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ANALYTIC FUNCTIONAL CALCULUS

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1. The spectral projection theorem. Functional calculus

1.1. The spectral projection theorem for self-adjoint matrices.

Let $A \in \mathcal{M}_n$, $A = A^*$. Then there is a unitary matrix U so that $U^*AU = \Lambda =$ a diagonal matrix with real entries. Write

$$\Lambda = \begin{bmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_n \end{bmatrix}$$

$$= \lambda_1 \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{bmatrix} + \lambda_2 \begin{bmatrix} 0 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{bmatrix} + \dots + \lambda_n \begin{bmatrix} 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{bmatrix}$$

$$\equiv \lambda_1 E_1 + \lambda_2 E_2 + \dots + \lambda_n E_n = \sum_{j=1}^n \lambda_j E_j$$

Then

$$A = U\Lambda U^* = U \left(\sum_{j=1}^n \lambda_j E_j \right) U^* = \sum_{j=1}^n \lambda_j \left(U E_j U^* \right) \equiv \sum_{j=1}^n \lambda_j P_j$$

where $P_j = UE_jU^* = \mathbf{u}_j\mathbf{u}_j^*$ is the orthogonal projection on (the span of) $\mathbf{u}_j$ (recall that if M is a matrix with orthonormal columns then MM^* is the orthogonal projection onto $\mathcal{R}(M)$). Therefore

$$A = \sum_{j=1}^n \lambda_j P_j, \text{ where } P_j = \mathbf{u}_j\mathbf{u}_j^* \tag{1}$$

where $\{\mathbf{u}_1, \dots, \mathbf{u}_n\}$ is an orthonormal set of eigenvectors of A.

Note that since $\sum_{j=1}^n E_j = I$ then also $\sum_{j=1}^n P_j = I$.

1.1.1. *Commuting normal operators.*

Recall:

Theorem 1. *Consider two square matrices A, B which are diagonalizable.*

Then $AB = BA$ if and only if they have a common set of independent eigenvectors (i.e. are diagonalizable by conjugation with the same matrix S, in other words, are simultaneously diagonalizable).

In particular:

Theorem 2. *Let A and B be normal. They commute, $AB = BA$, if and only if they have a common spectral resolution, that is, there are orthogonal projections P_j so that*

$$A = \sum_{j=1}^n \alpha_j P_j \quad \text{and} \quad B = \sum_{j=1}^n \beta_j P_j$$

where $\sigma(A) = \{\alpha_1, \dots, \alpha_n\},\ \sigma(B) = \{\beta_1, \dots, \beta_n\}$.

1.1.2. *Spectral Projections.* When we only care about about the location of the eigenvalues, and not about their multiplicity, we talk about:

Definition 3. *The* **spectrum** *of a matrix M is the set of all its eigenvalues:*

$$\sigma(M) = \{\lambda \,|\, \lambda \text{ is an eigenvalue of } M\}$$

Formula (1) is not very satisfactory when there are repeated eigenvalues. If, say, $\lambda_1 = \lambda_2 = \lambda_3$, then the 3 corresponding orthonormal eigenvectors $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3$ can be chosen otherwise arbitrarily in the 3-dimensional eigenspace $V_{\lambda_1} = V_{\lambda_2} = V_{\lambda_3}$. To eliminate this arbitrary choice, it is preferable to combine $\lambda_1 P_1 + \lambda_2 P_2 + \lambda_3 P_3 = \lambda_1(P_1 + P_2 + P_3)$ where $P_1 + P_2 + P_3$ is the orthogonal projection matrix on the 3-dimensional eigenspace V_{λ_1}. With this recombination of terms for all the repeated eigenvalues we can restate the decomposition (1) in the following canonical form:

Theorem 4. The spectral decomposition of self-adjoint matrices
If $A \in \mathcal{M}_n$ is a self-adjoint matrix, $A = A^*$ then

$$A = \sum_{\lambda \in \sigma(A)} \lambda \, P_\lambda \tag{2}$$

where P_λ is the orthogonal projection matrix onto the eigenspace V_λ.

The **spectral projections** *P_λ satisfy the* **resolution of the identity***:*

$$\sum_{\lambda \in \sigma(A)} P_\lambda = I \tag{3}$$

Theorem 4 states that a self-adjoint matrix can be decomposed as a linear combination of projection matrices P_λ onto its eigenspaces, with coefficients equal to the corresponding eigenvalue.

1.1.3. *Algebraic properties of the spectral projections.* It is relatively easy to work algebraically with the the spectral decomposition using (3) and the following two properties.

