LECTURE 17: SPECTRAL APPROXIMATIONS

1. Trigonometric basis

The monomial basis $\{1, t, t^2, \ldots\}$ for the vector space of all polynomials $P(\mathbb{R})$, and its derivatives (Lagrange, Newton, $B-$spline) allow the definition of an approximant $p \in P(\mathbb{R})$ for real functions $f: \mathbb{R} \to \mathbb{R}$, e.g., for smooth functions $f \in C^\infty(\mathbb{R})$. A different approach to approximation in infinite-dimensional vector spaces such as $P(\mathbb{R})$ or $C^\infty(\mathbb{R})$ is to endow the vector space with a scalar product (f, g) and associated norm $\|f\| = (f, f)^{1/2}$. The availability of a norm allows definition of convergence of sequences and series.

DEFINITION. *A sequence $\{f_n\}_{n \in \mathbb{N}}$ of elements of the normed vector space $\mathcal{F} = (F, \mathbb{C}, +, \cdot)$ converges to f, $f_n \to f$ if $\forall \varepsilon > 0$, $\exists N(\varepsilon)$ such that $\|f_n - f\| < \varepsilon$ for all $n > N(\varepsilon)$.*

DEFINITION. *The vector space $\mathcal{F} = (F, \mathbb{C}, +, \cdot)$ with a scalar product $(,): F \times F \to \mathbb{C}$ is a Hilbert space if the limit of all Cauchy sequences is an element of F.*

All Hilbert spaces have orthonormal bases, and of special interest are bases that arise Sturm-Liouville problems of relevance to the approximation task.

1.1. Fourier series - Fast Fourier transform

The $L^2([0, 2\pi])$ space of periodic, square-integrable functions is a Hilbert space (L^2 is the only Hilbert space among the L^p function spaces), and has a basis

$$\left\{\frac{1}{2}, \cos t, \sin t, \ldots, \cos kt, \sin kt, \ldots\right\}$$

that is orthonormal with respect to the scalar product

$$(f, g) = \frac{1}{\pi} \int_0^{2\pi} f(t)\, \overline{g(t)}\, \mathrm{d}t.$$

An element $f \in L^2([0, 2\pi])$ can be expressed as the linear combination

$$f(t) = \frac{a_0}{2} + \sum_{k=1}^{\infty} [a_k \cos kt + b_k \sin kt].$$

An alternative orthonormal basis is formed by the exponentials

$$\{e^{\pm int}\}, n \in \mathbb{N},$$

with respect to the scalar product

$$(f, g) = \frac{1}{2\pi} \int_0^{2\pi} f(t)\, \overline{g(t)}\, \mathrm{d}t.$$

The partial sum

$$S_N f(t) = \sum_{k=-N}^{N} c_k e^{ikt}$$

has coefficients c_k determined by projection

$$c_k = (f, e^{ikt}) = \frac{1}{2\pi} \int_0^{2\pi} f(t)\, e^{-ikt}\, \mathrm{d}t,$$

that can be approximated by the Darboux sum on the partition $t_j = 2\pi j / N$

$$c_k \cong \frac{1}{N} \sum_{j=1}^{N} f_j\, e^{-ikt_j} = \frac{1}{N} \sum_{j=1}^{N} f_j\, \omega_N^{-jk}$$

with

$$\omega = \exp\left[\frac{2\pi i}{N}\right],$$

denoting the N^{th} root of unity. The Fourier coefficients are obtained through a linear mapping

$$\boldsymbol{c} = \boldsymbol{W} \boldsymbol{f},$$

with $\boldsymbol{c}, \boldsymbol{f} \in \mathbb{C}^N$, and $\boldsymbol{W} \in \mathbb{C}^{N \times N}$ with elements

$$\boldsymbol{W} = [\omega^{-jk}]_{1 \leqslant j,k \leqslant N}.$$

The above discrete Fourier transform can be seen as a change of basis from the basis $\boldsymbol{I}$ in which the coefficients of f are $\boldsymbol{c}$ to the basis $\boldsymbol{W}$ in which the coefficients are $\boldsymbol{f}$.

