MA 580; Numerical Analysis I

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Part VIIIa: Eigenvalue Problems
Power Method and Rayleigh Quotient Iteration

Eigenvalue Problems

Problem: $\mathbf{x}$ and λ so that

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

- Sometimes you want them all,
- sometimes the largest or smallest,
- sometimes the ones nearest your favorite λ,
- ...

All norms are ℓ^2 in this part of the course.

Power Method for Largest Eigenvalue

We have been here before

$$\mathbf{x}_n = \frac{\mathbf{A}^n \mathbf{x}_0}{\|\mathbf{A}^n \mathbf{x}_0\|}$$

This is unstable as

$$\mathbf{A} = \begin{pmatrix} 10 & 0 \\ 0 & 1 \end{pmatrix}$$

illustrates.

Power Method done right

$$\mathbf{x}_n = \frac{\mathbf{A}\mathbf{x}_{n-1}}{\|\mathbf{A}\mathbf{x}_{n-1}\|}$$

Claim: In exact arithmetic it's the same iteration.

Proof: Either way gives you the unit vector in the direction $\mathbf{A}^n\mathbf{x}_0$.

PM Implementation

$x = x_0$
while not happy **do**
  $\mathbf{y} = \mathbf{A}\mathbf{x}$
  $\mathbf{x} \leftarrow \mathbf{y}/\|\mathbf{y}\|$
  $\mu = \mathbf{x}^T\mathbf{A}\mathbf{x}$
end while

Termination?

- $|\mu_n - \mu_{n-1}|$ small
- $\|\mathbf{A}\mathbf{x}_n - \mu_n\mathbf{x}_n\|$ small

So what do you get?

Let's try it with

$$\mathbf{A} = \begin{pmatrix} 10 & 0 \\ 0 & 1 \end{pmatrix} \text{ and } \mathbf{x} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

So

$$\mathbf{x}_1 = \frac{1}{\sqrt{11}} \begin{pmatrix} 10 \\ 1 \end{pmatrix} \text{ and } \mathbf{x}_2 = \frac{1}{\sqrt{10001}} \begin{pmatrix} 100 \\ 1 \end{pmatrix}$$

and it goes on ...

Convergence

$$\mathbf{x}_n = \frac{1}{\sqrt{10^{2n}+1}} \begin{pmatrix} 10^n \\ 1 \end{pmatrix} \approx \begin{pmatrix} 1 \\ 10^{-n} \end{pmatrix},$$

which is what you need and deserve.
What kind of things do we need to assume for this?
How about no Jordan blocks?

Convergence of the Power Method: I

Assumptions:

- $\mathbf{A}$ is diagonalizable.
    - $\mathbf{A}$ has N linearly independent unit eigenvectors $\{\mathbf{v}_i\}_{i=1}^N$
    - with corresponding eigenvalues $\{\lambda_i\}$.

$$|\lambda_1| \leq |\lambda_2| \leq \cdots \leq |\lambda_{N-1}| < |\lambda_N|$$

    - The largest eigenvalue in absolute value has geometric multiplicity one.
- $\mathbf{x}_0 = \sum_{i=1}^N \alpha_i \mathbf{v}_i$ with $\alpha_N \neq 0$.
- $\{\mathbf{x}_n\}$ are the power method iterations.

Convergence of the Power Method: II

Conclusions:

- The convergence rate to the eigen-manifold is r-linear

$$\min_{\mathbf{A}\mathbf{v}=\lambda_N \mathbf{v}} \|\mathbf{x}_n - \mathbf{v}\| = O\left(\left| \frac{\lambda_{N-1}}{\lambda_N} \right|^n \right),$$

$$\mu_n = \mathbf{x}_n^T \mathbf{A} \mathbf{x}_n = \lambda_N + O\left(\left| \frac{\lambda_{N-1}}{\lambda_N} \right|^n \right).$$

- Here, of course $\{\mathbf{v} \mid \mathbf{A}\mathbf{v} = \lambda_N \mathbf{v}\} = \{\pm \mathbf{v}_N\}$,but watch out for multiplicity later
- as is the convergence to the eigenvalue,

Proof: I

Since

$$\mathbf{x}_0 = \sum_{i=1}^{N} \alpha_i \mathbf{v}_i \text{ and } \alpha_N \neq 0$$

we have

$$\begin{aligned} \mathbf{A}^n \mathbf{x}_0 &= \alpha_N \lambda_N^n \mathbf{v}_N + \textstyle\sum_{i=1}^{N-1} \lambda_i^n \alpha_i \mathbf{v}_i \\ &= \alpha_N \lambda_N^n \left(\mathbf{v}_N + \textstyle\sum_{i=1}^{N-1} \frac{\lambda_i^n}{\alpha_N \lambda_N^n} \alpha_i \mathbf{v}_i \right) \end{aligned}$$

The sum is small relative to the rest because ...

Proof: II

$$\left\| \sum_{i=1}^{N-1} \frac{\lambda_i^n}{\alpha_N \lambda_N^n} \alpha_i \mathbf{v}_i \right\| \leq \left| \frac{\lambda_{N-1}^n}{\alpha_N \lambda_N^n} \right| \sum_{i=1}^{N-1} |\alpha_i|$$

$$\leq \left| \frac{\lambda_{N-1}^n}{\alpha_N \lambda_N^n} \right| \sqrt{N} \|\mathbf{x}_0\| = O\left(\left| \frac{\lambda_{N-1}}{\lambda_N} \right|^n \right)$$

So ...

