_{I_1 \setminus I_2}^\top \mathbf{L}_w \mathbf{P}_{I_2} \mathbf{y}_{known},$$



Actors similarity

Assume that we know that Jessica Chastain is female (label 1) and Will Ferrel male (label 0)

$$\mathbf{y}_{known} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

6x2 2x1

$$\mathbf{P}_{I_1 \setminus I_2}^\top \mathbf{L}_w \mathbf{P}_{I_1 \setminus I_2} \mathbf{y}_{unknown} = - \mathbf{P}_{I_1 \setminus I_2}^\top \mathbf{L}_w \mathbf{P}_{I_2} \mathbf{y}_{known},$$



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6x6 6x2 2x1



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4x6 6x6 6x2 2x1



Actors similarity

Assume that we know that Jessica Chastain is female (label 1) and Will Ferrel male (label 0)

$$\mathbf{y}_{known} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\begin{matrix} & 4 \times 1 & & 4 \times 6 & 6 \times 6 & 6 \times 2 & 2 \times 1 \\ \mathbf{P}_{I_1 \setminus I_2}^\top & \mathbf{L}_w & \mathbf{P}_{I_1 \setminus I_2} & \mathbf{y}_{unknown} & = & - \mathbf{P}_{I_1 \setminus I_2}^\top & \mathbf{L}_w & \mathbf{P}_{I_2} & \mathbf{y}_{known}, \end{matrix}$$



Actors similarity

Assume that we know that Jessica Chastain is female (label 1) and Will Ferrel male (label 0)

$$\mathbf{y}_{known} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\begin{matrix} 6 \times 4 & 4 \times 1 & & 4 \times 6 & 6 \times 6 & 6 \times 2 & 2 \times 1 \\ \mathbf{P}_{I_1 \setminus I_2}^\top & \mathbf{L}_w & \mathbf{P}_{I_1 \setminus I_2} & \mathbf{y}_{unknown} & = & - & \mathbf{P}_{I_1 \setminus I_2}^\top & \mathbf{L}_w & \mathbf{P}_{I_2} & \mathbf{y}_{known}, \end{matrix}$$



Actors similarity

Assume that we know that Jessica Chastain is female (label 1) and Will Ferrel male (label 0)

$$\mathbf{y}_{known} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\begin{matrix} 6 \times 6 & 6 \times 4 & 4 \times 1 & & 4 \times 6 & 6 \times 6 & 6 \times 2 & 2 \times 1 \\ \mathbf{P}_{I_1 \setminus I_2}^\top & \mathbf{L}_w & \mathbf{P}_{I_1 \setminus I_2} & \mathbf{y}_{unknown} & = & - & \mathbf{P}_{I_1 \setminus I_2}^\top & \mathbf{L}_w & \mathbf{P}_{I_2} & \mathbf{y}_{known}, \end{matrix}$$



Actors similarity

Assume that we know that Jessica Chastain is female (label 1) and Will Ferrel male (label 0)

$$\mathbf{y}_{known} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\begin{matrix} 4 \times 6 & 6 \times 6 & 6 \times 4 & 4 \times 1 & & 4 \times 6 & 6 \times 6 & 6 \times 2 & 2 \times 1 \\ \mathbf{P}_{I_1 \setminus I_2}^\top & \mathbf{L}_w & \mathbf{P}_{I_1 \setminus I_2} & \mathbf{y}_{unknown} & = & - & \mathbf{P}_{I_1 \setminus I_2}^\top & \mathbf{L}_w & \mathbf{P}_{I_2} \mathbf{y}_{known}, \end{matrix}$$



Actors similarity



Actors similarity

$$\mathbf{P}_{I_2} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Projects 2D vector in to 6D



Actors similarity

$$\mathbf{P}_{I_2} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Projects 2D vector in to 6D

$$\mathbf{P}_{I_1 \setminus I_2}^\top = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

Projects 6D vector in to 4D selecting the unknown targets

Actors similarity

$$\mathbf{P}_{I_1 \setminus I_2}^\top \mathbf{L}_w \mathbf{P}_{I_1 \setminus I_2} \mathbf{y}_{unknown} = - \mathbf{P}_{I_1 \setminus I_2}^\top \mathbf{L}_w \mathbf{P}_{I_2} \mathbf{y}_{known},$$

$$\mathbf{P}_{I_2} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Projects 2D vector in to 6D

$$\mathbf{P}_{I_1 \setminus I_2}^\top = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

Projects 6D vector in to 4D selecting the unknown targets

Actors similarity

Easy to find the solution

$$\begin{pmatrix} 89 & 0 & 0 & -25 \\ 0 & 117 & -36 & 0 \\ 0 & -36 & 121 & -49 \\ -25 & 0 & -49 & 99 \end{pmatrix} \tilde{v} = \begin{pmatrix} 64 \\ 0 \\ 0 \\ 25 \end{pmatrix} .$$

$$\hat{v} = (0.8912 \quad 0.0840 \quad 0.2732 \quad 1 \quad 0.6128 \quad 0)^T .$$

We can then impose a simple threshold $>0.5 \rightarrow 1$ $<0.5 \rightarrow 0$