The asymptotics of Wilkinson's shift iteration

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Abstract

We study the rate of convergence of Wilkinson's shift iteration acting on Jacobi matrices with simple spectrum. We show that for *AP-free* spectra (i.e., simple spectra containing no arithmetic progression with 3 terms), convergence is cubic. In order 3, there exists a tridiagonal symmetric matrix P_0 which is the limit of a sequence of a Wilkinson iteration, with the additional property that all iterations converging to P_0 are strictly quadratic. Among tridiagonal matrices near P_0, the set $\mathcal{X}$ of initial conditions with convergence to P_0 is rather thin: it is a union of disjoint arcs $\mathcal{X}_s$ meeting at P_0, where s ranges over the Cantor set of sign sequences $s : \mathbb{N} \to \{1, -1\}$. Wilkinson's step takes $\mathcal{X}_s$ to $\mathcal{X}_{s'}$, where s' is the left shift of s. Among tridiagonal matrices conjugate to P_0, initial conditions near P_0 but not in $\mathcal{X}$ converge at a cubic rate.

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1 Introduction

In this paper, we study of the asymptotics of the shifted QR iteration with the so called *Wilkinson's shift*, acting on Jacobi matrices. More precisely ([10], [4], [7]), for an $n \times n$ real symmetric tridiagonal matrix T and a real number s, write, if possible, the unique QR *factorization* $T - sI = QR$, where Q is orthogonal and R is upper triangular with positive diagonal. Wilkinson's shift strategy is the choice of $s = \omega(T)$ equal to the eigenvalue of the bottom 2×2 principal minor of T which is closest to the bottom entry T_{nn}. A *Wilkinson step* obtains a new matrix

$$\mathbf{W}(T) = Q^*TQ = RTR^{-1}.$$

From both defining formulae, $\mathbf{W}(T)$ is symmetric and upper Hessenberg, and thus, must also be a real, symmetric tridiagonal matrix, with the same spectrum as T, as well as the signs of the nontrivial off-diagonal elements.

As is well known ([7]), if the iterates $T_k = \mathbf{W}^k(T)$ of the Wilkinson step starting from a Jacobi matrix with simple spectrum exist for arbitrary k, then their lowest off-diagonal entry tend to 0: we are interested in the rate of convergence of this sequence. It has been conjectured ([7], [4]) that the rate is cubic, i.e., for any Jacobi matrix T there exists a constant C such that $|(T_{k+1})_{n,n-1}| \leq C|(T_k)_{n,n-1}|^3$. As we shall see, this is true for most matrices T but false in general. A Jacobi matrix T is an *AP-matrix* if its spectrum contains an arithmetic progression with three terms and is *AP-free* otherwise. For AP-free matrices, the conjecture is indeed true. On the other hand, there exist 3×3 AP-matrices for which the rate of convergence is, in the words of Parlett, merely quadratic.

We give an outline of the proof. A basic ingredient are the *bidiagonal coordinates*, consisting of eigenvalues λ_i, $i = 1, \ldots, n$, and additional variables β_i^π,

$i = 1, \dots, n-1$, defined on large open sets of tridiagonal matrices. As proved in [5], the set $\mathcal{T}_\Lambda$ of real, symmetric, tridiagonal matrices with fixed simple spectrum $\lambda_1 < \cdots < \lambda_n$ is covered by open dense subsets $\mathcal{U}_\Lambda^\pi$, indexed by permutations π and bidiagonal coordinates provide a diffeomorphism between each $\mathcal{U}_\Lambda^\pi$ and $\mathbb{R}^{n-1}$. The new coordinates are used to convert asymptotic issues of Wilkinson's iteration into local theory in an appropriate chart.

There are two subsets of $\mathcal{T}_\Lambda$ in which Wilkinson's step might break down. First, let $\mathcal{Z} \subset \mathcal{T}_\Lambda$ be the set of matrices T for which the shift $\omega(T)$ equals an eigenvalue of T: we are especially interested in $\mathcal{D}_{0,i} \subset \mathcal{Z}$, the set of matrices T with $(T)_{n,n} = \lambda_i$, $(T)_{n,n-1} = 0$. Second, the two eigenvalues $\omega_+(T) \geq \omega_-(T)$ of the bottom 2×2 block $\hat{T}$ may be equally distant from the corner entry $(T)_{n,n}$: let $\mathcal{Y} \subset \mathcal{T}_\Lambda$ be the set of such matrices T. It is clear that the function $\mathbf{W}$ is smoothly defined at least in $\mathcal{T}_\Lambda - \mathcal{Z} - \mathcal{Y}$ but using bidiagonal coordinates we shall see that the domain can be taken to be much larger. Indeed, for a matrix $T \in \mathcal{U}_\Lambda^\pi \subset \mathcal{T}_\Lambda$ with bidiagonal coordinates λ_i and β_i^π, $T \notin \mathcal{Z} \cup \mathcal{Y}$, the β_i^π's of $\mathbf{W}(T)$ are given by

$$\mathbf{W}_\pi(\beta_1^\pi, \dots, \beta_{n-1}^\pi) = \left(\left| \frac{\lambda_{\pi(2)} - \omega(T)}{\lambda_{\pi(1)} - \omega(T)} \right| \beta_1^\pi, \dots, \left| \frac{\lambda_{\pi(n)} - \omega(T)}{\lambda_{\pi(n-1)} - \omega(T)} \right| \beta_{n-1}^\pi \right).$$

In bidiagonal coordinates, points in $\mathcal{D}_{0,\pi(n)} \cap \mathcal{U}_\Lambda^\pi$ satisfy $\beta_{n-1}^\pi = 0$ and an inspection of the formula above shows that $\mathbf{W}_\pi$ extends smoothly to $\mathcal{D}_{0,\pi(n)} - \mathcal{Y}$. More generally, near $p_0 \in \mathcal{D}_{0,\pi(n)}$ the quotient $\beta_{n-1}^\pi / (T)_{n,n-1}$ is bounded above and below and rates of convergence are the same in both variables. We then expand $(\mathbf{W}_\pi(\beta_1^\pi, \dots, \beta_{n-1}^\pi))_{n-1}$ in a Taylor series around p_0. Notice that $\omega(T) \approx \lambda_{\pi(n)}$ near p_0 and oddness of this function in the variable β_{n-1}^π allows for

$$(\mathbf{W}_\pi(\beta_1^\pi, \dots, \beta_{n-1}^\pi))_{n-1} = G(\beta_1^\pi, \dots, \beta_{n-1}^\pi)(\beta_{n-1}^\pi)^3$$

for some smooth function G, yielding the cubic estimate

$$|(\mathbf{W}(T))_{n,n-1}| < C|(T)_{n,n-1}|^3$$

for some $C > 0$, T in a neighborhood of p_0.

Points of $\mathcal{Y}$ with $\beta_{n-1}^\pi \neq 0$ are step-like discontinuities for $\mathbf{W}$. The behavior of $\mathbf{W}$ near matrices $p_0 \in \mathcal{Y} \cap \mathcal{Z}$ is more complicated; in figure 2 we show what happens for $\Lambda = (1, 2, 4)$, a typical spectrum. The upshot from the figure is that typically the few points in $\mathcal{Y} \cap \mathcal{D}_{0,i}$, for which the cubic estimate does not hold, are isolated in the sequence of iterations $T_k = \mathbf{W}^k(T_0)$ and are irrelevant in the long run. More precisely, the argument holds for *AP-free* spectra, i.e., spectra which contain no three terms arithmetical progression. In such case, there exist positive constants C and K such that $|(T_{k+1})_{n,n-1}| > C|(T_k)_{n,n-1}|^3$ holds for at most K values of k (see theorem 3.4), yielding genuine cubic convergence of Wilkinson's iteration.

In the 3×3 AP case, instead, there exists a point $p_0 \in \mathcal{Y} \cap \mathcal{D}_{0,i}$ which is kept fixed by $\mathbf{W}$. The graphs of ω_+ and ω_- near p_0 resemble the two branches of the cone $z^2 = xz + y^2$ near the origin, x and y corresponding to β_1^π and β_2^π, respectively. Sections of the cone by planes $x = a$, $a \neq 0$, are hyperbola with a branch passing through $(a, 0, 0)$ and z is therefore of the order of y^2 for small y: this quadratic behavior of ω implies the cubic estimates for the $(n, n-1)$ entry under $\mathbf{W}$. For $a = 0$, however, the intersection of the cone with the plane $x = a$ is $z = \pm|y|$; z and therefore ω are of the order of $|y|$ and β_2^π, respectively: this entails a *quadratic* estimate for the $(n, n-1)$ entry under $\mathbf{W}$. Hence, the rate of convergence is dictated by whether T_k remains near p_0 when k goes to infinity. It turns out that T_k tends to p_0 (and cubic convergence fails) if and only if $T_0 \in \mathcal{X}$, where $\mathcal{X}$ is a remarkable set (see figure 7). A point $T_0 \in \mathcal{X}$ has a *sign sequence* $s : \mathbb{N} \to \{1, -1\}$, where $s(k)$ indicates whether $\omega(T_k)$ equals ω_+ or ω_-. The set $\mathcal{S}$ of sign sequences is a Cantor set and $\mathcal{X}$ is the disjoint union of graphs of Lipschitz functions $f_s : [-a^*, a^*] \to \mathbb{R}$ with $f_s(0) = 0$ for all $s \in \mathcal{S}$; a good reference for dynamically defined Cantor sets is [6]. For $y_0 \in [-a^*, a^*]$, $(f_s(y_0), y_0) \in \mathcal{X}$ has sign sequence s. There is an open set of points $T_0 \notin \mathcal{X}$ which are between branches of $\mathcal{X}$: for sufficiently large k, their iterates T_k will be either to the left or to the right of $\mathcal{X}$ and cubic convergence applies. Another application of dynamical systems to numerical spectral theory is the work of Batterson and Smillie ([1]) on the Rayleigh quotient iteration.

