Multimode algorithms for leaky modes in microstructured optical fibers

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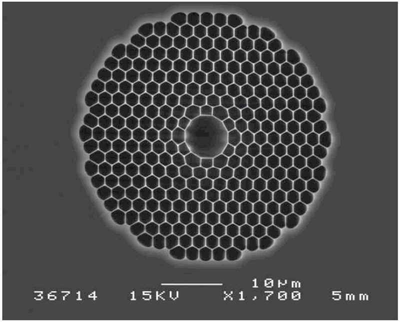
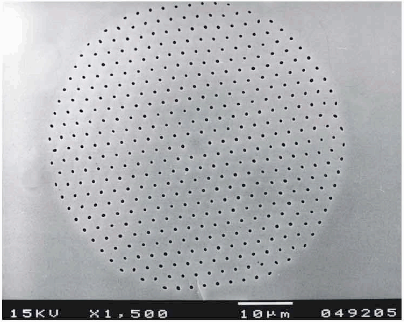
Outline

- Microstructured optical fibers (MOF)
- Properties of highly multi-moded fibers
- Numerical methods for finding leaky modes
- Algorithms for finding many modes in MOF
- Problems with standard techniques
- Othogonalization of leaky modes
- Summary

- Microstructured optical fibers (MOF) allow the properties of optical fiber to be taylored to suit a many different applications [Knight, 2003]
- Different materials of different shapes can be placed in the fiber
- Used for supercontinuum generation, endlessly single-moded fibers, sensing, dispersion engineering $\cdots$



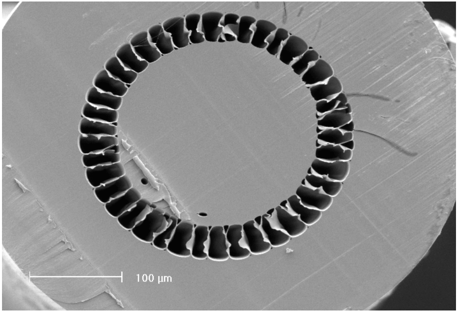


An example: High NA fiber

- Numeral Aperture quantifies the light capture of an optical fiber

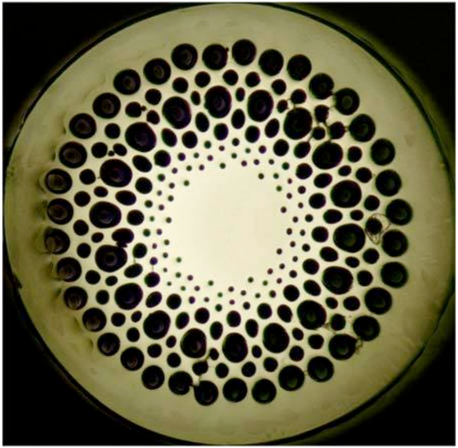
$$\mathrm{NA} = \sin(\theta_{\max}) = \sqrt{n_{\mathrm{core}}^2 - n_{\mathrm{clad}}^2}$$

- Highest NA attainable in air clad fiber
- Suspended core fibers are a way to approach this



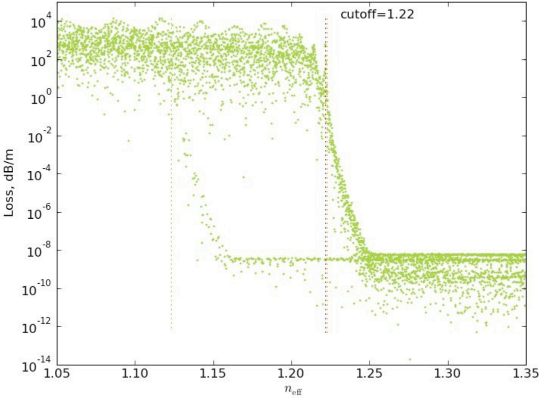
An example: High bandwidth polymer MOF

- Microstructures can be taylored to give high bandwidths in highly multimodes fibers
- Typically the higher the NA the lower the bandwidth, microstructures can be optimised to maximize both.



Fiber properties by modal analysis

- Many designs of interest in MOF are highly multi-moded
- Calculation of photonic bandgaps and density of states requires calculations of many modes over wavelength range of interest
- The effective NA and bandwidth require computation of all guided modes in the fiber



Microstructured fibers and leaky modes

- Each mode is defined by an effective index n_{eff} related to the eigenvalue
- In fibers with a low index cladding, the light falls of exponentially in the cladding,

$$\text{As } r \to \infty, \quad \Phi(r) \sim exp(-\gamma_b r)$$

$$n_{\mathrm{eff}} > n_{\mathrm{clad}}, \quad \gamma_b = \sqrt{n_{\mathrm{eff}}^2 - n_{\mathrm{clad}}^2}$$

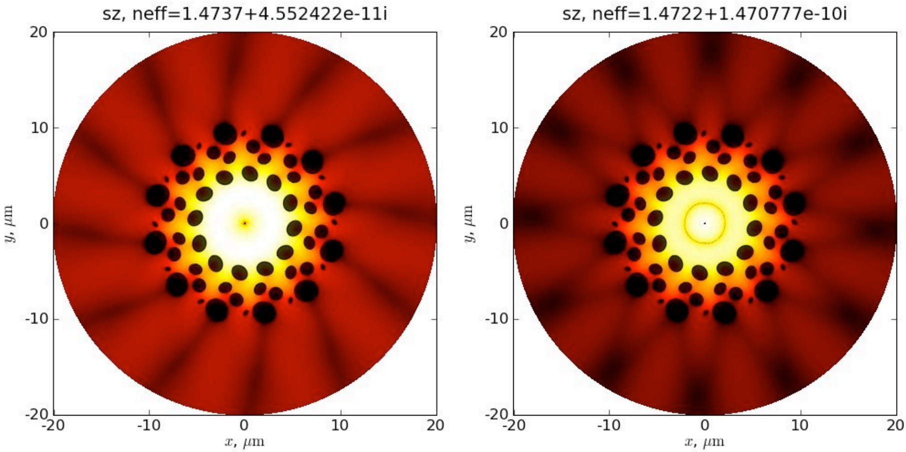
- In MOF structures the light is not bound within the core and leaks into the cladding

$$\text{As } r \to \infty, \quad \Phi(r) \sim exp(-i\gamma_l r)$$

$$n_{\mathrm{eff}} > n_{\mathrm{clad}}, \quad \gamma_l = \sqrt{n_{\mathrm{clad}}^2 - n_{\mathrm{eff}}^2}$$

