Overview

- Lanczos iteration
- Eigenvalue problem
- Orthogonal polynomials and Jacobi matrices
- Gauss Quadrature

- Consider $\boldsymbol{A} \in \mathbb{R}^{m \times m}$ symmetric positive definite (as often arises in physics)
- The reduced Hessenberg matrix $\boldsymbol{H}_n = \boldsymbol{Q}_n^T \boldsymbol{A} \boldsymbol{Q}_n$ is symmetric, positive definite, *tridiagonal*.

$$\boldsymbol{H}_n = \boldsymbol{T}_n = \begin{pmatrix} \alpha_1 & \beta_1 & & \\ \beta_1 & \alpha_2 & \beta_2 & \\ & \ddots & \ddots & \ddots \\ & & \beta_{n-1} & \alpha_n \end{pmatrix}, \tilde{\boldsymbol{T}}_n = \begin{pmatrix} \alpha_1 & \beta_1 & & \\ \beta_1 & \alpha_2 & \beta_2 & \\ & \ddots & \ddots & \ddots \\ & & \beta_{n-1} & \alpha_n \\ & & & \beta_n \end{pmatrix}$$

$$\boldsymbol{A}\boldsymbol{Q}_n = \boldsymbol{Q}_{n+1} \tilde{\boldsymbol{T}}_n \Rightarrow \boldsymbol{A}\boldsymbol{q}_n = \beta_{n-1}\boldsymbol{q}_{n-1} + \alpha_n \boldsymbol{q}_n + \beta_n \boldsymbol{q}_{n+1}$$

Algorithm Lanczos

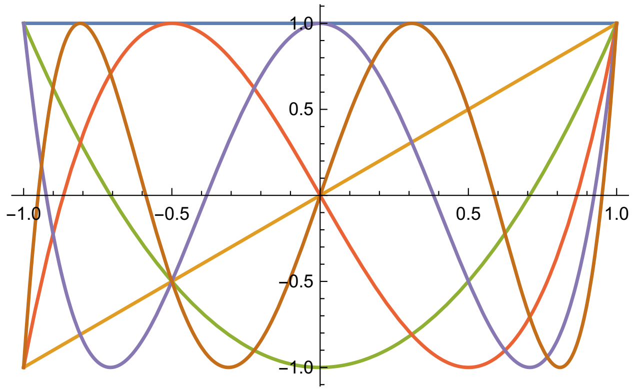
Given: $\boldsymbol{b}$, $\boldsymbol{A}$
$\beta_0 = 0$, $\boldsymbol{q}_0 = \boldsymbol{0}$, $\boldsymbol{q}_1 = \boldsymbol{b} / \|\boldsymbol{b}\|$
for $n = 1, 2, \ldots$
  $\boldsymbol{v} = \boldsymbol{A}\boldsymbol{q}_n$, $\alpha_n = \boldsymbol{q}_n^T \boldsymbol{v}$
  $\boldsymbol{v} = \boldsymbol{v} - \beta_{n-1}\, \boldsymbol{q}_{n-1} - \alpha_n\, \boldsymbol{q}_n$
  $\beta_n = \|\boldsymbol{v}\|$
  $\boldsymbol{q}_{n+1} = \boldsymbol{v} / \beta_n$

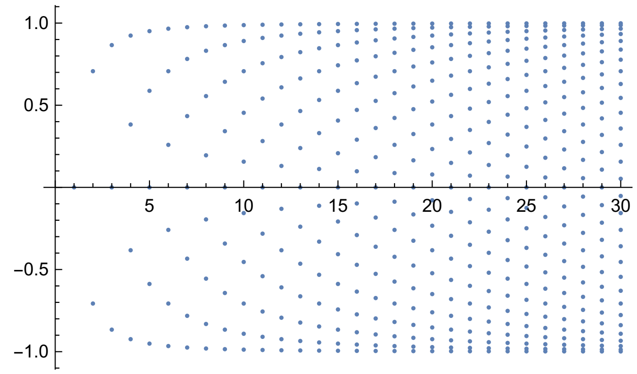
- Since Lanczos is a restriction of Arnoldi to s.p.d. matrices, all properties of Arnoldi localization of eigenvalues carry over, in particular solution $\min_{p^n \in P^n} \| p^n(\boldsymbol{A}) \boldsymbol{b} \|$ is characterisitic polynomial of $\boldsymbol{T}_n = \boldsymbol{Q}_n^* \boldsymbol{A} \boldsymbol{Q}_n$.
- Recall the definition of the Chebyshev polynomials for $x \in [-1, 1]$