Proof: III

$$\mathbf{A}^n \mathbf{x}_0 = \alpha_N \lambda_N^n \left(\mathbf{v}_N + O\left(\left| \frac{\lambda_{N-1}}{\lambda_N} \right|^n \right) \right)$$

and hence

$$\|\mathbf{A}^n \mathbf{x}_0\| = \alpha_N \lambda_N^n \left(1 + O\left(\left| \frac{\lambda_{N-1}}{\lambda_N} \right|^n \right) \right)$$

Set

$$\mathbf{w}_N = \frac{\alpha_N \lambda_N^n}{|\alpha_N \lambda_N^n|} \mathbf{v}_N = \operatorname{sign}(\alpha_N \lambda_N^n) \mathbf{v}_N$$

to get ...

Proof: IV

$$\mathbf{x}_n = \frac{\mathbf{w}_N + O\left(\left|\frac{\lambda_{N-1}}{\lambda_N}\right|^n\right)}{1 + O\left(\left|\frac{\lambda_{N-1}}{\lambda_N}\right|^n\right)} = \mathbf{w}_N + O\left(\left|\frac{\lambda_{N-1}}{\lambda_N}\right|^n\right)$$

So, we're halfway there since

$$\min_{\mathbf{A}\mathbf{v}=\lambda\mathbf{v}} \|\mathbf{x}_n - \mathbf{v}\| \le \|\mathbf{x}_n - \mathbf{w}\| = O\left(\left|\frac{\lambda_{N-1}}{\lambda_N}\right|^n\right).$$

Proof: V

The eigenvalue estimate is easy at this point. Set

$$\mathbf{x}_n = \mathbf{w} + \mathbf{e}$$

then

$$\mu_n = \mathbf{w}^T \mathbf{A} \mathbf{w} + O(\|\mathbf{e}\|) = \lambda + O\left(\left| \frac{\lambda_{N-1}}{\lambda_N} \right|^n \right).$$

If $\mathbf{A}$ is symmetric, there's more.

Rayleigh Quotients

Definition: Given a real symmetric $\mathbf{A}$ and $\mathbf{x} \in R^N$, the Rayleigh quotient

$$r(\mathbf{x}, \mathbf{A}) = \frac{\mathbf{x}^T \mathbf{A} \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \frac{\mathbf{x}^T \mathbf{A} \mathbf{x}}{\|\mathbf{x}\|^2}.$$

If $\mathbf{A}\mathbf{w} = \lambda \mathbf{w}$, the $r(\mathbf{w}, \mathbf{A}) = \lambda$.
What's Taylor's theorem look like near an eigenvector?

Taylor for scalar functions

Since r is a scalar, the conventional way to do this is

$$r(\mathbf{x}, \mathbf{A}) = r(\mathbf{w}, \mathbf{A}) + \nabla r(\mathbf{w}, \mathbf{A})^T (\mathbf{x} - \mathbf{w}) + \dots$$

where

$$\nabla r(\mathbf{x}, \mathbf{A}) = (\partial r(\mathbf{x}, \mathbf{A})/\partial x_1, \dots, \partial r(\mathbf{x}, \mathbf{A})/\partial x_N)^T$$

Remember: for scalar functions, the gradient is the transpose of the Jacobian.

Differentiability

If $\|\mathbf{w}\| \neq 0$ then r is infinitely differentiable with respect to $\mathbf{x}$, so

$$\begin{aligned} r(\mathbf{x}, \mathbf{A}) &= r(\mathbf{w}, \mathbf{A}) + \nabla r(\mathbf{w}, \mathbf{A})^T (\mathbf{x} - \mathbf{w}) + O(\|\mathbf{x} - \mathbf{w}\|^2) \\ &= \lambda + \nabla r(\mathbf{w}, \mathbf{A})^T (\mathbf{x} - \mathbf{w}) + O(\|\mathbf{x} - \mathbf{w}\|^2). \end{aligned}$$

Time to compute $\nabla r(\mathbf{w}, \mathbf{A})$ when $\mathbf{A}\mathbf{w} = \lambda \mathbf{w}$.

∇r

Begin with

$$r(\mathbf{x}, \mathbf{A}) = \frac{\sum_{k,l=1}^{N} x_k a_{kl} x_l}{\|\mathbf{x}\|^2}$$

Use the quotient rule and $\partial_i \equiv \partial / \partial x_i$ to get

$$\partial_i r(\mathbf{x}, \mathbf{A}) = \frac{\partial_i(\mathbf{x}^T \mathbf{A}\mathbf{x})\mathbf{x}^T\mathbf{x} - (\mathbf{x}^T\mathbf{A}\mathbf{x})\partial_i(\mathbf{x}^T\mathbf{x})}{\|\mathbf{x}\|^4}$$

The denominator is non-zero. Time to check out the numerator . . .

∂_i

Use $\mathbf{A} = \mathbf{A}^T$ to get

$$\begin{aligned}\partial_i(\mathbf{x}^T\mathbf{A}\mathbf{x}) &= \partial_i \sum_{k,l=1}^{N} x_k a_{kl} x_l \\ &= \sum_{k,l=1}^{N} a_{il} x_l + x_k a_{ki} = 2(\mathbf{A}\mathbf{x})_i\end{aligned}$$

Clearly

$$\partial_i \mathbf{x}^T \mathbf{x} = 2x_i$$

so . . .

