Approximation of Eigenvalue Problems I
Ritz–Galerkin discretization with finite elements

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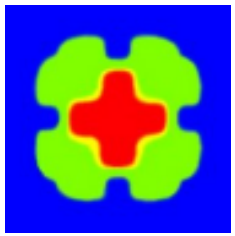

IWR School 2017: Mathematical Methods in Quantum Mechanics

1. Eigenvalue problems in Hilbert spaces
2. Introduction of the FEM
3. Ritz-Galerkin approximation of EVP
4. Additional improvements

1. **Eigenvalue problems in Hilbert spaces**
   - Schrödinger Equation
   - Variational EVP
   - Spectral analysis
   - Spectral transformations
   - Spectrum of the Schrödinger operator
   - The minimum-maximum principle
2. **Introduction of the FEM**
3. **Ritz-Galerkin approximation of EVP**
4. **Additional improvements**

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Literature: Hilbert spaces and linear operators

- W. Rudin: Functional Analysis, 2nd ed., 1991
- K. Yosida: Functional Analysis

$u = \psi$

Stationary Schrödinger equation in strong form

$$-\Delta u + V(u) = \lambda u$$

Assumptions

- u square integrable on $\mathbb{R}^3$

$$\Rightarrow \qquad |\mathbf{x}u(\mathbf{x})|^2 \to 0 \quad \text{as} \quad |\mathbf{x}| \to \infty$$

- $V(u)$ vanishes for $r \to \infty$

$$\text{Example:} \quad V(u) = \sum \frac{1}{|\mathbf{x}-\mathbf{x}_i|} u$$

- Single electron for the exposition

Erwin Schrödinger

$$\int_{\mathbb{R}^3} -\Delta u v + V(r) u v = \int_{\mathbb{R}^3} f v$$

1. Multiply with test function v
2. Integrate by parts
3. Boundary terms at infinity vanish

Schrödinger equation in weak form

$$\int_{\mathbb{R}^3} \nabla u \cdot \nabla v \, d\mathbf{x} + \int_{\mathbb{R}^3} V(u) v \, d\mathbf{x} = \lambda \int_{\mathbb{R}^3} uv \, d\mathbf{x}$$

Abstract formulation

Find $u \in H$ and $\lambda \in \mathbb{C}$ such that for all $v \in H$

$$a(u, v) = \lambda (u, v)$$

1. Symmetric bilinear form $a(u, v)$

$$a(u, v) = \int_{\mathbb{R}^3} \nabla u \cdot \nabla v \, d\mathbf{x} + \int_{\mathbb{R}^3} V(u) v \, d\mathbf{x}$$

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2. Inner product on $L^2(\mathbb{R}^3)$

$$(u, v) = \int_{\mathbb{R}^3} uv \, d\mathbf{x}$$

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$$(u,v) = \int_{\mathbb{R}^3} uv \, d\mathbf{x}$$

3. Target space

$$H = L^2(\mathbb{R}^3)$$

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Variational eigenvalue problem

Find $u \in H$ and $\lambda \in \mathbb{C}$ such that for all $v \in H$

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Source problem for given f

Find $u \in H$ such that for all $v \in H$

$$a(u, v) = (f, v)$$

Source problem

Find $u \in H$ such that for all $v \in H$

$$a(u, v) = (f, v)$$

Operator equation

$$a(u, v) =: (Au, v) = (f, v)$$
$$Au = f$$

A

H

The domain of the operator

[for the mathematically inclined]

$$a(u,v) = \int_{\mathbb{R}^3} \nabla u \cdot \nabla v \, d\mathbf{x} + \int_{\mathbb{R}^3} V(u) v \, d\mathbf{x}$$

- The form may not be defined for given $u \in H$
- The domain of A is

$$\mathcal{D}(A) := \left\{ u \in H \;\middle|\; a(u,v) < \infty \;\forall v \in \mathcal{D}(A) \right\}$$

- The domain of A is the space of functions with square integrable derivatives $H^1(\mathbb{R}^3)$

Density argument

$H^1(\mathbb{R}^3)$ is dense in $L^2(\mathbb{R}^3)$

$H^1 \ni u_n \to u \in L^2$

$a(u_n, v) \to a(u, v)$ if $u \in H^1$

$\to \infty$ if $u \notin H^1$

Restriction to the domain

$$a(u,v) = \lambda(u,v)$$

- We are interested in finite eigenvalues λ
  - Typically eigenvalues with low index
- All eigenfunctions of A are in the domain of A.
  - The only difficulties appear for infinite eigenvalues

Spectral properties of certain operators

- Compact operators
  - Countable, bounded set of eigenvalues
  - accumulating, if at all, at zero
  - typically found in finite element papers
- Self-adjoint operators
  - The spectrum is real and consists of
    - (discrete) eigenvalues and/or
    - continuous essential spectrum
  - Schrödinger operator

Compact operators

- Example: Laplacian with zero boundary values on Ω, bounded, convex domain

Since $D(A) = H^1_0(\Omega)$

$$a(u,v) = \int_\Omega \nabla u \cdot \nabla v \, d\mathbf{x} \qquad = D(A^*)$$

- A is unbounded on $L^2(\Omega)$ and thus not compact
- A is self-adjoint, positive definite

Solution operator

$$a(Tf, v) = (f, v) \qquad \forall v \in H^1(\Omega)$$

$H^1(\Omega) \subset L^2(\Omega)$ is the space on which $a(.,.)$ is bounded

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The operator T maps $L^2(\Omega)$ to $H^1(\Omega)$

Rellich-Kondrashov theorem

If Ω is bounded with Lipschitz boundary, the operator T is compact.

Franz Rellich

Vladimir Iosifovich Kondrashov

Eigenvalues of A and T

$$(Tf, v) = \mu(f, v)$$

A is self-adjoint, T is self-adjoint with respect to $(.,.)$ and $a(.,.)$

$$(u, v) = \mu\, a(u, v)$$

$$a(u, v) = \lambda (u, v)$$

$$\Longrightarrow \lambda = \frac{1}{\mu}$$

Spectrum of A and T

- The spectrum of T

$$\mu_1 \geq \mu_2 \geq \cdots > 0$$

- The spectrum of A

$$0 < \lambda_1 \leq \lambda_2 \leq \ldots$$

Eigenfunctions of A and T

- Eigenfunctions are mutually orthogonal
- The eigenfunctions form a (Schauder) basis for H:

$$v = \sum_{k=1}^{\infty} \alpha_k u_k \qquad Av = \sum_{k=1}^{\infty} \lambda_k \alpha_k u_k$$

