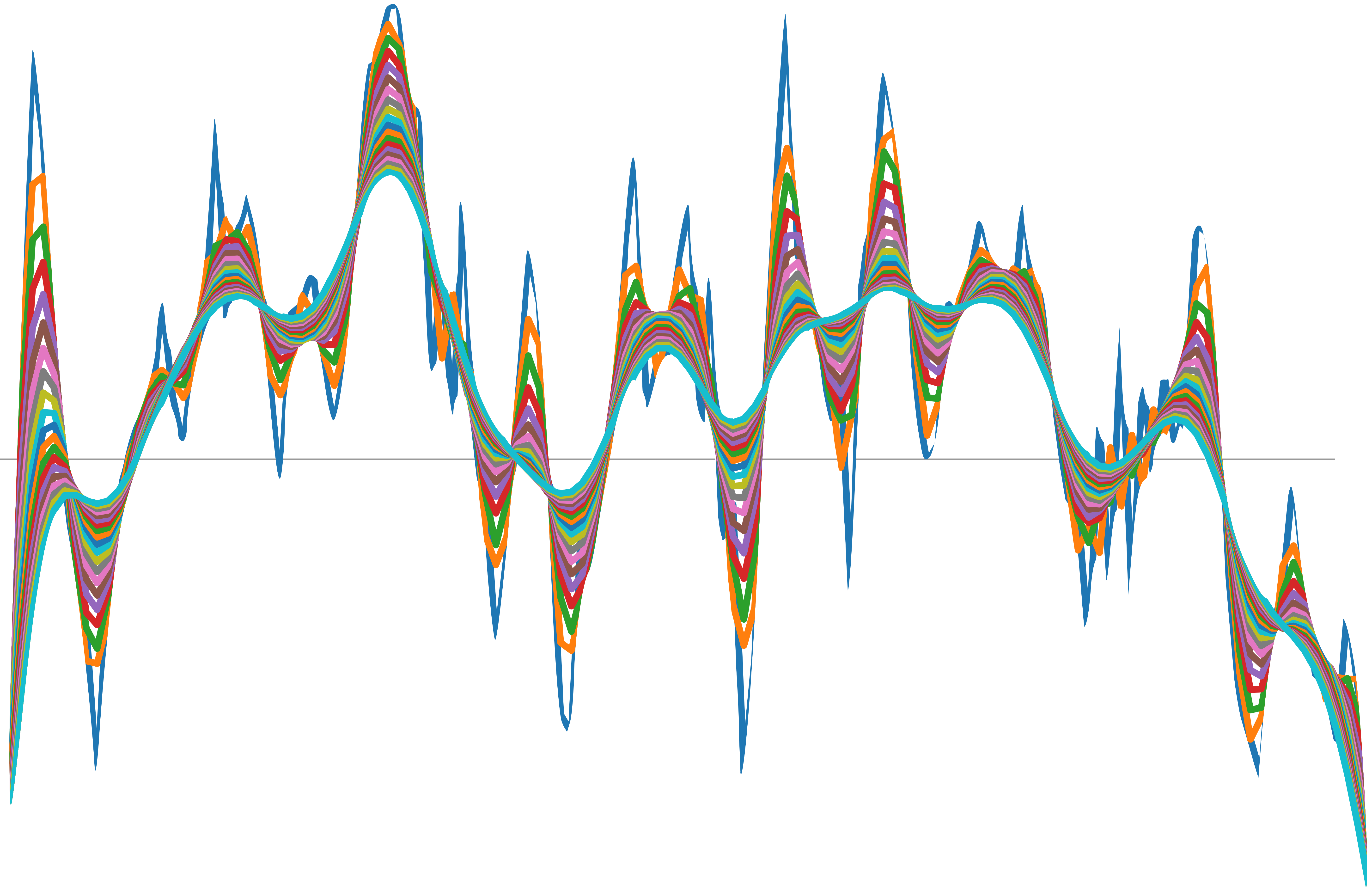
Multigrid Methods

The Basics



2023 Copper Multigrid Conference
April 16, 2023

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(slides by Luke Olson, Department of Computer Science, University of Illinois at Urbana-Champaign)

+ Notebooks 6, 7, 8, 9 , slides

What are we trying to do…

$A \in \mathbb{R}^{n \times n}$

- Solve problems of the form

$$Ax = b$$

GE : $W = O(n^3)$

MG : $W = O(n)$

- Solve this problem **iteratively**:

$$x_1 \leftarrow x_0 + v$$

- Solve this problem **inexpensively:**
  - The update should be “good” (small number of iterations)
  - Finding the update should be “cheap”

Objectives — high level

- Construct a multigrid method for **your** problem
- Interpret the effectiveness of a multigrid method
- Identify *why* a method works — or — *why* a method does not
- Recognize different forms of multigrid, their pitfalls and their uses

Objectives — this session

- **Create** a two level multigrid method
- **Illustrate** the main components of a multigrid method
- **Calculate** the effectiveness of a multigrid method
- **Highlight** some limitations of multigrid
- **Outline** some approaches to fixing multigrid (and why)
- **Identify** key pieces in moving to unstructured problems

A cautionary example (see slide 3)

Guess and look for and update $x_1 = x_0 + \text{update}$

Updating with the error would be **ideal** $x_1 = x_0 + e_0 = x_0 + (x^* - x_0) = x^*$

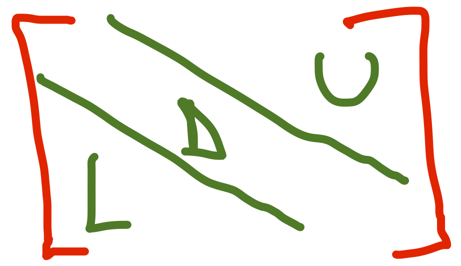
Or in another form $x_1 = x_0 + A^{-1} r_0 = x^*$

1 iteration

Not practical so… $x_1 = x_0 + D^{-1} r_0$

$\boxed{\text{Jacobi} \sim 1\ \text{SpMV}}$ ($W = O(n)$ per iteration)

note: $A = D + L + U$



x^* solution to $Ax = b$

$e_0 = x^* - x_0$ error

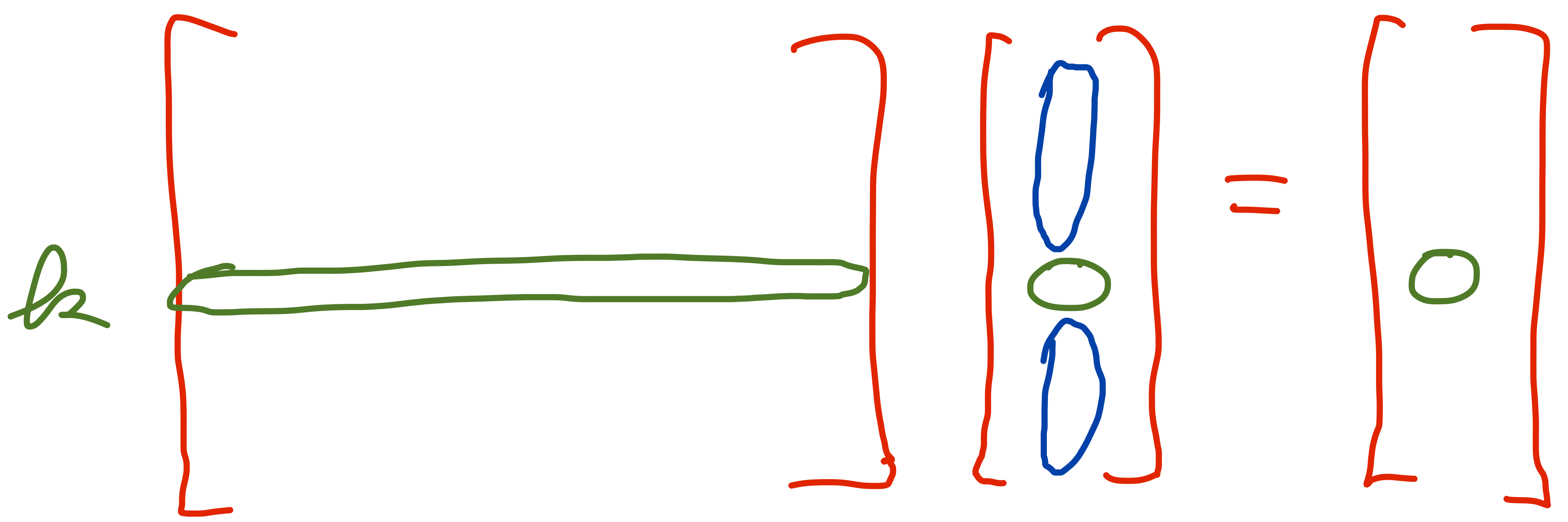
$r_0 = b - Ax_0$ residual

$= Ae_0 = A(x^* - x_0)$

$Ae_0 = r_0$ error equation

Jacobi iteration:

$$A\vec{x} = \vec{b}$$



eq. k: $\sum_j a_{kj} x_j = b_j$

Jacobi: $$x_k^{new} = \frac{1}{a_{kk}} \left(b_k - \sum_{j \neq i} a_{kj} x_j^{old} \right)$$

$$\vec{x}_1 = D^{-1} \left(\vec{b} - (L+U)\vec{x}_0 \right)$$

$$\vec{x}_1 = \vec{x}_0 + D^{-1} \left(\vec{b} - (D+L+U)\vec{x}_0 \right)$$

$$\vec{x}_1 = \vec{x}_0 + D^{-1} \left(\vec{b} - A\vec{x}_0 \right)$$

$$\vec{x}_1 = \vec{x}_0 + D^{-1} \vec{r}_0$$

A reminder — projection methods

- Take a guess

$$x_0$$

- Look for an update that is the "best":

$$x_1 \leftarrow x_0 + u$$

- Minimize over a smaller space

coarse grid

$$\min_{u\in span\{V\}} \|x^* - x_1\| = \|e_1\| = \|\underbrace{x^* - x_0}_{e_0} - u\|$$

$$= \|e_0 - Vy\|$$

- Then $u = Vy$

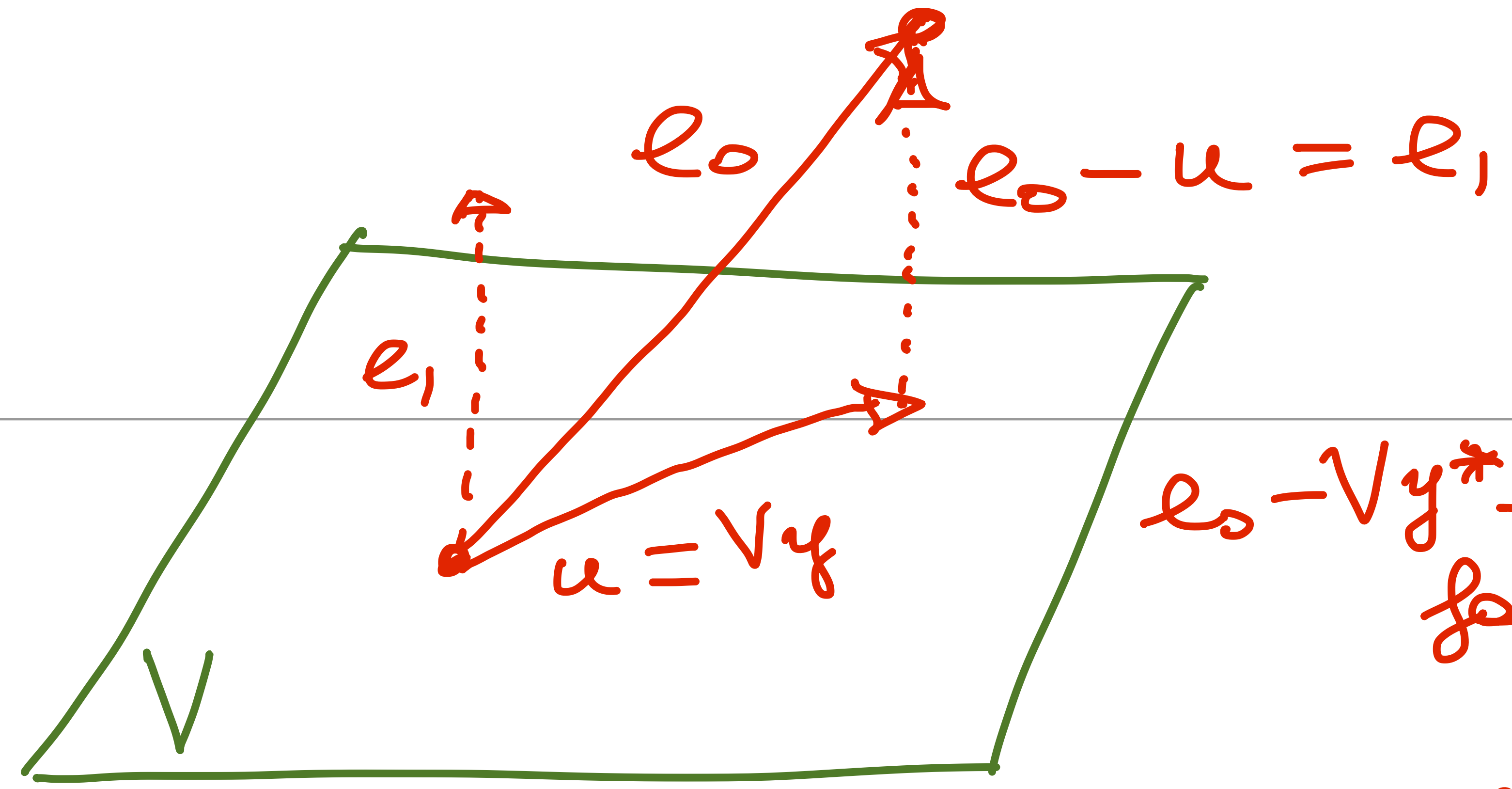
$$V^T V y = V^T e_0$$

normal equations

- So the update looks like

$$x_1 = x_0 + V\underbrace{(V^T V)^{-1} V^T e_0}_{y}$$

(coarse grid correction)



$e_0 - Vy^* \perp Vy$ for all y

$y^T V^T (e_0 - Vy^*) = 0$ for all y

→ optimal u = projection of e_0 on V, orthogonal

→ then remove u from e_0 to get e_1

A reminder — projection methods

- Instead, look at the A-norm (A s.p.d.):

$$\min_{u \in span\{V\}} \|x^* - x_1\|_A$$

- Then $u = Vy$

$$V^T A V y = V^T \underbrace{A e_0}$$

$$V^T A V y = V^T r_0$$

- So that

optimal coarse-grid operator

$$\underbrace{x_1}_{\text{A-optimal coarse-grid correction}} = x_0 + \underbrace{V \overbrace{(V^T A V)}^{}{}^{-1} V^T r_0}_{Vy}$$

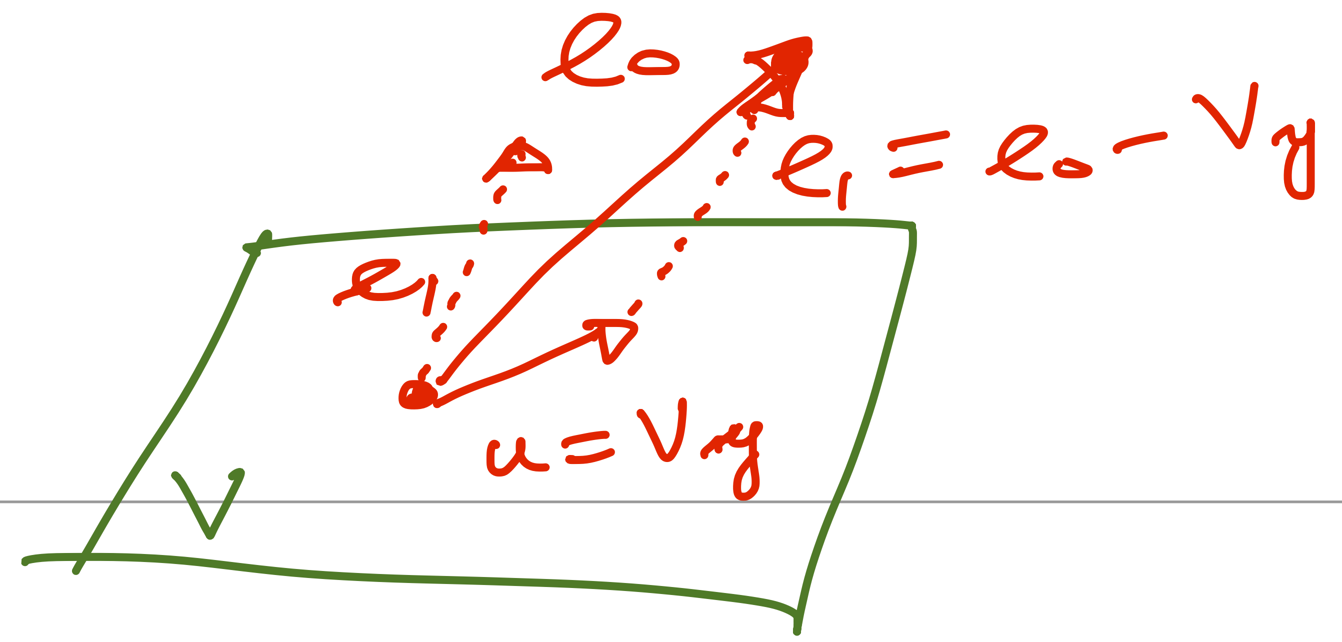
residual is cheaply computable $(O(n))$

A-orthogonal projection:

$$\min_u \|x^* - x_1\|_A = \|x^* - x_0 - u\|_A$$
$$= \|x^* - x_0 - Vy\|_A$$
$$= \|e_0 - Vy\|_A$$

$$\min_y (e_0 - Vy)^T A (e_0 - Vy)$$
$$= e_0^T A e_0 + (Vy)^T A Vy$$
$$- 2 e_0^T A Vy$$
$$\Rightarrow V^T A \underbrace{Vy}_{\text{A-orthogonal projection of } e_0} = V^T A e_0$$

A reminder — projection methods



$$x_1 = x_0 + u$$

$e_1 = e_0 - Vy^* \perp_A Vy$ for all y

$$x_1 = x_0 + V(V^TAV)^{-1}V^Tr_0$$

- What about the error

$$x^* - x_1 = x^* - x_0 - V(V^TAV)^{-1}V^Tr_0$$

$$e_1 = e_0 - V(V^TAV)^{-1}V^TAe_0$$

$$= \left(I - V(V^TAV)^{-1}V^TA\right)e_0$$

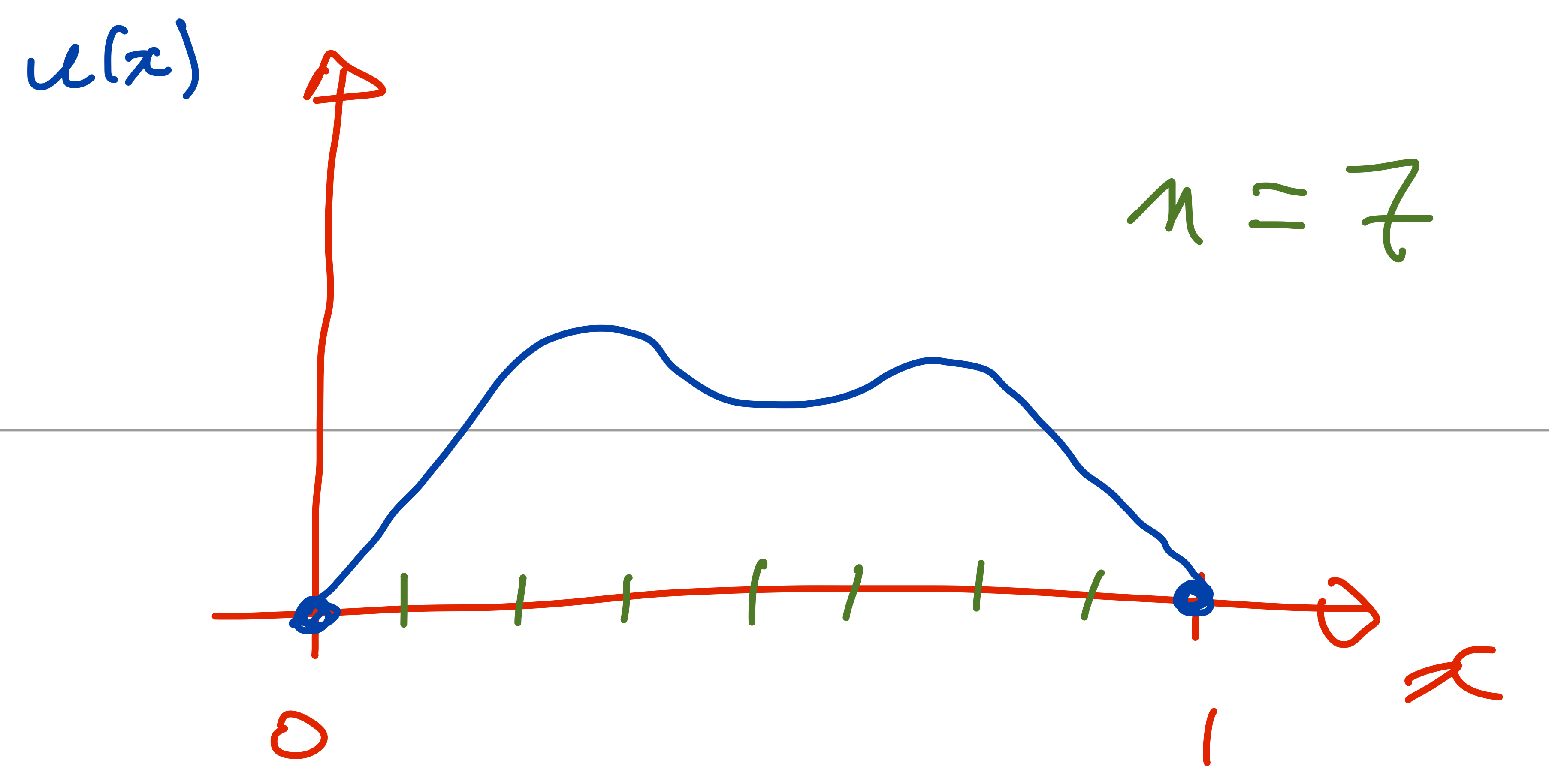
(optimal coarse-grid correction, given V)

A-orthogonal projection onto the range of V

Model Problem

- A model problem

$$-u_{xx} = f$$
$$u(0) = u(1) = 0$$



$n = 7$

$\underbrace{x_0, x_1 \qquad x_n,}_{} x_{n+1}$

n interior points

$h = \frac{1}{n+1} = \frac{1}{8}$

- Finite differences

$$\frac{-u_{i-1} + 2u_i - u_{i+1}}{h^2} = f_i \quad i = 1, \ldots, n \quad u_0 = u_{n+1} = 0$$

- A model matrix problem

$$A = \frac{1}{h^2} \begin{bmatrix} 2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & \ddots \\ & & \ddots & \end{bmatrix}$$

$A \in \mathbb{R}^{n \times n}$, sparse

$nnz(A) \approx 3n = O(n)$

$A \in \mathbb{R}^{n \times n}$ $h = \frac{1}{n+1}$

Model Problem

- A special matrix:

$$A = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & \ddots & & \\ & & & -1 & 2 \end{bmatrix}$$

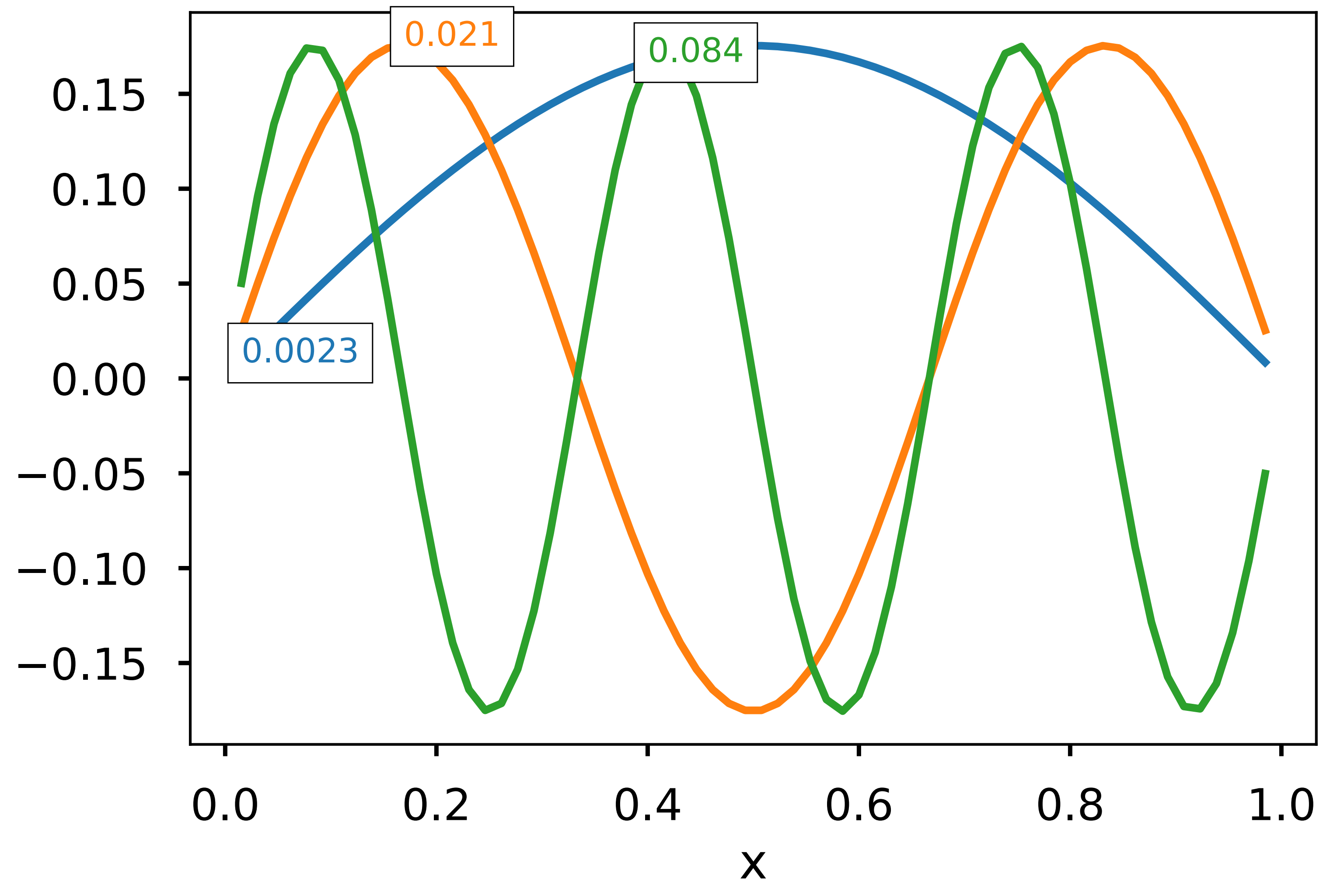
smoothest component = small λ_k $(O(h^2))$

The eigenvalues

$$\lambda_k = 4\sin^2\left(\frac{k\pi}{2(n+1)}\right)$$

$k = 1, \dots, n$

range from (0,4]
(or from c h^2 to ~4)



The eigenvectors are Fourier modes:

$\lambda_1 = 4\sin^2\left(\frac{\pi}{2(n+1)}\right) \approx 4\frac{\pi^2 h^2}{4}$

$$(v_k)_j = \sin\left(\frac{(j+1) * k\pi}{n+1}\right)$$

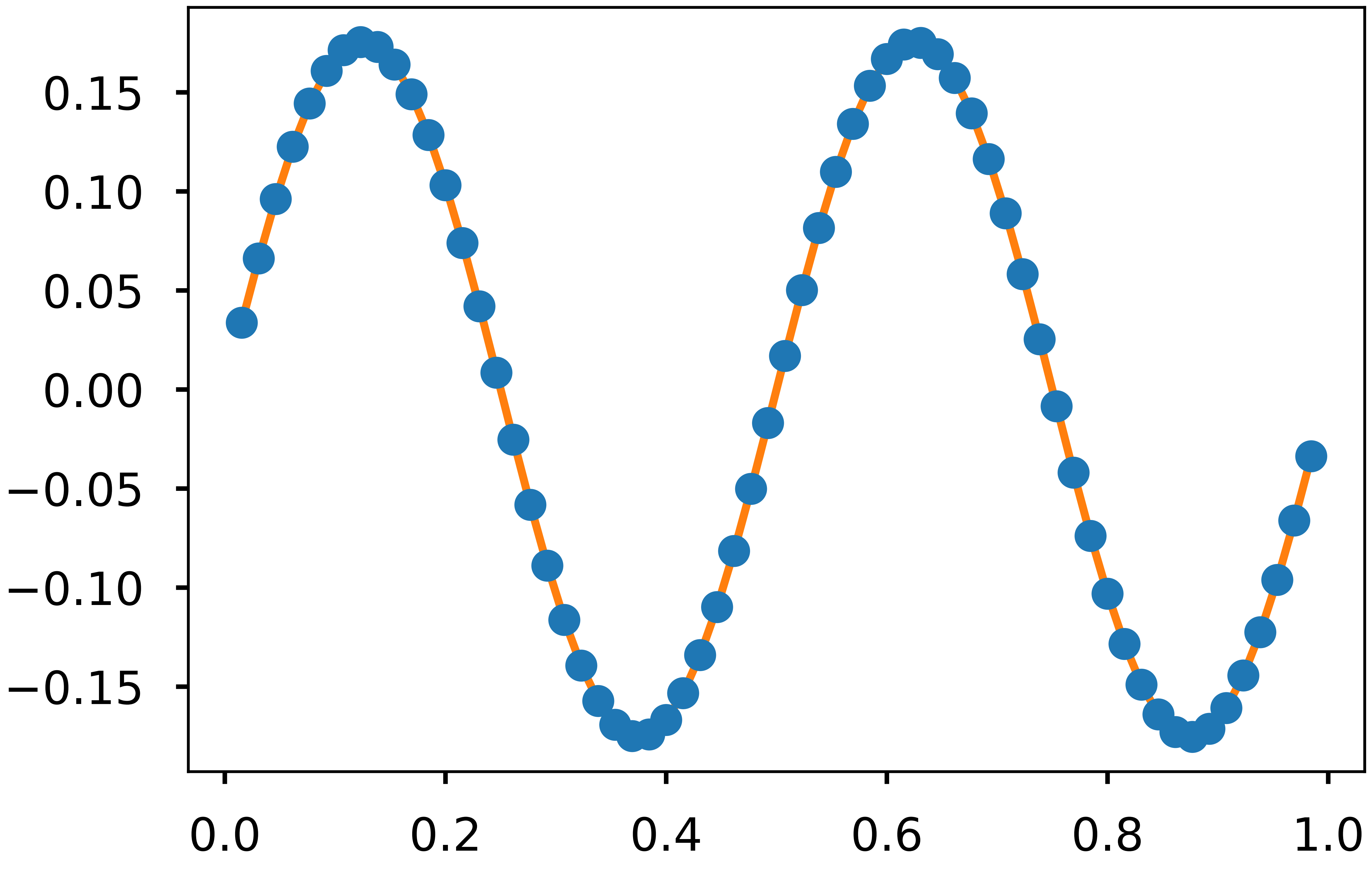
multigrid: (A) relaxation on the fine grid
(B) coarse-grid correction

Take a look: `01-model-problem.ipynb`

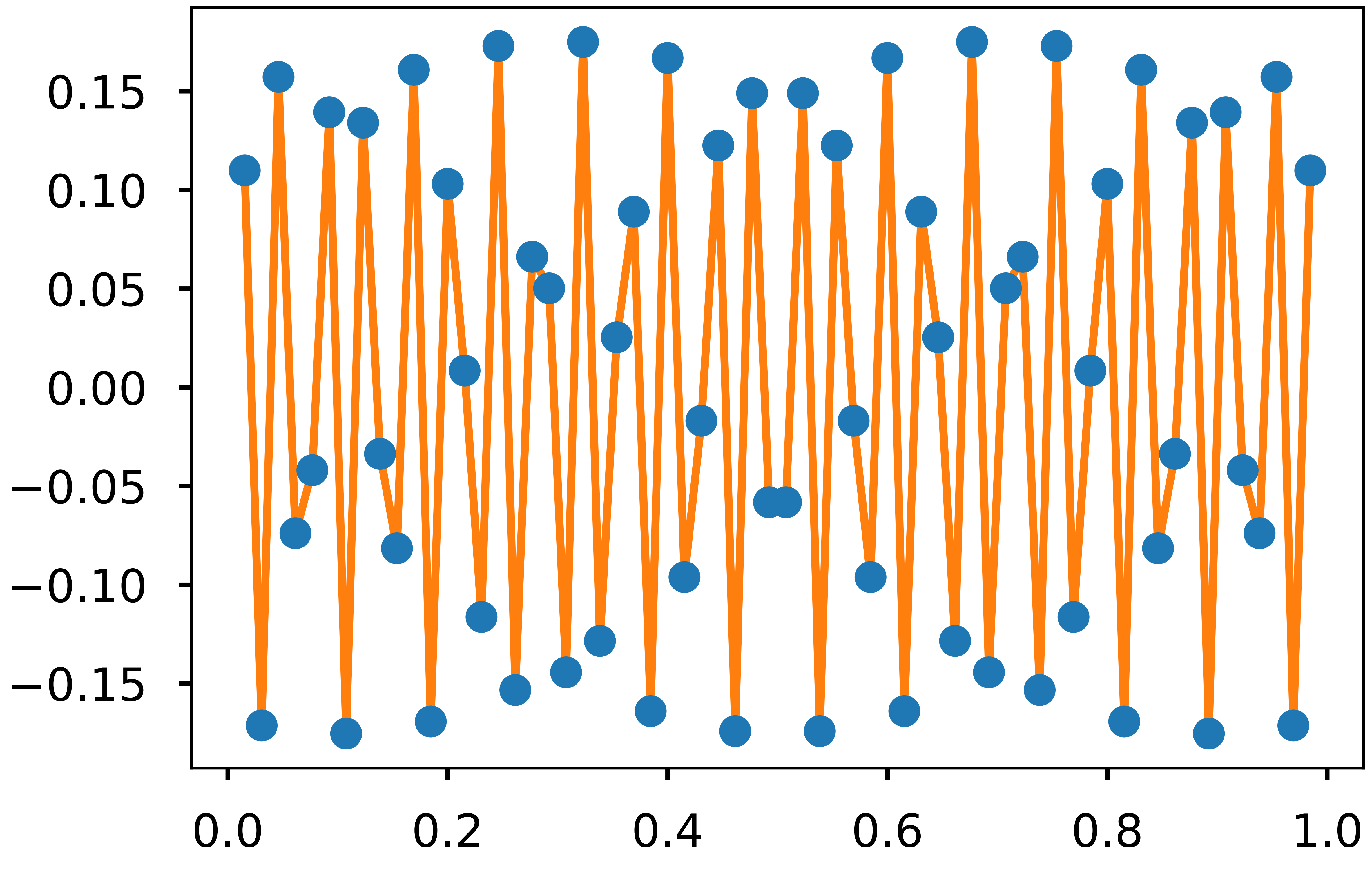
Smooth Mode ~ low Fourier Modes

(for ingredient (A))

- We will talk a lot about "smoothness" — how much variation there is **per** grid point.