∂_i: II

$$\partial_i(\mathbf{x}^T\mathbf{A}\mathbf{x})\mathbf{x}^T\mathbf{x} - (\mathbf{x}^T\mathbf{A}\mathbf{x})\partial_i(\mathbf{x}^T\mathbf{x}) = 2(\mathbf{A}\mathbf{x})_i\mathbf{x}^T\mathbf{x} - (\mathbf{x}^T\mathbf{A}\mathbf{x})2x_i$$

$$2(\mathbf{x}^T\mathbf{x})((\mathbf{A}\mathbf{x})_i - \mathbf{r}(\mathbf{x})x_i)$$

So

$$\nabla r(\mathbf{x}, \mathbf{A}) = \frac{2}{\mathbf{x}^T\mathbf{x}}(\mathbf{A}\mathbf{x} - r(\mathbf{x}, \mathbf{A})\mathbf{x})$$

∇r

Plug in $\mathbf{w}$ for which

$$\mathbf{A}\mathbf{w} = \lambda \mathbf{w}, \|\mathbf{w}\| = 1, \text{ and } r(\mathbf{x}, \mathbf{A}) = \lambda$$

and get

$$\nabla r(\mathbf{w}, \mathbf{A}) = 2(\mathbf{A}\mathbf{w} - \lambda \mathbf{w}) = 0!$$

So, back to Taylor and

$$r(\mathbf{x}, \mathbf{A}) = \lambda + O(\|\mathbf{x} - \mathbf{w}\|^2)$$

As for the power method

So, for real, symmetric **A**, we get

$$\mu_n = \mathbf{x}_n^T \mathbf{A} \mathbf{x}_n = \lambda_N + O\left(\left| \frac{\lambda_{N-1}}{\lambda_N} \right|^{2n} \right).$$

instead of

$$O\left(\left| \frac{\lambda_{N-1}}{\lambda_N} \right|^{n} \right).$$

as we got in the general case.

Inverse Power Method (IPM)

To find the smallest eigenvector, apply PM to $\mathbf{A}^{-1}$.

$$\mathbf{x}_n = \frac{\mathbf{A}^{-1}\mathbf{x}_{n-1}}{\|\mathbf{A}^{-1}\mathbf{x}_{n-1}\|} = \frac{(\mathbf{A}^{-1})^n\mathbf{x}_0}{\|(\mathbf{A}^{-1})^n\mathbf{x}_0\|}$$

You'd expect

$$\hat{\mu}_n = \mathbf{x}_n^T\mathbf{A}^{-1}\mathbf{x} = \lambda_1^{-1} + O\left(\left|\frac{\lambda_2^{-1}}{\lambda_1^{-1}}\right|^n\right) = \lambda_1^{-1} + O\left(\left|\frac{\lambda_1}{\lambda_2}\right|^n\right)$$

which means that

$$\mu_n = \mathbf{x}_n^T\mathbf{A}\mathbf{x} = \lambda_1 + O\left(\left|\frac{\lambda_1}{\lambda_2}\right|^n\right),$$

and you'd be right.

IPM Implementation

$\mathbf{x} = \mathbf{x}_0$
Factor $\mathbf{A} = \mathbf{LU}$
while not happy **do**
  Solve $\mathbf{LUy} = \mathbf{x}$
  $\mathbf{x} \leftarrow \mathbf{y}/\|\mathbf{y}\|$
  $\lambda = \mathbf{x}^T \mathbf{A} \mathbf{x}$
end while

Termination?

- $|\lambda_n - \lambda_{n-1}|$ small
- $\|\mathbf{A}\mathbf{x}_n - \lambda_n \mathbf{x}_n\|$ small

Convergence of IPM

Assumptions:

- **A** is diagonalizable.
  - **A** has N linearly independent unit eigenvectors $\{\mathbf{v}_i\}_{i=1}^N$
  - with corresponding eigenvalues $\{\lambda_i\}$.

$$|\lambda_1| < |\lambda_2| \leq \cdots \leq |\lambda_{N-1}| \leq |\lambda_N|$$

  - The smallest eigenvalue in absolute value has geometric multiplicity one.
- $\mathbf{x}_0 = \sum_{i=1}^N \alpha_i \mathbf{v}_i$ with $\alpha_1 \neq 0$.
- $\{\mathbf{x}_n\}$ are the inverse power method iterations.

Convergence of IPM: II

Conclusions:

- The convergence rate to the eigen-manifold is r-linear

$$\min_{\mathbf{A}\mathbf{v}=\lambda_1\mathbf{v}} \|\mathbf{x}_n - \mathbf{v}\| = O\left(\left| \frac{\lambda_1}{\lambda_2} \right|^n \right),$$

- as is the convergence to the eigenvalue,

$$\mu_n = \mathbf{x}_n^T \mathbf{A} \mathbf{x}_n = \lambda_1 + O\left(\left| \frac{\lambda_1}{\lambda_2} \right|^n \right).$$

Eigenvalue convergence is twice as fast if **A** is symmetric.