1.2. Fast Fourier transform

Carrying out the matrix vector product $\boldsymbol{W}\boldsymbol{f}$ directly would require $\mathcal{O}(N^2)$ operations, but the cyclic structure of the $\boldsymbol{W}$ matrix arising from the exponentiation of ω can be exploited to reduce the computational effort. Assume $N = 2P$ and separate even and odd indexed components of $\boldsymbol{f}$

$$c_k = \sum_{j=1}^{N} f_j \,\omega_N^{-jk} = \sum_{j=1}^{P} \left[f_{2j-1}\,\omega_N^{-(2j-1)k} + f_{2j}\,\omega_N^{-2jk} \right] = \sum_{j=1}^{P} f_{2j}\,\omega_P^{-jk} + \omega^k \sum_{j=1}^{P} f_{2j-1}\,\omega_P^{-jk}.$$

Through the above, the $\mathcal{O}(N^2)$ matrix-vector product is reduced to two smaller matrix-vector products, each requiring $\mathcal{O}(N^2/4)$ operations. For $N = 2^q$, recursion of the above procedure reduces the overall operation count to $\mathcal{O}(qN)$, or in general for N composed of a small numer of prime factors, $\mathcal{O}(N \log N)$. The overall algorithm is known as the fast Fourier transform or FFT.

1.3. Data-sparse matrices from Sturm-Liouville problems

One step of the FFT can be understood as a special matrix factorization

$$\boldsymbol{W}_N = \begin{bmatrix} \boldsymbol{I} & \boldsymbol{D}_N \\ \boldsymbol{I} & -\boldsymbol{D}_N \end{bmatrix} \begin{bmatrix} \boldsymbol{W}_P & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{W}_P \end{bmatrix} \boldsymbol{P}_N$$

where $\boldsymbol{D}_N$ is diagonal and $\boldsymbol{P}_N$ is the even-odd permutation matrix. Though the matrix $\boldsymbol{W}_N$ is full (all elements are non-zero), its factors are sparse, with many zero elements. The matrix $\boldsymbol{W}_N$ is said to be *data sparse*, in the sense that its specification requires many fewer than N^2 numbers. Other examples of data sparse matrices include:

Toeplitz matrices. $\boldsymbol{A} \in \mathbb{C}^{m \times m}$ has constant diagonal terms, e.g., for $m = 4$

$$\boldsymbol{A} = \begin{bmatrix} a & b & c & d \\ e & a & b & c \\ f & e & a & b \\ g & f & e & a \end{bmatrix},$$

or in general the elements of $\boldsymbol{A} = [a_{ij}]_{1 \leqslant i,j \leqslant m}$ can be specified in terms of $2m - 1$ numbers $a_{1-n}, \ldots, a_{n-1}$ through $a_{ij} = a_{i-j}$.

Exterior products. Rank-1 updates arising in the singular value or eigenvalue decompositions have the form

$$\boldsymbol{A} = \boldsymbol{u}\boldsymbol{v}^T = [\, v_1\boldsymbol{u} \;\; v_2\boldsymbol{u} \;\; \ldots \;\; v_m\boldsymbol{u} \,],$$

and the $2m$ components of $\boldsymbol{u}, \boldsymbol{v}$ are suficient to specify the matrix $\boldsymbol{A}$ with m^2 components. This can be generalized to any exterior product of matrices $\boldsymbol{B} \in \mathbb{C}^{n \times n}$, $\boldsymbol{C} \in \mathbb{C}^{p \times p}$ through

$$\boldsymbol{A} = \boldsymbol{B} \otimes \boldsymbol{C} = [\, \boldsymbol{b}_1 \otimes \boldsymbol{C} \;\; \boldsymbol{b}_2 \otimes \boldsymbol{C} \;\; \ldots \;\; b_n \otimes \boldsymbol{C} \,] = \begin{bmatrix} b_{11}\boldsymbol{C} & b_{12}\boldsymbol{C} & \ldots & b_{1n}\boldsymbol{C} \\ b_{21}\boldsymbol{C} & b_{22}\boldsymbol{C} & \ldots & b_{2n}\boldsymbol{C} \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1}\boldsymbol{C} & b_{n2}\boldsymbol{C} & \ldots & b_{nn}\boldsymbol{C} \end{bmatrix}.$$

The $m^2 = (np)^2$ components of $\boldsymbol{A}$ are specified through only $n^2 + p^2$ components of $\boldsymbol{B}, \boldsymbol{C}$.

The relevance to approximation of functions typically arises due basis sets that are solutions to Sturm-Liouville problems. In the case of the Fourier transform $e^{\pm ikt}$ are eigenfunctions of the Sturm-Liouville problem

$$w'' + \lambda w = 0, w = u + iv, u'(0) = u'(\pi) = 0, v(0) = v(\pi) = 0,$$

with eigenvalues $\lambda_n = k^2$. The solution set $\{\varphi_1, \varphi_2, \ldots\}$ to a general Sturm-Liouville problem to find $f\colon [a,b] \to \mathbb{R}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[p(t)\frac{\mathrm{d}f}{\mathrm{d}t}\right] + q(t)\,f = -\lambda\,w(t)\,f,$$