Semi-bounded operators

- Positive definite

$$a(u,u) \geq \alpha > 0$$

- Semi-bounded:

$$a(u,u) \geq \gamma$$

For any $\varepsilon > 0$, the bilinear form

$$b(u,v) = a(u,v) + (\gamma + \varepsilon)(u,v)$$

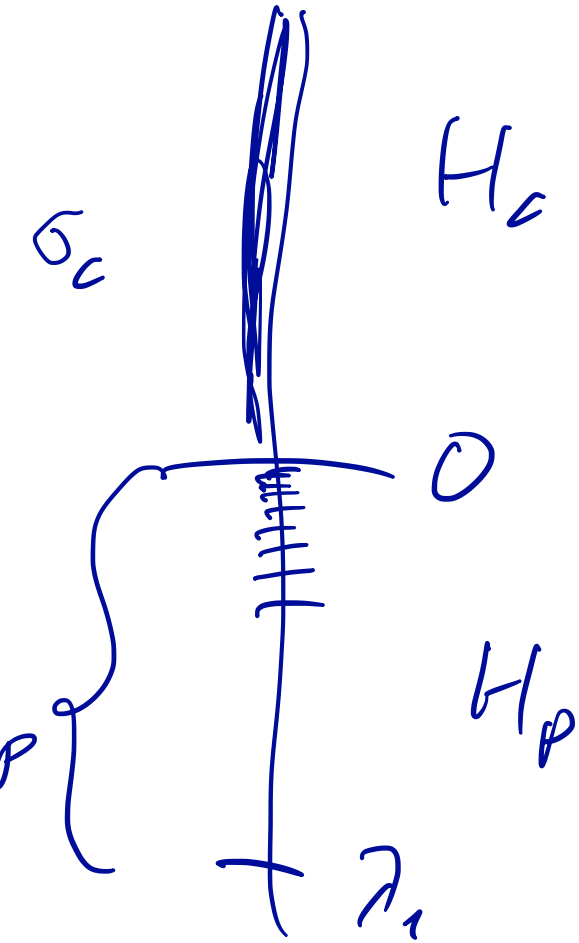
is positive definite. Let ν be an eigenvalue of the associated operator B with eigenfunction u, then $\lambda = \nu - \gamma - \varepsilon$ is an eigenvalue of A with the same eigenfunction.

Spectrum of the Schrödinger operator

- A is semi-bounded, self-adjoint
- $\Omega = \mathbb{R}^3$, no compactness of T
- Point spectrum with eigenfunctions u_k

$$\lambda_1 \leq \lambda_2 \leq \ldots \lambda_n < 0$$

- Essential spectrum: $\mathbb{R}^+$ with projectors $P(t)$
  - $P(t)u$ is "generalized eigenfunction"



Spectral representation

Any $v \in H$ is characterized by coefficients α_k and $\beta(t)$ through

$$v = \sum_{k=1}^{n} \alpha_k u_k + \int_0^\infty P(t) u \, dt$$

$$Av = \sum_{k=1}^{n} \lambda_k \alpha_k u_k + \int_0^\infty tP(t) u \, dt$$

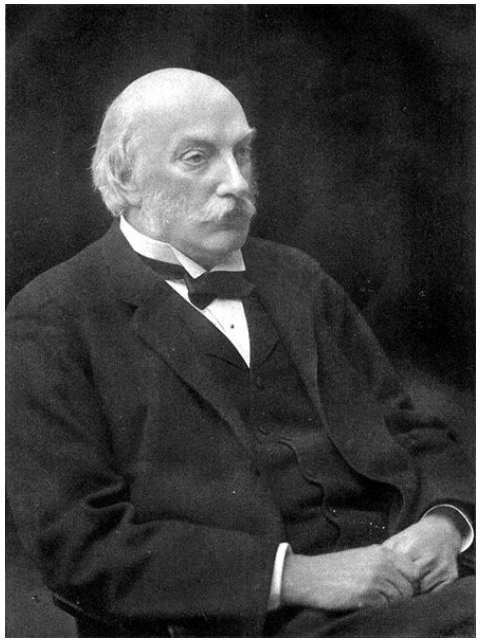
The Rayleigh quotient

Let u_k be an eigenfunction of the self-adjoint operator A. Then,

$$\lambda_k = \frac{a(u_k, u_k)}{(u_k, u_k)}$$

In particular, if A is bounded from below and above, then

$$\lambda_{\min} = \min_{u \in H} \frac{a(u,u)}{(u,u)} \qquad \lambda_{\max} = \max_{u \in H} \frac{a(u,u)}{(u,u)}$$



John William Strutt
3rd Baron Rayleigh

Corollary

If H is finite-dimensional, the extremal eigenvalues are characterized as minimum and maximum of the Rayleigh quotient.

How to characterize the second eigenvalue?

λ_1, u_1 by Rayleigh quotient

$$\lambda_2 = \min_{\substack{u \in V \\ u \perp u_1}} \frac{a(u,u)}{(u,u)}$$

The Courant-Fischer min-max theorem

Let the eigenvalues (below the essential spectrum if T is not compact) of A be sorted

$$\lambda_1 \leq \lambda_2 \leq \dots$$

Then, with subspaces $U \subset H$

$$\lambda_k = \min_{\substack{U \subset H \\ \dim U = k}} \max_{u \in U} \frac{a(u,u)}{(u,u)}$$

minimum is obtained for $U = \operatorname{span}\{u_1 \dots u_k\}$

Richard Courant

Ernst Sigismund Fischer

Images: Mathematisches Forschungsinstitut Oberwolfach (MFO)

Literature: the finite element method

- Ch. Grossmann, H.-G. roos, M. Stynes: Numerical Treatment of Partial Differential Equations, Springer 2007.
- G. Strang, G. Fix: An analysis of the finite element method, Prentice-Hall 1973.
- C. Johnson: Numerical Solutions of Partial Differential Equations by the Finite Element Method, Cambridge University Press 1987 (reprint at Dover Classics)
- S. C. Brenner, L. R. Scott: The Mathematical Theory of Finite Element Methods, Springer, 2002
- Ph. G. Ciarlet: The Finite Element Method for Elliptic Problems, North-Holland 1978.

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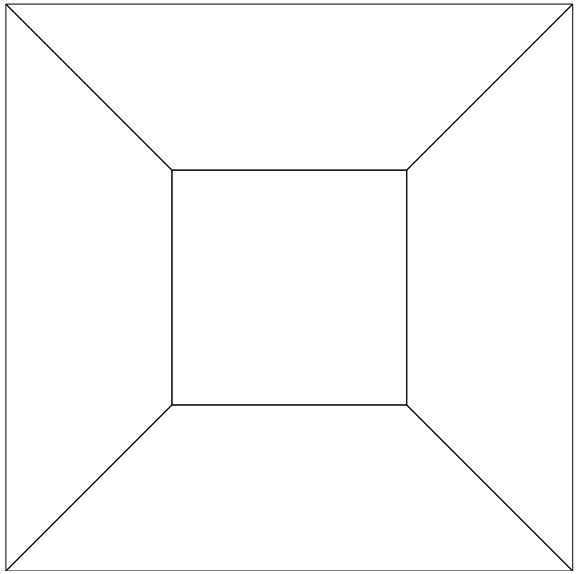
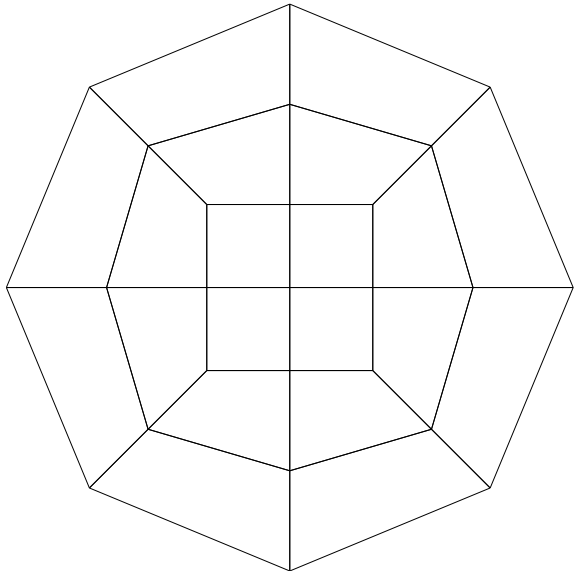
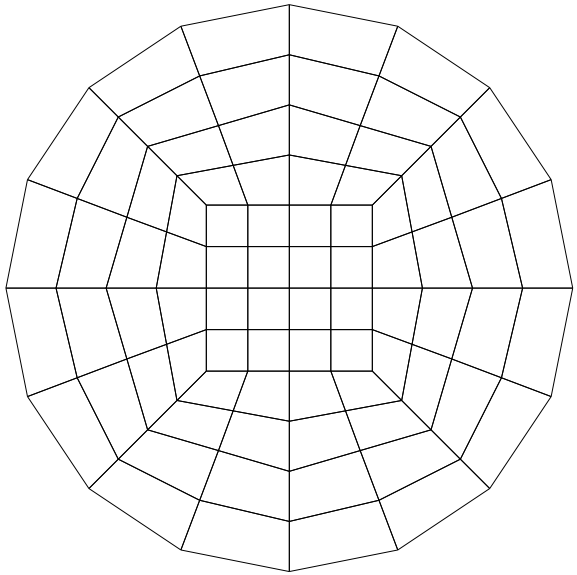
Ingredients to FEM