- Leaky modes loose power as the propagate,

$$\mathrm{loss} = 20\,\mathsf{Im}(n_{\mathrm{eff}}^2)\frac{2\pi}{\lambda \log 10}$$



Logarithmic intensity of the *z* component of the Poynting vector

Finding leaky modes in MOF numerically

Many techniques have been used to model light propagation in optical fibers. Some specific techniques for finding leaky modes in MOF are:

- Integral techniques using analytic solutions of waves in an unbounded homogeneous domain
  - Multipole method [Kuhlmey et al., 2002]
  - Surface Model Technique [Hochman and Leviatan, 2004]
- Use standard numerical techniques and a non-reflective boundary condition (NRBC)
  - Finite difference methods [Issa and Poladian, 2003]
  - Finite element methods [Uranus and Hoekstra, 2004] + commercial codes
- Non-reflective boundary condition required [Givoli, 1991]

$$\frac{\partial \Phi}{\partial r} = M\left[\Phi\right] \quad \text{on boundary}$$

Looking for a solution with explicit t and z dependance of the form

$$\tilde{\Psi}(r,\phi,z) = \Psi(r,\phi)\exp(i(\omega t - n_{\text{eff}}k_0)z)$$

The scalar wave equation can be written in cylindrical polar coords as,

$$\frac{\partial^2\Psi}{\partial r^2} + \frac{1}{r}\frac{\partial\Psi}{\partial r} + \frac{\partial^2\Psi}{\partial\phi^2} + \left[n(r,\phi)^2 - n_{\text{eff}}^2\right]k_0^2\Phi = 0$$

In homogeneous regions $n(r,\phi) = n_0$ is a constant the outward solution is

$$\Psi(r,\phi) = \sum_{m=-\infty}^{\infty} c_m H_m^{(1)}(\gamma r)e^{im\phi}$$

where $\gamma = \sqrt{n_0^2 - n_{\text{eff}}^2}k_0$, $k_0 = 2\pi/\lambda$ and $H^{(1)}$ is the Hankel functions of the first kind.

Taking the derivative of the solution in the external domain

$$\frac{\partial \Psi_j}{\partial r}(R,\phi) = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty} \hat{M}_m(\lambda_j, R)\int_{-\pi}^{\pi} \Psi_j(R,\tilde{\phi}) e^{im(\phi-\tilde{\phi})} d\tilde{\phi}$$
$$= M[\Psi_j(R,\phi), \lambda_j]$$

where with $H_n^{(1)'}(x) = \partial_x H_n^{(1)}(x)$

$$\hat{M}_m(\lambda, r) = \frac{\gamma(\lambda) H_m^{(1)'}(\gamma(\lambda) r)}{H_m^{(1)}(\gamma(\lambda) r)}$$

This is the Dirichlet-to-Neumann (DtN) map for the solution on a circle of radius R.

The nonlinear eigenvalue problem

- The boundary condition is dependent on the eigenvalue
- The discretized problem is thus also dependent on the eigenvalue
- This defines a nonlinear eigenvalue problem (NLEP)

$$\mathrm{T}(\lambda) = A(\lambda)\mathbf{x} - \lambda\mathbf{x} = 0$$

- For bound modes the fields are evanescent $\rightarrow$ a boundary can be found with field small and little dependence on the eigenvalue
- For leaky modes the loss is important and the boundary cannot be found with arbitrarily small field
- Confinement loss of the mode is highly dependent on accurate solution of the NLEP

Solving the NLEP: Fixed point iterations

- Start with an approximate eigenvalue of interest λ_0
- Solve linear eigenproblem for λ_1, the next guess

$$\mathrm{A}(\lambda_i)\mathbf{x}_{i+1} = \lambda_{i+1}\mathbf{x}_{i+1}$$

- Iterate until converged

Convergence dependent upon the loss of the mode. Defining the fixed point iterations as a function,

$$\lambda_{n+1} = f(\lambda_n)$$

Method converges for $|f'(\hat{\lambda})| < 1$

$$f'(\mu) = -\frac{\mathbf{y}^*\mathrm{A}'(\mu)\mathbf{x}}{\mathbf{y}^*\mathbf{x}}$$

$\mathrm{A}'(\lambda)$ is the Jacobian matrix of $\mathrm{A}(\lambda)$

Solving the NLEP: Nonlinear inverse iterations

Newton's method can be applied to both the eigenvector and eigenvalue together [Ruhe, 1973]

$$P(\xi) = P\begin{pmatrix}\mathbf{x}\\ \lambda\end{pmatrix} = \begin{bmatrix}\mathrm{T}(\lambda)\mathbf{x}\\ y^*\mathbf{x} - 1\end{bmatrix} = 0$$

Applying Newtown's method

$$\xi_{i+1} = \xi_i - P'(\xi_i)^{-1}P(\xi_i)$$

Gives the iterative method,

$$u_{i+1} = \mathrm{T}(\lambda_i)^{-1}\mathrm{T}'(\lambda_i)\mathbf{x}_i, \quad \lambda_{i+1} = \lambda_i - \frac{v_i^* x_i}{v_i^* u_{i+1}}, \quad x_{i+1} = c_i u_{i+1}$$

Nonlinear inverse iteration has the problem that the inverse operator must be updated with a new approximate shift at each iteration.

