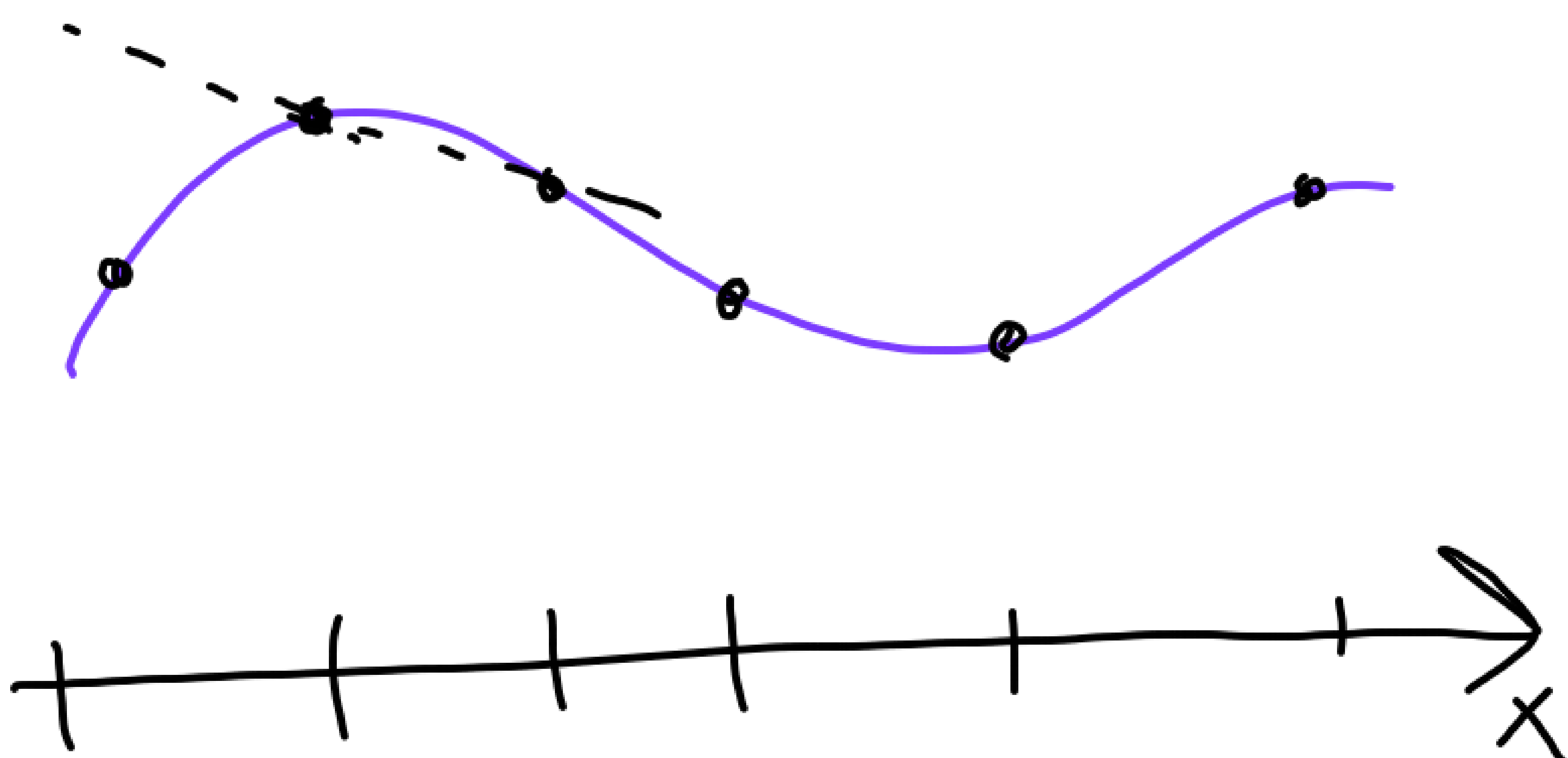
Finite Differences

Given $u(x)$:



Suppose we only know u at discrete points.

How to approximate $u'(x)$?