We begin the paper collecting from [5] the required information about bidiagonal coordinates, essentially, the description of Wilkinson's iteration in terms of bidiagonal variables. Section 2 also contains a key ingredient: the construction of a function $h(T)$ which grows along Wilkinson's iterations. The proof that $h(T)$ indeed satisfies this property is indirect: it requires the interpretation of a QR step as the time one map of a Toda flow. The monotonicity of h then follows by a simple differentiation argument.

In section 3 we prove cubic convergence of Wilkinson's shift iteration for AP-free matrices. In sections 4 and 5, we show that for 3×3 AP-matrices, the rate of convergence is usually cubic but strictly quadratic for a thin set of initial conditions.

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2 Preliminaries

Let $\mathcal{T}_\Lambda$ be the set of real, symmetric, tridiagonal matrices with simple spectrum $\lambda_1, \ldots, \lambda_n$ and set $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. For $T \in \mathcal{T}_\Lambda$, write $T = Q^*\Lambda Q$ for some $Q \in O(n)$. Write the PLU factorization of Q, i.e., $Q = PLU$ where P is a permutation matrix, L is lower unipotent and U is upper triangular. This is usually possible for $P = P_\pi$ for several permutations $\pi \in S_n$. Indeed, since Q is invertible, there is a matrix $P^{-1}Q$ obtained by permuting the rows of Q for which all the leading principal minors are invertible. For a permutation π, define $\mathcal{U}_\Lambda^\pi$ to be the set of matrices $T \in \mathcal{T}_\Lambda$ for which $P_\pi^{-1}Q$ admits an LU factorization. The following lemma provides other descriptions of $\mathcal{U}_\Lambda^\pi$. Let $\mathcal{E}$ be the set of diagonal matrices having the values 1 or -1 along the diagonal.

Lemma 2.1 ([5], lemma 3.1) *Take $T \in \mathcal{T}_\Lambda$ with unreduced blocks $T_1, \ldots, T_k$ of sizes $n_1, \ldots, n_k$ along the diagonal. Then $T \in \mathcal{U}_\Lambda^\pi$ if and only if the eigenvalues of T_i are*

$$\lambda^\pi_{n_1+\cdots+n_{i-1}+1}, \ldots, \lambda^\pi_{n_1+\cdots+n_{i-1}+n_i}.$$

Alternatively, $\mathcal{U}_\Lambda^\pi$ is the union of all open faces in $\mathcal{T}_\Lambda$ adjacent to Λ^π. Also, for $E \in \mathcal{E}$, if $T \in \mathcal{U}_\Lambda^\pi$ then $ETE \in \mathcal{U}_\Lambda^\pi$.

For $T \in \mathcal{U}_\Lambda^\pi$, we define the π-*normalized diagonalization* as the unique factorization $T = Q_\pi^*\Lambda^\pi Q_\pi$ for which the LU factorization of Q_π yields a matrix U with positive diagonal. Notice that $Q_\pi = EP_\pi^{-1}Q$ for some $E \in \mathcal{E}$.

We now construct charts for $\mathcal{T}_\Lambda$, $\phi_\pi : \mathbb{R}^{n-1} \to \mathcal{U}_\Lambda^\pi$ and $\phi_\pi^{-1} : \mathcal{U}_\Lambda^\pi \to \mathbb{R}^{n-1}$ with $\phi_\pi(0) = \Lambda^\pi \in \mathcal{U}_\Lambda^\pi$. For $T \in \mathcal{U}_\Lambda^\pi$, consider its π-normalized diagonalization $T = Q_\pi^*\Lambda^\pi Q_\pi$ and $Q = P_\pi Q_\pi$ so that $T = Q^*\Lambda Q$. Write $Q_\pi = L_\pi U_\pi$ (which is possible because the leading principal minors of Q_π are positive) and therefore $P_\pi L_\pi = QR_\pi$, where $R_\pi = U_\pi^{-1}$ is also upper triangular. Set

$$B_\pi = R_\pi^{-1} T R_\pi = L_\pi^{-1} \Lambda^\pi L_\pi.$$

Notice that the columns of L_π^{-1} are the eigenvectors of B_π. From $B_\pi = R_\pi^{-1}TR_\pi$, B_π is upper Hessenberg and from $B_\pi = L_\pi^{-1}\Lambda^\pi L_\pi$, it is lower triangular with diagonal entries $\lambda_1^\pi, \ldots, \lambda_n^\pi$. Summing up, B_π is lower bidiagonal:

$$B_\pi = \begin{pmatrix} \lambda_1^\pi & & & & \\ \beta_1^\pi & \lambda_2^\pi & & & \\ & \beta_2^\pi & \lambda_3^\pi & & \\ & & \ddots & \ddots & \\ & & & \beta_{n-1}^\pi & \lambda_n^\pi \end{pmatrix}.$$

Define ψ_π to be the map just constructed taking $T \in \mathcal{U}_\Lambda^\pi$ to $(\beta_1^\pi, \ldots, \beta_{n-1}^\pi)$. We call $\beta_1^\pi, \ldots, \beta_{n-1}^\pi$ (together with $\lambda_1^\pi, \ldots, \lambda_n^\pi$) the π-*bidiagonal coordinates* of T.

Theorem 2.2 ([5], theorem 3.4) *The map $\psi_\pi : \mathcal{U}_\Lambda^\pi \to \mathbb{R}^{n-1}$ is a diffeomorphism with inverse $\phi_\pi : \mathbb{R}^{n-1} \to \mathcal{U}_\Lambda^\pi$.*

The map ϕ_π takes open quadrants of $\mathbb{R}^{n-1}$ diffeomorphically to the connected components of $\mathcal{T}_\Lambda$ formed by irreducible matrices (connected components are indexed by signs of off-diagonal entries). Also, the hyperplanes $\beta_i^\pi = 0$ in $\mathbb{R}^{n-1}$ are taken diffeomorphically to the set of matrices T in $\mathcal{U}_\Lambda^\pi$ with $(T)_{i,i+1} = 0$. Indeed, it is shown in theorem 4.5 of [5] that the quotient $\beta_i^\pi/((T)_{i,i+1})$ is a smooth nonzero function in $\mathcal{U}_\Lambda^\pi$. The following lemma follows by compactness.

Lemma 2.3 *Given a compact subset $K_\pi \subset \mathcal{U}_\Lambda^\pi$, there exist positive constants $C < C'$ such that, for $T \in K_\pi$,*

$$C|(T)_{n,n-1}| \le |\beta_{n-1}^\pi| \le C'|(T)_{n,n-1}|.$$

We say that a function $\alpha : \mathcal{T}_\Lambda \to \mathbb{R}$ is *even* if $\alpha(ETE) = \alpha(T)$ for any $T \in \mathcal{T}_\Lambda$ and $E \in \mathcal{E}$. The following lemma translates this definition to bidiagonal coordinates.

Lemma 2.4 ([5], lemma 3.6) *If $E = \operatorname{diag}(\sigma_1, \ldots, \sigma_n) \in \mathcal{E}$, $T \in \mathcal{U}_\Lambda^\pi$, and $\psi_\pi(T) = (\beta_1^\pi, \ldots, \beta_{n-1}^\pi)$ then*

$$\psi_\pi(ETE) = (\sigma_1\sigma_2\beta_1^\pi, \ldots, \sigma_{n-1}\sigma_n\beta_{n-1}^\pi).$$

A function $\alpha : \mathcal{T}_\Lambda \to \mathbb{R}$ is even if and only if each $\alpha \circ \phi_\pi : \mathbb{R}^{n-1} \to \mathbb{R}$ is even in each coordinate.

As an example of bidiagonal coordinates, let $\Lambda = \operatorname{diag}(-1, 0, 1)$. Set $\pi(1) = 3$, $\pi(2) = 1$, $\pi(3) = 2$. Matrices will be described by their π-bidiagonal coordinates $x = \beta_1^\pi$ and $y = \beta_2^\pi$. Since $B_\pi = L_\pi^{-1}\Lambda^\pi L_\pi$, we obtain

$$\Lambda^\pi = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad B_\pi = \begin{pmatrix} 1 & 0 & 0 \\ x & -1 & 0 \\ 0 & y & 0 \end{pmatrix}, \quad L_\pi = \begin{pmatrix} 1 & 0 & 0 \\ -x/2 & 1 & 0 \\ -xy & y & 1 \end{pmatrix}$$

and writing $Q_\pi = L_\pi U_\pi$ we have

$$Q_\pi = \frac{1}{r_1 r_2} \begin{pmatrix} 2r_2 & 2x(1+2y^2) & xyr_1 \\ -xr_2 & 2(2+x^2y^2) & -2yr_1 \\ -2xyr_2 & y(4-x^2) & 2r_1 \end{pmatrix},$$

where $r_1 = \sqrt{4 + x^2 + 4x^2y^2}$ and $r_2 = \sqrt{4 + 4y^2 + x^2y^2}$. From $T = Q_\pi^* \Lambda^\pi Q_\pi$,

$$T = \frac{1}{r_1^2 r_2^2} \begin{pmatrix} (4-x^2)r_2^2 & 2xr_2^3 & 0 \\ 2xr_2^3 & -4(4 - x^2 - 4x^2y^4 + x^4y^4) & 2yr_1^3 \\ 0 & 2yr_1^3 & y^2(x^2-4)r_1^2 \end{pmatrix}.$$

This example will be revisited in sections 4 and 5.

For an invertible real matrix M, write the unique *QR factorization*

$$M = \mathbf{Q}(M)\mathbf{R}(M),$$

where $\mathbf{Q}(M)$ is orthogonal and $\mathbf{R}(M)$ is upper triangular with positive diagonal. For some function f taking nonzero values on the spectrum of a tridiagonal symmetric matrix T_0, the *QR step induced by* f is the map

$$F(T) = \mathbf{Q}(f(T))^* \, T \, \mathbf{Q}(f(T)) = \mathbf{R}(f(T)) \, T \, \mathbf{R}(f(T))^{-1}.$$

From both equalities, we learn that $F(T)$ is also tridiagonal, with same signs and zeroes along the off-diagonal entries than T. The standard QR step corresponds to $f(x) = x$ and taking a shift s means taking $f(x) = x - s$. The map F admits a simple description in terms of bidiagonal coordinates.

