Some observations on constructing Q

We have:

- $Q = I - \gamma u u^T$ with

$$u = x - y = \begin{bmatrix} \tau + x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad \gamma = 2/\|u\|_2^2.$$

- It is convenient (Why?) to normalize u so that 1st entry is 1.

$$u = (x - y)/(\tau + x_1) = \begin{bmatrix} 1 \\ x_2/(\tau + x_1) \\ \vdots \\ x_n/(\tau + x_1) \end{bmatrix}$$

- Choose sign of τ same as that of x_1 to avoid cancellation

Numerical Issues

Fact 7

Show that if $\tau = \pm\|x\|_2$ is choosen so that τ and x_1 have the same sign, then all entries of u in

$$u = (x - y) = \begin{bmatrix} 1 \\ x_2/(\tau + x_1) \\ \vdots \\ x_n/(\tau + x_1) \end{bmatrix}$$

satisfy $|u_i| \leq 1$, and $\gamma = (\tau + x_1)/\tau$.

Computing γ

Turna out that computing γ for new u is easy:

$$\begin{aligned}\|u\|_2^2 &= \frac{(\tau + x_1)^2 + x_2^2 + \cdots + x_n^2}{(\tau + x_1)^2} \\ &= \frac{\tau^2 + 2\tau x_1 + \|x\|_2^2}{(\tau + x_1)^2}\end{aligned}$$

Since $\tau^2 = \|x\|^2$,

$$\|u\|_2^2 = 2\tau(\tau + x_1)/(\tau + x_1)^2 = 2\tau/(\tau + x_1),$$

hence,

$$\gamma = 2/\|u\|_2^2 = (\tau + x_1)/\tau$$

Numerical Issues Continued

Fact 8

We need to compute $\|x\|_2 = \sqrt{x_1^2 + \cdots + x_n^2}$. Squaring can lead to overflow (underflow), if the number are large (small). Consider, the following example. Compute $\|x\|_2$ where

$$x = [10^{-49}, 10^{-50}, 10^{-50}, \cdots, 10^{-50}]^T \in \mathbb{R}^{11}$$

on a computer that underflows at 10^{-99}, that is any number smaller than that is set to zero.

Avoiding Overflow and Underflows

Overflow/Underflow can be avoided:

Let $\beta = \|x\|_\infty = \max_{1\le i\le n} |x_i|$.

- If $\beta = 0$, then $\|x\|_2 = 0$
- Otherwise, let $\hat{x} = (1/\beta)x$. Then $\|x\|_2 = \beta\|\hat{x}\|_2 = \beta\sqrt{\hat{x}_1^2 + \cdots + \hat{x}_n^2}$
- Now evaluate the norm for the previous example

Algorithm for calculating Q, such that $Qx = y$

$\beta \leftarrow \max_{1 \le i \le n} |x_i|$
if $(\beta = 0)$ **then**
    $\gamma \leftarrow 0$
else
    $x_{1:n} \leftarrow x_{1:n}/\beta$
    $\tau \leftarrow \sqrt{x_1^2 + \cdots + x_n^2}$
    if $(x_1 < 0)$ **then**
        $\tau = -\tau$
    end if
    $x_1 \leftarrow \tau + x_1$
    $\gamma \leftarrow x_1/\tau$
    $x_{2:n} \leftarrow x_{2:n}/x_1$
    $x_1 \leftarrow 1$
    $\tau \leftarrow \tau\beta$
end if

$A = QR$ using reflectors

Fact 9

Given $A \in \mathbb{R}^{n \times n}$, then A can be expressed as $A = QR$, where Q is orthogonal and R is upper triangular.

Proof.

The proof is by induction on n.