small k



large k $\approx$ n

First relaxation scheme: Jacobi

$(h^2 \text{ in it})$

$Au = f$

- The discretization at point i:

d_{ii}

$$-u_{i-1} + 2u_i - u_{i+1} = h^2 f_i$$

- Solving for the variable at this point (eliminating the residual):

$$u_i \leftarrow \frac{1}{2}\left(u_{i-1} + u_{i+1} + h^2 f_i\right)$$

$1/d_{ii}$

- In matrix form:

$$u \leftarrow (I - D^{-1}A)u + h^2 D^{-1} f$$

$$u \leftarrow u + D^{-1} r$$

$$u^* - u \leftarrow u^* - u - D^{-1} A e$$

$$e \leftarrow \underbrace{(I - D^{-1} A)}_{G} e$$

- And the error:

$$e \leftarrow Ge \qquad \boxed{G = I - D^{-1}A}$$

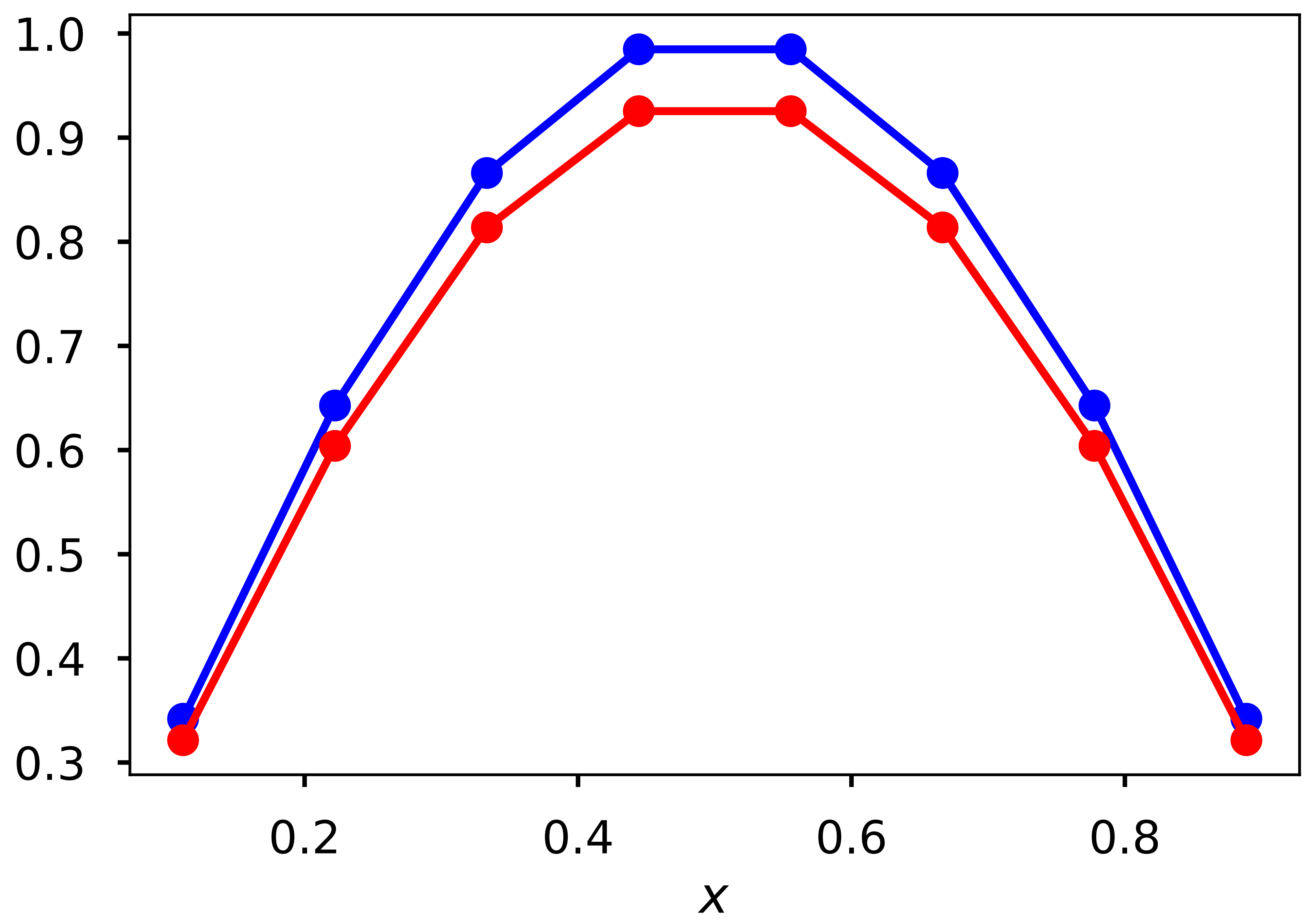
The "error propagation operator"

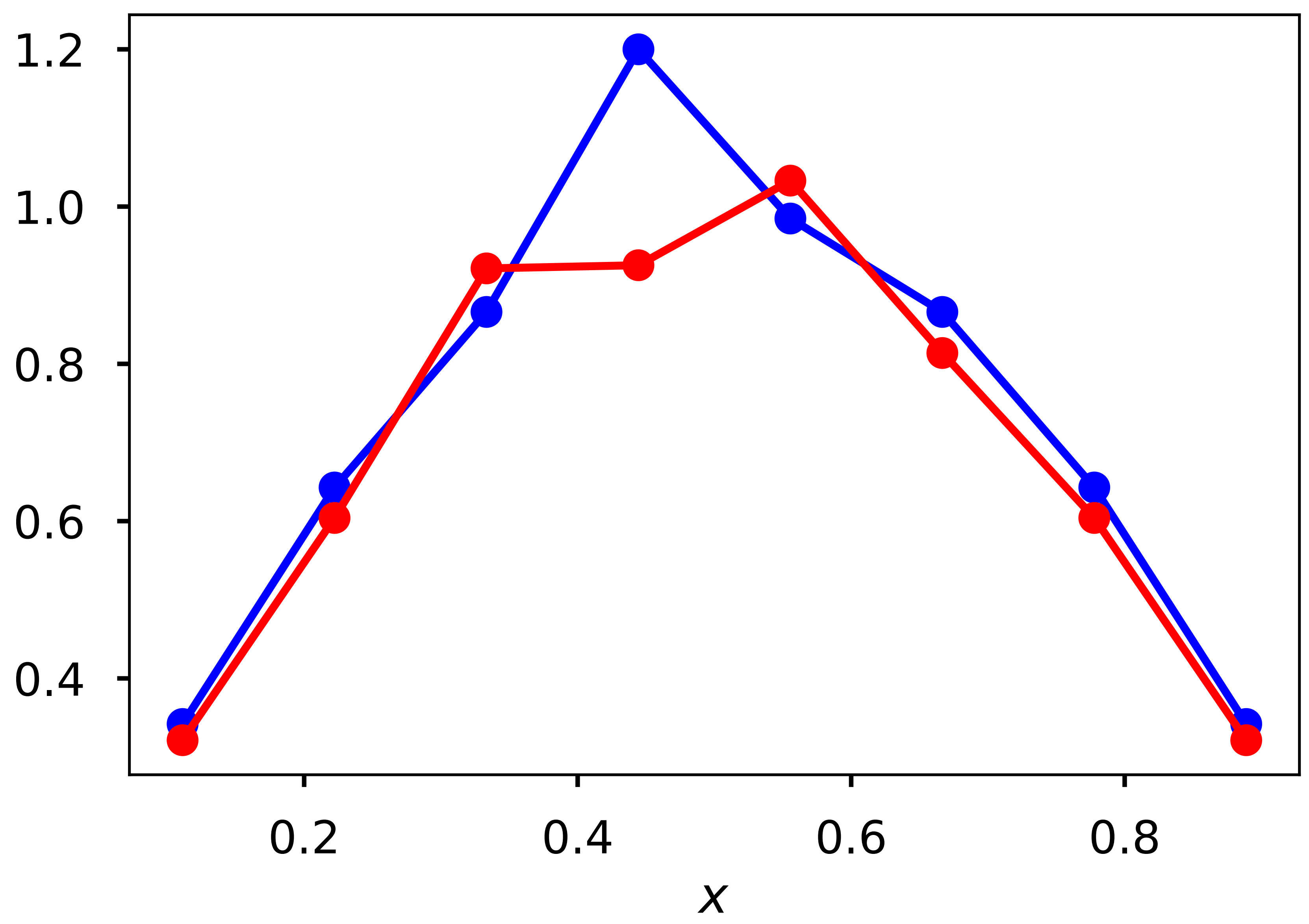
What does Jacobi do to error?

$$\color{red}{e^{new}} \leftarrow (I - D^{-1}A)\color{blue}{e^{old}}$$

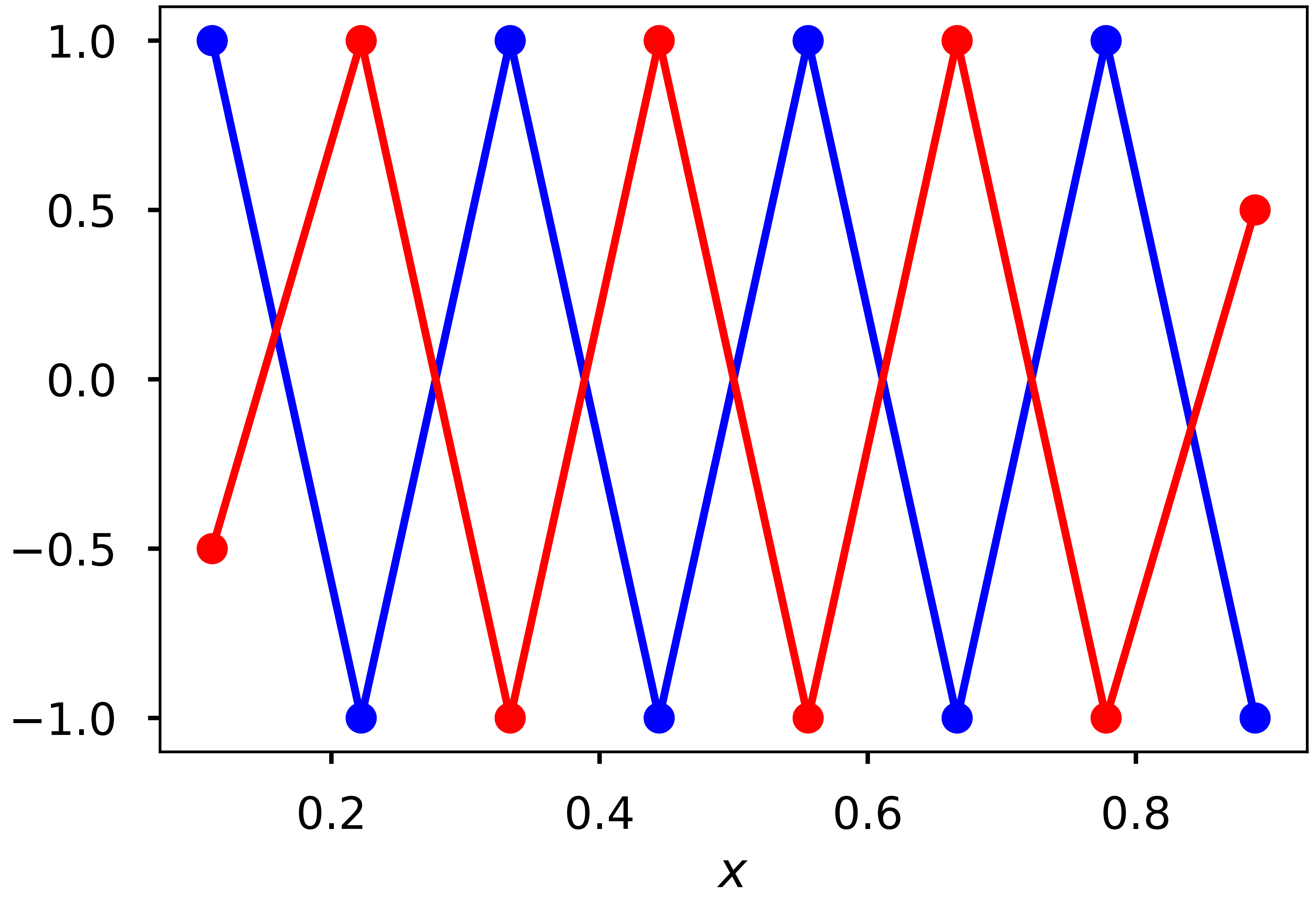
$$\color{red}{e_i^{new}} \leftarrow \frac{1}{2}\left(\color{blue}{e_{i-1}^{old}} + \color{blue}{e_{i+1}^{old}}\right)$$

- It averages…
- Consider smooth and oscillatory error:





But…

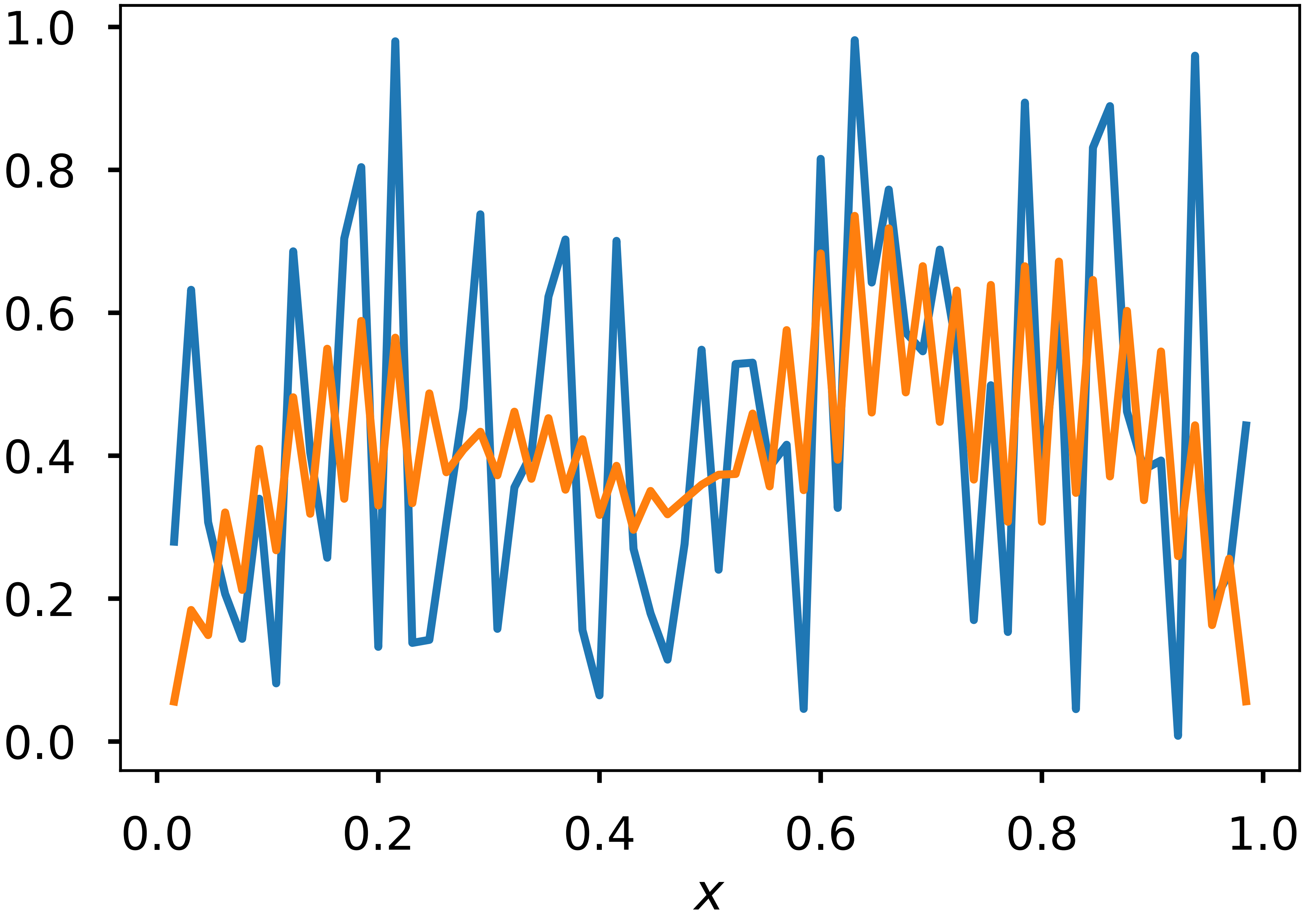


- Jacobi "averages out" certain error very quickly.
- But stagnates on very smooth error or very oscillatory error

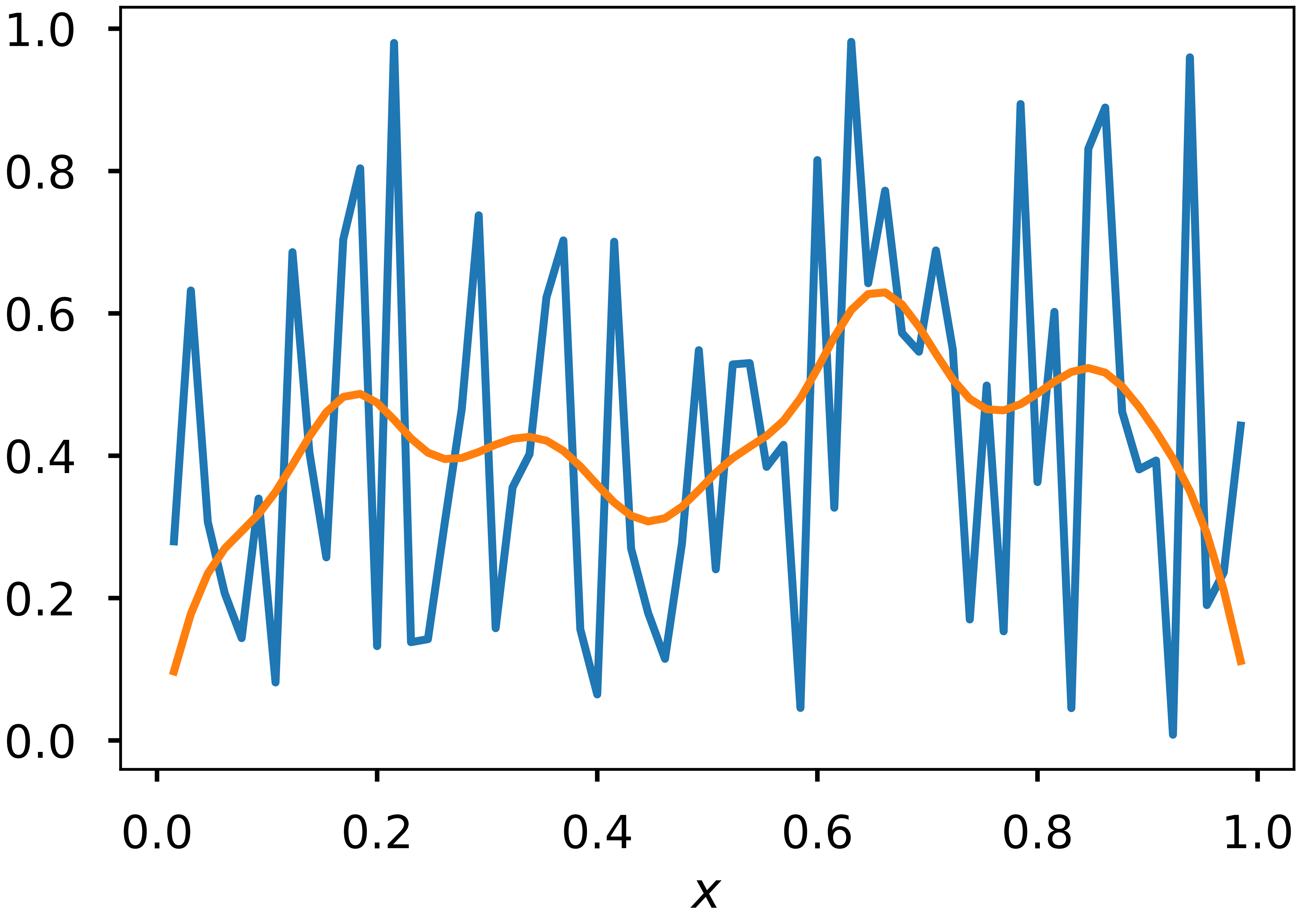
From Jacobi to weighted-Jacobi

- Random initial guess (random error):

$$u \leftarrow u + D^{-1}r$$



$$u \leftarrow u + (2/3)D^{-1}r$$



Weighted Jacobi

- Weighted Jacobi

$$u \leftarrow u + (2/3)D^{-1}r \;=\; \frac{1}{3}u + \frac{2}{3}(u + D^{-1}r)$$

$$= (1-\omega)u + \omega(u + D^{-1}r)$$

- What does this do to other modes?
  - Are smooth modes damped slowly?
  - What about oscillatory modes?

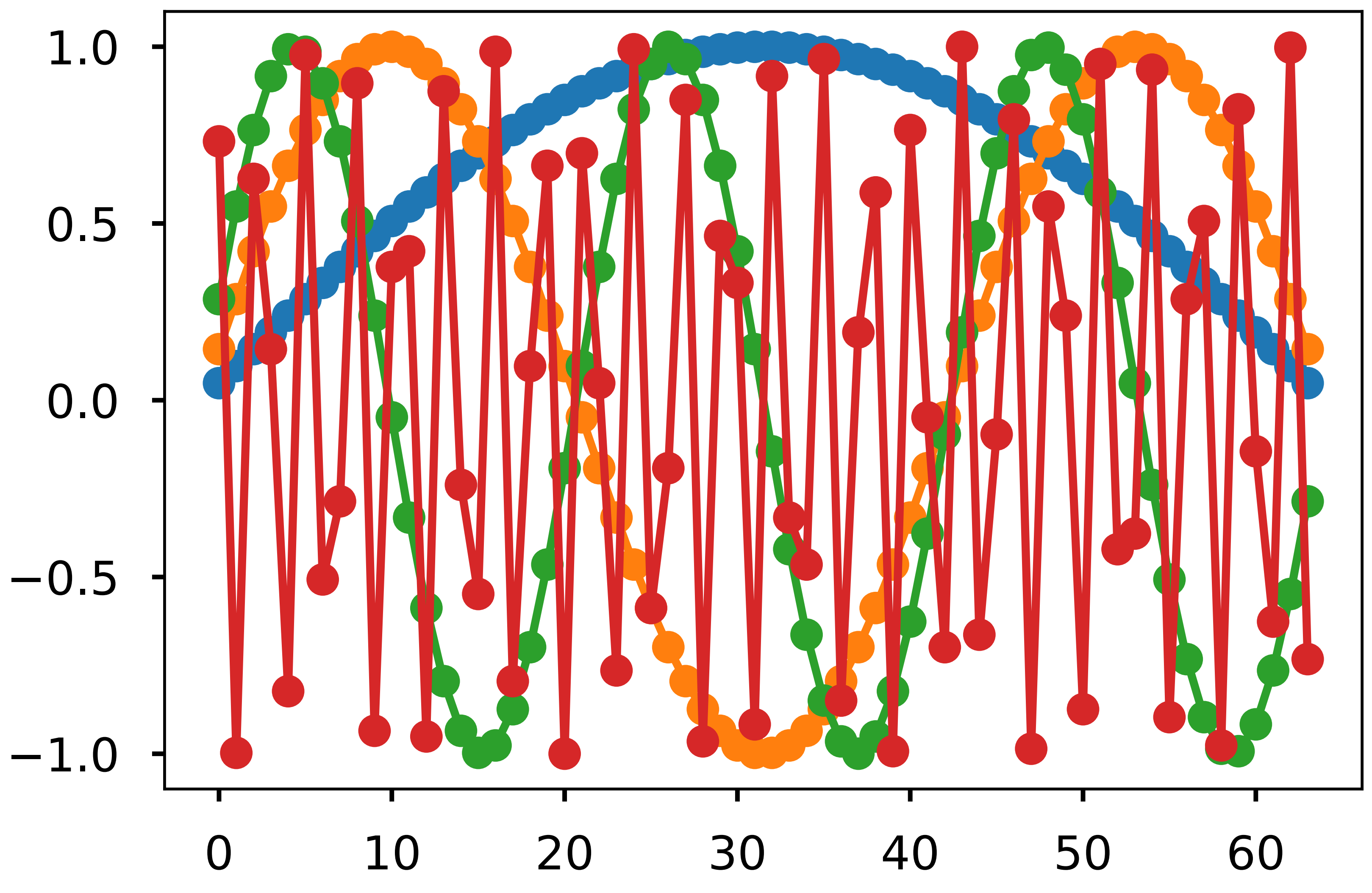
- Why did we pick 2/3 — that seemed like a lucky guess?!

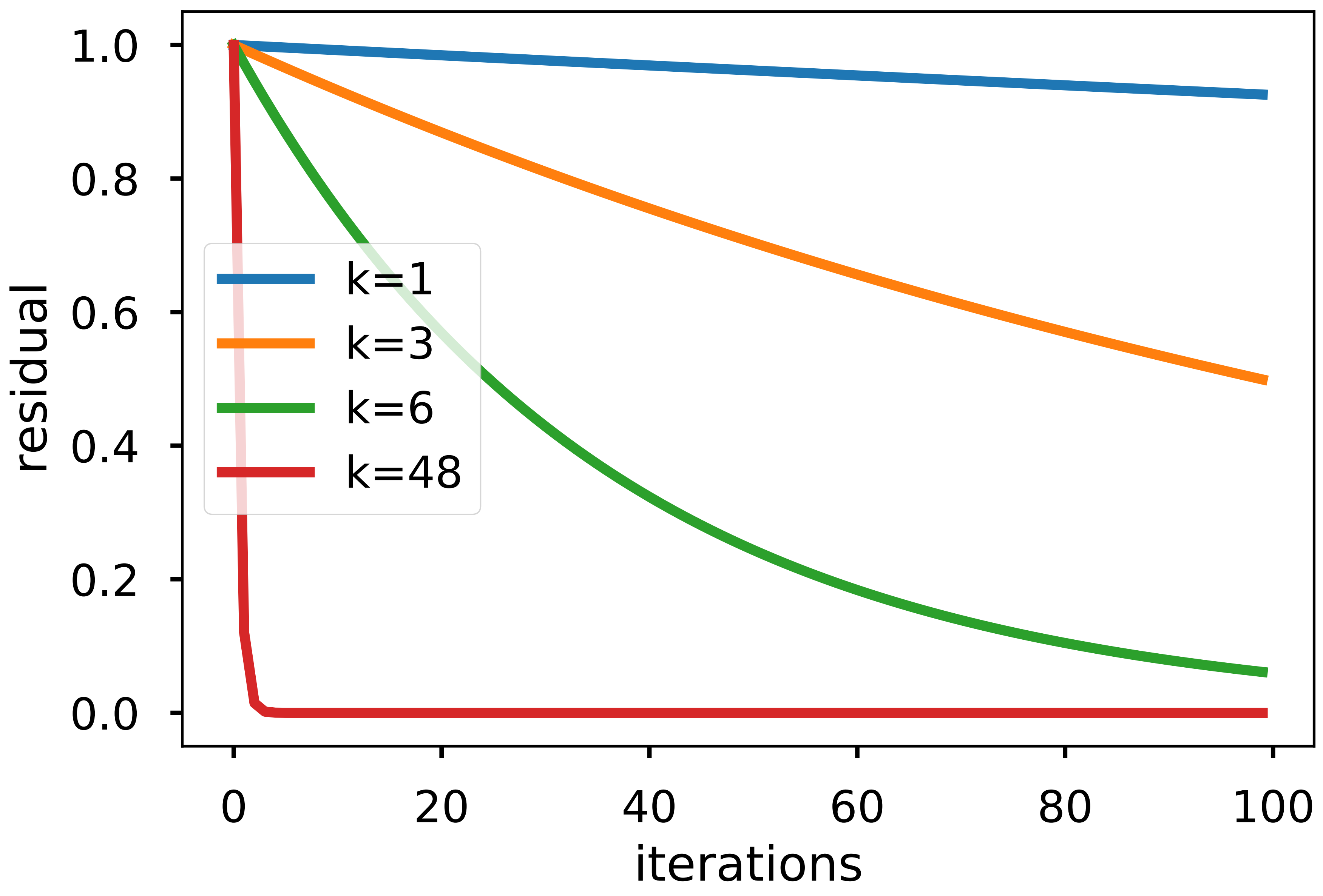
Weighted Jacobi

$n = 64$

$h = \frac{1}{65}$

- If we picked 4 modes, 1, 3, 6, and 48 (out of 64)
- Then smooth modes still dampen less quickly than higher ones





Error Propagation

- Let's consider an initial error

$$e_0 = \sum_{k=1}^{n} c_k v_k$$

- And the weighted Jacobi iteration matrix

$$e \leftarrow (I - \omega D^{-1}A)e = Ge$$

- From ν iterations we have

$$G^{\nu} e_0 = \sum_{k=1}^{n} c_k G^{\nu} v_k$$

$$= \sum_{k=1}^{n} c_k \lambda_k^{\nu} v_k$$

eigenvalues of G

- As a result, mode **k** is reduced by the magnitude of λ_k in every pass

(assume D has constant diagonal)

$Au = f$

$A\hat{u} = \hat{\lambda}\hat{u}$

$G = (I - \omega D^{-1}A)$

then $(I - \omega D^{-1}A)\hat{u}$

$= u - \omega D^{-1}A\hat{\lambda}\hat{u}$

$= (1 - \omega \frac{1}{d}\hat{\lambda})\hat{u}$

so $\lambda = 1 - \frac{\omega}{d}\hat{\lambda}$, $u = \hat{u}$

$k=1$: $\hat{\lambda}_1 = O(h^2)$

$\lambda_1 = O(1)$

Fundamental Theorem of Iteration

$$G = I - M^{-1}A$$

- Convergent ($G^n \to 0$) if and only if $\rho(G) < 1$

if $G = G^T$,

$\|G\| = \rho(G)$

$$\frac{\|e_n\|}{\|e_0\|} \leq \|G^n\| \leq \|G\|^n \approx 10^{-d}$$

$n \log_{10}(\rho(G)) \approx -d$

- How many iterations do we need to guarantee the reduction of the error by *d* digits?

$$n \approx -\frac{d}{\log_{10} \rho(G)}$$

Relaxation

- Convergence **factor**

$$\|G\| \text{ or } \rho(G)$$

- Convergence **rate**

$$-\log_{10}\rho(G)$$

(digits per iteration)

- For Jacobi:

$$G = I - D^{-1}A \longrightarrow \lambda_k = 1 - \frac{1}{2}\cdot 4 \cdot \sin^2\left(\frac{k\pi}{2(n+1)}\right)$$

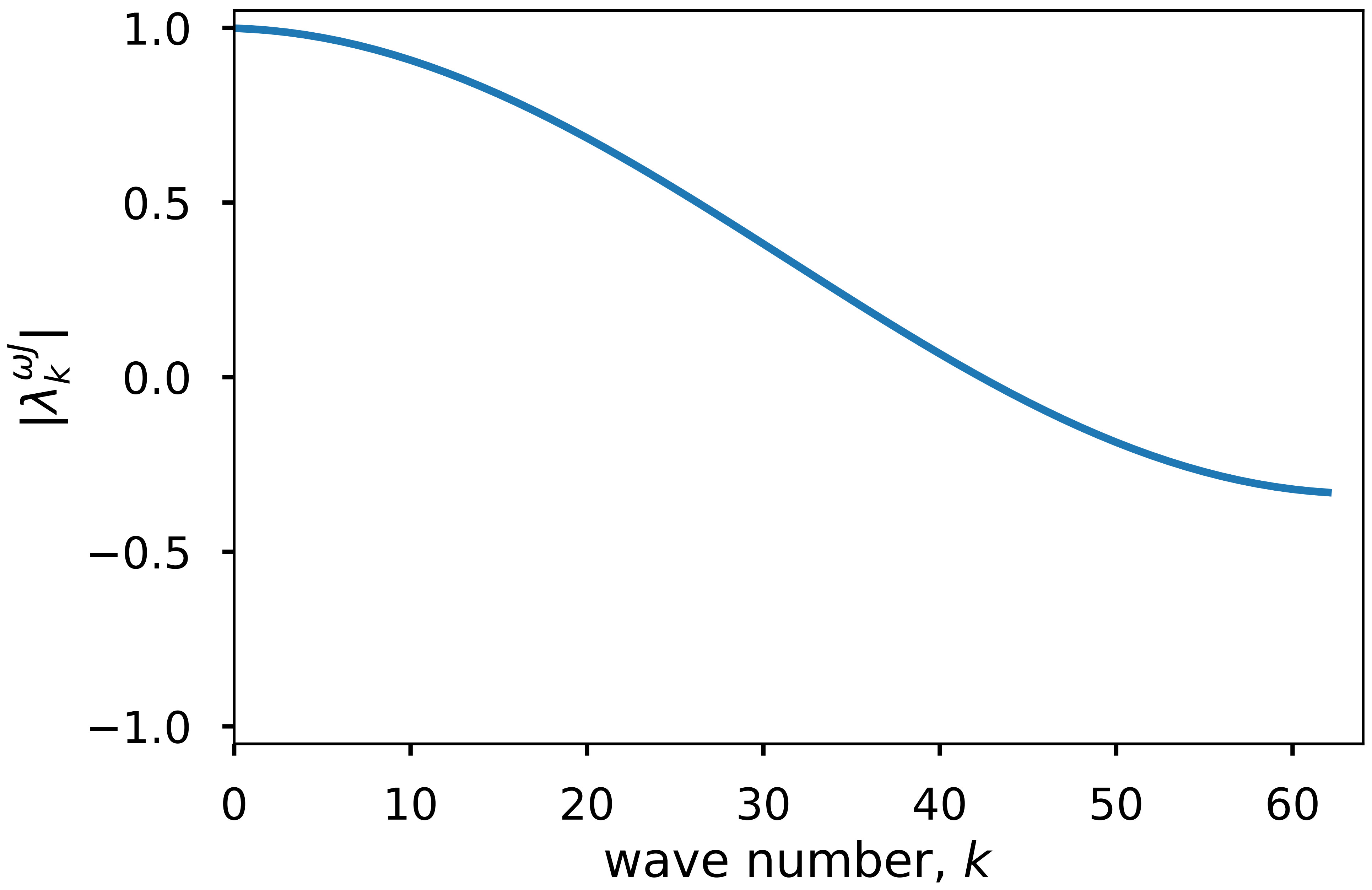
$$G = I - (2/3)D^{-1}A \longrightarrow \lambda_k = 1 - \frac{2}{3}\cdot\frac{1}{2}\cdot 4 \cdot \sin^2\left(\frac{k\pi}{2(n+1)}\right)$$

