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Lecture 1 Notes

Matrices, Moments and Quadrature

Bilinear Forms with Matrix Functions

Our goal is to develop methods for approximating expressions of the form

$$\mathbf{u}^T f(A)\mathbf{v}$$

where $\mathbf{u}$ and $\mathbf{v}$ are N-vectors and A is an $N \times N$ symmetric positive definite matrix. It is assumed that the function f is analytic on a domain containing the eigenvalues of A, meaning that it has a convergent Taylor series on such a domain. This problem arises in the following applications, among others:

- error estimation in the conjugate gradient method and least-squares problems
- selection of parameters in regularization of ill-conditioned least-squares problems
- estimation of the trace of the inverse, and the determinant
- approximation of the scattering amplitude
- spectral methods for PDEs

Because A is symmetric positive definite, it has real, positive eigenvalues

$$b = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N = a > 0,$$

and orthonormal eigenvectors $\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_N$ such that

$$A\mathbf{q}_j = \lambda_j \mathbf{q}_j, \quad j = 1, 2, \ldots, N.$$

It follows that we can write this bilinear form as a *Riemann-Stieltjes integral*

$$\begin{aligned}
\mathbf{u}^T f(A)\mathbf{v} &= \mathbf{u}^T f\left(\sum_{j=1}^N \lambda_j \mathbf{q}_j \mathbf{q}_j^T\right)\mathbf{v} \\
&= \sum_{j=1}^N f(\lambda_j)\mathbf{u}^T \mathbf{q}_j \mathbf{q}_j^T \mathbf{v} \\
&= \int_a^b f(\lambda)\, d\alpha(\lambda)
\end{aligned}$$

where the measure $\alpha(\lambda)$ is defined by

$$\alpha(\lambda) = \begin{cases} 0 & \lambda < a \\ \sum_{j=1}^{k} \mathbf{u}^T \mathbf{q}_j \mathbf{q}_j^T \mathbf{v} & \lambda_k \leq \lambda < \lambda_{k+1} \\ \sum_{j=1}^{N} \mathbf{u}^T \mathbf{q}_j \mathbf{q}_j^T \mathbf{v} & \lambda_N \leq b \end{cases}$$

Here we have used the fact that because f is analytic, and because A has the spectral decomposition

$$A = Q\Lambda Q^T, \quad Q = \begin{bmatrix} \mathbf{q}_1 & \cdots & \mathbf{q}_N \end{bmatrix}, \quad \Lambda = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_N \end{bmatrix},$$

we have

$$\begin{aligned} f(A) &= \sum_{k=0}^{\infty} c_k A^k \\ &= \sum_{k=0}^{\infty} c_k (Q\Lambda Q^T)^k \\ &= \sum_{k=0}^{\infty} c_k Q\Lambda^k Q^T \\ &= Q\left[\sum_{k=0}^{\infty} c_k \Lambda^k\right] Q^T \\ &= Qf(\Lambda)Q^T \\ &= \sum_{j=1}^{N} \mathbf{q}_j f(\lambda_j) \mathbf{q}_j^T. \end{aligned}$$

It is worth noting that if $\mathbf{u} = \mathbf{v}$, then the measure $\alpha(\lambda)$ is positive and increasing. For now, we will assume that this is the case.

Gaussian Quadrature

The purpose of expressing $\mathbf{u}^T f(A)\mathbf{u}$ as an integral is to develop approximation techniques based on quadrature. That is, we wish to compute nodes t_j and weights w_j, $j = 1, \ldots, n$, such that

$$\mathbf{u}^T f(A)\mathbf{u} = \int_a^b f(\lambda)\, d\alpha(\lambda) \approx \sum_{j=1}^{n} f(t_j)\, w_j.$$

As a primary goal in the development of any numerical integration technique is to achieve maximal accuracy with minimal computational expense, where such expense is measured in terms of evaluations of the integrand, we wish to choose the nodes and weights so that an accurate approximation can be obtained even if $n \ll N$.

Consider an integral

$$I[f] = \int_a^b f(\lambda)\, d\alpha(\lambda)$$

for a general measure $\alpha(\lambda)$ that is assumed to be positive and increasing. To minimize the number of nodes n, we attempt to choose them so that polynomials of as high a degree as possible can be integrated exactly using the resulting quadrature rule.