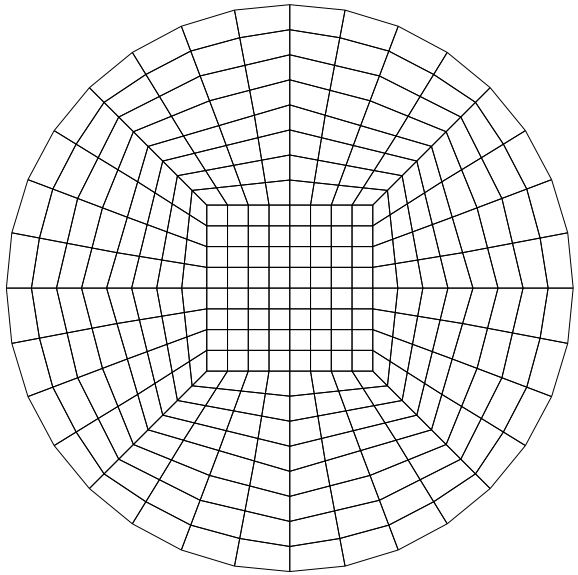
1. A variational formulation on a domain Ω
   - Ω must be bounded!
2. A "mesh" covering Ω by simple shapes (cells)
   - triangles, quadrilaterals in 2D
   - tertahedra, hexahedra in 3D
   - more complicated choices possible
3. A shape function space on each cell
4. A rule how to connect these functions between cells

Examples for meshes

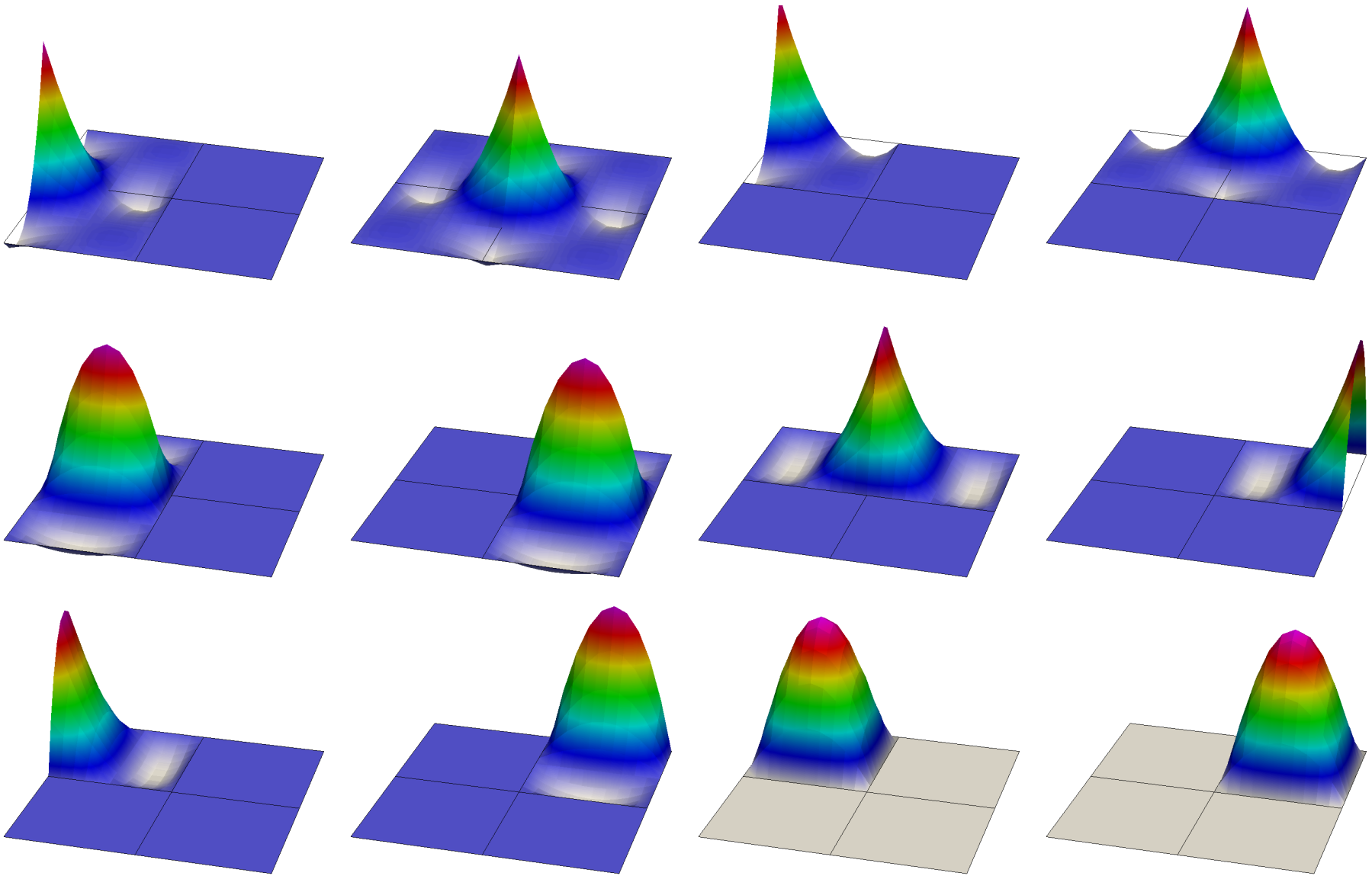








Example: Q_2 continuous basis (selection)