The spectral radius is almost the same, but…

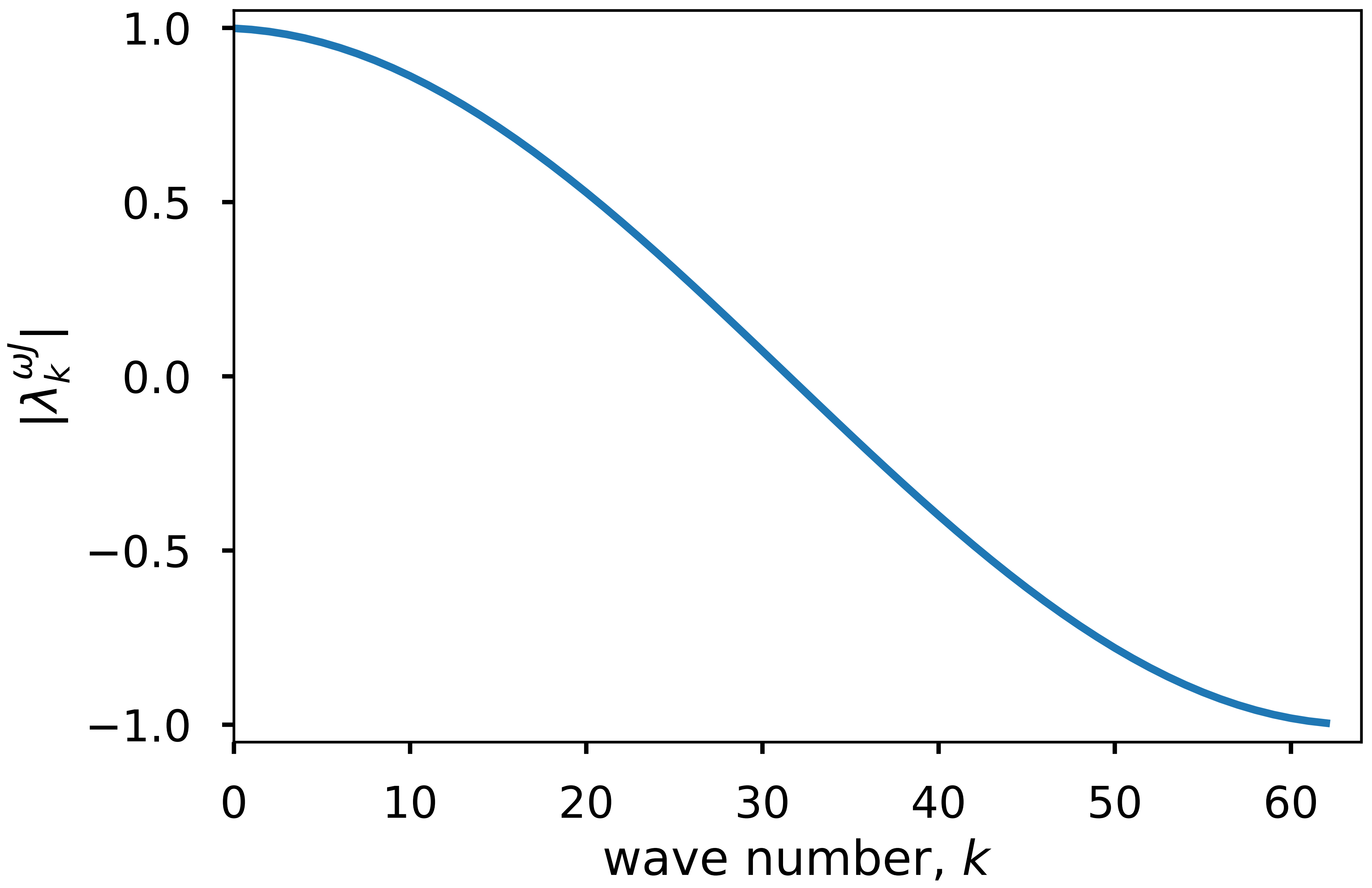
Weighted Jacobi

- If we look at the spectrum:
    - Weighted Jacobi dampens modes that are highly oscillatory

$$\omega = 2/3$$



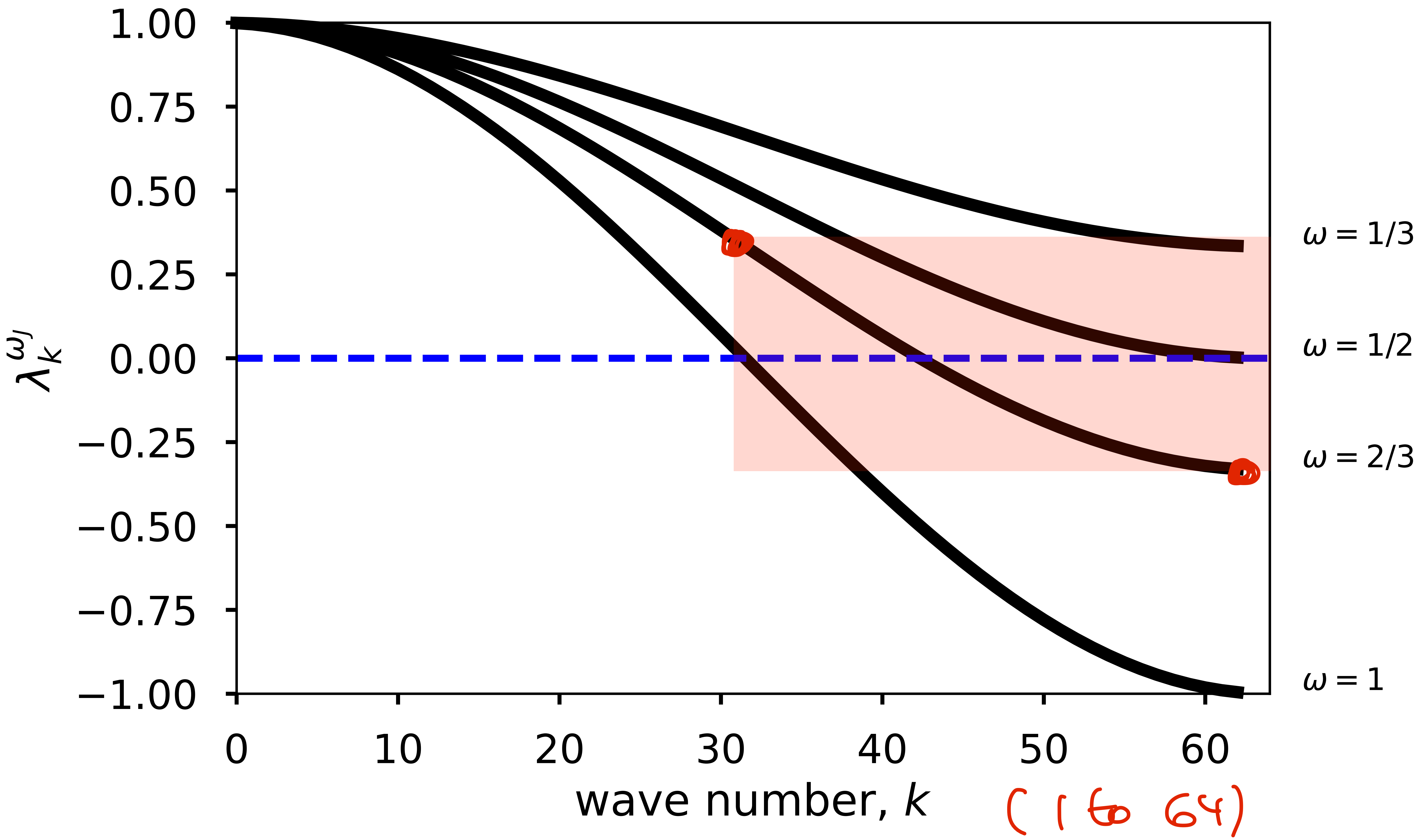
$$\omega = 1$$



Take a look: `02-relaxation-Jacobi.ipynb`

Weighted Jacobi

- Selecting 2/3 balances the reduction in error in the **high** modes

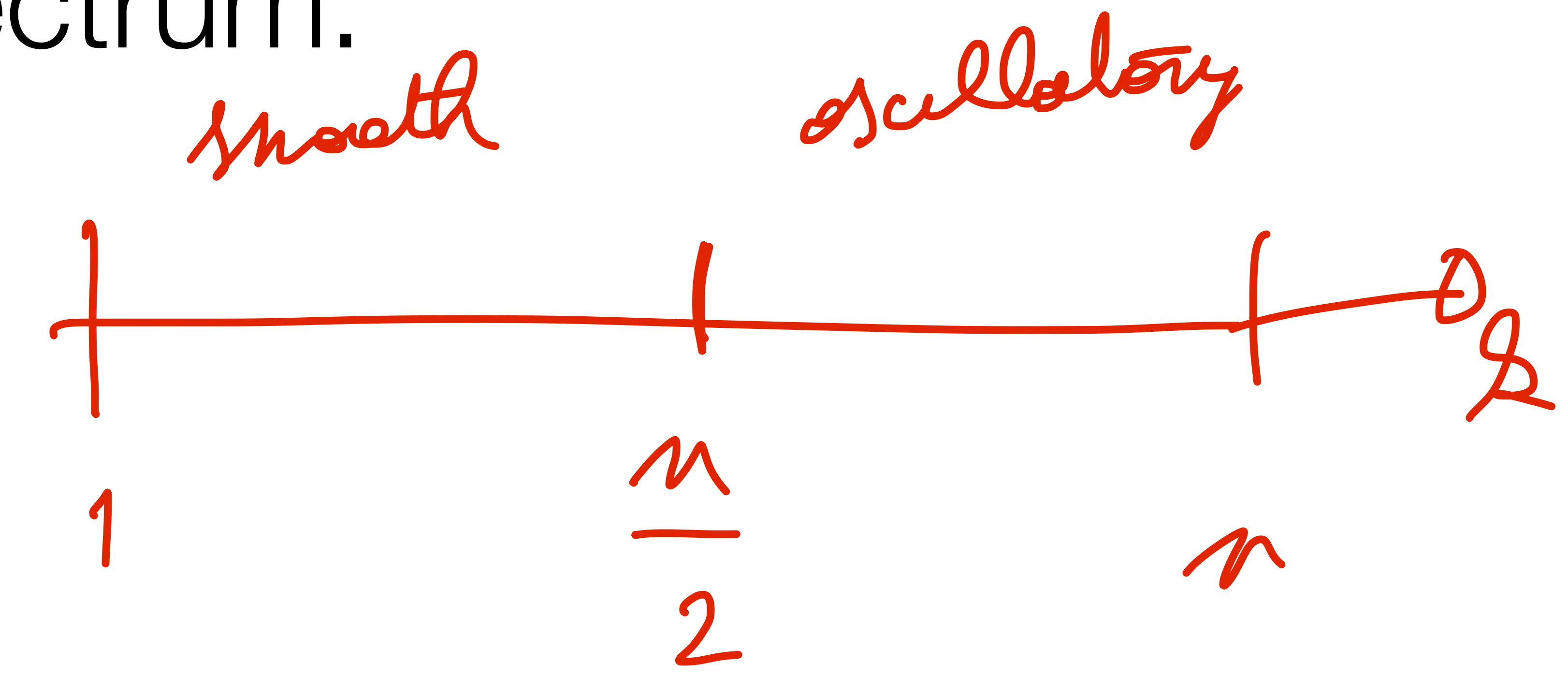


$(n = 64)$

The multigrid smoothing factor

- The **smoothing factor** of relaxation method G is the maximum magnitude of the upper half of the spectrum:

$$\max_{k \in [n/2, n]} |\lambda_k^G|$$



- A desired feature for relaxation:

$$\boxed{\begin{array}{c}\textbf{Oscillatory}\text{ modes are quick to converge}\\ \textbf{Smooth}\text{ modes are slow to converge}\end{array}}$$

Multigrid Step #1: pick a smoother

(A) relaxation on the fine grid

- For $\omega = 2/3$

$$|\lambda_{n/2}| = |\lambda_n| = 1/3$$

- For $\omega = 1$

$$|\lambda_{\cancel{n/2}}| = |\lambda_n| = 1$$

1

$$|\lambda_{\frac{n}{2}}| \approx 0$$

- Jacobi is not a smoother (weighted *is*)

Take a look: `03-smooth-error.ipynb`

An important observation on "smoothness"

- So far, we've mainly looked at

$$Au = 0$$

- In general we need to consider

$$Au = f$$

- If we **smooth** with

$$u \leftarrow u + \omega D^{-1} r$$

$e_1 = G e_0$

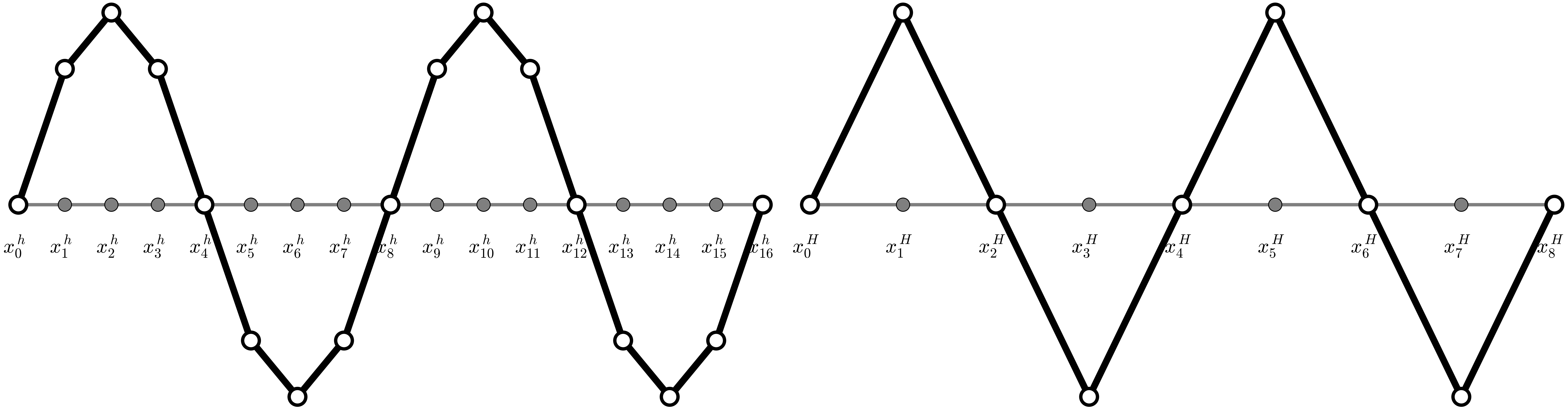
then the **error** is smooth, not (necessarily the solution).

Coarse Grids

B use coarse-grid correction to remove smooth fine-level error modes

- Smooth modes look like oscillatory modes when sampled on a coarse grid
- 4-mode of 15 **versus** 4-mode of 7

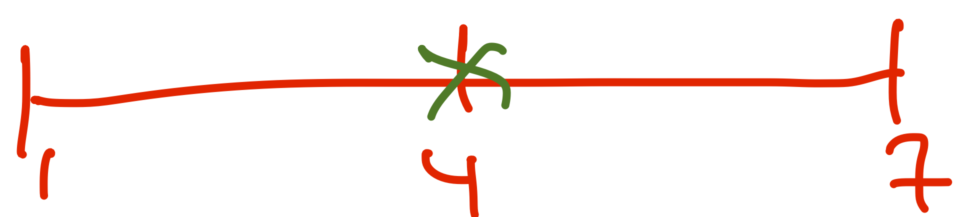
→ use relaxation on coarse grid ∇



$k=4,\ n=15$ $k=4,\ n=7$

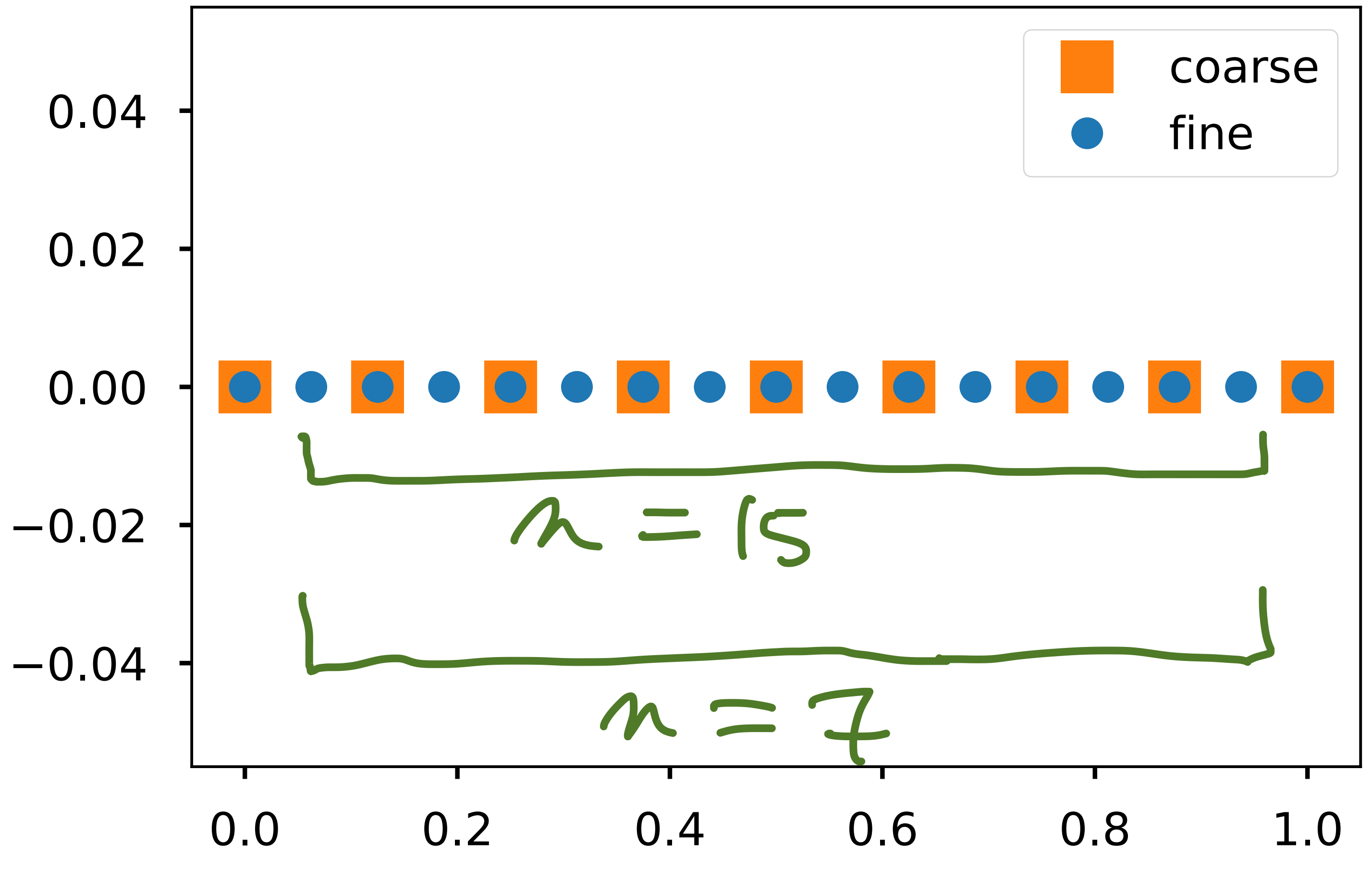
This looks like a “smooth” mode

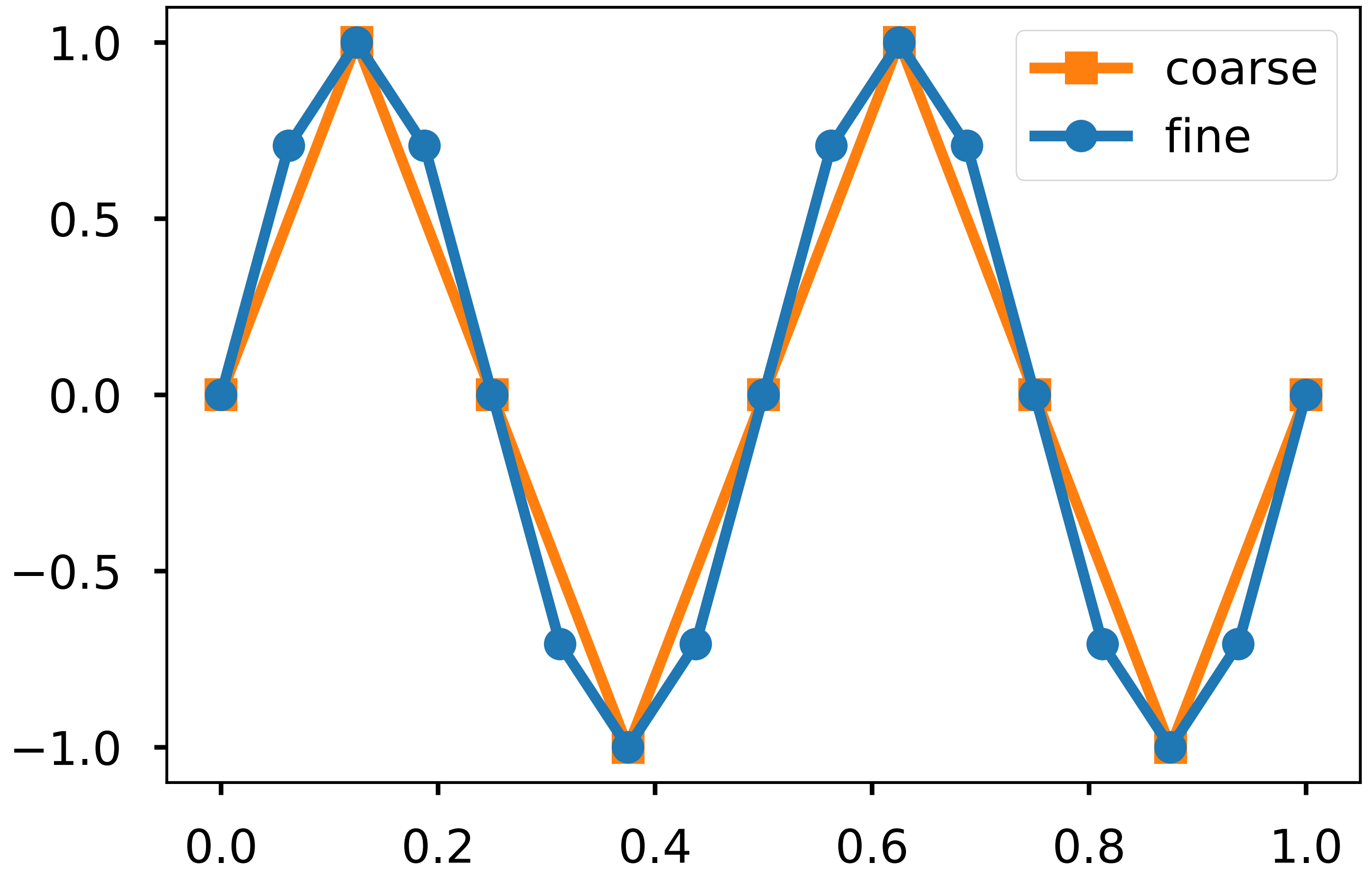
This looks like an “oscillatory” mode



Coarse modes $\left(k \in \left[1, \frac{n-1}{2}\right]\right)$

$h = \frac{1}{n+1}$





4 fine

4 coarse

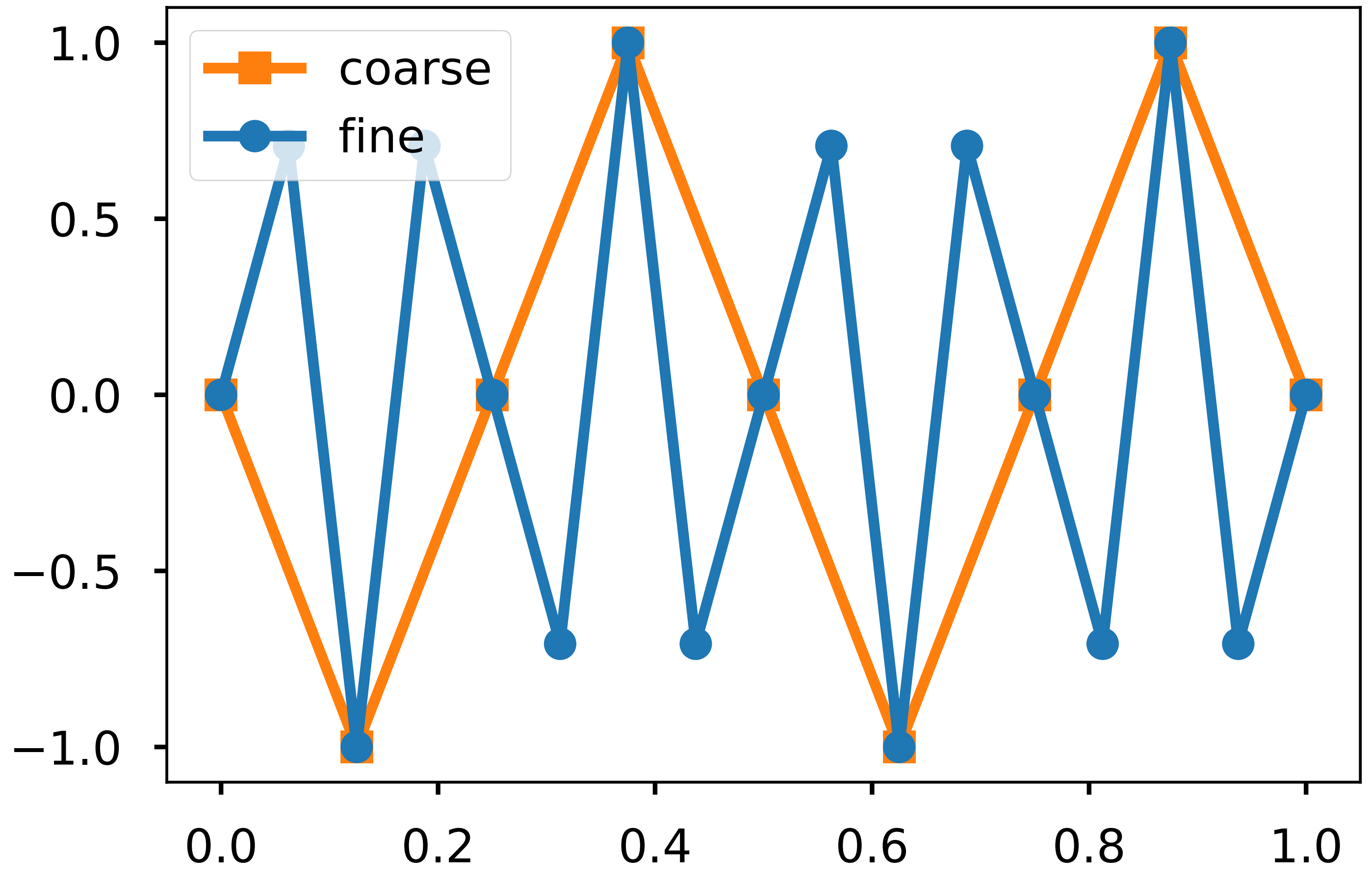
mode 4 of 15

$$(v_k)_j = \sin\frac{jk\pi}{n+1}$$ Fine mode

$$(v_k)_{2j} = \sin\frac{2jk\pi}{n+1}$$ Fine mode (every other)

$$= \sin\frac{jk\pi}{(n+1)/2}$$ Coarse mode

$$= (\hat{v}_k)_j$$



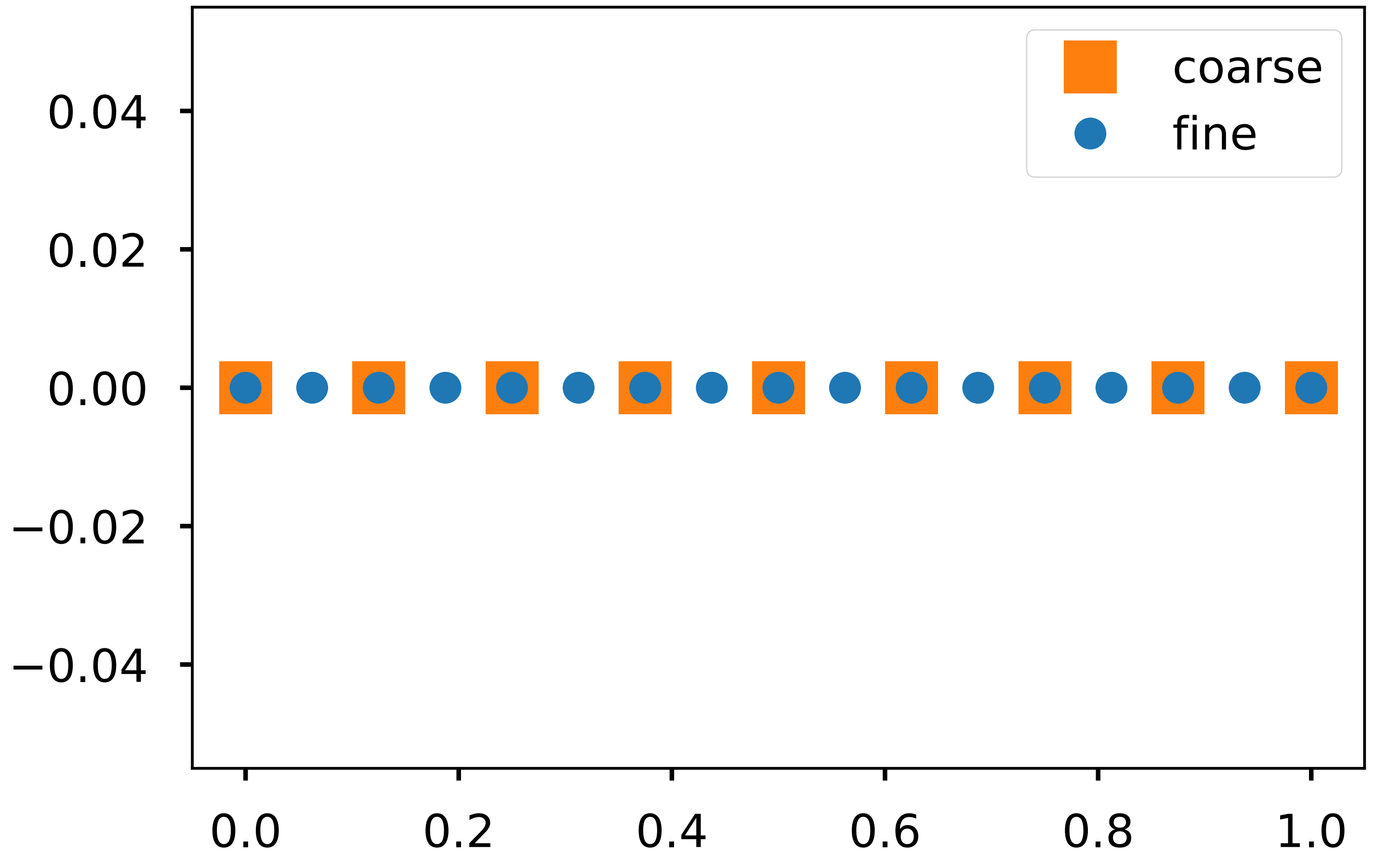
12 fine becomes −4 coarse

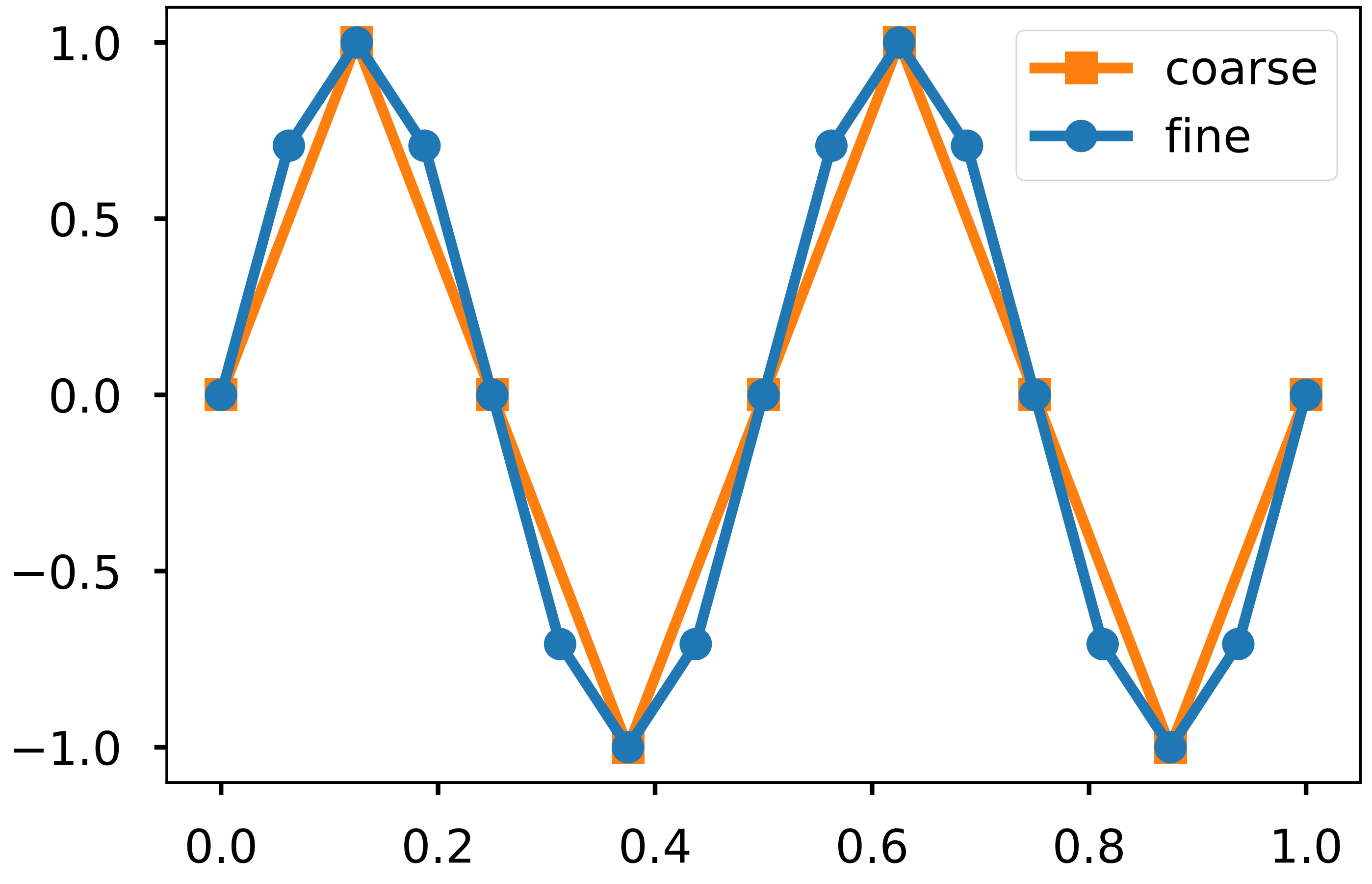
mode 12 of 15

For low modes, k-modes are preserved

Take a look: `04-coarse-modes.ipynb`

Coarse modes $\left(k \in \left[\frac{n+1}{2}, n\right]\right)$





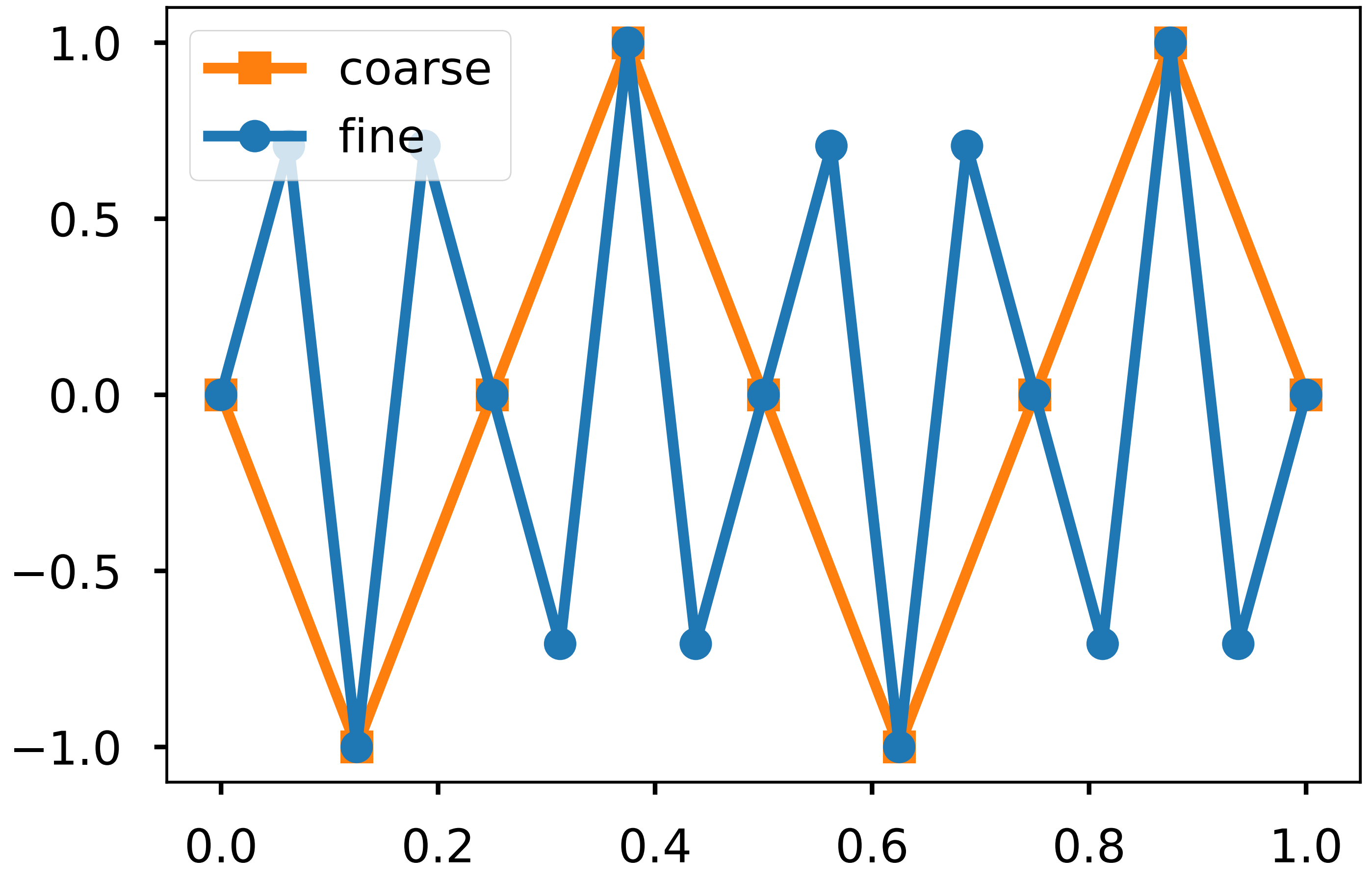
mode 4 of 15

$$(v_k)_{2j} = \sin\frac{2jk\pi}{n+1}$$ Fine mode

$$= -\sin\frac{2j(n-k)\pi}{n+1}$$ Fine mode (every other)