form an orthonormal basis under the scalar product

$$(f,g) = \int_a^b f(t)\,g(t)\,w(t)\,\mathrm{d}t,$$

and approximations of the form

$$\Phi_N f(t) = \sum_{k=1}^{N} c_k\,\varphi_k(t),$$

and Parseval's theorem states that

$$\|\boldsymbol{c}\|_2^2 = \sum_{k=1}^{\infty} c_k\,\bar{c_k} = \|f\|_2^2 = (f,f) = \int_a^b f(t)\,f(t)\,w(t)\,\mathrm{d}t,$$

read as an equality between the energy of f and that of $\boldsymbol{c}$. By analogy to the finite-dimensional case, the Fourier transform is unitary in that it preserves lengths in the $\|f\| + (f,f)^{1/2}$ norm with weight function $w(t) = 1$.

2. Wavelet approximations

The bases $\{\varphi_1, \varphi_2, \ldots\}$ arising from Sturm-Liouville problems are single-indexed, giving functions of increasing resolution over the entire definition domain. For example $\sin kx$ resolves ever finer features over $[0, 2\pi]$. When applied to a function with localized features, k must be increased with increased resolution in the entire $[0, 2\pi]$ domain. This leads to uneconomical approximation series $S_N f(t)$ with many terms, as exemplified by the Gibbs phenomenon in approximation of a step function, $f(t) = H(t - \pi/2) - H(t - 3\pi/2)$ for $t \in [0, 2\pi]$, and $f(t + 2\pi) = f(t)$. The approach can be represented as the decomposition of a space of functions by the direct sum

$$F = \Phi_1 \oplus \Phi_2 \oplus \ldots,$$

with $\Phi_k = \mathrm{span}(\varphi_k)$, for example

$$L^2 = E_0 \oplus E_1 \oplus E_{-1} \oplus E_2 \oplus E_{-2} \oplus \ldots,$$

with $E_k = \mathrm{span}\{e^{ikt}\}$ for the Fourier series.

Approximation of functions with localized features is more efficiently accomplished by choosing some generating function $\psi(t)$ and then defining a set of functions through translation and scaling, say

$$\psi_{jk}(t) = 2^{-j/2}\,\psi(2^{-j}t - k).$$

Such systems are known as *wavelets*, and the simplest example is the step function

$$\psi(t) = \begin{cases} 1 & 0 \leqslant t < 1/2 \\ -1 & 1/2 \leqslant t < 1 \\ 0 & \text{otherwise} \end{cases},$$

with ψ_{jk} having support on the half-open interval $h_{jk} = [k2^{-j}, (k+1)2^{-j})$. The set $\{\psi_{00}, \psi_{01}, \ldots\}$ is known as an Haar orthonormal basis for $L^2(\mathbb{R})$ since

$$(\psi_{jk}, \psi_{lm}) = \int_{-\infty}^{\infty} \psi_{jk}(t)\,\psi_{lm}(t)\,\mathrm{d}t = \delta_{jl}\,\delta_{km}.$$

Approximations based upon a wavelet basis

$$f(t) = \sum_{j\in\mathbb{Z}} \sum_{k\in\mathbb{Z}} (f, \psi_{jk})\,\psi_{jk}(t),$$

allow identification of localized features in f.

The costly evaluation of scalar products (f, ψ_{jk}) in the double summation can be avoided by a reformulation of the expansion as

$$f(t) = \sum_k c_{l,k}\, \varphi_l(t) + \sum_{j \leqslant l} \sum_k d_{j,k}\, \psi_{jk}(t), \tag{1}$$

with . In addition to the ψ ("mother" wavelet), an auxilliary φ scaling function ("father" wavelet) is defined, for example

$$\varphi(t) = \begin{cases} 1 & 0 \leqslant t < 1 \\ 0 & \text{otherwise} \end{cases},$$

for the Haar wavelet system.

The above approach is known as a *multiresolution* representation and is based upon a hierarchical decomposition of the space of functions, e.g.,

$$L^2 = V_l \oplus W_l \oplus W_{l-1} \oplus W_{l-2} \oplus \ldots$$

with

$$V_j = \text{span}\{\varphi_{jk} | k \in \mathbb{Z}\}, W_j = \text{span}\{\psi_{jk} | k \in \mathbb{Z}\}.$$

The hierarchical decomposition is based upon the vector subspace inclusions

$$\{0\} < \cdots < V_1 < V_0 < V_{-1} < V_{-2} < \cdots < L^2(\mathbb{R}),$$

and the relations

$$V_m \oplus W_m = V_{m-1},$$

that state that the orthogonal complement of V_m within V_{m-1} is W_m. Analogous to the FFT, a fast wavelet transformation can be defined to compute coefficients of (1).