Property 1. Since $V_\lambda \perp V_{\lambda'}$ for $\lambda \neq \lambda'$ then

$$P_\lambda P_{\lambda'} = 0 \quad \text{for } \lambda \neq \lambda' \tag{4}$$

Why: Geometrically this is clear; for an algebraic argument: for any $\mathbf{x}$ we have $P_\lambda \mathbf{x} \in V_\lambda \subset V_{\lambda'}^\perp$ therefore $P_{\lambda'}(P_\lambda \mathbf{x}) = \mathbf{0}$. $\Box$

Note that, as a consequence, all the spectral projections of a given matrix commute.

Property 2. The spectral projectors satisfy $P_\lambda^2 = P_\lambda$, and, therefore, moreover,

$$P_\lambda^k = P_\lambda \text{ for all } k \in \mathbb{Z}_+ \tag{5}$$

1.1.4. *Polynomial functional calculus.* Recall that for a polynomial $f(t) = a_N t^N + a_{N-1} t^{N-1} + \ldots + a_1 t + a_0$ we can define $f(A) = a_N A^N + a_{N-1} A^{N-1} + \ldots + a_1 A + a_0 I$ and if $A = U\Lambda U^*$ then $f(A) = U f(\Lambda) U^*$ where $f(\Lambda)$ is the diagonal matrix with the eigenvalues $f(\lambda_1), \ldots, f(\lambda_n)$ of $f(A)$ on the diagonal.

These facts are formulated in terms of spectral decomposition in Theorem 5, which simply states that $f(A)$ has the same eigenspaces V_λ as A, and the corresponding eigenvalues are $f(\lambda)$:

Theorem 5. Polynomial functional calculus

Let A be a self-adjoint matrix with spectral decomposition (2).

If $f(t)$ is a polynomial

$$f(t) = \sum_{k=0}^{N} a_k t^k \tag{6}$$

then $f(A)$ defined by

$$f(A) = \sum_{k=0}^{N} a_k A^k$$

has the spectral decomposition

$$f(A) = \sum_{\lambda \in \sigma(A)} f(\lambda)\, P_\lambda$$

Proof:

The proof was given in the paragraph before the statement of the theorem, by diagonalizing A.

It is instructive however to see another proof, which relies on algebraic calculations using only the properties in §1.1.3. Using them, a straightforward calculation gives

$$A^2 = \left(\sum_{\lambda \in \sigma(A)} \lambda\, P_\lambda \right) \left(\sum_{\lambda' \in \sigma(A)} \lambda'\, P_{\lambda'} \right) = \sum_{\lambda, \lambda' \in \sigma(A)} \lambda \lambda'\, P_\lambda P_{\lambda'} = \sum_{\lambda \in \sigma(A)} \lambda^2\, P_\lambda$$

and similarly (or by induction),

$$A^k = \sum_{\lambda \in \sigma(A)} \lambda^k\, P_\lambda \quad \text{for all } k \in \mathbb{Z}_+$$

For $f(t)$ given by (6) it follows that

$$f(A) = \sum_{k=0}^{N} a_k A^k = \sum_{k=0}^{N} a_k \sum_{\lambda \in \sigma(A)} \lambda^k\, P_\lambda = \sum_{\lambda \in \sigma(A)} \sum_{k=0}^{N} a_k \lambda^k P_\lambda = \sum_{\lambda \in \sigma(A)} f(\lambda)\, P_\lambda$$

which (re)proves the theorem. $\square$

1.1.5. *Analytic functional calculus (part I).* It is possible (and desirable) to define more general functions of matrices, just like the already defined exponential of a matrix.

A definition is useful at this point: the maximal absolute value of the eigenvalues of A is called the spectral radius of A:

Definition 6. *For any n-dimensional matrix M its* **spectral radius** *is the nonnegative number*

$$\rho(M) = \sup_{\lambda\in\sigma(M)} |\lambda|$$

Theorem 7. Analytic functional calculus theorem for self-adjoint matrices

Let A be a self-adjoint matrix with spectral decomposition (2).

Let $f(t)$ be an analytic function given by its Taylor series at 0:

$$f(t) = \sum_{k=0}^{\infty} a_k t^k \qquad \text{with radius of convergence greater than } \rho(A) \tag{7}$$

Then

$$f(A) = \sum_{\lambda\in\sigma(A)} f(\lambda)\, P_\lambda \tag{8}$$

Proof:

A straightforward proof can be given very similarly to the one used to define the exponential of a matrix. A self-contained and rigorous argument is as follows.