Proposition 2.5 ([5], proposition 4.2) *For f taking nonzero values on the spectrum of T,*

$$(F \circ \phi_\pi)(\beta_1^\pi, \ldots, \beta_{n-1}^\pi) = \phi_\pi \left(\left| \frac{f(\lambda_{\pi(2)})}{f(\lambda_{\pi(1)})} \right| \beta_1^\pi, \ldots, \left| \frac{f(\lambda_{\pi(n)})}{f(\lambda_{\pi(n-1)})} \right| \beta_{n-1}^\pi \right)$$

We now present some technical results concerning the dynamics QR type iterations which will be needed in the proof of theorem 3.4. The argument is rather indirect and seems to require the language of Toda flows. For a square matrix M, let $S = \Pi_a M$ be the skew symmetric matrix for which $(M)_{ij} = (S)_{ij}$ for $i > j$. The following result, which follows by direct computation, relates Toda flows and QR iterations.

Proposition 2.6 ([8]) *Let Λ be a diagonal matrix with simple spectrum, $g : \mathbb{R} \to \mathbb{R}$ be a smooth function, X_g be the vector field $X_g(T) = [T, \Pi_a g(T)]$ and $\mathbf{T} : \mathbb{R} \to \mathcal{T}_\Lambda$ be a path satisfying $\frac{d}{dt}\mathbf{T} = X_g(\mathbf{T})$, $\mathbf{T}(0) = T_0$. Then*

$$\mathbf{T}(t) = \mathbf{Q}(\exp(t\, g(T_0)))^* \, T_0 \, \mathbf{Q}(\exp(t\, g(T_0))) = \mathbf{R}(\exp(t\, g(T_0))) T_0 \mathbf{R}(\exp(t\, g(T_0)))^{-1},$$

or, in other words, $\mathbf{T}(t) = F(T_0)$ where $f(x) = \exp(t\, g(x))$.

The dynamics of Toda vector fields is rather simple: they are essentially gradients of Morse functions. The following result is known for $g(x) = x$ ([2], [3], [9]).

Theorem 2.7 *Let $g : \mathbb{R} \to \mathbb{R}$ satisfy $g(\lambda_i) \neq g(\lambda_j)$ for distinct eigenvalues λ_i, λ_j of Λ. Let X_g be the Toda vector field $[T, \Pi_a g(T)]$ on $\mathcal{T}_\Lambda$. Let $M = \operatorname{diag}(\mu_1, \mu_2, \ldots, \mu_n)$, $\mu_1 > \mu_2 > \cdots > \mu_n$; let $h_{M,g} : \mathcal{T}_\Lambda \to \mathbb{R}$ be the smooth function $h_{M,g}(T) = \operatorname{tr}(M g(T))$. Then the directional derivative $X_g h_{M,g}$ is strictly positive except at diagonal matrices.*

Proof: Define a path $\mathbf{T} : \mathbb{R} \to \mathcal{T}_\Lambda$ satisfying $\frac{d}{dt}\mathbf{T} = X_g$ as above. We first claim that $\frac{d}{dt}\tilde{g}(\mathbf{T}) = [\tilde{g}(\mathbf{T}), \Pi_a g(\mathbf{T})]$ for any smooth function $\tilde{g}$. Indeed, since Toda flows preserve spectra, $\tilde{g}$ may be replaced by a polynomial p which coincides with $\tilde{g}$ on the spectrum of Λ. By linearity, it suffices to consider $p_k(x) = x^k$, which is handled by induction on k:

$$\begin{aligned} \frac{d}{dt} p_{k+1}(\mathbf{T}) &= \frac{d}{dt}(\mathbf{T} p_k(\mathbf{T})) = \mathbf{T} \left(\frac{d}{dt} p_k(\mathbf{T}) \right) + \left(\frac{d}{dt}\mathbf{T} \right) p_k(\mathbf{T}) \\ &= \mathbf{T}[\mathbf{T}^k, \Pi_a f(\mathbf{T})] + [\mathbf{T}, \Pi_a f(\mathbf{T})]\mathbf{T}^k \\ &= \mathbf{T}^{k+1}(\Pi_a f(\mathbf{T})) - \mathbf{T}(\Pi_a f(\mathbf{T}))\mathbf{T}^k + \mathbf{T}(\Pi_a f(\mathbf{T}))\mathbf{T}^k - (\Pi_a f(\mathbf{T}))\mathbf{T}^{k+1} \\ &= [p_{k+1}(\mathbf{T}), \Pi_a f(\mathbf{T})]. \end{aligned}$$

Take $\tilde{g} = g$ and compute the derivative of $h_{M,g}$ along the path $\mathbf{T}$:

$$\begin{aligned} X_g h_{M,g} &= \frac{d}{dt} h_{M,g}(\mathbf{T}) = \frac{d}{dt} (\mathrm{tr}\ M g(\mathbf{T})) \\ &= \mathrm{tr}\ M \left(\frac{d}{dt} g(\mathbf{T}) \right) = \mathrm{tr}(M[g(\mathbf{T}), \Pi_a g(\mathbf{T})]) \\ &= \sum_{1 \le i < j \le n} 2(\mu_i - \mu_j)(g(\mathbf{T}))^2_{ij}. \end{aligned}$$

Since $g(T)$ has simple spectrum, it is diagonal only if T also is and we are done. ■

Corollary 2.8 *Let $f : \mathbb{R} \to \mathbb{R}$ be a function satisfying $|f(\lambda_i)| \neq |f(\lambda_j)| \neq 0$ for $i \neq j$ and let $F : \mathcal{T}_\Lambda \to \mathcal{T}_\Lambda$ be the QR step induced by f. Let $\mathcal{K} \subset \mathcal{T}_\Lambda$ be a compact set containing no diagonal matrices. Then there exists $K > 0$ such that, for all $T \in \mathcal{T}_\Lambda$,*

$$|\{k \in \mathbb{N} | F^k(T) \in \mathcal{K}\}| < K.$$

Proof: Consider $g(x) = \log|f(x)|$, X_g, $\mathbf{T}$, M and $h_{M,g}$ as in the previous theorem. Since $\mathcal{K}$ is compact and avoids diagonal matrices, $X_g h_{M,g} > \epsilon > 0$ on $\mathcal{K}$. From proposition 2.6, $F^k(T_0) = \mathbf{T}(k)$ and we are done. ■

It is not true that, given $\mathcal{K}$, there exists K_2 such that, for all $T_0 \in \mathcal{T}_\Lambda$, $F^k(T_0) \notin \mathcal{K}$ for all $k > K_2$. For instance, the exit time from a small neighborhood of a diagonal matrix T is not uniformly bounded; another situation is given in figure 3 below.

3 Wilkinson's shift and AP-free matrices

We consider iterations of shifted QR steps, induced by $f_s(x) = x - s$. The function $F_s : \mathcal{T}_\Lambda \to \mathcal{T}_\Lambda$ is defined whenever s is not an eigenvalue. Frequently, the shift s is taken to depend on T. We consider the asymptotic properties of a special choice of shift, which defines *Wilkinson's step* ([10]). For $T \in \mathcal{T}_\Lambda$, let $\omega_+(T) \ge \omega_-(T)$ be the two eigenvalues of the bottom 2×2 block of T and set $\omega(T)$ to be the one nearest to the entry $(T)_{n,n}$. This defines continuous maps $\omega_+, \omega_- : \mathcal{T}_\Lambda \to \mathbb{R}$ which are smooth in $\mathcal{T}_\Lambda - \mathcal{Y}_0$, where $\mathcal{Y}_0 \subset \mathcal{T}_\Lambda$ is the set of matrices T for which $(T)_{n,n} = (T)_{n-1,n-1}$ and $(T)_{n,n-1} = 0$. Indeed, $T \in \mathcal{Y}_0$ if and only if $\omega_+(T) = \omega_-(T)$. Also, $\omega : \mathcal{T}_\Lambda - \mathcal{Y} \to \mathbb{R}$ is smooth where $T \in \mathcal{Y} \subset \mathcal{T}_\Lambda$ if $(T)_{n,n} = (T)_{n-1,n-1}$. Indeed, $T \in \mathcal{Y}$ if and only if $(T)_{n,n}$ is equally distant from both eigenvalues of its bottom 2×2 block, which is the only way smoothness could fail. Also, $\omega_\pm$ and ω are even in the sense of lemma 2.4.

Lemma 3.1 *The functions $\omega_\pm : \mathcal{T}_\Lambda \to \mathbb{R}$ are Lipschitz.*

Proof: The function taking T to its bottom 2×2 block is clearly smooth. The function taking a 2×2 symmetric matrix A to its larger (resp. smaller) eigenvalue is Lipschitz in compact sets. The lemma follows from composition. ■

Let $\mathcal{Z}_k = \{T \in \mathcal{T}_\Lambda;\ \omega(T) = \lambda_k\}$, $\mathcal{Z} = \bigcup_k \mathcal{Z}_k$, $\hat{\mathcal{Z}}_k = \mathcal{Z} - \mathcal{Z}_k$. Notice that if $(T)_{n,n-1} = 0$ then $\omega(T) = (T)_{n,n} = \lambda_k$ for some k and therefore $T \in \mathcal{Z}_k$. Also, if $(T)_{n-1,n-2} = 0$ then again $\omega(T) = \lambda_k$ for some k. Define $\mathbf{W} : \mathcal{T}_\Lambda - \mathcal{Y} - \mathcal{Z} \to \mathcal{T}_\Lambda$ by $\mathbf{W}(T) = F_{\omega(T)}(T)$ for $f_s(x) = x - s$. Notice that $\mathbf{W}$ is an odd function.

Figure 1 shows $\bar{\mathcal{J}}_\Lambda$ for $\Lambda = \mathrm{diag}(1, 2, 4)$ and $\Lambda = \mathrm{diag}(-1, 0, 1)$. Labels indicate the diagonal entries and vertices are diagonal matrices. The set $\mathcal{Y}$, on which $\mathbf{W}$ is not defined, degenerates in the second example. Vertices are fixed points and edges are invariant under $\mathbf{W}$. A simple arrow indicates the order of the points $T, \mathbf{W}(T), \mathbf{W}^2(T), \ldots$ along the edge. For points T on an arc labeled with a double arrow, $\mathbf{W}(T)$ is a vertex. Arcs marked with a transversal segment consist of fixed points of $\mathbf{W}$.