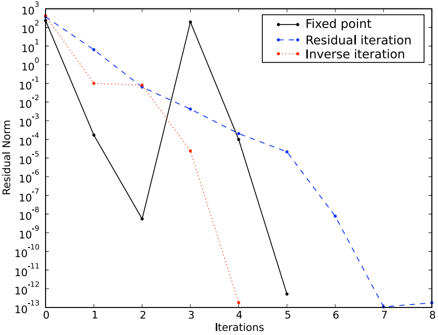
Residual inverse iteration

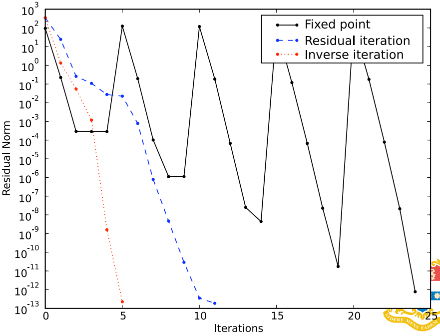
Replacing $T'(\lambda_i) = \frac{1}{\lambda_{i+1}-\lambda_i}\left[T(\lambda_{i+1}) - T(\lambda_i)\right]$ we get

$$u_{i+1} = \mathrm{T}(\lambda_i)^{-1}\left[T(\lambda_i) - T(\lambda_{i+1})\right]\mathbf{x}_i = \mathbf{x}_i - \mathrm{T}(\lambda_i)^{-1}T(\lambda_{i+1})\mathbf{x}_i$$

In fact the matrix inverse can now be given a constant shift, σ, and convergence is still achieved [Neumaier, 1985].

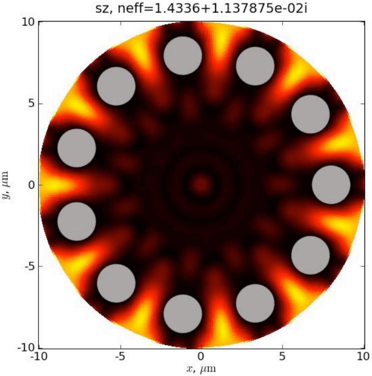
$$u_{i+1} = \mathbf{x}_i - \mathrm{T}(\sigma)^{-1}T(\lambda_{i+1})\mathbf{x}_i$$

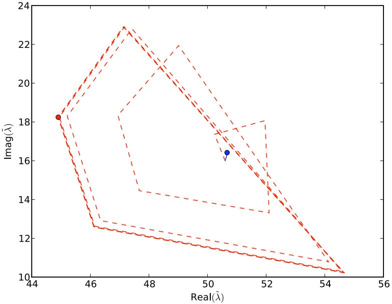




Problems: Spurious modes

- Modes may be guided between the microstructure and the imperfect boundary conditions
- These modes do not represent a physical solution
- They usually converge very slowly, or with the FP method not at all.





Eigenvectors of NLEP are not orthogonal

- The right $Au_i = \lambda_i u_i$ and left eigenvectors $A^* v_i = \bar{\lambda}_i v_i$ form a bi-orthogonal basis for the eigenspace

$$\langle v_i, u_j \rangle = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

- For the NLEP with $T(\lambda_i) x_i = 0$, $T(\lambda_i)^* y_i = 0$ this is usually not true,

$$y_i^* x_j \neq 0 \text{ for } i \neq j$$

- This is clear as y_i and x_j are eigenvectors of different linear matricies, however if $|\lambda_j - \lambda_i|$ is small, the eigenvectors are almost orthogonal.

Problems: Repeated modes

- For the non-Hermitian problem there is no deflation proceedure available so eigevectors are often found multiple times
- Thus multiple modes must be eliminated without eliminating degenerate modes
- Typically in large problems 30% of the eigenvectors are repeated

Inefficient computations are caused by slow convergence of unwanted solutions and calculation of already found modes

Extended Inner Product

- On the infinite domain the eigenvectors are orthogonal as they solve the wave equation.

$$I = \int_0^\infty \int_{-\pi}^{\pi} r\,\Psi_j(r,\phi)\Psi_k(r,\phi) = 0$$

- However for leaky modes the integration must be performed in the complex plane as the eigenmode does not decay as $r \to \infty$

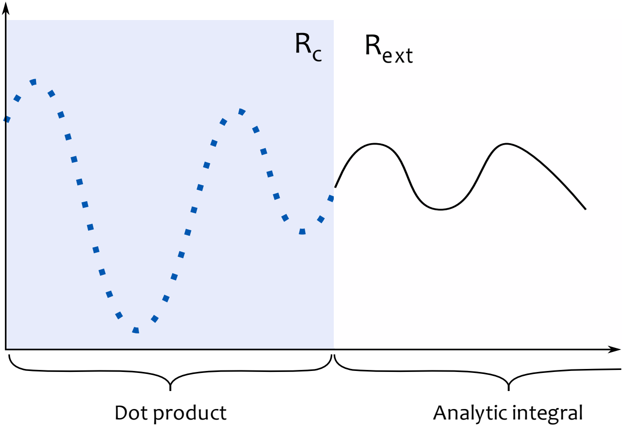
$$\Psi(r,\phi) = \sum_{m=-\infty}^{\infty} H_m^{(1)}(\gamma r) \sim \sum_{m=-\infty}^{\infty} exp(im\gamma_r r)exp(-m\gamma_i r)$$

which grows as $\gamma_i < 0$

- On the homogeneous external domain the contribution to the integral can be analytically derived

$$\int_{R_\infty} \int_{-\pi}^{\pi} r\,\Psi_j(r,\phi)\Psi_k(r,\phi) = f(\Psi_j(R,\phi), \Psi_k(R,\phi), \lambda_j, \lambda_k)$$