Shifted Power Method

Find eigenvalue nearest λ_t (the shift)
Method: Apply IPM to $\mathbf{A} - \lambda_t \mathbf{I}$.

$$\mathbf{x}_n = \frac{(\mathbf{A} - \lambda_t)^{-1} \mathbf{x}_{n-1}}{\|(\mathbf{A} - \lambda_t)^{-1} \mathbf{x}_{n-1}\|}$$

Assumptions:

$$|\lambda_k - \lambda_t| < |\lambda_l - \lambda_t| \le |\lambda_i - \lambda_t| \text{ for all } i \neq k, l.$$

Then, given the other things,

$$\mu_n = \mathbf{x}_n^T \mathbf{A} \mathbf{x}_n = \lambda_k + O\left(\left| \frac{\lambda_k - \lambda_t}{\lambda_l - \lambda_t} \right|^n \right).$$

Simple Example

$$\mathbf{V} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix} \text{ and } \mathbf{D} = \begin{pmatrix} 10 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Cook the books so that

$$\mathbf{A} = \mathbf{V}\mathbf{D}\mathbf{V}^{-1}.$$

A is diagonalizable, not symmetric, and the eigenvalues are $10, 5, 1$.

What to expect

We find the

- Largest eigenvalue (PM)
  expected convergence rate $= 5/10 = .5$
- Smallest eigenvalue (IPM)
  expected convergence rate $= 1/5 = .2$
- Nearest eigenvalue to $\lambda_t = 4$ (SPM)
  expected convergence rate $= |5-4|/|1-4| = 1/3$

Showtime!

PM		IPM		SPM	
$\lvert\mu_n - \lambda_3\rvert$	ratio	$\lvert\mu_n - \lambda_1\rvert$	ratio	$\lvert\mu_n - \lambda_2\rvert$	ratio
1.77e+00		8.98e-01		8.18e-01	
7.55e-01	0.43	1.28e-01	0.14	1.70e-01	0.21
3.47e-01	0.46	2.06e-02	0.16	8.28e-02	0.49
1.65e-01	0.48	3.66e-03	0.18	2.31e-02	0.28
8.05e-02	0.49	6.85e-04	0.19	8.52e-03	0.37
3.97e-02	0.49	1.33e-04	0.19	2.69e-03	0.32
1.97e-02	0.50	2.61e-05	0.20	9.23e-04	0.34
9.80e-03	0.50	5.17e-06	0.20	3.03e-04	0.33
4.89e-03	0.50	1.03e-06	0.20	1.02e-04	0.34
2.44e-03	0.50	2.05e-07	0.20	3.38e-05	0.33

Symmetric Case

$$\mathbf{A} = \mathbf{D} = \begin{pmatrix} 10 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Same computation.

- Largest eigenvalue (PM)
  expected convergence rate $= (5/10)^2 = .25$
- Smallest eigenvalue (IPM)
  expected convergence rate $= 1/25 = .04$
- Nearest eigenvalue to $\lambda_t = 4$ (SPM)
  expected convergence rate $= |5-4|^2/|1-4|^2 = 1/9$

Don't take my word for anything.

PM		IPM		SPM	
$\lvert\mu_n - \lambda_3\rvert$	ratio	$\lvert\mu_n - \lambda_1\rvert$	ratio	$\lvert\mu_n - \lambda_2\rvert$	ratio
1.06e+00		2.38e-01		2.68e-01	
2.95e-01	0.28	7.29e-03	0.03	4.49e-02	0.17
7.69e-02	0.26	2.65e-04	0.04	5.37e-03	0.12
1.95e-02	0.25	1.03e-05	0.04	6.07e-04	0.11
4.88e-03	0.25	4.10e-07	0.04	6.77e-05	0.11
1.22e-03	0.25	1.64e-08	0.04	7.52e-06	0.11
3.05e-04	0.25	6.55e-10	0.04	8.36e-07	0.11
7.63e-05	0.25	2.62e-11	0.04	9.29e-08	0.11
1.91e-05	0.25	1.05e-12	0.04	1.03e-08	0.11
4.77e-06	0.25	4.22e-14	0.04	1.15e-09	0.11

High Geometric Multiplicity

How about

$$\mathbf{A} = \begin{pmatrix} 10 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \mathbf{x}_0 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}?$$

You can see this coming

$$\mathbf{A}^n \mathbf{x}_0 = \begin{pmatrix} 10^n \\ 10^n \\ 1 \end{pmatrix} \text{ so } \mathbf{x}_n = \frac{\mathbf{A}^n \mathbf{x}_0}{\|\mathbf{A}^n \mathbf{x}_0\|} = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} + O(10^{-n})$$

is pretty close to something in $\{\mathbf{v} \,|\, \mathbf{A}\mathbf{v} = 10\mathbf{v}\}$

Convergence of PM

Assume:

- $\mathbf{A}$ is diagonalizable (basis of eigenvectors)
- There are K distinct eigenvalues

$$|\lambda_1| \leq \cdots < |\lambda_K|$$

Then everything looks almost the same ...

Convergence for high multiplicity

Conclusions: If $\mathbf{x}_0$ does the right thing (more later)

- The convergence rate to the eigen-manifold is r-linear

$$\min_{\mathbf{A}\mathbf{v}=\lambda_K \mathbf{v}} \|\mathbf{x}_n - \mathbf{v}\| = O\left(\left| \frac{\lambda_{K-1}}{\lambda_K} \right|^n \right),$$

- as is the convergence to the eigenvalue,

$$\mu_n = \mathbf{x}_n^T \mathbf{A} \mathbf{x}_n = \lambda_K + O\left(\left| \frac{\lambda_{K-1}}{\lambda_K} \right|^n \right).$$

And the symmetric case does better for the eigenvalue.