$$= -\sin\frac{j(n-k)\pi}{(n+1)/2}$$ Coarse mode

$$= -(\hat{v}_{n-k})_j$$

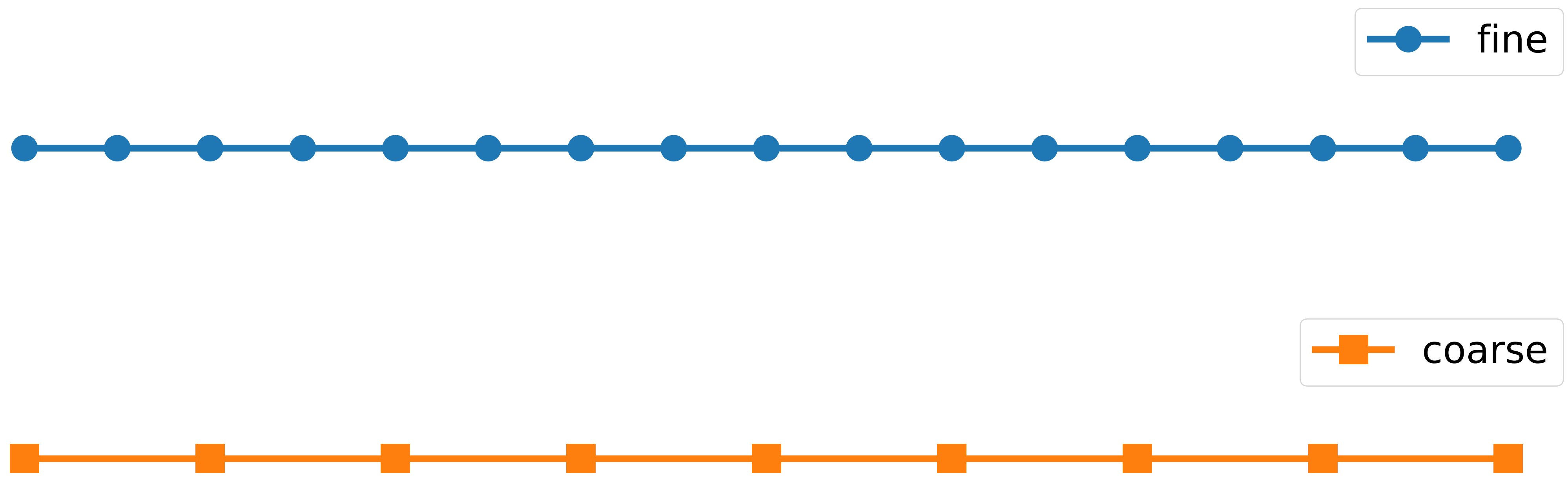


12 fine becomes −4 coarse

mode 12 of 15

For high modes, k-modes are *aliased*

Questions to resolve…



- How to transfer between **fine** and **coarse**?

(we want to use relaxation on coarse grid to correct fine grid)

- What do we do to "solve" on a coarse grid?

(relax to efficiently remove slow-to-converge fine-grid error)

What to use to transfer…

- Return to our projection problem: (optimal coarse-grid correction)

$$x_1 = \overbrace{x_0}^{\text{after five relaxation}} + \underbrace{V}_{15\times 7}\underbrace{(V^T A V)^{-1}}_{7\times 7}\underbrace{V^T}_{7\times 15}\underbrace{r_0}_{15\times 1}$$

- If we have a smoothing property, then smoothing a few times will leave smooth error.
- coarse-grid correction: project e_0 onto range of V, and subtract the projection
- Let’s construct V from say continuous piecewise linears

Interpolation P: from coarse to fine

- Consider coarse grid

$$\Omega^{2h}$$

- and fine grid

$$\Omega^{h}$$

- Construct an operator

$$P : \Omega^{2h} \to \Omega^{h}$$

$$P = \begin{array}{cc} & 7 \\ 15 & \begin{bmatrix} \quad & \quad \\ \quad & \quad \end{bmatrix} \end{array}$$

- Such that

$$Pv^{2h}$$

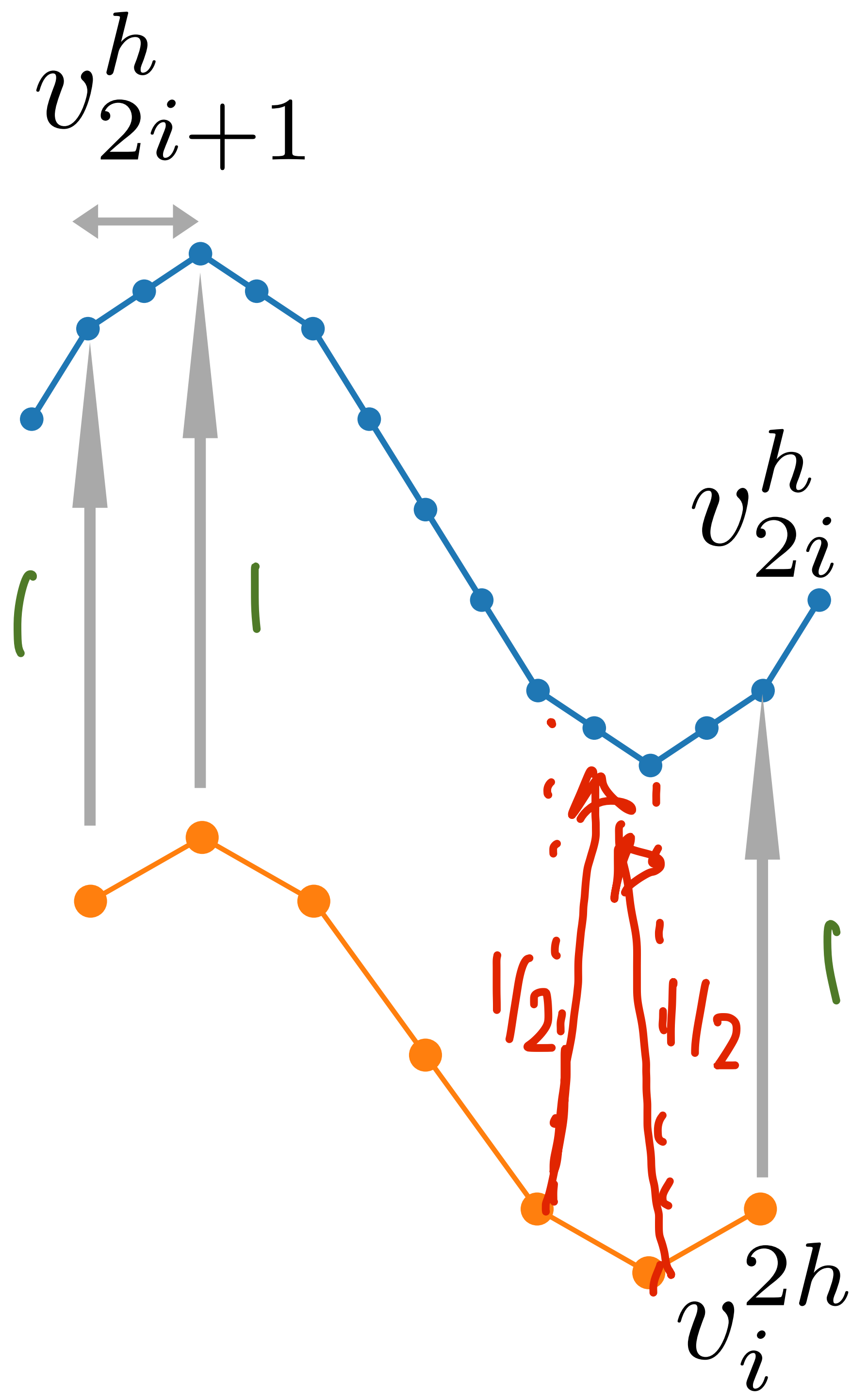
is continuous and piecewise linear

$(P = V)$

Interpolation P: from coarse to fine

$$v^h_{2i} = v^{2h}_i$$ Injection

$$v^h_{2i+1} = \frac{1}{2}(v^{2h}_i + v^{2h}_{i+1})$$ Average (linear interp)



15

4

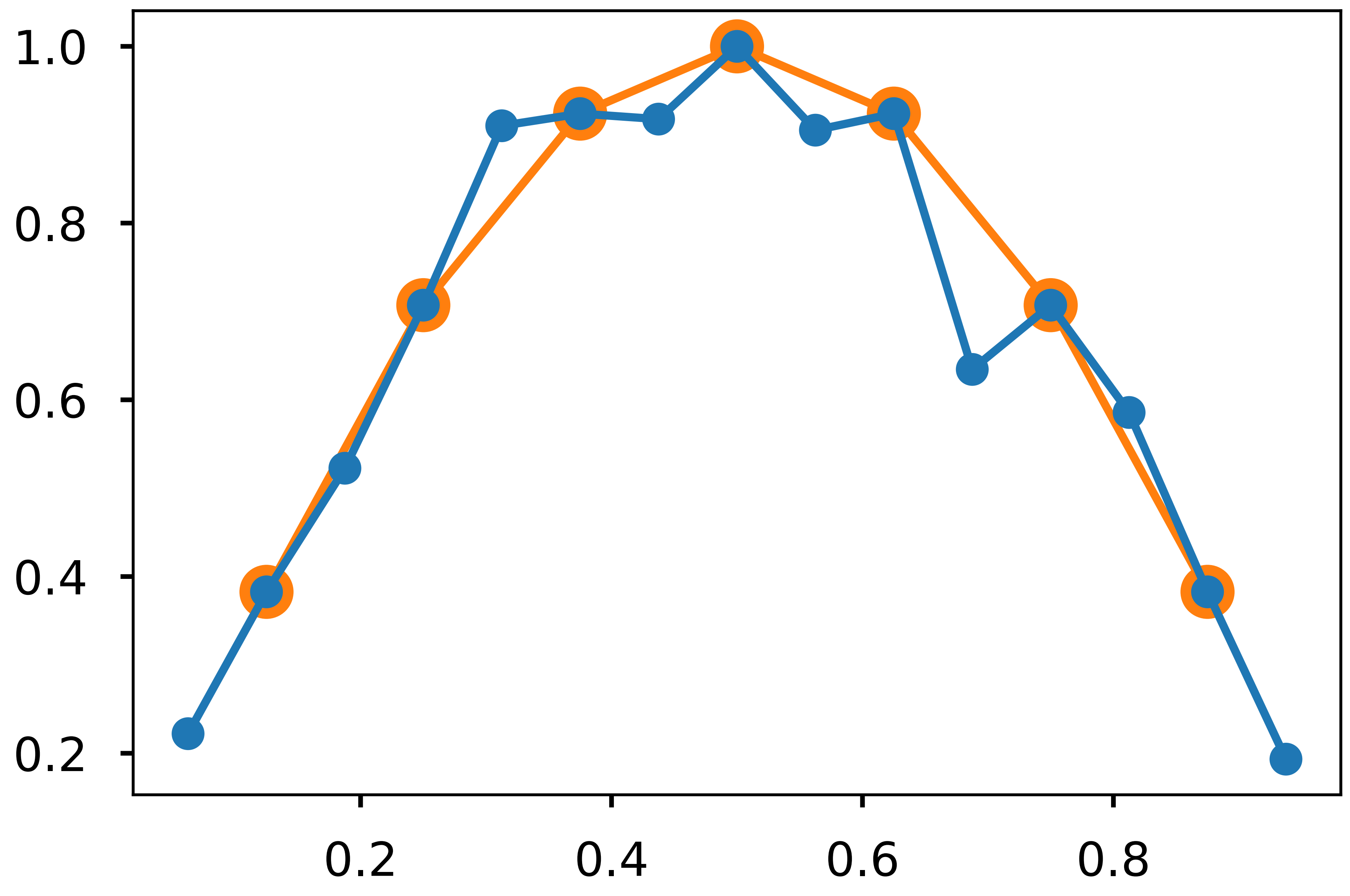
7

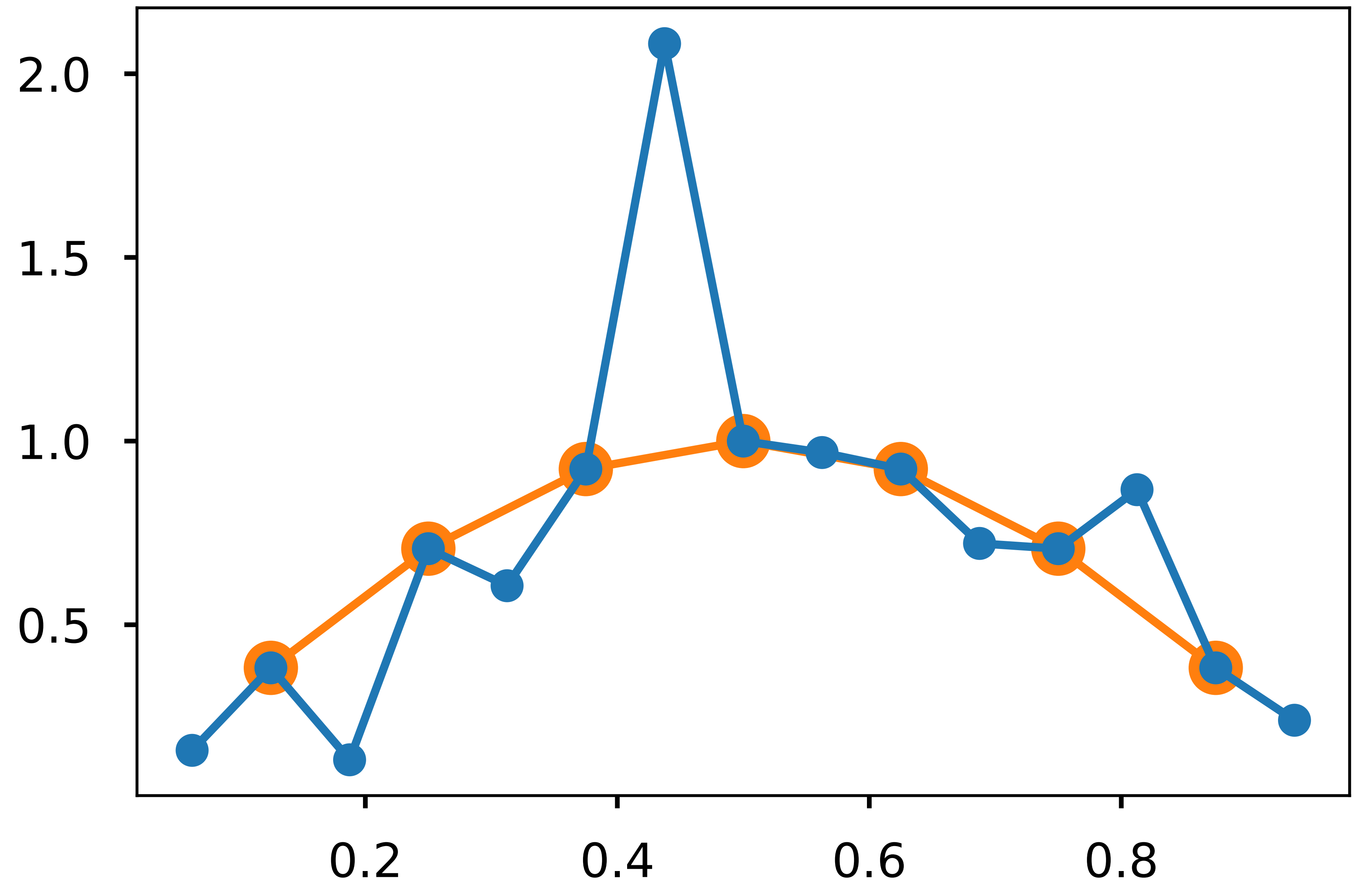
- Values at points common to both grids are reused (injected)

Interpolation

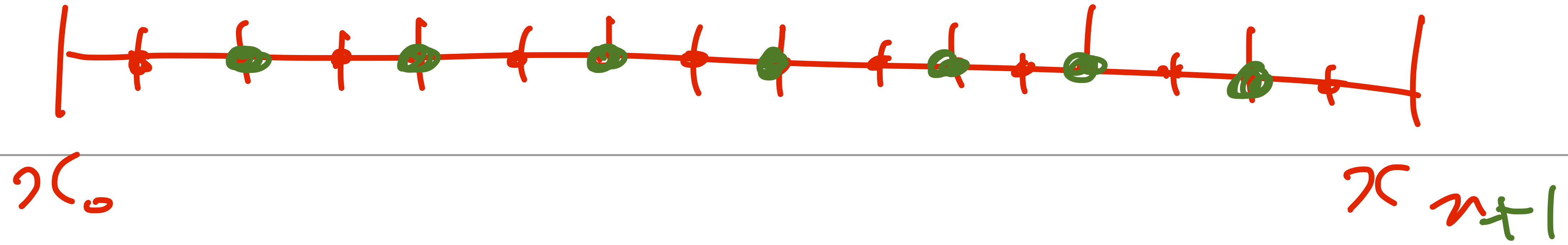
- interpolation gives smooth result

(we want to correct smooth error on the fine grid)

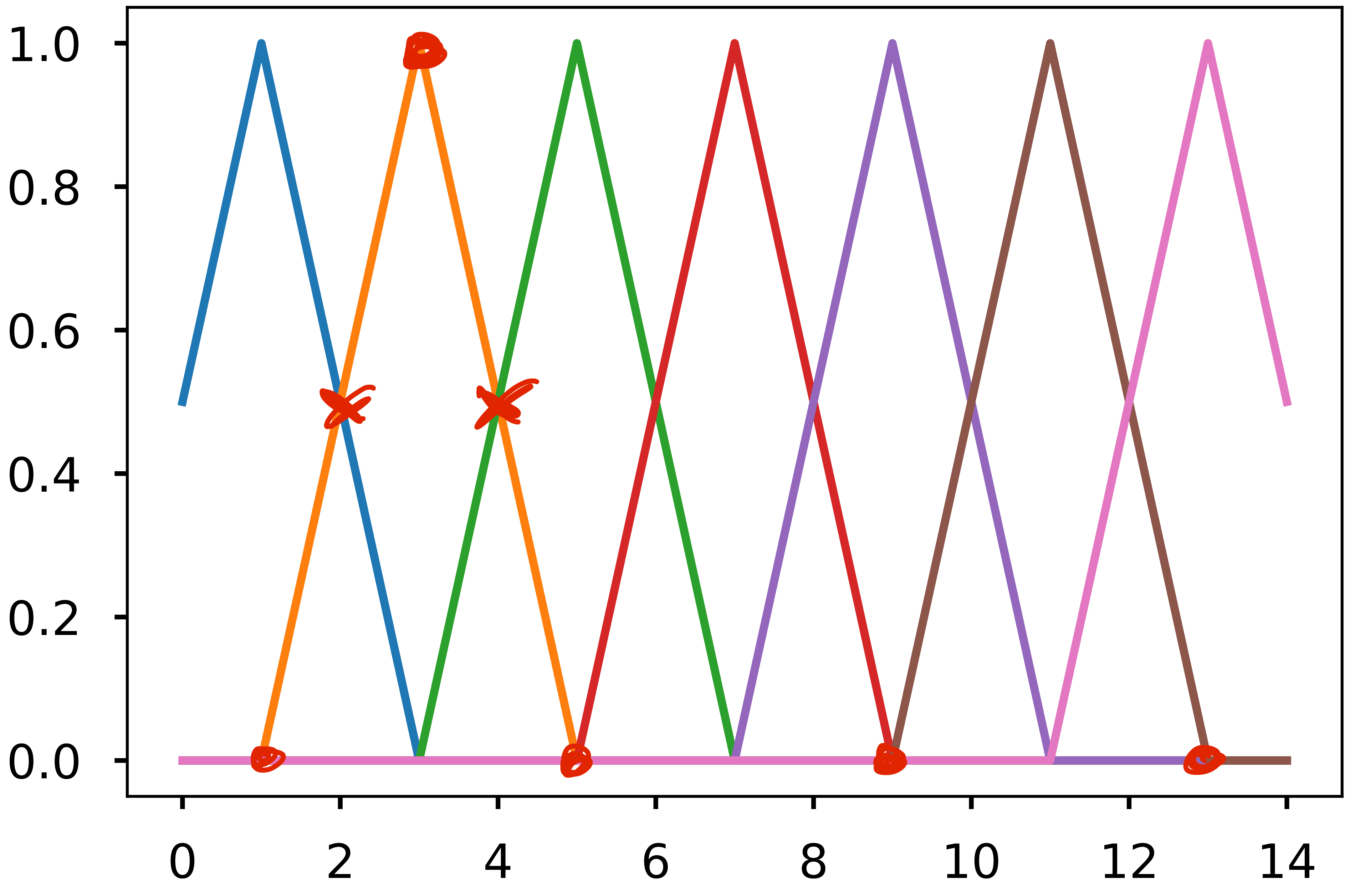




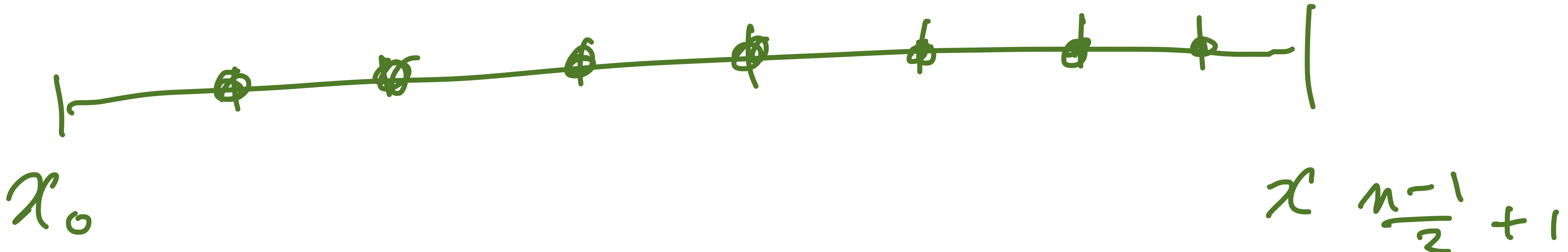
In matrix form



$$P = \frac{1}{2}\begin{bmatrix}
1. & & & & & & \\
2. & & & & & & \\
1. & 1. & & & & & \\
 & 2. & & & & & \\
 & 1. & 1. & & & & \\
 & & 2. & & & & \\
 & & 1. & 1. & & & \\
 & & & 2. & & & \\
 & & & 1. & 1. & & \\
 & & & & 2. & & \\
 & & & & 1. & 1. & \\
 & & & & & 2. & \\
 & & & & & 1. & 1. \\
 & & & & & & 2. \\
 & & & & & & 1.
\end{bmatrix}$$



- The columns of P are basis functions (right)
- The fine grid vectors, Pv, are linear combinations of these functions
- Notice: P is full rank!



The coarse grid operator

$$x_1 = x_0 + V(V^T AV)^{-1} V^T r_0$$

(sub)space defined by P

$x_1 = x_0 + P(P^T AP)^{-1} P^T r_0$

- If V is defined by $span\{P\}$ —or just P,

- Then V^T defines **restriction** as P^T

- And the **coarse level operator** is defined by $P^T AP$

└ optimal coarse-grid correction, given V
(minimizes $\|e_1\|_A$)

Take a look: `06-multigrid-two-level.ipynb`

Two level method

$$x_1 = x_0 + V(V^T A V)^{-1} V^T r_0$$

$$\downarrow$$

$$x_1 = x_0 + \underbrace{P(P^T A P)^{-1} P^T r_0}_{\hat{e}_c}$$

• Given	x_0		• What should this be?
• Smooth a few times	$x_0 \leftarrow x_0 + \omega D^{-1} A r_0$		• How many times
• Form residual	$r_0 = b - A x_0$		
• Restrict the residual	$P^T r_0$		
• Solve the coarse problem	$P^T A P \hat{e}_c = P^T r_0$	$A_c \hat{e}_c = r_c$	• What does this mean?
• Interpolate the approx error	$P\hat{e}_c$		• What are we interpolating?
• Correct the initial guess	$x_0 + P\hat{e}_0$		• Are we done?

$x_1 = x_0 + e_{CGC}$

find "good" e_{CGC} (to remove smooth fine-level error)

note $A e_0 = r_0$ (e_0 is smooth after fine-level relaxation)

$(x^* = x_0 + e_0)$

find coarse approximation of current e_0

$P^T A e_0 = P^T r_0$ let $e_0 \simeq P \hat{e}_c$

solve $\boxed{P^T A P \hat{e}_c = P^T r_0}$

(choose P such that its range contains smooth fine-level errors)

correct $x_1 \leftarrow x_0 + P \hat{e}_c$

$A_c = P^T A P$ or: $A_c = A_{2h}$

Notes on variants

- An alternative to restriction, is injection

$$\begin{bmatrix}
0 & 1 & 0 & & & & & & & & & & & & \\
 & & 0 & 1 & 0 & & & & & & & & & & \\
 & & & & 0 & 1 & 0 & & & & & & & & \\
 & & & & & & 0 & 1 & 0 & & & & & & \\
 & & & & & & & & 0 & 1 & 0 & & & & \\
 & & & & & & & & & & 0 & 1 & 0 & & \\
 & & & & & & & & & & & & 0 & 1 &
\end{bmatrix}$$

- Or a weighted transpose of linear interpolation (to restrict constants exactly)

$$\frac{1}{4}\begin{bmatrix}
1 & 2 & 1 & & & & & & & & & & & & \\
 & & 1 & 2 & 1 & & & & & & & & & & \\
 & & & & 1 & 2 & 1 & & & & & & & & \\
 & & & & & & 1 & 2 & 1 & & & & & & \\
 & & & & & & & & 1 & 2 & 1 & & & & \\
 & & & & & & & & & & 1 & 2 & 1 & & \\
 & & & & & & & & & & & & 1 & 2 & 1
\end{bmatrix}$$

- An alternative to $A_c = P^T A_h P$ is to rediscretize $A_c = A_{2h}$

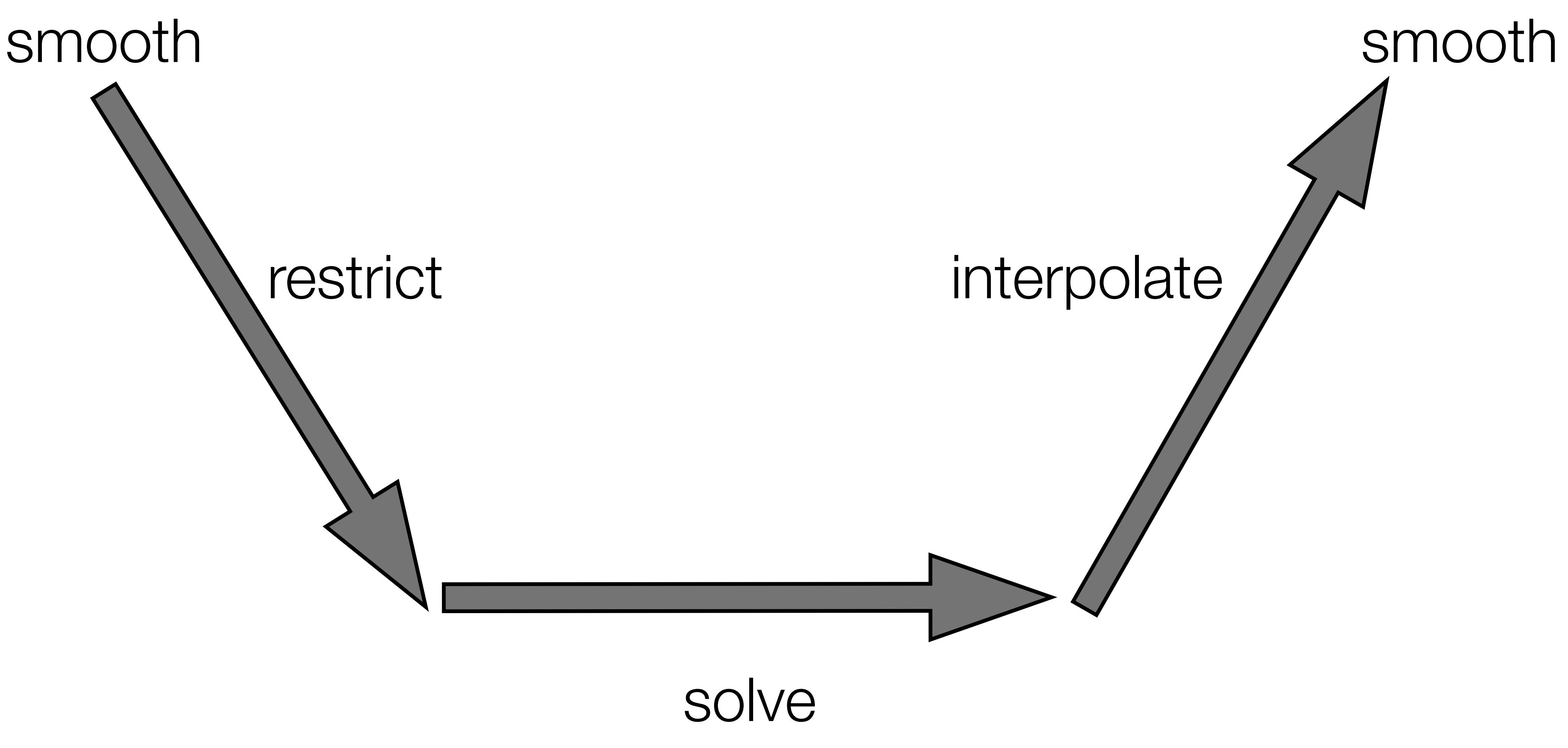
$$x_1 \leftarrow x_0 + P A_{2h}^{-1} R r_0$$

Take a look: `07-multigrid-two-level-matrix-form.ipynb`

Algorithm: two-level multigrid

Input: initial guess $P^T = R$

1. Smooth ν_{pre} times on $Au = f$
2. Compute $r = f - Au$
3. Compute $r_c = Rr$
4. Solve $A_c e_c = r_c$
5. Interpolate $\hat{e} = P e_c$
6. Correct $u \leftarrow u + \hat{e}$
7. Smooth ν_{post} times on $Au = f$



A two-level “V” cycle

How Accurate is Multigrid?

- Consider the exact solution to the PDE u^*

$$-u'' = f$$

- The exact solution to the **discrete** problem u_h^*

$$Au = b$$

- The approximate **discrete** solution $u_h \approx u_h^*$

- Define

$u^* - u_h^*$ Discretization error

$u_h^* - u_h$ Algebraic error

How Accurate should Multigrid aim to be?