To that end, let f be a polynomial of degree m, where $m \geq n$. We approximate $I[f]$ by constructing an interpolating polynomial p_{n-1}, of degree $n-1$, that interpolates f at the n nodes $t_1, t_2, \ldots, t_n$, and then integrate the interpolant exactly. It follows that

$$I[f] = \int_a^b f(\lambda)\, d\alpha(\lambda) \approx \int_a^b p_{n-1}(\lambda)\, d\alpha(\lambda) = \int_a^b \sum_{j=1}^n f(t_j) L_j(\lambda)\, d\alpha(\lambda) = \sum_{j=1}^n f(t_j)\, w_j,$$

where the weights w_j are given by

$$w_j = \int_a^b L_j(\lambda)\, d\alpha(\lambda),$$

and L_j is the jth Lagrange polynomial, of degree $n-1$, corresponding to the node t_j. That is,

$$L_j(t_k) = \delta_{jk}.$$

These are the weights for any *interpolatory* quadrature rule.

The error in this approximation is

$$\int_a^b f(\lambda) - p_{n-1}(\lambda)\, d\alpha(\lambda) = \int_a^b e_n(\lambda)\, d\alpha(\lambda),$$

where e_n is a polynomial of degree m. Because p_{n-1} agrees with f at the nodes $t_1, t_2, \ldots, t_n$, it follows that these are zeros of e_n, which we can then write in factored form

$$e_n(\lambda) = g_n(\lambda) r_{m-n}(\lambda)$$

where

$$g_n(\lambda) = (\lambda - t_1)(\lambda - t_2)\cdots(\lambda - t_n)$$

and r_{m-n} is a polynomial of degree $m-n$. In order to make the error be zero, we need $g_n(\lambda)$ to be *orthogonal* to $r_{m-n}(\lambda)$. That is,

$$\langle g_n, r_{m-n} \rangle = \int_a^b g_n(\lambda) r_{m-n}(\lambda)\, d\alpha(\lambda) = 0.$$

We want this to be true for as many polynomials r_{m-n} as possible, but this can only be assured if the degree of r_{m-n} is strictly less than that of g_n. That is, we must have $m \leq 2n-1$.

Therefore, if we can find a polynomial of degree n that is orthogonal to *all* polynomials of lesser degree, then its roots are the nodes that will allow all polynomials of degree $2n-1$ or less to be integrated exactly using the resulting quadrature rule. Furthermore, because the degree of each Lagrange polynomial L_j is $n-1$, it follows that $L_j(\lambda)^2$ can be integrated exactly using this quadrature rule. Therefore,

$$\int_a^b L_j(\lambda)^2 \, d\alpha(\lambda) = \sum_{k=1}^n L_j(t_k)^2 \, w_k = L_j(t_j)^2 \, w_j = w_j,$$

which means that the weights are positive. This is a *Gaussian* quadratue rule. It has the properties that its nodes have the maximum possible degree of accuracy, and it is robust, due to the positive weights.

Orthogonal Polynomials

It remains to obtain such a polynomial of degree n that is orthogonal to all polynomials of lesser degree. To that end, we assume that we have found a sequence $q_0, q_1, \ldots, q_{j-1}$ of *orthonormal* polynomials, meaning that

$$\langle q_i, q_j \rangle = \delta_{ij}, \quad i, j = 0, 1, \ldots, j-1,$$

where, as before,

$$\langle f, g \rangle = \int_a^b f(\lambda) g(\lambda) \, d\alpha(\lambda).$$

We also assume that for $k = 0, 1, \ldots, j-1$, q_k is of degree k.