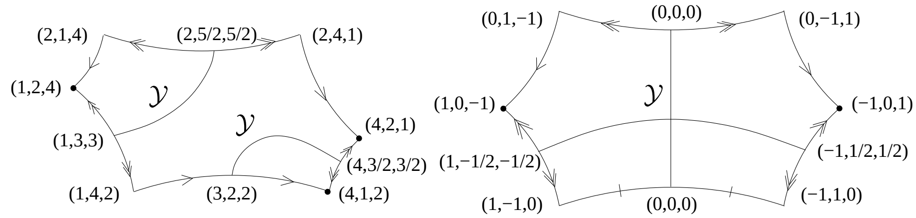

Figure 1: The phase space of Wilkinson's step for $n = 3$.

We apply proposition 2.5 to write down Wilkinson's step in bidiagonal coordinates. Define $\mathbf{W}_\pi$ by

$$\mathbf{W}_\pi(\beta_1^\pi, \ldots, \beta_{n-1}^\pi) = \left(\left| \frac{\lambda_{\pi(2)} - \omega}{\lambda_{\pi(1)} - \omega} \right| \beta_1^\pi, \ldots, \left| \frac{\lambda_{\pi(n)} - \omega}{\lambda_{\pi(n-1)} - \omega} \right| \beta_{n-1}^\pi \right)$$

where $\omega = \omega(\phi_\pi(\beta_1^\pi, \ldots, \beta_{n-1}^\pi))$. Thus, the natural domain for $\mathbf{W}_\pi$ is $\mathbb{R}^{n-1} - \phi_\pi^{-1}(\mathcal{Y} \cap \mathcal{U}_\Lambda^\pi) - \phi_\pi^{-1}(\hat{\mathcal{Z}}_{\pi(n)} \cap \mathcal{U}_\Lambda^\pi)$, where $\mathbf{W}_\pi$ is a smooth function, indicating that points in $\phi_\pi^{-1}(\mathcal{Z}_{\pi(n)})$ are removable singularities and that, despite absolute values in the formula, $\mathbf{W}_\pi$ is smooth at such points. Notice that $\mathbf{W}_\pi$ is odd, since ω is even in each variable β_i^π. Also, points in $\phi_\pi^{-1}(\mathcal{Z}_{\pi(n)})$ are of the form $\beta_{n-1}^\pi = 0$ or, equivalently, $(T)_{n,n-1} = 0$.

Points of $\mathcal{Y}$ with $\beta_{n-1}^\pi \neq 0$ are step-like discontinuities for $\mathbf{W}$. The behavior of $\mathbf{W}$ near matrices $p_0 \in \mathcal{Y} \cap \mathcal{Z}$ is more complicated; in figure 2 we show what happens for $\Lambda = (1, 2, 4)$, a typical 3×3 AP-free spectrum. Close to

$$p_0 = \begin{pmatrix} 3 & \sqrt{2} & 0 \\ \sqrt{2} & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \quad \pi(1) = 1, \pi(2) = 3, \pi(3) = 2, \quad \beta_1^\pi = 3\sqrt{2}, \beta_2^\pi = 0,$$

the set $\mathcal{Y}$ divides the plane into two sides $\mathcal{D}_+$ and $\mathcal{D}_-$, where we take ω_+ and ω_-, respectively, in the definition of $\mathbf{W}$. From each side $\mathcal{D}_\pm$, the function $\mathbf{W}$ can be continuously extended to $\mathcal{Y}$ but the two values thus obtained are quite different except at p_0.

The figure is drawn with a vertical stretching factor of 200. The thick vertical curve (which looks like a straight line due to stretching) is the set $\mathcal{Y}$. To the right, the curve BF (with a cusp at $\mathbf{W}(p_0)$) is the image of the arc in $\mathcal{Y}$ from $\beta_2^\pi = 0.1$ to $\beta_2^\pi = -0.1$ under $\mathbf{W}$ with the choice $\omega = \omega_-$; to the left, the curve CG is the image of the same arc, now with $\omega = \omega_+$. The dotted lines AB and CD are the image under $\mathbf{W}$ of the horizontal line $\beta_2^\pi = 0.1$: notice the jump discontinuity at $\mathcal{Y}$ from B to C. Oddness of $\mathbf{W}$ in the coordinate β_2^π explains the mirror symmetry in the horizontal axis.

The study of the asymptotic behavior of the iterations of Wilkinson's step becomes significantly simpler by taking into account the following result.

Theorem 3.2 ([7], p. 152) *If* $T_k = \mathbf{W}^k(T_0)$ *then* $\lim_{k\to\infty}(T_k)_{n,n-1} = 0$.

From this result, deflation is always possible in numerical implementations of Wilkinson's iteration: T will be truncated so as to split into blocks of size $n-1$ and 1. We will investigate the rate of convergence of $(T_k)_{n,n-1}$ to 0.

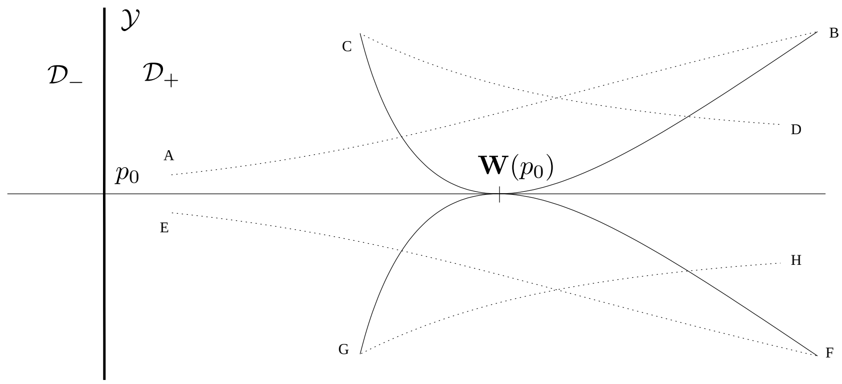

Figure 2: Image of $\mathcal{Y}$ under $\mathbf{W}_\pi$ for $\Lambda = \mathrm{diag}(1, 2, 4)$ (stretched vertically).

Proposition 3.3 *Let $\mathcal{D}(\epsilon) = \{T \in \mathcal{T}_\Lambda \mid |(T)_{n,n-1}| < \epsilon\}$. Given a spectrum $\lambda_1 < \cdots < \lambda_n$, there exists $\epsilon_q > 0$ and $C_q > 0$ such that $\mathbf{W}(\mathcal{D}(\epsilon)) \subset \mathcal{D}(\epsilon)$ for any $\epsilon \leq \epsilon_q$ and $|(\mathbf{W}(T))_{n,n-1}| \leq C_q |(T)_{n,n-1}|^2$ for $T \in \mathcal{D}(\epsilon_q)$.*

Furthermore, for any subset $\mathcal{D}_c \subset \mathcal{D}(\epsilon_q)$ satisfying $\overline{\mathcal{D}_c} \cap \mathcal{Y}_0 = \emptyset$ there exists $C_c > 0$ such that $|(\mathbf{W}(T))_{n,n-1}| \leq C_c |(T)_{n,n-1}|^3$ for $T \in \mathcal{D}_c$.

Proof: Define smaller open sets $\mathcal{V}^\pi \subset K_\pi \subset \mathcal{U}^\pi_\Lambda$ where each K_π is compact such that the open sets $\mathcal{V}^\pi$ still cover $\mathcal{T}_\Lambda$. Let $\mathcal{D}_0 \subset \mathcal{T}_\Lambda$ be the set of matrices T with $(T)_{n,n-1} = 0$. The set $\mathcal{D}_0$ is a compact submanifold of codimension 1. The set $\mathcal{D}_0$ is not contained in any $\mathcal{V}^\pi$ but is clearly covered by them and we can then write the π-bidiagonal coordinates $\beta^\pi_1, \cdots, \beta^\pi_{n-1}$ for $T \in \mathcal{V}^\pi$. Lemma 2.3 allows us to identify in $\mathcal{V}^\pi$ rates of decay for $(T)_{n,n-1}$ and β^π_{n-1}.

Let $\epsilon_1 < |\lambda_i - \lambda_j|/2$ for all $i \neq j$. We can take $\epsilon_0 > 0$ such that $T \in \mathcal{D}(\epsilon_0)$ implies $|(T)_{n,n} - \lambda_i| < \epsilon_1$ for some (unique) i (i depends on T). Call $\mathcal{D}^i(\epsilon_0) \subset \mathcal{D}(\epsilon_0)$ the set of such T. Assume without loss that $\mathcal{D}^i(\epsilon_0)$ is covered by $\mathcal{V}^\pi$ for permutations π satisfying $\pi(n) = i$. In $\mathcal{D}^i(\epsilon_0)$, $\mathbf{W}$ in π-bidiagonal coordinates is given by

$$\mathbf{W}_\pi(\beta^\pi_1, \ldots, \beta^\pi_{n-1}) = \left(\left| \frac{\lambda_{\pi(2)} - \omega}{\lambda_{\pi(1)} - \omega} \right| \beta^\pi_1, \ldots, \left| \frac{\lambda_i - \omega}{\lambda_{\pi(n-1)} - \omega} \right| \beta^\pi_{n-1} \right).$$

In each $\mathcal{V}^\pi \cap \mathcal{D}^i(\epsilon_0)$, ω is a continuous function taking the value λ_i when $\beta^\pi_{n-1} = 0$. Since $\omega_\pm$ are Lipschitz functions of T, $|\lambda_i - \omega| < L|\beta^\pi_{n-1}|$ for some $L > 0$, implying from the formula for $\mathbf{W}_\pi$ the quadratic rate of decay for β^π_{n-1}. By taking ϵ_0 even smaller, we can assume that $|\lambda_i - \omega| < \epsilon_1$ in this set so that the quotients

$$\frac{\lambda_{\pi(2)} - \omega}{\lambda_{\pi(1)} - \omega}, \cdots, \frac{\lambda_{\pi(n-1)} - \omega}{\lambda_{\pi(n-2)} - \omega}$$

have absolute value bounded and bounded away from zero and the first claim follows by compactness.