Analysis for high multiplicity

Let

$$M_k = \{\mathbf{v} \mid \mathbf{A}\mathbf{v} = \lambda_k \mathbf{v}\} \text{ for } 1 \le k \le K$$

Let M_k have dimension N_k. So

$$\sum N_k = N$$

because $\mathbf{A}$ is diagonalizable.
Linear independence implies that $\mathbf{x}_0$ has a unique expansion

$$\mathbf{x}_0 = \sum_{i=1}^{K} \alpha_i \mathbf{v}_i \text{ where } \mathbf{v}_i \in M_i \text{ and } \|\mathbf{v}_i\| = 1.$$

Analysis: II

So if $\alpha_K \neq 0$, then

$$\mathbf{A}^n \mathbf{x}_0 = \lambda_K^n \alpha_K \left(\mathbf{v}_K + O\left(\left| \frac{\lambda_{K-1}}{\lambda_K} \right|^n \right) \right).$$

So now we can proceed just like before. We get

$$\mathbf{x}_n - \text{sign}(\lambda_K^n \alpha_K) \mathbf{v}_K = O\left(\left| \frac{\lambda_{K-1}}{\lambda_K} \right|^n \right).$$

so the sequence $\{\mathbf{x}_n\}$ approaches M_K, but does so in an $\mathbf{x}_0$-dependent way.

Experiment for you to do

Use

$$\mathbf{D} = \begin{pmatrix} 10 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

and two different choices of $\mathbf{x}_0$

$$\mathbf{x}_0 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \text{ and } \mathbf{x}_0 = \begin{pmatrix} 1 \\ 1 \\ 3 \end{pmatrix}$$

What is $\lim \mathbf{x}_n$ for each choice? Does the final component of $\mathbf{x}_0$ make any difference?

But Tim, does high multiplicity have anything to do with me?

Recall that the eigenfunctions of

$$\frac{d^2}{dx^2} \text{ on } [0, 1] \text{ with zero boundary conditions}$$

are, for $n = 1, 2, \ldots$

$$u_n(x) = \sqrt{2}\sin(n\pi x) \text{ with eigenvalues } \lambda_n = n^2\pi^2$$

In two space dimensions you get ...

Laplacian in 2D

$$\nabla^2 u(x,y) = (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}) u(x,y) = \lambda u(x,y), \text{ for } 0 < x, y < 1,$$

subject to

$$u(0,y) = u(x,0) = u(1,y) = u(x,1) = 0.$$

Plug in to see that

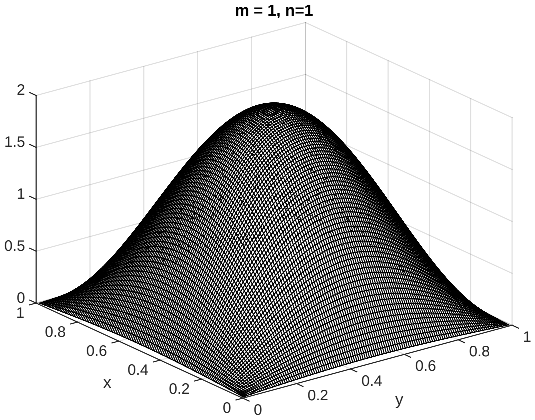
$$u_{m,n}(x,y) = u_m(x) u_n(y), \lambda_{m,n} = (m^2 + n^2)\pi^2$$

are eigenfunction/eigenvalue pairs.

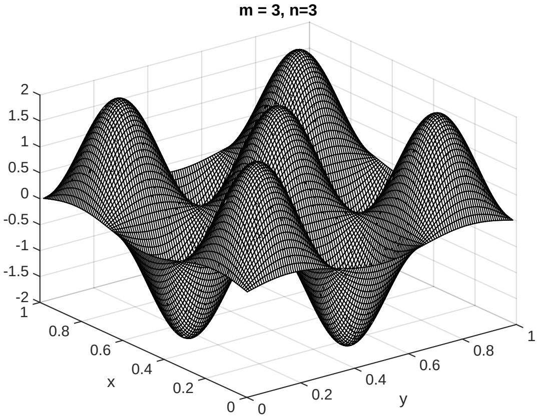
Managing the 2D to 1D map

```
x=h:h:1-h; x=x'; y=x;
lambda=(m*m*pi*pi+n*n*pi*pi);
U=2*sin(m*pi*x)*sin(n*pi*y)';
u=reshape(U,N^2,1);
D2=l2d(n);
r=(u'*D2*u)/(u'*u);
```

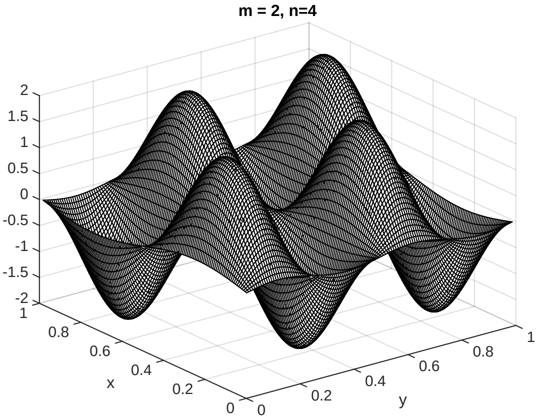
$m = n = 1$



$m = n = 3$



$m = 2, n = 4$



Applying IPM

```
D2=l2d(n);
L=chol(A,'lower');
x=ones(n*n,1);
while not happy
    w=L'\(L\x);
    x=w/norm(w);
end
```