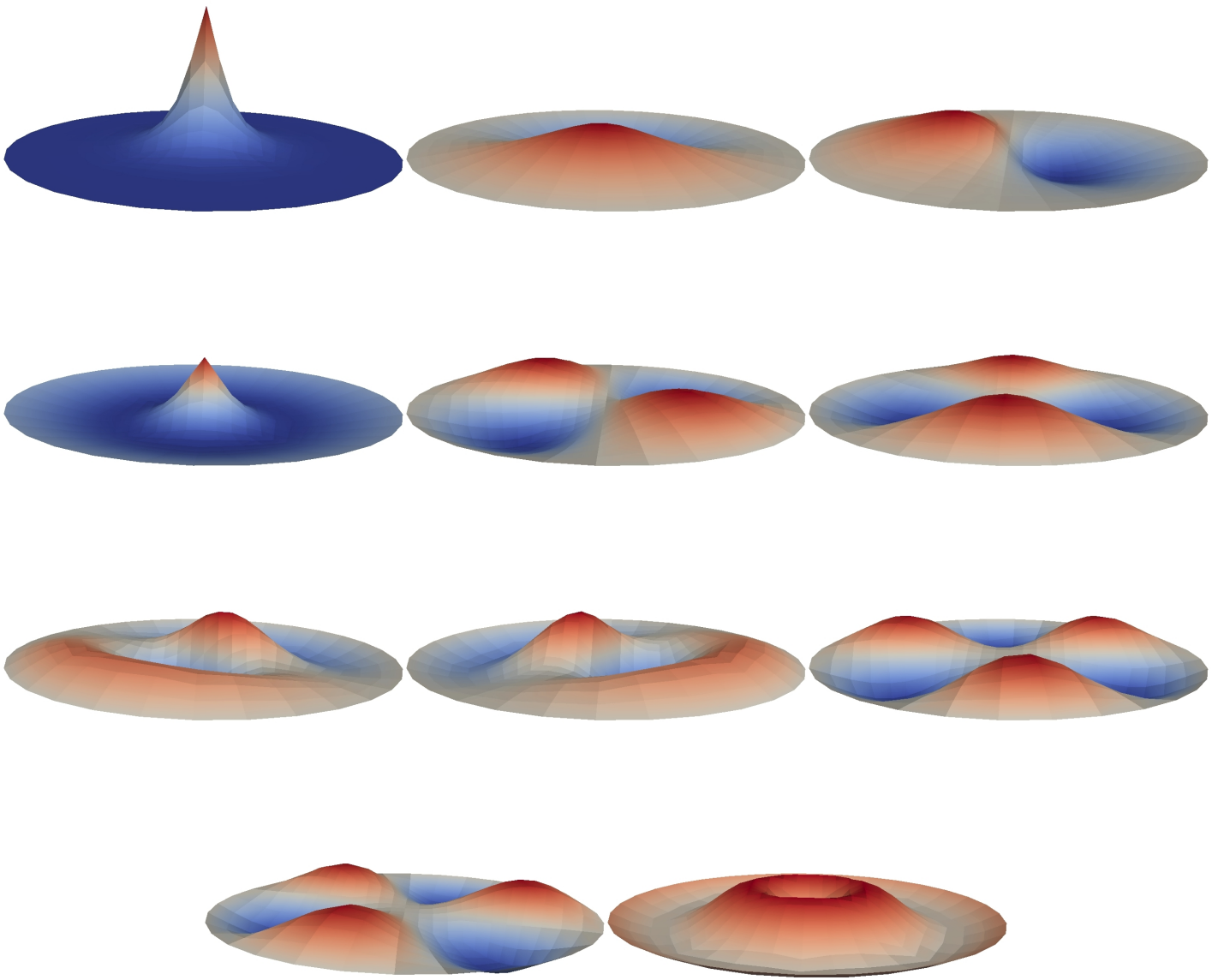


Finite element spaces

- Combining the mesh and the shape functions, we obtain a function space H_n
  - Localy described by shape functions
  - Globally described by mesh
  - Functions are identified by coefficient vectors

n = dimension of H_n

Example: eigenfunctions of 1D hydrogen atom



Interpolation estimates

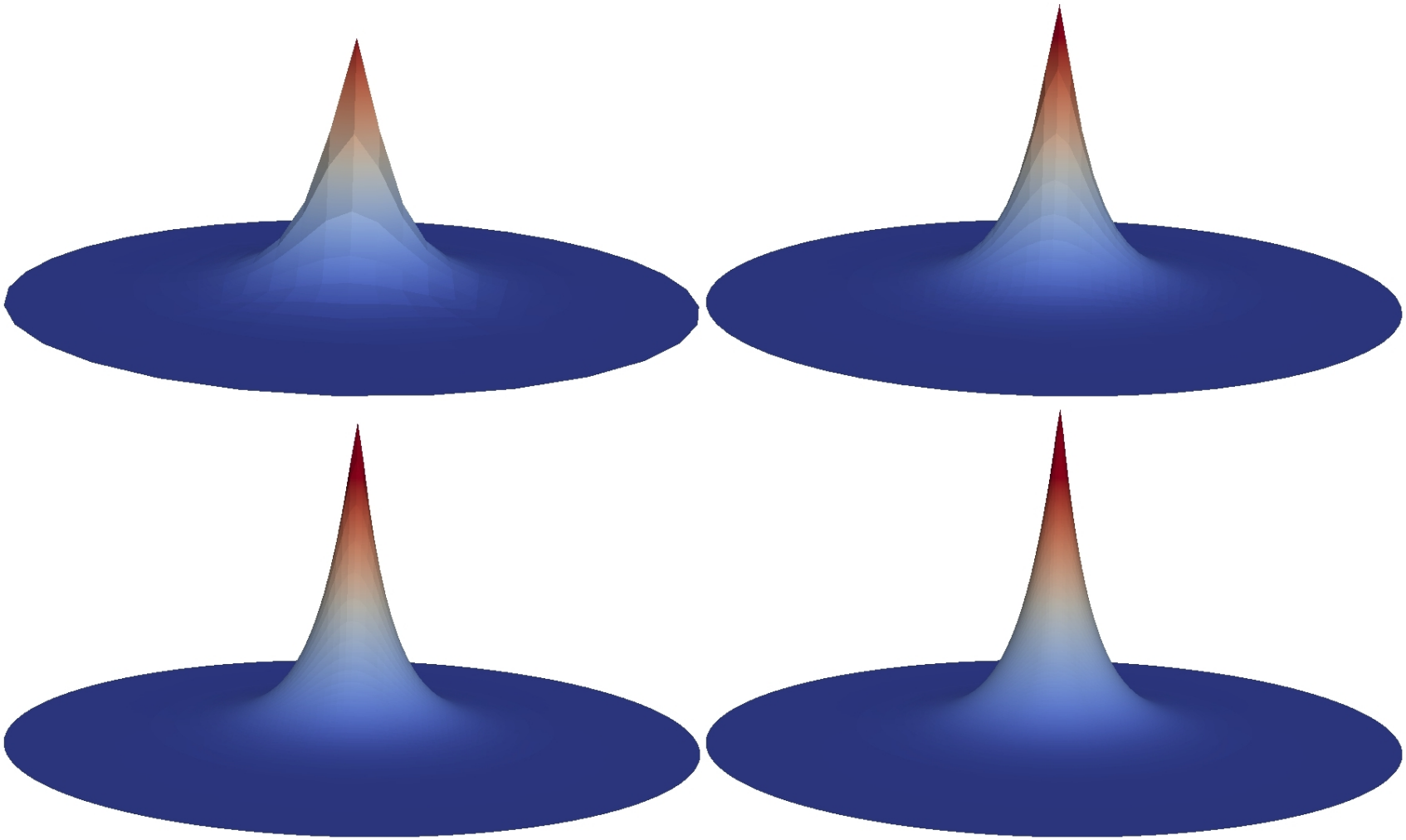
For shape function spaces of polynomial degree k and $j \leq k+1$ holds for meshes of maximum cell diameter h

$$\max_{u \in H} \min_{v \in H_h} \|u - v\| \lesssim h^j \left\|\nabla^j u\right\|$$

∇^j = tensor of derivatives of order j

- Estimate depends on smoothness of u.