Correct the numerical dot product with the contribution from the analytic solution in the external domain



$$I = \langle \mathbf{y}_j, \mathbf{x}_k \rangle \quad + \quad f(y_{r=r_c}, x_{r=r_c}, \lambda_j, \lambda_k)$$

Extended Projection

- Thus a new inner product can be defined,

$$\langle \mathbf{y}_j, \mathbf{x}_k \rangle_{\lambda_j,\lambda_k} = \langle \mathbf{y}_j, \mathbf{x}_k \rangle + f(y_{r=r_c}, x_{r=r_c}, \lambda_j, \lambda_k)$$

- The true eigenvectors fulfill a bi-orthonormal relation with respect to this inner product

$$\langle \mathbf{y}_j, \mathbf{x}_k \rangle_{\lambda_j,\lambda_k} = \delta_{j,k}$$

- Thus a spectral “projection” can be defined as,

$$P_j(\tilde{\lambda})\tilde{\mathbf{x}} = \frac{\langle \mathbf{y}_j, \tilde{\mathbf{x}} \rangle_{\lambda_j,\tilde{\lambda}}}{\langle \mathbf{y}_j, \mathbf{x}_j \rangle_{\lambda_j,\tilde{\lambda}}} \mathbf{x}_j$$

- A spectral projector must fulfill

$$P_j^2 = P_j \quad P_j P_k = 0 \quad \sum_{i=1}^{N} P_i = \mathrm{I}$$

Extended orthogonalization

- The Gram-Schmidt process doesn't work with the extended inner product
- Supposing we know eigenvalues λ_i and eigenvectors y_i, x_i for $i = 1 \dots k$ and a new eigenvalue λ_{k+1} with $\tilde{x} = \sum_{i=1}^{k+1} \alpha_i x_i$

$$\left\langle y_i, \tilde{x} \right\rangle_{\lambda_i, \lambda_{k+1}} = \sum_{i=j}^{k+1} \alpha_j \left\langle y_i, x_j \right\rangle_{\lambda_i, \lambda_{k+1}} = \sum_{i=j}^{k} \alpha_j \left\langle y_i, x_j \right\rangle_{\lambda_i, \lambda_{k+1}},$$

- This can be expressed as a matrix problem and $\alpha = [\alpha_j]_{j=1\dots k}$ found as

$$\alpha = Q(\lambda_{k+1})^{-1} \eta(\lambda_{k+1})$$

$$\text{where} \quad Q(\tilde{\lambda})_{i,j} = \left\langle y_i, x_j \right\rangle_{\lambda_i, \tilde{\lambda}}, \quad \eta(\tilde{\lambda})_{i,j} = \left\langle y_i, \tilde{x} \right\rangle_{\lambda_i, \tilde{\lambda}}$$

- Thus the orthogonalization against eigenvectors $1 \dots k$

$$\tilde{x} - \sum_{i=1}^{k} \alpha_i x_i = \alpha_{k+1} x_{k+1}$$

Algorithm

- Start with approximate eigensolution $\tilde{\lambda}^{(0)}$, $\tilde{x}^{(0)}$, $\tilde{y}^{(0)}$
- While $|r| < \epsilon$
  - Extended orthogonalize to previous vectors

$$u^{(i)} = x^{(i)} - \sum_j \alpha_j x_j$$
$$v^{(i)} = y^{(i)} - \sum_j \alpha_j^L y_j$$

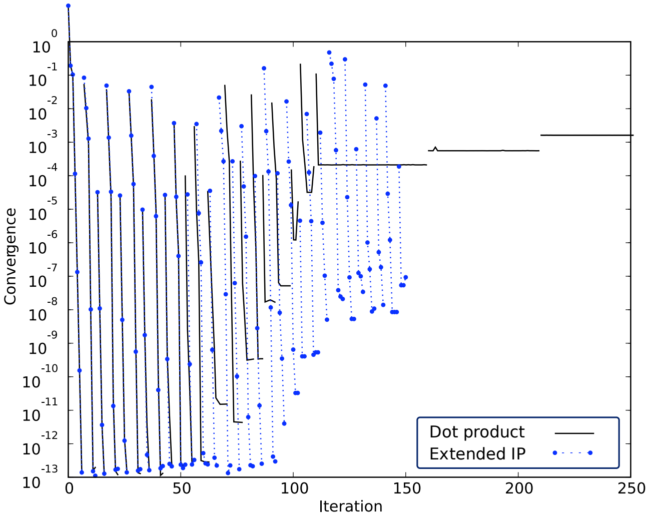
    Also giving new eigenvalue estimate $\tilde{\lambda}^{(i+1)}$
  - Apply RII operator

$$x^{(i+1)} = R(\tilde{\lambda}^{(i+1)})u^{(i)}$$
$$y^{(i+1)} = R(\tilde{\lambda}^{(i+1)})^* v^{(i)}$$

  - Calculate residual

$$r = T(\tilde{\lambda}^{(i+1)})x^{(i+1)}$$

Results



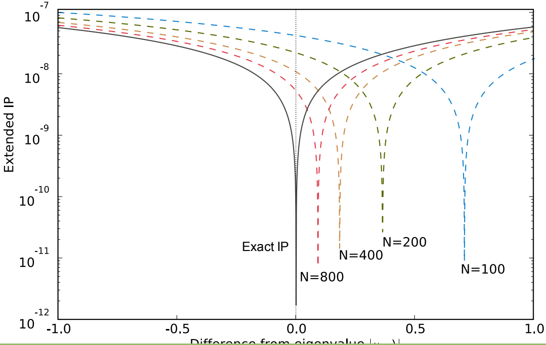
Convergence
Iteration
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
0
50
100
150
200
250
Dot product
Extended IP