To find the next polynomial in the sequence, q_j, we use Gram-Schmidt orthogonalization to orthogonalize $xq_{j-1}(x)$ against $q_0, q_1, \ldots, q_{j-1}$. We obtain

$$p_j(x) = xq_{j-1}(x) - \sum_{k=0}^{j-1} \langle xq_{j-1}, q_k \rangle q_k(x).$$

However, because $\langle xq_{j-1}, q_k \rangle = \langle q_{j-1}, xq_k \rangle$, it follows that $\langle xq_{j-1}, q_k \rangle = 0$ whenever $k+1 < j-1$, or $k < j-2$. Therefore, we have

$$p_j(x) = (x - \alpha_j) q_{j-1}(x) - \beta_{j-1} q_{j-2}(x),$$

where

$$\alpha_j = \langle xq_{j-1}, q_{j-1} \rangle, \quad \beta_j = \langle xq_{j-1}, q_j \rangle, \quad j \geq 1.$$

These numbers are called *recursion coefficients*. We see that orthogonal polynomials can be defined using a *3-term recurrence relation*, which allows them to be computed very efficiently. For this relation to make sense when $j = 1$, we define $q_{-1}(x) \equiv 0$.

The polynomial $p_j(x)$ is orthogonal to $q_0, q_1, \ldots, q_{j-1}$. To normalize it, we set

$$q_j(x) = \frac{p_j(x)}{\langle p_j, p_j \rangle^{1/2}},$$

and our sequence of orthonormal polynomials is extended. However, we note that

$$\begin{aligned}
\beta_j &= \langle x q_{j-1}, q_j \rangle \\
&= \langle p_j + \alpha_j q_{j-1} + \beta_{j-1} q_{j-2}, q_j \rangle \\
&= \langle p_j, q_j \rangle \\
&= \langle p_j, p_j \rangle^{1/2} \langle q_j, q_j \rangle \\
&= \langle p_j, p_j \rangle^{1/2}.
\end{aligned}$$

It follows that $p_j = \beta_j q_j$, and $\beta_j > 0$. For the base case of the induction, we set $p_0(x) = 1$, and define $\beta_0 = \langle p_0, p_0 \rangle^{1/2}$ for consistency with the definition of β_j for $j \geq 1$. Then, our sequence of orthonormal polynomials is begun with $q_0 = p_0/\beta_0$.

The Eigenvalue Connection

Now that we've found a polynomial of degree n that is orthogonal to all polynomials of lesser degree with respect to our chosen inner product, we could simply compute its roots to obtain the Gaussian quadrature nodes. However, it is not practical to accomplish this by using an iterative method such as Newton's method to find each root individually, or by computing the eigenvalues of an associated companion matrix, because these methods are not numerically robust.

As an alternative, we define the n-vector $\mathbf{Q}_n(x)$ by

$$\mathbf{Q}_n(x) = \begin{bmatrix} q_0(x) \\ q_1(x) \\ \vdots \\ q_{n-1}(x) \end{bmatrix}.$$

From the 3-term recurrence relation that defines the polynomials $q_0, q_1, \ldots, q_n$, we obtain

$$x q_{k-1}(x) = \beta_k q_k(x) + \alpha_k q_{k-1}(x) + \beta_{k-1} q_{k-2}(x), \quad k = 1, 2, \ldots, n.$$

Rewriting this system of equations in matrix-vector form yields

$$x\mathbf{Q}_n(x) = J_n \mathbf{Q}_n(x) + \beta_n q_n(x) \mathbf{e}_n,$$

where the tridiagonal *Jacobi matrix* J_n is defined by

$$J_n = \begin{bmatrix} \alpha_1 & \beta_1 & & \\ \beta_1 & \alpha_2 & \ddots & \\ & \ddots & \ddots & \beta_{n-1} \\ & & \beta_{n-1} & \alpha_n \end{bmatrix}.$$

Now, suppose that t_j is a root of $q_n(x)$; that is, $q_n(t_j) = 0$. We then have

$$t_j \mathbf{Q}_n(t_j) = J_n \mathbf{Q}_n(t_j).$$

That is, t_j is an eigenvalue of J_n, and a corresponding eigenvector is $\mathbf{Q}_n(t_j)$. This provides a much more effective method of computing the Gaussian quadrature nodes, because as the eigenvalues of the symmetric matrix J_n, they are guaranteed to be well-conditioned, and they can be computed quite efficiently using the symmetric QR algorithm.