Example: mesh refinement



Principle of Approximation

Find $u \in H$, such that

$$a(u, v) = f(v) \quad \forall v \in H$$

- Finite element methods are projection methods

Principle of Approximation

Find $u_n \in H_n$, such that

$$a(u_n, v_n) = f(v_n) \quad \forall v_n \in H_n$$

- Finite element methods are projection methods
- Replace the space H by a finite dimensional subspace $H_n \subset H$
  - Ritz-Galerkin method

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- Finite element methods are projection methods
- Replace the space H by a finite dimensional subspace $H_n \subset H$
  - Ritz-Galerkin method
- FEM refers to a special choice of subspaces

1. Eigenvalue problems in Hilbert spaces
2. Introduction of the FEM
3. **Ritz-Galerkin approximation of EVP**
   - Approximation of subspaces
   - Eigenvalue estimates
4. Additional improvements

Literature: Ritz-Galerkin approximation of EVP

- A. V. Knyazev, J. E. Osborn: New a priori FEM error estimates for eigenvalues, SIAM J. Numer. Anal. 43(6), pp. 2647–2667, 2006
- Older articles by Osborn and coauthors

Principle of Ritz-Galerkin approximation

- Replace the infinite dimensional function space H by a finite dimensional subspace H_n
- Use the same bilinear form

Approximating sequence

$$H_1 \subset H_2 \subset \cdots \subset H$$

such that for any $u \in H$

$$\inf_{v \in H_n} \|u - v\| =: \varepsilon_n(u) \to 0$$

Walter Ritz

Boris Grigoryevich Galerkin

Continuous EVP

Find $u_k \in H$ and $\lambda_k \in \mathbb{C}$
such that for all $v \in H$

$$a(u_k, v) = \lambda_k (u_k, v)$$

- λ_k: eigenvalue
- u_k: eigenvector, eigenfunction
- U_k: eigenspace

Ritz-Galerkin approximation

Find $u_k^{(n)} \in H_n$ and $\lambda_k^{(n)} \in \mathbb{C}$
such that for all $v \in H_n$

$$a(u_k^{(n)}, v) = \lambda_k^{(n)} \left(u_k^{(n)}, v\right)$$

- $\lambda_k^{(n)}$: Ritz value
- $u_k^{(n)}$: Ritz vector
- $U_k^{(n)}$: discrete eigenspace
- $n = \dim H_n$

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The Courant-Fischer min-max theorem

Let the Ritz values of A_n be sorted

$$\lambda_1^{(n)} \leq \lambda_2^{(n)} \leq \cdots \leq \lambda_n^{(n)}$$

Then, with subspaces $U \subset H_n \subset H$

$$\lambda_k^{(n)} = \min_{\substack{U \subset H_n \\ \dim U = k}} \max_{u \in U} \frac{a(u,u)}{(u,u)}$$

$$\lambda_k \leq \lambda_k^{(n)}$$

Separation theorem for single eigenvalues

Let the eigenvalues be real, single, and sorted such that

$$\lambda_1 < \lambda_2 < \dots$$

For each k there is an n such that

$$\lambda_k \leq \lambda_k^{(n)} < \lambda_{k+1}$$

Multiple eigenvalues

- All higher eigenvalues are degenerate
- The approximating Ritz values may or may not be equal

Separation theorem for multiple eigenvalues

Let the eigenvalues be sorted as before, but let λ_k be a j-fold eigenvalue,

$$\lambda_{k-1} < \lambda_k = \lambda_{k+1} = \cdots = \lambda_{k+j-1} < \lambda_{k+j}$$

Then, there is an n such that for the approximating Ritz values holds

$$\lambda_k \leq \lambda_k^{(n)} \leq \cdots \leq \lambda_{k+j-1}^{(n)} < \lambda_{k+j}$$

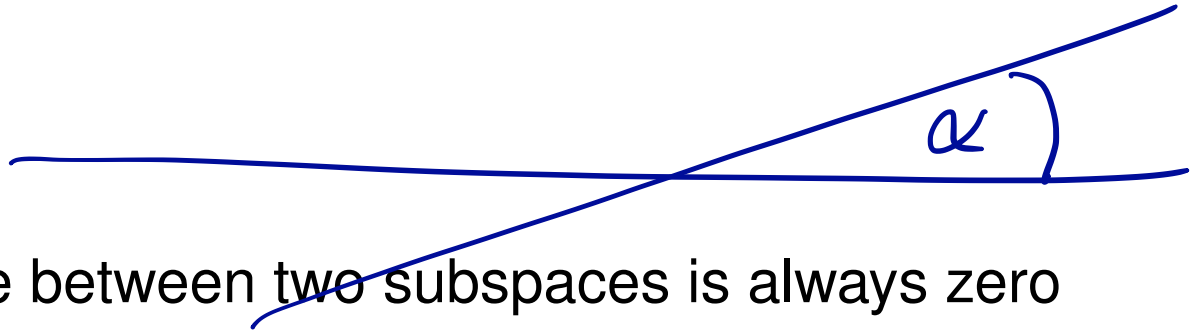
Reliability of small eigenvalues

If the approximation space H_n is rich enough, the lowest eigenvalues, single or multiple, will be approximated in the right order

Approximation of eigenvectors

- Eigenvectors are the wrong abstraction
  - Can be scaled and are still eigenvectors
  - May span multidimensional space for the same eigenvalue

Approximation of eigenspaces



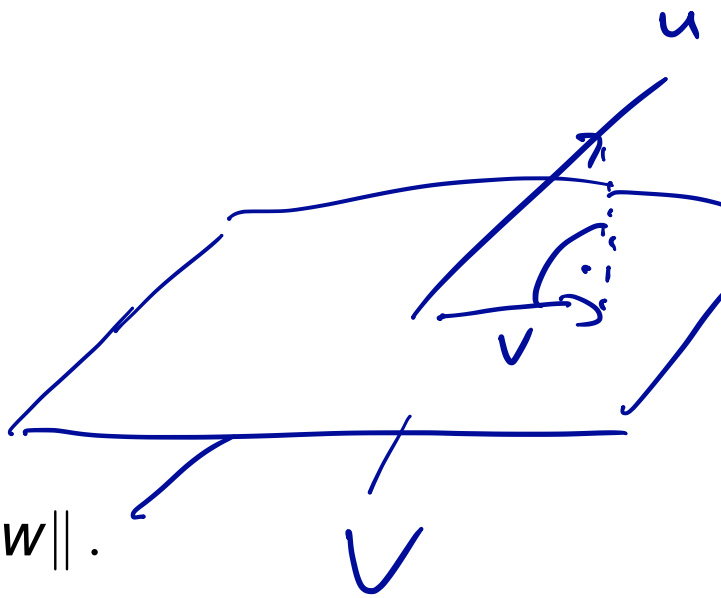
- The distance between two subspaces is always zero
  - both intersect at zero
- For any nonzero vector, the angle between the spaces determines the best approximation

Principal angle

Define the angle between arbitrary subspaces of a vector space such that they provide an estimate for the approximation of one subspace by the other.

Principal angles between vector and subspace

$$\angle(u, V) \qquad \|u\| = 1$$



1. Find $v \in V$ such that

$$\|u - v\| = \min_{w \in V} \|u - w\| .$$

2. v is the orthogonal projection

$$\begin{aligned} \|u\|^2 &= \|v\|^2 + \|u - v\|^2 \\ \sin \angle(u, v) &= \|u - v\| \\ \cos \angle(u, v) &= \|v\| \end{aligned}$$

Principal angles between subspaces

U, V finite dimensional subspaces of H

$$\angle(U, V)$$

1. Measure the angle between every vector from U and V
2. Take the worst case

Definition: largest principal angle

The largest principal angle between two subspaces U and V of H is defined by

$$\sin \angle(U, V) = \max_{u \in U} \min_{v \in V} \frac{\|u - v\|}{\|u\|}$$

Refined notion of principal angles

Sometimes, the worst case is not what we want!