Sanity Check: $h = 1/(n+1)$; $N = n^2$

- $D2$ is symmetric, so convergence rate should be

$$\left(\frac{\lambda_1}{\lambda_2}\right)^2 = \left(\frac{2\pi^2}{5\pi^2}\right)^2 = .04.$$

- $\lambda_1(h) = \lambda_1 + O(h^2)$

Convergence for $n = 63$

$\lvert\lambda - 2\pi^2\rvert$	$\lVert \mathbf{Ax} - \lambda \mathbf{x} \rVert$	$\lvert\lambda_n - \lambda_{n-1}\rvert$	ratio
8.95e-01	3.74e-01	2.06e+01	
2.52e-02	4.98e-02	8.70e-01	4.22e-02
2.83e-03	1.15e-02	2.80e-02	3.22e-02
3.92e-03	2.47e-03	1.09e-03	3.89e-02
3.96e-03	5.12e-04	4.35e-05	3.99e-02
3.96e-03	1.04e-04	1.74e-06	4.01e-02
3.96e-03	2.10e-05	6.98e-08	4.01e-02
3.96e-03	4.23e-06	2.80e-09	4.01e-02
3.96e-03	8.48e-07	1.12e-10	4.01e-02
3.96e-03	1.70e-07	4.44e-12	3.95e-02
3.96e-03	3.41e-08	1.81e-13	4.08e-02

$\lambda_1(h) = \lambda_1 + O(h^2)$?

Running from $n = 15$ to $n = 511$.

N	$\lvert\lambda - 2\pi^2\rvert$	ratio
15	6.33e-02	0.00e+00
31	1.58e-02	2.50e-01
63	3.96e-03	2.50e-01
127	9.91e-04	2.50e-01
255	2.48e-04	2.50e-01
511	6.19e-05	2.50e-01

More eigenvalues?

Table of λ_{mn}/π^2. $m \neq n$ means multiplicity ≥ 2.
$\lambda_{4,2}/\lambda_{3,3} \approx .94$ is not small at all.

m	n	λ_{mn}/π^2
1	1	2
1	2	5
2	2	8
3	1	10
3	2	13
4	1	17
3	3	18
2	4	20

Problems with more evals.

- $\mathbf{D}_2 - \lambda \mathbf{I}$ is not spd
  - Can't use Cholesky.
  - Your options are LDL or LU.
  - I'll use LU because it's simpler.
- Eigenvalues can be relatively close to each other.
  - Poor convergence for SPM?
- Experiment: $\lambda_{2,1} = 5\pi^2$ with $\lambda_t = 50$ expected convergence rate

$$\left(\frac{|\lambda_{2,1} - 50|}{|\lambda_{1,1} - 50|} \right)^2 \approx 4.6 \times 10^{-4}$$

SPM: $\lambda_{2,1} = 5\pi^2$ with SPM, $\lambda_t = 50$, $n = 63$

$\lvert\lambda - 5\pi^2\rvert$	$\lVert \mathbf{Ax} - \lambda \mathbf{x} \rVert$	$\lvert\lambda_n - \lambda_{n-1}\rvert$	ratio
2.27e+01	6.05e-01	2.66e+01	2.66e+00
2.70e+01	6.17e-01	4.32e+00	1.62e-01
2.86e+01	3.44e-01	1.56e+00	3.60e-01
2.92e+01	2.55e-01	6.17e-01	3.96e-01
2.95e+01	1.49e-01	2.42e-01	3.93e-01
2.96e+01	9.80e-02	9.46e-02	3.90e-01
2.96e+01	5.93e-02	3.67e-02	3.88e-01
2.94e+01	9.56e-02	2.27e-01	6.19e+00
1.77e+00	2.30e-01	2.76e+01	1.21e+02
3.46e-02	5.27e-03	1.73e+00	6.28e-02
3.37e-02	1.18e-04	9.44e-04	5.45e-04
3.37e-02	2.69e-06	4.85e-07	5.13e-04
3.37e-02	6.06e-08	2.49e-10	5.13e-04
3.37e-02	1.38e-09	2.84e-14	1.14e-04

Observations

- Results ok, but
  - convergence rate stabilizes late
  - poor performance early
- and it can get worse ...
- $\lambda_{4,1} = 17\pi^2$, $\lambda_t = 167$
  expected convergence rate

$$\left(\frac{|\lambda_{4,1} - 167|}{|\lambda_{3,3} - 167|} \right)^2 \approx .07.$$

SPM: $\lambda_{4,1} = 17\pi^2$ with SPM, $\lambda_t = 167$, $n = 255$

$\lvert\lambda - 17\pi^2\rvert$	$\lVert\mathbf{Ax} - \lambda\mathbf{x}\rVert$	$\lvert\lambda_n - \lambda_{n-1}\rvert$	ratio
3.68e+01	6.51e-01	1.31e+02	1.31e+01
8.79e+00	9.00e-02	4.56e+01	3.48e-01
9.83e+00	9.36e-03	1.04e+00	2.28e-02
9.85e+00	2.29e-03	2.01e-02	1.93e-02
9.85e+00	2.65e-04	4.67e-04	2.32e-02
9.85e+00	5.72e-05	1.13e-05	2.43e-02
9.85e+00	7.37e-06	2.76e-07	2.44e-02
9.85e+00	6.76e-06	3.57e-08	1.29e-01
9.85e+00	8.71e-05	8.50e-06	2.38e+02
9.85e+00	1.23e-03	1.70e-03	2.00e+02
9.52e+00	1.72e-02	3.29e-01	1.94e+02
1.21e+00	3.18e-02	8.31e+00	2.52e+01
2.47e-02	2.11e-03	1.24e+00	1.49e-01
3.18e-02	1.47e-04	7.07e-03	5.71e-03
3.18e-02	1.03e-05	3.54e-05	5.00e-03
3.18e-02	7.31e-07	1.77e-07	4.99e-03
3.18e-02	5.17e-08	8.84e-10	5.01e-03
3.18e-02	3.65e-09	5.12e-12	5.79e-03
3.18e-02	2.60e-10	1.11e-12	2.17e-01
3.18e-02	2.27e-11	1.36e-12	1.23e+00
3.18e-02	2.13e-11	1.25e-12	9.17e-01

Another free lunch: Rayleigh Quotient Iteration (RQI)

This is for real symmetric $\mathbf{A}$.