- For $n = 1$, take $Q = [1]$ and $R = [a_{11}]$ to get $A = QR$
- (Induction Hypothesis) Assume that the theorem is true for $(n-1)$.
- Claim: The theorem is true for n :

$\square$

- Let $Q_1 \in \mathbb{R}^{n\times n}$ be the reflector that creates zeros in the first column of A :

$$Q_1 \begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{n1} \end{bmatrix} = \begin{bmatrix} -\tau_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

- Recall that Q_1 is symmetric, we have

$$Q_1^T A = Q_1 A = \begin{bmatrix} -\tau_1 & \hat{a}_{12} & \cdots & \hat{a}_{1n} \\ 0 & * & \cdots & * \\ \vdots & * & \ddots & * \\ 0 & * & * & * \end{bmatrix}$$

- By induction hypothesis, the subblock $\hat{A}_2 = Q_1 A(2:n, 2:n)$ has QR decomposition: $\hat{A}_2 = \hat{Q}_2 \hat{R}_2$, where $\hat{Q}_2$ is orthogonal and $\hat{R}_2$ is upper triangular.

$A = QR$ finally!

- Define $\tilde{Q}_2 \in \mathbb{R}^{n\times n}$ by

$$\tilde{Q}_2 = \begin{bmatrix} 1 & 0 & \cdots & \cdots & 0 \\ 0 & q_2^{11} & q_2^{12} & \cdots & q_2^{1,n-1} \\ \vdots & \cdots & \ddots & \cdots & \vdots \\ 0 & q_2^{n-1,1} & \cdots & \cdots & q_2^{n-1,n-1} \end{bmatrix}$$

- Then it is easy to see that:

$$\tilde{Q}_2^T Q_1^T A = R \implies A = QR, Q = (\tilde{Q}_2^T Q_1^T)^T$$

Algorithm to compute QR of A

for $k = 1, \cdots, n-1$ **do**
  Determine a reflector $Q_k = I - u^{(k)}{u^{(k)}}^T$ such that
  $Q_k[a_{kk} \cdots a_{nk}]^T = [-\tau, 0 \cdots 0]^T$
  Store $u^{(k)}$ over $a_{k:n,k}$ as in previous algo (p237)
  $a_{k:n,k+1:n} \leftarrow Q_k a_{k:n,k+1:n}$
  $a_{kk} \leftarrow -\tau_k$
end for
$\gamma_n \leftarrow a_{nn}$

- Like LU, the Q and R of QR are overwritten in A
- Flop count $= 4n^3/3$, twice that of LU