Definition: the principal angles between subspaces

For subspaces U with $\dim U = k$ and V, we define the j-th principal angle as

$$\angle_j(U,V) = \min_{\substack{W \subset U \\ \dim W = j}} \angle(W,V)$$

or

$$\sin \angle_j(U,V) = \min_{\substack{W \subset U \\ \dim W = j}} \max_{w \in W} \min_{v \in V} \frac{\|w - v\|}{\|w\|}$$

The recursive meaning of principal angles

- The first principal angle describes the best approximation of a vector in U by a vector in V:

$$\sin \angle_1(U, V) = \min_{u \in U} \min_{v \in V} \frac{\|u - v\|}{\|u\|}$$

Let U_1 be the subspace generated by this vector $u_1 = u$.

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- The angle $\angle_2$ describes the best approximation of a vector in U orthogonal to U_1, yielding a subspace U_2.

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- The angle $\angle_2$ describes the best approximation of a vector in U orthogonal to U_1, yielding a subspace U_2.
- The angle $\angle_j$ describes the best approximation of a vector orthogonal to U_{j-1}, and defines a subspace U_j.

Preliminaries to eigenvalue estimates

- Derived for the eigenvalues μ_k of the solution operator T
- For positive definite A:

$$T = A^{-}1 \qquad \lambda_k = \frac{1}{\mu_k}$$

- For semi-bounded A choose σ such that $A - \sigma I$ is positive definite:

$$T = (A - \sigma I)^{-}1 \qquad \lambda_k = \frac{1}{\mu_k - \sigma}$$

- Eigenvalues of T are decreasing, beware of the use of “lower”!

First estimate

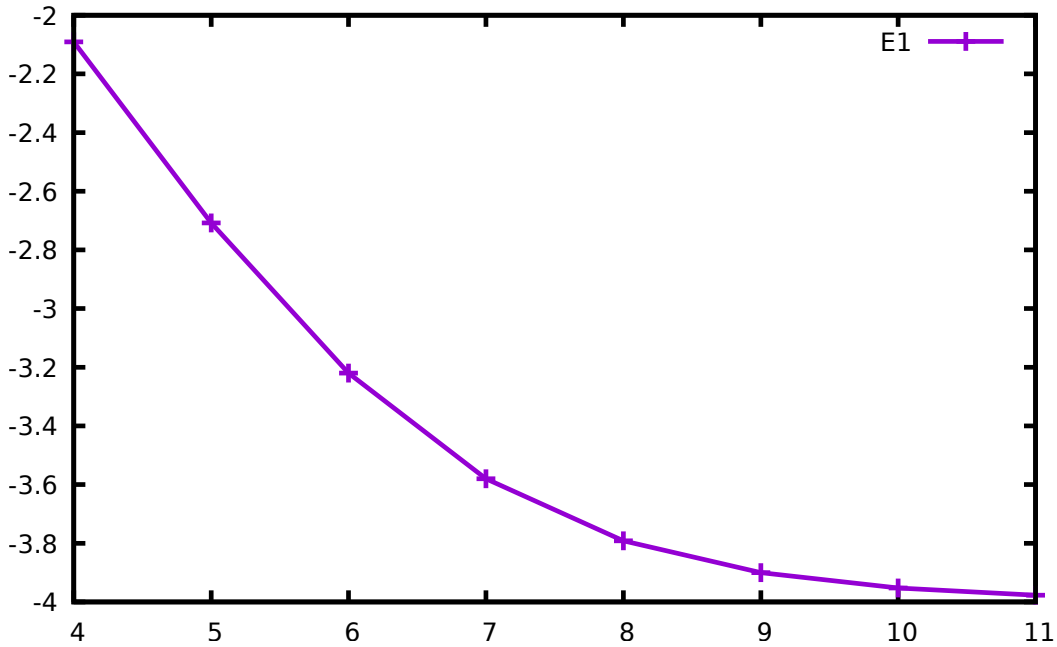
$$0 \leq \frac{\mu_k - \mu_k^{(n)}}{\mu_k} \leq \sin^2 \angle(U_{1,\dots,k}, H_n) \leq \sum_{j=1}^{k} \sin^2 \angle(U_j, H_n)$$

h^2 for FEM of lowest order

with $U_{1,\dots,k} = U_1 \oplus \cdots \oplus U_k$.

- Estimate is particularly simple
- Involves estimates for all previous eigenvalues
- Extends to multiple eigenvalues

Example: smallest Ritz value of A



$\lambda_1^{(n)}$ over $n = 5 \cdot 4^k$

Let

$$\mu_{k-1} > \mu_k = \mu_{k+1} = \cdots = \mu_{k+q-1} > \mu_{k+q}$$

with $k + q < n$.

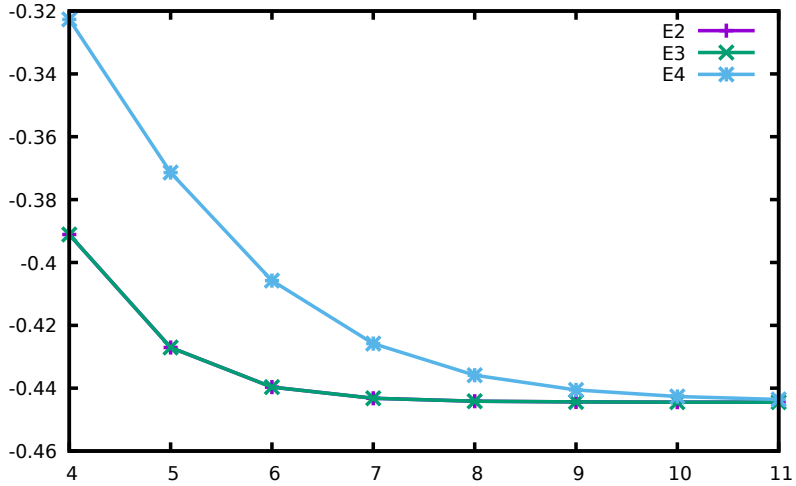
Refined estimate for multiple eigenvalues