$\mathbf{x} = \mathbf{x}_0$; $\mu = \lambda_t$
while not happy **do**
  Solve $(\mathbf{A} - \mu \mathbf{I})\mathbf{y} = \mathbf{x}$
  $\mathbf{x} \leftarrow \mathbf{y}/\|\mathbf{y}\|$
  $\mu = \mathbf{x}^T \mathbf{A} \mathbf{x}$
end while

Convergence

RQI converges for almost every $\mathbf{x}_0$. The limiting convergence rate is locally cubic. If $\mu_k \to \lambda$ for some $\lambda \in \sigma(\mathbf{A})$ then, for k sufficiently large

$$|\mu_{k+1} - \lambda| = O(|\mu_k - \lambda|^3)$$

and

$$\min_{\mathbf{A}\mathbf{v}=\lambda_N \mathbf{v}} \|\mathbf{x}_{k+1} - \mathbf{v}\| = O(\min_{\mathbf{A}\mathbf{v}=\lambda_N \mathbf{v}} \|\mathbf{x}_k - \mathbf{v}\|^3).$$

RQI Proof: I

We may assume **A** is diagonal without loss of generality. Since

$$\mathbf{A} = \mathbf{U}\Lambda\mathbf{U}^T \text{ with } \mathbf{U} \text{ orthogonal}$$

We have

$$(\mathbf{A} - \mu\mathbf{I}) = \mathbf{U}(\Lambda - \mu\mathbf{I})\mathbf{U}^T, \text{ and } r(\mathbf{x}, \mathbf{A}) = \frac{\mathbf{x}^T\mathbf{U}\Lambda\mu^T\mathbf{x}}{\mathbf{x}^t\mathbf{U}\mathbf{U}^T\mathbf{x}} = r(\mathbf{z}, \Lambda)$$

where $\mathbf{z} = \mathbf{U}^T\mathbf{x}$.
Hence we may replace $\mathbf{x}$ and $\mathbf{y}$ by $\mathbf{z} = \mathbf{U}^T\mathbf{x}$ and $\mathbf{w} = \mu^T\mathbf{y}$ and get an equivalent iteration for $\mathbf{A} \to \Lambda$

Proof: II

Track the iteration

$$\mathbf{w}_{k+1} = (\Lambda - r(\mathbf{z}_k, \Lambda)\mathbf{I})^{-1}\mathbf{z}_k$$

Suppose (no loss of generality):

- Our target eigenvalue is λ_1.
- $\mu_k \to \lambda_1$,
- $\mathbf{z}_k \to \mathbf{e}_1$, the corresponding eigenvector.
  This means that $\lambda_1 > 0$ so we don't have $\pm$ bookkeeping.

To make life simple, I will assume that λ_1 is simple.

Keeping Score

Let

$$\mathbf{z}_k = \mathbf{e}_1 + \mathbf{d}_k \text{ and } \|\mathbf{d}_k\| = \epsilon_k$$

We already proved that

$$r(\mathbf{z}_k, \Lambda) = \lambda_1 + O(\|\mathbf{z}_k - \mathbf{e}_1\|^2) = \lambda_1 + O(\epsilon_k^2).$$

We seek to show that $\epsilon_{k+1} = O(\epsilon_k^3)$.
$\mathbf{z}_k$ is a unit vector, so

$$1 = \mathbf{z}_k^T \mathbf{z} = 1 + 2\mathbf{e}_1^T \mathbf{d}_k + \mathbf{d}_k^T \mathbf{d}_k = 1 + 2\mathbf{d}_{k1} + \epsilon_k^2$$

So the first component of $\mathbf{d}_k$ is $-\epsilon_k^2/2$.

Chasing $\mathbf{w}$

By the formula

$$\begin{aligned} \mathbf{w}_{k+1} &= (\Lambda - \mu_k)^{-1}\mathbf{z}_k = \Big(\frac{1 + d_{k1}}{\lambda_1 - \mu_k}, \dots, \frac{d_{ki}}{\lambda_i - \mu_k}, \dots\Big)^T \\ &= \Big(\frac{1 - \epsilon_k^2/2}{\lambda_1 - \mu_k}, \dots, \frac{d_{ki}}{\lambda_i - \mu_k}, \dots\Big)^T = \frac{1 - \epsilon_k^2/2}{\lambda_1 - \mu_k}(\mathbf{e}_1 + \hat{\mathbf{d}}) \end{aligned}$$

Estimating the parts

Since $\mu_k = \lambda_1 + O(\epsilon_k^2)$ we have

$$p_k = \frac{1 - \epsilon_k^2/2}{\lambda_1 - \mu_k} = O(\epsilon_k^{-2}).$$

The error vector $\hat{\mathbf{d}}$ looks like

$$\left(0, \dots, \frac{d_{ki}/p_k}{\lambda_i - \mu_k}, \dots\right)^T = O(\epsilon_k^3)$$

because $\|\mathbf{d}_k\| = \epsilon_k$ and $p_k = O(\epsilon_k^2)$.
Normalize and that's it.