- Would like the total error bounded

$$\begin{aligned}\|u^* - u_h\| &\le \overbrace{\|u^* - u_h^*\|}^{\text{disc.}} + \overbrace{\|u_h^* - u^h\|}^{\text{alg.}} \\ &\le \varepsilon\end{aligned}$$

- To achieve this,

  —force the discretization (grid space) so that

$$\|u^* - u_h^*\| \le ch^2 \le \frac{\varepsilon}{2}$$

  —and the algebraic error (convergence) up to the discretization error

$$\|u_h^* - u^h\| \le \frac{\varepsilon}{2}$$

Multigrid convergence

- Convergence factor of a cycle — the factor by which the error (residual) is reduced (in some norm) in each iteration

$$\gamma$$

$$\gamma^m = c\, n^{-2}$$

…assume this is independent of n

$$m \log \gamma = \log c - 2 \log n$$

- Wish to have m cycles such that

$$\gamma^m \sim \mathcal{O}(n^{-2}) \leq \frac{\varepsilon}{2}$$

- Then we need

$$m \sim \mathcal{O}(\log n)$$

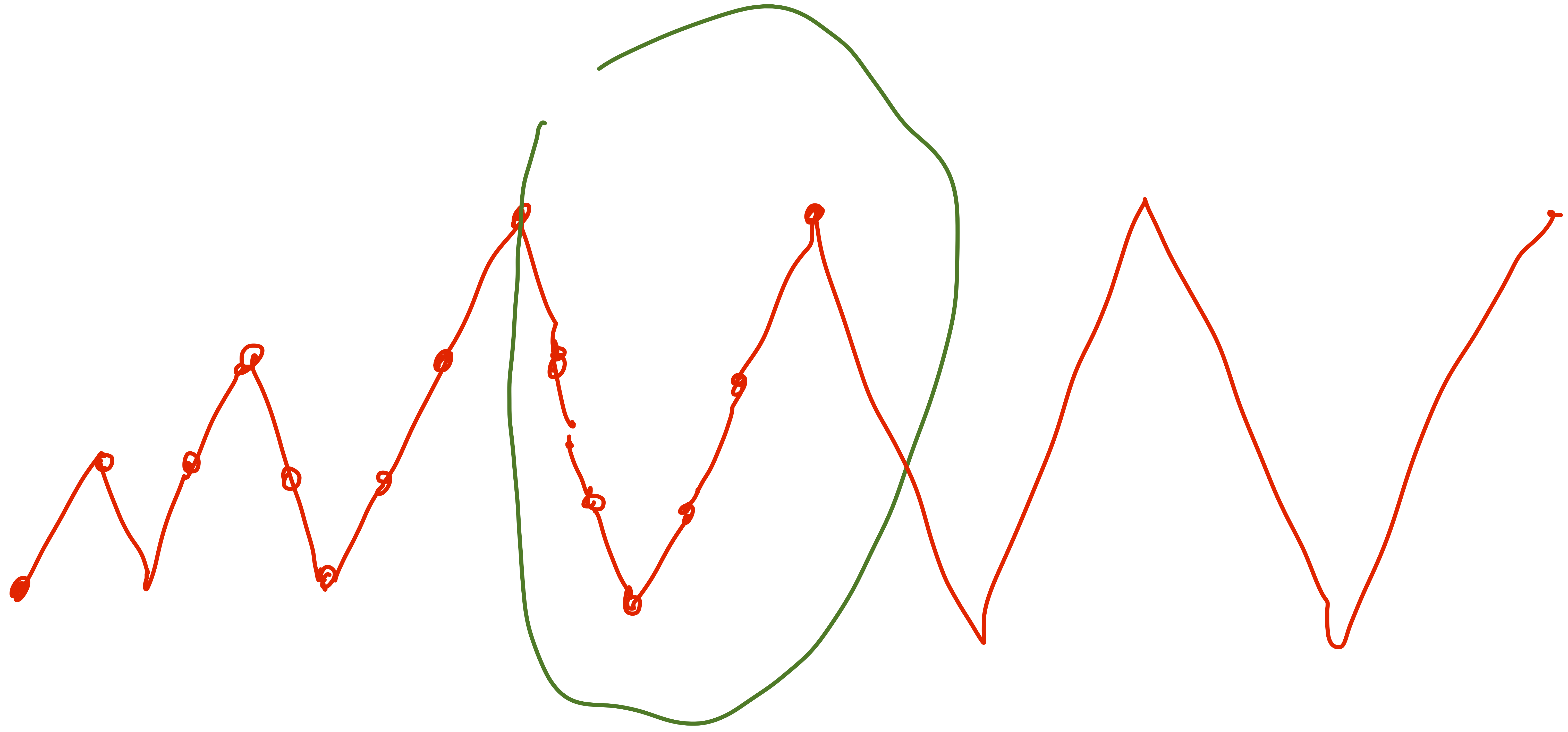
$$W = O(n \log n)$$

cycles

want $W = O(n)$

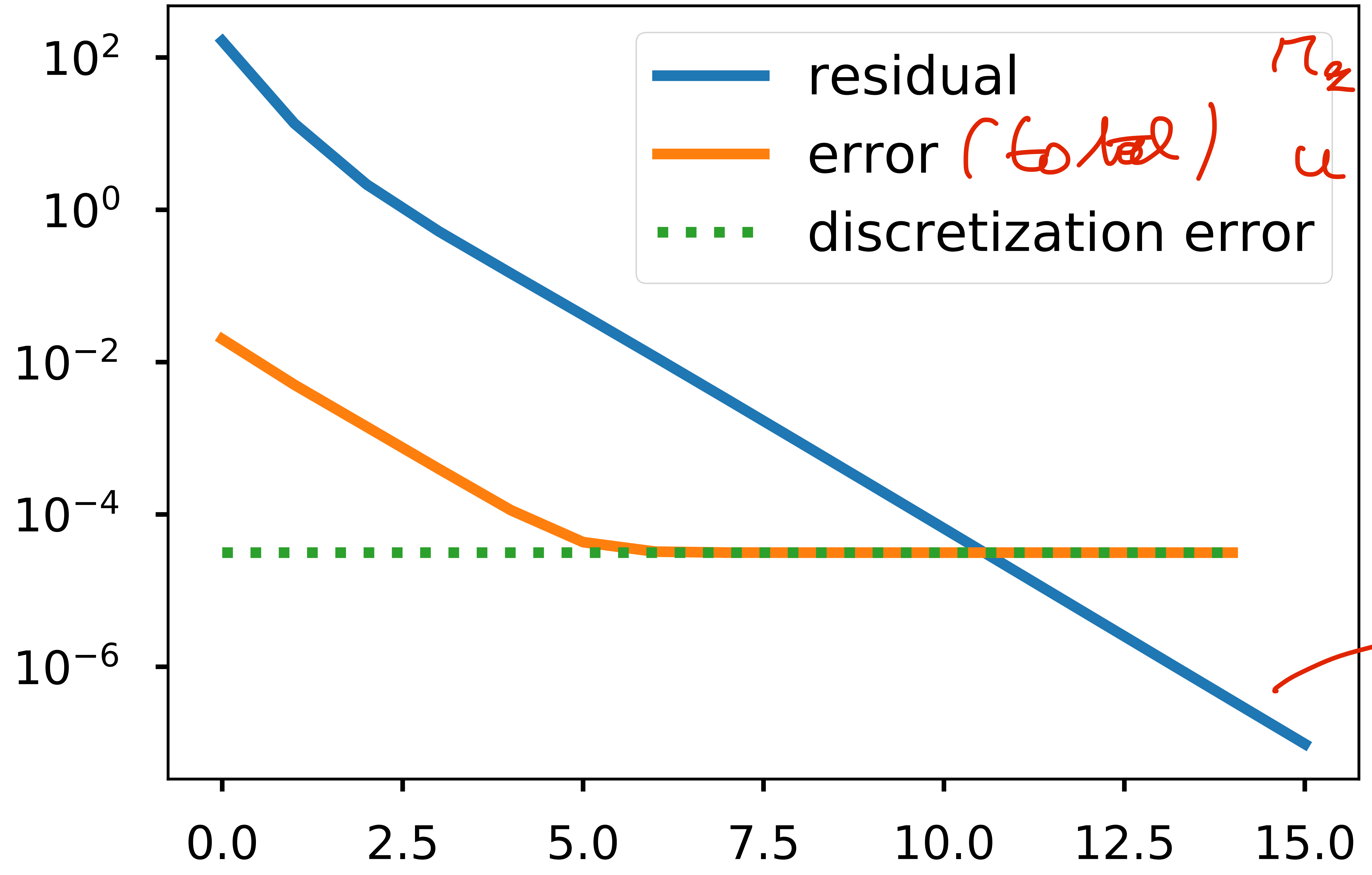
Full Multigrid (FMG)

$W = O(n)$



Take a look: `08-multigrid-v-cycle.ipynb`

Algebraic error



$r_\ell = b - A x_\ell$

$u^* - u_\ell$

$u^* - u^*_\ell$

$A(u^*_\ell - u_\ell)$

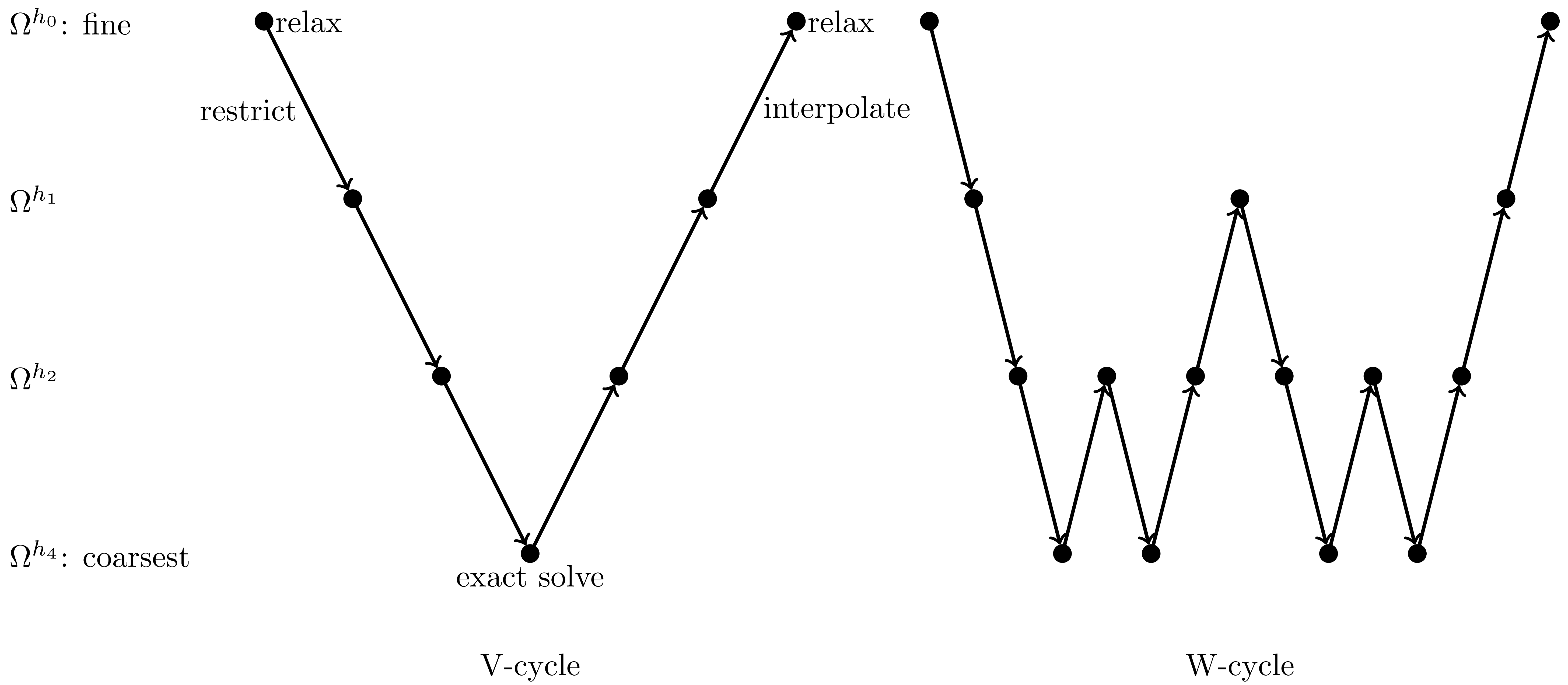
u^*

u^*_ℓ

u_ℓ

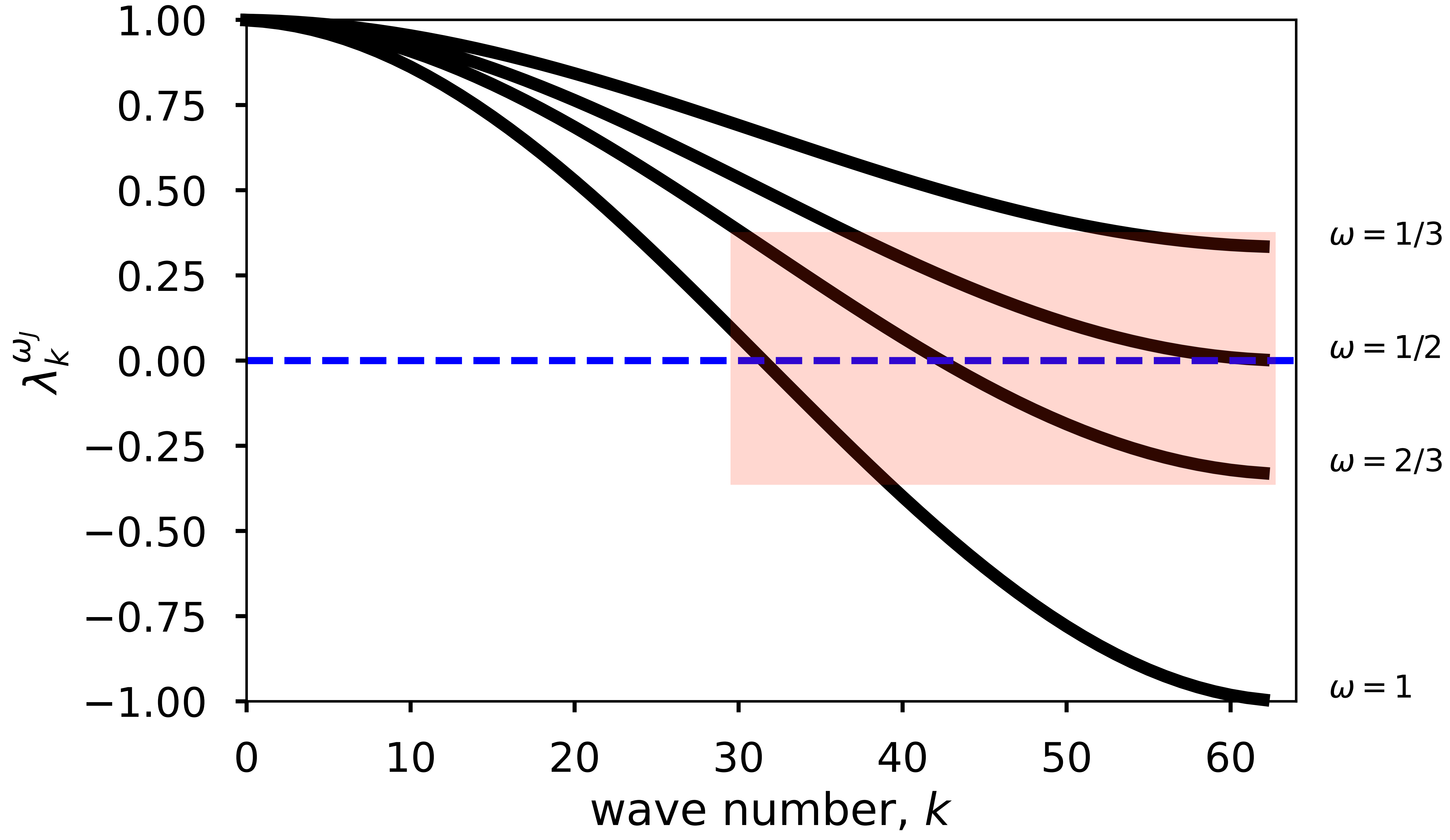
- The total error is limited by the discretization error

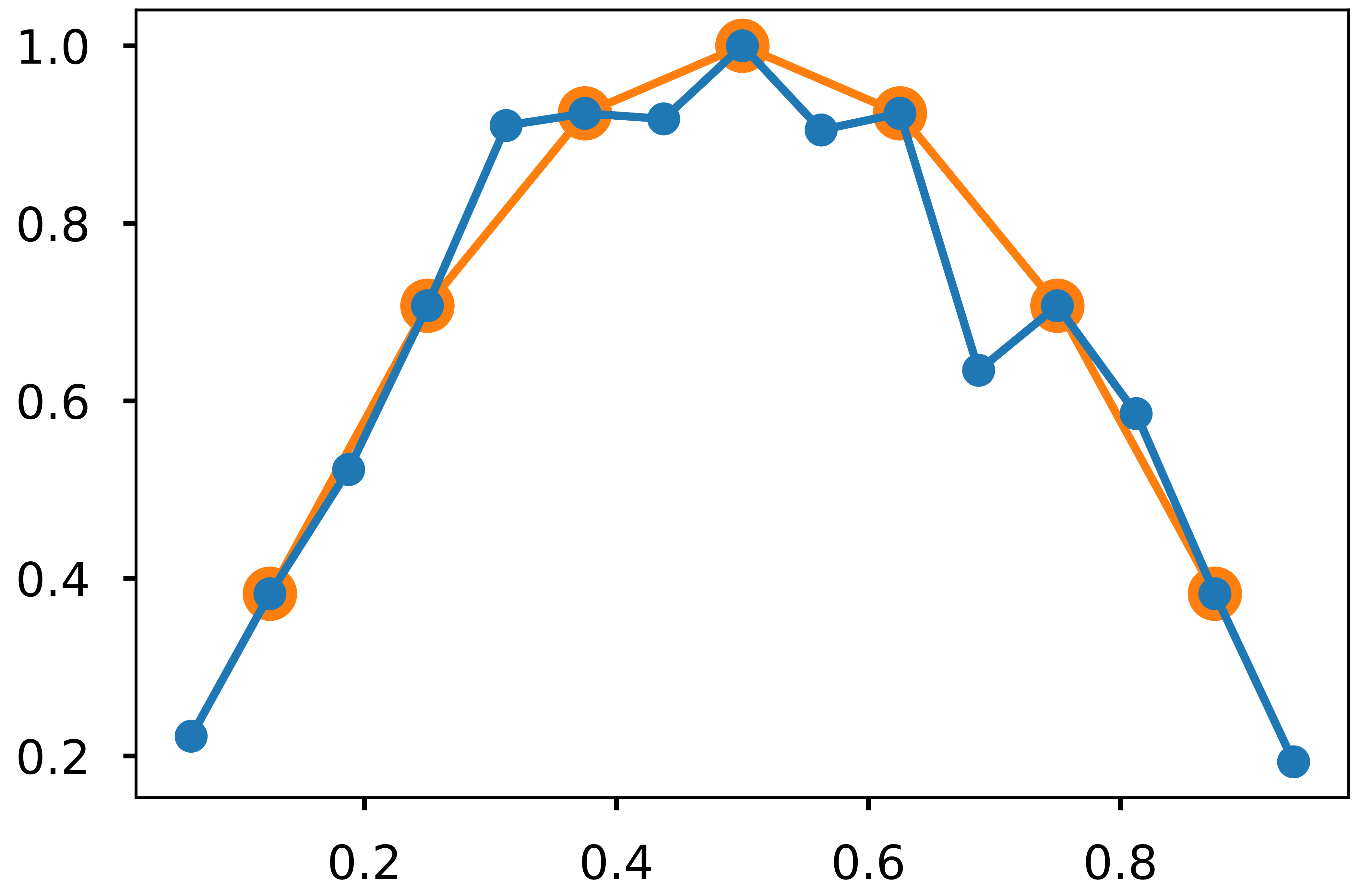
The Multigrid V-Cycle and W-Cycle



- W-Cycle can account for inadequate coarse level solves

Recap…



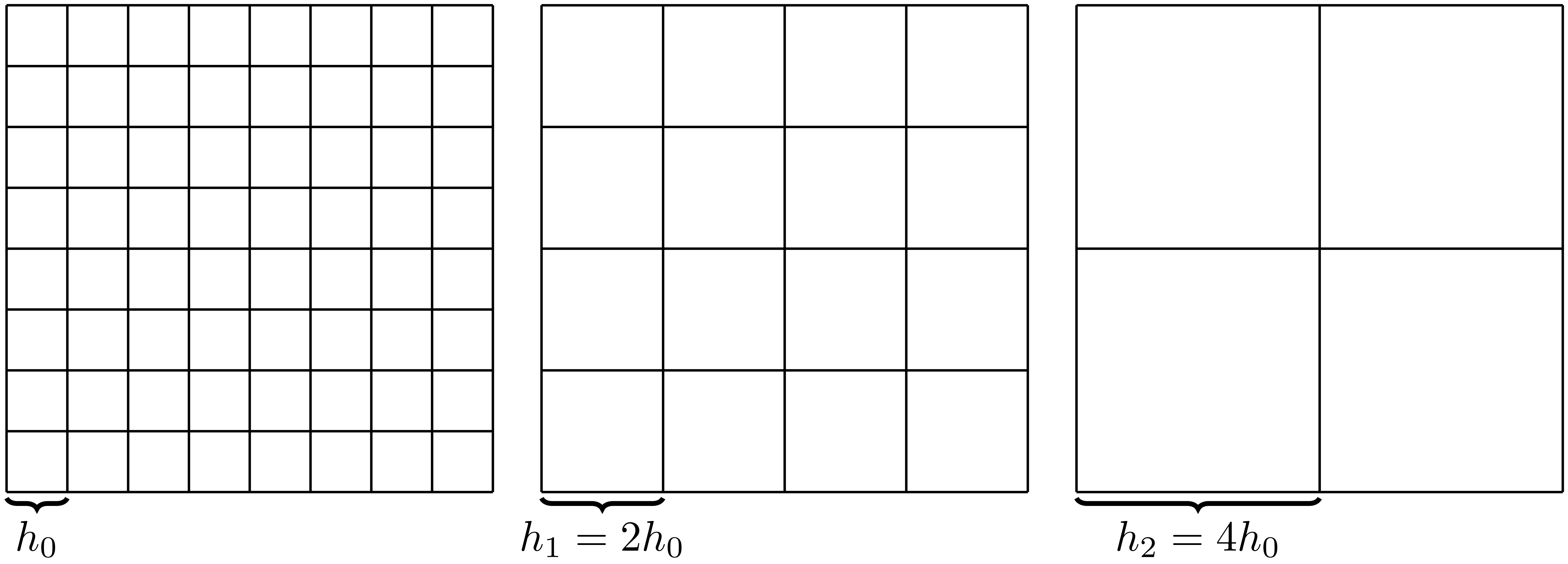


- Smoothing:
  Reduce high frequency error

- Coarse-grid correction:
  Reduce smooth-ish things in the range of interpolation

$$e_1 = e_0 - P(P^TAP)^{-1}P^TA\underbrace{Ge}_{e_0}$$

Multigrid in 2D



- Again, assume we have a sequence of uniform grids
- Relaxation remains the same (what is ω?)

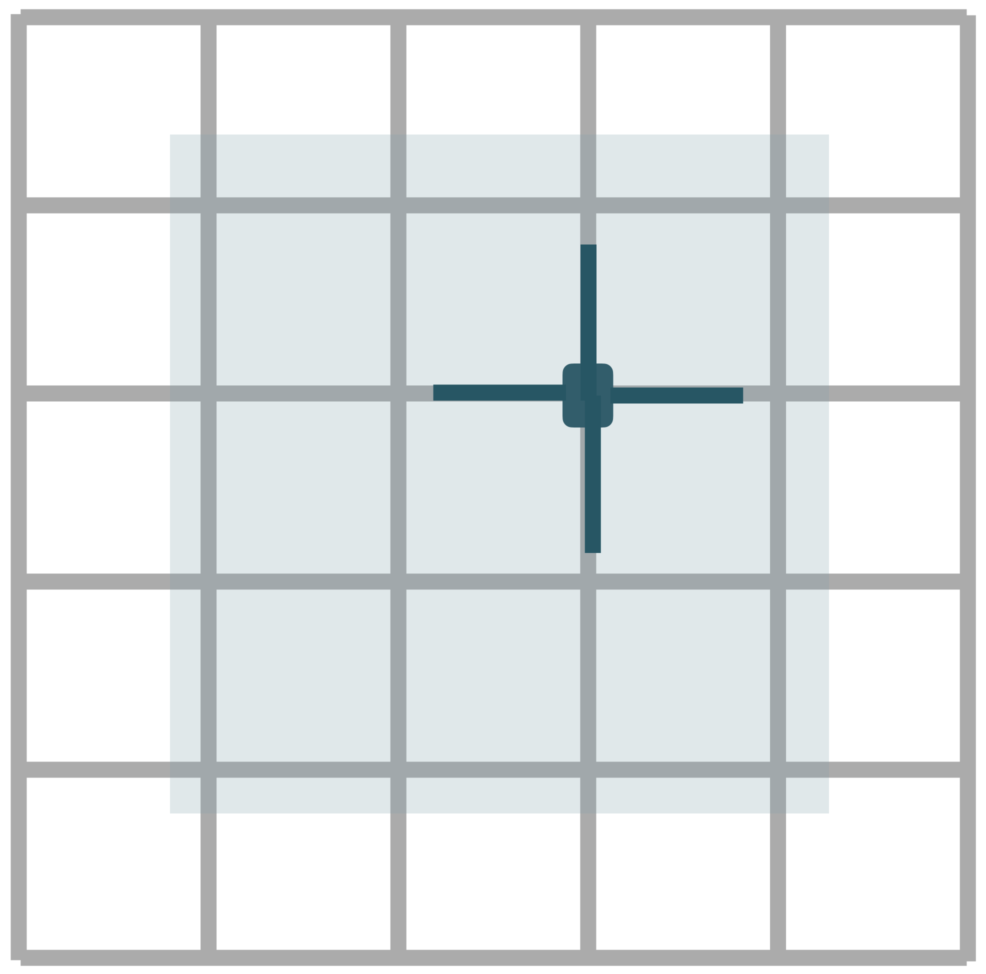
Multigrid in 2D

- Model problem

$$
\begin{aligned}
-u_{xx} - u_{yy} &= f \\
u &= 0 \qquad \text{on boundary}
\end{aligned}
$$

nnz $\approx$ 5n

- Results in the stencil / matrix

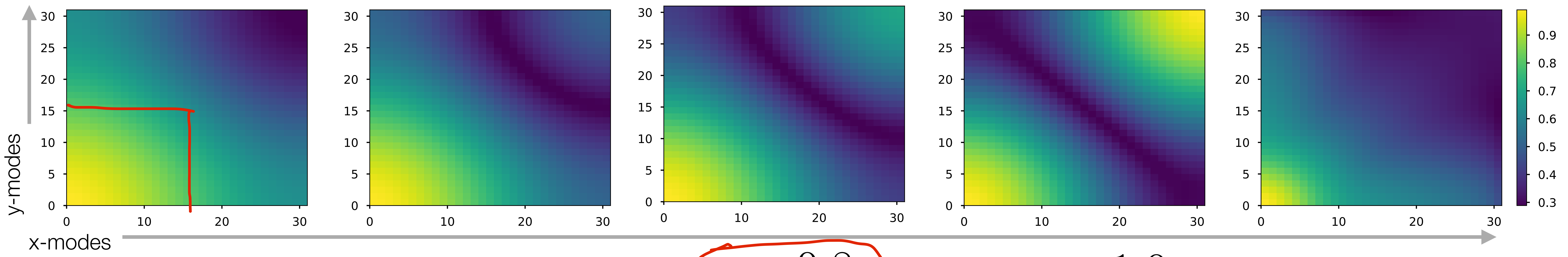


$$
\begin{bmatrix} & -1 & \\ -1 & 4 & -1 \\ & -1 & \end{bmatrix}
\rightarrow
\frac{1}{h^2}
\begin{bmatrix}
4 & -1 & & & -1 & & & & & & & & & & & \\
-1 & 4 & -1 & & & -1 & & & & & & & & & & \\
& -1 & 4 & -1 & & & -1 & & & & & & & & & \\
& & -1 & 4 & & & & -1 & & & & & & & & \\
-1 & & & & 4 & -1 & & & -1 & & & & & & & \\
& -1 & & & -1 & 4 & -1 & & & -1 & & & & & & \\
& & -1 & & & -1 & 4 & -1 & & & -1 & & & & & \\
& & & -1 & & & -1 & 4 & & & & -1 & & & & \\
& & & & -1 & & & & 4 & -1 & & & -1 & & & \\
& & & & & -1 & & & -1 & 4 & -1 & & & -1 & & \\
& & & & & & -1 & & & -1 & 4 & -1 & & & -1 & \\
& & & & & & & -1 & & & -1 & 4 & & & & -1 \\
& & & & & & & & -1 & & & & 4 & -1 & & \\
& & & & & & & & & -1 & & & -1 & 4 & -1 & \\
& & & & & & & & & & -1 & & & -1 & 4 & -1 \\
& & & & & & & & & & & -1 & & & -1 & 4
\end{bmatrix}
$$

Relaxation in 2D

$$\sin\left(\frac{k_x i\pi}{n+1}\right)\sin\left(\frac{k_y j\pi}{n+1}\right)$$

Convergence factor over 10 sweeps



$\omega = 0.5$ $\quad \omega = 0.667$ $\quad \omega = 0.8$ $\quad \omega = 1.0$ $\quad$ GS

$$I - \omega D^{-1}A \qquad\qquad I - (D-E)^{-1}A$$

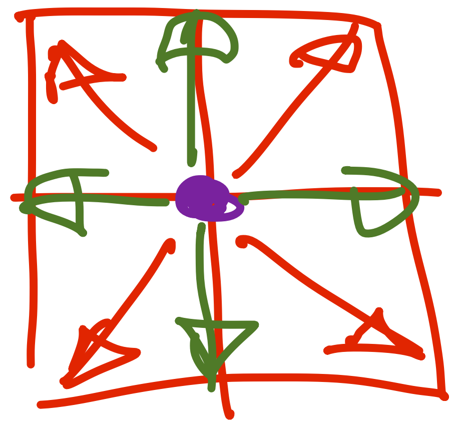
- weighted Jacobi: Same issue — need to select a parameter
- Gauss-Seidel improved
- Red-Black Gauss-Seidel and other schemes even more effective

Take a look: `09-multigrid-2d.ipynb`

Interpolation in 2D

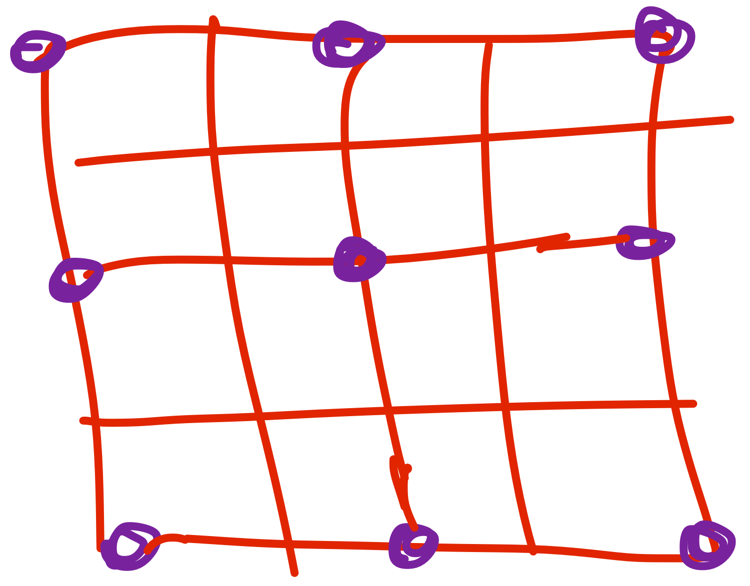
- Bilinear interpolation, tensor product of 1D interpolation

$$\frac{1}{2}\begin{bmatrix} 1 & 2 & 1 \end{bmatrix} \longrightarrow \frac{1}{4}\begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$$



• is coarse

- Example 3x3 -> 7x7



$$\begin{bmatrix} 0.5 & & \\ 1 & & \\ 0.5 & 0.5 & \\ & 1 & \\ & 0.5 & 0.5 \\ & & 1 \\ & & 0.5 \end{bmatrix} \otimes \begin{bmatrix} 0.5 & & \\ 1 & & \\ 0.5 & 0.5 & \\ & 1 & \\ & 0.5 & 0.5 \\ & & 1 \\ & & 0.5 \end{bmatrix} \longrightarrow \frac{1}{4}\begin{bmatrix} 1 & & & & & \\ 2 & & & & & \\ 1 & 1 & & & & \\ & 2 & & & & \\ & 1 & 1 & & & \\ & & 2 & & & \\ & & 1 & & & \\ 2 & & & & & \\ 4 & & & & & \\ 2 & 2 & & & & \\ & 4 & & & & \\ & 2 & 2 & & & \\ & & 4 & & & \\ & & 2 & & & \\ 1 & & & 1 & & \\ 2 & & & 2 & & \\ 1 & 1 & & 1 & 1 & \\ & 2 & & & 2 & \\ & 1 & 1 & & 1 & 1 \\ & & 2 & & & 2 \\ & & 1 & & & 1 \\ & & & 2 & & \\ & & & 4 & & \\ & & & 2 & 2 & \\ & & & & 4 & \\ & & & & 2 & 2 \\ & & & & & 4 \\ & & & & & 2 \\ & \vdots & & \vdots & & \end{bmatrix}$$

A few observations so far: **One**

- Let's consider a V(1,1) cycle — weighted Jacobi, etc.

smooth

smooth

- The **error** propagation for this looks like

$$e_1 = \underbrace{G\overbrace{(I - P(P^TAP)^{-1}P^TA)}^{\text{CGC}}G}_{M}e_0 \qquad G = I - \omega D^{-1}A$$

before smoothing

$$Me_k \not\to 0?$$

- One thing we can do, is consider bounds on each operation.