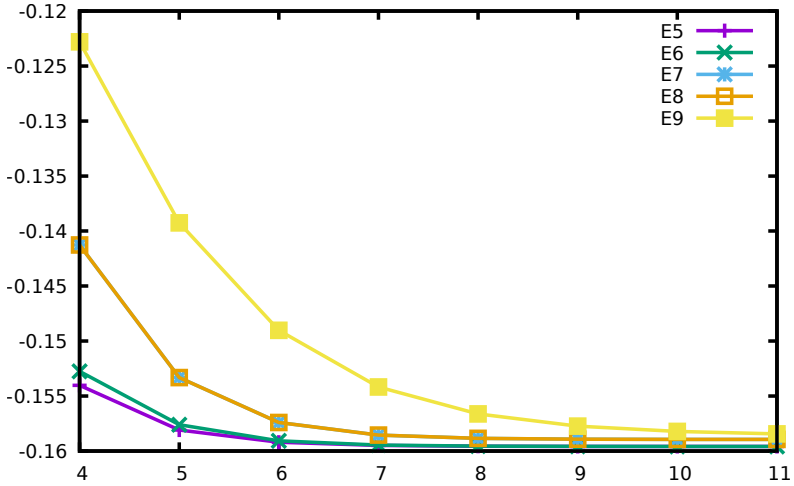
For any $j = 0, \ldots, q-1$ holds

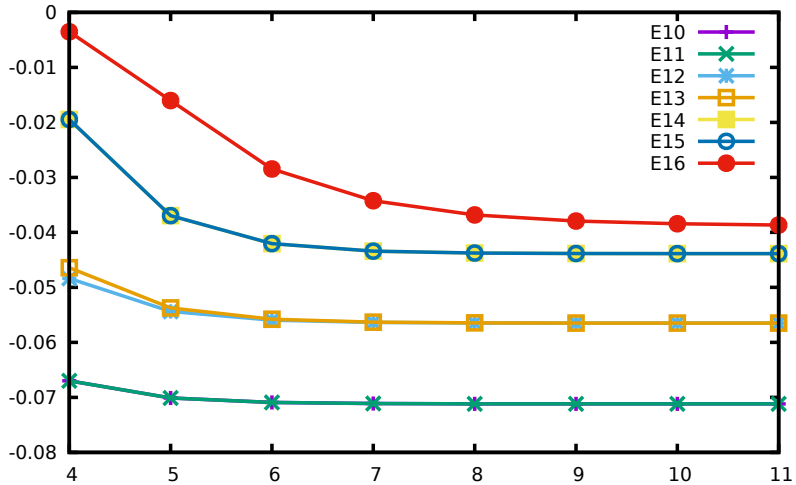
$$0 \leq \frac{\mu_k - \mu_{k+j}^{(n)}}{\mu_k} \leq \sum_{i=1}^{k-1} \sin^2 \angle(U_i, H_n) + \sin^2 \angle_j(U_k, H_n)$$

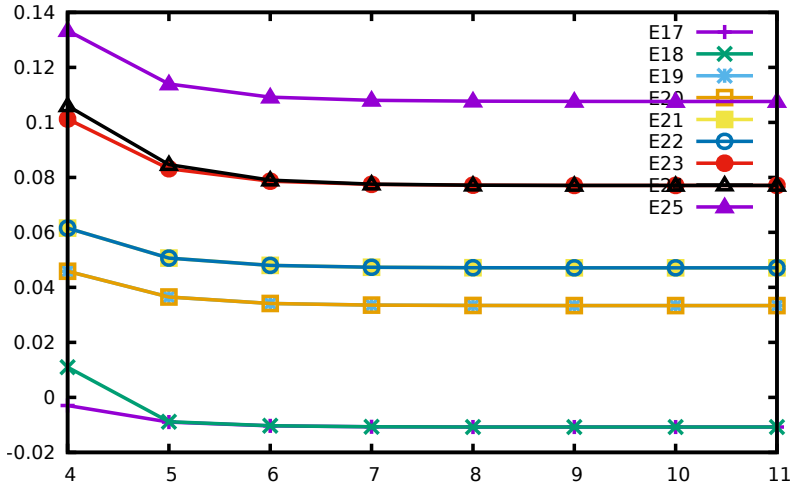
- q-dimensional eigenspace U_k
- Eigenvectors are sorted by approximability

Example: Ritz value of A



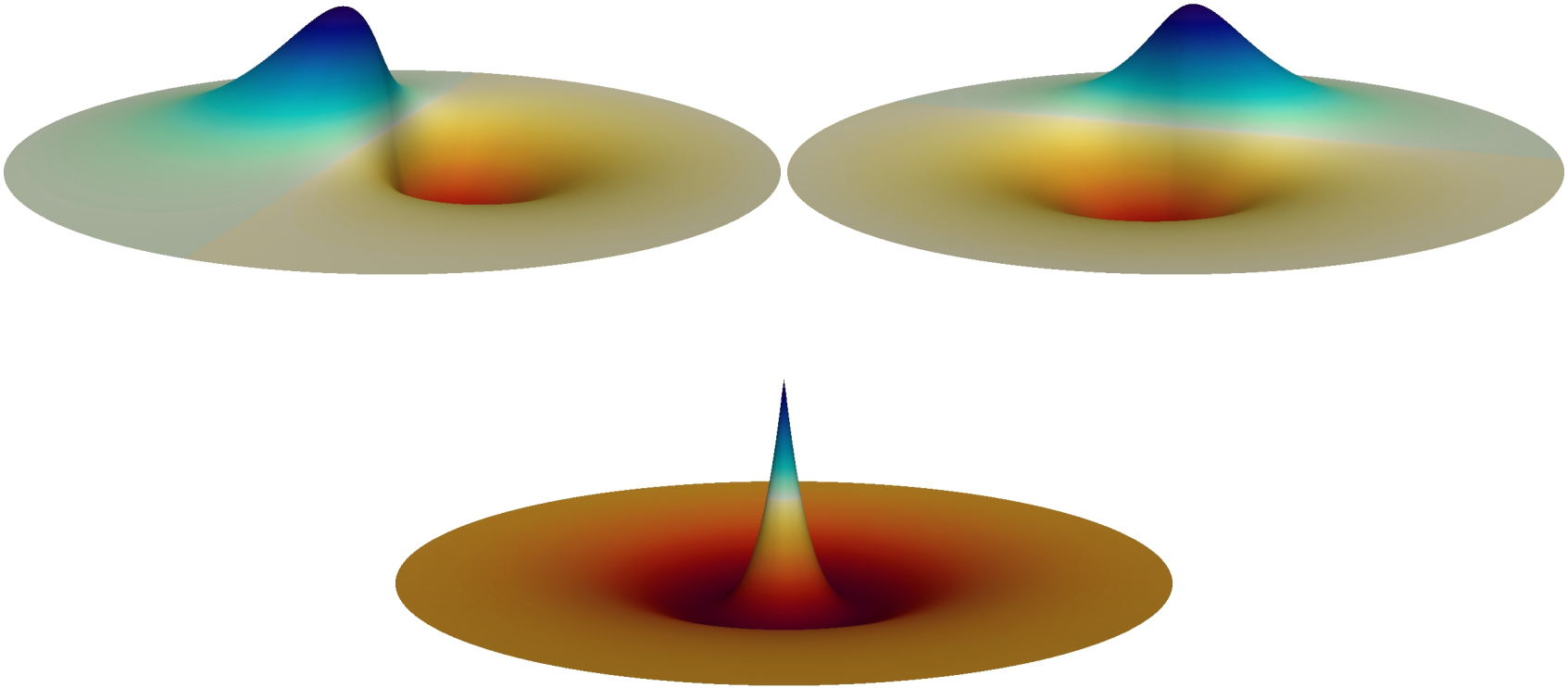






Example: eigenfunctions 2, 3, 4

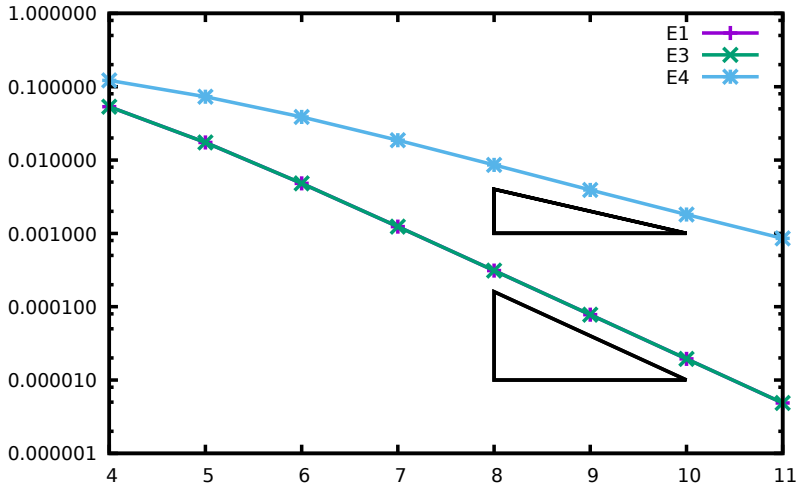
Ritz values: -0.44350691578878 -0.44350691578876
-0.43900523253881