It remains to compute the corresponding weights $w_1, \ldots, w_n$. While these can be obtained from the integrals of the Lagrange polynomials, it can be shown that for $j = 1, 2, \ldots, n$, w_j is equal to the square of β_0 times the first component of the normalized eigenvector of J_n corresponding to t_j.

Roots of Orthogonal Polynomials

The nodes $t_1, \ldots, t_n$ of Gaussian quadrature rule

$$\int_a^b f(\lambda)\, d\alpha(\lambda) \approx \sum_{j=1}^n f(t_j)\, w_j$$

are the roots of a polynomial $q_n(\lambda)$ that is orthogonal to all polynomials of lesser degree with respect to the inner product

$$\langle f, g \rangle = \int_a^b f(\lambda) g(\lambda)\, d\alpha(\lambda).$$

We now prove that these nodes are actually in $[a, b]$, as they should be for any quadrature rule for an integral defined on this interval.

Let $\tau_1, \ldots, \tau_k$ be the points in (a, b) at which $q_n(\lambda)$ changes sign, and let

$$\phi_k(\lambda) = (\lambda - \tau_1) \cdots (\lambda - \tau_k).$$

Then, $\phi_k(\lambda) q_n(\lambda)$ never changes sign on (a, b), and therefore

$$\langle \phi_k, q_n \rangle = \int_a^b \phi_k(\lambda) q_n(\lambda)\, d\alpha(\lambda) \neq 0.$$

We must have $k \leq n$, because a polynomial of degree n cannot change sign more than n times on the entire real line, let alone within (a, b). However, we must also have $k \geq n$, because if $k < n$, then $\langle \phi_k, q_n \rangle = 0$, due to the fact that q_n is orthogonal to any polynomial of degree less than n. We conclude that $k = n$, and that all of the roots of q_n lie within (a, b).

Connection to Hankel Matrices

Given a measure $\alpha(\lambda)$, the *moments* of the measure are the terms of the sequence defined by

$$\mu_k = \int_a^b \lambda^k \, d\alpha(\lambda).$$

If we define the *moment matrix* by

$$M_n = \begin{bmatrix} \mu_0 & \mu_1 & \mu_2 & \cdots & \mu_{n-1} \\ \mu_1 & \mu_2 & & & \mu_n \\ \mu_2 & & & & \vdots \\ \vdots & & & & \vdots \\ \mu_{n-1} & \mu_n & \cdots & \cdots & \mu_{2n-2} \end{bmatrix},$$

then it has been shown that M is positive definite if and only if the sequence $\{\mu_k\}_{k=0}^\infty$ is a sequence of moments corresponding to a positive Borel measure $\alpha(\lambda)$.

The matrix M is a *Hankel matrix*, because its "northeast-to-southwest" diagonals are constant. If it is positive definite, then its Cholesky decomposition can be used to obtain orthonormal polynomials with respect to the associated measure $\alpha(\lambda)$ in terms of the monomial basis.

Derivation of the Lanczos Algorithm

We have described how Jacobi matrices can be used to compute nodes and weights for Gaussian quadrature rules for a general positive, increasing measure $\alpha(\lambda)$, which ensures that the Jacobi matrix J_n is not only symmetric but also positive definite. Now, we consider the case of the specific inner product

$$\langle f, g \rangle = \int_a^b f(\lambda) g(\lambda) \, d\alpha(\lambda) = \mathbf{u}^T f(A) g(A) \mathbf{u},$$

with associated norm

$$\|f\|_\alpha = \langle f, f \rangle^{1/2} = (\mathbf{u}^T f(A)^2 \mathbf{u})^{1/2}.$$

The underlying measure $\alpha(\lambda)$ allows us to represent the quadratic form $\mathbf{u}^T f(A)\mathbf{u}$ as a Riemann-Stieltjes integral that can be approximated via Gaussian quadrature.