Cubic convergence is fast: 2D Laplacian

$\lambda_t = 20$, $n = 100$

μ_k	$\|\mu_k - \mu_{k-1}\|$	$\|\mathbf{Ax} - \mu\mathbf{x}\|_\infty$
2.00e+01		2.04e+04
1.97e+01	2.62e-01	3.20e-03
1.97e+01	2.38e-04	8.34e-09

- If you try one more iteration, Matlab complains about a singular matrix.
- If you do it, you'll get a better vector.
- Your value is as good as it'll get.

Some facts

- Cubic is real fast. Terminate when

$$\|\mathbf{A}\mathbf{x} - \mu\mathbf{x}\| = O(\epsilon_{mach}^{1/3})$$

  or risk whining from Matlab.
- You must do a factorization of $\mathbf{A} - \mu\mathbf{I}$ at each iteration.
- The near singularity of $\mathbf{A} - \mu\mathbf{I}$ is not a big deal.
  You're only after the direction.

RQI: $\lambda_{2,1} = 5\pi^2$ with SPM, $\lambda_t = 50$, $n = 63$

$$\mathbf{x}_0 = (1, 1, \ldots, 1)^T .$$

This is embarrassing! What went wrong?

μ_k	$\lvert \mu_k - \mu_{k-1} \rvert$	$\lVert \mathbf{Ax} - \mu \mathbf{x} \rVert_\infty$
5.00e+01	1.00e+00	8.14e+03
2.66e+01	2.34e+01	6.05e-01
1.98e+01	6.83e+00	8.59e-02
1.97e+01	6.30e-02	7.34e-05
1.97e+01	4.00e-08	1.39e-13

A couple bandaids

- $\lambda_t = 49$, $5\pi^2 = 49.35$
- $\mathbf{x}_0$ random

μ_k	$\lvert\mu_k - \mu_{k-1}\rvert$	$\lVert \mathbf{Ax} - \mu\mathbf{x} \rVert_\infty$
4.90e+01	1.00e+00	1.37e+04
4.07e+01	8.33e+00	7.84e-01
4.68e+01	6.17e+00	3.25e-01
4.93e+01	2.45e+00	2.28e-02
4.93e+01	2.28e-02	2.14e-05
4.93e+01	1.37e-08	1.70e-13

RQI: $\lambda_{4,1} = 17\pi^2$, $\lambda_t = 167$, $n = 255$

Yee-Hah! $17\pi^2 = 167.78$, $18\pi^2 = 177.65$

μ_k	$\lvert\mu_k - \mu_{k-1}\rvert$	$\lVert \mathbf{Ax} - \mu\mathbf{x} \rVert_\infty$
1.67e+02	1.00e+00	2.33e+05
1.42e+02	2.55e+01	7.78e-01
1.62e+02	2.05e+01	2.21e-01
1.68e+02	6.45e+00	4.21e-02
1.68e+02	6.66e-01	1.95e-03
1.68e+02	4.50e-03	7.65e-07
1.68e+02	9.40e-10	9.40e-13

Can you get a basis for the eigen-manifold?

How's this sound?

- Solve the problem to get λ and $\mathbf{u}$
- Use a random $\mathbf{x}_0$ with is orthogonal to $\mathbf{u}$
  ```
  x0=rand(N,1); x0 = x0 - (u'*x0)*u;
  ```
- and it was much better to orthogonalize twice.
- Solve it again.

What should λ_t be for the second solve?

So I did it with $\lambda_{4,1}$, and $\lambda_t = \mu_{final}$

The second solve said

```
Warning: Matrix is close to singular or badly scaled.
Results may be inaccurate. RCOND =  8.862787e-22.
> In rqi at 15
  In high_mult at 10
```

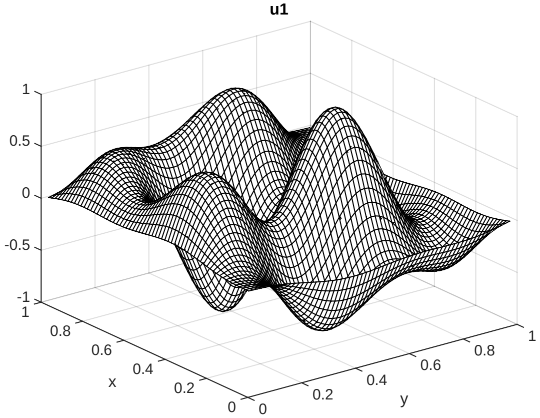
but I got something anyhow

μ_k	$\|\mu_k - \mu_{k-1}\|$	$\|\mathbf{Ax} - \mu\mathbf{x}\|_\infty$
1.68e+02	1.00e+00	2.43e+05
1.68e+02	7.11e-13	6.52e-10

Results?

- I got two linearly independent eigenvectors,
- which were kinda orthogonal $\mathbf{u}_1^T \mathbf{u}_2 \approx .005$,
- and were not the eigenvectors you derive by hand.
- If you only orthogonalize once, $\mathbf{u}_1^T \mathbf{u}_2 \approx .99$

First eigenvector



Second eigenvector