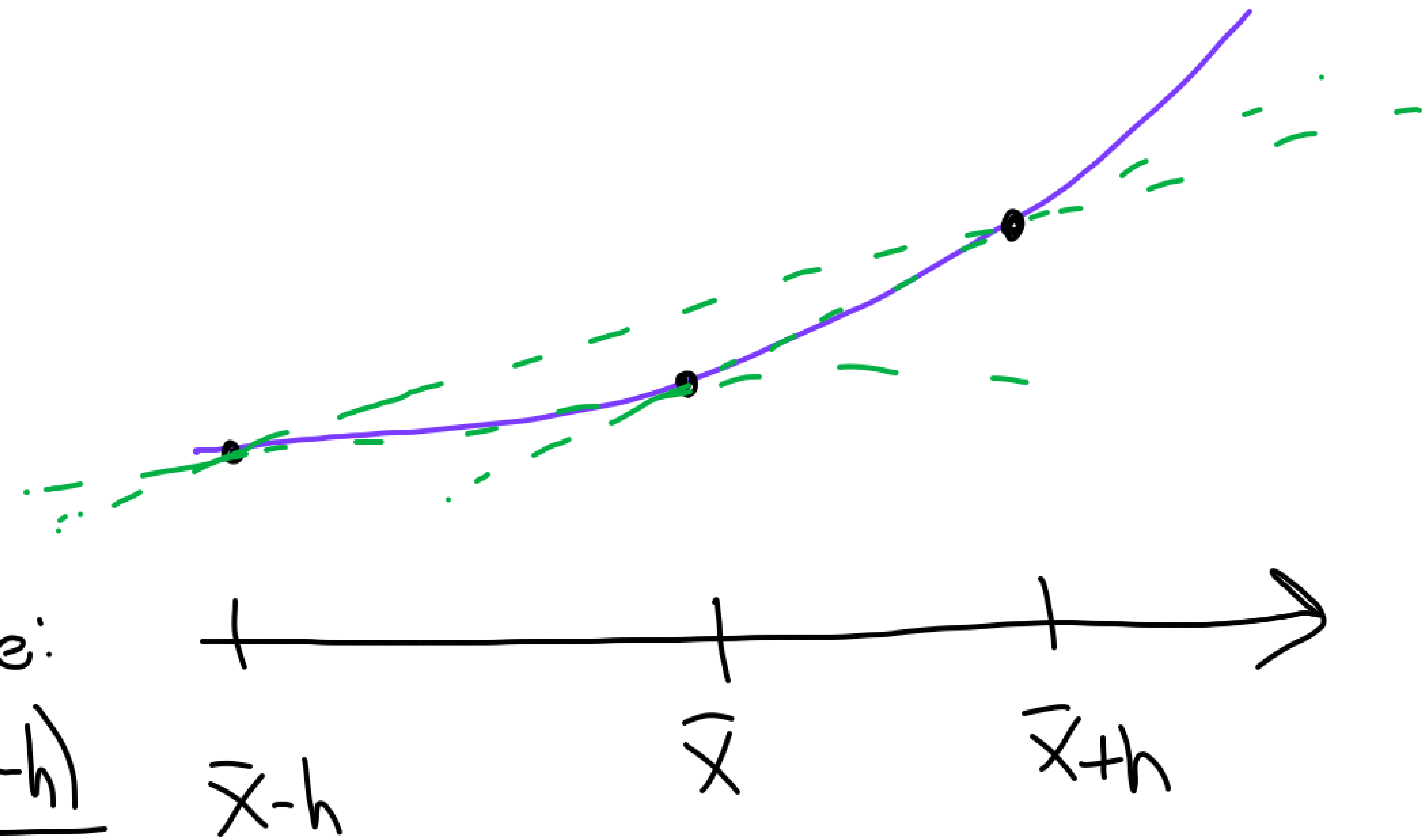
Recall: $u'(x) = \lim_{h \to 0} \frac{u(x+h) - u(x)}{h}$

This suggests the approximation

$$u'(\bar{x}) \approx \underbrace{D_+ u(\bar{x}) = \frac{u(\bar{x}+h) - u(\bar{x})}{h}}_{\text{Forward Difference}}.$$

We could also use a backward difference:

$$D_-u(\bar{x}) = \frac{u(\bar{x}) - u(\bar{x}-h)}{h}$$



Or a centered difference:

$$\frac{1}{2}\left(D_+u + D_-u\right) = \frac{u(\bar{x}+h) - u(\bar{x}-h)}{2h}$$

Error decreases as $h \to 0$.