- Another measure of orthogonality for NLEP is

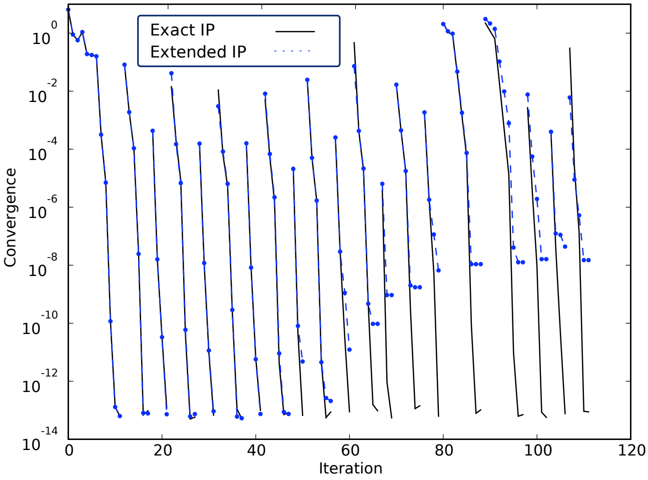
$$\left\langle \mathbf{y}, \mathbf{x} \right\rangle_{\lambda_j,\lambda_k} = \frac{\mathbf{y}^* \left[T(\lambda_j) - T(\lambda_k) \right] \mathbf{x}}{\lambda_j - \lambda_k}$$

- With $\mathbf{y}_i$, $\mathbf{x}_i$ left and right eigenvalues corresponding too λ_i clearly

$$\left\langle \mathbf{y}_j, \mathbf{x}_k \right\rangle_{\lambda_j,\lambda_k} = \left\langle \mathbf{y}_k, \mathbf{x}_j \right\rangle_{\lambda_j,\lambda_k} = 0$$



Convergence with Exact IP



Projection methods for eigenvalue problems

- The successive application of the matrix A to a starting vector v_0 gives a series of vectors $A\mathbf{v}_0$, $A^2\mathbf{v}_0$, $A^3\mathbf{v}_0 \ldots$
- These vectors $\mathbf{v}_i = A\mathbf{v}_{i-1}$ converge to the dominant eigenvector but also have information on other eigenvectors.
- Projection methods aim to extract this information

Given a bi-orthogonal basis $\mathbf{v}_0 \ldots \mathbf{v}_n$, $\mathbf{w}_0 \ldots \mathbf{w}_n$ for a right V and a left subspaces W,
For the linear eigenvalue problem

$$A\mathbf{v} = \lambda$$

Assume that a pair $\tilde{\lambda}$, $\tilde{\mathbf{v}} = \sum_{j=0}^{n} \alpha_j v_j$ for some $\alpha = [\alpha_0, \ldots, \alpha_n]$, is an approximate solution fulfilling the Galerkin condition

$$A\tilde{\mathbf{v}} - \tilde{\lambda}\tilde{\mathbf{v}} = AV\alpha - \tilde{\lambda}V\alpha \quad \perp \quad W$$

This gives a projected eigenproblem of dimension n

$$A_P\,\alpha = \tilde{\lambda}\alpha \quad A_P = W^* AV\alpha$$

For NLEP we can apply the Galerkin condition to the extended inner product, the residual is orthogonal to the left subspace

$$T(\tilde{\lambda})\tilde{\mathbf{v}} \quad \perp \quad W$$

$$\sum_{j=0}^{n} \alpha_j \langle w_i, T(\tilde{\lambda})\mathbf{v}_j \rangle_{\lambda_i,\tilde{\lambda}} = 0 \quad \forall i = 0 \ldots n$$

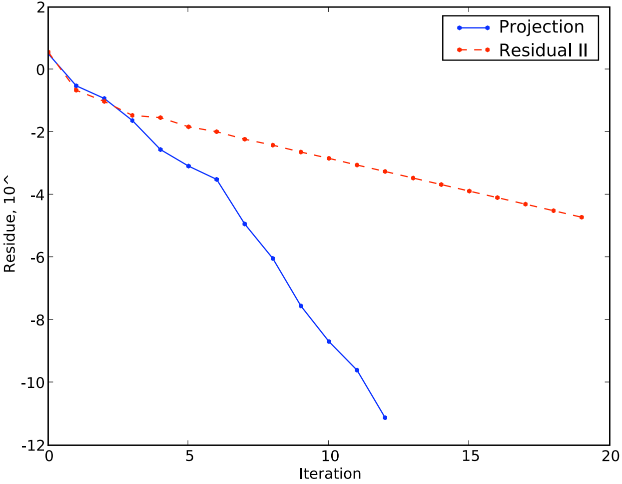
This gives the projected nonlinear eigenvalue problem.

$$T_P(\tilde{\lambda})\alpha = 0$$

where the (i,j) element in the projected matrix is given by

$$\left[T_P(\tilde{\lambda}) \right]_{i,j} = \langle w_i, T(\tilde{\lambda})\mathbf{v}_j \rangle_{\lambda_i,\tilde{\lambda}}$$

Single eigenvalue solution



Conclusion

- A general proscription for solving linear wave problems in unbounded domains has been applied to the vector wave equation
- Reduction of the wave problem onto a bounded domain by a Dirichlet to Neumann nonlocal boundary condition
- Solve the resulting nonlinear eigenvalue problem using extended orthogonalization
- Current algorithm allows the modal analysis of MOF with arbitrary cross-sectional profile quickly with little user intervention
- Algorithms using NLEP projection methods are hoped to be developed for automatic calculation of large numbers of modes

For Further Reading I

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Non-reflective boundary conditions

- Artificial absorbing material: Matched Layer & Perfectly Matched Layer

  [Bérenger, 1994]