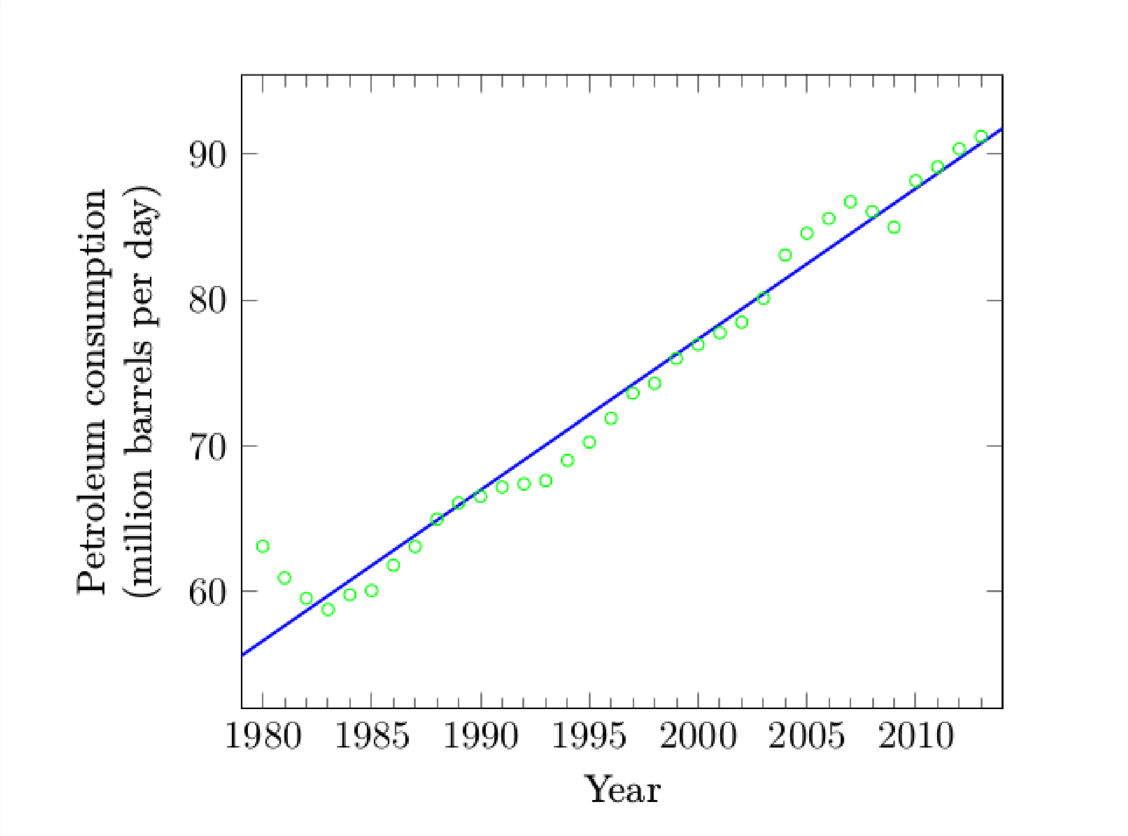
Solution of the least squares problem

The Least Squares Problem: Given

$$Ax = b, \quad A \in \mathbb{R}^{n \times m}, b \in \mathbb{R}^n, n > m.$$

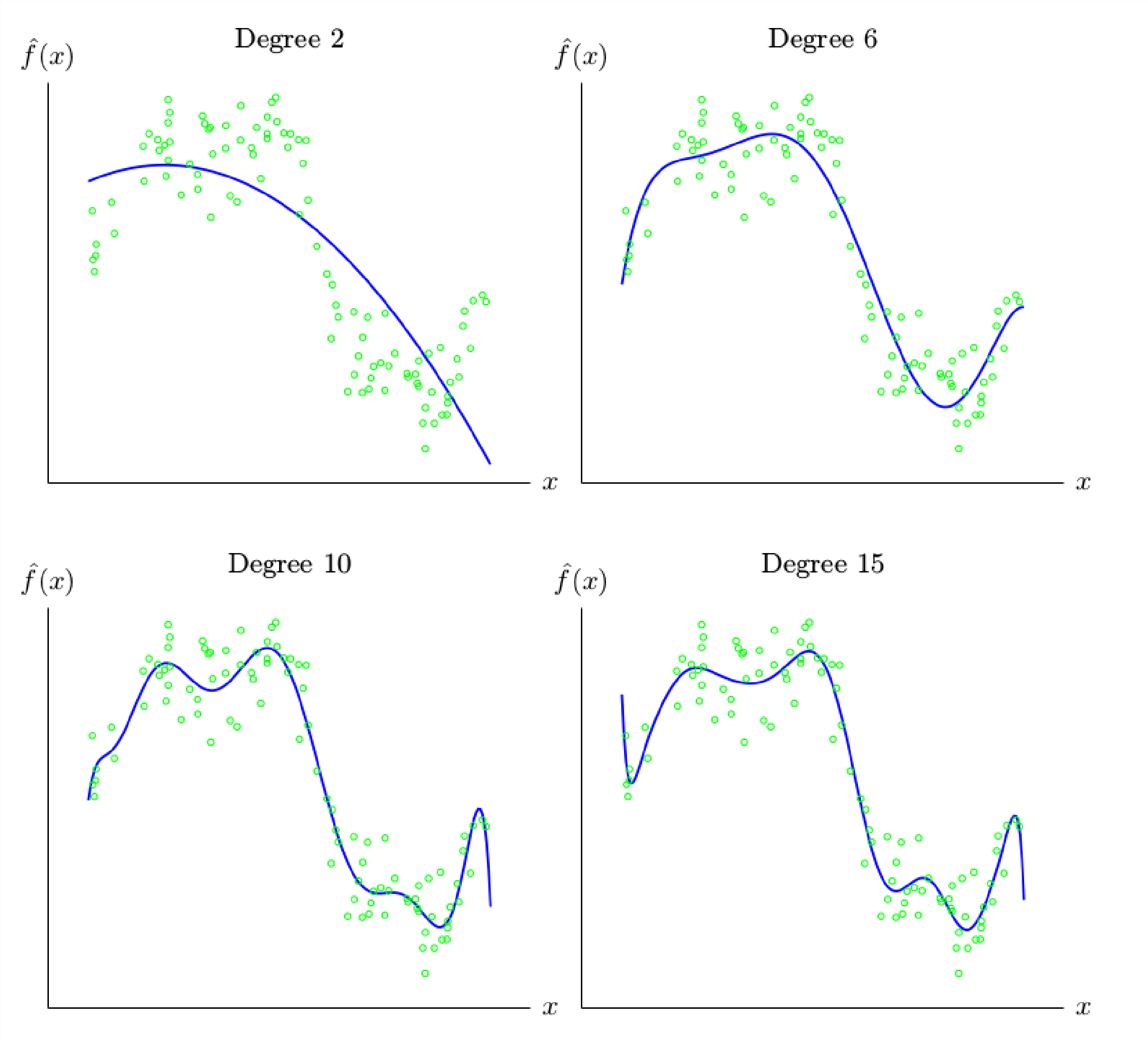
Find $x \in \mathbb{R}^m$ such that $\|r\|_2 = \|b - Ax\|_2$ is minimized.