We can estimate the error using Taylor series:

all terms go to zero at least as fast as h^4

$$u(\bar{x}+h) = u(\bar{x}) + h u'(\bar{x}) + \frac{1}{2}h^2 u''(\bar{x}) + \frac{1}{6}h^3 u'''(\bar{x}) + O(h^4)$$

$$u(\bar{x}) = u(\bar{x})$$

$$u(\bar{x}-h) = u(\bar{x}) - \underline{h u'(\bar{x})} + \frac{1}{2}h^2 u''(\bar{x}) - \frac{1}{6}h^3 u'''(\bar{x}) + O(h^4)$$

Taylor:

$$u(x+y) = \sum_{j=0}^{\infty} \frac{y^j}{j!} u^{(j)}(x)$$

$$D_+ u(\bar{x}) = \frac{u(\bar{x}+h) - u(\bar{x})}{h} = u'(\bar{x}) + \underbrace{\frac{1}{2} h u''(\bar{x})}_{\text{Leading truncation error}} + O(h^2)$$

$$D_- u(\bar{x}) = \frac{u(\bar{x}) - u(\bar{x}-h)}{h} = u'(\bar{x}) \underbrace{- \frac{1}{2} h u''}_{} + O(h^2)$$

$$D_0 u(\bar{x}) = \frac{u(\bar{x}+h) - u(\bar{x}-h)}{2h} = u'(\bar{x}) + \underbrace{\frac{1}{3}\frac{h^2}{2} u'''(\bar{x})}_{\text{Leading truncation error}} + O(h^4)$$

We say D_+, D_- are 1st-order accurate

D_0 is 2nd-order accurate.

Deriving F.D. Formulas

Suppose we know

$$u(\bar{x}),\ u(\bar{x}+h),\ u(\bar{x}+2h)$$

and we want to approximate

$$u''(\bar{x}).$$

If we add the 3 Taylor series multiplied by a, b, c we get an equation for each derivative of u.

$$\underline{u(\bar{x}+2h)} = u(\bar{x}) + 2h\,u'(\bar{x}) + \overbrace{\frac{4h^2}{2}}^{2h^2} u''(\bar{x}) + \overbrace{\frac{8h^3}{6}}^{\frac{4}{3}h^3} u'''(\bar{x}) + O(h^4)$$

We seek a formula

$$a\,u(\bar{x}) + b\,u(\bar{x}+h) + c\,u(\bar{x}+2h) \approx u''(\bar{x})$$

$$(a+b+c)u(\bar{x})=0$$

$$(bh+2ch)u'(\bar{x})=0$$

$$\left(\tfrac{1}{2}bh^2+2h^2c\right)u''(\bar{x})=u''(\bar{x})$$

$$\left.\begin{aligned} a+b+c&=0\\ b+2c&=0\\ \tfrac{1}{2}bh^2+2ch^2&=1 \end{aligned}\right\} \text{3 Eqns. for } a,b,c$$

$$b=-2c$$

$$\frac{1}{2}(-2c)h^2+2ch^2=1$$

$$ch^2=1$$

$$c=\frac{1}{h^2} \quad b=\frac{-2}{h^2} \quad a=-b-c=\frac{2}{h^2}-\frac{1}{h^2}=\frac{1}{h^2}$$

$$u''(\bar{x})\approx\frac{u(\bar{x})-2u(\bar{x}+h)+u(\bar{x}+2h)}{h^2}$$

$$\left(\tfrac{1}{6}h^3b+\tfrac{4}{3}h^3c\right)u'''(\bar{x})\stackrel{?}{=}0$$

$$\frac{-2}{6}+\frac{4}{3}\neq 0$$

We can't satisfy the next condition

The leading error will be proportional to $h\, u'''(\bar{x})$

Derivation of a general FD formula

$$u(x_j) = u(\bar{x}) + (x_j - \bar{x}) u'(\bar{x}) + \frac{1}{2}(x_j - \bar{x})^2 u''(\bar{x}) + \dots$$

$$u(x_j) = \sum_{i=0}^{\infty} \frac{(x_j - \bar{x})^i}{i!} u^{(i)}(\bar{x}) \qquad (1)$$

We want a formula

$$\sum_{j=1}^{n} c_j u(x_j) = u^{(k)}(\bar{x}) + O(h^p) \qquad (2)$$

We substitute (1) into (2) and obtain an equation involving the coefficients of each derivative

$$\sum_{j=1}^{n} c_j \sum_{i=0}^{\infty} \frac{(x_j-\bar{x})^i}{i!} u^{(i)}(\bar{x}) = \underline{u^{(k)}(\bar{x})} + O(h^p)$$ What is p?