The Taylor expansion of the last coordinate of $\mathbf{W}_\pi$ centered at points $T \in (\mathcal{V}^\pi \cap \mathcal{D}_0) - \mathcal{Y}_0$ with respect to the variable β^π_{n-1} is of the form

$$(\mathbf{W}_\pi(\beta^\pi_1, \ldots, \beta^\pi_{n-1}))_{n-1} = \sum_\ell a_\ell(\beta^\pi_1, \ldots, \beta^\pi_{n-2})(\beta^\pi_{n-1})^\ell.$$

The function $\mathbf{W}_\pi$ is odd, so $a_0 = a_2 = 0$. The factor $(\lambda_{\pi(n)} - \omega)/(\lambda_{\pi(n-1)} - \omega)$ equals 0 if $\beta^\pi_{n-1} = 0$ and therefore $a_1 = 0$. In other words,

$$(\mathbf{W}_\pi(\beta^\pi_1, \ldots, \beta^\pi_{n-1}))_{n-1} = G(\beta^\pi_1, \ldots, \beta^\pi_{n-1})(\beta^\pi_{n-1})^3$$

for some real analytic function G. Again by compactness, we are done. ■

A matrix T is an *AP-matrix* if its spectrum contains an arithmetic progression with 3 terms, i.e., some eigenvalue is the average of two others; otherwise, T is *AP-free*. We also refer to AP-free spectra, Jacobi cells, isospectral manifolds and so on, with the obvious meanings. The left hexagon in figure 1 is AP-free and the right hexagon is not.

Theorem 3.4 *For AP-free tridiagonal matrices, Wilkinson's iteration has cubic convergence. More precisely, given an AP-free spectrum $\lambda_1 < \cdots < \lambda_n$, there exist $C > 0$ and $K > 0$ such that, for any $T_0 \in \mathcal{T}_\Lambda$,*

(a) *if $k > K$ then $|(T_{k+1})_{n,n-1}| < 1/C$ and $|(T_{k+1})_{n,n-1}| \leq C|(T_k)_{n,n-1}|^2$;*

(b) *the set of positive integers k for which $|(T_{k+1})_{n,n-1}| > C|(T_k)_{n,n-1}|^3$ has at most K elements.*

Proof: We keep the notation of the proof of proposition 3.3. Item (a) follows from theorem 3.2, proposition 3.3 and compactness. Indeed, for any given $\epsilon > 0$ there exists K_1 such that for any $T_0 \in \mathcal{T}_\Lambda$ and for any $k > K_1$ we have $T_k \in \mathcal{D}(\epsilon)$. For item (b), we need to prove that, given an open $\mathcal{D}_c \subset \mathcal{T}_\Lambda$ containing the diagonal matrices, there exists K_2 such that, for any $T_0 \in \mathcal{T}_\Lambda$, the set of positive integers k for which $T_k \notin \mathcal{D}_c$ has at most K_2 elements. Notice that $\mathcal{Y}_0$ is removed from diagonal matrices and therefore such a set $\mathcal{D}_c$ exists.

As a warm-up case, let $\mathcal{D}_{0,i} \subset \mathcal{Z}_i$ be the set of matrices $T \in \mathcal{T}_\Lambda$ for which $(T)_{n,n} = \lambda_i$, $(T)_{n,n-1} = 0$. Clearly, $\mathcal{D}_{0,i}$ are the n connected components of $\mathcal{D}_0$ and the set $\mathcal{D}_{0,i}$ is diffeomorphic to $\mathcal{T}_{\Lambda_i}$, where

$$\Lambda_i = \mathrm{diag}(\lambda_1, \ldots, \lambda_{i-1}, \lambda_{i+1}, \ldots \lambda_n),$$

that is, Λ without λ_i. Points in $\mathcal{D}_{0,i}$ are removable singularities of $\mathbf{W}$ and there $\mathbf{W}$ is a QR step on $\mathcal{T}_{\Lambda_i}$ (the top $(n-1) \times (n-1)$ block) with $f(x) = x - \lambda_i$. Apply corollary 2.8 to conclude this special case: simplicity of Λ ensures that λ_i is not an eigenvalue of the top $(n-1) \times (n-1)$ block and the fact that Λ is AP-free ensures that $|lambda_j - \lambda_i| \neq |\lambda_{j'} - \lambda_i|$ for distinct eigenvalues λ_j and $\lambda_{j'}$ of said block. In general, we need to extend the reasoning in corollary 2.8 to a neighborhood of $\mathcal{D}_{0,i}$.

Let $b : \mathcal{T}_\Lambda \to \mathbb{R}$ be the smooth function defined by $b(T) = (T)_{n,n-1}$. From lemma 2.3, b is transversal to $\mathcal{D}_0$; let Z be a smooth vector field in $\mathcal{T}_\Lambda$ such that the directional derivative Zb satisfies $Zb = 1$ in $\mathcal{D}(\epsilon_Z)$ for some $\epsilon_Z > 0$, $\epsilon_Z < \epsilon_q$. The vector field Z can be integrated to yield a diffeomorphism $\zeta : \mathcal{D}_0 \times (-\epsilon_Z, \epsilon_Z) \to \mathcal{D}(\epsilon_Z)$. Let $\mathcal{D}_i(\epsilon_Z) = \zeta(\mathcal{D}_{0,i} \times (-\epsilon_Z, \epsilon_Z))$: we have a diffeomorphism $\tilde{\zeta} : \mathcal{T}_{\Lambda_i} \times (-\epsilon_Z, \epsilon_Z) \to \mathcal{D}_i(\epsilon_Z)$. Set $\hat{\mathbf{W}}_i : \mathcal{T}_{\Lambda_i} \times (-\epsilon_Z, \epsilon_Z) \to \mathcal{T}_{\Lambda_i} \times (-\epsilon_Z, \epsilon_Z)$, $\hat{\mathbf{W}}_i = (\tilde{\zeta})^{-1} \circ \mathbf{W} \circ \tilde{\zeta}$ and, for $\mathbf{t}_0 \in \mathcal{T}_{\Lambda_i} \times (-\epsilon_Z, \epsilon_Z)$, $\mathbf{t}_k$ is defined recursively by $\mathbf{t}_{k+1} = \hat{\mathbf{W}}_i(\mathbf{t}_k)$.

Let $g(x) = \log(|x - \lambda_i|)$ and $M = \mathrm{diag}(n-1, n-2, \ldots, 2, 1)$. Let X_g tangent to $\mathcal{T}_{\Lambda_i}$ and $h_{M,g} : \mathcal{T}_{\Lambda_i} \to \mathbb{R}$ be as in theorem 2.7. Extend $h_{M,g}$ to $h_{M,g} : \mathcal{T}_{\Lambda_i} \times (-\epsilon_Z, \epsilon_Z) \to \mathbb{R}$ by ignoring the second coordinate. Let $\mathbf{T} : \mathbb{R} \to \mathcal{T}_{\Lambda_i}$ with $\frac{d}{dt}\mathbf{T} = X_g$: from proposition 2.6 we have $\hat{\mathbf{W}}_i(\mathbf{T}(0), 0) = (\mathbf{T}(1), 0)$. Therefore, from theorem 2.7, $h_{M,g}(\hat{\mathbf{W}}_i(\mathbf{t}_0)) > h_{M,g}(\mathbf{t}_0)$ for any $\mathbf{t}_0 = (T_0, 0) \in \mathcal{T}_{\Lambda_i} \times \{0\}$, T_0 not a diagonal matrix. Set $\delta : \mathcal{T}_{\Lambda_i} \times (-\epsilon_Z, \epsilon_Z) \to \mathbb{R}$, $\delta(\mathbf{t}_0) = h_{M,g}(\hat{\mathbf{W}}_i(\mathbf{t}_0)) - h_{M,g}(\mathbf{t}_0)$; by compactness of the complement of $\mathcal{D}_c$, there exists $\epsilon > 0$ such that $\delta(\mathbf{t}_0) > \epsilon$ if $\mathbf{t}_0 \in (\mathcal{T}_{\Lambda_i} \times \{0\}) - (\tilde{\zeta}^{-1}(\mathcal{D}_c))$. Since δ is continuous in $\mathcal{T}_{\Lambda_i} \times \{0\}$, there exists $\epsilon' > 0$, $\epsilon' < \epsilon_Z$, such that $\mathbf{t}_0 \in (\mathcal{T}_{\Lambda_i} \times (-\epsilon', \epsilon')) - \tilde{\zeta}^{-1}(\mathcal{D}_c)$ implies $\delta(\mathbf{t}_0) > \epsilon/2$. Clearly, for any $\mathbf{t}_0$ in $\mathcal{T}_{\Lambda_i} \times (-\epsilon', \epsilon')$,

$$\sum_{k \geq 0} \delta(\mathbf{t}_k) \leq \max h_{M,g} - \min h_{M,g}$$

and therefore there are at most $2(\max h_{M,g} - \min h_{M,g})/\epsilon$ values of k for which $\mathbf{t}_k \notin \tilde{\zeta}^{-1}(\mathcal{D}_c)$ and we are done. ■

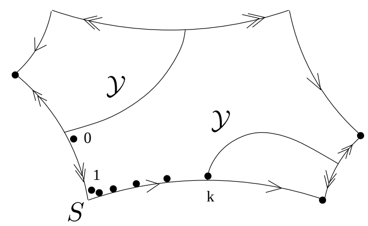

Figure 3: We may have $T_k \in \mathcal{Y}$ for large values of k.

On the other hand, it is *not* true that given an AP-free spectrum Λ there exist $C > 0$ and K such that $|(T_{k+1})_{n,n-1}| \leq C|(T_k)_{n,n-1}|^3$ for all $k > K$. A counterexample is indicated in figure 3: the orbit may spend an arbitrarily large number of steps near the saddle point S and we may therefore have $T_k \in \mathcal{Y}$ for arbitrarily large k.