Why Least Squares is Useful?



- Understand pattern in the underlying data

Model Selections



- Possible non-linear pattern in underlying data

Fitting a line to a given set of data:

- Data: Consider the following XY data:

X	y
x_1	y_1
x_2	y_2
$\vdots$	$\vdots$
x_n	y_n

- Fit a line $f(x) = mx + c$ to the given data
- We expect/force:

$$
\begin{aligned}
f(x_1) &= y_1 \\
f(x_2) &= y_1 \\
\cdots &= \cdots \\
f(x_n) &= y_n
\end{aligned}
$$

Line Fitting

We have:

$$\begin{aligned} mx_1 + c &= y_1 \\ mx_2 + c &= y_2 \\ \vdots &= \vdots \\ mx_n + c &= y_n \end{aligned}$$

In other words,

$$\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} m \\ c \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Solution to Least squares using QR

Solution to the following overdetermined system may not exist!

$$\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} m \\ c \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

- Find best possible solution, that is,

$$\min_x \|Ax - b\|_2$$

QR for least squares

We have:

$$\begin{aligned}\min_x \|Ax - b\|_2 &= \min_x \|QRx - b\|_2 \\ &= \|Rx - Q^T b\|\end{aligned}$$

Now solve: $Rx = Q^T b$

From Line to More Generalized Models

When fitting a line to a given (X, y), we used the following model:

$$\hat{f}(x) = \theta_1 f_1(x) + \theta_1 f_2(x), \quad \text{where } \theta_1 = m,\ \theta_2 = c$$

Consider the generalized linear (why?) model:

$$\hat{f}(x) = \theta_1 f_1(x) + \theta_2 f_2(x) + \cdots + \theta_p f_p(x)$$

Here:

- c_i are constants and θ_i are called model parameters
- $f_i(x)$ are real valued functions: $f_i : \mathbb{R}^n \to \mathbb{R}$
- f_i are called basis functions or feature mappings
- $\hat{f}$ is called prediction function
- This model is linear as a function of the parameters (Why?)