The coefficient of $u^{(i)}(\bar{x})$ is

$$\underbrace{\frac{1}{i!}\sum_{j=1}^{n}(x_j-\bar{x})^i}_{m_{ij}} c_j = \sum_{j=1}^{n} m_{ij} c_j = Mc$$

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_1-\bar{x} & x_2-\bar{x} & \cdots & x_n-\bar{x} \\ \frac{1}{2}(x_1-\bar{x})^2 & \cdots & & \frac{1}{2}(x_n-\bar{x})^2 \\ \vdots & & & \\ \frac{1}{n-1}(x_1-\bar{x})^{n-1} & \cdots & & \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ \vdots \\ c_n \end{bmatrix} = \begin{array}{c} \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \end{array} \begin{array}{l} \leftarrow u^{(0)}(\bar{x}) \\ \leftarrow u^{(1)}(\bar{x})h^1 \\ \\ \leftarrow u^{(k)}(\bar{x})h^k \\ \\ \leftarrow u^{(n-1)}(\bar{x})h^{n-1} \end{array}$$

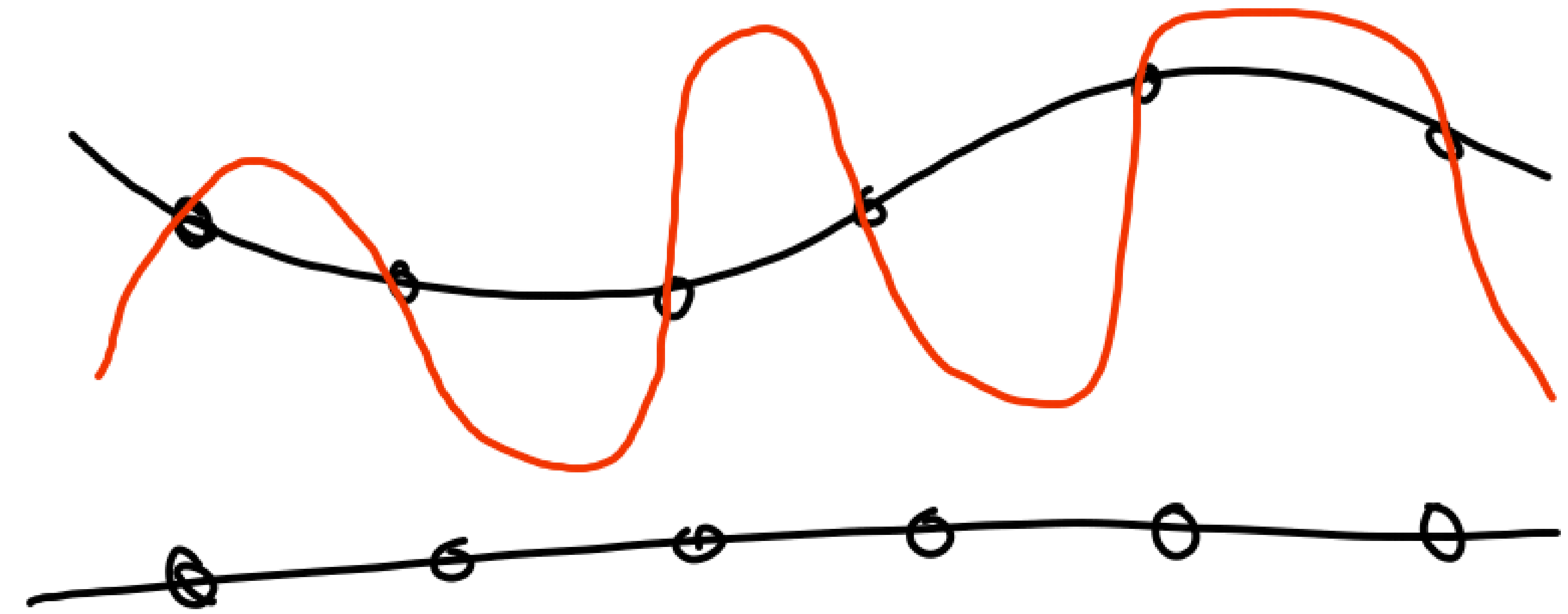
If $x_i \neq x_j \ \forall (i,j)$ then M is non-singular

M is a Vandermonde matrix

The leading error term will be proportional to

$$\frac{u^{(n)}(\bar{x})h^n}{h^k} = O(h^{n-k})$$

$$p = n-k$$



Runge Phenomenon

Polynomial interpolants on evenly-spaced grids are highly oscillatory.

Two solutions:

1. Don't use polynomials
   Use Fourier modes

2. Use a Chebyshev
   grid