4 Wilkinson's step for 3×3 AP-matrices

In this and the following sections we prove that for any spectrum of the form $\{a-b, a, a+b\}$ there exist matrices T_0 for which

$$\lim_{k\to\infty} T_k = \begin{pmatrix} a & b & 0 \\ b & a & 0 \\ 0 & 0 & a \end{pmatrix}$$

and that the convergence of $(T_k)_{n,n-1}$ towards 0 is still quadratic but not cubic. For $a = 0$, $b = 1$, this limit is the point labeled $(0,0,0)$ at the bottom of the right hexagon in figure 1.

Up to normalizations, a 3×3 AP-matrix is isospectral to $\Lambda = \mathrm{diag}(-1, 0, 1)$. We use the π-bidiagonal coordinates for matrices in $\mathcal{U}_\Lambda^\pi$ computed in section 2 for an appropriate permutation π. The bottom 2×2 block of $T \in \mathcal{U}_\Lambda^\pi$ is

$$\hat{T} = \frac{1}{r_1^2 r_2^2} \begin{pmatrix} -4(x^2-4)(x^2y^4-1) & 2yr_1^3 \\ 2yr_1^3 & y^2(x^2-4)r_1^2 \end{pmatrix}$$

where $r_1 = \sqrt{4 + x^2 + 4x^2y^2}$, $r_2 = \sqrt{4 + 4y^2 + x^2y^2}$. Let $\omega_+ \geq \omega_-$ be the (real) eigenvalues of $\hat{T}$; by interlacing, $-1 \leq \omega_- \leq 0 \leq \omega_+ \leq 1$, with equality only when $x = 0$ or $y = 0$. The discriminant of the characteristic polynomial of $\hat{T}$ is $\Delta = ((x+2)^2 + 8x^2y^2)((x-2)^2 + 8x^2y^2) \geq 0$ which is zero exactly at the points $\pm p_0$, $p_0 = (2, 0)$. These points correspond to the matrices $\pm P_0$,

$$P_0 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

and the origin to the matrix Λ^π.

The eigenvalue closest to the bottom element $(\hat{T})_{2,2} = (T)_{3,3}$ is ω_+ if and only if $(T)_{3,3} > (\omega_+ + \omega_-)/2$. A straightforward computation yields

$$(T)_{3,3} - \frac{\omega_+ + \omega_-}{2} = \frac{(2-x)(2+x)(4 - 4y^2 - x^2y^2 - 8x^2y^4)}{2r_1^2 r_2^2}$$

which indicates that the xy-plane is divided by $\mathcal{Y}$ into regions, the choice between ω_+ and ω_- being as in figure 4 (where only the region $x > 0$ is shown). The hexagon of matrices on the right of figure 1 is the image under ϕ_π of the first quadrant (of π-bidiagonal coordinates) in figure 4; the reader may check, for instance, that $\phi_\pi(2,0) = P_0$ and that

$$\phi_\pi(0,1) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1/2 & 1/2 \\ 0 & 1/2 & -1/2 \end{pmatrix}.$$

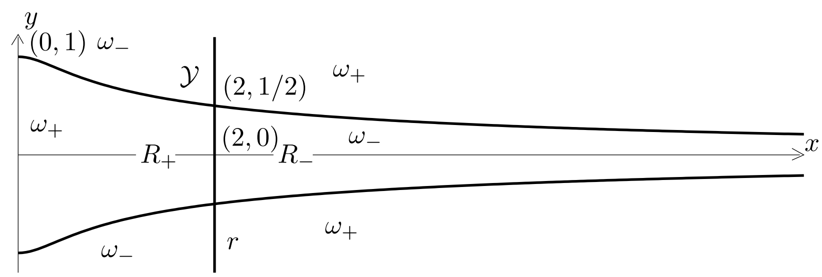

Figure 4: The choice of ω.

We consider the region

$$R = \{(x,y)|x > 0, 4 - 4y^2 - x^2y^2 - 8x^2y^4 \geq 0\}$$

and the subsets $R_+ = R \cap ((0,2] \times \mathbb{R})$, $R_- = R \cap ([2,+\infty) \times \mathbb{R})$. For $0 < a \leq 1/10$, define the *wedge of height* a to be

$$V_a = \{(x,y)||y| \leq a, |y| \geq |x-2|/10\}.$$

Lemma 4.1 *The functions $\omega_\pm$ are smooth in $(x,y) \in R$ except at the point p_0, where they have a cone-like behavior:*

$$\omega_\pm = \frac{(x-2) \pm \sqrt{(x-2)^2 + 32y^2}}{4} + O((x-2)^2 + 32y^2).$$

For $(x,y) \in R_+$ (resp. R_-), $0 \leq \omega_+ \leq 2|y|$ (resp. $-2|y| \leq \omega_- \leq 0$). There exists a positive constant C such that $|\omega_\pm| \geq C|y|$ for $(x,y) \in V_a$.

Proof: We have

$$\omega_\pm = \frac{-4 + x^2 \pm \sqrt{\Delta}}{2r_1^2}.$$

The displayed estimate for $\omega_\pm$ follows directly from

$$\lim_{(x,y)\to(2,0)} \frac{\Delta}{16((x-2)^2 + 32y^2)} = 1.$$

The signs of $\omega_\pm$ follow from interlacing and the other estimates are now easy. ■

Lemma 4.2 *The partial derivatives $(\omega_\pm)_x$ and $(\omega_\pm)_y$ are uniformly bounded in $R - \{p_0\}$. For all $(x,y) \in R_\pm - \{p_0\}$ we have $(\omega_\pm)_x \geq 0$, with equality exactly when $y = 0$. Also, $(\omega_\pm)_x > 1/120$ in any wedge V_a. Furthermore, for $y \neq 0$, $\pm y(\omega_\pm)_y > 0$.*

Proof: A straightforward computation yields

$$(\omega_\pm)_x = \frac{8x}{r_1^4\sqrt{\Delta}}\left(\left((1+2y^2)\sqrt{\Delta}\right) \pm \left(-4+x^2+8y^2+6x^2y^2+16x^2y^4\right)\right),$$
$$(\omega_\pm)_y = \frac{4x^2y}{r_1^4\sqrt{\Delta}}\left(\left((4-x^2)\sqrt{\Delta}\right) \pm \left(16+24x^2+x^4+32x^2y^2+8x^4y^2\right)\right).$$

Also,

$$\left((1+2y^2)\sqrt{\Delta}\right)^2 - \left(-4+x^2+8y^2+6x^2y^2+16x^2y^4\right)^2 = 8y^2r_1^4 \geq 0$$

whence

$$(1+2y^2)\sqrt{\Delta} \geq \left|-4+x^2+8y^2+6x^2y^2+16x^2y^4\right|,$$

where the equality holds if and only if $y=0$. In order to prove the estimate in V, write

$$(\omega_\pm)_x = \frac{8x}{r_1^4\sqrt{\Delta}}\;\frac{8y^2r_1^4}{\left(\left((1+2y^2)\sqrt{\Delta}\right) \mp (-4+x^2+8y^2+6x^2y^2+16x^2y^4)\right)}$$
$$\geq \frac{32x}{(1+2y^2)((x+2)^2+8x^2y^2)}\;\frac{y^2}{(x-2)^2+8x^2y^2} > 1/120.$$

Since

$$\left((4-x^2)\sqrt{\Delta}\right)^2 - \left(16+24x^2+x^4+32x^2y^2+8x^4y^2\right)^2 = -64x^2r_1^4 \leq 2$$

we have

$$\left|(4-x^2)\sqrt{\Delta}\right| \leq 16+24x^2+x^4+32x^2y^2+8x^4y^2,$$

which yields the sign of $(\omega_\pm)_y$.

Boundedness near $x=\infty$ follows from the rates in x since y is bounded. For (x,y) near p_0, expand the formula for $(\omega_\pm)_x$ as a sum of two terms. The first term is bounded since $\sqrt{\Delta}$ simplifies; from the computations above, the absolute value of the second term is no larger. Since $y/\sqrt{\Delta}$ is bounded near p_0, so is $(\omega_\pm)_y$. ■

In bidiagonal coordinates, Wilkinson's step is given by

$$\mathbf{W}(x,y) = \left(\frac{1+\omega}{1-\omega}x, \frac{|\omega|}{1+\omega}y\right).$$

Since from interlacing $\omega_\pm$ does not change sign, the restrictions $\mathbf{W}_+ : R_+ \to R \subset \mathbb{R}^2$ and $\mathbf{W}_- : R_- \to R \subset \mathbb{R}^2$, are continuous in their respective domains and smooth except at p_0. The restrictions of $\mathbf{W}$ to the the left and to the right of the vertical line r given by $x=2$ coincide with $\mathbf{W}_+$ and $\mathbf{W}_-$ and the restrictions of these two functions to r yield different values. Figure 5 shows the images of $\mathbf{W}_+$ and $\mathbf{W}_-$, clearly contained in R. As we shall see, both $\mathbf{W}_+$ and $\mathbf{W}_-$ are homeomorphisms onto their respective images.

The line r is taken by $\mathbf{W}_+$ (resp. $\mathbf{W}_-$) to an arc contained in R_- (resp. R_+), with a cusp at p_0. The horizontal axis is a common tangent to the four smooth subarcs in the images of r. A straightforward computation verifies that the preimage of the vertical line r under $\mathbf{W}$ consists of the two smooth arcs

$$\left(x, \pm\frac{(x-2)\sqrt{x(x^2+2x+4)}}{4x^2}\right),$$

shown in figures 5 and 6, which are tangent to the lines $y = \pm\frac{\sqrt{6}}{8}(x-2)$.