It is known that the partial sums $f^{[N]}(t) = \sum_{k=0}^{N} a_k t^k$ of the convergent power series (7) converge absolutely to the limit $f(t)$ for all t. Then by Theorem 5

$$f^{[N]}(A) = \sum_{\lambda\in\sigma(A)} f^{[N]}(\lambda)\, P_\lambda$$

converges to (8), entry by entry. $\square$

Remark. Note that in above the proof it is essential that the radius of convergence of the power series be larger than $\rho(A)$. We will soon see that this is not necessary, as it is apparent that only the values $f(\lambda)$ for $\lambda \in \sigma(A)$ are necessary in (8).

Example: the exponential of a self-adjoint matrix A has the spectral decomposition

$$e^A = \sum_{\lambda\in\sigma(A)} e^\lambda\, P_\lambda$$

1.2. **The spectral projection theorem and functional calculus for normal matrices.** All the results of §1.2 hold for normal matrices, the *only difference* being that the spectrum of a normal matrix is complex, not necessarily real.

2. Analytic functional calculus

2.1. **The resolvent matrix.**

The resolvent matrix appears in many applications (for example in solving differential equations) and is a building block for extending functional calculus to more general functions.

Definition 8. *Given a square matrix M its* **resolvent** *is the matrix-valued function $R_M(z) = (zI - M)^{-1}$, defined for all $z \in \mathbb{C} \setminus \sigma(M)$.*

In infinite dimensions the resolvent is also called *the Green's function.*

Note that the resolvent of A is simply is $f(A)$ for $f(t) = (z-t)^{-1}$, which has the power series

$$\frac{1}{z-t} = \frac{1}{z}\,\frac{1}{1-\frac{t}{z}} = \frac{1}{z}\sum_{k=0}^{\infty}\frac{t^k}{z^k} \quad \text{for } |t| < |z|$$

having radius of convergence $|z|$. On the other hand, $(zI - A)^{-1}$ exists for all $z \in \mathbb{C} \setminus \sigma(A)$.

The spectral decomposition of the resolvent $R_M(z)$ is as expected:

Theorem 9. Spectral decomposition of the resolvent

Let A be a self-adjoint matrix, $A = A^*$ with spectral decomposition (2). Then

$$(zI - A)^{-1} = \sum_{\lambda \in \sigma(A)} \frac{1}{z-\lambda} P_\lambda, \quad \text{for all } z \in \mathbb{C} \setminus \sigma(A) \tag{9}$$

For numbers z with $\rho(A) < |z|$ the result follows from Theorem 7. But Theorem 9 states the result for any number z for which all $(z - \lambda_j)^{-1}$ are defined: it is a stronger result.

Proof:

The matrix $z - A$ is normal (it is self-adjoint only for $z \in \mathbb{R}$), and so is $(z - A)^{-1}$ for $z \notin \sigma(A)$. It can be easily checked that A, $z - A$, $(z - A)^{-1}$ commute and therefore they diagonalize simultaneously, by Theorem 2 of §1.1. (In fact it can be easily checked directly that if λ is an eigenvalue of A with eigenvector $\mathbf{v}$ then $z - \lambda$ is an eigenvalue of $z - A$ with the same eigenvector $\mathbf{v}$, and $(z-\lambda)^{-1}$ is an eigenvalue of $(z-A)^{-1}$ corresponding also to $\mathbf{v}$.)

Therefore A, $z-A$ and $(z-A)^{-1}$ have the same eigenspaces (the spectral projector P_λ of A equals the spectral projector $P_{(z-\lambda)^{-1}}$ of $(z - A)^{-1}$), and therefore spectral decomposition of $(z - A)^{-1}$ is (9). $\square$

2.2. **Motivation for a more general analytic functional calculus.**

The condition on the radius of convergence in (7) is too strong, and more general functions of matrices are needed in many applications. For example, if a matrix A has positive eigenvalues, then we would expect to be able to define $\ln A$ and $\sqrt{A}$, even if the functions $\ln t$ and $\sqrt{t}$ do not have Taylor series at $x = 0$.

And indeed, many analytic function of matrices can be defined using the resolvent combine with the Cauchy's integral formula.

2.3. **A brief review of functions of one complex variable.** A sequence of complex numbers $z_n = x_n + iy_n$ is said to converge to $z = x + iy$ if the sequence of real numbers $|z_n - z|$ converges to zero. Note that this is the same as the sequence of points in the plane $(x_n, y_n) \in \mathbb{R}^2$ converges to the point (x, y): if the distance between them goes to zero.