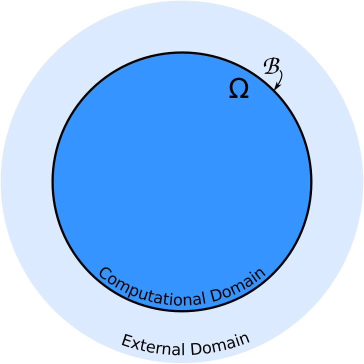
- Radiation boundary conditions & one-way wave equations [Bayliss et al., 1982]

$$\lim_{r\to\infty} r^{\left(\frac{d-1}{2}\right)} \left[\frac{\partial\Phi}{\partial r} - ik\Phi\right] = 0$$

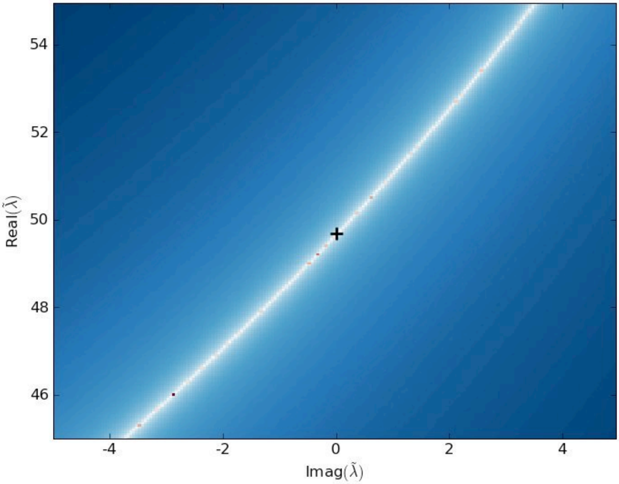
- Dirichlet to Neumann maps as boundary conditions [Givoli, 1991]

$$\frac{\partial\Phi}{\partial r} = M[\Phi]$$

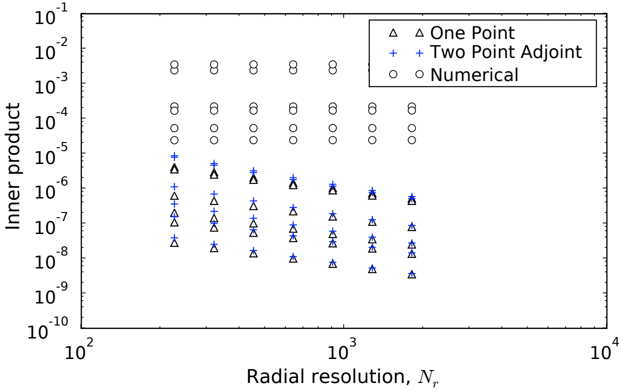
Where $M[\cdot]$ is typically a nonlocal operator.



The extended inner product



- The extended IP is only approximately valid, depends on the accuracy of the numerical solution.
- Typically obtain first order convergence.



Extended Projection

However for the extended projection,

$$P_j(\tilde{\lambda})^2\tilde{\mathbf{x}} = P_j(\tilde{\lambda})\tilde{\mathbf{x}} = \sigma_j\mathbf{x}_j$$

$$P_j(\tilde{\lambda})P_k(\tilde{\lambda})\tilde{\mathbf{x}} = \frac{\left\langle \mathbf{y}_j, \sigma_k\mathbf{x}_k \right\rangle_{\lambda_j,\tilde{\lambda}}}{\left\langle \mathbf{y}_j, \mathbf{x}_j \right\rangle_{\lambda_j,\tilde{\lambda}}}\mathbf{x}_j \neq 0$$

However using a different parameter for the projector would give what we expect,

$$P_j(\lambda_j)P_k(\tilde{\lambda})\tilde{\mathbf{x}} = \frac{\left\langle \mathbf{y}_j, \sigma_k\mathbf{x}_k \right\rangle_{\lambda_j,\lambda_j}}{\left\langle \mathbf{y}_j, \mathbf{x}_j \right\rangle_{\lambda_j,\lambda_j}}\mathbf{x}_j = 0$$

Taking $\tilde{x}$ as a combination of eigenvectors $\tilde{x} = \sum_i \alpha_i x_i$ then clearly the sum of the spectral projectors does not recover $\tilde{x}$,

$$\sum_j P_j(\lambda_j)\tilde{\mathbf{x}} = \sum_j \sum_i \alpha_i \frac{\left\langle \mathbf{y}_j, \mathbf{x}_i \right\rangle_{\lambda_j,\tilde{\lambda}}}{\left\langle \mathbf{y}_j, \mathbf{x}_j \right\rangle_{\lambda_j,\tilde{\lambda}}}\mathbf{x}_j \neq \tilde{\mathbf{x}}, \quad \forall\tilde{\lambda} \in \mathbb{C}$$

Extended orthogonalization

- If $\tilde{x}$ contains more than one unknown eigenvector then this orthogonalization doesn't work, $\tilde{x} = \sum_{i=1}^{n} \beta_i x_i$, $n > k+1$

$$\begin{aligned}
\langle y_i, \tilde{x} \rangle_{\lambda_i, \lambda_{k+1}} &= \sum_{i=j}^{n} \beta_j \langle y_i, x_j \rangle_{\lambda_i, \lambda_{k+1}} \\
&= \sum_{i=j}^{k} \beta_j \langle y_i, x_j \rangle_{\lambda_i, \lambda_{k+1}} + \sum_{i=k+2}^{n} \beta_j \langle y_i, x_j \rangle_{\lambda_i, \lambda_{k+1}}
\end{aligned}$$

- The calculated $\alpha_i \neq \beta_j$ and the orthogonalization will give components of $x_1 \ldots x_k$

$$\tilde{x} - \sum_{i=1}^{k} \alpha_i x_i = \alpha_{k+1} x_{k+1} + \sum_{i=1}^{k} (\beta_i - \alpha_i) x_i$$