A few observations so far: **One**

- Take the operator

$$M = G(I - P(P^T AP)^{-1} P^T A)G$$

- And makes some bounds

$$\underbrace{\|I - P(P^T AP)^{-1} P^T A\|}_{\text{approximation property}} \underbrace{\|G\|^2}_{\text{smoothing property}}$$

- General $\|G\| \le 1$

1D over [n/2,n]: $\|G\| \le \dfrac{1}{3}$

2D over [n/2,n]: $\|G\| \le \dfrac{3}{5}$

"Multigrid tutorial"

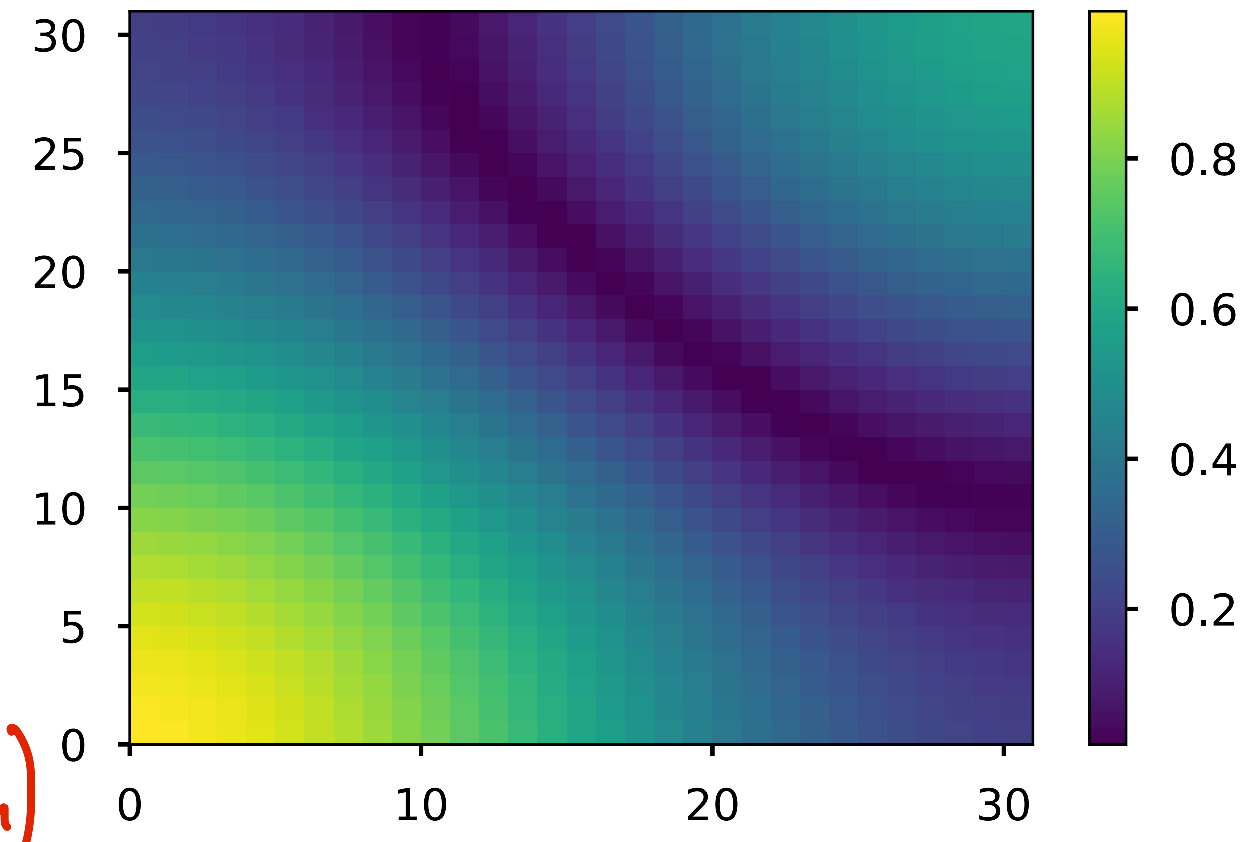
A few observations so far: **One**

$$\underbrace{\|I - P(P^TAP)^{-1}P^TA\|}_{\text{approximation property}}\underbrace{\|G\|^2}_{\text{smoothing property}}$$

- General $\|G\| \leq 1$

1D over [n/2,n]: $\|G\| \leq \frac{1}{3}$

2D over [n/2,n]: $\|G\| \leq \frac{3}{5}$



- Also, if w s.t. $Aw \in \mathcal{N}(P^T)$ (null space of restriction)

then $(I - P(P^TAP)^{-1}P^TA)w = w$

$\| \cdot \| \geq 1$

L error

A few observations so far: **Two**

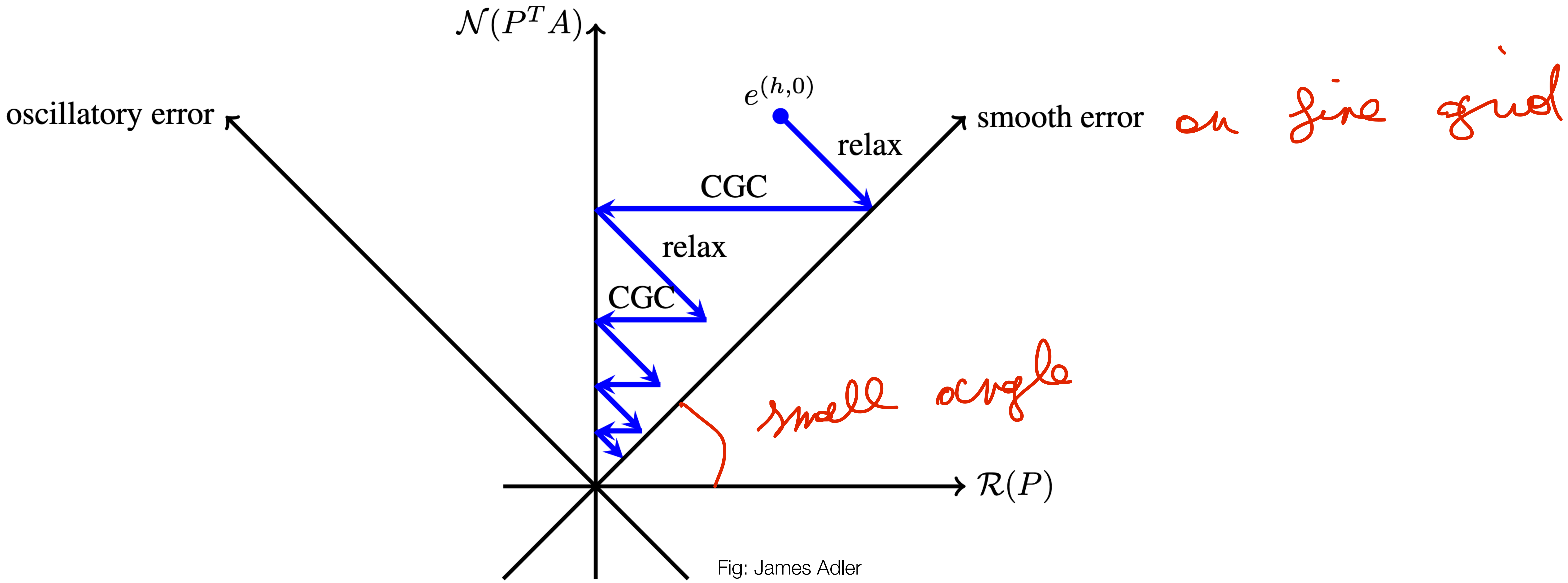


Fig: James Adler

- Complementary processes:
  - **relaxation:** targets (Fourier) smoothing
  - **coarse grid correction:** targets things in the range of interpolation

A few observations so far: **Three**

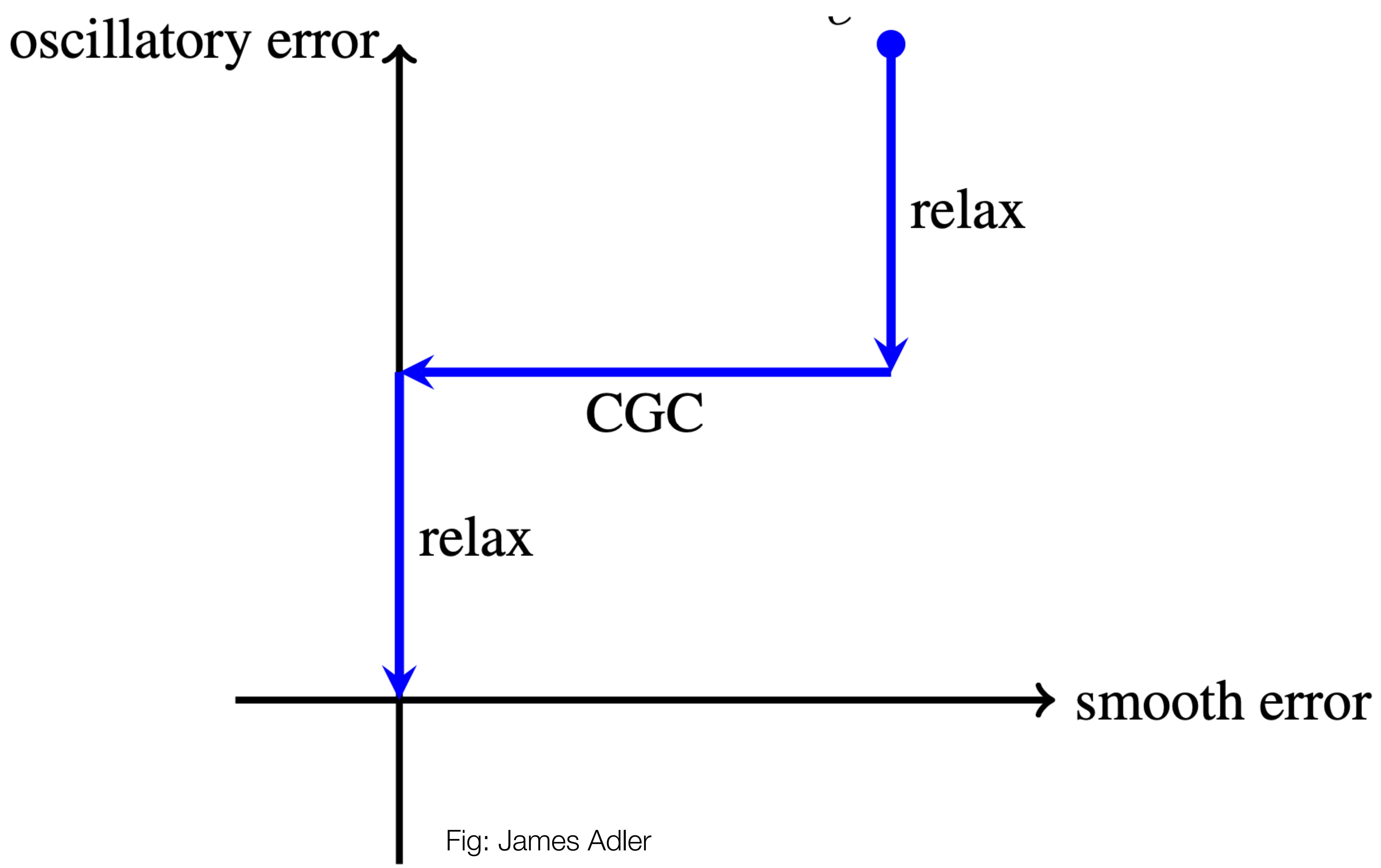


Fig: James Adler

$$e_1 \leftarrow (I - P(P^TAP)^{-1}P^TA)Ge_0$$

$$Ge_0 \in \mathcal{R}(P) \quad \Rightarrow \quad e_1 = 0$$

interpolation should capture what relaxation misses

Take a look: `10-multigrid-anisotropy.ipynb`

What can go wrong?!

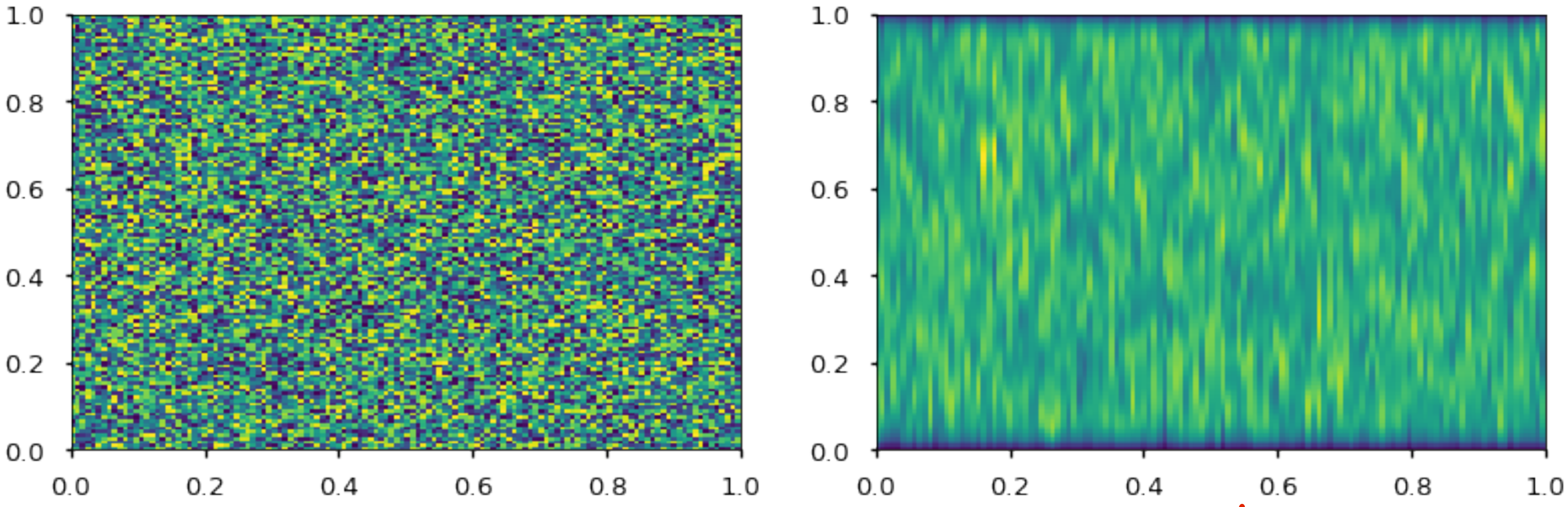
- Consider an *anisotropic problem*

after relaxation: smooth in y, not in x

$$-\varepsilon u_{xx} - u_{yy} = f$$

$$u = 0 \qquad \text{on boundary}$$

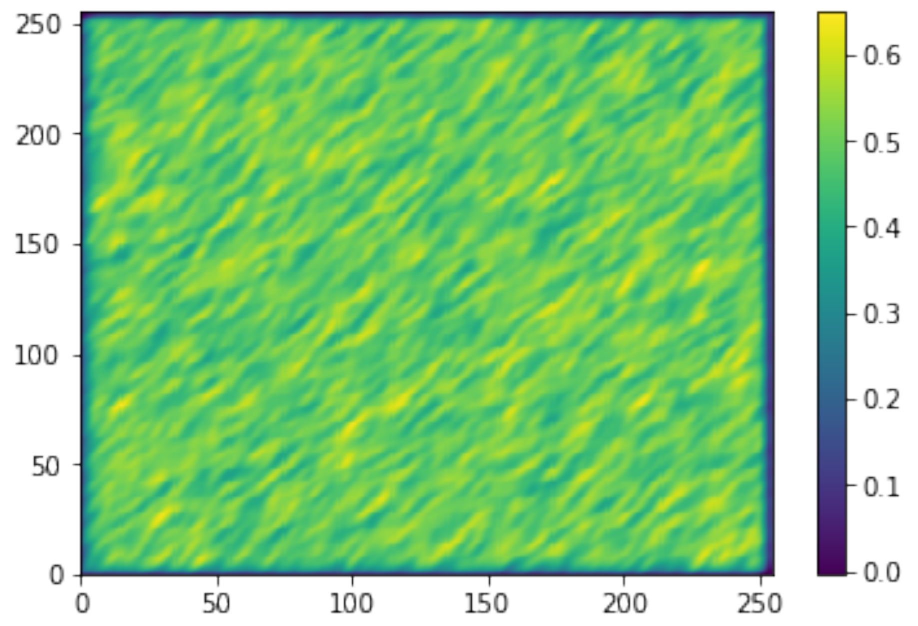
$$\begin{bmatrix} & -1 & \\ -\varepsilon & 2+2\varepsilon & -\varepsilon \\ & -1 & \end{bmatrix}$$

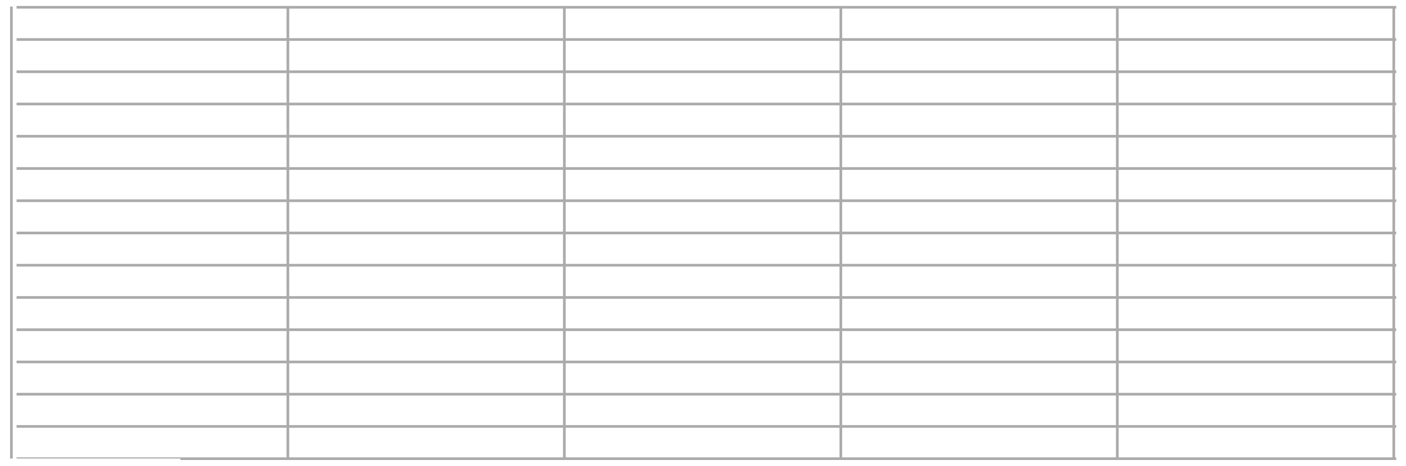


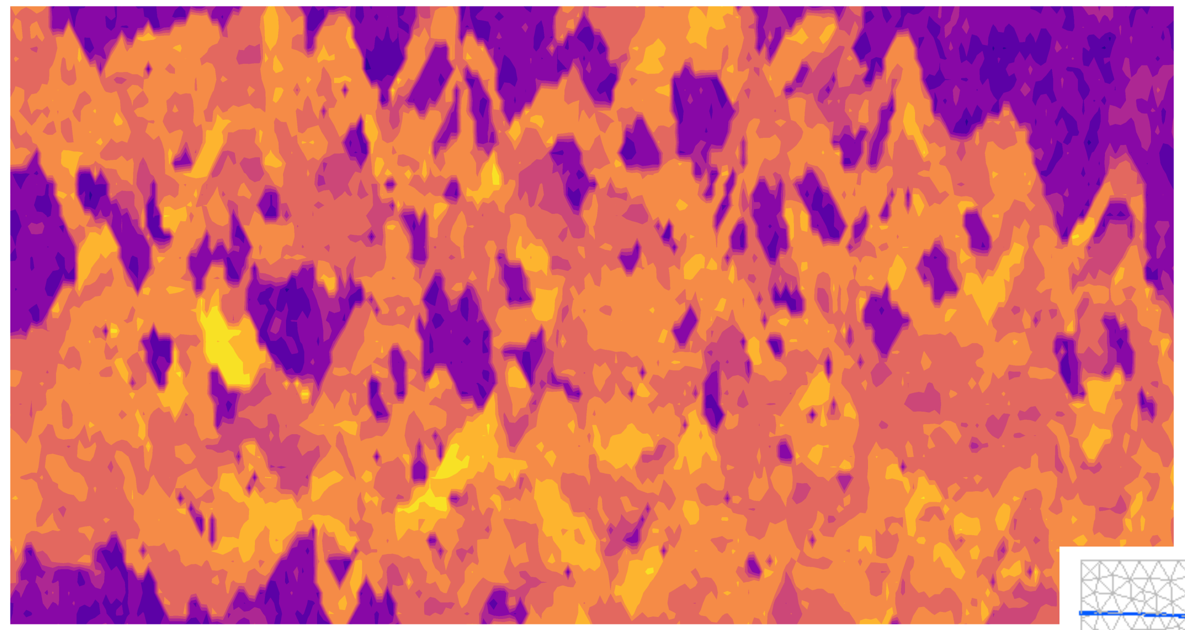
we cannot coarsen in x !

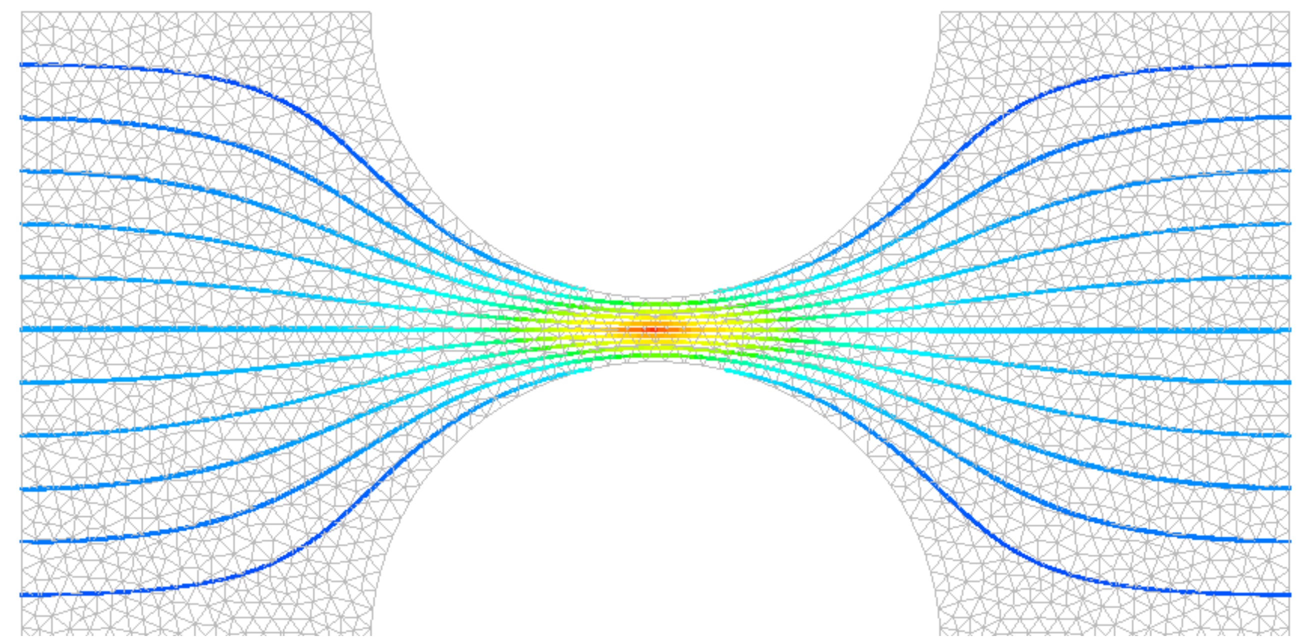
What can go wrong?!

- Anisotropy
- Mesh stretching
- Jumping coefficients
- Non-elliptic







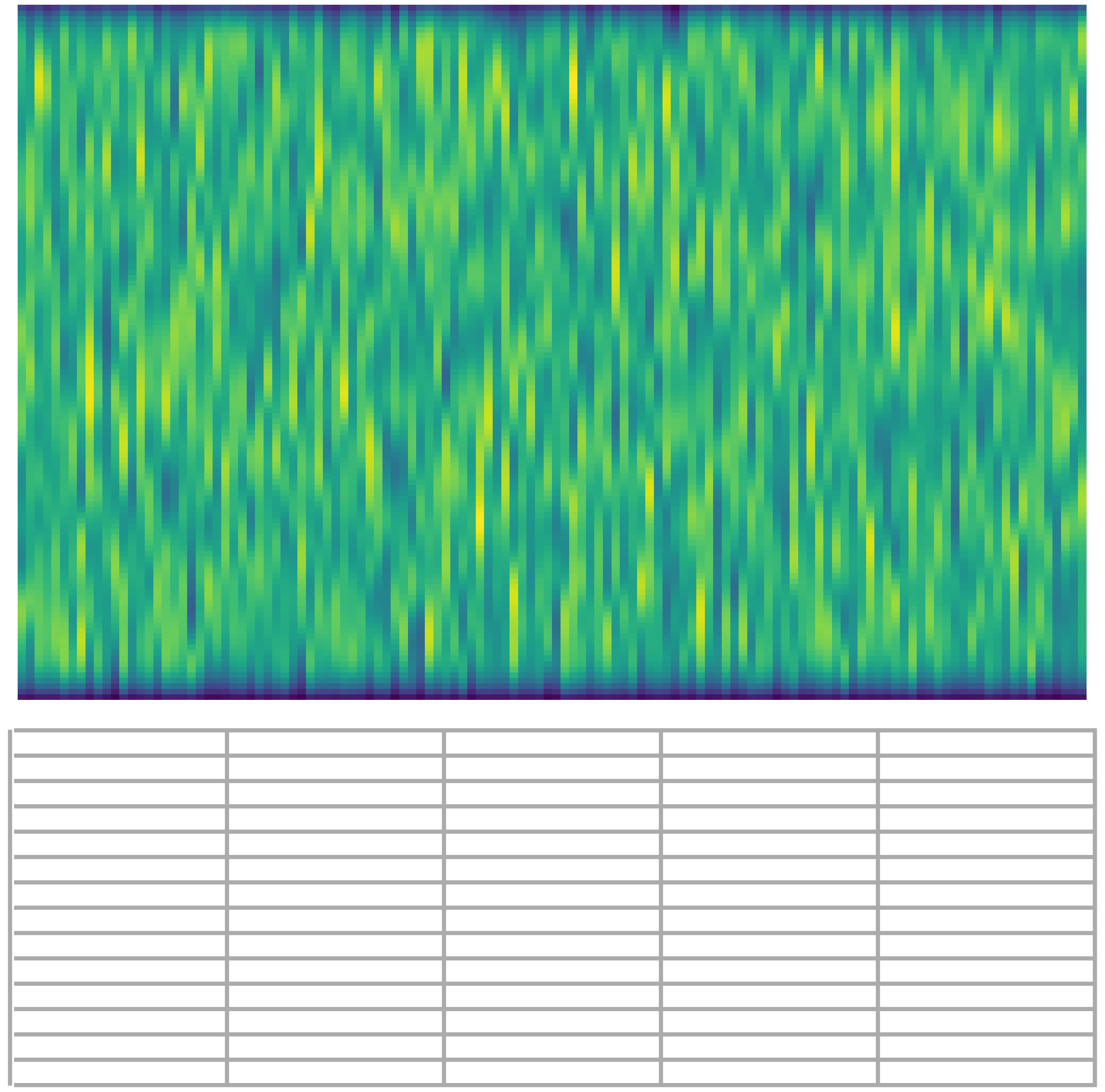


Options for more robust Multigrid

$-\varepsilon u_{xx} - u_{yy} = f$

- **Semicoarsening:** Coarsen in the direction of smoothness

(change coarsening)

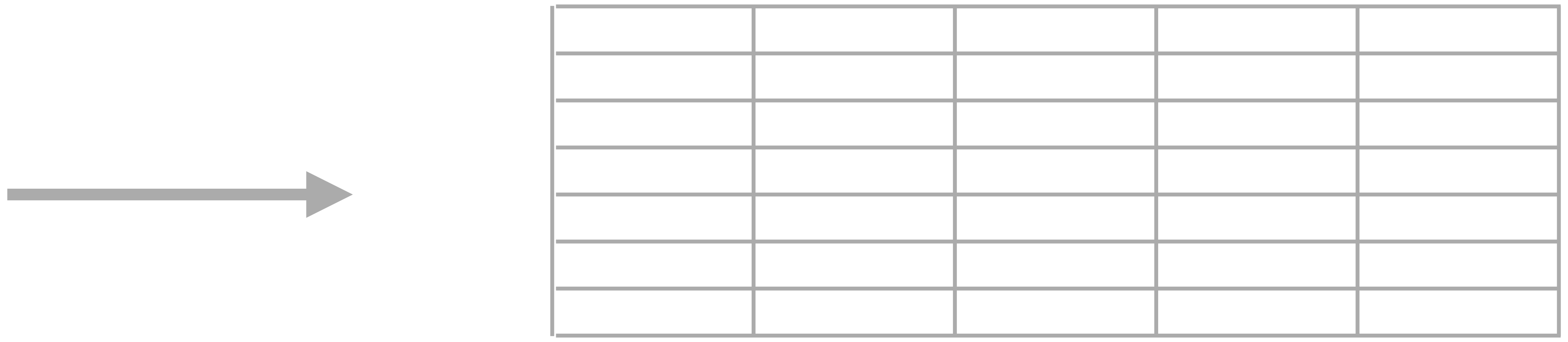


don't coarsen in x

only coarsen in y

(then CGC will be OK)

(on special coarse grid)



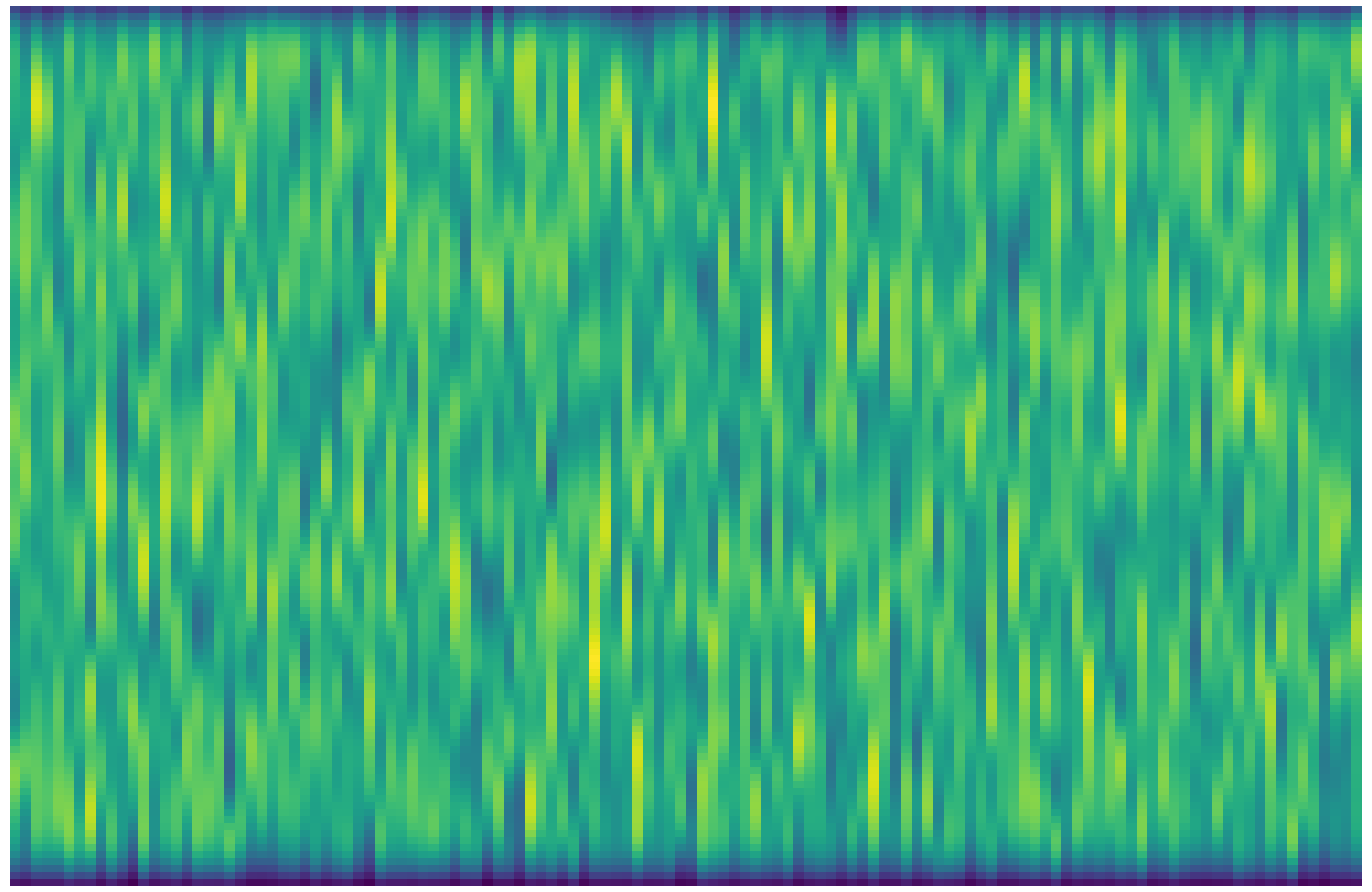
- Downside: if anisotropy varies in another direction, we need a different grid

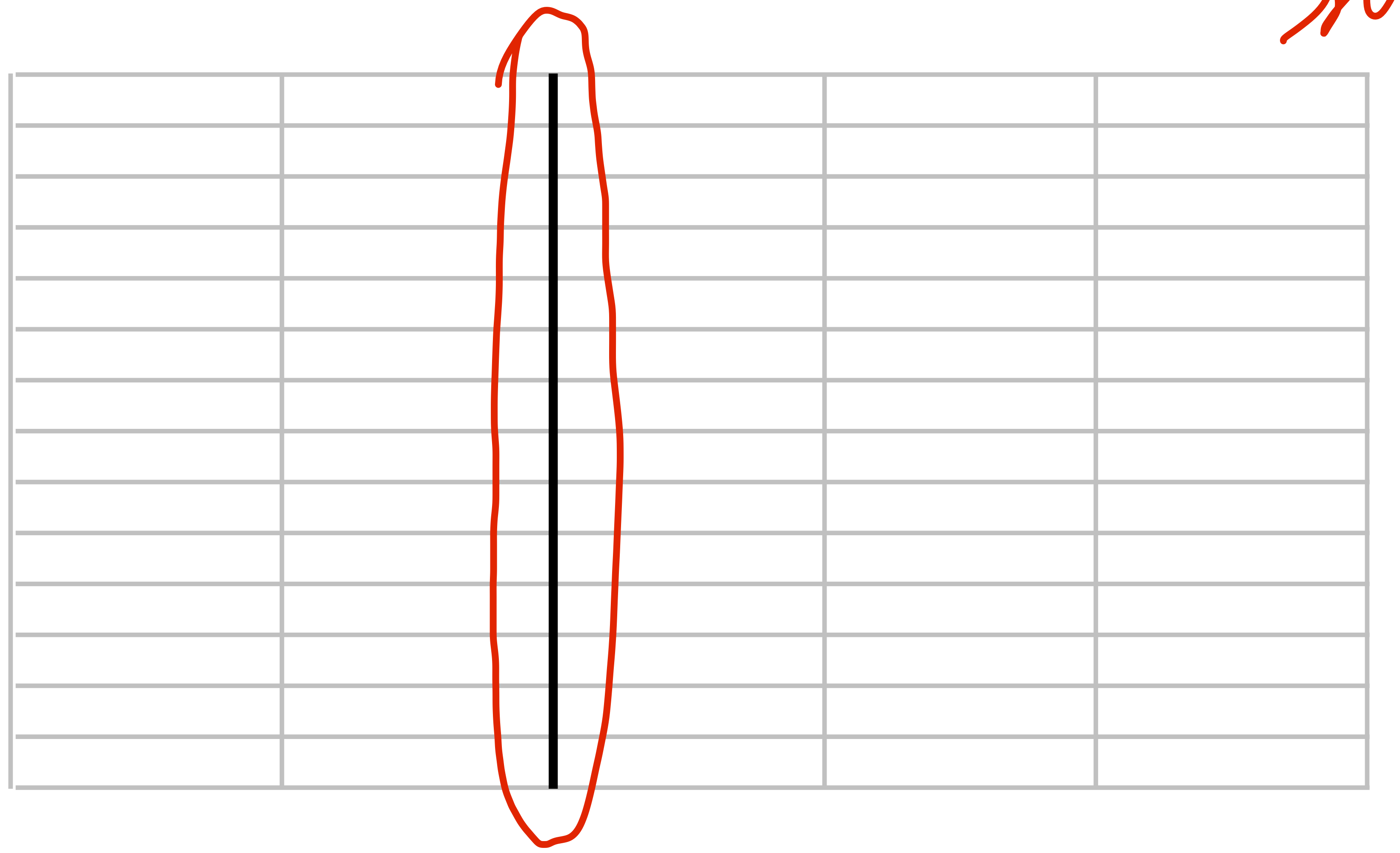
$-\varepsilon u_{xx} + u_{yy} = f$

Options for more robust Multigrid

- **Line/plane relaxation** (or: change relaxation)
  Perform relaxation in groups (in a line)

smooth these together (direction of strong connections)