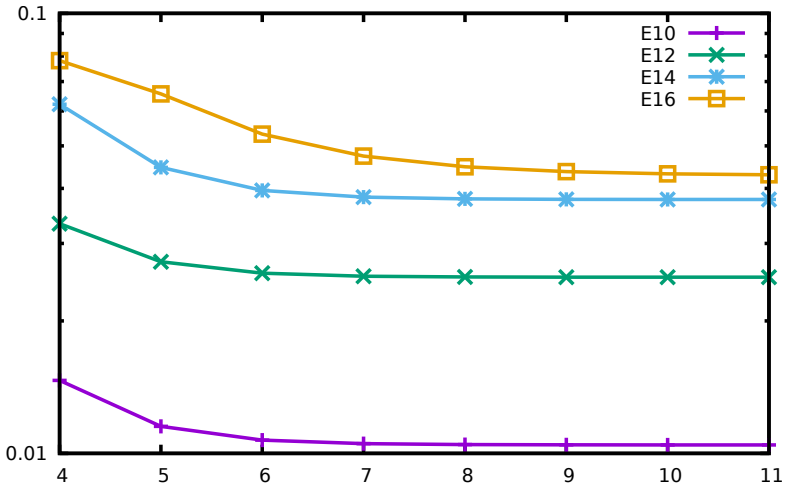


Can you explain the order?

1. Eigenvalue problems in Hilbert spaces
2. Introduction of the FEM
3. Ritz-Galerkin approximation of EVP
4. **Additional improvements**
   - The artificial boundary
   - Adaptive methods
   - Numerical quadrature

Observed errors do not follow the theory!



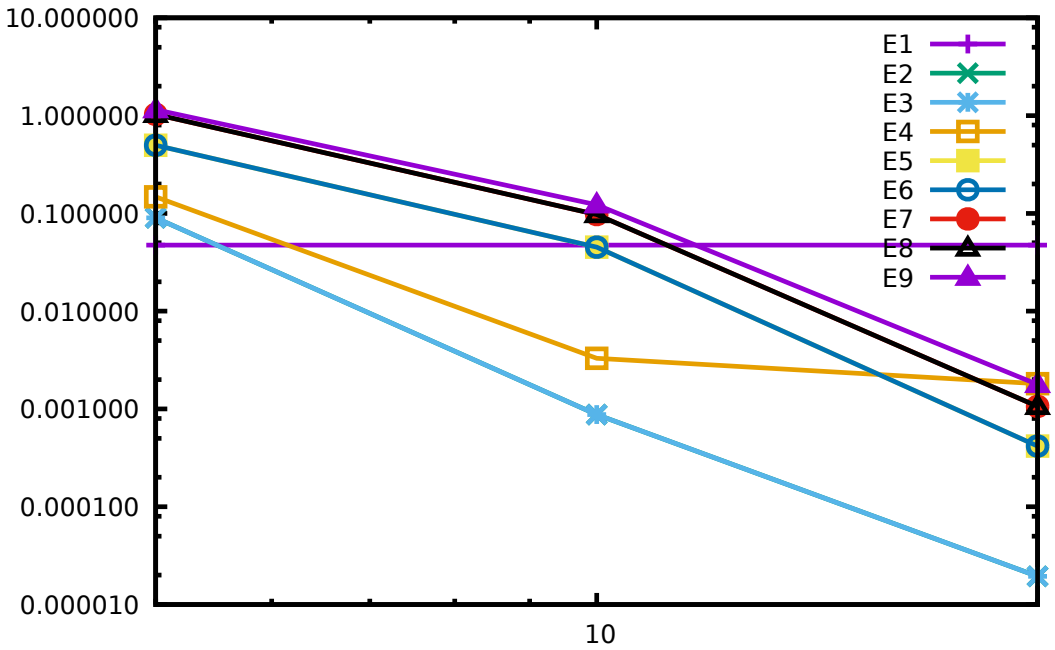


The Dirichlet boundary approximation

FEM/BEM

- With the finite element method, we cannot compute on infinite domains
  - There are tricks to do so — infinite element method
- We had to cut off the domain at a certain radius R
  - Justification: Eigenfunctions converge to zero due to $e^{-r/n}$
  - Laguerre polynomials grow slowly
  - But: worse for large n, thus $R \gtrsim 1/n$
- Effort for similar accuracy is R^3!

Example: approximaton with equal mesh size



Eigenvalue error over domain radius

Ritz-Galerkin property of Dirichlet boundary

- Functions with zero boundary conditions can be extended by zero

$$H^1(\Omega) \subset \mathcal{D}(A).$$

- Therefore, the Dirichlet boundary approximation is of Ritz-Galerkin type
- But still, very large radii may be needed for higher eigenvalues

Can we do better?

Radiation boundary condition

- Solutions to the atomic Schrödinger equation have the form

$$u(\mathbf{x}) = \varphi(r) Y_l^m(\theta, \varphi)$$

- Boundary values depend on all three variables, but

$$\frac{\partial}{\partial r} u / u = \frac{\varphi'(r)}{\varphi(r)}$$

- Use (known) radial solution to prescribe boundary condition

$$\partial_n u = \alpha u$$

Robin type

Radiation boundary for molecules

- No separation in radial ad angular functions
- No known radial solution
- But: solution converges to separable as $r \to \infty$
- Approximate this radial function to obtain boundary condition

Properties of radiation boundary conditions

- Typically much more accurate than Dirichlet
  - Smaller radius for same accuracy
- Specific to certain eigenfunctions
  - In a given computation, some eigenvalues may be approximated worse
- Not a subspace approximation anymore
  - Not in the Ritz-Galerkin framework

Defeating the R^3 effort

- It is difficult to quantify the error introduced by cutting the domain at radius R
  - We would like to choose R large to be safe
  - Too expensive!
- Wave functions decay when far from the nuclei
  - High resolution only needed in a small area
  - Meshes should be locally fine
- How to determine where to put resolution

A posteriori error estimation

- Intrinsic estimation based on computed solution
- Possible error measures
  - Local roughness
  - Local residuals
  - Effect of local residuals on eigenvalues
- Refine the mesh iteratively where estimator indicates

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Warning!

Refining for the secod Ritz value approximating an eigenvalue will make it the first!

Computation of the local integrals

- The finite element method requires integrals of the form

$$a_K(u,v) = \int_K \nabla u \cdot \nabla v \, d\mathbf{x} + \int_K V(u) v \, d\mathbf{x}$$

  where K is a single grid cell and u, v are local shape functions
- shape functions are polynomials
- typically (Gauß) quadrature

$$int_K \varphi(\mathbf{x}) \, d\mathbf{x} \approx \sum_{i=1}^{n_q} \omega_i \varphi(\mathbf{x}_i)$$

- Introduces quadrature error

Assumptions

- Smooth coefficients, smooth right hand side
- Shape functions: polynomials of order k
- k-point Gauß formula: exact for polynomials of degree $2k-1$

Quadrature error for standard FEM

Under these assumptions, the error introduced in the equation by quadrature does not change the asymptotic approximation rate of the solution.

Application to Schrödinger equation

- Coulomb potential is not smooth!
- Specialized quadrature formulas needed

Variational crimes

Any method that violates the conditions of the Ritz-Galerkin approach

1. $H_n \subset H$
2. $a(u^{(n)}, v^{(n)}) = \lambda^{(n)} \left(u^{(n)}, v^{(n)}\right)$

is called a variational crime.

- Such crimes may be useful
  - increase accuracy
  - make the method work at all
- They change the fundamental property

$$\lambda_k \leq \lambda_k^{(n)}$$

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ε = error beyond Galerkin