Predictions, Prediction Errors, and Residuals

Goal: Choose the model $\hat{f}$ so that it is consistent with the data, i.e.,

$$\hat{y}^{(i)} = \hat{f}(x^{(i)}), \quad \forall i = 1, \cdots, N$$

For data sample i, our model predicts the value $\hat{y}^{(i)}$, so the prediction error or residual is:

$$r^{(i)} = y^{(i)} - \hat{y}^{(i)}$$

Vector Notation: Outcomes, Predictions, Residuals

We have the following notations.

- Observed Response:

$$y^d = (y^{(1)}, \cdots, y^{(N)})$$

- The prediction:

$$\hat{y}^d = (\hat{y}^{(1)}, \cdots, \hat{y}^{(N)})$$

- The Residuals:

$$r^d = y^{(i)} - \hat{y}^{(i)} = (r^{(1)}, \cdots, r^{(N)})$$

How to know whether the model predicts well?

- Check the norm of r^d

Least Squares Model Fitting

Recall the prediction function:

$$\hat{f}(x) = \theta_1 f_1(x) + \theta_2 f_2(x) + \cdots + \theta_p f_p(x)$$

Write the predicted output for the ith data $x^{(i)}$ as follows:

$$\hat{y}^{(i)} = \hat{f}(x^{(i)})$$

as follows:

$$\begin{aligned} \hat{y}^{(i)} &= A_{i1}\theta_1 + \cdots A_{ip}\theta_p, \quad i = 1, \cdots N,\ j = 1, \cdots, p, \\ A_{ij} &= \hat{f}_j(x^{(i)}), \quad i = 1, \cdots, N, \quad j = 1, \cdots, p \end{aligned}$$

LS Model Fitting: Matrix Vector Notation

We observe:

- Let $\theta = [\theta_1, \theta_2, \cdots, \theta_p]^T$
- The jth column of A is the jth basis function evaluated at data points $x^{(1)}, \cdots, x^{(N)}$
- The i row gives the values of the pth basis functions on the ith data points $x^{(i)}$

In Matrix-Vector Notation:

$$A\theta = \hat{y}^d$$

Here θ is the unknown, and A and $\hat{y}^d$ are given

Least Squares Fitting on the Data set

We wish to minimize the residual, r^d over θ, where

$$\|r^d\|^2 = \|y^d - \hat{y}^d\|^2 = \|y^d - A\theta\|^2 = \|A\theta - y^d\|^2$$

The solution may not exist, as there are more rows then columns, so our best bet is:

$$\min_\theta \|r^d\|^2 = \min_\theta \|A\theta - y^d\|^2$$

- $\|r^d\|$ is called minimum sum square error
- $\|r^d\|/N$ is called minimum mean square error
- Normal Equations Approach: $\hat{\theta} = (A^T A)^{-1} A^T y^d$
- QR Factorization (seen before)

Linear to Non-Linear Models

What are non-linear models?

- Models where prediction function is a non-linear function of parameter (or weights) θ

Examples of non-linear models:

- Most successful non-linear model is Neural Networks

Why Neural Networks are non-linear?

- The prediction function in NN are of the form:

$$\hat{f}(x;\theta) = f_m(\cdots(f_2(f_1(\theta)))\cdots)$$

- Moreover, f_i are non-linear. Hence, $\hat{f}$ cant be written as $A\theta$. It cant be solved using linear system solver!