$$T_m(x) = \cos(m\theta), x = \cos\theta$$

- Lanczos iteration converges rapidly if (scaled and centered) eigenvalue distribution of $\boldsymbol{A}$ differs substantially from that of the Chebyshev roots

$$x_j = \cos\theta_j, \theta_j = \frac{\pi}{m}\left(j - \frac{1}{2}\right), j = 1, \dots, m$$





- Vectors $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^m$ are functions, $\boldsymbol{u}, \boldsymbol{v} \colon \{1, \ldots, m\} \to \mathbb{R}$. As $m \to \infty$, vectors $\boldsymbol{u}, \boldsymbol{v}$ can be considered as samples from real functions $u, v \colon \mathbb{R} \to \mathbb{R}$
- $\boldsymbol{A} \in \mathbb{R}^{m \times m}$ encodes a linear transformation between vector spaces, $\boldsymbol{A} \colon \mathbb{R}^m \to \mathbb{R}^m$, $\boldsymbol{b} = \boldsymbol{A}\boldsymbol{x}$. As $m \to \infty$, $\boldsymbol{A}$ can be considered as an approximation (sample) of a linear operator between function spaces
- A *Banach space* $\mathcal{B}$ is a linear (vector) space endowed with a norm $\|\| \colon \mathcal{B} \to \mathbb{R}_+$
- A *Hilbert space* $\mathcal{H}$ is a linear (vector) space endowed with a scalar product $(,) \colon \mathcal{H} \times \mathcal{H} \to \mathbb{R}$
- The scalar product can be used to induce a 2-norm, $\|u\| = (u, u)^{1/2}$
- Consider $\mathcal{H}$ to be the space of square-integrable functions defined on $[-1, 1]$, $\mathcal{H} = L^2[-1, 1]$

$$(u, v) = \int_{-1}^{1} u(x)\, v(x)\, \mathrm{d}x,$$

- Introduce operator $\mathcal{A}$ that when sampled leads to multiplication of a vector by a diagonal matrix

$$(\mathcal{A}\,[u])(x) = x\, u(x) = v(x)$$

- Consider the continuum generalization of a Krylov space
  - Replace $\boldsymbol{b} \in \mathbb{R}^m$ by the function $1 \in L^2[-2, 2]$ with norm $\|1\| = (1, 1)^{1/2} = \sqrt{2}$
  - Replace $\boldsymbol{A}\boldsymbol{b}$ by aplication of operator $\mathcal{A}$, e.g., $(\mathcal{A}\,[1])(x) = x \cdot 1$, $(\mathcal{A}\,[x])(x) = x \cdot x, \ldots$
  - Arrive at Krylov space $\operatorname{span}\{1, x, x^2, \ldots\}$
  - Interpret sampling of operator relationship $(\mathcal{A}[u])(x) = x\,u(x) = v(x)$ at x_i as

$$\boldsymbol{A}\,\boldsymbol{u} = \boldsymbol{v},\, v_i = x_i\,u_i,\, \boldsymbol{A} = \operatorname{diag}(x_1, \ldots, x_m) = \boldsymbol{A}^T$$

- Construction of an orthogonal set of (Legendre) polynomials is identical to Lanczos iteration

Algorithm Lanczos: discrete and continuum

$\beta_0 = 0$, $\boldsymbol{q}_0 = \boldsymbol{0}$, $\boldsymbol{q}_1 = \boldsymbol{b} / \|\boldsymbol{b}\|$
for $n = 1, 2, \ldots$
  $\boldsymbol{v} = \boldsymbol{A}\,\boldsymbol{q}_n$, $\alpha_n = \boldsymbol{q}_n^T \boldsymbol{v}$
  $\boldsymbol{v} = \boldsymbol{v} - \beta_{n-1}\,\boldsymbol{q}_{n-1} - \alpha_n\,\boldsymbol{q}_n$
  $\beta_n = \|\boldsymbol{v}\|$
  $\boldsymbol{q}_{n+1} = \boldsymbol{v} / \beta_n$