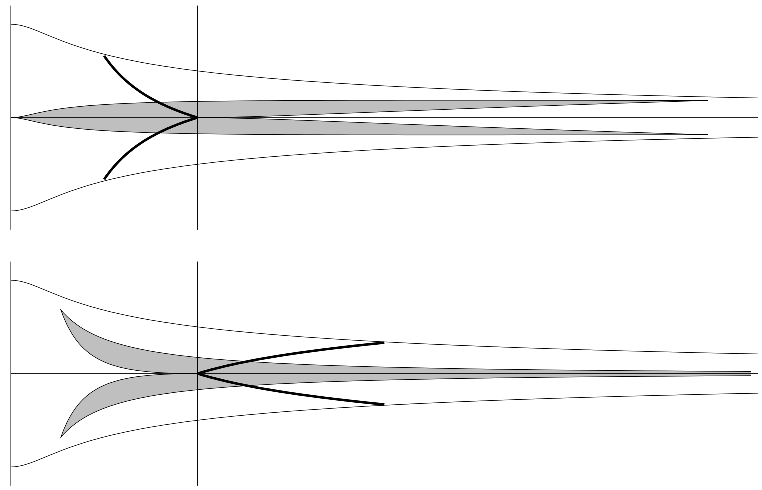

Figure 5: $\mathbf{W}_\pm(R_\pm)$ (shaded) and $\mathbf{W}_\pm^{-1}(r)$ (thick); in scale.

Proposition 4.3 *The functions $\mathbf{W}_\pm$ are orientation preserving homeomorphisms onto their respective images.*

Proof: The Jacobian matrix of $\tilde{\mathbf{W}}_\pi$ is

$$D\mathbf{W}_\pm(x,y) = \begin{pmatrix} \dfrac{2(\omega_\pm)_x}{(1-(\omega_\pm))^2}x + \dfrac{1+(\omega_\pm)}{1-(\omega_\pm)} & \dfrac{2(\omega_\pm)_y}{(1-(\omega_\pm))^2}x \\ \\ \pm\dfrac{(\omega_\pm)_x}{(1+(\omega_\pm))^2}y & \pm\dfrac{(\omega_\pm)_y}{(1+(\omega_\pm))^2}y \pm \dfrac{(\omega_\pm)}{1+(\omega_\pm)} \end{pmatrix},$$

with determinant given by

$$\det D\mathbf{W}_\pm(x,y) = \pm\frac{1}{1-\omega_\pm^2}\left(\frac{2(\omega_\pm)_x\omega_\pm x}{1-\omega_\pm} + (\omega_\pm)_y y + \omega_\pm(1+\omega_\pm)\right).$$

It follows from lemmas 4.1 and 4.2 that each term in the sum between parenthesis have the same sign and $\det D\mathbf{W}_\pm(x,y) > 0$ if $y \neq 0$.

Points in the horizontal axis are fixed points of $\mathbf{W}_\pm$. Figure 5 indicates that the boundary of the domains are taken to simple closed curves, which in turn implies the result, from standard degree theory. A more rigorous and rather lengthy proof is possible using estimates and a little topology, but will be omitted. ■

Notice that $\tilde{\mathbf{W}}_\pi$ reverses orientations for $(x,y) \in R_-$ but $\mathbf{W}_-$ preserves orientations.

5 Quadratic convergence for Wilkinson's iteration

Theorem 5.1 *There exists an open neighborhood $\mathcal{A} \subset \mathcal{T}_\Lambda$ of P_0 and a closed set $\mathcal{X} \subset \mathcal{A}$ of zero measure, invariant under $\mathbf{W}$, on which the iteration converges quadratically to P_0. The part of $\mathcal{X}$ with positive y coordinate is homeomorphic to the Cartesian product of a Cantor set and an open interval.*

Numerical evidence indicates that we can take $\mathcal{A} = \mathcal{U}_\Lambda^\pi$. Figure 7 shows $\mathcal{X}$ in π-bidiagonal coordinates: $\mathcal{X}$ and its mirror image at the y axis map the set of *all* matrices in $\mathcal{T}_\Lambda$ for which Wilkinson's iteration converges quadratically. Since the

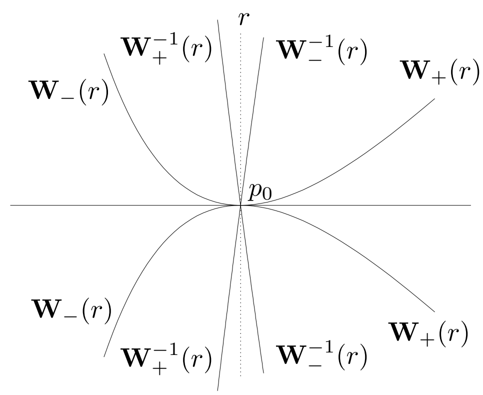

Figure 6: Images and preimages of the line $x = 2$; not in scale.

Cantor set is extremely thin, the fine structure of the set $\mathcal{X}$ is invisible in the figure; the curves $\mathbf{W}_\pm^{-1}(r)$ fit inside the largest gaps of $\mathcal{X}$ in each quadrant. As we shall see, an equivalent characterization of $\mathcal{X}$ is *wedge invariance*: $\mathcal{X}$ is the set of points whose forward orbit under $\mathbf{W}$ is eventually contained in V_a. Propositions 5.4 and 5.5 below imply the theorem and provide additional, more technical information about $\mathcal{X}$.

In a self-evident notation, we speak of the upper and lower half-wedges and of the NE, NW, SE and SW faces of a wedge V_a. Given $z_0 \in R$, set $z_{k+1} = \mathbf{W}(z_k)$; this is well defined unless $z_k \in r$. The sequence $(z_k)_{k\in\mathbb{N}}$ is the $\mathbf{W}$-*orbit* of z_0.

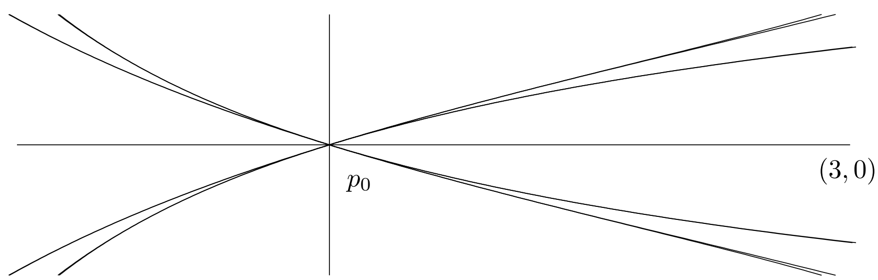

Figure 7: The set $\mathcal{X}$ near p_0; in scale

Lemma 5.2 *For sufficiently small $a > 0$, if $(x, y) \notin V_a$, $|y| \le a$, then $\mathbf{W}(x, y) \notin V_a$. Furthermore, a $\mathbf{W}$-orbit tends to p_0 if and only if it is eventually contained in a wedge.*

Proof: Consider a short segment in the upper half plane starting at p_0 with argument θ. It is easy to see that for $\theta > \pi - \arctan(\sqrt{6}/8)$, the image under $\mathbf{W}_+$ of this segment is a curve tangent to the horizontal axis at p_0 and to the left of the vertical line r. Similarly, if $\theta < \pi - \arctan(\sqrt{6}/8)$, the curve is to the right of r. An example of this is $\mathbf{W}_+(r)$, shown in figure 6. We remind the reader that $-\sqrt{6}/8$ is the slope of $\mathbf{W}_+^{-1}(r)$ at p_0. Since $-1/6 < -\sqrt{6}/8 < 0$, the images of the NW face and of the line r are to the left and right, respectively, of the wedge. A similar remark holds for $\mathbf{W}_-$ and the NE face.

Near the horizontal axis, $|\omega|/(1 + \omega)$ can be assumed to be smaller than 1 and therefore the absolute value of the second coordinate of z_k is decreasing. The slope of the line joining $z_0 = (x, y)$ and z_1 is

$$\frac{y}{\omega_\pm} \frac{(1-\omega_\pm)(1+\omega_\pm \mp \omega_\pm)}{-2x(1+\omega_\pm)}.$$

Since $|\omega_\pm| \le 2|y|$ (lemma 4.2) and the second fraction tends to $1/4$ when (x, y) tends to p_0, the slope can be assumed to have absolute value greater than $1/9$, i.e., to be steeper than the faces of the wedge. Thus, V_a is further from z_{k+1} than from z_k. ■

The set $\mathcal{X}$ can now be defined either as the set of points whose orbit is eventually contained in a wedge or as the set of points z for which $\lim_{k\to\infty} \mathbf{W}^k(z) = p_0$.

An *L-flat arc* in V_a is the graph $\Gamma \subset V_a$ of a L-Lipschitz function $f : I \to \mathbb{R}$.

Lemma 5.3 *There exist a wedge V_{a^*} and a positive constant $L^* < 1/6$ with the following properties. Suppose Γ_0^+ is an L^*-flat arc in V_{a^*}, with left endpoint belonging to the NW face of V_{a^*} and right endpoint in the vertical line r. Then $\mathbf{W}_+(\Gamma_0^+)$ contains Γ_1, also an L^*-flat arc in V_{a^*} with left (resp. right) endpoint in the NW (resp. NE) face of V_{a^*}. Moreover, such arcs are uniformly pushed towards the horizontal axis:*

$$\max_{(x,y)\in\Gamma_1} y < 1/4 \min_{(x,y)\in\Gamma_0^+} y.$$

Furthermore, $\mathbf{W}_+$ stretches the horizontal coordinate. More precisely, let the endpoints of Γ_1 be $\mathbf{W}_+(x_\pm, y_\pm)$ and for $x \in [x_+, x_-]$, let $\phi(x)$ be the first coordinate of $\mathbf{W}_+(x, y)$ where $(x, y) \in \Gamma_0^+$; then $\phi'(x) > 1$ for all x.

An analogous statement holds for the action of $\mathbf{W}_-$ on an L^*-flat arc Γ_0^- with endpoints now belonging to r and the NE face of the wedge.

Symmetry with respect to the horizontal axis implies similar results for arcs in the lower half wedge.

Notice that on smaller wedges, the lemma still holds for the same Lipschitz constant but given a wedge, the Lipschitz constant cannot be taken arbitrarily small.