Power series are defined using complex numbers just as they are defined for real numbers: a power series at $z = z_0$ is a series of the form

$$\sum_{k=0}^{\infty} a_k (z - z_0)^k \tag{10}$$

where $a_k, z_0 \in \mathbb{C}$ and z is a complex variable.

We are interested in the values of z for which the series (10) converges *absolutely*, by which we mean that the series of nonnegative (real) numbers

$$S(z) = \sum_{k=0}^{\infty} |a_k|\, |z - z_0|^k \tag{11}$$

converges.

The series (11) is a series of nonnegative numbers; it can be shown that if (11) converges then (10) (with a proof essentially the same as for series of real numbers).

Recall that there are three cases:
(i) $S(z)$ converges only for $z = z_0$ and diverges for all other z.
(ii) $S(z)$ converges for all $z \in \mathbb{C}$.
(iii) $S(z)$ converges for some $z \neq z_0$ but not for all z. In this case it can be shown that the series converges for all z in a disk $\{z \in \mathbb{C} \,|\, |z - z_0| < r\}$. If r is the largest such number, r is called the *radius of convergence* of (10).

In case (i) we say that (10) is divergent (and write $r = 0$).

In the other cases we say that the series converges. In case (ii) we conventionally write $r = \infty$.

It can be shown that if r is the radius of convergence, then for some z on the circle $\{z \in \mathbb{C} \,|\, |z - z_0| = r\}$ the series (10) diverges.

Examples.

1. The geometric series $\sum_{k=0}^{\infty} z^k$ has radius of convergence $r = 1$. It converges absolutely for all $z \in \mathbb{C}$ with $|z| < 1$. Its sum, for $|z| < 1$, is the function $\frac{1}{1-z}$ which is not defined at $z = 1$.

2. The geometric series $\sum_{k=0}^{\infty} (-1)^k z^{2k}$ also has radius of convergence $r = 1$. Its sum, for $|z| < 1$, is the function $\frac{1}{1+z^2}$ which is not defined at $z = \pm i$. The function $\frac{1}{1+z^2}$ is defined for all real numbers z, and the reason for which its Maclaurin series has radius of convergence of only 1 is revealed only if we look in the complex plane!

Power series (10) can be differentiated or integrated term-by-term for $z \in \mathbb{C}$ inside the circle of convergence, obtaining series *with the same radius of convergence*:

Theorem 10. *If the radius of convergence of (10) is $r > 0$ then for all $z \in \mathbb{C}$ with $|z - z_0| < r$ we have*

$$\frac{d}{dz} \sum_{k=0}^{\infty} a_k (z - z_0)^k = \sum_{k=0}^{\infty} a_k \, k \, (z - z_0)^{k-1}$$

and

$$\int_{z_0}^{z} \sum_{k=0}^{\infty} a_k (s - z_0)^k \, ds = \sum_{k=0}^{\infty} a_k \frac{1}{k+1} (z - z_0)^{k+1}$$

and both series converge also for $|z - z_0| < r$.

Definition 11. *A function $f : D \to \mathbb{C}$ is called* **analytic** *(or* **holomorphic***) on the domain $D \subset \mathbb{C}$ if for all $z_0 \in D$ $f(z)$ it is the sum of a convergent power series at z_0:*

$$f(z) = \sum_{k=0}^{\infty} a_k (z - z_0)^k \quad \text{with a nonzero radius of convergence} \tag{12}$$

The power series (12) turns out to be the Taylor expansion of $f(z)$ at $z = z_0$:

$$a_k = \frac{1}{k!} \, f^{(k)}(z_0)$$

In particular, an analytic function on D is infinitely many times differentiable at all points of D.

Throughout this section γ will denote *a piecewise smooth closed curve.*

Recall the following result on real vector fields in the plane: suppose a planar vector field is conservative (or, irrotational) on a *simply connected* (i.e. "without holes") domain. Then its integral along a closed curve is zero.

This result can be reformulated in terms of analytic functions (a bit of work is needed), yielding one of the most powerful results for analytic functions:

Theorem 12. Cauchy's integral theorem

Let f is analytic on a simply connected domain D. Then

$$\oint_{\gamma} f(\zeta) \, d\zeta = 0$$

for any γ in D.