$\beta_0 = 0$, $q_0(x) = 0$, $q_1(x) = 1 / \sqrt{2}$
for $n = 1, 2, \ldots$
  $v(x) = \mathcal{A}[q_n](x) = x\,q_n(x)$, $\alpha_n = (q_n, v)$
  $v(x) = v(x) - \beta_{n-1}\,q_{n-1} - \alpha_n\,q_n$
  $\beta_n = \|v\|$
  $q_{n+1} = v / \beta_n$

- Properties of orthogonal polynomials can be obtained from linear algebra operations
- Define Krylov matrix as the sample of the continuum Krylov space at $x_i = ih$, $h = 2/(m-1)$

$$\boldsymbol{x}^k = \left(\begin{array}{ccc} x_1^k & \ldots & x_m^k \end{array} \right)^T, \boldsymbol{K}_n = \left(\begin{array}{cccc} \boldsymbol{1} & \boldsymbol{x} & \ldots & \boldsymbol{x}^{n-1} \end{array} \right)$$

- Tridiagonal matrices $\boldsymbol{T}_n = \boldsymbol{Q}_n^T \boldsymbol{A} \boldsymbol{Q}_n$ from Lanczos iteration are known as *Jacobi matrices*

$$(\boldsymbol{T}_n)_{ij} = (q_i(x), x\, q_j(x)), \boldsymbol{Q}_n = \left(\begin{array}{ccc} q_1(\boldsymbol{x}) & \ldots & q_n(\boldsymbol{x}) \end{array} \right)$$

- Exploit the relationship between discrete and continuum formulations by applying knowledge of the solution to polynomial approximation problem $\min_{p^n \in P^n} \|p^n(\boldsymbol{A})\boldsymbol{b}\|$ for $\boldsymbol{A}$ a sample of $\mathcal{A}[u] = x\, u$, and $\boldsymbol{b}$ a sample of 1. Conclude that

$$\operatorname{argmin}_{p^n \in P^n} \|p^n(x)\| = p_{\boldsymbol{T}_n}, i.e.,$$

  solution to the polynomial minimization problem is the characteristic polynomial of $\boldsymbol{T}_n$
- $\forall p \in P^n$, $p(x) = C q_{n+1}(x) + \boldsymbol{Q}_n(x)\, \boldsymbol{y}$, $\boldsymbol{Q}_n = \left(\begin{array}{ccc} q_1(\boldsymbol{x}) & \ldots & q_n(\boldsymbol{x}) \end{array} \right)$, $\|p\| = (C^2 + \|\boldsymbol{y}\|^2)^{1/2}$
- Conclude that roots of the orthogonal polynomial $q_{n+1}(x)$ are the eigenvalues of $\boldsymbol{T}_n$

- Gauss quadrature for $f \in L^2[-1,1]$

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = \sum_{j=1}^{n} w_j\, f(x_j)$$

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \cong \int_{-1}^{1} p_{n-1}(x)\,\mathrm{d}x = \int_{-1}^{1} \sum \mathcal{L}_i(x) y_i\,\mathrm{d}x = \sum \left[\int_{-1}^{1} \mathcal{L}_i(x)\,\mathrm{d}x\right] y_i$$

$$w_i = \int_{-1}^{1} \mathcal{L}_i(x)\,\mathrm{d}x = \int_{-1}^{1} \prod_{j=1}^{n}{}' \frac{(x-x_j)}{(x_i-x_j)}\,\mathrm{d}x$$

with nodes x_j given by roots of Legendre polynomials.

- Find the orthogonal eigendecomposition of the Jacobi matrices $\boldsymbol{T}_n$, $\boldsymbol{T}_n = \boldsymbol{V}\boldsymbol{D}\boldsymbol{V}^T$
  - The nodes of the Gauss quadrature are eigenvalues of $\boldsymbol{T}_n$, $x_j = \lambda_j$
  - The weights of the Gauss quadrature are $w_j = 2\,[(\boldsymbol{v}_j)_1]^2$, $\boldsymbol{V} = (\ \boldsymbol{v}_1\ \ \ldots\ \ \boldsymbol{v}_n\ )$