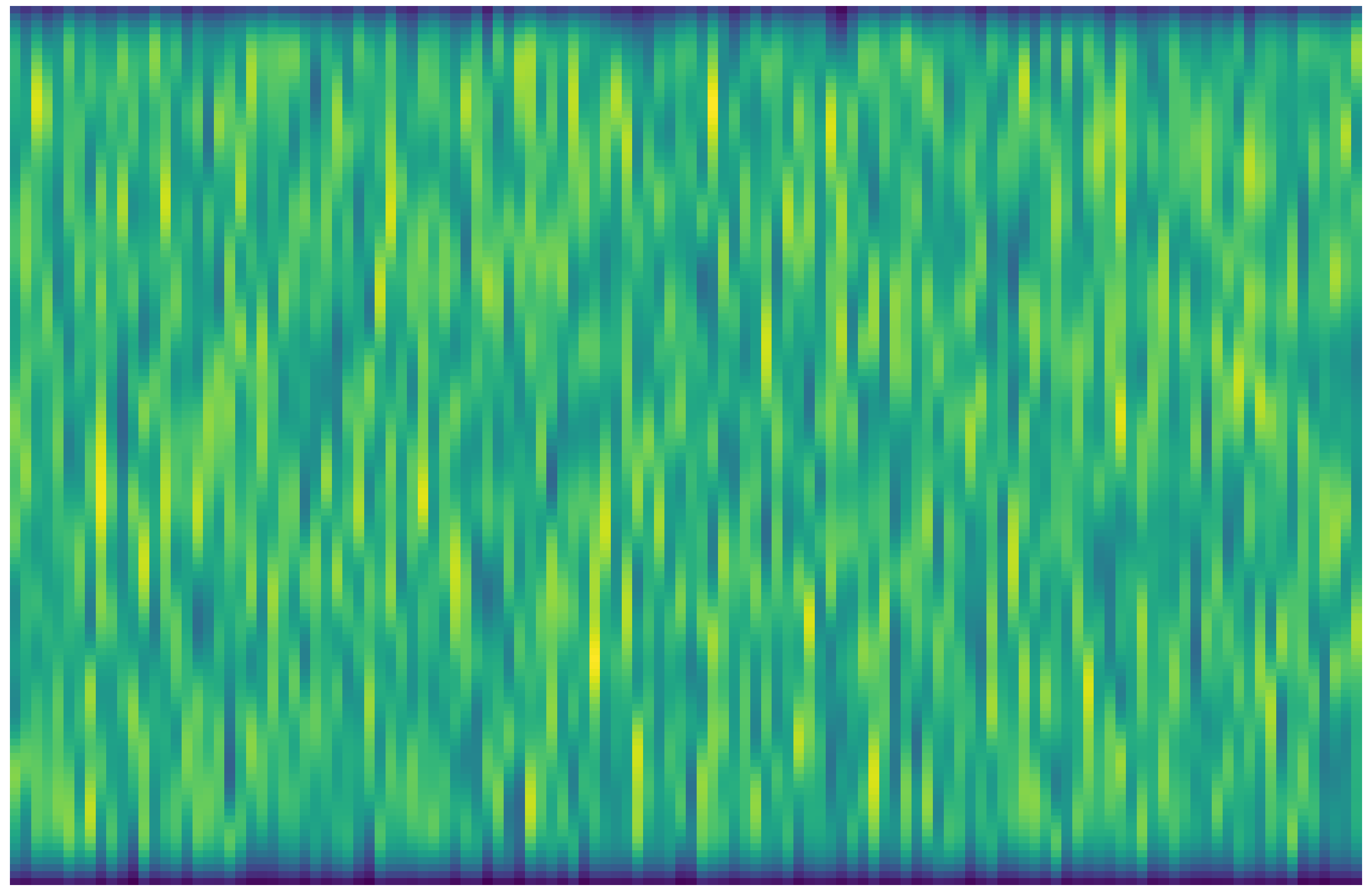


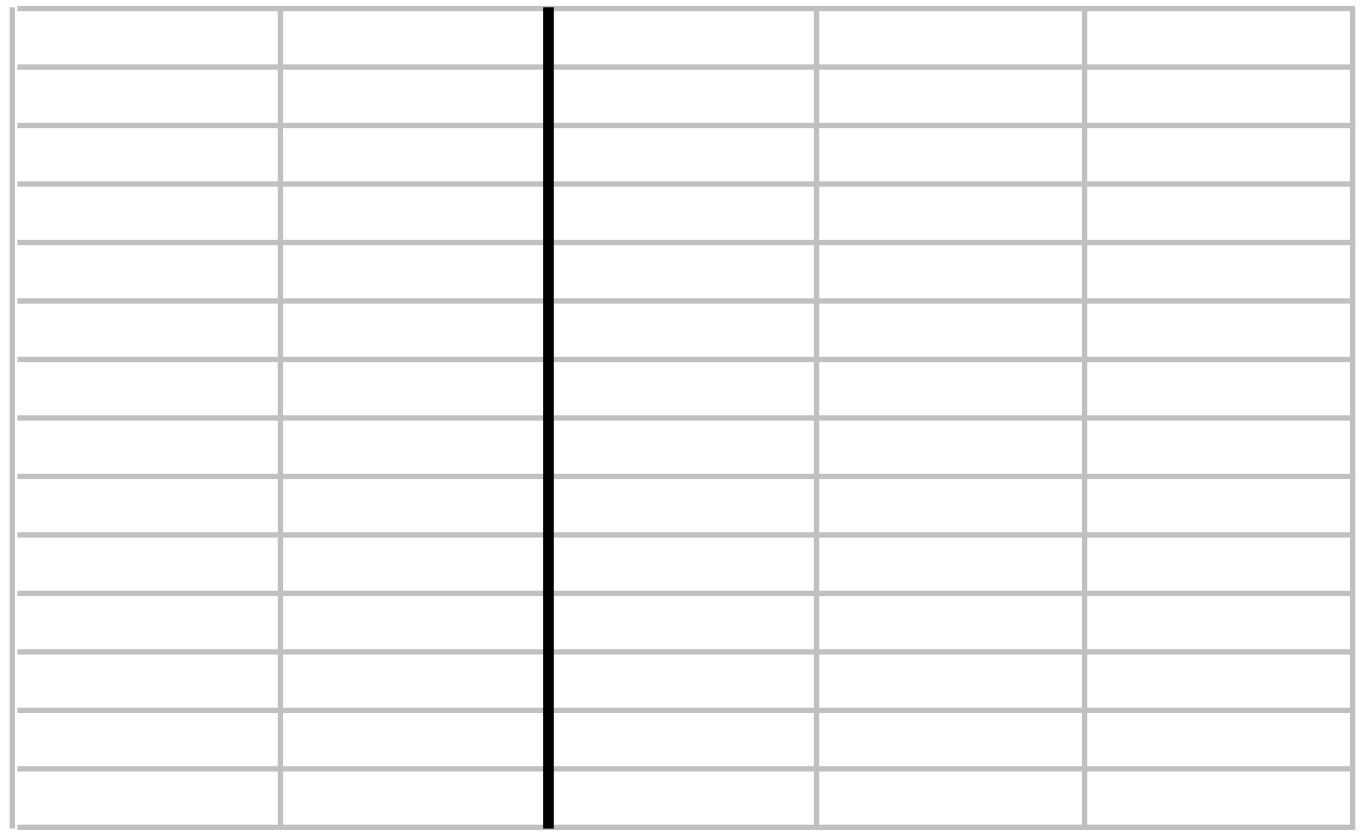
- Example:
  - relax error in block in the y-direction (constant x-lines)
  - no (block) smoothing in the x-direction (constant y-lines)

(then CGC will be OK on fully coarsened grid)

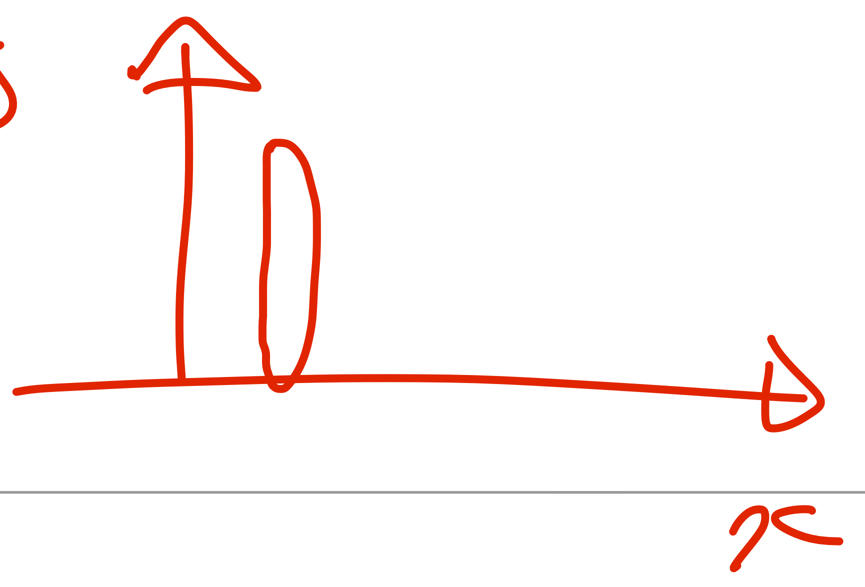
Options for more robust Multigrid

- **Line/plane relaxation**
- For each x-line (lines of strong anisotropy):
  - Eliminate the residual on the entire line
  - (Gauss-Seidel, by lines)





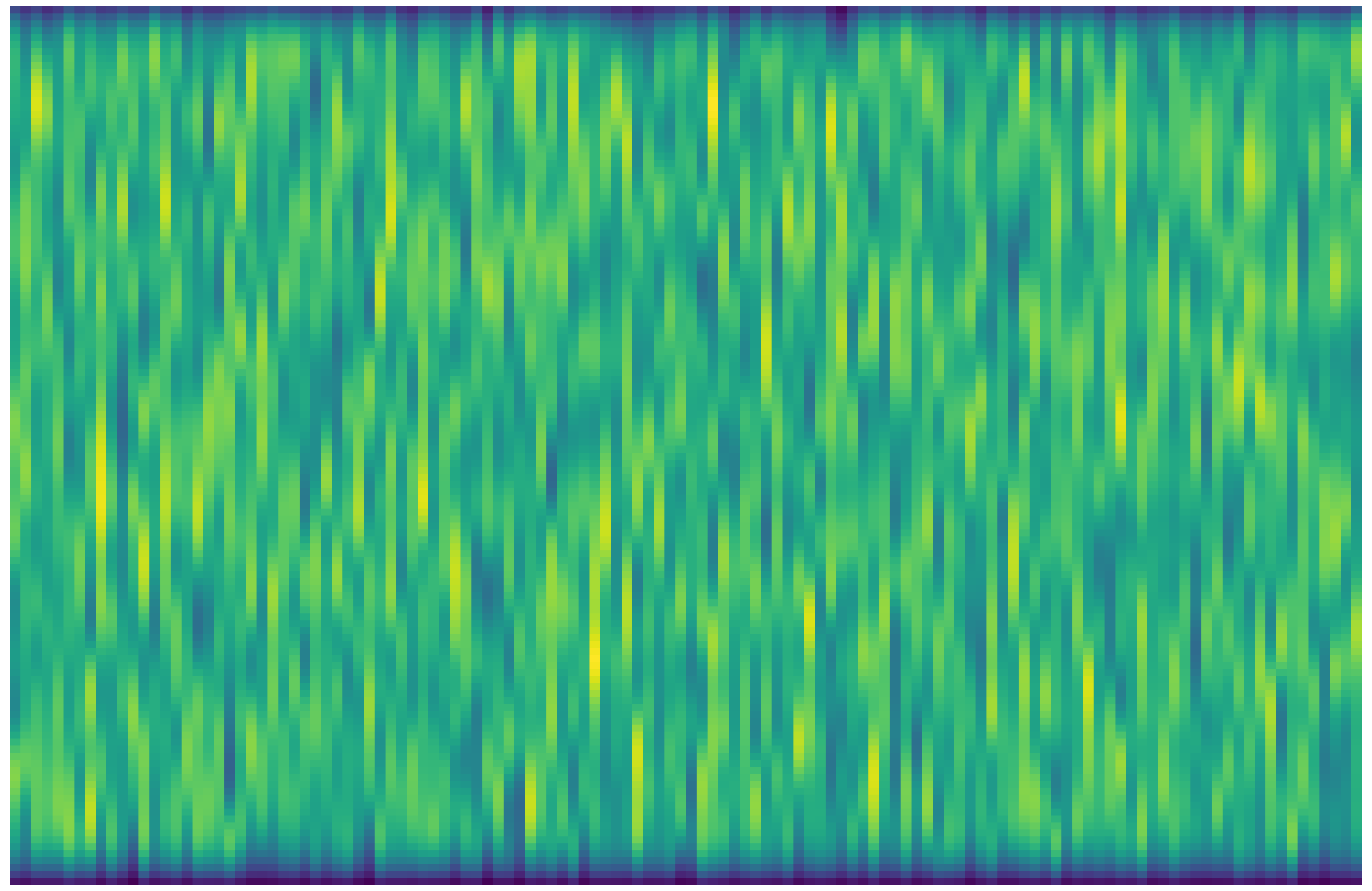
$-\varepsilon u_{xx} + u_{yy} = f$



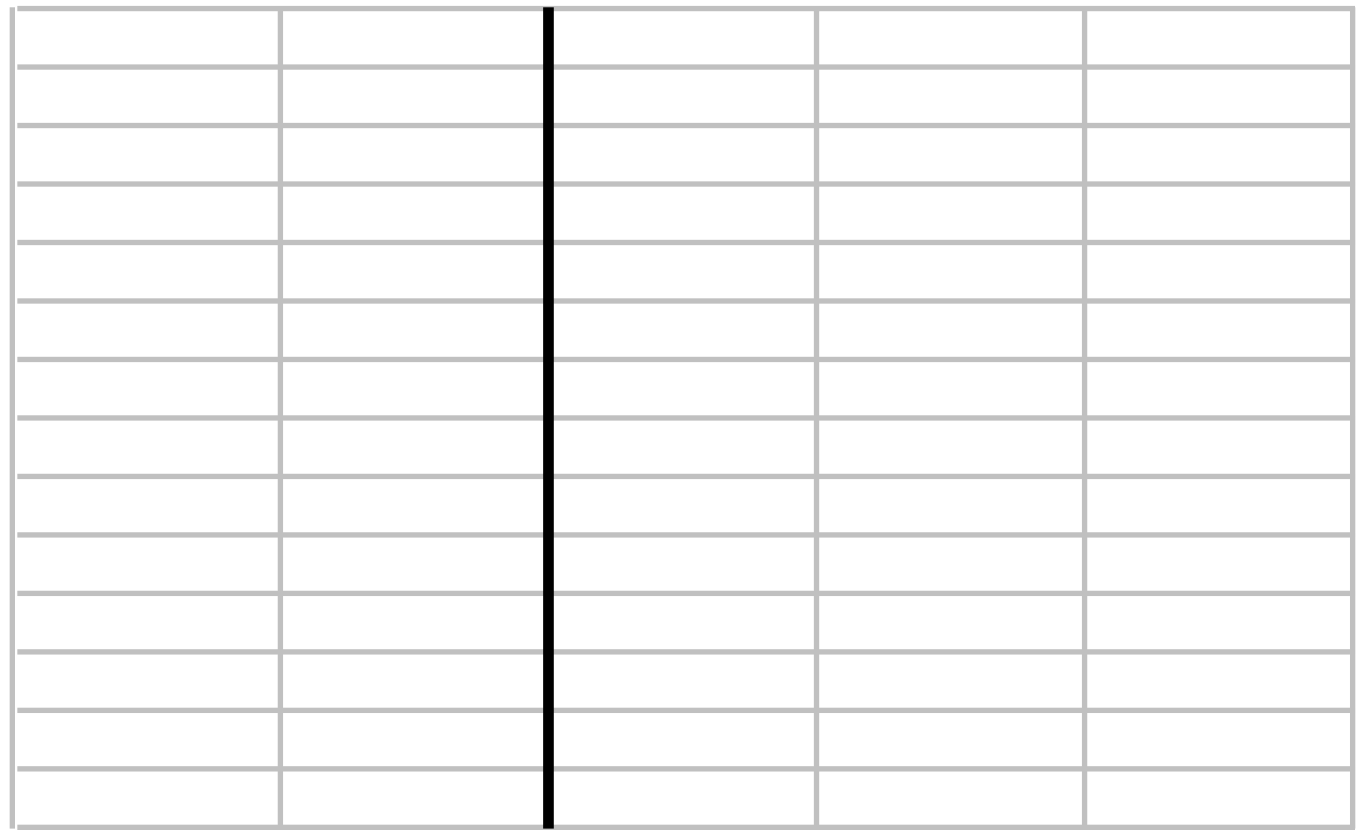
column - lexicographic

Options for more robust Multigrid

- **Line/plane relaxation**
- $$A = \frac{1}{(n+1)^2}\begin{bmatrix} A_{1D} & -\varepsilon I & & & \\ -\varepsilon I & A_{1D} & -\varepsilon I & & \\ & -\varepsilon I & A_{1D} & -\varepsilon I & \\ & & \ddots & & \\ & & & -\varepsilon I & A_{1D} \end{bmatrix}$$



$$A_{1D} = \frac{1}{(n+1)^2}\begin{bmatrix} 2+2\varepsilon & -1 & & \\ -1 & 2+2\varepsilon & -1 & \\ & & \ddots & \\ & & -1 & 2+2\varepsilon \end{bmatrix}$$



Take a look: `11-multigrid-2d-line-relaxation.ipynb`

Options for more robust Multigrid

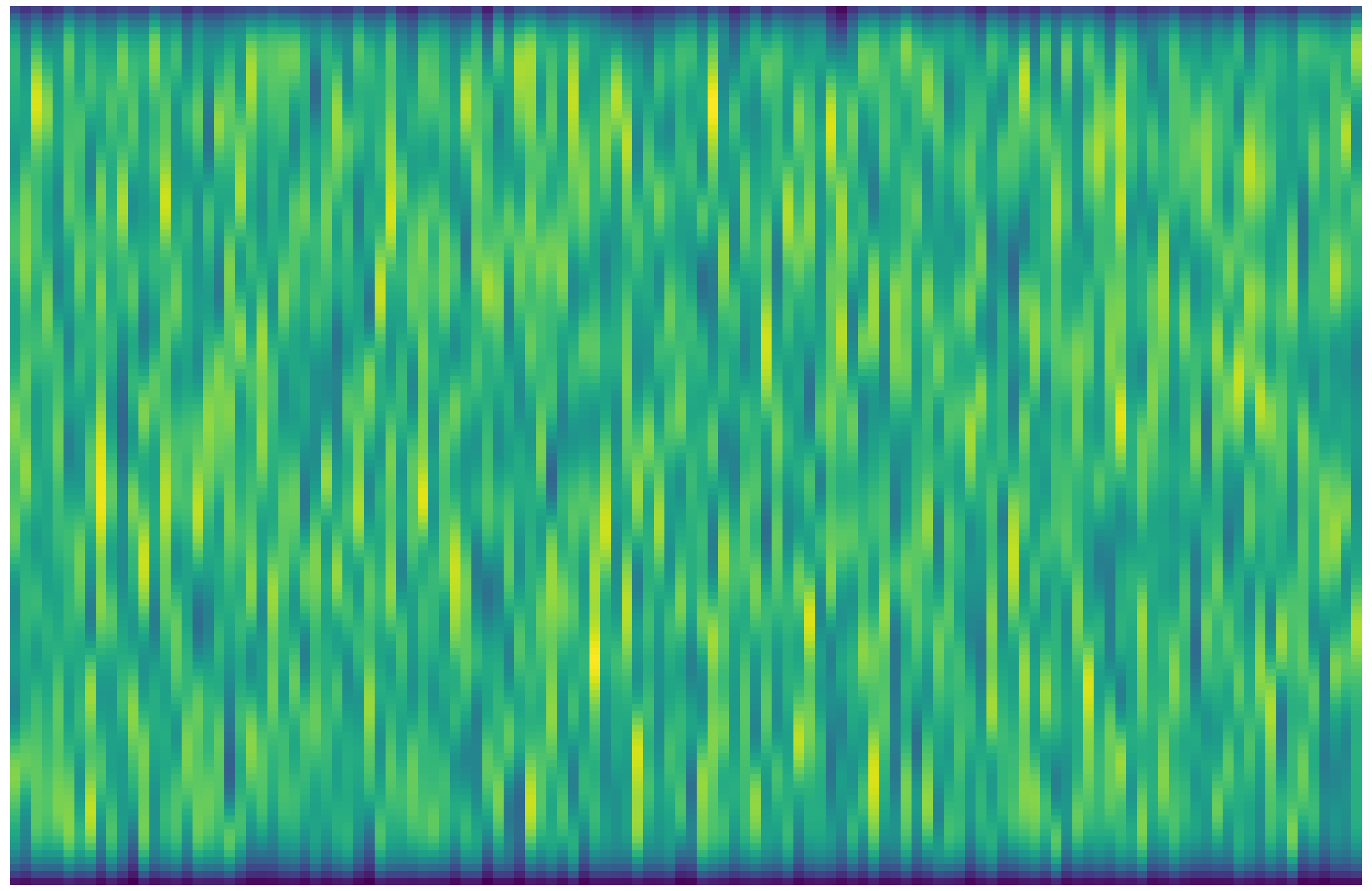
- **Line/plane relaxation**
- For each line, solve

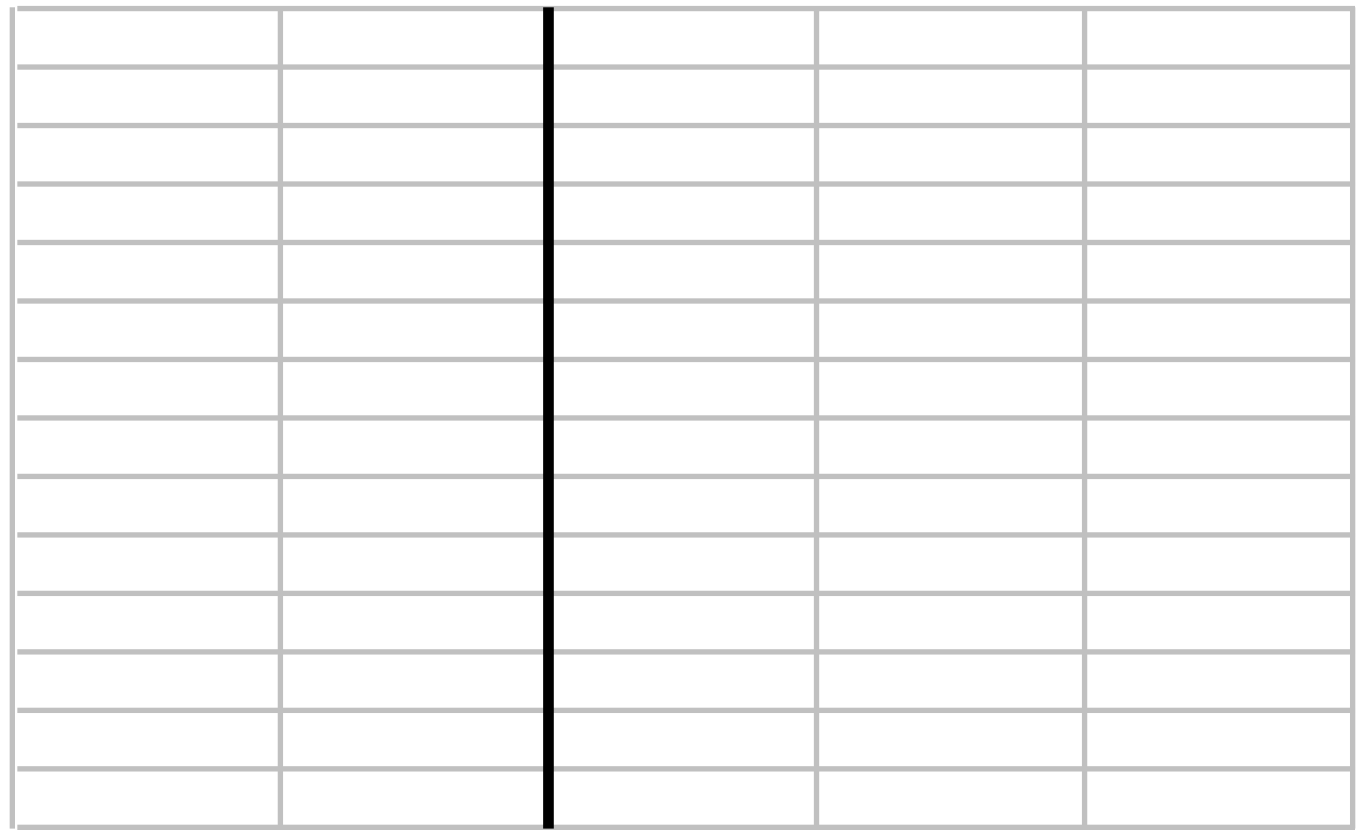
$$A_{1D} v_k = g_k$$

L x constant

$$v_k = \begin{bmatrix} \vdots \\ v_{k,j-1} \\ v_{k,j} \\ v_{k,j+1} \\ \vdots \end{bmatrix} \quad g_k = \begin{bmatrix} \vdots \\ f_{k,j-1} + \varepsilon\left(v_{k-1,j-1} + v_{k+1,j-1}\right) \\ f_{k,j} + \varepsilon\left(v_{k-1,j} + v_{k+1,j}\right) \\ f_{k,j+1} + \varepsilon\left(v_{k-1,j+1} + v_{k+1,j+1}\right) \\ \vdots \end{bmatrix}$$

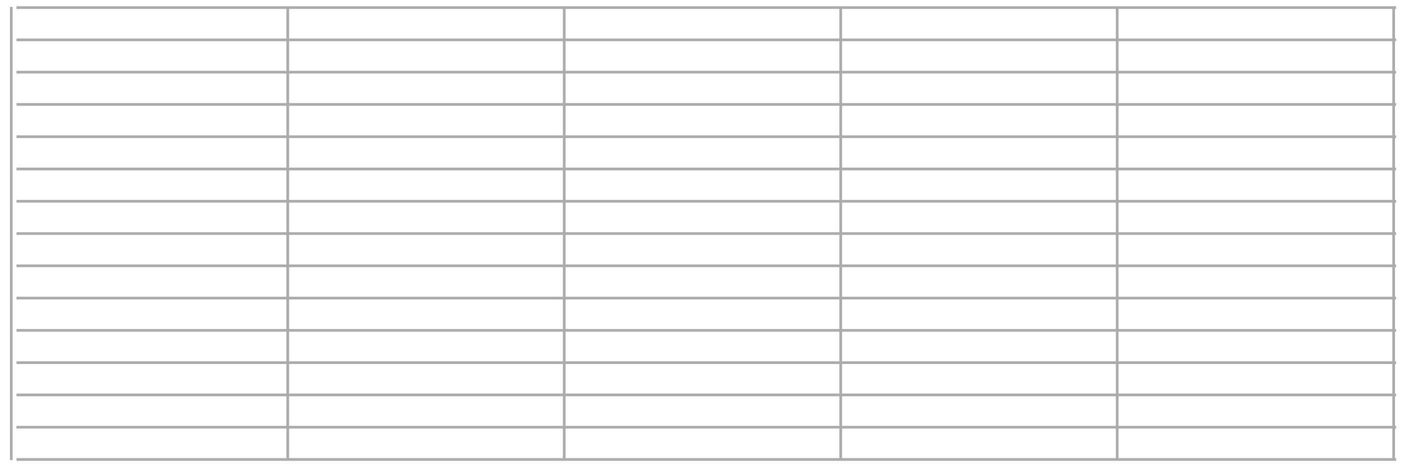
- In 3D, lines become planes…

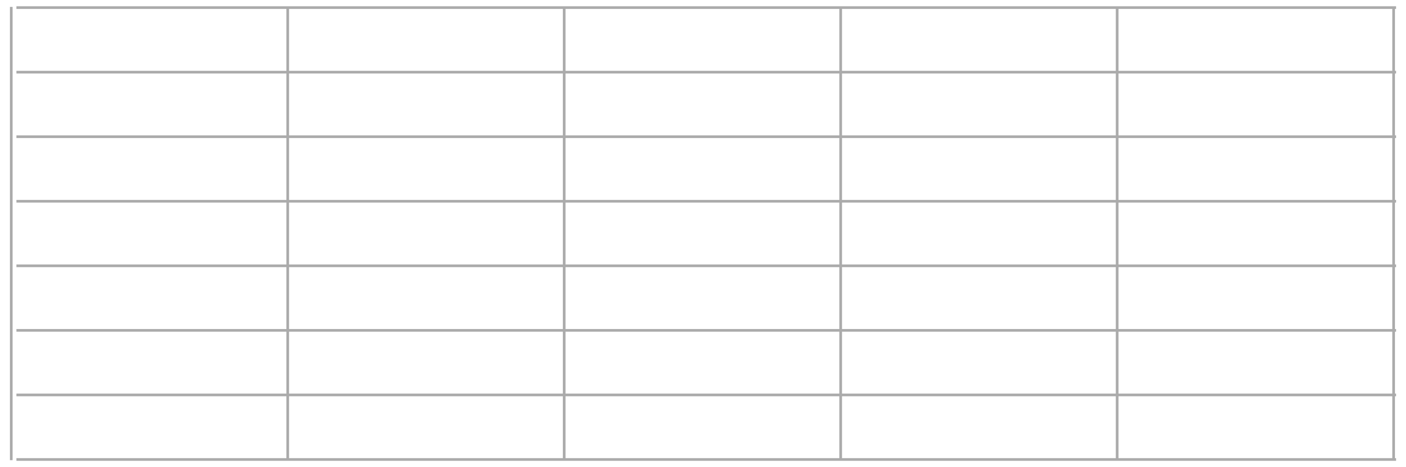




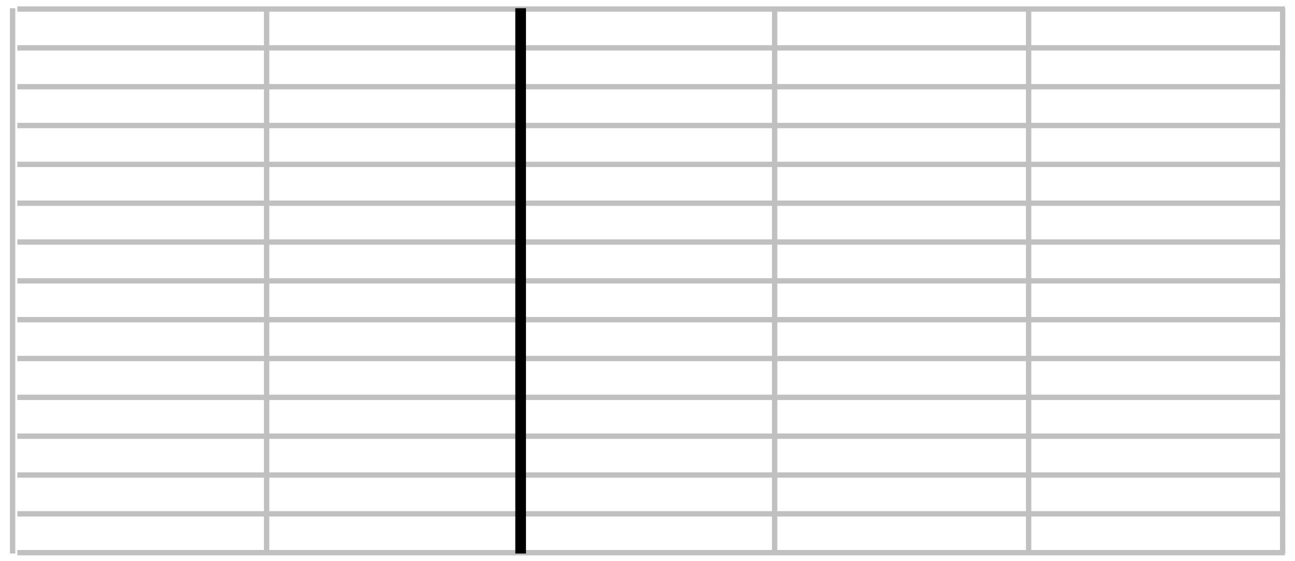
Options for more robust Multigrid

- **Semicoarsening**
  Coarsen in the direction of smoothness





- **Line/plane relaxation**
  Perform relaxation in groups (in a line)



- **Operator based Interpolation** (e.g. BoxMG)

$$Ae = 0$$

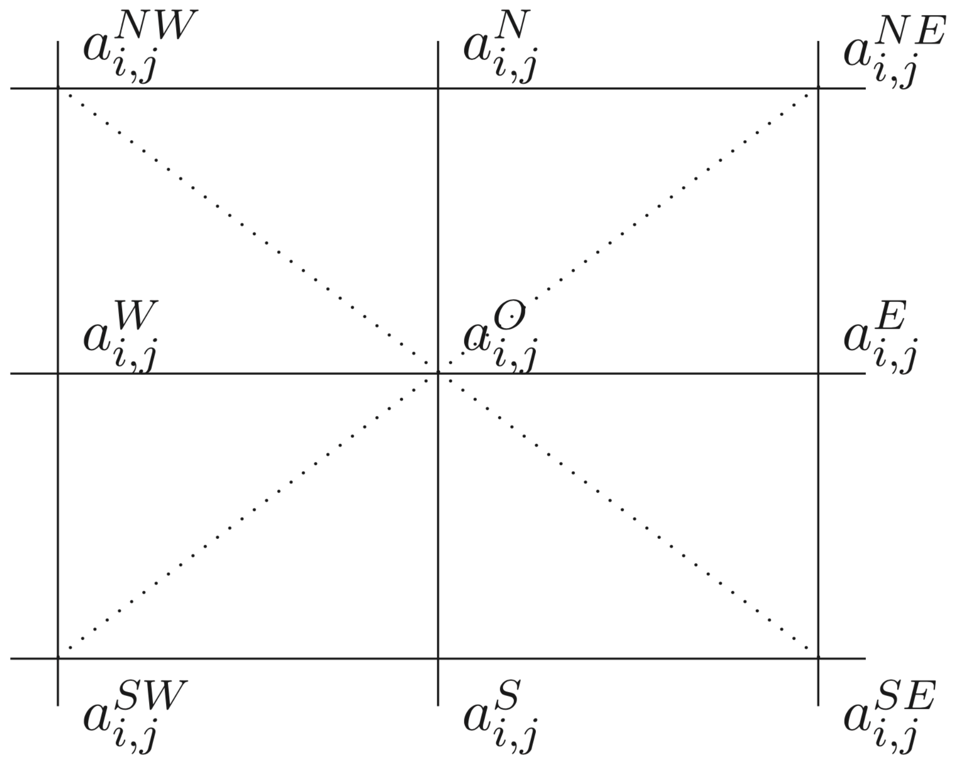
J. E. Dendy, Black box multigrid, J. Comput. Phys., 1982

J. E. Dendy and J. D. Moulton, Black box multigrid with coarsening by a factor of three, J. Numer. Lin. Alg. App., 2010

BoxMG

Math and figures from:
Robust and adaptive multigrid methods: comparing structured and algebraic approaches, MacLachlan, Moulton, Chartier

- Node (i,j) stencil:

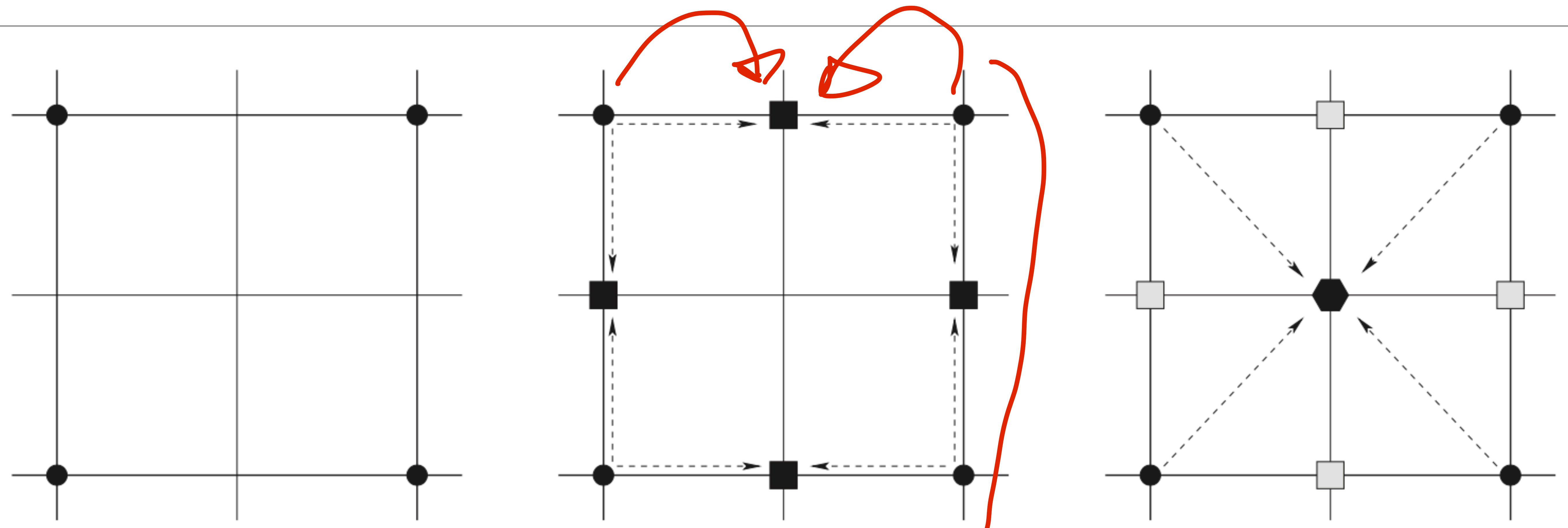


$$Ax = b$$

$$a_{i,j}^{SW} x_{i-1,j-1} + a_{i,j}^{S} x_{i,j-1} + a_{i,j}^{SE} x_{i+1,j-1} + a_{i,j}^{W} x_{i-1,j} + a_{i,j}^{O} x_{i,j} + a_{i,j}^{E} x_{i+1,j} + a_{i,j}^{NW} x_{i-1,j+1} + a_{i,j}^{N} x_{i,j+1} + a_{i,j}^{NE} x_{i+1,j+1} = b_{i,j}$$