From this it is not hard to obtain another central result:

Theorem 13. Cauchy's integral formula
Let f be analytic in a simply connected domain D.
If γ is any closed curve in D, with no self-intersections, then

$$f(z) = \frac{1}{2\pi i} \oint_\gamma \frac{f(\zeta)}{\zeta - z}\, d\zeta \quad \text{for all } z \text{ inside } \gamma \tag{13}$$

where γ is oriented counterclockwise.

Cauchy's integral formula recovers the values of the analytic function *inside* the curve γ from its values on γ! Analytic functions are very special.
It should also be noted that

$$0 = \oint_\gamma \frac{f(\zeta)}{\zeta - z}\, d\zeta \quad \text{for all } z \in D,\ z \text{ outside } \gamma$$

Note that that if γ_1 and γ_2 are two closed curves encircling z, then the values of the two corresponding integrals in (13) are equal.

2.4. **Analytic functions of matrices.** Assume that A is a self-adjoint (or normal) matrix. In view of (8) and (9) it is reasonable to be expect that if an analytic function f is defined at all the eigenvalues of A, then we could define $f(A)$.
Indeed, let f be an analytic function on a domain D which includes $\sigma(A)$.
Formula (13) suggests the following definition for $f(A)$:

$$f(A) = \frac{1}{2\pi i} \oint_\gamma f(\zeta)(\zeta - A)^{-1}\, d\zeta \tag{14}$$

where $(\zeta - A)^{-1}$ is the resolvent of A. Formula (14) clearly makes sense for γ a closed curve in $D \setminus \sigma(A)$ (i.e. γ must avoid the eigenvalues of A).
If A has the spectral decomposition (2), then from (9)

$$f(A) = \frac{1}{2\pi i} \oint_\gamma f(\zeta) \left(\sum_{\lambda \in \sigma(A)} \frac{1}{z - \lambda} P_\lambda \right) d\zeta$$

$$= \sum_{\lambda \in \sigma(A)} \left(\frac{1}{2\pi i} \oint_\gamma \frac{f(\zeta)}{\zeta - \lambda}\, d\zeta \right) P_\lambda \tag{15}$$

If an eigenvalue λ is inside the curve γ then

$$\frac{1}{2\pi i} \oint_\gamma \frac{f(\zeta)}{\zeta - \lambda}\, d\zeta = f(\lambda)$$

while if λ is *not* inside the curve γ, then the integral is zero.
Assuming that all eigenvalues are inside γ (γ must contain $\sigma(A)$ in its interior) the sum in (15) becomes

$$f(A) = \sum_{\lambda \in \sigma(A)} f(\lambda)\, P_\lambda \quad \text{for any } f \text{ analytic in a neighborhood of } \sigma(A)$$

Note that:
1. $f(A)$ is a normal matrix (it is self-adjoint if all $f(\lambda) \in \mathbb{R}$),
2. $f(A)$ has the same eigenvectors as A, hence it commutes with A, and
3. the eigenvalues of $f(A)$ are $f(\lambda)$ where λ are the eigenvalues of A.

A few applications.

1. *The logarithm* $\ln A$.

Recall that, as a function of a real variable, $\ln t$ is defined for all $t > 0$. Moreover, it is an analytic function since it has a convergent Taylor series at any point $a > 0$:

$$\ln t = \ln(a) + \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k\, a^k}\,(t-a)^k \quad \text{for } |t-a| < a$$

which has radius of convergence a.

In fact, the same series converges for any $t \in \mathbb{C}$ with $|t-a| < a$, defining the logarithm for complex numbers. Moreover, $a \neq 0$ can be any complex number. (*Caution:* the logarithm cannot be defined on a domain in the complex plane which contains the origin.)

Assuming that A is a self-adjoint matrix with all eigenvalues $\lambda_j > 0$, can we define $\ln A$? In other words, is there a matrix B (self-adjoint, perhaps) so that $e^B = A$? Yes: since the eigenvalues of A are strictly positive, the logarithm is analytic at all eigenvalues of A, therefore $\ln A$ is defined, and

$$\ln A = \sum_{\lambda \in \sigma(A)} \ln(\lambda)\ P_\lambda$$

2. *The radical* $\sqrt{A}$.

Similarly, if A has positive eigenvalues we can define its radical:

$$\sqrt{A} = \sum_{\lambda \in \sigma(A)} \sqrt{\lambda}\, P_\lambda \tag{16}$$

which is a matrix $B = \sqrt{A}$ with nonnegative eigenvalues so that $B^2 = A$. Note that there are many other matrices B so that $B^2 = A$ (having some negative eigenvalues).