We now examine the computation of the required recursion coefficients

$$\alpha_j = \langle x q_{j-1}, q_{j-1} \rangle, \quad \beta_j = \langle p_j, p_j \rangle^{1/2}, \quad j \geq 1.$$

If we define the vectors

$$\mathbf{x}_j = q_{j-1}(A)\mathbf{u}, \quad \mathbf{r}_j = p_j(A)\mathbf{u}, \quad j \geq 1,$$

then it follows that

$$\alpha_j = \mathbf{x}_j^T A \mathbf{x}_j, \quad \beta_j = \|\mathbf{r}_j\|_2.$$

Furthermore,

$$\mathbf{r}_j = p_j(A)\mathbf{u} = (A - \alpha_j I)q_{j-1}(A)\mathbf{u} - \beta_{j-1}q_{j-2}(A)\mathbf{u} = (A - \alpha_j I)\mathbf{x}_j - \beta_{j-1}\mathbf{x}_{j-1}.$$

Putting all of these relations together yields the algorithm

$\mathbf{r}_0 = \mathbf{u}$
$\mathbf{x}_0 = \mathbf{0}$
for $j = 1, 2, \ldots, n$ **do**
    $\beta_{j-1} = \|\mathbf{r}_{j-1}\|_2$
    $\mathbf{x}_j = \mathbf{r}_{j-1}/\beta_{j-1}$
    $\alpha_j = \mathbf{x}_j^T A\mathbf{x}_j$
    $\mathbf{r}_j = (A - \alpha_j I)\mathbf{x}_j - \beta_{j-1}\mathbf{x}_{j-1}$
end

This is precisely the *Lanczos algorithm* that is often used to approximate extremal eigenvalues of A, and is closely related to the conjugate gradient method for solving symmetric positive definite systems. The vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n$ are called the *Lanczos vectors*. The matrix $X_n = \begin{bmatrix} \mathbf{x}_1 & \cdots & \mathbf{x}_n \end{bmatrix}$ satisfies the relations

$$X_n^T X_n = I_n, \quad X_n^T A X_n = J_n.$$

The second relation follows from the above formula for α_j, as well as the relation

$$\beta_j = \langle x q_{j-1}, q_j \rangle = \mathbf{x}_{j-1}^T A\mathbf{x}_j, \quad j \geq 1.$$

From Large to Small Matrix Functions

The Lanczos vectors allow us to express our approximation of the quadratic form $\mathbf{u}^T f(A)\mathbf{u}$, that involves a function of an $N \times N$ matrix, in terms of a function of an $n \times n$ matrix. We have

$$\begin{aligned}
\mathbf{u}^T f(A)\mathbf{u} &= (\beta_0\mathbf{x}_1)^T f(A)(\beta_0\mathbf{x}_1) \\
&= \beta_0^2 (X_n\mathbf{e}_1)^T f(A)(X_n\mathbf{e}_1) \\
&= \langle p_0, p_0 \rangle \mathbf{e}_1^T X_n^T f(A) X_n \mathbf{e}_1 \\
&\approx \langle 1, 1 \rangle \mathbf{e}_1^T f(X_n^T A X_n)\mathbf{e}_1 \\
&\approx \mathbf{u}^T\mathbf{u}\mathbf{e}_1^T f(J_n)\mathbf{e}_1 \\
&\approx \|\mathbf{u}\|_2^2 [f(J_n)]_{11}.
\end{aligned}$$

It follows that if the particular function f is conducive to computing the $(1, 1)$ entry of a tridiagonal matrix efficiently, then there is no need to compute the nodes and weights for Gaussian quadrature explicitly.

Now, suppose that J_n has the spectral decomposition

$$J_n = U_n \Lambda_n U_n^T,$$

where U_n is an orthogonal matrix whose columns are the eigenvectors of J_n, and Λ_n is a diagonal matrix that contains the eigenvalues. Then we have

$$\begin{aligned}
\mathbf{u}^T f(A)\mathbf{u} &\approx \|\mathbf{u}\|_2^2 \mathbf{e}_1^T f(U_n \Lambda_n U_n^T)\mathbf{e}_1 \\
&\approx \|\mathbf{u}\|_2^2 \mathbf{e}_1^T U_n f(\Lambda_n) U_n^T \mathbf{e}_1 \\
&\approx \|\mathbf{u}\|_2^2 \sum_{j=1}^n f(t_j) u_{1j}^2 \\
&\approx \sum_{j=1}^n f(t_j)\, w_j.
\end{aligned}$$

Thus we have recovered the relationship between the quadrature weights and the eigenvectors of J_n.