Proof: We prove the statements concerning the action of $\mathbf{W}_+$ on the upper half wedge, the others being similar.

In order to control the slope of images of L-flat arcs, we proceed to prove the following claim. Given $L > 0$, there exists $a > 0$ such that if $(x, y) \in V_a$ then:

1. the eigenvalues λ_0 and λ_1 of $D\mathbf{W}_+(x, y)$ satisfy $|\lambda_0| < 1/4$, $\lambda_1 > 1/2$;
2. for the associated eigenvectors v_i, $|\cot \arg v_0| < 1/L$ and $|\tan \arg v_1| < L$.

Indeed, from lemma 4.2 and the formula for $D\mathbf{W}_+$ in the proof of proposition 4.3, the entries in the second row of $D\mathbf{W}_+$ tend to zero when (x, y) tends to p_0, the $(1, 2)$ entry is bounded and the $(1, 1)$ entry is larger than $3/4$. In a suggestive notation,

$$D\mathbf{W}_+ = \begin{pmatrix} a_1 & a_2 \\ \epsilon_1 & \epsilon_2 \end{pmatrix}$$

has eigenvalues

$$\frac{(a_1 + \epsilon_2) \pm \sqrt{(a_1 - \epsilon_2)^2 + 4a_2\epsilon_1}}{2},$$

from which the estimates for λ_0 and λ_1 follow. The eigenvectors can be written as $v_0 = C_0(a_2, \lambda_0 - a_1)$ and $v_1 = C_1(\epsilon_2 - \lambda_1, -\epsilon_1)$, from which estimates for the arguments also follow, completing the proof of the claim.

Assume without loss of generality that L^* is so small that

$$\max_{(x,y)\in\Gamma} y < 2 \min_{(x,y)\in\Gamma} y$$

for any L^*-flat arc Γ in V_{a^*}. Assume also that $\omega_+ < 1/8$ for all $(x,y) \in V_{a^*}$. From

$$\mathbf{W}_+(x,y) = (x_1, y_1) = \left(\frac{1+\omega_+}{1-\omega_+} x, \frac{\omega_+}{1+\omega_+} y \right)$$

we have $y_1 < y/8$ proving

$$\max_{(x,y)\in\Gamma_1} y < 1/4 \min_{(x,y)\in\Gamma_0^+} y.$$

The claim implies that for all $(x,y) \in V_a$, v_1 is in the east sector $|\arg v_1| < \arctan L$ and v_0 is in the north sector $\arctan L < \arg v_0 < \pi - \arctan L$. Thus, the east sector is taken by $D\mathbf{W}_+(x,y)$ to a subset of itself. Setting $L = L^*$ and $a^* = a$, this in turn implies that the image under $\mathbf{W}_+$ of the arc Γ_0^+ in the statement of the lemma is an arc for which the Lipschitz constant L^* still holds. As seen in the beginning of the proof, the endpoints of $\mathbf{W}_+(\Gamma_0^+)$ are to the left and right of V_{a^*}. The intersection of $\mathbf{W}_+(\Gamma_0^+)$ with V_{a^*} is Γ_1.

Write

$$a_1 = \frac{1 + 2(\omega_\pm)_x x - \omega_\pm^2}{(1-\omega_\pm)^2}.$$

Take V_{a^*} so that $(1-\omega_\pm)^2 < 1.01$, $\omega_\pm^2 < 0.01$, $2(\omega_\pm)_x x > 0.1$ from which we learn that $a_1 > 1.05$, completing the proof. ■

A *sign sequence* is a function $s : \mathbb{N} \to \{\pm 1\}$ or $(s_0, s_1, s_2, \ldots)$. The distance between two distinct sign sequences s and $\tilde{s}$ is 3^{-k}, where k is the smallest number for which $s_k \neq \tilde{s}_k$. There is a natural bi-Lipschitz homeomorphism between the set $\mathcal{S}$ of all sign sequences and the middle third Cantor set $\mathcal{K}_3 \subset [0,1]$: take s to $\sum_{k\geq 0}(1+s_k)/3^{k+1}$. More generally, a closed subset $\mathcal{K}$ of a Lipschitz graph Γ is a *Cantor set* if it has empty interior (in the induced topology in Γ) and no isolated points. As is well known, a subset of a Lipschitz graph Γ is a Cantor set if and only if it is homeomorphic to $\mathcal{S}$.

Given $z_0 \in R$, the z_0*-sign sequence* s^{z_0} is such that $s_k^{z_0} = +1$ iff $z_k \in R_+$ (where $z_{k+1} = \mathbf{W}(z_k)$).

Proposition 5.4 *Let L^* and a^* be as in lemma 5.3. Let Γ_0 be an L^*-flat arc in V_{a^*} with endpoints in the NW and NE faces. The set $\mathcal{X} \cap \Gamma_0$ is a Cantor set and the map taking z_0 to the z_0-sign sequence is a bijection from $\mathcal{X} \cap \Gamma_0$ to $\mathcal{S}$.*

The set $\mathcal{X}$ is the disjoint union of graphs of Lipschitz functions $f_s : [0, a^*] \to \mathbb{R}$ (one for each sign sequence s) taking y_0 to the x coordinate of the unique point in the intersection of $\mathcal{X}$ with the arc $y = y_0$ with sign sequence s.

Numerical analysis gives, for example,

$$f_{(+,+,+,+,\ldots)}(1/10) \approx 1.7083176575931057990364676076125577647675348497797 6.$$

Proof: Let $\Gamma_0^\pm = \Gamma_0 \cap R_\pm$. From lemma 5.3, the image of $\Gamma_0^\pm$ under $\mathbf{W}_\pm$ contains an L^*-flat arc in V_{a^*} with endpoints in the NW and NE faces. For a sign sequence $s = (s_0, s_1, s_2, \ldots)$, let Γ_1 be such an arc contained in $\mathbf{W}_{s_0}(\Gamma_0^{s_0})$, and, more generally, Γ_{k+1} be an arc contained in $\mathbf{W}_{s_k}(\Gamma_k^{s_k})$. Define intervals $I_k = [a_k, b_k] \subset \Gamma_0$ (see figure 8 for $s = (+,-,-,\ldots)$) by

$$I_0 = \Gamma_0^{s_0}, \quad \mathbf{W}_{s_{k-1}} \cdots \mathbf{W}_{s_1} \mathbf{W}_{s_0} I_k = \mathbf{W}^k I_k = \Gamma_k^{s_k}.$$

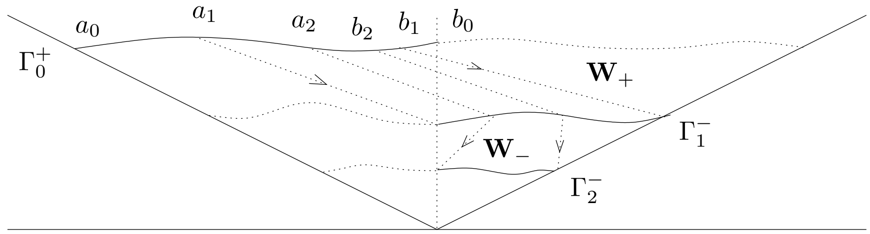

Figure 8: Some curves Γ_i; schematic.

Again from lemma 5.3, $|I_{k+1}| \leq |I_k|/4$ and the intersection of the nested family of intervals $\cap_k I_k$ consists of the unique point in $\mathcal{X} \cap \Gamma_0$ with sign sequence s. Thus the map from $\mathcal{S}$ to $\mathcal{X} \cap \Gamma_0$ taking s to the point with sign sequence s is injective and continuous, whence $\mathcal{X} \cap \Gamma_0$ is a Cantor set.

Now fix a sign sequence s. Since the arc $y = y_0$ is L^*-flat, the function f_s is well defined. We show that f_s is Lipschitz with constant $1/L^*$. Indeed, assume by contradiction that y_1 and y_2 satisfy

$$|f_s(y_1) - f_s(y_2)| > \frac{1}{L^*}|y_1 - y_2|;$$

the line through the points $(f_s(y_1), y_1)$ and $(f_s(y_2), y_2)$ has slope smaller than L^* and is therefore L^*-flat. Thus, there are two points on the intersection of $\mathcal{X}$ with an L^*-flat arc with the same sign sequence, a contradiction. ■

The set $\mathcal{X}$ is rather thin, with Hausdorff dimension (at least in a neighborhood of p_0) equal to 1; we do not present a proof of this fact. Numerics suggests that $\mathcal{X}$ is a union of smooth curves $\mathcal{X}_s$, $s \in \mathcal{S}$, parametrized by $(f_s(y), y)$. The curve $\mathcal{X}_s$ is taken by $\mathbf{W}$ to $\mathcal{X}_{s'}$, where s' is the left shift of s: $s' = (s(1), s(2), s(3), \ldots)$.

Proposition 5.5 *For $z_0 = (x_0, y_0) \in \mathcal{X}$, there exists positive constants c, C such that, for $z_n = (x_n, y_n)$, $c|y_n|^2 \leq |y_{n+1}| \leq C|y_n|^2$, i.e., the convergence of z_n to p_0 is strictly quadratic. On the other hand, for $z_0 \in R - \mathcal{X}$ the convergence of z_n is strictly cubic.*

Proof: Recall that $y_{n+1} = \frac{|\omega|}{1+\omega} y_n$. From lemma 4.1, there exist positive constants c_1, C_1 such that $c_1|y| \leq |\omega| \leq C_1|y|$ for any point $(x, y) \in V_a$. Also, we may assume that $1/2 < 1 + \omega < 2$ and therefore

$$\frac{c_1}{2}|y|^2 \leq \frac{|\omega|}{1+\omega}|y| \leq 2C_1|y|^2$$

and the first claim follows.

If the limit point is some $p = (x, 0)$, $x \neq 0$, then there exists positive constants c_1, C_1 such that, in a neighborhood of p, $c_1|y|^2 \leq |\omega| \leq C_1|y|^2$. This follows from the fact that ω is smooth and even near p we may write a Taylor expansion as in theorem 3.4. The second claim now follows easily. ■

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