Eigenvalues and Eigenvectors

$A \in \mathbb{R}^{n\times n}$. A vector $v \in \mathbb{R}^n, v \neq 0$ is called an eigenvector of A, if there exists a $\lambda \in \mathbb{C}$ such that

$$Av = \lambda v$$

Here λ is called the eigenvalue of A

- The pair (λ, v) is called an eigenpair of A
- Each eigenvector has unique eigenvalue associated with it
- Each eigenvalue is associated with many eigenvectors
- Set of all eigenvalues of A is called the spectrum of A

Facts about Eigenvalues and Eigenvectors

- λ is an eigenvalue of A if and only if

$$\det(\lambda I - A) = 0$$

- The above equation is called characteristic equation of A
- Useful theoretical device, but of little value for computing eigenvalues
- Not hard to see that $\det(\lambda I - A) = 0$ is a polynomial of degree n
- Here $\det(\lambda I - A) = 0$ is called characteristic polynomial of A

Computing Eigenvalues and Eigenvectors

- Eigenvalue problem and problem of finding root is equivalent
- (Abel) No general formula for the roots of equation of degree > 4
- Hence no general formula for computing eigenvalues for $n > 4$

Division of numerical methods:

- Direct: Result in finite number of steps. Examples: LU, QR
- Iterative: Produces sequence of approximations towards the required result

Power method and extensions

Assume:

- $A \in \mathbb{R}^{n \times n}$
- A is semi-simple: A has n linearly independent eigenvectors, which forms the basis of $\mathbb{R}^n$
- Eigenvalues are ordered: $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$
- λ_1 is called dominant eigenvalue

Power Method: If A has a dominant eigenvalue, then we can find it and an associated eigenvector.

Power Method: Basic Idea

Idea: Generate the following sequence

$$q, Aq, A^2 q, \cdots$$

Claim: The above sequence converges to largest eigenvector of A regardless of the initial vector q. Why?

Power Method Finds the Largest Eigenvector

Proof: Given a vector q, since $v_1, v_2, \cdots, v_n$ forma a basis for $\mathbb{R}^n$, there exists constants $c_1, \cdots, c_n$ such that

$$q = c_1 v_1 + c_2 v_2 + \cdots + c_n v_n$$

In general c_1 will be non-zero. Multiplying q by A, we have

$$\begin{aligned}
Aq &= c_1 A v_1 + c_2 A v_2 + \cdots + c_n A v_n \\
&= c_1 \lambda_1 v_1 + c_2 \lambda_2 v_2 + \cdots + c_n \lambda_n v_n \\
A^2 q &= c_1 \lambda_1 v_1 + c_2 \lambda_2 v_2 + \cdots + c_n \lambda_n v_n \\
A^j q &= c_1 \lambda_1^j v_1 + c_2 \lambda_2^j v_2 + \cdots + c_n \lambda_n^j v_n \\
&= \lambda_1^j (c_1 v_1 + c_2 (\lambda_2/\lambda_1)^j v_2 + \cdots + c_n (\lambda_n/\lambda_1)^j v_n)
\end{aligned}$$

Second term onwards goes to zero as $j \to \infty$

Power Method Algorithm

Let $q_j = A^j q/\lambda_1^j$, then $q_j \to c_1 v_1$ as $j \to \infty$. We have

$$\begin{aligned}\|q_j - c_1 v_1\| &= \|c_2(\lambda_2/\lambda_1)^j v_2 + \cdots + c_n(\lambda_n/\lambda_1)^j v_n\| \\ &\le |c_2||\lambda_2/\lambda_1|^j \|v_2\| + \cdots + |c_n||\lambda_n/\lambda_1|^j \|v_n\| \\ &\le (|c_2|\|v_2\| + \cdots + |c_n|\|v_n\|)|\lambda_2/\lambda_1|^j\end{aligned}$$

Note: We used $|\lambda_i \le |\lambda_2||, i = 3, \cdots, n$.
Let $C = |c_2|\|v_2\| + \cdots + |c_n|\|v_n\|$, we have

$$\|q_j - c_1 v_1\| \le C|\lambda_2/\lambda_1|^j, \quad j = 1, 2, 3, \ldots$$

Clearly, since, $|\lambda_1| > |\lambda_2|$, it follows that

$$|\lambda_2/\lambda_1| \to 0 \quad \text{as } j \to \infty$$

Algorithm: Power Method

Find largest eigenvector of A

```
Choose a random vector q
for i = 1, ··· , do
    q_{j+1} = Aq_j / ||Aq_j||_∞
    if ||q_{j+1} − q_j|| ≤ tol then
        break
    end if
end for
```