- Applying the RII operator to a vector $\tilde{x} = x_{k+1} + \sum_{i=1}^{k} \beta_i x_i$

$$R(\mu)\tilde{x} = \left[I - T(\sigma)^{-1} T'(\mu) \right] \tilde{x}$$

- For eigenvectors close to σ and μ

$$\frac{R(\mu)\tilde{x}}{y_i^* R(\mu)\tilde{x}} \simeq x_i + \sum_i \beta_i \frac{\sigma - \lambda_{k+1}}{\sigma - \lambda_i} x_i$$

- Thus contributions from other eigenvectors are reduced at a rate $\frac{\sigma - \lambda_{k+1}}{\sigma - \lambda_i}$

Orthogonalization and the Rayleigh Functional

- However to orthogonalize a vector pair $\tilde{y}$, $\tilde{x}$ close to an eigenpair y_{k+1}, x_{k+1} we need an approximation to the eigenvalue
- The eigenvalue will solve the equation

$$\tilde{y}^* T(\tilde{\lambda})\tilde{x} = 0$$

- With an approximate $\tilde{\lambda}^{(0)}$ Newtown's method gives an updated approximate

$$\tilde{\lambda}^{(1)} = \tilde{\lambda}^{(0)} - \frac{\tilde{y}^* T(\tilde{\lambda}^{(0)})\tilde{x}}{\tilde{y}^* T'(\tilde{\lambda}^{(0)})\tilde{x}}$$

- Therefore EO seeks a solution $\tilde{\lambda}$, $\mathbf{x} = \tilde{\mathbf{x}} - \sum_j \alpha_j \mathbf{x}_j$, $\mathbf{y} = \tilde{\mathbf{y}} - \sum_j \alpha_j^{(L)} \mathbf{y}_j$

$$\left\langle \mathbf{y}_i, \mathbf{x} \right\rangle_{\lambda_i, \tilde{\lambda}} = 0$$
$$\left\langle \mathbf{y}, \mathbf{x}_i \right\rangle_{\tilde{\lambda}, \lambda_i} = 0$$
$$\mathbf{y}^* T(\tilde{\lambda})\mathbf{x} = 0$$

$$\nabla^2 \mathbf{H}(\mathbf{r}, z) - k^2 n^2(\mathbf{r}) \mathbf{H}(\mathbf{r}, z) = -(\nabla \ln n^2(\mathbf{r})) \times \left[\nabla \times \mathbf{H}(\mathbf{r}, z)\right] \tag{1a}$$

and for the corresponding electric field

$$\nabla^2 \mathbf{E}(\mathbf{r}, z) - k^2 n^2(\mathbf{r}) \mathbf{E}(\mathbf{r}, z) = -\nabla \left[\mathbf{E}(\mathbf{r}, t) \cdot (\nabla \ln n^2(\mathbf{r}))\right] \tag{1b}$$

assuming an implicit time dependence and where ∇^2 is the vector Laplacian, $\mathbf{E}$ and $\mathbf{H}$ are the electric and magnetic vector fields, $n = n(\mathbf{r})$ is the refractive index, $\mathbf{r}$ is the transverse coordinate vector and $k = \omega\sqrt{\varepsilon_0 \mu_0} = 2\pi/\lambda$ is the wave number in free space [Snyder and Love, 1983].

The SWE operator in polar coordinates can be written as,

$$S = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} + (n^2(r,\phi)k^2 - \beta^2)$$

Considering two solutions of the SWE $S[y_j] = 0$ and $S[y_k] = 0$ with different eigenvalues β_j, β_k we form the combination $y_k S y_j - y_j S y_k = 0$ giving,

$$\frac{\partial}{\partial r}(rW_r[y_j, y_k]) + \frac{\partial}{\partial \phi}(rW_\phi[y_j, y_k]) = (\beta_j - \beta_k) r y_j y_k$$

where the Wronksians in r and ϕ are given by $W_r[y_j, y_k] = \frac{\partial y_j}{\partial r} y_k - y_j \frac{\partial y_k}{\partial r}$ and $W_\phi[y_j, y_k] = \frac{\partial y_j}{\partial \phi} y_k - y_j \frac{\partial y_k}{\partial \phi}$
Integrating over r and ϕ and using the periodicity of $y(r,\phi)$ in ϕ we arrive at

$$\int_0^\infty \int_0^{2\pi/\mu} r y_j(r,\phi) y_k(r,\phi) dr d\phi = \Big[Wr[y_j, y_k]\Big]_0^\infty$$

when $\beta_j \neq \beta_k$. For all bound modes it is clear that $\Big[Wr[y_j, y_k]\Big]_0^\infty = 0$ however for leaky modes this is not true.

Substituting the Fourier series for $y_j(r,\phi) = \sum_{m=-\infty}^{\infty} Y_m^{(j)} \exp(im\mu\phi)$ into this equation we have

$$\int_0^\infty \int_0^{2\pi/\mu} r y_j(r,\phi) y_k(r,\phi)$$
$$= \int_0^\infty \int_0^{2\pi} r \left(\sum_{m=-\infty}^{\infty} Y_m^{(j)}(r) e^{i(m\mu + m_0^{(j)})\phi} \right)$$
$$\cdot \left(\sum_{n=-\infty}^{\infty} Y_k^{(k)}(r) e^{i(n\mu + m_0^{(k)})\phi} \right) d\phi dr$$
$$= \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \int_0^\infty \int_0^{2\pi} r Y_n^{(j)}(r) Y_{m-n}^{(k)}(r) e^{i(m\mu + m_0^{(j)} + m_0^{(k)})\phi} d\phi dr$$

Clearly the only contribution comes from when $n = 0$ and $m_0^{(j)} = -m_0^{(k)}$ as $\mu/2 < m_0 < \mu/2$. In that case the orthogonality relation reduces to,

$$\int_0^\infty \int_0^{2\pi} y_j(r,\phi) y_k(r,\phi) = \sum_{m=-\infty}^{\infty} \frac{2\pi}{\mu} \int_0^\infty Y_m^{(j)}(r) Y_{-m}^{(k)}(r) dr = 0 \qquad (2)$$

This relationship is true for all solutions of the SWE of Eq.**??** that decay to zero as $r \rightarrow \infty$, for leaky modes this is not true as long as r is real and this orthogonality relation must me modified for leaky modes, as detailed in the following sections.