BoxMG

Math and figures from:
Robust and adaptive multigrid methods: comparing structured and algebraic approaches, MacLachlan, Moulton, Chartier



1. Inject coarse points (left)
2. Assume the error is constant along x-lines (and y-lines)
3. Infer interpolation from the edges (right)

constant

Example: Assuming Ae=0 and constant y-lines:

$$(a^S + a^O + a^N)e = -(a^{SW} + a^W + a^{NW})e^c_{w}$$
$$- (a^{SE} + a^E + a^{NW})e^c_{E}$$

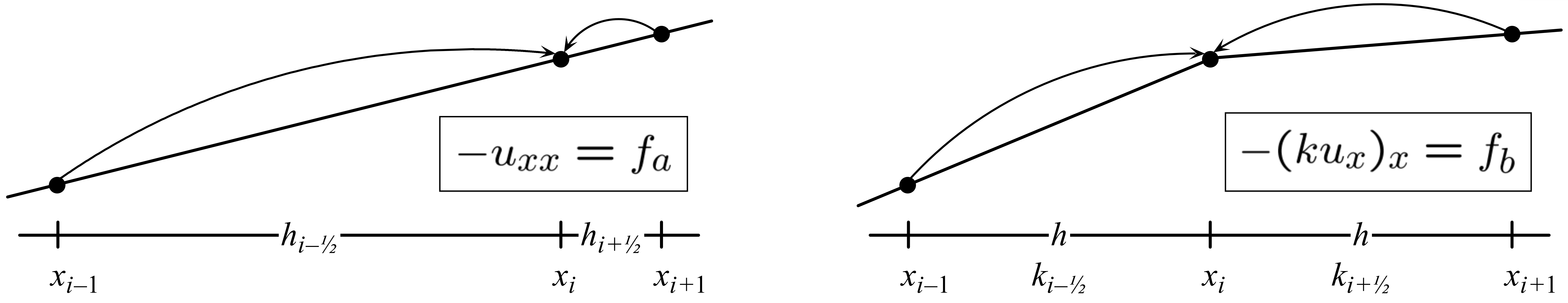
Interpolation based on entries in A

Algebraic Multigrid (AMG) uses matrix coefficients

- Geometric information alone is not sufficient

Linear Interpolation　　Operator-Dependent Interpolation

Slide credit: R. Falgout, 2/1/2016



- AMG does not use geometric information, but captures both linear & operator-dep interpolation

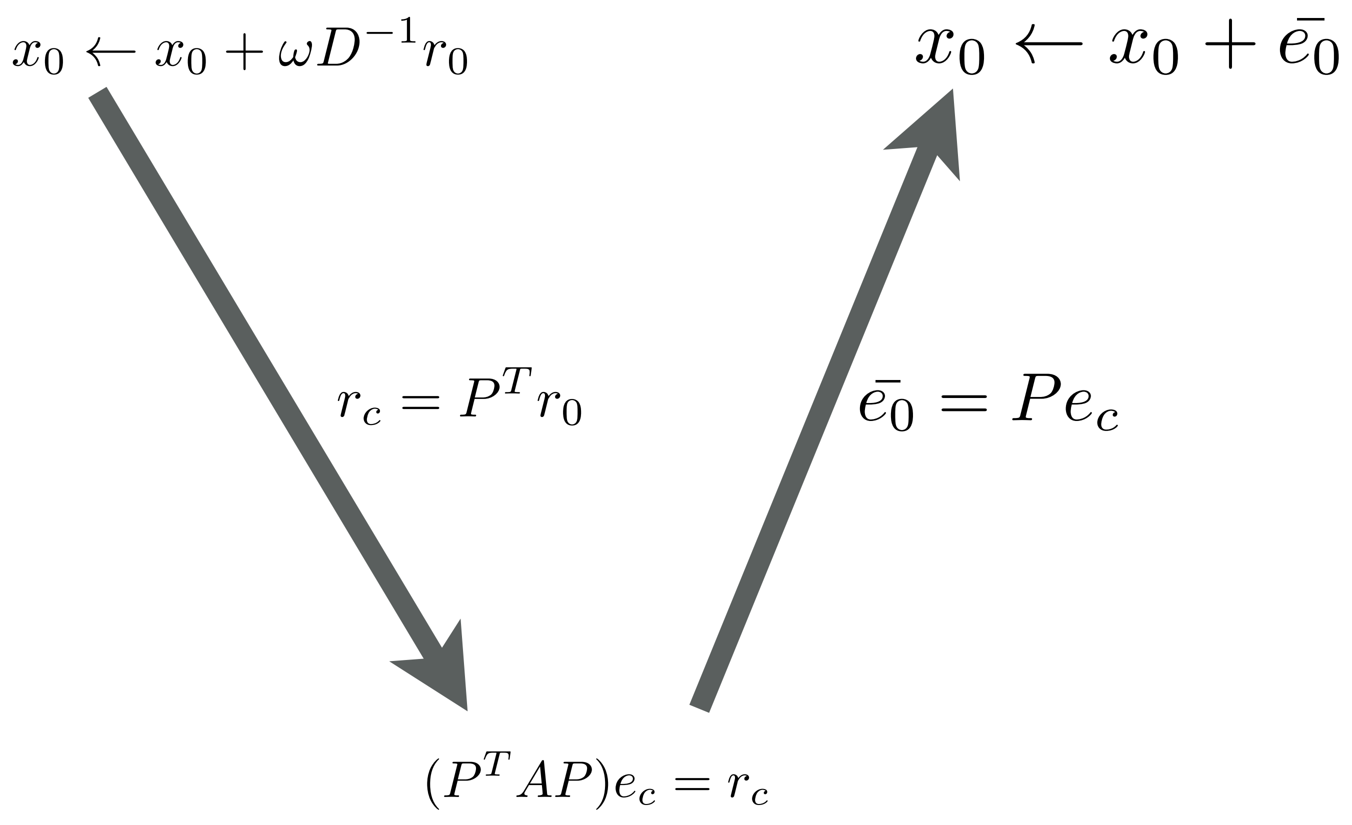
C　F　C

$$(A\mathbf{u})_i = a_{i,i-1}u_{i-1} + a_{i,i}u_i + a_{i,i+1}u_{i+1} \approx 0$$

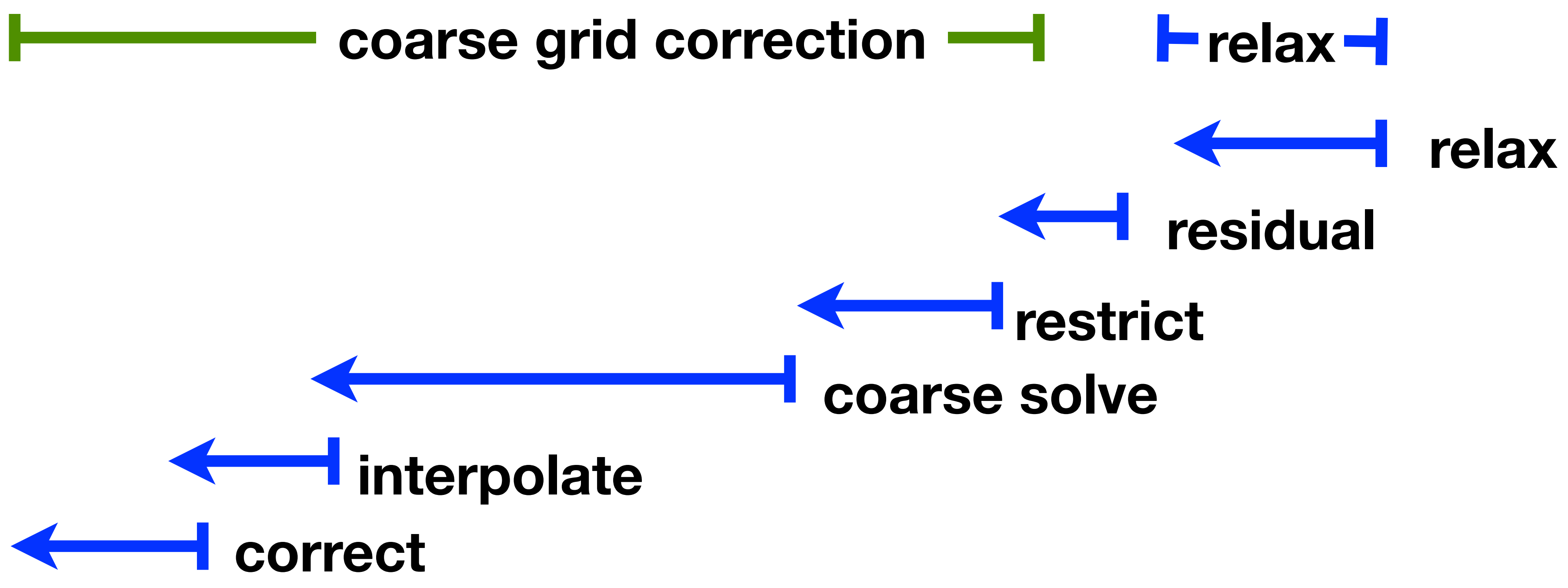
(slow modes are close to constant)

$$u_i = \left(-\frac{a_{i,i-1}}{a_{i,i}}\right) u_{i-1} + \left(-\frac{a_{i,i+1}}{a_{i,i}}\right) u_{i+1}$$

Algebraic Observation



$$e_1 \leftarrow (I - P(P^T A P)^{-1} P^T A) G e_0$$



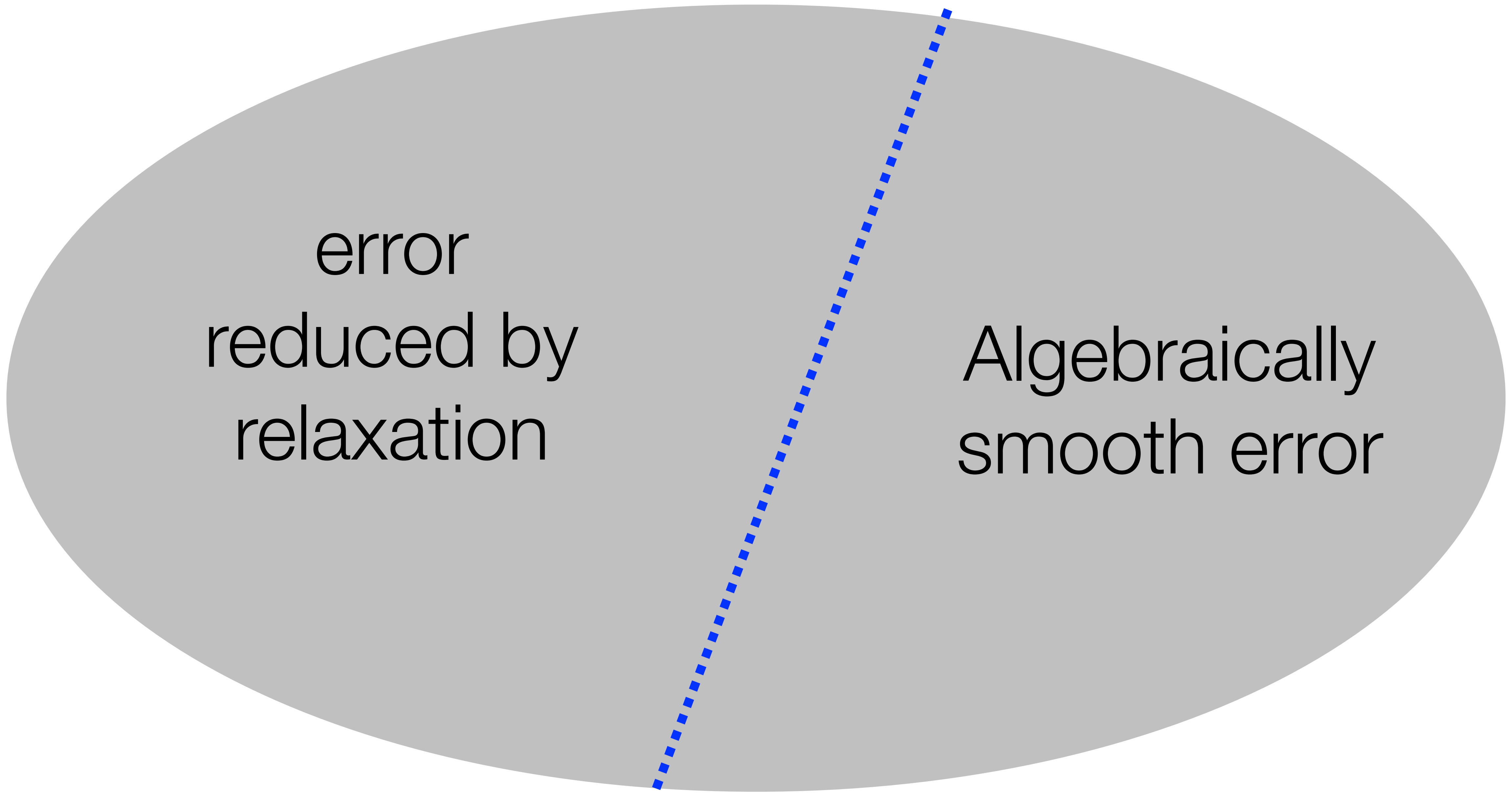
$$Ge_0 \in \mathcal{R}(P) \quad \Rightarrow \quad e_1 = 0$$

interpolation should capture what relaxation misses

determine coarse grid and interpolation based on A

Algebraically Smooth Error

- **"Algebraically smooth" error may not be geometrically smooth**

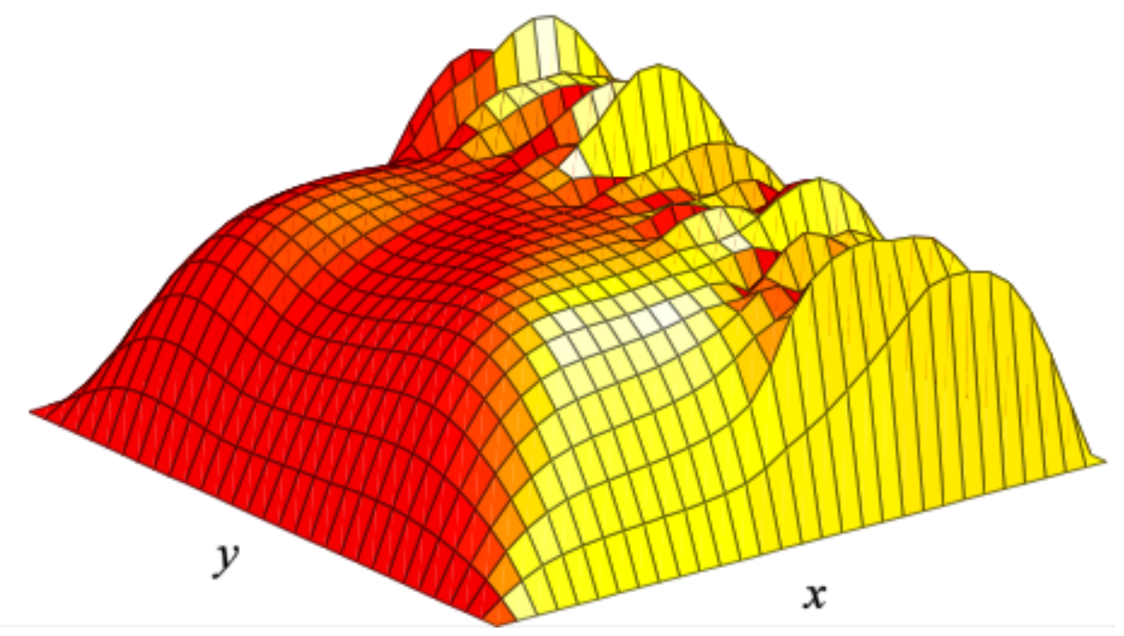


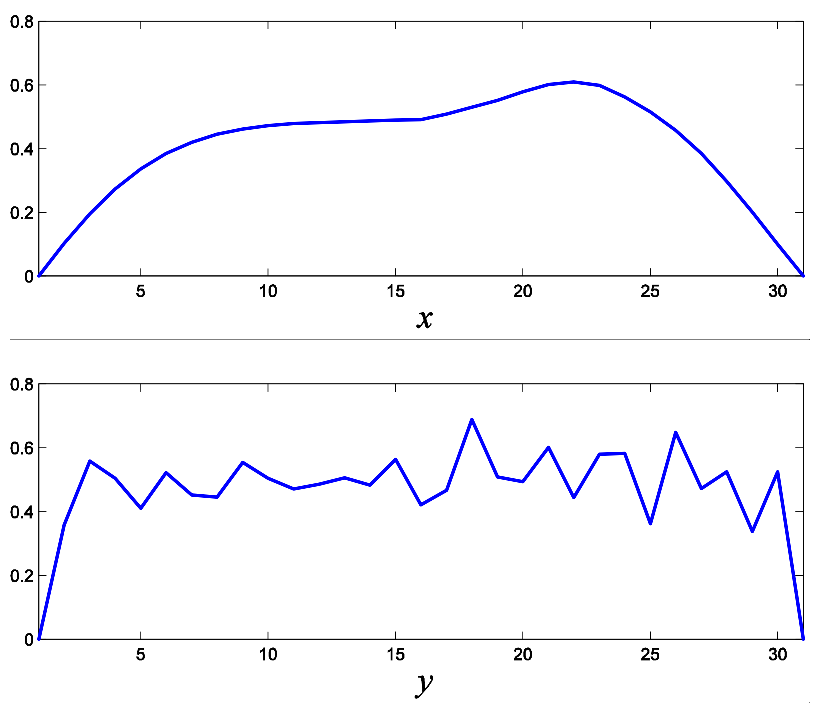
Error left by relaxation can be geometrically oscillatory

- 7 GS sweeps on

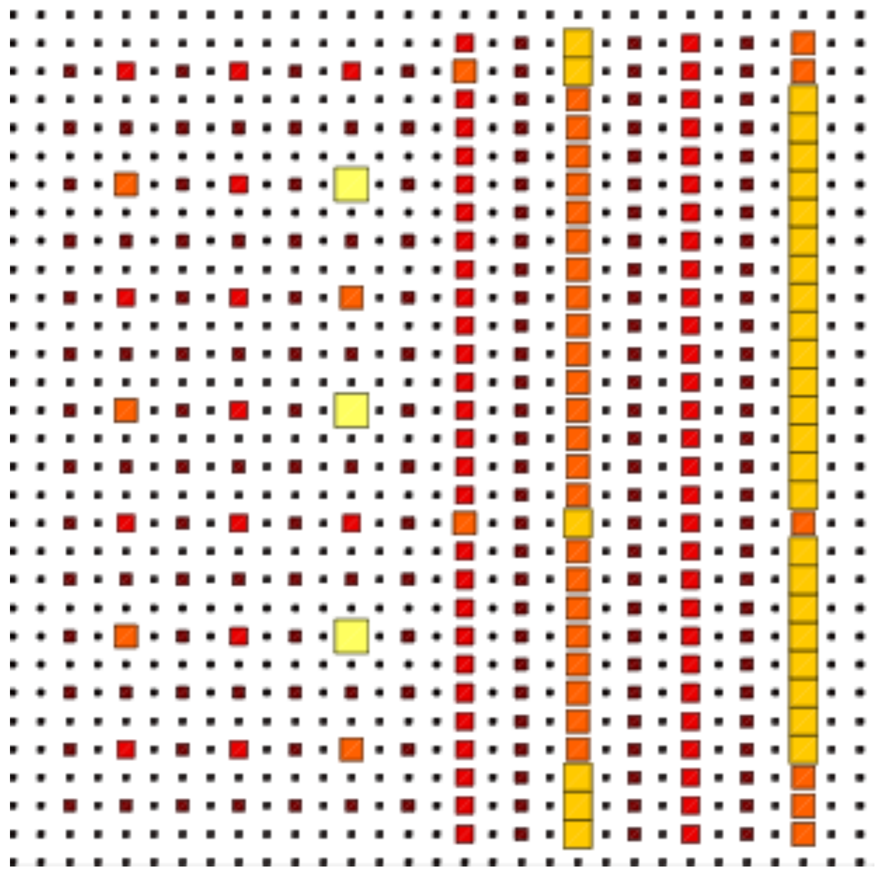
$$-au_{xx} - bu_{yy} = f$$

$a = b$	$a \gg b$





- Caution: this example
  - targets geometric smoothness
  - uses pointwise smoothers



don't coarsen in y, because b is very small, error is oscillatory in y

Slide credit: R. Falgout, 2/1/2016

AMG coarsens grids in the direction of geometric smoothness

"coarsen in the direction of strong connections"

Main idea: Algebraically smooth error

- Take a relaxation scheme such as w-Jacobi

$$e \leftarrow (I - M^{-1}A)e$$

- If relaxation stagnates, then the remaining error exhibits poor convergence, so

error component with small eigenvalues of A converge slowly

- Formally (characterized by small eigenvalues)

$$(I - M^{-1}A)e \approx e \Rightarrow M^{-1}Ae \approx 0 \Rightarrow r \approx 0$$

(small residual)

$$\langle Ae, e \rangle << 1$$

(small eigenvalues of A)

(if $\|e\| = 1$)

Main idea: Algebraically smooth error

- We then have

$$
\begin{aligned}
\langle Ae, e\rangle &= \sum_i e_i(A_{ii}e_i + \sum_{j\neq i} A_{ij}e_j) \\
&= \sum_i e_i \left(\sum_{j\neq i} -A_{ij}(e_i - e_j) \right) \\
&= \sum_{i<j} -A_{ij}\cdot e_i \cdot (e_i - e_j) + \sum_{i>j} -A_{ij}\cdot e_i \cdot (e_i - e_j) \\
&= \sum_{i<j} -A_{ij}\cdot e_i \cdot (e_i - e_j) - \sum_{i<j} -A_{ij}\cdot e_j \cdot (e_i - e_j) \\
&= \sum_{i<j} -A_{ij}\cdot (e_i - e_j)^2 \ll 1
\end{aligned}
$$

assume zero row sum $A_{ii} = -\sum_{i\neq j} A_{ij}$

swap i, j

A_{ji}

- Ok, so smooth error varies **slowly** in the direction of large matrix coefficients

when A_{ij} is large,
$e_i \simeq e_j$ after relaxation

Briggs, William L. and Henson, Van Emden and McCormick, Steve F., A Multigrid Tutorial (2Nd Ed., 20000

Take a look: `12-AMG-coarse-mesh.ipynb`

Main idea: Algebraically smooth error

- We have assumed **geometric** smoothness to show

$$\mathbf{e}^T A \mathbf{e} = \sum_{i<j} (-a_{ij})(e_i - e_j)^2 \ll 1$$

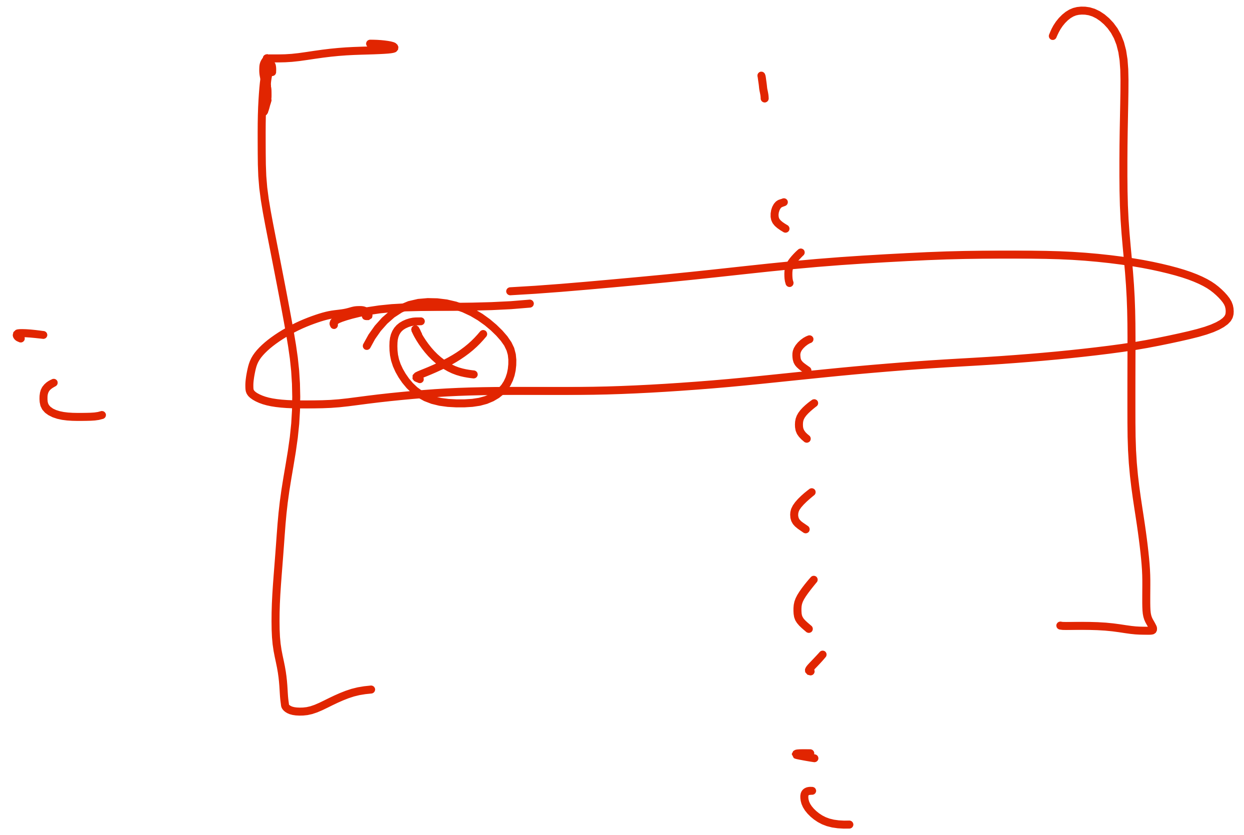
assume $a_{ij} < 0$ if $i \neq j$

- **CF AMG**: Smooth error varies slowly in the direction of "large" matrix coefficients
- **Strength of connection**: Given a threshold $0 < \theta \leq 1$, we say that variable u_i strongly depends on variable u_j if

$$-a_{ij} \geq \theta \max_{k \neq i} \{-a_{ik}\}$$

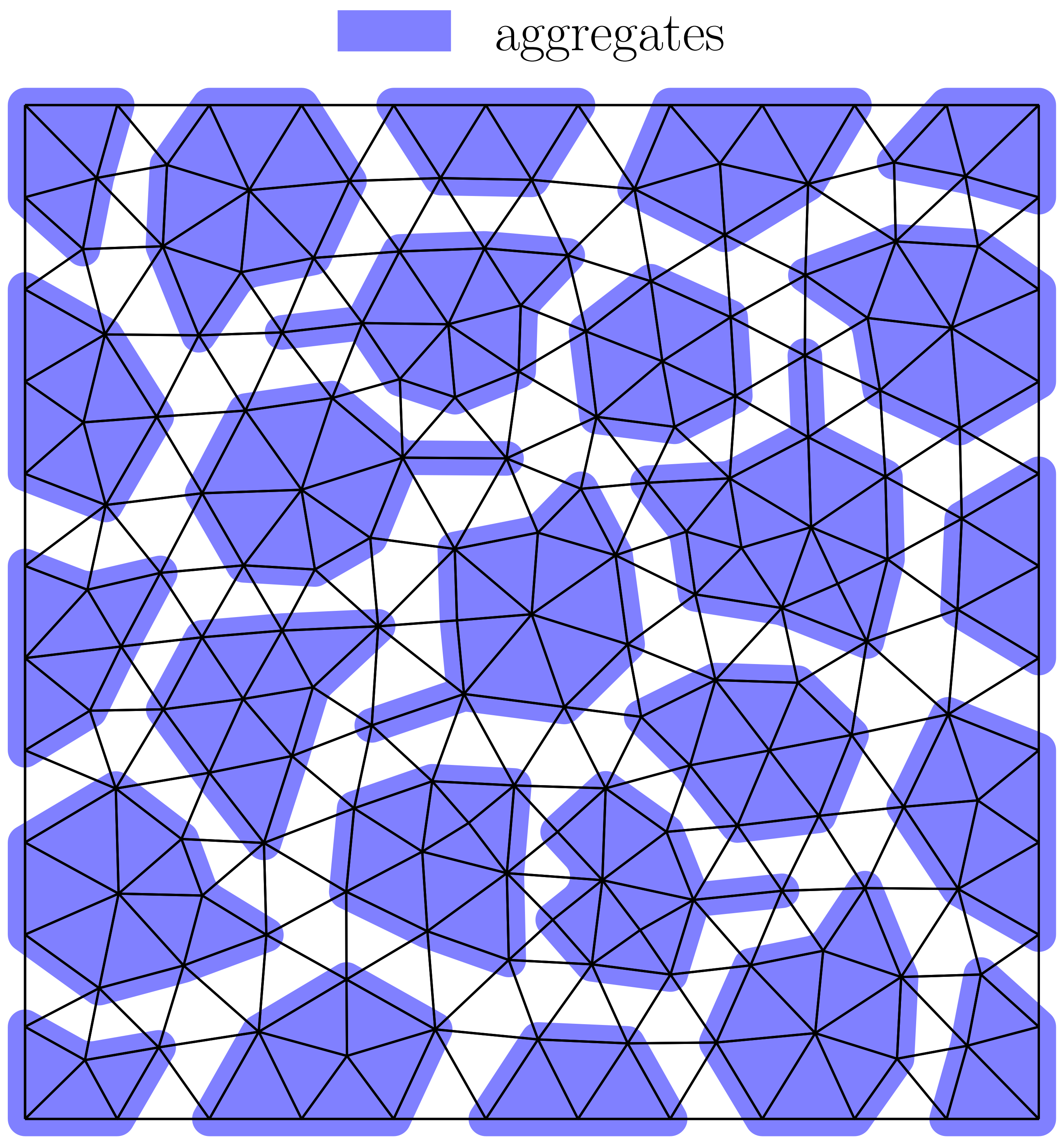
$<$ in row i

- Often positive off-diagonals are treated as weak
- This definition of strength of connection is not symmetric

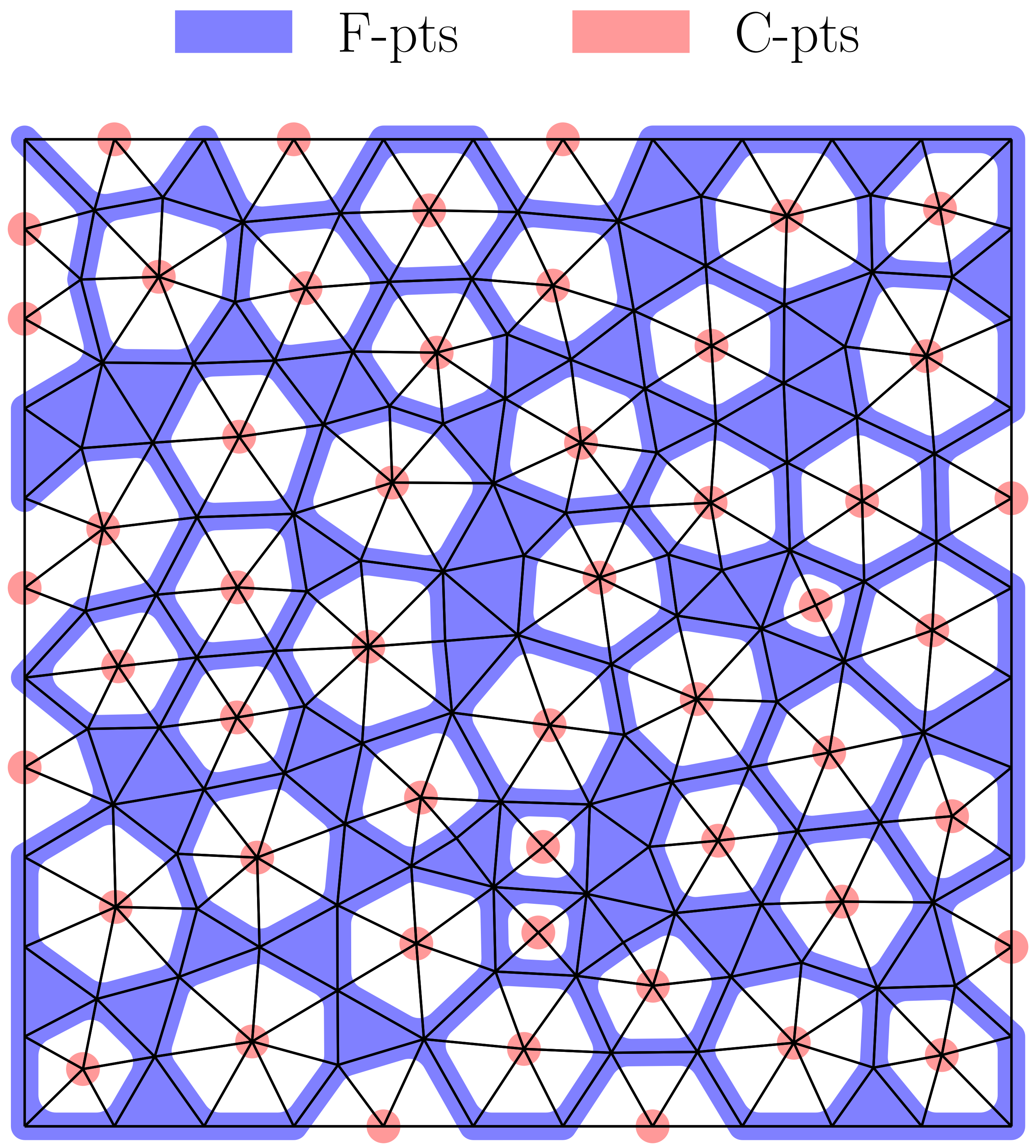


Slide credit: R. Falgout, 2/1/2016

Two (general) forms of AMG



- Smoothed Aggregation AMG (SA-AMG)
- Interpolation constructed from candidate vectors
- Clear approach to *optimize* interpolation



- Coarse-Fine AMG (CF-AMG) or Ruge-Stüben
- Coarse grid points are a subset of the fine grid points
- Edge-wise construction of interpolation, allowing straightforward control of sparsity
- Incorporating near-nullspace is not straightforward