- Flops: $2n^2$ assuming A is not a sparse matrix
- Flops for sparse matrices is considerably less
  - If A has five non-zero entries per row, then cost of Aq_j is only $10n$ Flops

Inverse Iteration and Shift-and-Invert Strategy

Assumption: Let $A \in \mathbb{R}^{n\times n}$ is semisimple with linearly independent eigenvectors $v_1, \cdots, v_n$ and associated eigenvalues $\lambda_1, \cdots, \lambda_n$, arranged in descending order.

Fact 10

If A is non-singular, then all the eigenvalues of A are non-zeros. Show that if v is an eigenvector of A associated with eigenvalue λ, then v is also an eigenvector of A^{-1} associated with eigenvalue λ^{-1}.

Proof in class.

Inverse Iteration

Find smallest eigenvector of A

Key Idea: Smallest eigenvector of A is the largest eigenvector of A^{-1}

1: Choose random vector q, tolerance *tol*
2: **for** $i = 1, 2, \ldots$ **do**
3: $\quad q_{j+1} = A^{-1} q_j / \|Aq_j\|_\infty$
4: **end for**
5: **if** $\|q_{j+1} - q_j\| \leq tol$ **then**
6: $\quad$ break
7: **end if**

- Only change compared to power method is in line 3.

Towards Shift-and-Invert Iteration

Fact 11

Let $\rho \in \mathbb{R}$. Show that v is an eigenvector of A with eigenvalue λ, then v is also an eigenvector of $A - \rho I$ with eigenvalue $\lambda - \rho$.

Proof in class.

Shift-and-Invert Idea

- Let $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_n$ be the eigenvalues of A
- $A - \rho I$ has eigenvalues $\lambda_1 - \rho, \lambda_2 - \rho, \ldots, \lambda_n - \rho$, here ρ is the shift
- To find eigenvector corresponding to eigenvalue λ_i, choose a shift, such that the smallest eigenvalue of $A - \rho I$ is $\lambda_i - \rho$
- Now apply inverse power method to find the smallest eigenvalue $\delta_i = \lambda_i - \rho$ of $A - \rho I$
- The ith eigenvalue λ_i of A is $\delta_i + \rho$
- How to guess ρ?

Rayleigh Quotient Iteration

Idea: Use Rayleigh quotient as a shift for the next iteration.

Choose random vector q
for for $i = 1, \cdots$ **do**
    $\rho_j = \dfrac{q_j^* A q_j}{q_j^* q_j}$
    $(A - \rho_j I)\hat{q}_{j+1} = q_j$
    $q_{j+1} = \sigma_{j+1}^{-1} \hat{q}_{j+1}$
    if $\|q_{j+1} - q_j\| \le tol$ **then**
        break
    end if
end for

- ρ_j is a suitable scaling factor

Computing All Eigenvalues of a Matrix

Fact 12

Two matrices A and B are said to be similar if there exists a nonsingular $S \in \mathbb{R}^{n\times n}$ such that

$$B = S^{-1}AS$$

It is called a similarity transform, and S is called the transforming matrix. It is equivalent to:

$$AS = SB$$

Key Idea: Do a series of similarity transform such that B is a simple matrix, whose eigenvalues can be computed easily

Similar Matrices have Same Eigenvalues

Fact 13

Similar matrices have same eigenvalues.

Proof done in class.

Fact about Similar Matrices

Fact 14

Suppose $B = S^{-1}AS$. Then v is an eigenvector of A with eigenvalue λ if and only if $S^{-1}v$ is an eigenvector of B with associated eigenvalue λ.

Proof done in class.