Due to the exponential growth of the leaky mode in the direction orthogonal to the fiber axis the orthogonality condition of Eq. **??** is invalid, however an alternate condition can be found by modifying the integral to occur in the complex r plane [Snyder and Love, 1983].

The complex integration path can be specified so that the field exponentially decreases along this path, thus introducing $r = r_r + ir_i$ and using the asymptotic expression of Eq. **??**

$$\int_R r y_j(r,\phi) y_k(r,\phi) dr \sim \int_R e^{+\left[|\gamma_r^{(j)}|+|\gamma_r^{(k)}|\right] r_r - \left[|\gamma_i^{(j)}|+|\gamma_i^{(j)}|\right] r_i} \times e^{+i\left(\left[|\gamma_r^{(j)}|+|\gamma_r^{(j)}|\right] r_i + \left[|\gamma_i^{(j)}|+|\gamma_i^{(j)}|\right] r_r\right)} e^{i\beta_r z - \beta_i z} \tag{3}$$

so we choose a path so that $\lim_{r\to\infty} H_j(r,\phi) = 0$, namely $\frac{r_i}{r_r} > \left[|\gamma_r^{(j)}| + |\gamma_r^{(k)}|\right] / \left[|\gamma_i^{(j)}| + |\gamma_i^{(k)}|\right]$ as $r_r \to \infty$. This can be acheived by choosing the path illustrated in Fig. **??** where the integration is performed along the real axis until a point where the path diverts into the imaginary axis with an angle

$$\theta > \tan^{-1} \frac{|\gamma_r^{(j)}| + |\gamma_r^{(k)}|}{|\gamma_i^{(j)}| + |\gamma_i^{(k)}|} \tag{4}$$

Using this path the orthogonality relationship may be expressed as

$$\int_R \int_0^{2\pi/\mu} r y_j(r,\phi) y_k(r,\phi) dr d\phi = 0$$

where now y_j and y_k can be leaky modes and the integration path R is in the complex plane.
Now if a mode is computed numerically on a finite numerical domain $0 < r < r_{\text{max}}$ representing the numerically calculated solution as $\tilde{y}$ and the associated extended solution outside the computational domain as y we can break the orthogonality integral into two parts, one inside the computational domain and one outside. Assuming wlog that the integration path extends into imaginary r only outside of the numerical region we arrive at,

$$I = \int_R \int_0^{2\pi/\mu} r y_j(r,\phi) y_k(r,\phi) dr d\phi = I_n + I_\infty = 0$$

where

$$I_n = \int_0^{r_{\max}} \int_0^{2\pi/\mu} r\tilde{y}_j(r,\phi)\tilde{y}_k(r,\phi)drd\phi$$

$$I_\infty = \int_{R'} \int_0^{2\pi/\mu} ry_j(r,\phi)y_k(r,\phi)drd\phi = 0$$

where R' is the integration path of Fig. **??** starting from $r = r_{\max}$ and continuing to infinity.

The second part of this expression can be calculated analytically, assuming the region $r > r_{\max}$ has constant refractive index using the analytic expression for the outward travelling wave field of Eq. **??** and the orthogonality relation in the Fourier coefficients of Eq. **??**.

$$I_\infty = \frac{2\pi}{\mu} \sum_{m=-\infty}^{\infty} \int_{R'} rY_m^{(j)}(r)Y_{-m}^{(k)}(r)dr$$

$$= \frac{2\pi}{\mu} \sum_{m=-\infty}^{\infty} a_m^{(j)} a_{-m}^{(k)} \int_{R'} rH^{(1)}_{m\mu+m_0+p}(\gamma_j r)H^{(1)}_{-m\mu-m_0-p}(\gamma_k r)dr$$

Using the Bessel identity $H_{-n}^{(1)}(x) = e^{in\pi} H_n^{(1)}(x)$ and the analytic representation of the integral, [Abramowitz and Stegun, 1965] we obtain

$$I_\infty = \frac{2\pi}{\mu} \sum_{m=-\infty}^{\infty} \left[(-1)^{\tilde{m}} r \frac{a_m^{(j)} a_{-m}^{(k)}}{\gamma_j^2 - \gamma_k^2} \left(\gamma_j H_{\tilde{m}+1}^{(1)}(\gamma_j r) H_{\tilde{m}}^{(1)}(\gamma_k r) \right.\right. \\ \left.\left. - \gamma_k H_{\tilde{m}}^{(1)}(\gamma_j r) H_{\tilde{m}+1}^{(1)}(\gamma_k r) \right) \right]_{r_{\max}}^{r_\infty}$$

This expression is accurate for real and complex r and as the integration path has been chosen so that the integrand vanishes as

$r \to r_\infty$ the contribution to the integral from that point is zero and we obtain the analytic contribution to the orthogonality relation as

$$I_\infty = \frac{2\pi}{\mu} \sum_{m=-\infty}^{\infty} (-1)^{\tilde{m}} r_{\max} \frac{a_m^{(j)} a_{-m}^{(k)}}{\gamma_j^2 - \gamma_k^2} \Big(\gamma_j H_{\tilde{m}+1}^{(1)}(\gamma_j r_{\max}) \times H_{\tilde{m}}^{(1)}(\gamma_k r_{\max}) - \gamma_k H_{\tilde{m}}^{(1)}(\gamma_j r_{\max}) H_{\tilde{m}+1}^{(1)}(\gamma_k r_{\max}) \Big)$$